

## Chapter 2

# Quantum-Electrodynamics Approach to Description of Bremsstrahlung of a Fast Charged Particle on an Atom with Account for the Polarization Channel

In this chapter with the use of the consistent quantum-electrodynamic approach the cross-section of bremsstrahlung of a fast charged particle on a one-electron and multielectron atom was obtained and analyzed within the framework of the first Born approximation.

In this section, unless otherwise indicated, we use the relativistic system of units, in which  $\hbar = c = 1$  ( $\hbar$  is the Planck constant,  $c$  is the velocity of light in vacuum).

### 2.1 Amplitude of Bremsstrahlung of a Relativistic Charged Particle on a One-Electron Atom

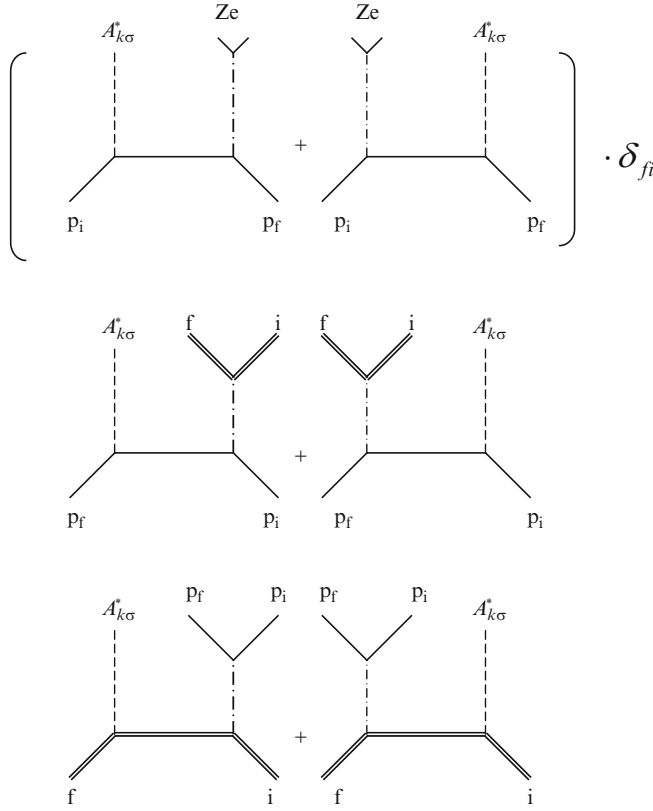
In this paragraph the expression for the amplitude of Bs of a relativistic incident particle (IP) on a one-electron (hydrogen-like) atom is derived within the framework of the consistent quantum-electrodynamic approach.

Let us consider the collision of a relativistic charged particle (the charge  $e_0$ , the mass  $m_0$ , the initial energy  $\varepsilon_i = \sqrt{p_i^2 + m_0^2}$ ) in the state  $|p_i\rangle$  with a hydrogen-like atom being in the state  $|n_i\rangle$  with the energy  $E_i$ . (It will be recalled that the symbol  $|\psi\rangle$  means the Dirac ket vector corresponding to the wave function  $\psi$ .)

As a result of collision, the IP goes to the state  $|n_f\rangle$  with the energy  $\varepsilon_f = \sqrt{p_f^2 + m_0^2}$ , a bremsstrahlung photon with the frequency  $\omega$  and the wave vector  $\mathbf{k}$  is emitted, and the atom goes to the state  $|n_f\rangle$  with the energy  $E_f$ .

We assume that the incident particle satisfies the Dirac equation. Besides, we consider satisfied the Born condition for IP velocities before ( $v_i$ ) and after ( $v_f$ ) collision with a target ( $Z$  is the atomic nucleus charge):

$$Z e_0 \ll v_{i,f}. \quad (2.1)$$



**Fig. 2.1** The diagrams describing the amplitude of bremsstrahlung on an atom in the third order of the perturbation theory

In this case the IP is described by a plane wave in contrast to the exact solution of the Dirac equation in the external nuclear field that is necessary to describe a bound electron of an atom. In the case that an incident particle is an electron, this makes it possible also to neglect exchange summands in the process amplitude.

Let us use the standard quantum-electrodynamics perturbation theory for a scattering operator [1]. In its lower order of interaction between an IP and an atomic electron with an electromagnetic field we have a graphic expression for the Bs amplitude (Fig. 2.1).

In Fig. 2.1 the single lines correspond to the wave functions and the propagator of an incident particle, the double lines correspond to an atomic electron in the nuclear field,  $\delta_{fi}$  is the Kronecker symbol. It will be recalled that the propagator (or the propagation function) describes the amplitude of probability of particle propagation from one spatio-temporal point to another. The wavy line means the electromagnetic field: the photon propagator and the wave function of a free photon  $A_{\mathbf{k}\sigma}$  ( $\mathbf{k}$  is the wave vector,  $\sigma$  is the photon polarization index).

The analytical expression for the amplitude of total Bs corresponding to the diagrams shown in Fig. 2.1 represents the sum of static and polarization terms:

$$M_{fi} = M_{fi}^{st} + M_{fi}^{pol} \quad (2.2)$$

The first summand in Eq. 2.2 corresponds to the ordinary (static) channel, its expression looks like:

$$M_{fi}^{st} = -\frac{4\pi e_0^2 e}{q^2} A_{\mathbf{k},\sigma}^{\mu*} \left[ Z g^{0\nu} \langle f|i \rangle - j_{fi}^\nu(\mathbf{q}) \right] G_{\nu\mu}(p_1, p_2), \quad (2.3)$$

where

$$G_{\nu\mu}(p_1, p_2) = \frac{\bar{u}_f}{\sqrt{2\varepsilon_f}} \left[ \gamma_\nu \frac{\gamma p_2 + m_0}{p_2^2 - m_0^2} \gamma_\mu + \gamma_\mu \frac{\gamma p_1 + m_0}{p_1^2 - m_0^2} \gamma_\nu \right] \frac{u_i}{\sqrt{2\varepsilon_i}} \quad (2.4)$$

is the propagator of a free electron. In the formulas (2.3) and (2.4) the following designations are used:

$$\begin{aligned} q_1 &= p_f - p_i, \quad q = q_1 + k, \quad p_2 = p_f + k, \quad p_1 = p_i - k, \quad A_{\mathbf{k},\sigma} = \sqrt{2\pi/\omega} e_{\mathbf{k},\sigma}, \\ |p\rangle &= \frac{u(p,s)}{\sqrt{2\varepsilon}} \exp(-ipx), \quad j_{n'n}^\mu(\mathbf{k}) = \langle n' | \gamma^\mu \exp(-i\mathbf{k}\mathbf{r}) | n \rangle, \quad a = a^\mu = \{a^0, \mathbf{a}\}, \\ ab &= a^\mu b_\mu = a^0 b_0 - \mathbf{a}\mathbf{b}, \quad \mu, \nu = 0 \div 3. \end{aligned}$$

The metric, normalization and designations in the formula (2.3) are analogous to those used in the book [1]:  $g_{\mu\nu}$  is the metric tensor,  $\gamma^\mu$  are the Dirac matrices. The normalization of bispinors:  $\bar{u}u = u^+ \gamma^0 u = 2m_0$  corresponds to the normalization of the wave function of an incident charge to one particle in the main region with a unit volume. The wave function of a photon  $A_{\mathbf{k},\sigma}$  is also normalized to one photon in the main region,  $e_{\mathbf{k},\sigma}$  is the polarization 4-vector that in the laboratory system of coordinates satisfies the three-dimensionally transverse gauge:  $e_{\mathbf{k},\sigma} = \{0; \mathbf{e}_{\mathbf{k},\sigma}\}$ ,  $\mathbf{k}\mathbf{e}_{\mathbf{k},\sigma} = 0$ .  $n, f, i$  is the set of quantum numbers defining a stationary state of an atom.

The second summand in the formula (2.2) corresponds to the polarization channel. We have for it [2, Chap. 5]:

$$M_{fi}^{pol} = \frac{4\pi}{q_1^2} A_{\sigma\nu\mathbf{k}}^* \sum_n \left[ \frac{j_{nfn}^\nu(\mathbf{k}) j_{nni}^\mu(\mathbf{q}_1)}{E_f - E_n + \omega \pm i0} + \frac{j_{nfn}^\mu(\mathbf{q}_1) j_{nni}^\nu(\mathbf{k})}{E_i - E_n - \omega \pm i0} \right] \frac{\bar{u}_f \gamma_\mu u_i}{2\sqrt{\varepsilon_f \varepsilon_i}} \quad (2.5)$$

The sum over intermediate states extends both to the positive (+i0) and to the negative (-i0) energy spectrum of an atomic electron.

Let us analyze the diagrams of Fig. 2.1 and their associated formulas (2.3) and (2.5). The first four graphic summands and their associated expression for the static amplitude (Eq. 2.3) in the case that an atomic electron does not change its state give the classical Bethe-Heitler result [3] – bremsstrahlung of a relativistic electron in

the static nuclear field and the atomic electron field screening it (the screening approximation). If in these terms of the process amplitude all possible final states of an atomic electron are taken into account, we will obtain the Lamb and Wheeler result [4]. The Fourier transform of the time part of the transitional current 4-vector at  $f = i$  gives an ordinary form factor of charge screening. Its space part is a current (magnetic) summand of screening and can be essential in Bs with excitation of deep atomic shells for high nuclear charges.

It should be noted that the consistent electrodynamic approach to the relativistic problem of Bs on an atom even in the ordinary static part of the process amplitude leads to results supplementing the Bethe-Heitler theory: to taking into account a possibility of change of an atomic state and to appearance of a current additive in the form factor caused by the space components of the transitional current 4-vector for an atomic electron.

The last two graphic summands in Fig. 2.1 and their associated expression (2.5) describe the emission of a bremsstrahlung photon by an atomic electron in collision of an IP with an atom. These terms appear if an atomic electron is considered as a peer dynamic particle interacting with an electromagnetic field, including the electromagnetic field of vacuum. The contribution to total bremsstrahlung given by these summands is called polarization bremsstrahlung since it is defined by the dynamic polarization of an atom in the IP field.

A characteristic feature of the polarization summand of the amplitude of Bs on an atom is the presence of sums over intermediate states of an atomic electron with resonant energy denominators. And the relativistic (for a bound electron) problem in addition to the resonance in the electronic spectrum of atomic states has a resonant denominator in the positron part of the sum, when  $\omega = \varepsilon_i - \varepsilon_n^{(-)} \approx 2m$ . However, we will restrict ourselves to the frequency range  $\omega \ll m$ .

The total Bs cross-section contains also the interference contribution of the static and polarization channels. But, as it will be seen from the following, its value for a relativistic IP is small.

It is of interest to trace two passages to the limit in the expression (2.2). Let us assume at first that a nucleus is absent ( $Z = 0$ ). In this case the first two diagrams presented in Fig. 2.1 will disappear. In the remaining four diagrams it is necessary to replace the double lines describing an atomic electron in the nuclear field by single lines (describing a free electron). Then these diagrams go to the graphic representation of the process of IP emission on a free electron that is well known in quantum electrodynamics. In this case the first pair of diagrams describes the contribution of an incident particle to Bs in its scattering by an electron, and the second pair of diagrams describes the contribution of a recoil electron to the process.

In the high-frequency range ( $\omega \gg m$ ) in case of an incident electron a result is obtained that is known from quantum electrodynamics: recoil electron emission can be neglected, in this case a fast electron emits at a slow unit charge as at an immobile one. It should be noted that to obtain the said passage to the limit, it is

necessary to take into account all possible excitations of an atom both in the discrete spectrum and in the continuous spectrum.

In another limiting case, when an atomic electron is absent, the last four diagrams in Fig. 2.1 disappear, and the process amplitude comes to bremsstrahlung on a “bare” nucleus.

From the diagrams of Fig. 2.1 it is seen that the ordinary (static or Bethe-Heitler) and polarization summands of the amplitude differently depend on the mass and charge of an IP. Really,  $M_{fi}^s \propto e_0^2 e / m_0$ , and  $M_{fi}^{pol} \propto e_0 e^2 / m$ , and static Bs disappears with the IP mass tending to infinity, while the polarization summand remains finite. The change of the sign of the incident particle charge does not change the static amplitude and changes the sign of the polarization amplitude, which results in changing sign of the interference summand of the total cross-section of Bs on an atom.

Let us consider a case of a nonrelativistic atomic electron ( $Z \ll 137$ ,  $|E_{i,f} - m| \ll m$ ). If, besides,  $\omega \ll m$ , the expression (2.5) can be transformed to the form containing only nonrelativistic characteristics of an atomic electron.

Really, at  $Z \ll 137$  we have the following passage to the limit for the components of the current 4-vector:

$$\begin{aligned} j_{fn}^\mu(\mathbf{q}_1) &= \int d\mathbf{r} \varphi_f^* \{1, \vec{\alpha}\} \varphi_n \exp(-i \mathbf{q}_1 \mathbf{r}) \\ &\approx \left\{ \int d\mathbf{r} \varphi_f^* \exp(-i \mathbf{q}_1 \mathbf{r}) \varphi_n; \int d\mathbf{r} \varphi_f^* \hat{j}(\mathbf{q}_1) \varphi_n \right\}, \end{aligned} \quad (2.6)$$

here

$$\hat{j}(\mathbf{q}) = \exp(-i \mathbf{q} \mathbf{r}) \frac{(-i \nabla)}{2m} + \frac{(-i \nabla)}{2m} \exp(-i \mathbf{q} \mathbf{r}) \quad (2.7)$$

is the nonrelativistic expression for the spatial Fourier transform of the current density operator,  $\nabla$  is the vector differential operator.

The approximate Eq. 2.6 corresponds to the formal expansion of atomic bispinors to the large ( $\sim 1$ ) and small ( $\sim v_a$ ) spinors and to following neglect of spin additives.

Thus in the polarization term of the amplitude (Eq. 2.5) in the sum over intermediate states with positive energy the transition to the nonrelativistic description comes to replacement of relativistic expressions for transitional currents by their nonrelativistic analogs. The sum over intermediate states with negative energy can be transformed if it is assumed that the main contribution to it is made by states, the energy of which satisfies the inequality  $||E_n^{(-)}| - m| \ll m$ . In view of the fact that  $|E_{f,i} - m| \ll m$  and  $\omega \ll m$ , the energy denominators in the summands with negative energy can be replaced by the value  $2m$ . Further, using the projection operator  $(m - \hat{H}_a)/2m$  ( $\hat{H}_a$  is the atomic Hamiltonian) for the space of wave

functions with negative energy, it is possible to extend summation to the whole energy spectrum of an atomic electron. For this purpose we assume:

$$(m - \hat{H}_a)/2m = (1 - \gamma^0)/2$$

$$\gamma^0 |n^\pm\rangle = \pm |n^\pm\rangle,$$

then

$$\sum_{E_n < 0} \approx \frac{1}{2m} \langle f | \exp(-i \mathbf{q} \mathbf{r}) \left( \gamma^\mu \frac{(1 - \gamma^0)}{2} \gamma^\nu + \gamma^\nu \frac{(1 - \gamma^0)}{2} \gamma^\mu \right) | i \rangle, \quad (2.8)$$

and in view of the permutation relation  $\gamma^\mu \gamma^\nu + \gamma^\nu \gamma^\mu = 2 \delta^{\mu\nu}$  we will obtain:

$$\sum_{E_n < 0} \approx \frac{\delta^{\mu\nu}}{m} \langle f | \exp(-i \mathbf{q} \mathbf{r}) | i \rangle = \frac{\delta^{\mu\nu}}{m} j_{fi}^{(0)}(\mathbf{q}). \quad (2.9)$$

Thus the polarization term of the amplitude for a nonrelativistic atomic electron looks like:

$$M_{fi}^{pol} = \frac{4 \pi e_0 e^2}{q_1^2} A_{\mathbf{k}\sigma}^* \sum_{E_n > 0} \left[ \frac{j_{fn}^\nu(\mathbf{k}) j_{ni}^\mu(\mathbf{q}_1)}{\omega_{fn} + \omega + i0} + \frac{j_{fn}^\mu(\mathbf{q}_1) j_{ni}^\nu}{\omega_{in} - \omega + i0} + \frac{\delta^{\mu\nu}}{m} j_{fi}^0(\mathbf{q}) \right] \frac{\bar{u}_f \gamma_\mu u_i}{2 \sqrt{\epsilon_f \epsilon_i}}. \quad (2.10)$$

The expression (2.10) in case of a nonrelativistic IP leads to the known result of the nonrelativistic theory of PBs [2]:

$$M_{fi}^{pol} = \frac{4 \pi e_0 e^2}{q_1^2} \sqrt{\frac{2 \pi}{\omega}} \sum_n \left\{ \frac{\mathbf{e}_{\mathbf{k}\sigma} \mathbf{j}_{fn}(\mathbf{k}) j_{ni}^0(\mathbf{q}_1)}{\omega_{fn} + \omega + i0} + \frac{j_{fn}^0(\mathbf{q}_1) \mathbf{e}_{\mathbf{k}\sigma} \mathbf{j}_{ni}(\mathbf{k})}{\omega_{in} - \omega + i0} \right\}. \quad (2.11)$$

To derive the formula (2.11) from (2.10), it is necessary to suppose (neglecting spin effects):

$$\bar{u}_f \gamma^\mu u_i / 2 \sqrt{\epsilon_i \epsilon_f} \approx \{1, \mathbf{v}_0\}, \quad |\mathbf{q}_1| \ll |\mathbf{p}_{i,f}|.$$

## 2.2 Amplitude of Bremsstrahlung of a Fast Charged Particle on a Multielectron Atom

The consistent quantum-electrodynamic consideration of PBs of a relativistic IP on a multielectron atom is complicated by the necessity to take into account the interaction between atomic electrons in the relativistic formalism as well as by

the problem of summation over states with negative energy for a multielectron system. At the same time calculation for nonrelativistic atomic electrons can be considerably simplified if from the very beginning a nonrelativistic atomic Hamiltonian is used and an incident particle is replaced by the electromagnetic field it produces (by a set of virtual photons).

Let us justify a possibility of such a replacement. Let the free IP field operator  $\hat{\varphi}(x)$  ( $x = \{t, \mathbf{r}\}$ ) satisfy the Dirac equation:

$$(\gamma p - m_0)\hat{\varphi}(x) = 0. \quad (2.12)$$

We will assume that for the operator of the electron-positron field of atomic electrons  $\hat{\psi}(x)$  the Dirac equation with interaction is true:

$$\left[ \gamma \left( p + e A^{ext}(x) + e \hat{A}^{ae} \right) - m \right] \hat{\psi}(x) = 0, \quad (2.13)$$

where  $A^{ext}(x)$  is the potential of the external nuclear field,  $\hat{A}^{ae}(x)$  is the operator of the electromagnetic field produced by atomic electrons that satisfies the Maxwell equation:

$$\partial^\nu \partial_\mu \hat{A}^{ae\mu}(x) - \partial^\mu \partial_\mu \hat{A}^{ae\nu}(x) = 4\pi e \hat{j}^\nu(x), \quad (2.14)$$

where  $\hat{j}^\nu(x) = \hat{\bar{\psi}}(x) \gamma^\nu \hat{\psi}(x)$  is the operator of atomic electron current, summation is supposed over twice-repeating indices.

Thus it is supposed that the interaction between atomic electrons is taken into account in  $\hat{\psi}(x)$ .

Let us represent the state vectors for the system of fields (of atomic electrons, an incident particle, an electromagnetic field) as the product:  $|\Phi_j\rangle = |j\rangle |\varphi_j\rangle |n_{\mathbf{k}\sigma}\rangle$ , where  $|j\rangle$  is the state vector for atomic electrons interacting among themselves,  $|\varphi_j\rangle$  is the state vector for a free incident particle,  $|n_{\mathbf{k}\sigma}\rangle$  is the state vector for an electromagnetic field. The equation for the system state vector  $|\Phi\rangle$  in the interaction representation looks like:

$$i\partial|\Phi\rangle/\partial t = \int dr \left[ e_0 \hat{J}^\nu(x) - e \hat{j}^\nu(x) \right] \hat{A}_\nu(x) |\Phi\rangle,$$

where

$$\hat{J}^\nu(x) = \ddot{\varphi}(x) \gamma^\nu \hat{\varphi}(x)$$

is the four-dimensional vector of the operator of incident particle current density.

$$\hat{S} = T \exp \left\{ -i \int dx \hat{A}_\nu(x) \left[ e_0 \hat{J}^\nu(x) - e \hat{j}^\nu(x) \right] \right\}, \quad (2.15)$$

where  $T$  is the chronological ordering symbol.

The PBs amplitude in the lower order of the perturbation theory is described by the third term in the expansion of the scattering operator  $\hat{S}$  (here for short we use the designation  $x_i \equiv i$ ):

$$\hat{S}_3 = (-i)^3 e^2 e_0 \int d1 d2 d3 T \left\{ \hat{A}_v(1) \hat{j}^v(1) \hat{A}_\mu(2) \hat{j}^\mu(2) \hat{A}_\lambda(3) \hat{j}^\lambda(3) \right\}. \quad (2.16)$$

In obtaining this formula similar summands resulting from rearrangement of integration variables were reduced. Hereafter we consider that there is no exchange between an incident particle and atomic electrons. Using the commutativity of corresponding operators, the expression (2.16) for the scattering operator in the third order of the perturbation theory can be rewritten as:

$$\hat{S}_3 = (-i)^2 \int d1 d2 \hat{A}_v(1) T \left\{ e^2 \hat{j}^v(1) \hat{j}^\mu(2) \right\} \int d3 e_0 D_{\mu\lambda}(2, 3) \hat{j}^\lambda(3), \quad (2.17)$$

where  $D_{\mu\lambda}(2, 3) = iT \langle 0 | \hat{A}_\mu(2) \hat{A}_\lambda(3) | 0 \rangle$  is the photon propagator.

In the formula (2.17) one unpaired  $\hat{A}$ -operator is retained, which corresponds to the one-photon change of the electromagnetic field.

By matrixing the scattering operator  $\hat{S}$  with respect to the initial and final states of the system we obtain:

$$S_{3fi}^{pol} = (-i)^2 \int d1 d2 A_{\mathbf{k}\sigma v}^*(1) L_{fi}^{v\mu}(1, 2) A_{\mu fi}^{(0)}(2), \quad (2.18)$$

where

$$L_{fi}^{v\mu}(1, 2) = e^2 \langle f | T \left\{ \hat{j}^v(1) \hat{j}^\mu(2) \right\} | i \rangle \quad (2.19)$$

is the relativistic analog of the tensor of electromagnetic field scattering by an atom;

$$A_{\mu fi}^{(0)}(2) = -e_0 \int d3 D_{\mu\nu}(2, 3) \langle \varphi_f | \hat{j}^\nu(3) | \varphi_i \rangle \quad (2.20)$$

is the 4-potential of a virtual photon produced by an incident particle in the process of scattering:  $|\varphi_i\rangle \rightarrow |\varphi_f\rangle$ . It should be noted that the potential of a virtual photon  $A_{fi}^{(0)}$  could be found from the Maxwell equations (2.14) if on their right side the matrix element of the IP transitional current operator  $\langle \varphi_f | \hat{j}^\mu(3) | \varphi_i \rangle$  is substituted.

The formula (2.18) for the amplitude of PBs allows its interpretation as a process of scattering (conversion) of a virtual photon  $A_{fi}^{(0)}$  by atomic electrons to a real photon.



It is easy to show that the same expression for the PBs amplitude can be obtained from another form of the interaction Hamiltonian:

$$V' = -e \int d\mathbf{r} \left\{ \hat{A}_v(x) + A_{fi,v}^{(0)}(x) \right\} \hat{j}^v(x). \quad (2.21)$$

Here an incident particle is replaced by the electromagnetic field  $A_{fi}^{(0)}$  it produces and thus it is excluded from consideration as a dynamical degree of freedom. The field  $A_{fi}^{(0)}$  can be considered a specified field determined by the Eq. 2.20 – the prescribed current approximation. Then the PBs amplitude is obtained by the standard method in the second order of the perturbation theory. After calculation of a corresponding matrix element we find for it:

$$S_{2,fi}^{pol} = (-i)^2 \int d1 d2 A_{\mathbf{k}\sigma,v}^*(1) \langle f | T \left\{ e^2 \hat{j}^v(1) \hat{j}^\mu(2) \right\} | i \rangle A_{fi}^{(0)}(2). \quad (2.22)$$

From comparison of the formulas (2.18) and (2.22) it follows:

$$S_{3,fi}^{pol} = S_{2,fi}^{pol}.$$

Thus the PBs amplitude can be calculated (with fixed initial and final IP states) with replacing an incident particle by the field it produces with the help of formula (2.20). Then in the case under consideration for nonrelativistic atomic electrons a single relativistic degree of freedom – an incident particle – will be excluded, and it is possible to use the nonrelativistic formalism to calculate the Bs amplitude.

It should be noted that replacement of a particle by its field is widely used also in calculation of Bethe-Heitler Bs by the equivalent photon method, when in the IP rest frame the atomic field is replaced by equivalent photons that are Compton-scattered to bremsstrahlung photons by an incident particle.

Let us calculate, replacing an IP by its field, the PBs amplitude for a nonrelativistic multielectron atom ( $Z < 137$ ) with neglected exchange of incident and bound electrons. We use the axial gauge of the electromagnetic potential ( $A_0 = 0$ ). The nonrelativistic Hamiltonian of perturbation of atomic electrons by the electromagnetic field looks like:

$$V = \frac{e}{2m} \sum_j \left\{ \hat{\mathbf{p}}_j \hat{\mathbf{A}}(\mathbf{r}_j, t) + \hat{\mathbf{A}}(\mathbf{r}_j, t) \hat{\mathbf{p}}_j + e \hat{\mathbf{A}}^2(\mathbf{r}_j, t) \right\}, \quad (2.23)$$

where  $\hat{\mathbf{p}}_j = -i \nabla_j$ ,  $\hat{\mathbf{A}} = \hat{\mathbf{A}}^{ph} + \mathbf{A}_{fi}^{(0)}$  is the sum vector-potential, the operator  $\hat{\mathbf{A}}^{ph}$  describes the photon field ( $kx = \omega t - \mathbf{k}\mathbf{r}$ ,  $\omega = |\mathbf{k}|$ ),

$$\hat{\mathbf{A}}^{ph}(x) = \sum_{\mathbf{k}, \sigma} \sqrt{\frac{2\pi}{\omega}} \left\{ \mathbf{e}_{\mathbf{k}, \sigma} \hat{c}_{\mathbf{k}, \sigma} \exp(-ikx) + \mathbf{e}_{-\mathbf{k}, \sigma}^* \hat{c}_{-\mathbf{k}, \sigma}^+ \exp(ikx) \right\}, \quad (2.24)$$

where  $\mathbf{e}_{\mathbf{k},\sigma}$  is the unit vector of photon polarization,  $c_{\mathbf{k},\sigma}^+, c_{\mathbf{k},\sigma}$  are the operators of birth and destruction of photons;  $\mathbf{A}_{fi}^{(0)}$  is given by the formula (2.20) – this is an external field produced by an incident particle.

Going to the interaction representation  $\hat{V}_{\text{int}} = \exp(i\hat{H}_a t) V \exp(-i\hat{H}_a t)$  (the photon field is already written in the interaction representation), we have for the scattering operator:

$$\hat{S} = T \exp \left\{ -i \int_{-\infty}^{\infty} \hat{V}_{\text{int}}(t) dt \right\}. \quad (2.25)$$

The contribution to the PBs amplitude in the lower order of the perturbation theory (in the second order with respect to an electron charge) is made by the first and second terms of the expansion  $S$ , the zeroth term of this expansion – one – corresponds to the unchanged state of the system. In the first-order term the contribution to the process is made by the summand containing the squared sum vector potential, in the first-order term in perturbation the contribution is made by the summand containing  $\hat{\mathbf{p}}\hat{\mathbf{A}} + \hat{\mathbf{A}}\hat{\mathbf{p}}$ . According to the physical picture of PBs, it is necessary to take into account terms containing the mixed product  $\hat{\mathbf{A}}_{ph}$  and  $\mathbf{A}_{fi}^{(0)}$ . So the matrix element of the process is represented as

$$S_{fi}^{pol} = S_{fi}^{(1)} + S_{fi}^{(2)},$$

here

$$S_{fi}^{(1)} = -i \langle \Phi_f | \int_{-\infty}^{\infty} dt \exp(iH_a t) \frac{e^2}{2m} \sum_{j=1}^N 2\hat{\mathbf{A}}^{ph}(\mathbf{r}_j, t) \mathbf{A}_{fi}^{(0)}(\mathbf{r}_j, t) \exp(-iH_a t) | \Phi_i \rangle, \quad (2.26)$$

with  $|\Phi_j\rangle = |j\rangle |n_{\mathbf{k},\sigma}\rangle$  since an incident particle is already taken into account in  $\mathbf{A}_{fi}^{(0)}$ .

From the relation (2.26) we find

$$S_{fi}^{(1)} = -2i\pi\delta(\varepsilon_f + E_f + \omega - \varepsilon_i - E_i) \sqrt{\frac{2\pi}{\omega}} \mathbf{e}_{\mathbf{k},\sigma}^* \mathbf{A}_{fi}^{(0)}(q_1) \langle f | \sum_{j=1}^N \exp(-i\mathbf{q}\mathbf{r}_j) | i \rangle \frac{e^2}{m}, \quad (2.27)$$

where  $\mathbf{A}_{fi}^{(0)}(q_1)$  is the spatio-temporal Fourier transform of the incident particle field calculated on the four-dimensional vector  $q_1 = \{\varepsilon_f - \varepsilon_i, \mathbf{p}_f - \mathbf{p}_i\}$ . Spin effects are neglected. By analogy, for  $S_{fi}^{(2)}$  we have the expression:

$$S_{fi}^{(2)} = -\frac{1}{2} \langle \Phi_f | T \int \int dt dt' \hat{V}_{\text{int}}(t) \hat{V}_{\text{int}}(t') | \Phi_i \rangle. \quad (2.28)$$

After simple transformations the matrix element of the scattering operator  $S_{fi}^{(2)}$  is brought to the form:

$$S_{fi}^2 = -e^2 2\pi \delta(\Delta E_i) \sqrt{\frac{2\pi}{\omega}} e_{k,\sigma,1}^* A_{fi,s}^{(0)}(q_1) \langle f | \int d\tau \exp(i\omega\tau) \hat{j}^l(\mathbf{k}, \tau) \hat{j}^s(\mathbf{q}_1) | i \rangle, \quad (2.29)$$

where

$$\hat{j}^l(\mathbf{k}, \tau) = \exp(iH_a\tau) \frac{1}{2m} \sum_{j=1}^N \left\{ \hat{p}_j^l \exp(-i\mathbf{k}\mathbf{r}_j) + \exp(-i\mathbf{k}\mathbf{r}_j) \hat{p}_j^l \right\} \exp(-iH_a\tau)$$

is the spatial Fourier transform of the operator of atomic electron current in the interaction representation.

Summing the matrix elements  $S_{fi}^{(1)}$  and  $S_{fi}^{(2)}$ , we obtain the PBs amplitude as:

$$S_{fi}^{\text{pol}} = 2\pi i \delta(\varepsilon_f + E_f + \omega - \varepsilon_i - E_i) (q_1^0)^2 \sqrt{\frac{2\pi}{\omega}} e_{k,\sigma,t}^* A_{fi,s}^{(0)}(q_1) \langle f | \hat{c}^{ls}(k, \mathbf{q}_1) | i \rangle, \quad (2.30)$$

where

$$q_1^0 = \varepsilon_f - \varepsilon_i$$

is the change of IP energy during the process.

In the expression (2.30)  $\hat{c}^{ls}(k, \mathbf{q}_1)$  is the operator of electromagnetic field scattering by an atom in the nonrelativistic (for atomic electrons) approximation that can be represented in the following form:

$$\hat{c}^{ls}(k, \mathbf{q}_1) = \frac{e^2}{m(q_1^0)^2} \left[ im \int_{-\infty}^{\infty} d\tau \exp(i\omega\tau) T \{ \hat{j}^l(\mathbf{k}, \tau) \hat{j}^s(\mathbf{q}_1, 0) \} - \delta^{ls} \hat{n}(\mathbf{q}) \right], \quad (2.31)$$

where  $\hat{n}(\mathbf{q}) = \sum_{j=1}^N \exp(-i\mathbf{q}\mathbf{r}_j)$  is the Fourier transform of the operator of atom electron density.

Analyzing the initial relativistic expression, from which Eq. 2.31 follows, it can be said that the first summand in the square brackets in Eq. 2.31 arises from the sum over the positive part of the atomic electron spectrum and describes scattering of an electromagnetic field by the atomic electron current. The second summand in

Eq. 2.31 arises after folding of the sum over states of the negative energy spectrum and describes field scattering by the atomic electron charge.

Let us write the matrix element  $c_{fi}^{ls}(k, \mathbf{q}_1)$  in terms of the sum over intermediate states of atomic electrons:

$$c_{fi}^{ls}(k, \mathbf{q}_1) = \frac{e^2}{m(q_1^0)^2} \left\{ m \sum_n \left[ \frac{j_{fn}^l(\mathbf{k}) j_{ni}^s(\mathbf{q}_1)}{\omega_{fn} + \omega + i0} + \frac{j_{fn}^s(\mathbf{q}_1) j_{ni}^l(\mathbf{k})}{\omega_{in} - \omega + i0} \right] - \delta^{ls} n_{fi}(\mathbf{q}) \right\}. \quad (2.32)$$

In case of the spherically symmetric state  $|i\rangle$  and within the framework of the dipole approximation (for  $f = i$ ,  $\mathbf{k} = \mathbf{q}_1 = 0$ ), from the formula (2.32) it follows:

$$c_{ii}^{ls}(\mathbf{q}_1, \mathbf{k} \rightarrow 0) \rightarrow \alpha(\omega) \delta^{ls} = \delta^{ls} \frac{e^2}{m} \sum_n \frac{f_{in}}{\omega_{in}^2 - \omega^2}, \quad (2.33)$$

where  $\alpha(\omega)$  is the dipole polarizability of an atom,  $f_{in}$  is the oscillator strength for the transition  $i \rightarrow n$ . In the formulas (2.30), (2.31), (2.32) and (2.33) it is implied that the bremsstrahlung photon frequency detuning  $\Delta$  from resonance is great enough, so that:  $\Delta = |\omega - \omega_{f(i)n}| \gg \Gamma_{f(i)n}$ , where  $\Gamma_{f(i)n}$  is the line width for the transition  $n \rightarrow f(i)$ . Otherwise in these expressions it is necessary to take into account the line width for corresponding transitions.

It is well seen that the obtained expression for the PBs amplitude (Eq. 2.30) corresponds to its interpretation as a process of scattering of the incident particle eigenfield by atomic electrons to a bremsstrahlung photon.

Now let us calculate the amplitude of static (ordinary) bremsstrahlung (due to emission of a photon by an incident particle) taking into account possible excitation of atomic electrons. We use again the interpretation of bremsstrahlung as a process of scattering of a virtual photon to a real photon. Now virtual photons are produced by an atom (by a nucleus and bound electrons). For an atom at rest and nonrelativistic atomic electrons, virtual photons produced by them are mainly longitudinal. In this case it is convenient to use the Coulomb gauge of the electromagnetic potential ( $\text{div} \mathbf{A} = 0$ ) since then it is possible to take into account only its time component. The space components describe in the Coulomb gauge the transverse part of the field and in the case under consideration are small. The time component of the potential of a virtual photon produced by an atom according to Eq. 2.20 is

$$A_{fi}^0 = - \int d1' D_{00}(1, 1') \langle f | \hat{J}^0(1') | i \rangle, \quad (2.34)$$

where

$$\hat{J}^0(1) = Ze\delta(\mathbf{r}_1 - \mathbf{r}_0) - e \sum_{j=1}^N \delta(\mathbf{r}_1 - \mathbf{r}_j)$$

is the atomic charge density operator in the coordinate representation ( $\mathbf{r}_0$  is the radius vector of a nucleus). According to the standard rules of quantum electrodynamics [1], it is easy to obtain the expression for the static bremsstrahlung amplitude:

$$S_{fi}^{st} = -2\pi i \sqrt{\frac{2\pi}{\omega}} e_0^2 e_{k,\sigma,\nu}^* T^v(p_{f,i}; k) A_{fi}^0(q) \delta(\varepsilon_f + E_f + \omega - \varepsilon_i - E_i). \quad (2.35)$$

Here the following designations are introduced:

$$T^v = \frac{\bar{u}_f}{\sqrt{2\varepsilon_f}} \left\{ \gamma^v \frac{p_f \gamma + \gamma k + m_0}{(p_f + k)^2 - m_0^2} \gamma^0 + \gamma^0 \frac{p_i \gamma - \gamma k + m_0}{(p_i - k)^2 - m_0^2} \gamma^v \right\} \frac{\bar{u}_i}{\sqrt{2\varepsilon_i}}, \quad (2.36)$$

$$A_{fi}^0(\mathbf{q}) = (4\pi/\mathbf{q}^2) \{ \delta_{fi} Z e - e n_{fi}(\mathbf{q}) \}. \quad (2.37)$$

Physically Eq. 2.37 describes the screened potential of a nucleus, and Eq. 2.36 describes scattering of an electromagnetic field by an incident particle.

Thus the total amplitude of Bs of a relativistic incident particle on a nonrelativistic atom ( $Z \ll 137$ ) in view of the polarization mechanism and possible excitation of atomic electrons with neglected spin effects looks like:

$$S_{fi}^{Br} = S_{fi}^{st} + S_{fi}^{pol}, \quad (2.38)$$

where  $S_{fi}^{pol}$  and  $S_{fi}^{st}$  are given respectively by the formulas (2.30) and (2.35).

## 2.3 Total Bremsstrahlung of a Fast Charged Particle on an Atom

### 2.3.1 General Expression for the Process Cross-Section

Based on the obtained expression for the amplitude, we will write the expression for the spectral Bs cross-section [1]:

$$\frac{d\sigma^{Br}(\omega)}{d\omega} = \frac{\varepsilon_i}{|\mathbf{p}_i|} \sum_{f,\sigma} \frac{d\Omega_{\mathbf{k}}}{(2\pi)^3} \frac{d\mathbf{q}}{(2\pi)^3} \lim_{T \rightarrow \infty} \frac{|S_{fi}^{Br}(\sigma; \mathbf{p}_{f,i}; \mathbf{k})|}{T}, \quad (2.39)$$

here  $d\Omega_{\mathbf{k}}$  is the solid angle around the direction of the photon wave vector  $\mathbf{k}$ ,  $T$  is the parameter having time meaning, summation is made over polarizations of an emitted photon ( $\sigma$ ) and final states of an atom ( $|f\rangle$ ). As before, we consider an

incident particle to be a Born particle, and the initial state of an atom to be nondegenerate.

In view of the explicit form of  $S_{fi}^{Br}$  the formula (2.39) can be rewritten:

$$\begin{aligned} \frac{d\sigma^{Br}(\omega)}{d\omega} &= \frac{\varepsilon_i}{|\mathbf{p}_i|} \sum_{f,\sigma} \omega^2 \frac{d\Omega_{\mathbf{k}}}{(2\pi)^3} \frac{d\mathbf{q}}{(2\pi)^3} 2\pi\delta(\Delta E) \\ &\times \frac{2\pi}{\omega} \left| e_{\mathbf{k}\sigma,l}^* \left\{ e_0^2 T^l \frac{4\pi}{q^2} (Ze\delta_{fi} - en_{fi}(\mathbf{q})) + (q_1^0)^2 c_{fi}^{ls} A_{fi,s}^0 \right\} \right|^2 \end{aligned} \quad (2.40)$$

or

$$\frac{d\sigma^{Br}(\omega)}{d\omega} = \frac{d\sigma^{st}}{d\omega} + \frac{d\sigma^{pol}}{d\omega} + \frac{d\sigma^{int}}{d\omega}. \quad (2.41)$$

The last term in Eq. 2.41 describes the interference of the static and polarization Bs,  $T^l$  and  $c_{fi}^{ls}$  are given by the formulas (2.36) and (2.32) of the previous paragraph.

Hereafter we assume that  $|\mathbf{q}_1| \ll |\mathbf{p}_{f,i}|$  – the motion of an IP is weakly disturbed during bremsstrahlung. So in the following formulas we use one value of IP velocity:  $\mathbf{v}_i \cong \mathbf{v}_f \equiv \mathbf{v}_0$ . Then for the vector potential of the virtual photon field  $A_{fi}^{(0)}$  we have the expression:

$$\mathbf{A}^{(0)}(q) \simeq \frac{4\pi e_0}{q^0} \frac{\mathbf{v}_0 q^0/c^2 - \mathbf{q}}{(q^0/c)^2 - \mathbf{q}^2} \delta(q^0 - \mathbf{q}\mathbf{v}), \quad (2.42)$$

where  $\mathbf{v}_0$  is the velocity of an incident particle.

In the same approximation for the function  $T$  (see the definition (2.36)) we obtain:

$$\mathbf{T} = \frac{\mathbf{q}_1}{m_0 \gamma (\omega - \mathbf{k}\mathbf{v}_0)}, \quad \gamma = \varepsilon_i/m_0. \quad (2.43)$$

The obtained expression (2.40) for the cross-section of bremsstrahlung on an atom is the most general. With neglected internal degrees of freedom for an IP and an atomic nucleus it describes consistently the contribution of atomic electrons to the Bs process.

For the static Bs cross-section from Eq. 2.40 after simple transformations we find:

$$\begin{aligned} \frac{d\sigma^{st}}{d\omega} &= \frac{\omega}{v_0} \int \frac{d\Omega_{\mathbf{k}} d\mathbf{q}}{(2\pi)^4} \int dt e^{it(\omega+q_1^0)} \sum_{\sigma} \left| \mathbf{e}_{\mathbf{k},\sigma}^* \mathbf{T} \right|^2 \\ &\times \frac{e_0^4 e^2}{q^2} \langle i | (Z - \hat{n}(-\mathbf{q})) (Z - \hat{n}(\mathbf{q}, t)) | i \rangle. \end{aligned} \quad (2.44)$$

If the energy of excitation of atomic electrons can be neglected in comparison with the frequency of an emitted photon  $\omega$ , then in the formula (2.44) it is possible to assume  $\hat{n}(\mathbf{q}, t) \approx \hat{n}(\mathbf{q}, 0)$ :

$$\frac{d\sigma^{st}}{d\omega} = \frac{\omega}{v_0} \int \frac{d\Omega_{\mathbf{k}} d\mathbf{q}}{(2\pi)^3} \delta(q_1^0 + \omega) [\mathbf{n} \mathbf{T}]^2 \frac{e_0^4 e^2}{\mathbf{q}^2} \langle i | |Z - \hat{n}(\mathbf{q})|^2 | i \rangle, \quad \mathbf{n} = \frac{\mathbf{k}}{k}. \quad (2.45)$$

In derivation of (2.45) the equation was used:  $\sum_{\sigma} e_{\mathbf{k}\sigma,l}^* e_{\mathbf{k}\sigma,s} = \delta_{ls} - n_l n_s$ .

The expression (2.45) agrees with the result of Lamb and Wheeler [4] who for the first time consistently took into consideration the contribution of excitation of atomic electrons to static bremsstrahlung.

In case of a heavy IP ( $m_0 \gg m$ ) the first summand under the modulus sign in the formula (2.40) can be neglected in comparison with the second summand since  $|\mathbf{T}| \propto 1/m_0$ , while  $\mathbf{A}^{(0)}(\mathbf{q})$  and  $\hat{c}^{ls}(k, \mathbf{q}_1)$  do not depend on the IP mass. Then the total cross-section of Bs on an atom comes to the PBs cross-section, for which from Eq. 2.40 we find:

$$\frac{d\sigma^{pol}}{d\omega} = \frac{\omega}{v_0} \int \frac{d\Omega_{\mathbf{k}} d\mathbf{q}}{(2\pi)^5} (\delta_{ls} - n_l n_s) (q_1^0)^4 A_{fi,s'}^{(0)}(q_1) A_{fi,r'}^{(0)}(q_1) \int dt e^{iq_1^0 t} \langle i | \hat{c}^{sl'*}(0) \hat{c}^{ls'}(t) | i \rangle, \quad (2.46)$$

where

$$\hat{c}^{ls}(t) = \exp(i H_a t) \hat{c}^{ls}(0) \exp(-i H_a t) \quad (2.47)$$

is the operator of electromagnetic field scattering by an atom in the Heisenberg representation.

Thus the polarization bremsstrahlung cross-section summed over all final states of atomic electrons is expressed in terms of the correlation function of the operator of electromagnetic field scattering by an atom that can be written as

$$Kc_{ii}(t) \equiv \langle i | \hat{c}^{ls'*}(0) \hat{c}^{ls'}(t) | i \rangle,$$

where summation is supposed over twice-repeating indices.

### 2.3.2 PBs Without Excitation of a Target

Let us consider PBs without excitation of an atom ("elastic" PBs). Its cross-section is given by the summand with  $f = i$  in the second term under the modulus sign in the formula (2.40):

$$\frac{d\sigma_{ii}^{pol}}{d\omega} = \frac{\omega}{v_0} \int \frac{d\Omega_{\mathbf{k}} d\mathbf{q}}{(2\pi)^4} (\delta_{ls} - n_l n_s) (q_1^0)^4 A_h^{(0)}(q_1) A_r^{(0)}(q_1) \delta(q_1^0 + \omega) \langle i | \hat{c}^{lh} | i \rangle \langle i | \hat{c}^{sr*} | i \rangle. \quad (2.48)$$

At first we consider the spectral range  $\omega \ll p_a v_0$  ( $p_a \approx Z^{1/3} m e^2$  is the characteristic atomic momentum). Then the main contribution to the process under consideration will be made by the moduli  $|\mathbf{q}_1| \ll p_a$  permitted by the energy conservation law. Otherwise ( $|\mathbf{q}_1| > p_a$ ) PBs with excitation and ionization of an atom should prevail. So in this case for the scattering tensor the dipole approximation can be used:

$$c_{ii}^{lh}(k, \mathbf{q}_1) \rightarrow \delta^{lh} \alpha_i(\omega) \theta(p_a - |\mathbf{q}_1|), \quad (2.49)$$

and instead of Eq. 2.48 we will obtain:

$$\frac{d\sigma_{ii}^{pol}}{d\omega} \approx \frac{\omega}{v_0} \int \frac{d\Omega_{\mathbf{k}} d\mathbf{q}}{(2\pi)^4} \left[ \mathbf{n} \mathbf{A}^{(0)}(q_1) \right]^2 \delta(q^0) \theta(p_a - |\mathbf{q}_1|) |\omega^2 \alpha_i(\omega)|^2, \quad \omega < p_a v_0. \quad (2.50)$$

It should be noted that the used approximation corresponds to the Born-Bethe approximation in the theory of atomic excitation by electron impact.

From the formula (2.50) we find the following expression for the frequency-angular distribution of elastic PBs in the frequency range under consideration:

$$\frac{d\sigma_{ii}^{pol}(\omega, \vartheta)}{d\omega} = \frac{2 e_0^2}{v_0^2} \frac{d\omega}{\omega} |\omega^2 \alpha_i(\omega)|^2 (1 + \cos^2 \vartheta) \sin \vartheta d\vartheta \ln \left( \frac{\gamma p_a v_0}{\omega} \right), \quad (2.51)$$

where  $\vartheta$  is the angle between the initial IP velocity vector and the bremsstrahlung photon wave vector (radiation angle).

In derivation of the formula (2.51) summands of the order of one were neglected in comparison with the large logarithm (the large logarithm approximation).

From the expression (2.51) two corollaries follow:

1. In contrast to static Bs, polarization Bs of an ultrarelativistic IP ( $\gamma \gg 1$ ) in the frequency range  $\omega < p_a v_0$  is not directional, but is of a dipole nature,
2. The PBs cross-section grows logarithmically with IP energy in the ultrarelativistic limit at  $\omega < p_a v_0$ .

These characteristic features of PBs of a relativistic IP allow descriptive physical interpretation. The logarithmic growth of the PBs cross-section with IP energy is connected with the features of the spatial structure of the electromagnetic eigenfield of a relativistic charged particle. The spatial distribution of the potential of this field at the frequency  $\omega$  is given by the formula:

$$A^{(0)}(\omega) \propto \exp \left( i \frac{\omega}{v_0} (z - v_0 t) - i \frac{\omega \rho}{\gamma v_0} \right), \quad (2.52)$$

here  $z, \rho$  are the cylindrical coordinates of the IP field.



Thus we obtain the lateral dimension of the field  $\rho_{\max} \approx \gamma v_0/\omega$ , and accordingly for the minimum transferred transverse momentum we have  $|\mathbf{q}_\perp|_{\min} \approx \omega/\gamma v_0$ . Hence from the formula for the spectral PBs cross-section (in the Born approximation):  $d\sigma^{pol}(\omega) \propto \ln(|\mathbf{q}_\perp|_{\max}/|\mathbf{q}_\perp|_{\min})$  the second PBs property follows that is noted here. It should be noted that in case of static Bs on a neutral atom the maximum size of a field scattered by an IP to a bremsstrahlung photon is defined by the size of an atom.

### 2.3.3 High-Frequency Limit

Now we will consider “elastic” PBs (without change of an atomic state) in the frequency range  $I \ll \omega \ll m$  ( $I$  is the atomic ionization potential). In this case it is possible to use the high-frequency asymptotics for the scattering operator:

$$\hat{c}^{ls}(k, \mathbf{q}_1) \approx -\frac{e^2}{m(q_1^0)^2} \hat{n}(\mathbf{q}) \left\{ \delta^{ls} + \frac{q_1^l q_1^s}{2m\omega} \right\}, \quad I \ll \omega \ll m. \quad (2.53)$$

The formula (2.53) is obtained with the use of the expansion into a series of the matrix element  $c_{fi}^{ls}$  (Eq. 2.32) in terms of the powers of the ratio  $|\omega_{jn}|/\omega$  ( $j = f, i$ ), the summands in the sum over intermediate states with  $|\omega_{jn}| > \omega$  making a small contribution to  $c_{fi}^{ls}$  at  $\omega \gg I$ . Substituting the formula (2.53) in Eq. 2.48, we find:

$$\frac{d\sigma_{ii}^{pol}}{d\omega} = \frac{\omega}{v_0} \int \frac{d\Omega_{\mathbf{k}} d\mathbf{q}}{(2\pi)^4} \delta(q^0) \left( \frac{e^2}{m} \right)^2 |n_{ii}(\mathbf{q})|^2 \left[ \mathbf{n}, \left( \mathbf{A}^{(0)}(\mathbf{q}) + \frac{\mathbf{q}_1 (\mathbf{q}_1 \mathbf{A}^{(0)}(\mathbf{q}_1))}{2m\omega} \right) \right]^2, \quad I \ll \omega \ll m. \quad (2.54)$$

To simplify the calculations, we consider that  $\gamma \gg 1$ , then the IP field is mainly transverse and  $\mathbf{q}_1 \mathbf{A}^{(0)}(\mathbf{q}_1) = 0$ . We use the approximation of *exponential* screening of an atomic nucleus to calculate the spectral PBs cross-section. Then:

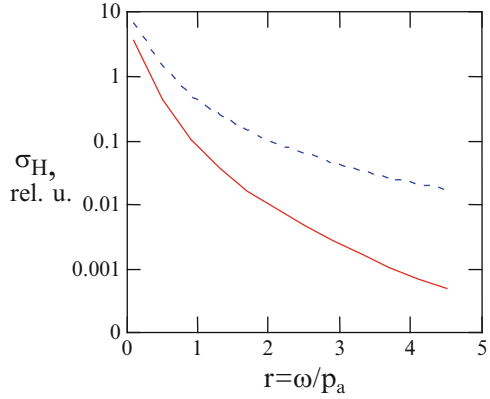
$$n_{ii}(\mathbf{q}) = \frac{N}{(1 + \mathbf{q}^2/p_a^2)}. \quad (2.55)$$

Here  $N$  is the number of atomic electrons (for a neutral atom, naturally,  $N = Z$ ).

The value  $n_{ii}(\mathbf{q})$  represents the (static) form factor of the atomic core in the state  $|i\rangle$ .

Using Eq. 2.55 and the relation  $\alpha_i(\omega) \rightarrow \alpha_\infty(\omega) = -N e^2/m\omega^2$  to estimate the spectral PBs cross-section in a high-frequency range, we find for three spectral

**Fig. 2.2** The spectral cross-section of PBs of a relativistic electron on a hydrogen atom in the high-frequency region  $\omega \gg I = 0.5$  a.u. as a function of the parameter  $r = \omega/p_a$  for two values of the relativistic factor:  $\gamma = 2$  (solid line),  $\gamma = 10$  (dotted line)



ranges after integration with respect to the solid angle of photon escape and the transferred momentum the following expressions:

$$\frac{d\sigma_{ii}^{pol}}{d\omega} = \frac{16}{3} N^2 \frac{e^4 e_0^2}{m^2 \omega} \ln\left(\frac{\gamma p_a}{\omega}\right) \quad I \ll \omega \ll p_a, \quad (2.56)$$

$$\frac{d\sigma_{ii}^{pol}}{d\omega} = 2 N^2 \frac{e^4 e_0^2}{m^2 \omega} \left(\frac{p_a}{\omega}\right)^2 \ln(\gamma) \quad p_a \ll \omega \ll \gamma^2 p_a, \quad (2.57)$$

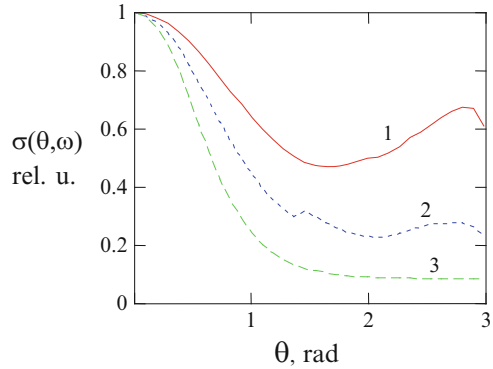
$$\frac{d\sigma_{ii}^{pol}}{d\omega} = 4 N^2 \frac{e^4 e_0^2}{m^2 \omega} \left(\frac{p_a}{\omega}\right)^2 \left(\frac{\gamma^2 p_a}{\omega}\right)^2 \quad \gamma^2 p_a \ll \omega \ll m. \quad (2.58)$$

The formulas (2.56), (2.57), and (2.58) are low-sensitive to a specific type of nucleus screening by atomic electrons. The spectral cross-section (2.56) can be obtained from the formula (2.51) since in this frequency range the dipole approximation for interaction of an IP with an atomic core (and especially with a photon) is still true.

The spectral cross-section of PBs of a relativistic electron on a hydrogen atom in a high-frequency range calculated by the formulas (2.56) and (2.57) is presented in Fig. 2.2 for two values of the relativistic factor  $\gamma$ .

From the given figure it follows that the cross-section of PBs of a relativistic electron in the high-frequency range  $\omega > p_a$  decreases with growing frequency. Physically this is a consequence of coherence loss for interaction of a virtual photon of the IP field with an atomic electron. From mathematical point of view, this decrease is defined by reduction of the atomic form factor  $n_{ii}(\mathbf{q})$  with growing magnitude of the transferred wave vector  $|\mathbf{q}| > p_a$ . Another conclusion of Fig. 2.2 is the growth of the PBs cross-section with increasing energy of a relativistic incident particle (of the relativistic factor  $\gamma$ ).

**Fig. 2.3** The angular dependence of PBs on an atom ( $Z = 30$ ) in the high-frequency approximation for different frequencies of a bremsstrahlung photon:  $\omega = 5$  keV (curve 1),  $\omega = 15$  keV (curve 2),  $\omega = 50$  keV (curve 3), the IP velocity is:  $v = 0.9 c$



The frequency range of Eq. 2.57 is characteristic for ultrarelativistic incident particles. In this range the compensation of a momentum transferred from an IP to an atom due to a photon momentum is possible. As the analysis shows, this is true only for small enough radiation angles:  $\vartheta \leq \sqrt{p_a/\omega} \approx \sqrt{\lambda/R_a}$ ,  $R_a \approx p_a^{-1}$ . This inequation follows from the condition of smallness of a momentum transferred to a target during Bs in comparison with an atomic momentum:  $\omega(1 - v_0 \cos(\vartheta)) \leq p_a v_0$ .

Thus in the frequency range of Eq. 2.57 PBs gains directionality, and in calculation of the process cross-section it is necessary to take into account a photon momentum.

The angular diagram of PBs of a relativistic electron on a hydrogen atom in the high-frequency limit is presented in Fig. 2.3 for different values of bremsstrahlung photon energy.

It is seen that with growing energy of a bremsstrahlung photon the angular distribution of PBs of a relativistic electron is narrowed.

In the frequency range of Eq. 2.58 (if it exists) a momentum transferred from an IP to the atomic core at any radiation angles is more than the characteristic atomic momentum, and PBs is strongly suppressed as it follows from the form of the static atomic form factor (2.57). Physically this means that with large momenta transferred to an atom ( $|\mathbf{q}| \gg p_a$ ) that are characteristic for this frequency range inelastic PBs channels prevail that are accompanied by excitation and ionization of an atomic electron.

It should be noted that in the above “elastic” PBs the contribution of all atomic electrons to radiation is coherent, so the process cross-section is proportional to the squared number of atomic electrons. This circumstance can be explained as follows. During elastic PBs, when the state of the atomic core does not change, an electron charge, remaining localized in the atom, shows itself as the charge of one particle  $Ne$  (at  $\lambda > R_a$ ). Therefore the amplitude of its interaction with an electromagnetic field is proportional to  $Ne$ , and the cross-section is proportional to  $(Ne)^2$ .

Let us return to the total PBs cross-section that takes into account excitation of atomic electrons – the formula (2.46). To obtain the spectral PBs cross-section in the explicit form in the general case does not seem possible. Let us consider some particular, but practically important situations.

Let the frequency  $\omega$  be such that the main contribution to the cross-section that is differential with respect to a transferred momentum is made by  $|\mathbf{q}_1| < p_a$ . (This in particular takes place in experiments on agreement (see [5]) if a scattered electron is observed at small scattering angles). Then the dipole approximation for interaction of an IP with the atomic core is true, and it is possible to integrate with respect to  $\mathbf{q}$  in view of the explicit form of  $\mathbf{A}^{(0)}(q)$  (Eq. 2.42). Taking into account the spherical symmetry of the state  $|i\rangle$ , we obtain after a number of transformations for the spectral PBs cross-section the following expression (we assume that  $\omega_{si} < p_a v_0 - \omega$ ):

$$\frac{d\sigma_{fi}^{pol}}{d\omega} = \frac{16 e_0^2}{9 v_0^2} \sum_{m,l,f} \omega^3 |\langle f | \hat{c}_{ml}(\omega) | i \rangle|^2 \ln \left( \frac{\gamma p_a v_0}{\omega + \omega_{fi}} \right). \quad (2.59)$$

It should be noted that the summand in the formula (2.59) with  $f = i$  gives the spectral cross-section of elastic PBs following also from the formula (2.51) after integration with respect to the angle of photon escape.

### 2.3.4 Near-Resonant PBs

Let us consider a case of the near-resonance frequency  $\omega$ , when the following inequation is satisfied:  $\Gamma_{nf} < |\omega - \omega_{nf}| < \omega$ , here  $\omega_{nf}$  and  $\Gamma_{nf}$  are the eigenfrequency and the line width for the transition  $n \rightarrow f$  between two states of the discrete spectrum of the atomic core. Then in the expression for the matrix element from the operator of electromagnetic field scattering by an atom (Eq. 2.32) one resonant summand can be separated that makes the main contribution to the amplitude, and the imaginary part of the scattering tensor can be neglected in comparison with the real part. Then in the sum over  $f$  on the right side of the Eq. 2.59 one resonant summand remains.

After summation over the projections of the total momentum of resonant states we find for a singlet initial state:

$$\begin{aligned} \frac{d\sigma_{fi}^{res}}{d\omega} &= \frac{4 e_0^2 e^4}{3 v_0^2 m^2} \left( \frac{\omega}{\Delta} \right)^2 \frac{f_{in}}{\omega_{ni}} (2J_f + 1) f_{fn} \ln \left( \frac{\gamma p_a v_0}{\omega + \omega_{fi}} \right) \quad \Delta = \omega - \omega_{nf} \\ &\quad \omega \gg |\Delta| \gg \Gamma_{fn}, \end{aligned} \quad (2.60)$$

here  $f_{ik}$  is the oscillator strength for the transition  $i \rightarrow k$ ,  $J_f$  is the quantum number of the total angular momentum of an atom in the state  $|f\rangle$ .

Following from the expression (2.60) for  $f = i$  is the formula for “elastic” near-resonance PBs that was studied in detail earlier [2].

The case  $f \neq i$  was studied in the paper of V.M. Buimistrov and L.I. Trakhtenberg [6] from the standpoint of the prospect of obtaining radiation amplification based on the PBs effect.

Given in the author's work [7] is the generalization of the spectrum of near-resonant PBs to the case of the energy-band structure of a target in the elementary isotropic effective mass approximation.

In this situation the scattering tensor can be represented as:

$$c^{hl}(k, q) = \int_{\Omega_{Br}} \frac{d\vec{k}}{(2\pi)^3} \frac{e^2}{\omega^2} \frac{j_{vc}^h(\mathbf{k}, \vec{k}) j_{cv}^l(\mathbf{q}, \vec{k})}{\omega - \omega_{cv}(\vec{k}) + i\Gamma_{cv}/2}. \quad (2.61)$$

Here integration is performed with respect to the quasi-momentum of electrons  $\vec{k}$  in the Brillouin zone  $\Omega_{Br}$ ,  $\omega_{cv}(\vec{k}) = \varepsilon_c(\vec{k}) - \varepsilon_v(\vec{k})$  is the difference of electron energies in the conduction band and in the valence band. Then we will assume that transitional current weakly depends on an electron quasi-momentum. In the general case it is necessary to perform integration in the formula (2.61) in view of the dispersion law  $\varepsilon_{c,v}(\vec{k})$ . We will consider the approximation of parabolic bands, in which:  $\varepsilon_{v,c}(\vec{k}) = \varepsilon_{v,c}^0 \mp \vec{k}^2/2m_{v,c}$ ,  $m_{v,c}$  are the effective masses of electrons near the valence band top and the conduction band bottom. Then after averaging over photon polarizations for the spectral intensity of PBs the following expression can be obtained:

$$\frac{dW^{pol}}{d\omega} = B(\omega) |J(\Delta)|^2, \quad (2.62)$$

where

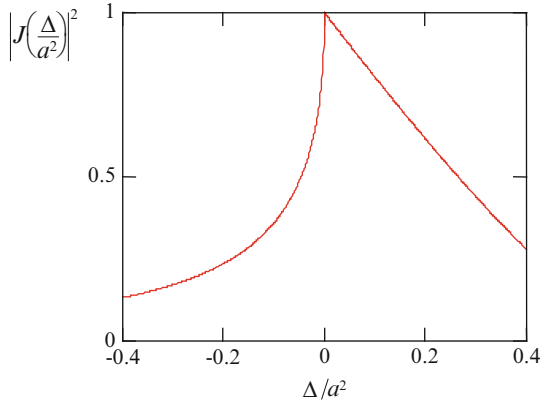
$$B(\omega) = \int \frac{d\mathbf{q}}{(2\pi)^{10}} \mu_{cv}^3 e^4 [\mathbf{n} \mathbf{j}_{vc}(\mathbf{k})]^2 (\mathbf{A}(q) \mathbf{j}_{cv}(\mathbf{q}))^2,$$

$$J(\Delta) = \begin{cases} 1 - \frac{\sqrt{|\Delta|}}{a} \operatorname{arctg}\left(\frac{a}{\sqrt{|\Delta|}}\right), & \Delta < 0 \\ 1 + \frac{\sqrt{\Delta}}{2a} \ln \left| \frac{a - \sqrt{\Delta}}{a + \sqrt{\Delta}} \right|, & \Delta > 0 \end{cases}$$

$$\Delta = \omega - (\varepsilon_c^0 - \varepsilon_v^0), \quad \mu_{cv}^{-1} = m_c^{-1} + m_v^{-1}, \quad a \approx N_v^{1/3} / \mu_{cv}^{1/2}, \quad \mathbf{n} = \mathbf{k}/|\mathbf{k}|,$$

$N_v$  is the concentration of the valence band electrons. The target parameter is  $a^2$ , it is proportional to the energy of localization of a quasi-particle with the reduced mass  $\mu_{cv}$  in the volume  $N_v^{-1}$ , its value is accordingly of the order of the permitted band width.

**Fig. 2.4** The plot of the function  $|J(x)|^2$  describing the spectrum of near-resonance PBs for a case of the energy-band structure of a target in the isotropic effective mass approximation



In the formula (2.62) it is assumed that  $a^2 \neq |\Delta|$ , otherwise it is necessary to take into account the imaginary additive in the expression for the scattering tensor (2.61).

The function  $B(\omega)$  has no resonance peculiarities for the case under consideration:  $\omega < v_0/d$  ( $d$  is the lattice constant), so the frequency peculiarities of the PBs spectrum are described by the function  $|J(\Delta)|^2$ , the plot of which is presented in Fig. 2.4 for the case of practical interest  $\Delta < a^2$  ( $a^2 = N_v^{2/3}/\mu_{cv}$ ).

From this figure it follows in particular that the spectrum of near-resonance PBs for the energy-band structure of a target has a pronounced asymmetry: for frequencies smaller than the energy gap width (negative detunings from resonance  $\Delta$ ) the PBs intensity falls more steeply than for positive detunings. This circumstance is quite expected since positive detunings correspond to the virtual transition to the conduction band, and negative detunings correspond to the virtual transition to the band gap.

The function  $J(\Delta)$  itself for detunings under consideration is positive ( $\Delta < a^2$ ), which corresponds to destructive interference with the static Bs channel. For high detunings  $\Delta > a^2$  this function is negative, and interchannel interference is constructive.

It should be noted that in the limit  $a^2 \ll |\Delta|$  in the expression (2.62) the multiplier  $|\omega_{cv}/\Delta|^2$  appears that is characteristic for near-resonant PBs on one atom.

It is significant that if  $\omega < \omega_{cv}$  and  $|\Delta| > \Gamma_{cv}$ , a cascade process connected with real filling of the conduction band is impossible.

### 2.3.5 PBs with Target Excitation

Now we will calculate the PBs cross-section with excitation (including ionization) of an atom for  $m \gg \omega \gg I$ . Substituting the expression for  $\hat{c}^{lh}$  in this spectral range Eq. 2.53 in the formula (2.48), we find

$$\frac{d\sigma_{ii}^{pol}}{d\omega} = \frac{\omega}{v_0} \int \frac{d\Omega_{\mathbf{k}} d\mathbf{q}}{(2\pi)^4} \left(\frac{e^2}{m}\right)^2 \left[ \mathbf{n}, \left( \mathbf{A}^{(0)}(q_1) + \frac{\mathbf{q}_1 (\mathbf{q}_1 \mathbf{A}^{(0)}(q_1))}{2m\omega} \right) \right]^2 S_{ii}(q). \quad (2.63)$$

Here the value is introduced:

$$S_{ii}(q) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dt \exp(iq^0 t) \langle i | \hat{n} | (-\mathbf{q}) \hat{n}(\mathbf{q}, t) | i \rangle \quad (2.64)$$

that we will call the dynamic form factor according to the terminology accepted for description of effects in a media. For simplicity we assume further  $q_1 \approx q$ , so neglecting summands of the order of  $(p_a/\omega)^2$  in comparison with one at  $\omega \gg p_a$ ; at  $\omega < p_a$  the dipole approximation is true, so the magnitudes  $|\mathbf{q}|$  and  $|\mathbf{k}|$  can be neglected in comparison with  $p_a$ . As seen from Eq. 2.63, for calculation of the spectral PBs cross-section it is necessary to know the explicit form of the  $\mathbf{q}$  and  $q^0$  functional dependence of  $S_{ii}$ .

With further tracing only qualitative moments in mind, here we use for calculations the simplest analytical approximation of  $S_{ii}(q)$ :

$$S_{ii}(q) \approx \theta(|\mathbf{q}| - p_a) \delta\left(q^0 + \frac{\mathbf{q}_1^2}{2m}\right) N + \theta(p_a - |\mathbf{q}|) \delta(q^0) N^2, \quad (2.65)$$

where  $N$  is the number of electrons in an atom.

The approximate Eq. 2.65 can be obtained after a number of transformations, taking into account the explicit form of the electron density operator being an operator of shift in the momentum space and corresponding permutation relations.

The physical meaning of two summands in Eq. 2.65 is transparent: the first summand describes processes with ionization of the atomic core, when a transferred momentum is large, in this case the contribution of bound electrons is incoherent and part of energy is carried away by a knocked-on electron. The second summand describes the coherent process, when a momentum transferred to the core from an IP is small, and the atom remains in the former state. In the latter case the recoil momentum takes over a massive nucleus, and coherence takes place since the phase of electromagnetic interaction of the IP with the target core changes little at distances of the order of the atomic radius.

From the formulas (2.63) and (2.65) it is easy to find the spectral PBs cross-section in the approximation under consideration:

$$\begin{aligned} \frac{d\sigma_{ii}^{pol}}{d\omega} = \frac{16e_0^2 e^4}{3m^2 v_0^2} \left\{ \theta(p_a v_0 - \omega) \left[ N^2 \ln\left(\frac{\gamma p_a v_0}{\omega}\right) + N \ln\left(\frac{m_0 v_0}{p_a}\right) \right] \right. \\ \left. + \theta(\omega - p_a v_0) N \ln\left(\frac{\gamma m_0 v_0^2}{\omega}\right) \right\}. \end{aligned} \quad (2.66)$$

The obtained expression allows descriptive physical interpretation. At  $\omega < p_a v_0$  (the summand in the square brackets) PBs proceeds both without excitation of an atom (if  $|\mathbf{q}| < p_a$ ) and with its ionization (at  $|\mathbf{q}| > p_a$ ). And in the first case PBs is coherent by the contribution of atomic electrons to the process (the cross-section is proportional to  $N^2$ ), in the second case PBs is incoherent (the cross-section is proportional to the number of atomic electrons  $N$ ). In the spectral range  $\omega > p_a v_0$  – the second summand in the braces in Eq. 2.66 – the law of conservation of energy-momentum permits only  $|\mathbf{q}| > p_a$ , so PBs proceeds mainly with atomic ionization, and its cross-section is proportional to  $N$ .

It is essential that the total PBs cross-section (2.66) taking into account excitation and ionization of an atom admits a correct passage to the limit to the case  $Z = 0$ , corresponding to which is the equation  $p_a = 0$  in the formula (2.66). Then the summand in the square brackets describing “elastic” PBs disappears, and the remaining last term in the braces describes emission of a slow free recoil electron in collision with a relativistic charged particle as it must be according to the physical picture of the process. It should be noted that this passage to the limit does not take place for the “elastic” PBs cross-section since in the absence of a nucleus the process becomes fundamentally inelastic – an atomic electron takes over a momentum excess and increases its energy.

Let us compare integrated (with respect to the scattering and radiation angles) cross-sections of the polarization and static Bs channels. Corresponding cross-sections look most simple in the quasi-classical ( $\varepsilon_{f,i} \gg \omega$ ) and ultrarelativistic ( $\gamma \gg 1$ ) limits and in the region of frequencies exceeding the atomic ionization potential.

Thus in the spectral range  $p_a v_0 > \omega \gg I$  the main contribution to both Bs channels is made by the “elastic” summands (without excitation of the atomic core) (we assume  $Z, N \gg 1$ ):

$$\frac{d\sigma_{ii}^{pol}}{d\omega} = \frac{16N^2 e^6}{3m^2 \omega} \ln\left(\frac{\gamma p_a}{\omega}\right), \quad (2.67)$$

$$\frac{d\sigma_{ii}^{st}}{d\omega} = \frac{16Z^2 e^6}{3m^2 \omega} \ln\left(\frac{m}{p_a}\right), \quad (2.68)$$

that (in case of  $Z = N$ ) differ only by logarithmic factors, though they have (in the ultrarelativistic case) essentially different radiation patterns.

Let us write out the cross-sections of inelastic static and polarization Bs in the spectral range where the main contribution to PBs is made by the processes with atomic ionization:

$$\frac{d\sigma_{nonel}^{pol}}{d\omega} = \frac{16Ne^6}{3m^2 \omega} \ln\left(\frac{\varepsilon}{\omega}\right), \quad (2.69)$$



$$\frac{d\sigma_{nonel}^{stl}}{d\omega} = \frac{16Ne^6}{3m^2\omega} \ln\left(\frac{m}{p_a}\right), \quad \gamma \gg \sqrt{\frac{\omega}{p_a}}. \quad (2.70)$$

Thus in the frequency range  $p_a v_0 \ll \omega \ll m$  the cross-sections of elastic static and elastic polarization Bs differ only by logarithmic factors, and inelastic summands of the cross-section corresponding to them are close in value up to  $\omega \approx m$ .

At  $\omega \gg m$  the space part of the 4-momentum transferred to an atom is great, and atomic electrons can to a good accuracy be considered free, which gives the result known in quantum electrodynamics when a recoil electron emits  $\omega/m$  times less than a fast electron. Thus the contribution of the polarization summand to the total cross-section of Bs of an electron on an atom in the region of high ( $\omega \gg m$ ) frequencies is negligibly small in comparison with the contribution of the static summand.

All aforesaid is true also for the case of Bs of an ultrarelativistic positron on an atom, when the sign of the polarization summand of the amplitude changes to the opposite. But, as for an electron, due to different dependences of the static and polarization summands on radiation angles their interference can be neglected and thereby the total cross-section of Bs of an ultrarelativistic particle can be represented as the sum of two summands (polarization and static).

### 2.3.6 Channel Interference

Now let us consider the summand in the cross-section of Bs on a neutral atom describing the interference of the static and polarization channels. As follows from the analysis of angular dependences, this interference is low for an ultrarelativistic incident particle. So here we will consider an incident particle to be nonrelativistic, but still a Born particle. Let us neglect excitation of an atom during bremsstrahlung. Then from Eq. 2.40 in view of Eqs. 2.42 and 2.43 it can be obtained for the interference summand in the cross-section:

$$\frac{d\sigma_{ii}^{int}}{d\omega} \approx \frac{32 e_0^2 \omega^3}{3 v_0^2} \int_{\omega/v_0}^{|\mathbf{q}_1|_{\max}} \frac{|e e_0|}{m_0 \omega} \operatorname{Re}\{c_{ii}(\omega; |\mathbf{q}_1|)\} (Z - n_{ii}(\mathbf{q}_1)) \frac{d|\mathbf{q}_1|}{|\mathbf{q}_1|}. \quad (2.71)$$

In derivation of Eq. 2.71 it was taken into account that for a nonrelativistic IP  $|\mathbf{q}_1| \geq \omega/v_0 \gg |\mathbf{k}|$ . We call attention to the fact that the contribution to interference is made only by the real part of the diagonal matrix element from the operator of electromagnetic field scattering by an atom (Eq. 2.31). For the elementary approximation of the scattering tensor (2.49) from the formula (2.71) we have approximately:

$$\frac{d\sigma_{ii}^{\text{int}}}{d\omega} \approx \frac{32|e_0^2 e|}{3m_0 v_0^2} \omega^2 \{\text{Re}[\alpha_i(\omega)]\} \int_{p^*}^{p_a} \frac{(Z - n_{ii}(|\mathbf{q}_1|))}{|\mathbf{q}_1|} d|\mathbf{q}_1|, \quad (2.72)$$

$p^* = \max\{p_{\min}, \omega/v_0\}$ , where  $p_{\min}$  is the characteristic momentum of outer shell electrons,  $p_a$  is the characteristic momentum of atomic electrons making the main contribution to atomic polarizability at the frequency under consideration  $\omega$ . From Eq. 2.72 it follows that the interference term in the Bs cross-section can be noticeable if the greatest contribution to polarizability is made by the inner atomic shell with comparable cross-sections of PBs and SBs. This takes place, for example, for Bs of electrons on neutral xenon for frequencies near the potential of ionization of the 4f -subshell.

The radiation spectrum of xenon in case of passage of an electron beam through it was recorded in the work [8]. A shift of the frequency maximum from the value calculated without considering interference to 20 eV was found. This discrepancy was explained by the fact that the velocity of electrons in a beam is probably not high enough for the Born approximation to work “well”. On the other hand, a reason of shift can be an interference term in the total Bs cross-section that was not taken into account. And if an IP is heavy or ultrarelativistic, the expected value of shift should be small due to the smallness of the interference summand in these cases.

For an ultrarelativistic IP the theory results in an additional possibility of interest: the value of shift of the Bs frequency maximum relative to the potential of ionization of a corresponding atomic subshell sharply depends on the angle of photon emission, which is caused by essentially different patterns of the static and polarization Bs channels in the ultrarelativistic case.

It should be noted that the above brief analysis of channel interference relates to Bs of a Born IP on a neutral atom, where, generally speaking, interference effects in the Bs cross-section integrated with respect to the angle of incident particle scattering are low due to different regions of space of channel formation: corresponding to the static channel are large angles of IP scattering and respectively small distances to a nucleus, corresponding to the polarization channel are small scattering angles and large distances.

Thus interference effects in Bs on a neutral atom can show themselves most strongly in the Bs cross-section differential with respect to the angle of IP scattering, which was shown in the work [9]. The situation is different for Bs on ions for strongly inelastic scattering of electrons of moderate energies, when channel interference is found to be essential also in the integrated process cross-section.

## 2.4 Polarization Bremsstrahlung of a Fast Charged Particle on an Atom in the Local Plasma Approximation

The spectral PBs cross-sections in the high-frequency limit obtained in the previous paragraph in Eqs. 2.56, 2.57, and 2.58 are true for the frequencies  $\omega \gg I$ , where  $I$  is the characteristic atomic ionization potential (it will be recalled that in this chapter

we use the relativistic system of units, in which  $\hbar = c = 1$ ). In case of a multielectron atom this value is of rather indefinite nature, so the domain of applicability of the high-frequency approximation requires its refinement.

At the same time it is for a multielectron atom that polarization effects in Bs should be the most essential. And the calculation of the dynamic polarizability of a multielectron atom defining the PBs cross-section is an intricate quantum-mechanical problem that has to be solved anew for each specific target.

In this connection it seems to be useful to apply simple universal models suitable for estimation of the value of the polarization Bs cross-section and for revealing general qualitative regularities of this process.

One of such models is the method of local electron density (or local plasma frequency) that was first proposed by Brandt and Lundqvist for calculation of the cross-section of photoabsorption by multielectron atoms [10].

In this section this method is used to describe PBs of a fast (including relativistic) charged particle on a neutral multielectron atom, the distribution of electron density in which is given by the statistical Thomas-Fermi model.

It should be noted that the use of the local plasma frequency method for calculation of the polarizability of a Thomas-Fermi atom is intrinsically consistent since the physical representations underlying both models are analogous.

The advantages of the used approach are also that it is most adequate just for those frequencies and distances, at which the significant role is played by multielectron effects, the description of which within the framework of the consistent quantum-mechanical consideration is difficult and laborious.

### 2.4.1 Polarizability of a Thomas-Fermi Atom in the Local Plasma Frequency Approximation

Within the framework of the Brandt-Lundqvist model the expression for the dynamic polarizability of an atom looks like:

$$\alpha(\omega) = \int_0^{\infty} \frac{\omega_p^2(r) r^2 dr}{\omega_p^2(r) - \omega^2 - i0}, \quad (2.73)$$

where  $\omega_p(r) = \sqrt{4\pi e^2 n(r)/m}$  is the local plasma frequency depending on the local electron density of the electron core  $n(r)$ ,  $r$  is the distance from a point under consideration to an atomic nucleus.

Hereafter for the function  $n(r)$  the Thomas-Fermi approximation will be used that gives [11]:

$$n(r) = n_{TF}(r) = Z^2 f(r/r_{TF}), \quad f(x) = \frac{32}{9\pi^3} \left( \frac{\chi(x)}{x} \right)^{3/2}, \quad (2.74)$$

where  $r_{TF} = b a_0 / Z^{1/3}$  is the Thomas-Fermi radius ( $b = (9 \pi^2 / 128)^{1/3} \cong 0.8853$ ,  $a_0$  is the Bohr radius,  $Z$  is the nuclear charge),  $\chi(x)$  is the Thomas-Fermi function.

The expression (2.71) can be transformed to the form revealing the scaling law (scaling) with respect to the parameter  $v = \hbar \omega / 2 R y Z$  ( $R y = 13.6$  eV) having the meaning of dimensionless (reduced) frequency:

$$\alpha(v) = r_{TF}^3 \beta(v) = \frac{b^3 a_0^3}{Z} \beta(v). \quad (2.75)$$

Here the dimensionless complex function  $\beta(v)$  (the reduced polarizability of a Thomas-Fermi atom) is introduced, the imaginary part of which is (the prime means differentiation with respect to the argument  $x$ ):

$$\text{Im}\{\beta(v)\} = \pi \frac{f(x_v) x_v^2}{|f'(x_v)|}, \quad (2.76)$$

and the real part can be calculated by the “punctured” Kramers-Kronig relation:

$$\text{Re}\{\beta(v)\} = \frac{2}{\pi} \int_0^\infty \frac{[\text{Im}\{\beta(v)\} - \text{Im}\{\beta(\tilde{v})\}] \tilde{v} d\tilde{v}}{v^2 - \tilde{v}^2}. \quad (2.77)$$

In the formulas (2.76), (2.77) the value  $x_v$  is determined by solution of the equation:

$$4 \pi f(x) = v^2 \quad (2.78)$$

that describes the resonance of the radiated frequency with the local plasma frequency at some value of the parameter  $x$  (the reduced distance to a nucleus).

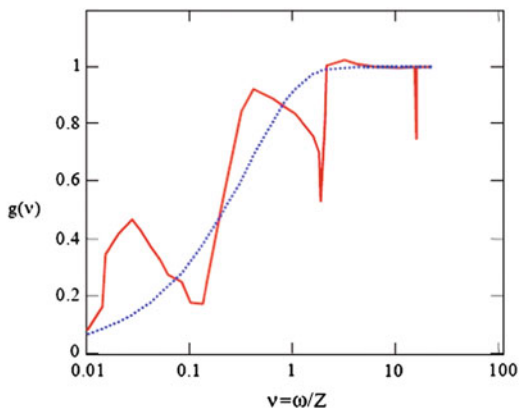
The expression (2.76) is obtained from the determination of the dynamic (Eq. 2.73) and reduced (Eq. 2.75) polarizabilities with the use of the known Sokhotsky formula.

It should be noted that the numerical calculation of dimensionless polarizability directly by the formulas (2.73), (2.74), and (2.75) is found to be difficult for low frequencies ( $v < 1$ ) in view of the singularity of a corresponding integrand and slow decrease of Thomas-Fermi electron density (2.74) with distance. As a result, the numerical integration loses accuracy. So it is proved to be preferably to use the formulas (2.76), (2.77), and (2.78) for calculation of the reduced polarizability  $\beta(v)$ .

The ratio  $g(v)$  of the modulus of the function  $\beta(v)$  to the modulus of its high-frequency limit ( $\beta_\infty(v) = -b^{-3} v^{-2}$ ) is presented in Fig. 2.5.

Given in the same figure is the corresponding ratio for a krypton atom restored by the data of the work [12], in which the dynamic polarizability of an atom was calculated by the quantum-mechanical method within the framework of the random phase exchange approximation.

**Fig. 2.5** The dynamic polarizability moduli normalized to their high-frequency limit as functions of the dimensionless frequency  $\nu = \hbar \omega / 2 Z R y$  for a krypton atom: *solid curve* – by the data of the work [12], *dotted curve* – calculation for a Thomas-Fermi atom in the local electron density model



It is seen that the function  $g(\nu) = \nu^2 |\beta(\nu)|$  for a Thomas-Fermi atom smoothly describes the spectral peculiarities of the dynamic polarizability of a krypton atom connected with the shell structure of an atom and approaches its high-frequency limit for  $\nu > 10$ .

However, it should be remembered that in the range of low frequencies  $\nu < 0.1$  the used approximation becomes inadequate since, on the one hand, the local plasma frequency approximation “works” badly for polarizability of an atom Eq. (2.73), and on the other hand, the contribution to polarizability at these frequencies is made by the peripheral regions of an atom, where the statistical model is inapplicable. Really, calculation by the formula (2.78) gives:  $x_{0.1} = 3.4$ ,  $x_1 = 0.64$ , and  $x_{10} = 0.053$ , at the same time the region of truth of the statistical model in the variable  $x$  is determined by the inequation  $Z^{-2/3} \ll x \ll Z^{1/3}$ .

So in further consideration we will restrict ourselves to the range  $\nu > 0.1$ . It should be noted that for  $Z \approx 50$  this corresponds to the photon energies  $\omega > 130$  eV, which exceeds considerably the potential of ionization of the outer electron shell of a neutral atom, so the electron core can be considered “defrozen”. Besides, in this frequency range, as seen from the above values of  $x_\nu$ , the inequation  $x_\nu \leq 3.4$  is true. The boundary reduced radius of a neutral atom calculated in the Thomas-Fermi-Dirac model (with consideration for exchange) according to the paper [13] is well approximated by the formula  $x_0 = 4 Z^{0.4}$ . Thus in our case ( $Z \gg 1$ )  $x_\nu \ll x_0$ , and conclusions of further consideration practically do not depend on refinements of the initial statistical Thomas-Fermi model, they are also true for ions with low enough degree of ionization if the condition  $x_0(Z_i/Z) \gg x_\nu$  is satisfied, which is confirmed by calculations carried out.

Good agreement of the magnitude of the dynamic polarizability of a Thomas-Fermi atom calculated in the local electron density approximation with the results of quantum-mechanical calculations [12], as seen from Fig. 2.5, takes place for the values of the dimensionless frequency:  $\nu > 2$ . Both approaches give the same value of frequency for the maximum of the function  $g(\nu)$ :  $\nu_{\max} \approx 0.5$  or  $\hbar \omega_{\max} \approx 490$  eV,

so that  $\hbar \omega_{\max} \gg I_p(Kr) = 14 \text{ eV}$ , and the electron core of a krypton atom can be considered “defrozen”.

The latter circumstance serves as a qualitative justification of adequacy of using the local plasma frequency approximation for calculation of the dynamic polarizability of an atom in the spectral range under consideration:  $v \geq v_{\max}$ .

It is interesting to note that even in the region of the maximum of the function  $g(v) = v^2 |\beta(v)|$  ( $v_{\max} \approx 0.5$ ), where, generally speaking, the quantum features of motion of atomic electrons are essential, the distinction in the results of quantum-mechanical and statistical calculations of the dynamic polarizability of a krypton atom is less than 30 %.

The most distinction in results (about 47 %), as seen from Fig. 2.5, takes place for  $v \approx 1$ , that is, for frequencies near the potential of ionization of the  $2p$ -subshell of a krypton atom. This fact is quite natural since neither the statistical model of a Thomas-Fermi atom nor the local plasma frequency approximation takes into account the shell structure of an atom, but they render the smoothed behavior of corresponding dependences.

Thus it can be stated that the model approximations used in this section for calculation of the dynamic polarizability of an atom are in good conformity with the results of quantum-mechanical calculations and at the same time are of a universal nature.

### 2.4.2 Cross-Section of Polarization Bs of a Fast Charged Particle on a Thomas-Fermi Atom

The spectral cross-section of polarization Bs of a fast electron on an atom within the framework of the first Born approximation is described by the expression (2.46) that for a process without excitation of a target, as it was shown in the previous paragraph, can be simplified to the form:

$$\frac{d\sigma^{PB}}{d\omega} = \frac{\omega^5}{(2\pi)^3 v} \int d\Omega_{\mathbf{n}} d\mathbf{q} |\alpha(\omega, \mathbf{q} + \mathbf{k})|^2 [\mathbf{n} \mathbf{A}(q)]^2 \delta(\omega + \mathbf{q}\mathbf{v}), \quad (2.79)$$

here  $d\Omega_{\mathbf{n}}$  is the solid angle in the direction of photon emission,  $\mathbf{k}$ ,  $\omega$  are the wave vector and the frequency of a bremsstrahlung photon,  $\mathbf{q} = \mathbf{p}_f - \mathbf{p}_i$  is the change of an incident particle momentum,  $\mathbf{A}(q)$  is the spatio-temporal Fourier transform of the vector-potential of the incident particle electromagnetic field that in the axial gauge ( $A_0 = 0$ ) is given by the expression (2.42).

The key value in the formula (2.79) –  $\alpha(\omega, \mathbf{q} + \mathbf{k})$  – is the nondipole dynamic polarizability of an atom, to calculate which the above approach is used.

It should be noted that the formula (2.79) is of a classical nature, it does not include the Planck constant, and it can be obtained within the framework of the

classical calculation of the PBs cross-section for a uniformly moving charge after summation over the impact parameter.

Hereafter for calculation of the Bs cross-section we will restrict ourselves to the Born-Bethe approximation, in which it can be assumed:

$$\alpha(\omega, q) = \alpha(\omega) \theta(p_a - q), \quad (2.80)$$

here  $\theta(x)$  is the Heaviside function (a unit “step”). As a characteristic atomic momentum, we will use the Thomas-Fermi momentum  $p_a = Z^{1/3} / (b a_0)$ .

In the Born-Bethe approximation (2.80) the integral in the formula (2.79) is calculated analytically. The result, however, is found to be cumbersome. So we will give here the formula in the general writing representing the spectral cross-section of polarization Bs in terms of the single integral with respect to the value of a transferred momentum. In this expression there are two characteristic frequency ranges that are explicitly separated:  $\omega < p_a v$  is the “low-frequency” range and  $\omega > p_a v$  is the “high-frequency” range:

$$\begin{aligned} \frac{d\sigma^{PB}}{d\omega} = \frac{4\omega^3}{v^2} |\alpha(\omega)|^2 & \left\{ \theta \left( \frac{p_a v}{1+v} - \omega \right) [H_1(\omega, p_a - \omega) + H_2(\omega)] \right. \\ & \left. + \theta \left( \omega - \frac{p_a v}{1+v} \right) H_1 \left( \omega, \frac{\omega}{v} \right) \right\}, \end{aligned} \quad (2.81)$$

where

$$\begin{aligned} G_1 = \frac{p_a^2 - (q - \omega)^2}{2\omega q} & \left[ \omega^2 v^2 + q^2 - \frac{5}{2} \omega^2 + \frac{\omega^4}{2q^2 v^2} \right] \\ & - \frac{1}{3} \left[ \left( \frac{p_a^2 - (q - \omega)^2}{2\omega q} \right)^3 + 1 \right] \left[ q^2 - \frac{5}{2} \omega^2 + \frac{3\omega^4}{2q^2 v^2} \right] \end{aligned}$$

and

$$G_2 = 2\omega^2 \left( v^2 - \frac{5}{3} \right) + \frac{4}{3} q^2.$$

The formula (2.81) in the frequency range  $\omega < p_a v$ , when the contribution to the cross-section is made by the first summand in the braces, is reduced to the known expression for the spectral cross-section of polarization Bs of a relativistic incident electron [2] (see also the formula (2.51) for the spectral-angular PBs cross-section):

$$\frac{d\sigma^{PB}}{d\omega} = \frac{16\omega^3 |\alpha(\omega)|^2}{3v^2} \ln \left( \frac{2\gamma p_a v}{\omega(1+v)} \right), \quad \omega < p_a v. \quad (2.82)$$

Here  $\gamma = (1 - v^2)^{-1/2}$  is the relativistic factor,  $\alpha(\omega)$  is the *dipole* dynamic polarizability of a target atom.

Going in the formula (2.82) to dimensionless variables with the use of the Eq. 2.75 and the determination of the Thomas-Fermi radius, we obtain the following expression for the spectral cross-section of polarization Bs:

$$d\sigma^{PB}(v) = \frac{16Z^2 b^6}{3v^2} |v^2 \beta(v)|^2 \frac{dv}{v} \ln \left( \frac{2\gamma v}{v a_0 (1+v) Z^{2/3}} \right) = Z^2 d\tilde{\sigma}^{PB}(v). \quad (2.83)$$

In the formula (2.83) the function  $d\tilde{\sigma}^{PB}(v)$  is introduced that is naturally can be called the *reduced cross-section* of the process since for this function in the case under consideration for polarization Bs of a fast incident particle approximate scaling with respect to the parameter  $\omega/Z$  takes place, while the nuclear charge dependence is only logarithmic.

From the expression (2.83) it follows in particular that the spectral cross-section of polarization Bs of a Thomas-Fermi atom (accurate to the logarithmic factor) grows quadratically with increasing nuclear charge if in this case the dimensionless frequency  $v$  does not change.

It should be noted that in case of a hydrogen-like ion, when scaling with respect to the parameter  $v_H = \omega/Z^2$  takes place, the spectral cross-section of PBs of a fast particle in the Born approximation does not depend at all on a nuclear charge for the specified value of the dimensionless frequency  $v_H$ , while the spectral cross-section of static Bs grows quadratically with increasing  $Z$  (accurate to the logarithmic factor).

Thus the used model predicts amplification of polarization effects in Bs of a fast particle on a neutral atom with increasing charge of the nucleus of the latter.

The spectral cross-section of ordinary (static) Bs in view of screening of the nuclear field [2] in case of weakly inelastic electron scattering is given by the expression:

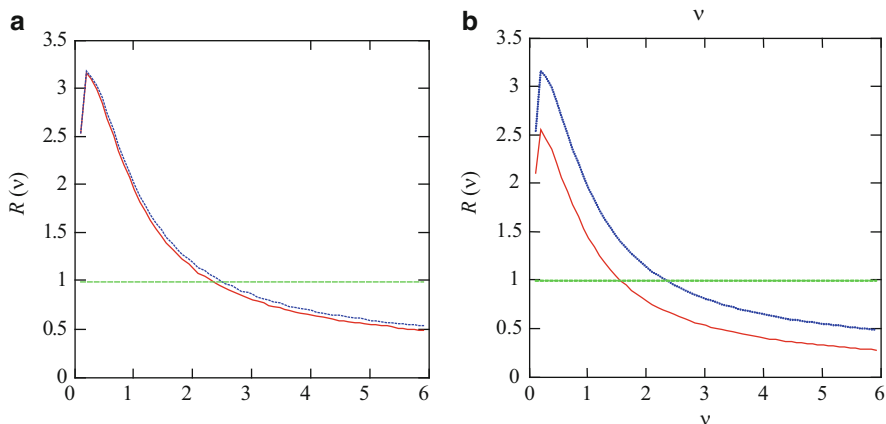
$$d\sigma^{OB}(\omega) = \frac{16Z^2}{3v^2} \frac{d\omega}{\omega} \ln \left\{ \frac{v}{p_a} \right\}, \quad \omega < p_a v. \quad (2.84)$$

The ratio of the cross-sections determined by the formulas (2.83) and (2.84) makes it possible to find the  $R$ -factor in the frequency range under consideration ( $\omega < p_a v$ ) and in the relativistic limit ( $v \cong 1$ ):

$$R(v, Z, \gamma) \equiv \frac{d\sigma^{PB}}{d\sigma^{OB}} = b^6 |v^2 \beta(v)|^2 \frac{\ln \left\{ \frac{137\gamma}{v Z^{2/3}} \right\}}{\ln \left\{ \frac{137}{Z^{1/3}} \right\}}, \quad v < \frac{137}{Z^{2/3}}. \quad (2.85)$$

The results of calculation of the  $R$ -factor as a function of the dimensionless frequency  $v$  for different values of the charge  $Z$  and the relativistic factor  $\gamma$  in the





**Fig. 2.6** The dependences of the  $R$ -factor on the reduced frequency  $\nu$  calculated for Bs of a fast electron on a Thomas-Fermi atom with the nuclear charge  $Z$ : (a) solid curve –  $\gamma = 10$ ,  $Z = 60$ ; dotted curve –  $\gamma = 10$ ,  $Z = 30$ ; (b) solid curve –  $Z = 60$ ,  $\gamma = 3$ ; dotted curve –  $Z = 60$ ,  $\gamma = 10$

range  $\nu < 137/Z^{2/3}$  are presented in Fig. 2.6. It should be noted that corresponding to these values of the dimensionless frequency  $\nu$  (for the nuclear charges  $Z \approx 50$ ) are the photon energies  $\hbar\omega < 14$  keV.

It is seen that the value of the  $R$ -factor of a relativistic incident electron in a wide frequency range is about one and for  $\omega \approx ZR\gamma$  ( $\nu = 0.5$ ) reaches its maximum value about  $2.5 \div 3$ . In this case the “sublogarithmic” influence of a nuclear charge on scaling with respect to  $Z$  is vanishingly small, and the influence of the relativistic factor is more significant.

It should be noted that the interference of the polarization and static Bs channels in case of a relativistic charged particle is small in view of different radiation patterns: the ordinary channel gives high-directivity radiation to a cone with an angle of the order of  $1/\gamma$  [1], and the angular distribution of polarization Bs for the frequencies  $\omega < p_a \nu$  is of a dipole nature [2].

In the case under consideration for weakly inelastic scattering of a Born charged particle in the frequency range  $\omega < p_a \nu$  the main contribution to Bs is made by small scattering angles, when the influence of effects of penetration of an incident particle into the electron core of an atom is small.

The said circumstance results in different frequency dependences of the polarization Bs cross-section for different degrees of inelasticity of incident electron scattering. In case of the process considered in this chapter, the spectral maximum of the polarization Bs cross-section is considerably shifted to the region of high frequencies and falls with growing Bs frequency more slowly than corresponding spectral dependences in emission of photons of threshold energies.

In the frequency range  $\omega > p_a \nu$  the law of conservation of energy-momentum conditions the necessity of penetration of an incident charged particle into the electron core of a target. So reradiation of a virtual photon of the scattered electron

eigenfield to a real photon on atomic electrons loses coherent behavior. As a result, the spectral cross-section of polarization Bs is found to be suppressed in comparison with the cross-section of ordinary Bs.

It should be noted that in the high-frequency region  $\omega > p_a v$  the dimensionless frequency  $v$  satisfies the inequation  $v > 10$  (we assume that  $Z \geq 30$ ), and, as seen from Fig. 2.5, the reduced polarizability of a Thomas-Fermi atom is close to its high-frequency limit:  $\beta(v) \approx \beta_\infty(v) = -b^{-3}v^{-2}$ . The frequency dependence of the polarization Bs cross-section in this case is defined mainly by the integral with respect to the angular variables and the value of the transferred momentum  $q$  in the formula (2.79).

The formula (2.82) in the frequency range  $\omega > p_a v$  becomes untrue, and for determination of the polarization Bs cross-section it is necessary to proceed from the general expression (2.81). In this case the contribution is made by the second summand in the braces of Eq. 2.81. The analysis shows that in the expression for the spectral cross-section the multiplier  $(p_a/\omega)^2$  appears that defines the smallness of the polarization channel contribution to the total spectral Bs cross-section. However, the spectral-angular cross-section of polarization Bs in the region of photon emission angles  $\gamma^{-1} < \vartheta \leq \sqrt{p_a/\omega}$  exceeds the corresponding cross-section of the static channel.

The carried out consideration shows in particular that the characteristic potential of ionization of a multielectron atom included in the definition of the region of truth of the high-frequency approximation (see Eq. 2.53) can be represented as:  $I(Z) = 2\zeta ZRy$ , that is, increases linearly with growing charge of the nucleus of a target atom. In this formula the constant  $\zeta \geq 5$  is introduced, the exact value of which is not determined and depends on accuracy, with which it is required to calculate the process cross-section.

Thus in this paragraph within the framework of the local electron density method and the Thomas-Fermi model the universal description of polarization Bs of a fast Born charged particle on a multielectron atom ( $Z \gg 1$ ) in the region of energies of bremsstrahlung photons  $\omega > 100$  eV is given. It is shown that the  $R$ -factor defining the relative value of the polarization channel contribution to the total Bs cross-section has approximate scaling with respect to the parameter  $\omega/Z$  and at the frequencies  $\omega_{\max} \approx ZRy$  reaches its maximum value  $R_{\max}(\gamma) = 2.5 \div 3$  that grows logarithmically with the energy of an incident particle.

The decrease of the  $R$ -factor with growing energy of an emitted photon in the low-frequency region  $\omega < p_a v$  is most pronounced up to frequencies of the order of  $20 ZRy$ , when the magnitude of the polarizability of a Thomas-Fermi atom decreases when going to its high-frequency asymptotics.

In the spectral range  $10 ZRy < \omega < p_a v$  the decrease of the  $R$ -factor and polarization Bs intensity has weak logarithmic behavior and is caused by reduction of the maximum impact parameter.

In the high-frequency range  $\omega > p_a v$  the frequency change of polarization Bs intensity is defined mainly by kinematic factors and by violation of coherence of reradiation of a virtual photon to a real photon on atomic electrons. In this case the

decrease of spectral intensity becomes power-like. At the same time the pattern of radiation by the polarization channel is narrowed, so that  $\vartheta \leq \sqrt{p_a/\omega}$ , and in the frequency range  $p_a < \omega < \gamma^2 p_a$  there is the region of Bs angles:  $\gamma^{-1} < \vartheta \leq \sqrt{p_a/\omega}$ , in which the polarization mechanism prevails over the ordinary (static) mechanism of radiation.

## 2.5 Incoherent Polarization Bremsstrahlung of a Fast Charged Particle on an Atom in the High-Frequency Approximation

In this paragraph within the framework of the high-frequency approximation for the operator of electromagnetic field scattering the universal description of incoherent polarization Bs of a fast charged particle on a multielectron atom is obtained. The PBs cross-section is expressed in terms of the Compton profile of X-ray scattering, for which a voluminous calculation material is available. The obtained universal representation for the process cross-section is justified both for the statistical atom model and on the basis of established approximate scaling of Hartree-Fock Compton profiles.

This paragraph is the refinement, supplement, and generalization of the consideration of PBs with atomic ionization carried out in the Sect. 2.3 to the case of taking into account atomic electron binding in the initial state.

### 2.5.1 *Connection of the Dynamic Form Factor with the Compton Profile of an Atom*

In Sect. 2.3 the expression (2.63) was obtained for the cross-section of high-frequency PBs ( $m \gg \omega \gg I$ ) of a fast charged particle in terms of the dynamic form factor (DFF) of a target (Eq. 2.64).

The approximate expression for the DFF (2.65) and the formula following from it for the PBs cross-section (2.66) give a qualitative idea of the process, separating two characteristic frequency ranges.

In the low-frequency range ( $\omega < p_a v_0$ ) PBs is coherent by the contribution of atomic electrons, the process proceeds without excitation of a target, and the cross-section is proportional to the squared number of atomic electrons.

In the high-frequency range ( $\omega > p_a v_0$ ) radiation with ionization of a target prevails, and the PBs cross-section is proportional to the number of electrons in an atom.

In the latter case the (incoherent) DFF of an atom is represented as the sum of the DFF of electron subshells of the atom:

$$S(q) = \sum_{n,l} S_{nl}(q). \quad (2.86)$$

Let us transform the expression for the dynamic form factor of the electron subshell (Eq. 2.64) using the expansion in terms of the total system of wave functions.

Then we will use the fact that in the frequency range under consideration  $\omega > p_a v_0$  momenta transferred from an incident particle to a target far exceed the characteristic atomic momentum. Then the wave functions of the continuous spectrum making the main contribution to the DFF can be to a good accuracy approximated by plane waves, and the expression for the DFF of the electron subshell is represented as:

$$S_{nl}(q) = \int \frac{d\mathbf{p}}{4\pi} \delta\left(q^0 + \frac{(\mathbf{p} - \mathbf{q})^2}{2} - \varepsilon_{nl}\right) |R_{nl}(p)|^2, \quad (2.87)$$

here  $q^0 = \omega + \mathbf{q}_1 \mathbf{v} + \mathbf{q}_1^2/2m$  is the energy of a nonrelativistic IP transferred to the target, ( $m$  is its mass);  $\mathbf{q}_1 = \mathbf{p}_f^{IP} - \mathbf{p}_i^{IP}$  is the change of the incident particle momentum (here the upper index is introduced for IP momenta to distinguish them from atomic electron momenta),  $\mathbf{q} = \mathbf{q}_1 + \mathbf{k}$  is the momentum transferred to the target;  $\varepsilon_{nl}$  is the energy of the electron subshell under consideration ( $n, l$  are the principal and orbital quantum numbers). In the formula (2.87) the function  $R_{nl}(p)$  is introduced that represents the spatial Fourier transform of a normalized radial wave function of the  $nl$ -state determined by the formula:

$$R_{nl}(p) = \sqrt{\frac{2}{\pi}} \int_0^\infty R_{nl}(r) j_l(pr) r^2 dr, \quad (2.88)$$

$j_l(pr)$  is the spherical Bessel function of the first kind.

### 2.5.2 Impulse Approximation

The delta function in the formula (2.86) describes the law of conservation of energy in the PBs process with target ionization. In the expression (2.86) we went from summation over the finite momentum of an atomic electron to summation over the momentum of the Fourier expansion of the wave function of the electron subshell under consideration. In the impulse approximation this value coincides with the initial momentum of an atomic electron. Thus, if it is assumed that:

$$p^2/2 = \varepsilon_{nl}, \quad (2.89)$$

we come to the impulse approximation widely used in calculations of the Compton effect on atoms.

Really, in fulfilment of Eq. 2.89 the DFF of the electron subshell (Eq. 2.86) can be represented as:

$$S_{nl}^{(IA)}(q) = \frac{1}{|\mathbf{q}|} J_{nl} \left( Q = -\frac{q^0 + \mathbf{q}^2/2}{|\mathbf{q}|} \right). \quad (2.90)$$

Here the Compton profile of the electron subshell  $J_{nl}(Q)$  [14, 15] is introduced that is determined according to the formula:

$$J_{nl}(Q) = \frac{1}{2} \int_Q^\infty |R_{nl}(p)|^2 p dp. \quad (2.91)$$

This value is tabulated for all subshells of all elements in [14] with the use of the Hartree-Fock and Dirac-Hartree-Fock wave functions.

The formulas (2.86) and (2.90) give the representation of an incoherent DFF in terms of the Compton profile in the impulse approximation.

Beyond the framework of the impulse approximation instead of the formula (2.90) it is possible to obtain from Eq. 2.86 the following representation for the dynamic form factor of an atom in terms of its Compton profile:

$$S_{nl}(q) = \frac{1}{2|\mathbf{q}|} \left\{ J_{nl} \left( -|\mathbf{q}| + \sqrt{2(-q^0 + \varepsilon_{nl})} \right) - J_{nl} \left( |\mathbf{q}| + \sqrt{2(-q^0 + \varepsilon_{nl})} \right) \right\}. \quad (2.92)$$

Using the tabulated values of the Compton profile [14] makes it possible with the formulas (2.86), (2.92), and (2.63) to calculate the cross-sections of incoherent PBs of various elements.

### 2.5.3 Compton Profile Within the Framework of Statistical Atom Models

For universalization of the dependence of PBs cross-sections on the charge of an atomic nucleus, it is of interest to obtain an expression for the Compton profile within the framework of the statistical model.

Let us introduce an “effective” one-electron radial wave function of an atom in the statistical model, connecting it with the radial density of distribution of the electron charge  $\rho_{stat}(r)$  by the formula:

$$R_{stat}(r) = \sqrt{\rho_{stat}(r)/Z}. \quad (2.93)$$

Then, considering the distribution of electron density in an atom spherically symmetrical, it is possible to obtain from Eqs. 2.88, 2.91, and 2.93 for the Compton profile in the statistical approximation (in terms of one electron) the following expression:

$$J_{stat}^{(1)}(q) = \frac{1}{\pi Z} \int_q^\infty \frac{dp}{p} \left| \int_0^\infty \sqrt{\rho_{stat}(r)} \sin(pr) r dr \right|^2. \quad (2.94)$$

In the elementary case of exponential screening, when the radial electron density in an atom looks like:

$$\rho_{exp}(r) = \frac{4Z}{r_{TF}^3} e^{-2r/r_{TF}}, \quad (2.95)$$

the following expression for the Compton profile (Eq. 2.94) can be obtained:

$$J_{exp}^{(1)}(q) = \frac{8 r_{TF}}{3\pi} \frac{1}{\left(1 + (q r_{TF})^2\right)^3}. \quad (2.96)$$

By analogy, for the reduced Compton profile of an atom in the Thomas-Fermi model we have:

$$\tilde{J}_{TF}(\tilde{q}) = \frac{1}{\pi} \int_{\tilde{q}}^\infty \frac{|g_{TF}(\tilde{p})|^2}{\tilde{p}} d\tilde{p}, \quad (2.97)$$

introduced here is the spatial Fourier transform of the square root of the normalized Thomas-Fermi density:

$$g_{TF}(\tilde{p}) = \int_0^\infty (\chi(x))^{3/4} \sin(\tilde{p}x) x^{1/4} dx. \quad (2.98)$$

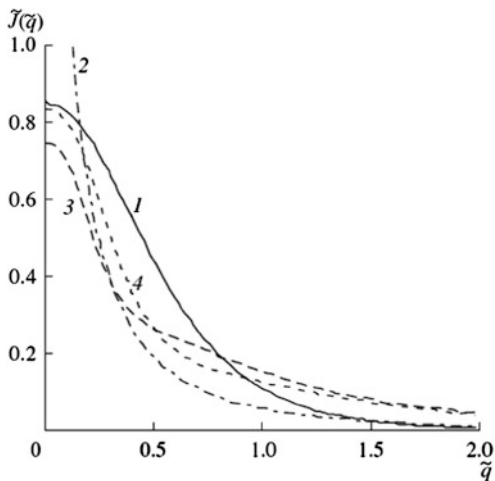
The obtained reduced Compton profiles satisfy the necessary normalizing condition:

$$\int_0^\infty \tilde{J}_{stat}(\tilde{q}) d\tilde{q} = \int_0^\infty J_{stat}^{(1)}(q) dq = 0.5. \quad (2.99)$$

As seen from the formulas (2.96), (2.97), the normalized Compton profile of an atom in statistical models depends only on the reduced momentum  $\tilde{q} = q r_{TF} = q/p_{TF}$ .

Presented in Fig. 2.7 are the dependences of normalized Compton profiles of an atom on the reduced momentum  $\tilde{q}$  calculated within the framework of statistical models and by the data of the Hartree-Fock calculations [14] for argon and krypton atoms. It is seen that the Thomas-Fermi Compton profile in the region of small transferred momenta exceeds appreciably values obtained within the framework of other models, which is explained by not fast enough decrease of the Thomas-Fermi electron density with distance. At the same time the exponential screening model

**Fig. 2.7** The dependences of the normalized Compton profile on the reduced transferred momentum obtained within the framework of different models: (1) exponential screening; (2) Hartree-Fock calculation for an argon atom; (3) Hartree-Fock calculation for a krypton atom; (4) Thomas-Fermi model



gives quite satisfactory approximation to the results of more exact calculations [14] with the use of the Hartree-Fock wave functions.

Following from this figure, in particular, is approximate scaling of normalized Hartree-Fock Compton profiles as functions of the reduced momentum.

### 2.5.4 Cross-Section of Incoherent PBs of a Nonrelativistic Born Particle

The expression for the spectral cross-section of PBs of a nonrelativistic Born charged particle in the high-frequency range  $m \gg \omega \gg I$  integrated with respect to the solid angle of photon emission can be obtained from the formula (2.63). In the ordinary (Gaussian) system of units it looks like:

$$d\sigma(\omega) = \frac{8}{3\pi} \frac{e^4 e_0^2}{m_e^2 v \hbar c^3} \frac{d\omega}{\omega} \int \int d\Omega_{\mathbf{q}} dq S(q^0, \mathbf{q}), \quad (2.100)$$

where  $e_0 = Z_0 e$  is the IP charge.

In derivation of (Eq. 2.100) the expression for the vector potential of the eigenfield of a nonrelativistic IP in the axial gauge was used, and it was assumed that  $\mathbf{q} = \mathbf{q}_1$ .

It should be noted that in the approximation of quasi-free (at rest) atomic electrons the incoherent DFF of a target is given by the equation:

$$S_{free}^{ncoh}(q) = \frac{Z}{q v} \delta\left(\frac{\omega + \mathbf{q} \mathbf{v} + \mathbf{q}^2/(2\mu)}{q v}\right), \quad (2.101)$$

where  $\mu$  is the reduced mass of an electron and an IP,  $Z$  is the number of atomic electrons equal to the nuclear charge.

Substituting the expression (2.92) for the incoherent DFF summed over all electron subshells of an atom in the formula (2.100), we come to the following representation of the spectral PBs cross-section in the frequency range  $\omega > p_a v_0$ :

$$d\sigma(\omega, v, m) = \sqrt[3]{Z} Z_0^2 d\tilde{\sigma}\left(\frac{\omega}{p_{TF}^2}, \frac{v}{p_{TF}}, m\right). \quad (2.102)$$

Introduced here is the reduced cross-section  $d\tilde{\sigma}$  depending on the frequency of an emitted photon and the IP velocity normalized accordingly to the characteristic momentum of a Thomas-Fermi atom.

The reduced cross-section is expressed in terms of the normalized Compton profile of an atom by the formulas:

$$d\tilde{\sigma}(\tilde{\omega}, \tilde{v}, m) = \sigma_0 \frac{b^2}{\tilde{\omega}^2} \frac{d\tilde{\omega}}{\tilde{\omega}} I(\tilde{\omega}, \tilde{v}, m) \quad (2.103)$$

$$I(\tilde{\omega}, \tilde{v}, m) = \int_{q_{\min}}^{q_{\max}} \frac{d\tilde{q}}{\tilde{q}} \int_{-v}^{-v_m} \left\{ \tilde{J}\left(-\tilde{q} + \sqrt{-2\tilde{q}^0}\right) - \tilde{J}\left(\tilde{q} + \sqrt{-2\tilde{q}^0}\right) \right\} d(v \cos(\mathbf{q} \mathbf{v})), \quad (2.104)$$

here  $v_m = (\tilde{\omega} + \tilde{q}^2/2m)/\tilde{q}$ ,  $b = 0.8853$ .

The upper and lower limits of integration with respect to the magnitude of the transferred momentum in the integral (2.104) are defined by the condition  $v_m < v$ .

The dimensional cross-section  $\sigma_0$  included in the expression (2.103) is:

$$\sigma_0 = \frac{16}{3} \frac{e^6}{m_e^2 \hbar c^3} = 2.074 \cdot 10^{-6} \text{ a.u.} \quad (2.105)$$

Here we used the Gaussian system of units.

Thus the formulas (2.102), (2.103), (2.104), and (2.105) reveal the scaling law for the cross-section of incoherent PBs of a fast (but nonrelativistic) charged particle on a multielectron atom and express the process cross-section in terms of the normalized Compton profile of X-ray scattering. This cross-section (accurate to the multiplier  $\sqrt[3]{Z}$ ) depends on the frequency of an emitted photon and the IP velocity nondimensionalized with the use of the Thomas-Fermi momentum.

It should be noted that though, strictly speaking, scaling Eqs. 2.102, 2.103, 2.104, and 2.105 is obtained within the framework of the statistical model of an atom, it is also approximately true for a Hartree-Fock atom in view of the above approximate scaling of normalized Compton profiles (see Fig. 2.7).



We will give for comparison a corresponding expression for the cross-section of incoherent PBs on a hydrogen-like ion with the charge  $Z$ :

$$d\sigma_H(\omega, v, m) = Z^{-1} b^{-2} d\tilde{\sigma}\left(\frac{\omega}{p_H^2}, \frac{v}{p_H}, m\right), \quad (2.106)$$

where  $p_H = Z$  a.u. is the characteristic momentum of a hydrogen-like atom.

The found expression (2.102) for the cross-section of high-frequency PBs with atomic ionization refines and supplements the result of Eq. 2.69 obtained with the use of the DFF in the model of free atomic electrons (Eq. 2.101) that can also be represented in the form (2.102) and (2.103), if it is assumed that:

$$I_{free}(\tilde{\omega}, \tilde{v}, \mu) = \ln \left\{ \frac{1 + \sqrt{1 - 2\tilde{\omega}/(\mu\tilde{v}^2)}}{1 - \sqrt{1 - 2\tilde{\omega}/(\mu\tilde{v}^2)}} \right\}. \quad (2.107)$$

Shown in Fig. 2.8 are the spectral dependences of the value  $\omega \frac{d\sigma}{d\omega}$  calculated within the framework of different approximations, including the model of free atomic electrons, for incoherent PBs of a proton. It is seen that the main difference of the models shows itself in the frequency range  $\omega > \omega^* = \mu v^2/2$ , that is, behind the “cutoff” frequency for PBs on free electrons.

From kinematic considerations it is clear that the “cutoff” frequency for PBs of an electron, other things being equal, is half the value for PBs of a proton (because of the difference in reduced masses), this situation supplements the conclusion drawn earlier about the PBs cross-section independence of the mass of an incident particle.

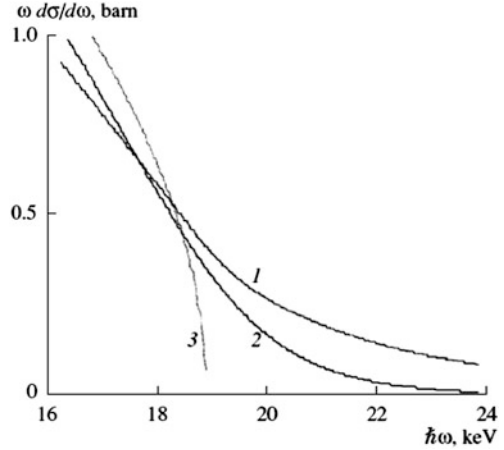
The reduction of the cross-section with growing PBs frequency in the exponential screening model occurs appreciably faster than for the Hartree-Fock Compton profile, which follows also from Fig. 2.7. For frequencies smaller than the “cutoff” frequency the Hartree-Fock consideration of binding of atomic electrons in the initial state results in a somewhat smaller cross-section value in comparison with the model of free atomic electrons.

Let us note the close similarity of the dependences in Fig. 2.8 with corresponding spectral cross-sections for radiation ionization from the theoretical work [16]. In this work for description of incoherent PBs (radiation ionization) a similar approach was used, based on the use of the nondiagonal atomic form factor  $F_{n,W}(q)$  that was calculated earlier in connection with the problem of ionization of atoms and excitation of characteristic X-rays.

Shown in Fig. 2.9 are the dependences of the value  $\omega d\sigma/d\omega$  of incoherent PBs of a proton on a krypton atom on the proton velocity for three values of bremsstrahlung photon energy – 3.78 keV, 7.57 keV, and 11.35 keV.

It is seen that the velocity dependences of cross-section have maxima. These maxima are shifted to the region of higher velocities with growing bremsstrahlung

**Fig. 2.8** The spectral cross-section of incoherent PBs of a proton with an energy of 34 MeV on a krypton atom near the “cutoff” frequency calculated within the framework of different approximations for the electron density of an atom: Hartree-Fock calculation (curve 1), exponential screening (curve 2), approximation of free atomic electrons (curve 3)



photon energy. A corresponding formula relating the bremsstrahlung photon frequency and the optimum value of proton velocity in atomic units looks like:

$$v_{\text{opt}} = 1.89 \sqrt{\omega} \quad (2.108)$$

It is essential that the relation (2.108) does not depend on the charge of an atomic nucleus in contrast to the analogous dependence for coherent PBs, when there is a linear connection between the optimum velocity and radiated frequency through the radius of the atomic subshell making the greatest contribution to the process.

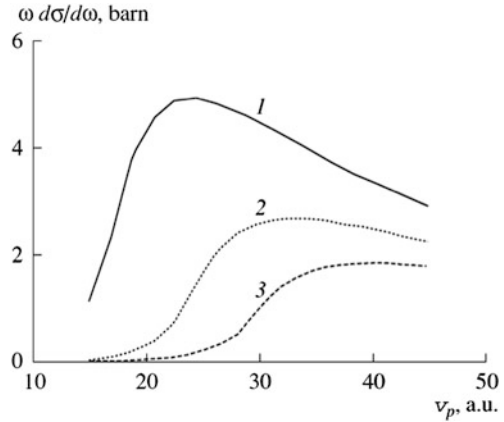
### 2.5.5 Comparison of Cross-Sections of Incoherent and Coherent PBs

Now we will analyze the relation between the cross-sections of coherent and incoherent PBs.

We will calculate the cross-section of the coherent process within the framework of the exponential screening model for the electron density of the target core. A corresponding expression can be obtained from the formula (2.63) if it is taken into account that the DFF of an atom in this case is reduced to the ordinary static form factor being a Fourier transform of electron density.

After standard transformations including integration with respect to the solid angles of an emitted photon and a transferred momentum, for the cross-section of coherent PBs of a nonrelativistic Born particle we have the following expression (in atomic units):

**Fig. 2.9** Incoherent PBs of a proton on a krypton atom as a function of the proton velocity for three values of bremsstrahlung photon energy:  $\hbar\omega = 3.78$  keV (curve 1),  $\hbar\omega = 7.57$  keV (curve 2),  $\hbar\omega = 11.35$  keV (curve 3)



$$d\sigma_{coh}^{(exp)}(\omega) = \frac{16}{3} \frac{Z^{4/3}}{\tilde{v}^2 c^3} b^2 \int_{\tilde{q}_{min}}^{\tilde{q}_{max}} \frac{1}{(1 + \tilde{q}^2/2)^4} \frac{d\tilde{q}}{\tilde{q}} \frac{d\omega}{\omega}. \quad (2.109)$$

In the integral of the expression (2.109) there are the same limits of integration with respect to the transferred momentum as in the formula (2.104). “Tilde” above the sign of the transferred momentum and of the IP velocity, as before, means normalization to the momentum (velocity) of a Thomas-Fermi atom.

The integral in the Eq. 2.109 is taken in quadratures, but a corresponding expression is rather cumbersome. For a heavy IP the upper limit of integration can be replaced by infinity, then for the integral with respect to the reduced transferred momentum we have:

$$I_{coh}^{(exp)}(\tilde{\omega}, \tilde{v}) = \frac{11 + 54 \left(\frac{\tilde{v}}{\tilde{\omega}}\right)^2 + 72 \left(\frac{\tilde{v}}{\tilde{\omega}}\right)^4}{12 \left(1 + 2 \left(\frac{\tilde{v}}{\tilde{\omega}}\right)^2\right)^3} - \frac{11}{12} + \frac{1}{2} \ln \left(1 + 2 \left(\frac{\tilde{v}}{\tilde{\omega}}\right)^2\right). \quad (2.110)$$

It should be noted that in the limit  $v p_{TF} \ll \omega$  (\*) from the formula (2.110) the asymptotics follow:

$$I_{coh}^{(exp)}(\tilde{\omega}, \tilde{v}) \cong 2 \left(\tilde{v}/\tilde{\omega}\right)^8. \quad (2.111)$$

The inequation (\*) can be rewritten as:  $\omega \gg 0.125 Z^{2/3}$  keV, whence it follows that it is satisfied for all  $Z$  in the kiloelectron-volt range of bremsstrahlung photon energies.

From the formulas (2.109), (2.110), and (2.111) we obtain for the coherent PBs cross-section in the exponential screening approximation and the high-frequency limit  $\omega \gg 0.125 Z^{2/3}$  keV:

$$d\sigma_{coh}^{(exp)}(\omega) = \frac{32 b^2}{3 c^3} Z^{4/3} \frac{\tilde{v}^6}{\tilde{\omega}^8} \frac{d\omega}{\omega}. \quad (2.112)$$

For correct estimation of the relation between the cross-sections of coherent and incoherent processes it is important to emphasize that a simple exponential approximation underestimates considerably the contribution of the  $K$ -shell to coherent PBs on a multielectron atom in a high-frequency range. Really, the radius of the orbit nearest to the nucleus is approximately  $Z^{2/3}$  times less than the Thomas-Fermi radius, so the corresponding integral in the formula (2.109) results in reduction of the spectral cross-section at higher frequencies than this takes place for the Thomas-Fermi radius.

To take into account the contribution of the  $K$ -shell, we rewrite the formula (2.109) as follows ( $Z \gg 1$ ):

$$d\sigma_{coh}^{(exp)}(\omega) = \frac{16}{3} \frac{Z^{4/3}}{\tilde{v}^2 c^3} b^2 \frac{d\omega}{\omega} \left\{ I_{coh}^{(exp)}(\tilde{\omega}, \tilde{v}) + \frac{4}{Z^2} I_{coh}^{(exp)}(\tilde{\omega}, \tilde{v} (p_K(Z)/p_{TF})) \right\}, \quad (2.113)$$

introduced here is the momentum of the atomic  $K$ -shell  $p_K(Z)$ .

The expression (2.113) is a universal (common for all nuclear charges) representation of the cross-section of coherent PBs of a fast particle obtained in the exponential electron density model with individual consideration of the contribution of the  $K$ -shell to radiation.

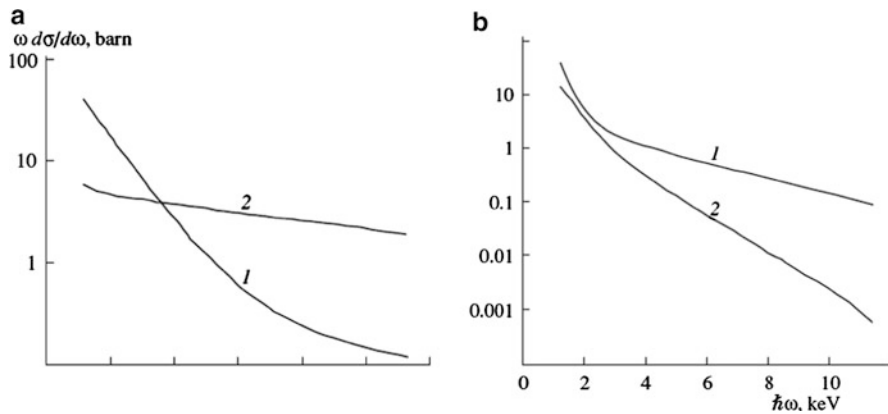
The results of calculation of the spectral cross-sections of coherent and incoherent PBs of a proton on a krypton atom for two values of proton velocity are presented in Fig. 2.10.

From this figure it follows in particular that the prevalence of the incoherent process over the coherent process can take place at high enough velocities of an incident particle since in this case the “cutoff frequency” for radiation ionization is shifted to the region of high frequencies, in which the contribution of most of atomic electrons to coherent PBs is already small.

Thus in this paragraph within the framework of the high-frequency approximation for the operator of electromagnetic field scattering the universal description of incoherent PBs of a fast charged particle on a multielectron atom was obtained. The process cross-section is expressed in terms of the Compton profile of X-ray scattering.

The basis for the obtained universal description is approximate scaling of the reduced Compton profile of X-ray scattering by a neutral atom for high enough nuclear charges ( $Z \geq 20$ ) that was found in this work.

Based on the derived formulas and within the framework of different approximations for electron density of the electron core of a target, the spectral and velocity dependences of the cross-section of incoherent PBs of a proton on a multielectron atom were analyzed.



**Fig. 2.10** The spectral cross-sections of coherent (curves 1) and incoherent (curves 2) polarization bremsstrahlung of a proton on a krypton atom for different proton velocities: (a)  $v^{IP} = 10 v_{TF} = 7.3$  a.u., (b)  $v^{IP} = 3 v_{TF} = 11.2$  a.u.

It was shown that for a specified PBs frequency there is an optimum velocity of an incident particle, at which the process cross-section has maximum. The value of optimum velocity grows as the square root of frequency.

The carried out comparison of the cross-sections of coherent and incoherent processes has shown that for high enough velocities of an incident particle there is a frequency range of prevalence of PBs with atomic ionization over coherent PBs.

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