# APPLICABILITY OF THE BORN APPROXIMATION TO COLLISIONS BETWEEN ELECTRONS AND EXCITED ATOMS

A. N. STAROSTIN

Moscow Power Engineering Institute

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The problem of the limits of applicability of first-order perturbation theory for the calculation of the cross sections for electron scattering on excited atoms is considered. Criteria for the validity of the Born approximation for elastic and inelastic collisions of electrons and excited atoms are formulated on the basis of the requirement that the second-order amplitude of perturbation theory be small.

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m HE}$  exact calculation of the cross section for elastic and inelastic collisions between electrons and excited atoms is connected with considerable difficulties. Therefore the majority of the calculations of recent years, even for collisions with hydrogen atoms, [1-6] have been carried out in Born approximation. However, an open question remains: what are the energies beyond which the quantitative results of the Born approximation can be trusted? For elastic scattering on the ground state and for excitation of the lowest levels the criterion for the applicability of the Born approximation is taken from a comparison with experiment. It is commonly assumed [7,8] that Born approximation is good for such processes at energies larger than 100 eV.

For transitions between excited states a comparison of the calculations with experiment can only be made indirectly, since direct measurements are not available. It is natural to assume that for transitions with transition energies  $\Delta E$ the first order perturbation theory is valid if  $E \gg \Delta E$ .<sup>[9]</sup> Unfortunately, it is not clear what "much larger" means in the present case. The point is that for n, n'  $\gg \Delta = |n - n'|$ , where n and n' are the principal quantum numbers of the initial and final states, the quantity  $\Delta E \sim n^{-3} \Delta \cdot Ry$  is small, and there are in general several possibilities:  $E \gg n^{-3}Ry$ ,  $\Delta E \gg n^{-2}Ry$ ,  $E \gg n^{-1}Ry$ , etc. On the other hand,  $\Delta E = 0$  for elastic scattering, and the inequality  $E \gg \Delta E$  becomes meaningless.

In the present paper we attempt to formulate criteria for the applicability of the Born approximation to elastic and inelastic collisions of electrons and excited atoms. It is assumed that the Born approximation is valid if the second-order amplitude of perturbation theory is small in comparison with the first. This condition is easily obtained from the usual requirement that the firstorder corrections to the wave function be small compared with the zeroth order functions. Indeed, multiplying both sides of the inequality  $\psi^{(1)} \ll \psi^{(0)}$ by the interaction potential and the wave function of the final state of the noninteracting system and integrating over the coordinates of the particles, we find the condition  $|f^{(2)}| \ll |f^{(1)}|$ . Since in Born approximation the forward scattering amplitude is maximal for elastic and inelastic scattering and the cross sections are mainly determined by the behavior of the amplitude at small angles, we compare the forward scattering amplitudes calculated in first and second order of perturbation theory.

An explicit calculation of the first Born amplitude for arbitrary transitions and momentum transfers is possible for hydrogen, using parabolic coordinates. The scattering amplitude has a complicated form so that an estimate of the second order of perturbation theory is not realistic. For the forward scattering amplitude the situation is much simpler, so that criteria for the applicability of the Born approximation can be formulated in explicit form. The estimates are made for hydrogenlike levels. This does not affect the generality of our results, since the excited states of different atoms are analogous to the states of the hydrogen atom.

Usually one is interested in transitions  $n \rightarrow n'$ ; we therefore do not give criteria for the applicability of the Born approximation for the amplitudes of the separate transitions  $n, l \rightarrow n', l'$ , but for the amplitudes averaged over the orbital angular momenta.

#### 1. ELASTIC SCATTERING

In Born approximation the amplitude for elastic scattering of electrons on atoms in the n-th excited state is, neglecting the recoil of the nucleus, [10]

$$f_n^{(1)}(E,\vartheta) = \frac{2me^2}{\hbar^2 q^2} [Z - F_n(q)], \quad q = 2k \sin\frac{\vartheta}{2}, \quad (1)$$

where k is the wave number of the electron,  $\vartheta$  is the scattering angle, Ze is the charge of the atom, and  $F_n(q)$  is the atomic form factor,

$$F_n(q) = \int e^{-i(\mathbf{k}-\mathbf{k}_0)\mathbf{r}} \psi^*_{nlm}(\mathbf{r}) \psi_{nlm}(\mathbf{r}) d\mathbf{r}, \qquad (2)$$

where  $\mathbf{k}_0$  and  $\mathbf{k}$  are the wave vectors of the electron before and after the collision. For a hydrogen-like atom Z = 1, and the integration in (2) goes over the coordinates of the valence electron. The total cross section for elastic scattering averaged over all l, m has the form

$$\sigma_n^{(1)}(E) = \frac{1}{n^2} \sum_{l,m} \int d\Omega |f_n^{(1)}(E, \vartheta)|^2.$$
(3)

When the approximation (1) is valid, the cross section is determined by the behavior of the amplitude at small angles. In the region of small angles the amplitude has the following form:

$$f_n^{(1)}(E,\vartheta) \approx \frac{q_i q_j}{q^2 a_0} \langle nlm | x_i x_j | nlm \rangle.$$
 (4)

Here  $a_0$  is the Bohr radius, and dummy indices are to be summed over.

For not too small energies  $k^2$  a simple estimate of the cross section shows that (3) is determined by the averaged square of (4) multiplied by the interval of solid angles where this last expression is valid. The order of magnitude of these angles is determined by the condition that the exponent of the exponential in (2) be close to unity. Since distances of order  $r_n \sim a_0 n^2$  give the main contribution to the integrals determining the form factor, we have the inequality  $k \mathfrak{s} a_0 n^2 \leq 1$  for the angles. We thus find in order of magnitude

$$\sigma_n^{(1)}(E) \sim \frac{\pi}{(ka_0)^{2n}} \frac{1}{a^2} \sum_{l,m} \left| \frac{\langle nlm | r^2 | nlm \rangle}{3a_0} \right|^2.$$
 (5)

This estimate of the total cross section  $\sigma$  shows that the latter increases with increasing principal quantum number according to the law  $\sim n^4$  and decreases in proportion to the inverse first power of the energy. The exact calculation of the form factors is cumbersome for arbitrary values of n, *l*, m and all values of momentum transfer. For small energies  $(k^2 \rightarrow 0)$  Eq. (5) does not hold. Returning to the original expression (3), we find easily that the scattering is isotropic and the cross section increases proportional to  $n^8$ . This increase is implausible and indicates that the Born approximation is not applicable at small energies.

We note further that the amplitude (1) is real in the physical region of scattering angles. This is not in agreement with the optical theorem, according to which the imaginary part of the forward elastic scattering amplitude is proportional to the total cross section. The imaginary part of the elastic scattering amplitude appears in second order and is for  $\vartheta = 0$  proportional to the total cross section calculated in first order.

We use this circumstance to estimate the forward elastic scattering amplitude in second-order perturbation theory. Let us denote the scattering amplitude in this order by  $f_n^{(2)}(E, \vartheta)$ ; according to what has been said above,

$$\operatorname{Im} f_{n}^{(2)}(E,0) = \frac{k}{4\pi} \sigma_{n, \ tot}^{(1)}(E).$$
(6)

The total cross section is the sum of the elastic and inelastic cross sections averaged according to (3). The quantity on the left-hand side of (6) should therefore be averaged in this way.

The estimate of the elastic scattering cross section is simplified if we replace the averaging of the cross section over l and m by the average of the amplitude (1). This replacement in the crude estimate (5) leads to an error not exceeding 10% for  $n \gg 1$ :

$$\frac{1}{n^2} \sum_{l,m} |\langle nlm | r^2 | nlm \rangle|^2 \approx 3.25n^8,$$
$$\left| \frac{1}{n^2} \sum_{l,m} \langle nlm | r^2 | nlm \rangle \right|^2 \approx 3.06n^8; \quad n \sim 10.$$

This is connected with the fact that the matrix elements of the type  $\langle nlm | r^k | nlm \rangle$  (k > 0) depend mainly on the principal quantum number n and more weakly on l for  $n \gg 1$ .

A certain justification for this kind of summation can be seen in the fact that the Born approximation is determined by the Fourier transform of the static potential of the atom. The latter is determined by the quantum numbers n, l, and m. It is natural to assume that the elastic scattering cross section for scattering on an atom with given n is obtained by averaging the potential over the orbital quantum numbers.

The average of the form factor (2) for hydrogen over l and m was first introduced by Fock<sup>[11]</sup> in the momentum representation of the wave functions  $\psi n l m$ :

$$\frac{1}{n^2} \sum_{l,m} F_n(q) = \frac{1}{4n^4} T_n'(x) \left(1+x\right)^2 \left[P_n'(x) + P_{n-1}'(x)\right].$$
(7)

Here  $T_n(x) = \cos(n \arccos x)$  is a Tschebyshev polynomial,  $P_n(x)$  is a Legendre polynomial, and  $x = (4 - n^2q^2a_0^2)/(4 + n^2q^2a_0^2)$ .

For  $n \gg 1$  we can use the asymptotic forms  $(|x| \leqslant 1)$ 

$$T_{n'}(x) \approx \frac{n}{\sqrt{2(1-x)}} \sin\left(2n\sqrt{\frac{1-x}{2}}\right)$$
$$P_{n'}(x) \approx \frac{n}{\sqrt{2(1-x)}} J_{1}\left(2n\sqrt{\frac{1-x}{2}}\right), \qquad (8)$$

here  $J_1(\boldsymbol{x})$  is the Bessel function. As a result we have for the differential elastic scattering cross section

$$\frac{d\sigma_n}{d\Omega} = \frac{4}{a_0^2 q^4} \left[ 1 - \frac{(1+x)^2}{4n^2(1-x)} \right]_{\times} \sin\left(2n\sqrt[4]{\frac{1-x}{2}}\right) J_1' 2n\sqrt[4]{\frac{1-x}{2}} \left(\frac{1-x}{2}\right) \right].$$
(9)

Introducing the new variable  $t^2 = 2n^2(1-x)$ , we obtain for the total elastic scattering cross section

$$\sigma_n^{(1)}(E) = \frac{8\pi a_0^2 n^4 \operatorname{Ry}}{E} \int_0^{t_m} \frac{dt}{t^3} \left[ 1 - \frac{2(1 - t^2/4n^2)^2 \sin t J_1(t)}{t^2} \right]^2,$$
$$t_m = 2k a_0 n^2 / \sqrt{1 + n^2 k^2 a_0^2}.$$
 (10)

This expression reproduces correctly the Born approximation of the elastic cross section as a function of n and E.

The inelastic scattering cross section has been estimated in Born approximation in <sup>[10]</sup>:

$$\sigma_{n,in}^{(1)}(E) = \frac{8\pi \operatorname{Ry}}{3E} \overline{r_n^2} \ln\left(\frac{\beta_n \hbar v}{e^2}\right); \quad (11)$$

here  $\overline{r_n^2}$  stands for the following quantity:

$$\overline{r_n^2} = \frac{1}{n^2} \sum_{l,m} \langle nlm | r^2 | nlm \rangle;$$
(12)

 $\beta_n$  is a dimensionless constant which is in general very difficult to estimate.

When the Born approximation is valid, the inelastic scattering cross section (11) is larger than the elastic scattering cross section (10), owing to the presence of the logarithmic term. Therefore we do not require an accurate estimate of the elastic scattering cross section in (6). We use the simplest approximation which takes account of the main features of the elastic cross section in Born approximation:

$$\sigma_n^{(1)}(E) = \frac{4\pi (r_n^2)^2}{9a_0^2 [1 + 4n^4 E \gamma_n / \text{Ry}]},$$
(13)

where  $\gamma_n$  is a constant analogous to  $\beta_n$ . When  $4n^4E \gg Ry/\gamma_n$ , the cross section (13) behaves similarly to (10). This similarity is preserved for  $E \rightarrow 0$ . Using (11) and (13) we have for the total cross section

$$\sigma_{n,tot}^{(1)}(E) = \frac{8\pi \operatorname{Ry}}{3E} \overline{r_n^2} \ln\left(\frac{\beta_n \hbar v}{e^2}\right) + \frac{4\pi (r_n^2)^2}{9a_0^2 [1 + 4n^4 E \gamma_n / \operatorname{Ry}]}.$$
(14)

The knowledge of the imaginary part of the forward elastic scattering amplitude in second order perturbation theory allows us to use the dispersion relation<sup>1)</sup>

$$\bar{f}_{n}^{(2)}(E,0) = \frac{1}{\pi} \int_{0}^{\infty} \frac{\operatorname{Im} \bar{f}_{n}^{(2)}(E',0) dE'}{E' - E - i\varepsilon}.$$
(15)

Using (6), (14), and (15), and calculating the integral with logarithmic accuracy, we obtain

$$f_n^{(2)}(E,0) = \frac{2i\,\sqrt{2m}}{3\hbar\,\sqrt{E}} \operatorname{Ry}\overline{r_n^2} \ln\left(\frac{\beta_n\hbar\nu}{e^2}\right) + \frac{\sqrt{2m}\,(\overline{r_n^2})^2\,(i\,\sqrt{E} + \frac{1}{2}n^{-2}\,\sqrt{\mathrm{Ry}}/\gamma_n)}{9a_0^2\hbar\,(1 + 4n^4E\gamma_n/\mathrm{Ry})}.$$
(16)

The averaged forward elastic scattering amplitude in first-order perturbation theory has the form

$$\overline{f}_{n}^{(1)}(E,0) = \overline{r_{n}^{2}}/3a_{0}.$$
 (17)

We assume that the Born approximation is valid if the following inequality is fulfilled:

$$|\bar{f}_n^{(1)}(E,0)| \gg |\bar{f}_n^{(2)}(E,0)|,$$

which yields, using (17) and (16),

$$\frac{4e^2}{\hbar v}\ln\frac{\beta_n\hbar v}{e^2} \ll 1.$$
(18)

In deriving (18) we have neglected the contribution to (16) from the elastic scattering, which under

<sup>&</sup>lt;sup>1)</sup>In order to avoid misunderstanding we note that here and later on for the inelastic scattering we use a dispersion relation for the scattering amplitude in second-order perturbation theory. The analytic properties of this amplitude are established in an elementary way from the general expression for the second Born approximation. The problem of the existence of a dispersion relation for the exact amplitudes is not considered. Although the Born approximation is wrong for small energies, the construction of the second-order amplitude from its imaginary part obtained by the unitarity relation (6), in which the cross section is determined in first approximation, is correct for all energies.

the condition (18) is small compared with the contribution from the inelastic processes. This justifies the simplified form (13), since the final answer is insensitive to it.

The condition for the applicability of the Born approximation for elastic scattering depends weakly on the principal quantum number n. In our estimates we have not taken exchange effects into account. This is permitted if (18) is satisfied, since the exchange amplitude is, according to [12]

$$f_n^{\mathbf{ex}} \sim k^{-2} F_n(q);$$

under the same conditions we have for the direct scattering amplitude

$$f_n^{\rm dir} \sim q^{-2} (1 - F_n(q))$$

For forward scattering the direct amplitude is larger than the exchange amplitude if  $E \gg Ry/n^4$ , which is always the case when (18) is satisfied.

### 2. INELASTIC SCATTERING

The inelastic scattering amplitude in Born approximation has the form [10]

$$f_{nn'}^{(1)}(E,\vartheta) = \frac{2me^2}{\hbar^2 q^2} \langle n'l'm' | \exp\{-i(\mathbf{k}_j - \mathbf{k}_i)\mathbf{r}\} | nlm \rangle.$$
(19)

For small angle scattering the momentum transfer q is small compared to  $1/a_n$ ; we may therefore expand the exponent in (19) in a series, and keeping only the first nonvanishing term we obtain (Bethe approximation)

$$f_{nn'}^{(1)}(E, \vartheta) \approx \frac{2i \langle n'l'm' | x | nlm \rangle}{qa_0}.$$
 (20)

For forward scattering  $q=\Delta E_{nn^{\prime}}/\hbar v,$  and we find from (20)

$$f_{nn'}^{(1)}(E,0) = \frac{2i\hbar v \langle n'l'm' \mid x \mid nlm \rangle}{\Delta E_{nn'} a_0}, \qquad (21)$$

this holds for  $\Delta E_{nn'}a_n/\hbar v \ll 1$ , where  $a_n$  is the radius of the n-th orbit  $(n, n' \gg \Delta = |n - n'|)$ .

Since we are not interested in the detailed description of the cross section for the different transitions  $n, l, m \rightarrow n', l', m'$ , we average the quantity  $\langle n'l'm' | x | nlm \rangle$  in (21) over all l, m and l', m':

$$\bar{x}_{nn'} = \left(\frac{1}{n^2} \sum_{l,m,\,l'm'} |\langle n'l'm' \,|\, x \,|\, nlm \rangle |^2\right)^{1/2}.$$
(22)

This averaging procedure allows us to obtain a simple formula which characterizes (21) as function of n, n' and  $\Delta = |n - n'|$ . To this end we use the definition of the dipole oscillator strength averaged over l, m and summed over l', m': <sup>[13]</sup>

$$|\bar{f}_{nn'}| = \frac{2m|\omega_{nn'}|}{\hbar} |\bar{x}_{nn'}|^2 = \frac{3.92nn'^3}{|n^2 - n'^2|^3}, \quad (23)$$

From this we obtain for  $\overline{x}_{nn'}$ 

$$\bar{x}_{nn'} = \left(\frac{\hbar^2 |\bar{f}_{nn'}|}{2m |\Delta \bar{E}_{nn'}|}\right)^{1/2} \approx \frac{n^2 a_0}{2\Delta^2}, \qquad (24)$$

where  $\Delta = |\mathbf{n} - \mathbf{n'}| \ll \mathbf{n}, \mathbf{n'}$ .

In order to estimate the inelastic forward scattering amplitude in second-order perturbation theory we use the unitarity relation:

$$\operatorname{Im} f_{nn'}^{(2)}(E,0) = \frac{1}{4\pi} \sum_{r} k_r \int d\Omega' f_{n'r}^{\bullet(1)}(q) f_{nr}^{(1)}(q). \quad (25)$$

The main contribution to the integral on the righthand side of (25) comes from the region of small angles. The sum in (25) contains amplitudes of elastic and inelastic processes. The calculations in first-order perturbation theory show that in the region of small angles the inelastic scattering amplitude is larger than the elastic amplitude; <sup>[10]</sup> this property holds the better, the larger the value of the principal quantum number n ( $\Delta \ll$  n, n').

Keeping in (25) only the inelastic contributions, we write the latter in the form [cf. (20)]

$$\operatorname{Im} f_{nn'}^{(2)}(E, 0) = \frac{1}{\pi a_0^2} \sum_r k_r x_{n'r}^* x_{nr} \int \frac{d\Omega}{q_{n'r} q_{nr}} \,.$$
(26)

Here  $q_{ab} = (k_a^2 - 2k_ak_b \cos \vartheta + k_b^2)^{1/2}$ , where  $k_a$  and  $k_b$  are connected by the relation

$$\frac{\hbar^2 k_a^2}{2m} + E_a = \frac{\hbar^2 k_b^2}{2m} + E_b; \quad x_{ab} = \langle (nlm)_b | x | (nlm)_a \rangle.$$

For large values of the quantum numbers n, n' > 1 the inequality  $E > \Delta E_{nn'}$  is already satisfied for small (of order 1 eV) energies of the electrons. In this region we may assume  $k_n \approx k_{n'}$ . On account of what has been said above, (26) takes the form

$$\operatorname{Im} f_{nn'}^{(2)}(E, 0) = \frac{1}{\pi a_0^2} \sum_r k_r x_{n'r}^* x_{nr} \int \frac{d\Omega}{k_n^2 - 2k_n k_r \cos \vartheta + k_r^2}$$

$$= 2 \sum_{r} \frac{x_{n'r}^{*} x_{nr}}{a_0^2 k_n} \ln \left| \frac{k_n + k_r}{k_n - k_r} \right|.$$
 (27)

Let us use the dispersion relation for  $f_{nn'}^{(2)}(E, 0)$ :

$$f_{nn'}^{(2)}(E_{\star} 0) = \frac{1}{\pi} \int_{\Delta E_{nn'}}^{\infty} \frac{\operatorname{Im} f_{nn'}^{(2)}(E', 0) dE'}{E' - E - i\varepsilon}.$$
 (28)

Calculating the integral in (28) with logarithmic accuracy in the region  $E \gg \Delta E_{nn'}$  we obtain

$$f_{nn'}^{(2)}(E,0) = \frac{2i\hbar}{a_0^2 \sqrt{2m}} \sum_r \frac{x_{n'r}^* x_{nr}}{\sqrt{E}} \ln \left| \frac{k_n + k_r}{k_n - k_r} \right| + O\left(\frac{\Delta E}{E}\right).$$

The argument of the logarithm is independent of the quantum numbers l, m. We average the sum in (29) in analogy to (22):<sup>2)</sup>

$$\bar{f}_{nn'}^{(2)}(E,0) = \frac{2i\hbar}{a_0^2 \sqrt{2mE}} x_{nn'}^2 \ln \frac{4E}{\bar{J}_n}, \qquad (30)$$

where

$$\ln \frac{4E}{\bar{J}_n} = \frac{\sum_{j,r} x_{n'r}^* x_{nr} \ln |(k_n + k_r)/(k_n - k_r)|}{\sum_{r} x_{n'r}^* x_{nr}} .$$
 (31)

The constant  $\overline{J}_n$  is defined in analogy to the quantity I, which characterizes the "effective braking" of the electrons by the atoms;<sup>[10]</sup> the quantity  $x_{nn'}^2$  is by definition equal to

$$\overline{x_{nn'}^{2}} = \left(\frac{1}{n^{2}} \sum_{l, m, l', m'} |\langle n'l'm' | x^{2} | nlm \rangle|^{2}\right)^{l_{2}}.$$
 (32)

As in the case of elastic scattering, the condition for the applicability of perturbation theory follows from the inequality

$$|\bar{f}_{nn'}^{(1)}(E,0)| \gg |\bar{f}_{nn'}^{(2)}(E,0)|.$$
 (33)

Using (21) and (30), we obtain from (33)

$$\frac{E}{\ln\left(4E/\bar{J}_{n}\right)} \gg \frac{x_{nn'}^{2} |\Delta E_{nn'}|}{2a_{0}\bar{x}_{nn'}}.$$
(34)

To determine the character of the dependence of this condition on the quantum numbers n and n' we must calculate the quantity (32).

The matrix element  $x_{nn'}^2$  can be estimated in the following form:

$$\frac{1}{n^{2}} \sum_{l, m, l', m'} |x_{nlm, n'l'm'}^{2}|^{2} = \frac{4}{45n^{2}} \sum_{l} [|(l'||C^{(2)}||l)|^{2} + \frac{5}{4}(2l+1)\delta_{ll'}]|\langle n'l'|r^{2}|nl\rangle|^{2}.$$
(35)

Here we have used the notation of [9]: the quantity  $(l' \parallel C^{(2)} \parallel l)$  is the reduced matrix element of the function

$$C_m^{(2)}(\vartheta,\varphi) = \sqrt{4\pi/5} Y_{2m}(\vartheta,\varphi),$$
$$\langle n'l' | r^2 | nl \rangle = \int_0^\infty R_{n'l'} r^2 R_{nl} r^2 dr,$$

where  $R_{nl}(r)$  is the radial wave function of the hydrogen atom.

The first term in (35) can be expressed through the quadrupole oscillator strength  $f_{nn'}^{(2)}$ , since

$$f_{nn'}^{(2)} = \frac{\omega_{nn'}^3}{30\hbar c^3} \frac{1}{2n^2} \sum_{l, l'} |(l' \| C^{(2)} \| l) |^2 |\langle n'l' | r^2 | nl \rangle |^2.$$
(36)

The calculation of the quadrupole oscillator strength is presented in the Appendix. The result is for  $n, n' \gg 1$ :

$$f_{nn'}^{(2)} = \frac{7.15 \cdot 10^{-5}}{n^5 n'^3 (n^{-2} - n'^{-2})^{7/3}}.$$
 (37)

For  $n, n' \gg \Delta = |n - n'|$ , formula (37) has the form

$$f_{nn'}^{(2)} = \frac{1.42 \cdot 10^{-5}}{\Lambda^{7/_{3}} n}.$$
 (38)

The second term in (35) is determined by a matrix element of the type  $\langle n'l | r^2 | nl \rangle$ . This can be calculated using the results of <sup>[10]</sup>. If n, n'  $\gg \Delta$  we have

$$|\langle n'l|r^2|nl\rangle|^2 \approx 4a_0^4 n^8 / \Delta^4 \Gamma^2 (1+\Delta). \tag{39}$$

Using (36), (38), and (39), we can obtain the following expression for (35):

$$\frac{1}{n^2} \sum_{l, m, l', m'} |x_{nlm, n'l'm'}^2|^2 = \frac{4a_0^4 n^8}{45} \Big[ \frac{16}{\Delta^{16/3}} + \frac{5}{\Delta^4 \Gamma^2 (1+\Delta)} \Big].$$
(40)

For the case of practical importance  $\Delta \sim 1$ , we obtain, using (40),

$$x_{nn'}^2 \approx 1.4a_0^2 n^4.$$
 (41)

Let us use for  $|\Delta E_{nn'}|$  the expression

$$\left|\Delta E_{nn'}\right| = \operatorname{Ry}\left|\frac{1}{n^2} - \frac{1}{n'^2}\right|,\qquad(42)$$

where Ry is the ionization potential of the hydrogen atom. We now substitute (24), (41), and (42) in (34) with  $\Delta \sim 1$ :

$$E/\ln\frac{4E}{\bar{J}_n} \gg \frac{\mathrm{Ry}}{n}.$$
 (43)

The inequality (43) is the final condition for the applicability of the Born approximation as a function of the principal quantum number n for n, n'  $\gg \Delta \sim 1$ . The quantity  $\bar{J}_n$  remains undetermined, but in estimates one can regard it as equal to the ionization potential of the n-th level, since the logarithm is rather insensitive to such an approximation.

If (43) is satisfied, then the conditions already used,

$$\Delta E_{nn'}a_n / \hbar v \ll 1, \qquad E \gg \Delta E_{nn'}$$

are fulfilled. The inverse for large n is not true in general. As in the case of elastic scattering,

<sup>&</sup>lt;sup>2)</sup>The quantities  $\langle n'l'm' | x | nlm \rangle$  and  $\langle n'l'm' | x^2 | nlm \rangle$  cannot be simultaneously different from zero, since they satisfy different selection rules in l and m. We compare the amplitudes (21) and (30) in which an average over all l and m is taken and where the quantities  $\overline{x}_{nn'}$  and  $\overline{x}_{nn'}^2$  are simultaneously finite. Without such an average, one must compare (21) and (29), where in the later expression one cannot use a representation of the type (30).

we may convince ourselves that the neglect of exchange effects is permitted under the condition (43), for the direct forward scattering amplitude is much larger than the exchange forward scattering amplitude if  $(\Delta E_{nn'}/E)^2 \ll 1$ , which is a much weaker condition than (43).

In conclusion we note that, for inelastic transitions in collisions of electrons with atoms in the ground state, the approximation for the scattering amplitude (20) leads generally to a larger value than the more accurate expression (19). Since we have used such an approximation for the estimate in second order perturbation theory, it may turn out that the condition for the applicability of the Born approximation is somewhat weaker than condition (43).

#### APPENDIX

## CALCULATION OF THE QUADRUPOLE OSCIL-LATOR STRENGTH

To calculate the quadrupole oscillator strength we use an approach analogous to the one used for the calculation of the dipole oscillator strength (cf., for example, <sup>[14]</sup>). We consider the classical problem of the quadrupole radiation of an electron in an attractive Coulomb field. The intensity of the radiation is determined by the sum of the square moduli of the Fourier components of the quadrupole moment. Since the orbit of the electron is a plane curve (we shall regard it as lying in the x, y plane) the components  $(xy)_{\omega}$ ,  $(x^2)_{\omega}$ , and  $(y^2)_{\omega}$  of the quadrupole tensor will be different from zero, where

$$a_{\omega} = \frac{1}{2\pi} \int_{-\infty}^{\infty} a(t) e^{i\omega t} dt$$

We use the following relations:

$$(xy)_{\omega} = \frac{i(\dot{x}y + \dot{y}x)_{\omega}}{\omega}, \qquad (A.1)$$

$$(x^2)_{\omega} = -\frac{2i}{\omega} (x\dot{x})_{\omega}, \qquad (A.2)$$

$$(y^2)_{\omega} = \frac{2i}{\omega} (y\dot{y})_{\omega}.$$
 (A.3)

According to [15], we use for x, y, and t the parametric representation  $(-\infty < \xi < \infty)$ 

$$x = a(\varepsilon - \operatorname{ch} \xi), \quad y = a\gamma \varepsilon^{2} - 1 \operatorname{sh} \xi,$$
  
$$t = \sqrt{ma^{3}/e^{2}}(\varepsilon \operatorname{sh} \xi - \xi),$$
  
(A.4)

where

$$a = \frac{e^2}{mv_0^2}, \quad \varepsilon = \sqrt{1 + \frac{2EM^2}{me^4}}, \quad E = \frac{mv_0^2}{2}, \quad M = m\rho v_0$$

 $v_0$  is the initial velocity, and  $\rho$  is the impact parameter. Calculating (A.1), (A.2), and (A.3) with the help of (A.4), we obtain  $(\gamma = \omega e^2/mv_0^2)$ :

$$(xy)_{\omega} = \frac{a^2 \gamma \varepsilon^2 - 1}{\omega} H_{i\gamma}^{(1)\prime\prime}(i\gamma \varepsilon), \qquad (A.5)$$

$$(x^2)_{\omega} = -(y^2)_{\omega} = -\frac{a^2}{\omega} \left(\varepsilon - \frac{1}{\varepsilon}\right) H_{i\gamma}^{(j)}(i\gamma\varepsilon).$$
 (A.6)

For the intensity of the radiation, integrated over all impact parameters  $\rho$  (or, what is the same, over all eccentricities  $\epsilon$ ) we obtain from (A.5) and (A.6)

$$\frac{dI_{\omega}}{d\omega} = \frac{4\pi^2 e^{14} \omega^4}{5c^5 m^6 v^{12}} \int_1^{\infty} \varepsilon \left(\varepsilon^2 - 1\right) d\varepsilon \left\{-\left[H_{i\gamma}^{(1)\prime\prime}(i\gamma\varepsilon)\right]^2 + \frac{\varepsilon^2 - 1}{\varepsilon^2} \left[H_{i\gamma}^{(1)\prime}(i\gamma\varepsilon)\right]^2\right\}.$$
(A.7)

Let us consider (A.7) in the limit  $\gamma \gg 1$ . This corresponds to the condition for quasiclassical motion in the Coulomb field  $e^2/\hbar v \gg 1$  with  $\hbar \omega \sim E$ . Using the asymptotic form of the Hankel functions for  $\gamma \gg 1$ ,

$$H_{i\gamma}^{(1)}(i\gamma\varepsilon) \approx -\frac{2ix}{\pi\sqrt{3}} K_{1/3}\left(\frac{\gamma}{3}x^3\right), \quad x = \sqrt{\varepsilon^2 - 1},$$
$$H_{i\gamma}^{(1)\prime}(i\gamma\varepsilon) \approx \frac{2x^2}{\pi\sqrt{3}} K_{2/3}\left(\frac{\gamma}{3}x^3\right), \quad (A.8)$$

and taking into account that for  $\gamma \gg 1$  the integrals in (A.7) are determined by the small values of the parameter x, we find

$$\frac{dI_{\omega}}{d\omega} = \frac{4\pi^2 e^{14} \omega^4}{5c^5 m^6 v^{12}} a(\gamma),$$

$$a(\gamma) = \frac{4}{3\pi^2} \int_0^\infty x^3 dx \left\{ \frac{x^4}{\gamma^2} K_{2/3}^2 \left( \frac{\gamma}{3} x^3 \right) + \frac{2x^5}{\gamma} K_{2/3}^2 \left( \frac{\gamma}{3} x^3 \right) K_{1/3}^{1/3} \left( \frac{\gamma}{3} x^3 \right) + x^6 K_{2/3}^2 \left( \frac{\gamma}{3} x^3 \right) \right\}.$$
(A.9)

The integrals appearing in (A.9) are given in [16].

Keeping the first nonvanishing term for  $\gamma \gg 1$ , we obtain

$$\frac{dI_{\omega}}{d\omega} = b \frac{\omega^{2/3} e^8}{c^5 m^3 v^2} \left(\frac{m}{e^2}\right)^{1/3}, \qquad (A.10)$$

where

$$b = \frac{32 \sqrt[3]{6} \pi \Gamma(^2/_3)}{5 \sqrt{3} \Gamma(^1/_3)} = 10,56.$$

The cross section for quadrupole recombination  $\sigma_{\rm rec}^{(2)}(\nu)$  is determined from (A.10) by the relation

$$\sigma_{\rm rec}^{(2)}(\mathbf{v}) = \frac{1}{h\mathbf{v}} \left( \frac{dI_{\mathbf{v}}}{d\mathbf{v}} \right) \frac{\Delta \mathbf{v}}{\Delta n}, \quad \frac{h\Delta \mathbf{v}}{\Delta n} = \frac{4\pi^2 m e^4}{h^2 n^3}, \quad (A.11)$$

where  $dI_{\nu}(\nu) = 2\pi dI_{\omega}(\nu)$ .

The cross section for quadrupole photo ionization  $\sigma_{\rm ph}^{(2)}(\nu)$  is connected with  $\sigma_{\rm rec}^{(2)}(\nu)$  by the principle of detailed balance:

$$\sigma_{\rm ph}^{(2)}(v) = \frac{m^2 c^2 v^2}{h^2 v^2 2 n^2} \sigma_{\rm rec}^{(2)}(v). \tag{A.12}$$

Let us extend this expression to a bound-bound state transition:

$$\mathbf{v} \to \mathbf{v}_{nn'} = \frac{2\pi^2 m e^4}{h^3} \left( \frac{1}{n^2} - \frac{1}{n'^2} \right).$$

The quadrupole oscillator strength is connected with the probability for the transition  $n \rightarrow n'$  per unit time through the relation

$$W_{nn'}^{(2)} = \frac{2\omega_{nn'}^2 e^2}{mc^3} |f_{nn'}^{(2)}|.$$
 (A.13)

On the other hand, the quadrupole absorption cross section  $\bar{\sigma}_{nn}^{(2)}$ , averaged over the frequencies and summed over the interval of final states, is connected with  $f_{nn}^{(2)}$ , by the equation

$$\overline{\sigma}_{nn'}^{(2)} = \frac{\Delta n'}{\Delta v} \int \sigma_{nn'}^{(2)} dv = \frac{\pi e^2}{mc} f_{nn'}^{(2)} \frac{\Delta n'}{\Delta v}.$$
 (A.14)

Using (A.10) to (A.14), we obtain

$$f_{nn'}^{(2)} = \frac{(12)^{\frac{1}{3}} \cdot 32\Gamma(\frac{2}{3})}{5\sqrt{3}\pi\Gamma(\frac{1}{3})} \frac{\alpha^2}{n^5 n^{\frac{3}{3}}(n^{-2} - n^{\frac{1}{2}})^{\frac{1}{3}}}$$
(A.15)

$$=\frac{110^{-10}}{n^5 n'^3 (n^{-2} - n'^{-2})^{7/3}}$$

where  $\alpha = e^2/\hbar c = 7.3 \times 10^{-3}$ .

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