Elastic scattering of electrons and positrons by complex atoms at medium energies

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The transport cross sections have been obtained for elastic scattering of electrons and positrons by complex atoms in the quasiclassical approximation, in the energy range from several tens of electron-volts to several tens of kiloelectron-volts. A simple analytical formula has been found for the transport cross section, which goes over to the well known Born approximation result at high energies. For the first time, the transport cross section for elastic scattering of electrons has been shown to be a universal function of the reduced particle energy in the medium energy range. The values of this function have been tabulated. It is shown that the stopping power of matter for slow ions, attributable to elastic collisions, can be determined by measuring the transport cross section for scattering of positrons by complex atoms. The theoretical conclusions are in good agreement with the abundant experimental data and with the results of computer calculations.

1. INTRODUCTION

Many problems of modern electron physics and astrophysics require the study of elastic scattering of electrons and positrons by atoms at energies ranging from several tens of electron-volts to several tens of kiloelectron-volts. In particular, electron scattering plays an important role in interpretation of the data obtained through the use of various approaches have been used to compute the differential cross sections, such as the R-matrix method, the polarized orbitals method, and the optical model with exchange and correlation interaction energy of a particle in the screened field of a nucleus.

2. QUASICLASSICAL APPROXIMATION

The condition for the applicability of the quasiclassical approximation to scattering of electrons (or positrons) with energy $E$ by the screened Coulomb field of a nucleus has the form

$$ Z^2 e^2 E e < Z^2, \quad (1) $$

where $Z$ is the nuclear charge of the target atoms (it is assumed, that $Z > 1$) and, for simplicity, atomic units have been used. The right inequality in expression (1) ensures applicability of the quasiclassical description in the range of order $E \ll Z^{-1}$, where the screening of the nucleus by atomic electrons is small and the potential of interaction is close to the Coulomb potential (see Ref. 15). The left inequality in expression (1) means that the particle wavelength $\lambda$ is small compared to the screening radius $r_\text{Fermi} \equiv Z^{-1}$, which coincides with the characteristic length over which the Thomas-Fermi potential varies. Besides condition (1), for the quasiclassical approximation to be applicable, the uncertainty $\Delta \sigma$ of the scattering angle should be much smaller than $\theta$—the scattering angle itself. That yields the inequality

$$ 4 \pi b/\lambda \Delta \sigma > 1, \quad (2) $$

where $\lambda$ is the orbital quantum number and $\sigma$ is the corresponding phase shift. Thus, the phase shifts $\sigma$ found in the quasiclassical approximation should, generally speaking, satisfy condition (2). However, it will be shown below that due to the properties of the Thomas-Fermi potential, the quasiclassical phase shifts can still be used to determine the transport cross sections, even when inequality (2) is not satisfied.

We shall show, that the effects of both exchange interaction (for electron scattering) and correlation interaction on the transport cross section are negligible in the energy range (1). The value of the exchange interaction is of the order of the reciprocal of the mean atomic electron radius and is proportional to $\rho^{1/2}$, where $\rho$ is the charge density. Let $V$ denote the absolute value of the potential interaction energy of a particle in the screened field of a nucleus. Since $\rho^{1/2} \sim V^{1/2}$, it is obvious that the exchange interaction is of order $V$ only at the distances $r \geq 1$, when $V \sim V^{1/2} \sim 1$. Small scattering angles, whose contributions to the transport cross section are insignificant in the energy range (1), correspond to impact parameters $b \gg 1$. It is convenient to consider the short-range ($r < 1$) and the long-range ($r > 1$) parts of the correlation interaction separately. The long-range correlation interaction mainly reduces to the polarization of the high-lying atomic shells,
and has an order of magnitude $1/v < 1$, where $v$ is the velocity of an incident particle. Hence, the polarization correction to the potential becomes significant only in the region $r \approx 1$, which is unimportant for calculations of $\sigma_{el}$. The short-range interaction has been shown in Ref. 12 to be less than $V/\langle E \rangle$ everywhere in the region $r \approx 1$. This comes as little surprise, since the correlation interaction at such distances consists of deviations of the potential from its statistical mean due to fluctuations, which should be small for the system with the large number of particles.\textsuperscript{16}

Since the scattering takes place against a background of inelastic processes, it is important to estimate the effect of the inelastic channels on the probability of inelastic interaction. We shall show that the cross section $\sigma_{el}$ for elastic scattering is significantly larger than $\sigma_{el}$ for the total energy range (1). To derive this estimate, we will use the explicit form of the cross section for elastic interaction between fast electrons and complex atoms. It is given in Ref. 15

$$\sigma_{el} = 2\alpha Z^2/\langle E \rangle.$$

Correspondingly, for inelastic scattering we have\textsuperscript{16}:

$$\sigma_{in} = \sum_{i=1}^{N} n_i \int \frac{E}{U_i} f_i \left( E / U_i \right).$$

where $U_i$ and $n_i$ are the binding energy and the number of electrons in the $i$th atomic shell, $N$ is the total number of shells and $f_i(E/U_i)$ is a function which grows proportional to $\ln(E/U_i)$\textsuperscript{15} for large values of the argument. Weakly bound electrons, with binding energy $U_i \approx 1$, provide the main contribution to $\sigma_{in}$. According to the Thomas-Fermi model, their number is of the order of $Z^2/\alpha^2$. Hence, the cross section for inelastic interaction is of the order of magnitude

$$\sigma_{in} \approx n Z^2/\langle E \rangle.$$

One can easily deduce from this that the ratio of the cross sections over the full range of energy (1) is

$$\sigma_{el}/\sigma_{in} = Z^{-2} \approx 1.$$

To calculate $\sigma_{el}$, we have used the expression for elastic cross section, which, generally speaking, had been derived for fairly fast electrons, so it will be helpful to compare the obtained estimate with the results of numerical calculations\textsuperscript{6,11} in the energy range $E \approx Z^2/\alpha^2$. In particular, in the case of electrons with energy 100 eV the inelastic cross section for scattering by neon ($Z = 10$) is $\sigma_{in} = 0.88$\textsuperscript{11}, while the elastic cross section is $\sigma_{el} = 8.0$\textsuperscript{11}. These results hold also for other elements\textsuperscript{11} at energies $E \approx Z^2/\alpha^2$.

Thus, even at moderate energies, the probability of inelastic scattering still remains far smaller than the probability of elastic scattering. One can expect the effect of inelastic processes on the value of transport cross sections to be even less pronounced. In fact, inelastic scattering leads mainly to the ionization of an atom, which is accompanied by the emergence of the slow secondary electrons with speeds $v \approx 1$. Collisions which cause scattering at small angles $\theta < 1$ (Ref. 15) play a major role here. This is why inelastic processes will mainly affect those partial amplitudes $f_i$ with large numbers of particles, which correspond to scattering at small angles. The contribution of these members to the sum over $l$ determining the transport cross section is insignificant. Taking into consideration the above arguments, we shall neglect inelastic processes when calculating $\sigma_{el}$.

Making use of the estimates of the potential energy of interaction, we can set

$$U = \langle 0 \rangle |U(0) = U_{rin},$$

where the averaging is taken over the wave functions of electrons in the ground state of the atom and $U_{rin}$ is the kinetic energy in the Thomas-Fermi model. Next, using the expression for $U_{rin}$ in the approximation of Lindhard, et al.,\textsuperscript{14}

$$U_{tin} = -e^2 \chi_{tin}(z)/r, \quad \chi_{tin}(z) = 1 - e^2 Z^2/\alpha_1 Z^2, \quad \chi_{tin} = 1,$$

$$X(z) = \left\{ \begin{array}{ll}
1 - e^{-1/\alpha_1} & z < 1 \\
1 - e^{-1/\alpha_1} & z > 1
\end{array} \right.$$

we obtain for the transport cross section

$$\sigma_{tin} = \frac{4\pi}{\alpha_1^2} \sum_{l=1}^{l=1} \langle l+1 \rangle \sin^2 \Delta_{in},$$

where

$$\Delta_{in} = \begin{cases}
\text{arcsec} \left( \frac{1}{\sqrt{2}} + \frac{1}{\sqrt{2}} \right) \sqrt{1 + \frac{1}{\sqrt{2}}}, & \frac{1}{\sqrt{2}} \leq x^2 + 1 - 1 \\
\text{arcsec} \left( \frac{1}{\sqrt{2}} + \frac{1}{\sqrt{2}} \right) \sqrt{1 + \frac{1}{\sqrt{2}}}, & \frac{1}{\sqrt{2}} > x^2 + 1 - 1
\end{cases}$$

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\text{arcsec} \left( \frac{1}{\sqrt{2}} + \frac{1}{\sqrt{2}} \right) \sqrt{1 + \frac{1}{\sqrt{2}}}, & \frac{1}{\sqrt{2}} > x^2 + 1 - 1
\end{cases}$$

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\text{arcsec} \left( \frac{1}{\sqrt{2}} + \frac{1}{\sqrt{2}} \right) \sqrt{1 + \frac{1}{\sqrt{2}}}, & \frac{1}{\sqrt{2}} \leq x^2 + 1 - 1 \\
\text{arcsec} \left( \frac{1}{\sqrt{2}} + \frac{1}{\sqrt{2}} \right) \sqrt{1 + \frac{1}{\sqrt{2}}}, & \frac{1}{\sqrt{2}} > x^2 + 1 - 1
\end{cases}$$

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here \( k \) is the particle momentum, 

\[
w = 0.885 a, Z^{\text{eff}} = k/v, \quad \mu = (1/\gamma^4)Z^{\text{eff}}(1+1/\gamma), \quad (8)
\]

signs "+" and "−" correspond to positrons and electrons. The dimensionless parameters \( \gamma \) and \( \mu \) have an obvious physical meaning. Specifically, \( \gamma \) is the reduced particle momentum, i.e., the momentum expressed in the characteristic units for fixed electrons in a Thomas-Fermi atom. Similarly, \( \mu \) is the impact parameter corresponding to the quantum number \( l \) and the Fermi momentum \( v_F \), divided by the screening radius \( a_s \).

It follows from Eqs. (6) and (7), that the quasiclassical phase differences \( \Delta_{\gamma} = \Delta_{\gamma}^{+} - \Delta_{\gamma}^{-} \) are essentially different for positrons (+) and electrons (−). This difference is totally attributable to the sign of the interaction potential energy. In view of this fact, it is of interest to analyze the results in more detail. Expression (6a) is meaningful only when \( \gamma = |\gamma| \geq 1 \). A positron with such values of \( \gamma \) can approach the nucleus to within the distance \( r \leq Z^{-1/2} \). It is clear that at such short distances the field is close to the Coulomb field, and for this reason, the phase difference is close to the Coulomb value as well. We note, that for \( x < (3 - 1) \), a positron is unable to penetrate the region \( r < Z^{-1/2} \), due to the strong Coulomb repulsive force from the positively charged nucleus. The phase difference is entirely determined by Eq. (6b). It can be readily observed, that in fact this expression coincides with the phase difference for scattering by the potential field, inversely proportional to the squared radius. This result is in complete agreement with the functional dependence of the potential energy on radius specified in (3). The same is true for Eq. (7c) applied to electrons.

The fact that electrons can penetrate the region \( r < Z^{-1/2} \) around the nucleus due to their negative charge, regardless of the values of their kinetic energy, constitutes an important property of electron elastic scattering. This is why there always exists range of impact parameters corresponding to scattering by a nearly-Coulomb nuclear field if the particle momentum is \( k > Z^{-1/2} \). The number of values such that the phase differences \( \Delta_{\gamma}^{+} \) are still close to the Coulomb ones increases with increasing electron energy (i.e. increasing parameter \( \gamma \)). Expressions (7a) and (7b) correspond to these values of \( \gamma \). Thus the values of \( \Delta_{\gamma}^{+} \) are comprised of the Coulomb phase differences and the phase differences corresponding to scattering by a field varying as \( 1/r^2 \), as expected.

We note that for \( l \geq Z^{-1/2} \), the phase differences \( \Delta_{\gamma} \), defined by formulas (6) and (7), become much less than unity 

\[
\Delta_{\gamma} = \Delta_{\gamma}/l - Z^{-1}/l < 1.
\]

In this last case condition (2) is violated, and the expressions derived earlier for \( \Delta_{\gamma} \), formally, cease to hold. However, the phases \( \Delta_{\gamma}^{+} \) are easy to find in the Born approximation for the values \( \gamma > Z^{-1/2} \) (See Ref. 15). The appropriate calculations show that the values of \( \Delta_{\gamma}^{+} \) obtained from perturbation theory, coincide with the values of \( \Delta_{\gamma} \), accurate to within 2%. Since the transport cross section \( \sigma_T \) depends only on the absolute value of the phase differences, this discrepancy can be neglected, and the summation over \( l \) in formula (5) can be extended to arbitrary values of \( l \), however large.

3. TRANSPORT CROSS SECTION

In subsequent discussions it will be advantageous to go over to the ordinary units and introduce the reduced particle energy 

\[
\varepsilon = E_{\text{Boh}}/Z = 0.885 a, Z^{\text{eff}} e^2 a^{-2}.
\]

where \( a \) and \( e \) are the Bohr radius and the electron charge. For \( \varepsilon > 1 \), the incident particles energy exceeds the average kinetic energy of the atomic electrons. Then expression (5) simplifies significantly, and we obtain for the transport cross section

\[
\sigma_T = 2 a \left( Z e^2 \right) \left( (\varepsilon e^2 Z e^2) + (0.885 a, Z^{\text{eff}} e^2 Z e^2) \right)^{-2} Z^3 (Y^3 - 1) \left( (\varepsilon e^2 Z e^2) + 1 \right)^{1/2} \left( (Y - 1)^{1/2} \right)^{1/2}, \quad \varepsilon > 1.
\]

Here \( m \) is the electron mass. If the reduced particle energy is sufficiently large \( \varepsilon > 1 \), the difference between the transport cross sections for electrons and positrons becomes negligible. Making use of expression (9), we find

\[
\sigma_T = 8 a (Z e^2/m)^2 \ln (1.085 a, Z^{\text{eff}} e^2 Z e^2), \quad 1 < \varepsilon < Z^3.
\]

which agrees with the results of Ref. 16, obtained by a qualitative approach.

We stress here, that even though expression (9) has been derived under the assumption \( \varepsilon < Z^{-1/2} \), it holds true for any \( \varepsilon > 1 \), including \( \varepsilon < Z^{-1/2} \) (for non-relativistic values of energy). This follows from the fact that scattering of high-energy particles takes place mostly in the nuclear Coulomb field. However, as is well known, both the classical and quantum-mechanical approaches to scattering by the Coulomb field yield identical results.14 In connection with this, it is of interest to analyze Eq. (9) in the limiting case \( \varepsilon > Z^{3/2} \).

Expression (9) gives for the energy range in question

\[
\sigma_T = 4 a (Z e^2/m)^2 \ln (1.085 a, Z^{\text{eff}} e^2 Z e^2), \quad \varepsilon > Z^3.
\]

In essence, Eq. (11) coincides with the formula for the transport cross section for elastic scattering obtained in Ref. 15 in the Born approximation. We note that in the intermediate region of velocities \( \varepsilon \sim Z^{-1/2} e^2/m (e^{-1/2} ) \) expressions (10) and (11) yield practically the same values of \( \sigma_T \). Thus, formula (9) describes the behavior of the transport cross sections for electrons and positrons in a wide range of non-relativistic energies.

In the limit \( \varepsilon < 1 \) the transport cross sections can be presented in the form

\[
\sigma_T = a_2 S^{*}(\varepsilon),
\]

where \( a_2 = 0.885 a, Z^{\text{eff}} e^2 \) is the Thomas-Fermi screening radius, \( S^{*}(\varepsilon) \) is the reduced energy function, which is tabulated in Table I. The functions \( S^{*}(\varepsilon) \) have been obtained by going from summation over \( l \) in Eq. (5) to integration over the continuous variable \( \mu \). It follows from Table I, that the transport cross section for electrons is approximately 2.5 times larger, than the corresponding value for positrons. Thus, for example, for \( \varepsilon = 1 \) we have \( S^{*}(\varepsilon) \approx 1.7/\varepsilon \), while \( S^{*}(\varepsilon) \approx 0.7/\varepsilon \). It is interesting to note, that the functional dependence of \( a_2 \) on energy is essentially different for the
TABLE I. Values of the function $S^*$ ($\varepsilon$).

<table>
<thead>
<tr>
<th>$\varepsilon$</th>
<th>$S^*$</th>
<th>$\varepsilon$</th>
<th>$S^*$</th>
<th>$\varepsilon$</th>
<th>$S^*$</th>
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ranges of small $\varepsilon \ll 1$ and large $\varepsilon \gg 1$ energies. While for $\varepsilon \ll 1$ we have $\sigma_\varepsilon \sim \varepsilon^{-1/2} \ln \varepsilon$, for $\varepsilon < 1$, the cross section is inversely proportional to the reduced energy, $\sigma_\varepsilon \sim 1/\varepsilon$. The relationship (12) has a universal nature. Namely, for any arbitrary combination of the nuclear charge of the target atom $Z$ and the energy of the incident particle $E$, the value of $\sigma_\varepsilon/\sigma_{TF}$ depends only on the reduced energy $\varepsilon$. This makes expression (12) very useful indeed for practical computations of the transport cross sections in the range of small and medium $\varepsilon$.

4. COMPARISON OF THE THEORY WITH EXPERIMENT AND WITH OTHER CALCULATIONS

At the present time, measurements of the transport cross sections for elastic scattering of electrons have been carried out mainly for the noble (He, Ne, Ar, Xe) and molecular (O, N, N$_2$, O$_2$) gases. As it was pointed out earlier, the ratio of the transport cross section to the cross section of the Thomas-Fermi atom is a universal function of $\varepsilon$ in the range of moderate energies $\varepsilon \sim 1$. The function $S^*(\varepsilon)$, calculated by using Eq. (5), is plotted on Fig. 1, together with the experimental results.$^1$ The values of $\sigma_\varepsilon/\sigma_{TF}$, calculated in Refs. 8, 19, 20 for various elements of the periodic tables, are also listed there. One can see that the same curve fits to the vast majority of data points in the region $\varepsilon < 1$ (taking into account that the measuring errors for transport cross sections $\sigma_\varepsilon$ are of order 20–30%). When $\varepsilon \gg 2$, the function $S^*(\varepsilon)$ lies approximately 10% higher than the data obtained by other authors, which can be accounted for by the fact that the universal relationship is violated when $\varepsilon$ grows larger.

It is important to note, that the transport cross section $\sigma_\varepsilon$ at the fixed value of $Z$ is determined only by the reduced energy $\varepsilon$ and does not explicitly depend on the mass of the incident particle in the region $\varepsilon \ll 1$. This indicates that Eq. (12) is applicable for calculations of $\sigma_\varepsilon$ for both negatively and positively charged particles with arbitrary masses. In particular, the function $S^+*(\varepsilon)$ describes elastic scattering of slow ions by complex atoms. The problem of elastic scattering of ions by complex atoms has been considered using the classical approach in Refs. 18 and 21. For the function $S^+*(\varepsilon)$ Firsov$^{22}$ found the following approximation

$$S^+ \sim \varepsilon^{-2} \ln (1 + 0.7\varepsilon),$$

which is in good agreement with our result, obtained for $\varepsilon < 1$. At the same time, the values of $S^+$ differ from $S^*$ by roughly 30–40%. This difference gets smaller again with the increase in $\varepsilon$.

In the paper of Lindhard, et al. (Ref. 18) the average energy losses by slow ions, incurred through elastic scattering by atoms, have been tabulated as a function of the values of $S^+$.
of $k$. Since these losses are unambiguously related to the transport cross section for elastic scattering, one can easily construct the corresponding function $S^+(k)$ using the results obtained in Ref. 18. The values of $S^+(k)$ and $S^+(k)$ differ only slightly, the maximum discrepancy being less than 15%. This implies an interesting conclusion: it is possible to determine the stopping power of matter for slow atomic particles attributable to elastic scattering by measuring the transport cross section for positrons in the region of medium energies.

In the region $k > 1$ the results of the calculations of $\sigma^{\prime}$ using Eq. (9), are in good agreement with the data from Ref. 19, obtained numerically. For instance, when the electron energy is $E = 8.0$ keV the transport cross sections for aluminum ($k = 8.58$) and copper ($k = 2.94$), obtained through the use of Eq. (9), coincide with those quoted in Ref. 19 through the third decimal place. The same energy for the case of silver ($k = 1.54$) yields, using (9), $\sigma^{\prime} = 3.17 \times 10^{-18}$ cm$^2$, while Ref. 19 gives $\sigma^{\prime} = 3.10 \times 10^{-18}$ cm$^2$.

In conclusion, I take pleasure in thanking S. I. Nefedov, V. B. Dudarev, D. B. Rovinskii, M. I. Ryazanov, O. B. Firsov for useful discussions of the present results.

1V. I. Nefedov, Poverkhnost’ 1, 4 (1982).