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Potential and Glauber Scattering of Electrons
by Complex Atoms

by

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Abstract

Some simple models for scattering of electrons in the 1 keV energy region by complex atoms are considered. For a static potential consisting of a sum of Yukawa functions approximate solutions to the scattering problem are compared with the results obtained by a numerical solution of the radial wave equation. The effects due to the separate scatterers in the target are introduced in a non-relativistic Glauber model where the target electrons are taken to be in a common spherically symmetric state. The resulting scattering amplitude is then used to generate an optical potential, which is modified by a method based on the eikonal-Born series and used to calculate differential and total cross sections for scattering on rare gases.

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1. Introduction

The scattering of electrons and positrons by complex atoms at intermediate energies has been the subject of a great number of recent experimental and theoretical investigations. We refer to Bransden and McDowell [1] for a review of pertinent contributions to the field during the last years.

On the theoretical side there are basically two types of difficulties that must be resolved, those connected with the scattering process itself and those which are due to the complexities of atomic structure. In the present paper the latter is described in terms of exponential density functions fitted either to the statistical Thomas-Fermi distribution [2] or to the actual atomic radius. Indeed, this misses many details contained e.g. in the Hartree-Fock wave function, but gives a reasonable reproduction of the main features of the electron distribution in complex atoms. This work is therefore aimed at a description of the elastic scattering process which, albeit of limited accuracy, is simple to use and can be applied to all except the lightest atoms. In inelastic scattering, which we do not consider here, it is of course important to use good wave functions for the initial and final states that are directly involved in the transition, but the rest of the atom could still be described in terms of the simpler model described above.

The simplest way to deal with the elastic scattering process is to treat it as scattering in a static, central potential, in our case a sum of Yukawa potentials. This can be done either by using the partial-wave expansion, or

by one of several approximate methods, some of which will be considered later. However, at intermediate energies it becomes important to take into account the fact that the scattering takes place on separate scatterers rather than in an overall potential. This effect may be introduced e.g. through the Glauber model [3], which has already been considered by several authors working in the field [4]. A general method for calculating the Glauber cross section in a complex atom described by product wave functions was given by Franco [5] and re-formulated by Thomas and Chan [6]. In practice, such calculations have only been performed for light atoms [7-10]. In the case of heavier atoms Glauber calculations have, to our knowledge, been made for alkalis only, and then in the so-called frozen-core approximation [11,12]. Here, the scattering is treated as though it takes place on a two-body system consisting of an inert core plus a valence electron.

One of the problems associated with the Glauber model is that it gives a rather poor approximation to the intermediate-energy large-angle cross section when applied to scattering in the atomic potential, although it reproduces the Rutherford cross section for scattering on a point charge exactly. This defect is carried over to the case in which one considers scattering on separate particles. One can at least to some extent overcome this difficulty by using the Glauber phase-shift function to generate an optical potential, and then solve the Schrödinger equation for scattering in this potential by the partial-wave

method or some suitable approximation. The absorptive part of the Glauber optical potential can in turn be modified by methods inspired by the eikonal-Born series, as done already by Byron and Joachain [13] for scattering on He and Ne. The potential derived by these authors, which is very carefully constructed, is based on realistic Hartree-Fock wave functions and contains exchange and polarization terms. In the energy region considered in the present paper exchange is of minor importance, whereas the polarization potential should indeed be included, at least for scattering at small angles. Our main efforts are, however, concentrated on the absorption potential, and we aim for a potential which is simple to use yet contains the essential features of the absorptive effects in complex atoms.

2. Some approximations to potential scattering

In this section we briefly consider some approximate scattering amplitudes that have been presented in the literature, as applied to a simple static potential. The idea is to see to what extent the various approximations reproduce the exact scattering cross section obtained from a partial-wave expansion for the same potential, rather than just making the usual test of comparing with the experimental results.

Considering elastic scattering of particles with charge $Z_1 e$ ($e > 0$) on a neutral atom with Z electrons we

write the corresponding scattering potential as

$$V_{st}(r) = Z_1 Z \alpha r^{-1} \phi_0(t),$$

$$t = r/\mu, \quad \mu = 0.8853 a_0 Z^{-1/3}, \quad (1)$$

where $\alpha = 1/137$ and where a_0 is the hydrogen Bohr radius (we use units for which $\hbar = c = 1$). The radius parameter μ is that appearing in the Thomas-Fermi model, and we write the function ϕ_0 as a sum of exponentials,

$$\phi_0(t) = \sum_{j=1}^N a_j \exp(-t_j),$$

$$t_j = \alpha_j t, \quad \sum_{j=1}^N a_j = 1. \quad (2)$$

A four-term least-squares fit to the Thomas-Fermi function at the points of Table 1 in [2] gives

$$\begin{aligned} a_1 &= 0.696, & \alpha_1 &= 1.274, \\ a_2 &= 0.264, & \alpha_2 &= 0.313, \\ a_3 &= 0.037, & \alpha_3 &= 0.114, \\ a_4 &= 0.003, & \alpha_4 &= 0.0354. \end{aligned} \quad (3)$$

The corresponding electron density is

$$\rho(r) = (4\pi\mu r^2)^{-1} \rho_0(t),$$

$$\rho_0(t) = \sum_{j=1}^N a_j \alpha_j t_j \exp(-t_j). \quad (4)$$

In addition to the fit to the Thomas-Fermi distribution we consider a one-term potential, where the parameter α_1 is chosen so that the density (4) reproduces the rms radius for the atom in question, as determined from the magnetic susceptibility.

Looking then at various approximate scattering amplitudes for particles with momentum $\underline{k}$ scattered through an angle θ by the potential (1)-(2), i.e. with momentum transfer $\underline{q} = 2k\sin(\theta/2)$, we mention initially that the first Born approximation gives the amplitude

$$f_{B1}(x) = 2\eta k^{-1} \sum_{j=1}^N a_j (\beta_j^2 + x^2)^{-1},$$

$$x = q/k, \quad \eta = Z\eta_1, \quad \eta_1 = Z_1\alpha/\beta, \quad \beta_j = \alpha_j/(k\mu), \quad (5)$$

where β is the velocity of the projectile (in units $\underline{c}$). Adding the contribution from the second Born approximation we have

$$f_{B12}(x) = f_{B1}(x) + f_{B2}(x),$$

$$f_{B2}(x) = \sum_{j=1}^N \sum_{j'=1}^N a_j a_{j'} f_{B2jj'}(x), \quad (6)$$

in which

$$f_{B2jj}(x) = 4\eta^2 k^{-1} (A_j x)^{-1} \left[\text{Arctan}\left(\frac{\beta_j x}{2A_j}\right) + \frac{1}{2} i \ln\left(\frac{A_j + x}{A_j - x}\right) \right],$$

$$A_j = (\beta_j^4 + 4\beta_j^2 + x^2)^{\frac{1}{2}}, \quad (7)$$

but where we refrain from presenting the rather more complicated cross terms ($\underline{j}' + \underline{j}$).

The Glauber [3] phase-shift function and scattering amplitude are for the static potential

$$\chi_G(v) = -2\eta \sum_{j=1}^N a_j K_0(\beta_j v), \quad v = kb,$$

$$f_G(x) = ik^{-1} \int_0^\infty v dv J_0(xv) \{1 - \exp[i\chi_G(v)]\}, \quad (8)$$

where $\underline{b}$ is the impact parameter. Variations on this theme are represented by the Glauber-angle approximation [14], which in the present case involves the addition of a quantity

$$\Delta\chi_{GA}(v) = 2\eta \sin\gamma(v) \sum_{j=1}^N a_j \exp(-\beta_j \tilde{v}),$$

$$\gamma(v) = \eta \sum_{j=1}^N a_j \beta_j K_1(\beta_j v), \quad \tilde{v} = v[1 + \tan^2 \gamma(v)], \quad (9)$$

to the Glauber phase-shift function, and the second-order eikonal approximation [15,16] which instead gives the additional phase

$$\Delta\chi_{SE}(v) = -\eta^2 \sum_{j=1}^N \sum_{j'=1}^N a_j a_{j'} (\beta_j + \beta_{j'}) K_0[(\beta_j + \beta_{j'})v]. \quad (10)$$

We also include two cross breeds between the Born and Glauber methods, viz. the eikonal-Born series [17] and the modified Glauber approach [18], the corresponding scattering amplitudes being

$$f_{EB} = f_{B1} + f_{B2} + f_{G3} ,$$

$$f_{MG} = f_G - f_{G2} + f_{B2} , \quad (11)$$

respectively, where

$$f_{Gn} = i^{n-1} (n!k)^{-1} \int_0^\infty v dv J_0(xv) [\chi_G(v)]^n. \quad (12)$$

The reader is referred to Sect. 6 for some numerical applications and a further discussion of these results.

3. The Glauber scattering amplitude and optical potential

We should now take into consideration that the scattering of the projectile takes place on individual scatterers (the nucleus and electrons of the target atom) rather than in an average static potential. Using the Glauber approximation to describe this effect and choosing the $\underline{z}$ direction perpendicular to the momentum transfer $\underline{q}$ we can write the scattering amplitude as [5]

$$\begin{aligned} f(\underline{q}) = & (2\pi)^{-1} i k \int d^2 \underline{b} \exp(i \underline{q} \cdot \underline{b}) d^3 r_1 \dots d^3 r_Z \\ & \times |\Psi(\underline{r}_1, \underline{r}_2, \dots, \underline{r}_Z)|^2 \left[1 - \prod_{j=1}^Z (b/b_j)^{2i\eta_1} \right], \\ \underline{b}_j = & \underline{b} - \underline{s}_j, \end{aligned} \quad (13)$$

where Ψ is the wave function of the electrons. The impact

parameter $\underline{b}$ and the components $\underline{s}_j$ of the electron coordinates $\underline{r}_j = (\underline{s}_j, z_j)$ are perpendicular to the $\underline{z}$ axis.

The calculation of the amplitude (13) is simplified considerably in the common-density approximation, which has been very widely used in applications of the Glauber theory to nuclear scattering. This approach consists in neglecting correlations between the target particles and writing

$$|\Psi(\underline{r}_1, \dots, \underline{r}_Z)|^2 = \prod_{j=1}^Z \rho(\underline{r}_j),$$

$$\int d^3r \rho(\underline{r}) = 1, \quad (14)$$

where the spherically symmetric density function $\rho(\underline{r})$ is an average over the filled target states. In this approximation the scattering amplitude becomes

$$f(x) = ik^{-1} \int_0^\infty v dv J_0(xv) [1 - S(v)],$$

$$S(v) = \exp[i\chi(v)] = [M(v)]^Z,$$

$$M(v) = \int d^3r \rho(\underline{r}) (v/v')^{2i\eta_1},$$

$$v' = kb', \quad \underline{b}' = \underline{b} - \underline{s}, \quad \underline{r} = (\underline{s}, z), \quad (15)$$

where the phase-shift function $\chi(\underline{v})$ replaces the corresponding quantity $\chi_G(\underline{v})$ (eq. (8)) which applies to Glauber scattering in the static potential.

Using the density (4) we can write the integral over the electron coordinates as

$$M(v) = v^2 \sum_{j=1}^N a_j \beta_j^2 \int_0^\infty u du I(u) K_0(\beta_j v u),$$

$$I(u) = (2\pi)^{-1} \int_0^{2\pi} d\phi (1+u^2-2u \cos \phi)^{-i\eta_1},$$

$$u = s/b. \quad (16)$$

Here, the modified Bessel function K_0 comes from the $\underline{z}$ -integration, and ϕ is the angle between $\underline{b}$ and $\underline{s}$. Since [19]

$$I(u) = -2^{-2\eta_1} \exp[-2i\sigma(\eta_1)] \int_0^\infty \tau^{2i\eta_1} d\tau (d/d\tau) J_0(u\tau) J_0(\tau),$$

$$\sigma(\eta_1) = \arg[\Gamma(1+i\eta_1)], \quad (17)$$

we can write

$$M(v) = -2^{-2\eta_1} \exp[-2i\sigma(\eta_1)] v^2 \sum_{j=1}^N a_j \beta_j^2 \times \int_0^\infty \tau^{2i\eta_1} d\tau (d/d\tau) J_0(\tau) (\tau^2 + \beta_j^2 v^2)^{-1}, \quad (18)$$

or, in terms of generalized hypergeometric functions [20],

$$M(v) = \sum_{j=1}^N a_j \{ [\Gamma(1-i\eta_1)]^2 z_j^{i\eta_1} [{}_1F_2(1+i\eta_1; i\eta_1, 1; z_j)$$

$$+(i/\eta_1) z_j {}_0F_1(2; z_j)]$$

$$-(i/\eta_1)(1-i\eta_1)^{-1} z_j [{}_1F_2(1; 2-i\eta_1, 1-i\eta_1; z_j)$$

$$-(1-i\eta_1)^{-1} {}_1F_2(2; 2-i\eta_1, 2-i\eta_1; z_j)] \},$$

$$z_j = \frac{1}{4} \beta_j^2 v^2. \quad (19)$$

An asymptotic expansion applicable to large impact parameters can be obtained by writing [19]

$$I(u) = {}_2F_1(in_1, in_1; 1; u^2), \quad (20)$$

and eq. (16) then yields [20]

$$M(v) = \sum_{j=1}^N a_j \sum_{n=0}^{\infty} [(in_1)_n]^2 z_j^{-n},$$

$$(z)_0 = 1, (z)_n = z(z+1)\dots(z+n-1). \quad (21)$$

Thus, $M(\underline{v}) \rightarrow 1$ as $\underline{v} \rightarrow \infty$, in such a manner that the integral (15) for the scattering amplitude is convergent, except for forward scattering ($\underline{x} = 0$).

The Glauber phase-shift function $\chi(\underline{v})$ can now be used to generate an equivalent optical potential

$$V_{\text{opt}}(r) = \pi^{-1} \beta k \int_{\rho}^{\infty} dv (v^2 - \rho^2)^{-\frac{1}{2}} (d/dv) \chi(v),$$

$$\rho = kr, \quad (22)$$

which has the property that the Glauber approximation to the scattering amplitude for this potential is identical to the amplitude (15) for scattering on the individual particles, i.e.

$$\chi(v) = -\beta^{-1} \int_{-\infty}^{\infty} V_{\text{opt}}(b, z) dz. \quad (23)$$

On the other hand, an exact solution of the scattering

problem for a particle moving in the optical potential no longer reproduces the Glauber amplitude (15), and by using the optical potential in this way one can avoid some of the drawbacks of the Glauber approximation, in particular the problems appearing at large scattering angles [3, 13].

It is convenient to write the optical potential as

$$V_{\text{opt}}(r) = Z_1 Z \alpha r^{-1} \phi_{\text{opt}}(t), \quad (24)$$

where the function ϕ_0 of the static potential (1) is replaced by the complex quantity ϕ_{opt} . In practice, we shall not use the Glauber phase-shift function $\chi(\underline{y})$ as given by eq. (15) to generate the optical potential, but rather apply a series expansion of ϕ_{opt} in terms of the parameter $\eta_1 = Z_1 \alpha / \beta$. The term of the lowest order then becomes the static potential function ϕ_0 , whereas the term of order η_1 is imaginary and acts as an absorption potential. We write

$$\begin{aligned} \phi_{\text{opt}}(t) &= \phi_0(t) + i\phi_{\text{abs}}(t), \quad \phi_{\text{abs}}(t) = -2\eta_1 \tilde{\phi}_{\text{abs}}(t), \\ \tilde{\phi}_{\text{abs}}(t) &= \sum_{j=1}^N a_j \phi_j(t_j), \end{aligned} \quad (25)$$

and obtain

$$\begin{aligned} \phi_j(t_j) &= -[\gamma + \ln(t_j/2)] e^{-t_j - K_0(2t_j) + \phi_j^{(1)}(t_j)}, \\ \phi_j^{(1)}(t_j) &= -\int_0^\infty u du \ln u (1+u^2)^{-3/2} J_0(t_j u), \end{aligned} \quad (26)$$

where $\underline{t}_j = \alpha_j \underline{t}$ and γ is Euler's constant. The absorption potential is influenced by the projectile charge and energy through its explicit dependence on η_1 , whereas the influence of the charge and density of the target atom is contained in the variables $\underline{t}_j$. We note that the function $\phi_j(\underline{t}_j)$ becomes $2(1-\ln 2)\underline{t}_j$ as $\underline{t}_j \rightarrow 0$ and $\underline{t}_j^{-2}$ as $\underline{t}_j \rightarrow \infty$.

4. A modification of the absorption potential

As it is well known, the Glauber scattering amplitude represents, in principle, a small-angle and high-energy approximation. For example, in Sect. 6 it is indeed seen that for electron scattering in a Yukawa potential the agreement between the exact and Glauber cross sections becomes progressively poorer as the scattering angle increases. This situation is also familiar in hadronic scattering on nuclei, even when one considers scattering on separate nucleons rather than in an overall potential. However, Coulomb scattering is pathological in many respects, and there is no doubt that the Glauber approximation suffers from serious defects not only at large but also at very small scattering angles when applied to electron scattering in the fields of the separate atomic particles. This shows up as a divergence in the scattering amplitude (15) for the forward direction, and we refer the reader to Byron and Joachain [13] (and references therein) for a further discussion of this shortcoming of the Glauber approximation. From a mathematical point of view the forward divergence in the scattering amplitude is due to the fact that for large $\underline{b}$ the Glauber

phase-shift function χ has a $\underline{b}^{-2}$ dependence on the impact parameter rather than the correct $\underline{b}^{-1} \exp(-\delta \underline{b})$ behaviour, and this in turn gives an $\underline{r}^{-3}$ instead of the true $\underline{r}^{-3/2} \exp(-\delta \underline{r})$ radial dependence in the absorptive part of the optical potential at large distances [13].

The parameter δ which is introduced above can be interpreted in terms of an average excitation energy Δ for the intermediate states in the scattering process. In our units $\delta = 2m\Delta/k$, where m is the electron mass, and in terms of the variables $\underline{t}_j = \alpha_j \underline{t}$ in the original static potential (2) we have $\delta \underline{r} = \delta_j \underline{t}_j$ with $\delta_j = 243Z^{-1/3} \Delta / (\alpha_j k)$. To correct the Glauber optical potential we apply the procedure in [13] to our simple model of the atomic system, i.e. in the spirit of the eikonal-Born series we replace the second-order Glauber term in the scattering amplitude by the imaginary part of the second Born term and transform the new amplitude into coordinate space to obtain the optical potential. We emphasize that the second Glauber and Born terms we are considering here are not the ones that apply to scattering in the static potential but those that appear in the model with separate scatterers, and with the average excitation energy Δ introduced in the Born amplitude. The result of this procedure is that the function ϕ_j of eq. (26) now becomes

$$\begin{aligned} \phi_j(\delta_j, t_j) = & -[\gamma + \ln(\delta_j t_j / 4)] e^{-t_j - K_0(2t_j)} \\ & + \phi_j^{(1)}(t_j) + \phi_j^{(2)}(t_j) + \phi_j^{(3)}(\delta_j, t_j), \end{aligned} \quad (27)$$

where $\phi_j^{(1)}$ is defined in eq. (26) and

$$\begin{aligned}\phi_j^{(2)}(t_j) &= (2/\pi) \int_0^\infty u du \ln u (1+u^2)^{-1} \sin(t_j u), \\ \phi_j^{(3)}(\delta_j, t_j) &= -(2/\pi) \int_0^\infty u^2 du (1+u^2)^{-1} (\delta_j^2 + u^2)^{-\frac{1}{2}} \\ &\quad \times \ln\{\delta_j^{-1} [(\delta_j^{-1} + u^2)^{\frac{1}{2}} + u]\} \sin(t_j u).\end{aligned}\quad (28)$$

For large t_j the integral $\phi_j^{(2)}$ cancels the t_j^{-2} behaviour introduced by $\phi_j^{(1)}$; in fact, $\phi_j^{(1)} + \phi_j^{(2)}$ is zero to all orders in the asymptotic expansion, but has the finite value $-\gamma - \ln(2t_j)$ for small t_j . The behaviour of the absorption potential at large distances ($\delta_j t_j \gg 1$) is now determined by $\phi_j^{(3)}$, which has the required behaviour

$$\begin{aligned}\phi_j^{(3)}(\delta_j, t_j) &\rightarrow \delta_j^2 [K_0(\delta_j t_j) + (\delta_j t_j)^{-1} K_1(\delta_j t_j)] \\ &\rightarrow \delta_j^{3/2} (\frac{1}{2}\pi/t_j)^{\frac{1}{2}} \exp(-\delta_j t_j).\end{aligned}\quad (29)$$

The small- t_j dependence is similar to that of the Glauber absorption potential, for small δ_j we have as $t_j \rightarrow 0$

$$\begin{aligned}\phi_j(\delta_j, t_j) &\rightarrow A_j t_j, \\ A_j &= 2(1 - \ln 2) - \frac{1}{4} \delta_j^2 [1 + 2 \ln(\delta_j/2)].\end{aligned}\quad (30)$$

This means that the actual absorption potential, including the factor in eq. (24), approaches a constant as $\underline{r} \rightarrow 0$.

The absorption potential defined by eq. (27) is still somewhat cumbersome to use. However, it is possible to fit ϕ_j by simple expressions based on the behaviour of this function at large and small t_j . Considering the simplifications involved in our model we have found, e.g., that the two-parameter fit

$$\phi_j(\delta_j, t_j) = A_j t_j e^{-y t_j + \delta_j^2 [K_0(\delta_j t_j) + (\delta_j t_j)^{-1} K_1(\delta_j t_j)] e^{-z/t_j}} \quad (31)$$

is quite satisfactory. While eq. (31) actually does not do too well in reproducing the calculated absorption potential itself (see Sect. 6) it is nevertheless very useful when it comes to calculating the scattering cross section, the important thing being that it has the correct behaviour at large and small distances, and more or less the correct overall strength. For the values of δ_j that we have occasion to consider we find that the parameters which give the best fit to the calculated absorption potential are $y = 2.9$ and $z = 2.3$.

5. The polarization potential

In addition to the static and absorptive parts we shall include a polarization term in the optical potential. The appropriate method for deriving the polarization potential is explained in [13] and references therein, and again

the average excitation energy Δ appears as a parameter. In our units and in accordance with the notation in previous sections we write the polarization potential as

$$V_{\text{pol}}(r) = Z_1 Z_2 a r^{-1} \phi_{\text{pol}}(t), \quad (32)$$

where

$$\begin{aligned} \phi_{\text{pol}}(t) &= -2\eta_1 \tilde{\phi}_{\text{pol}}(t), \\ \tilde{\phi}_{\text{pol}}(t) &= \frac{1}{4\pi} \sum_{j=1}^N a_j \delta_j^2 \bar{\phi}(\delta_j t_j). \end{aligned} \quad (33)$$

The function $\bar{\phi}$ can be expressed in terms of the modified Bessel functions I_n and Struve functions L_n of order $n = 0$ and 1 [13], for computational purposes it is, however, simpler to write

$$\bar{\phi}(x) = 4\pi^{-1} \int_0^{\pi/2} e^{-x \cos \theta} \cos^2 \theta d\theta, \quad (34)$$

where $\bar{\phi}(0) = 1$ and $\bar{\phi}(x) \rightarrow 8\pi^{-1} x^{-3}$ as $x \rightarrow \infty$.

We find that the function (34) can be reproduced very well by the two-parameter fit

$$\bar{\phi}(x) = e^{-y'x} + 8\pi^{-1} x^{-3} e^{-z'/x}, \quad (35)$$

with $y' = 0.84$ and $z' = 6.4$.

The polarization potential behaves as $\underline{r}^{-4}$ as $\underline{r} \rightarrow \infty$ and is therefore the dominating part of the optical potential at large distances. This, in turn, means

that this part of the potential is the major contributor to the scattering amplitude at small momentum transfers.

6. Numerical results and discussion

6.1. Potential parameters for rare gases.

Our numerical examples will be concerned with electron scattering on the rare gases from Ne to Xe, at various energies in the keV region. A Z -independent model is obtained by using the fit (1)-(3) to the Thomas-Fermi static potential as a basis for the optical potential. It is, however, possible to describe the scattering process in an equally satisfactory manner by starting from a one-term potential $V_{st}(\underline{r}) = Z_1 Z \alpha \underline{r}^{-1} \exp(-\alpha_1 \underline{t})$, where we are still using the Thomas-Fermi radial variable $\underline{t}$. The parameter α_1 is chosen in accordance with the actual atomic radius $\langle \underline{r}^2 \rangle^{\frac{1}{2}}$, as obtained from the diamagnetic susceptibility χ . The connection between χ and α_1 becomes

$$-\chi = 3.72 Z^{1/3} \alpha_1^{-2} \times 10^{-6} \text{ cm}^3, \quad (36)$$

where we use the values of χ quoted in [21].

A similar phenomenological model is used to obtain the average excitation energy Δ which appears in the optical potential. The experimental quantity in question is this time the atomic polarizability $\bar{\alpha}$, which in the closure approximation can be expressed in terms of Δ and

$\langle \underline{r}^2 \rangle$, i.e. in terms of Δ and χ . We find

$$\Delta = 22.9 \frac{-\chi/10^{-6} \text{ cm}^3}{\bar{\alpha}/a_0^3} \text{ eV} \quad (37)$$

and take the experimental values of the polarizability $\bar{\alpha}$ from [22]. The resulting radius parameters α_1 and excitation energies Δ are shown in Table I.

We note that for Ne our excitation energy is $\Delta = 58\text{eV}$, as compared with the value $\Delta = 41\text{eV}$ (1.5 a.u.) quoted in [13]. The reason for the difference is that in [13] $\langle \underline{r}^2 \rangle$ is obtained from the Hartree-Fock wave function rather from the experimental magnetic susceptibility.

6.2. Scattering in the static potential

The various approximations to potential scattering considered in Sect. 2 have been tested for electron scattering on Ne at 0.8 and 3keV, see Fig. 1-2. In order to display the influence of the target electrons on the scattering cross section we have divided the results by the Rutherford cross section for scattering on the bare nucleus. This reduced cross section is then conveniently presented on linear rather than the usual logarithmic scale.

The curves marked B1(first Born), B12(first and second Born), G(Glauber), GA(Glauber angle), SE(second-order eikonal), EB(eikonal-Born series) and MG(modified Glauber) should here be compared with the SP(static potential) curve, which shows the exact cross section

obtained by the partial-wave method; in all these cases we have used a one-term potential with a value of α_1 as given in Table I. We stress that the location of the experimental points is irrelevant as far as this comparison is concerned; for example, the fact that the Glauber approximation reproduces the 3keV experimental cross section very well cannot be taken as a point in favour of this approach. For comparison with the SP curve we have also shown the very similar curve SP_{TH-F} , which corresponds to a four-term potential with the parameters (3).

We see that the Born cross section B1 is too large at small angles and too small at large angles compared with the exact SP cross section. The GA and SE cross sections are, respectively, larger and smaller than their parent Glauber cross section, which in turn is smaller than the B1 cross section as well as the exact one of the SP curve, in particular at large angles.

At the energies in question the curves B12 and EB give cross sections that are much too large. This may seem surprising if one thinks of the amplitude $\underline{f}_{B2}$ as a correction of the order $\underline{k}^{-1}$ to $\underline{f}_{B1}$. It should be remembered, however, that the relevant parameter in the expansion actually is $\eta \propto Z_1 Z \underline{k}^{-1}$, where for electron scattering on Ne $|\eta|$ is 1.31 at 0.8keV and 0.68 at 3keV. Except at very small angles the B12 and EB cross sections are dominated by the imaginary part of the B2 amplitude, for instance, at 0.8keV the ratio $\text{Im}(\underline{f}_{B2})/\underline{f}_{B1}$ increases from 0.6 at 0° to 4.5 at 180° . The large imaginary part of $\underline{f}_{B2}$ also

appears in the MG amplitude, but it is there largely cancelled by the second Glauber term f_{G2} . Again, it may off-hand seem unlikely that there should be such a large difference between the EB and MG cross sections, since in terms of the successive Glauber amplitudes (12) the difference between the MG and EB amplitudes is just $f_{MG} - f_{EB} = \sum_{n=4}^{\infty} f_{Gn}$. But the point is that whereas the total Glauber amplitude f_G is well defined by eq. (8) for any n , it can not be written as a convergent series of amplitudes f_{Gn} unless $|n| < 1$, and for $Z = 10$ the series converges rather slowly even at 3keV.

Since neither of the approximations that we have considered does too well when it comes to reproducing the exact cross section it is clear that any comparison between the theoretical cross section for the static potential and the experimental one should be based on the SP curve itself. From Fig. 1-2, as well as from Fig. 5-8 which apply to scattering of 1-3keV electrons on the various rare gases, it is then seen that the static potential gives cross sections that are too large compared with the experimental ones, in particular at large angles. We emphasize that we have here used one-term potentials with parameters α_1 as shown in Table I.

6.3. Scattering in the optical potential

The cross sections that are obtained when the process is treated as Glauber scattering on separate particles are shown by the GSEP curves of Fig. 1-2 and 5-8; as

mentioned before we are here using a common spherical density for the target electrons. Since we have already seen that the Glauber cross section lies below the exact cross section for potential scattering (G versus SP), it follows that the GSEP curves can be expected to represent underestimates of the cross section in the model with separate scatterers.

As explained in Sect. 3 we can instead use the Glauber phase shift function to generate the absorption potential (25)-(26), as an example the function $\tilde{\phi}$ is shown by curve G in Fig. 3 for scattering on Ne at 0.8keV. The difference between this curve and the corresponding one obtained by the methods of Sect. 4 is not very pronounced in this figure, but as explained previously their different asymptotic behaviour has important consequences for the small-angle scattering amplitude. In Fig. 3 we also show the fit (31) to the absorption potential, which gives a $\tilde{\phi}$ that indeed is too large or too small depending on $\underline{r}$, but still gives a very good overall measure of the effects of absorption on the scattering cross section. The absorption potential that we are using in the actual calculations is thus

$$V_{\text{abs}}(r) = Z_1 Z \alpha r^{-1} \phi_{\text{abs}}(t),$$

$$\phi_{\text{abs}}(t) = -2\eta_1 \tilde{\phi}_{\text{abs}}(t),$$

$$\begin{aligned} \tilde{\phi}_{\text{abs}}(t) = A_1 \alpha_1 t e^{-2.9\alpha_1 t} \\ + (\bar{\delta}/\alpha_1)^2 [K_0(\bar{\delta}t) + (\bar{\delta}t)^{-1} K_1(\bar{\delta}t)] e^{-2.3(\alpha_1 t)^{-1}}, \end{aligned}$$

$$A_1 = 2(1 - \ln 2) - \frac{1}{4}(\bar{\delta}/\alpha_1)^2 [1 + 2 \ln(\frac{1}{2}\bar{\delta}/\alpha_1)],$$

$$\bar{\delta} = 243Z^{-1/3}\Delta/k, \quad (38)$$

where α_1 and Δ are given in Table I.

Similarly, the polarization potential is written as

$$V_{\text{pol}}(r) = Z_1 Z \alpha r^{-1} \phi_{\text{pol}}(t),$$

$$\phi_{\text{pol}}(t) = -2\eta_1 \tilde{\phi}_{\text{pol}}(t),$$

$$\tilde{\phi}_{\text{pol}}(t) = \frac{1}{4}\pi(\bar{\delta}/\alpha_1)^2 [e^{-0.84\bar{\delta}t} + 8\pi^{-1}(\bar{\delta}t)^{-3}e^{-6.4(\bar{\delta}t)^{-1}}]. \quad (39)$$

In Fig. 4 we have shown the various parts of the optical potential for electron scattering on Ne at 0.2keV, where in this case V_{abs} and V_{pol} are calculated as explained in Sect. 4 and 5 and not fitted by the expressions (38)-(39). The energy and units in Fig. 4 have been chosen so that our optical potential is directly comparable with that of Fig. 9 in [13], the latter potential having been obtained by rather more complicated methods (Hartree-Fock wave functions and different densities for the electrons in different states). It is seen that the potentials are quite similar in the two cases.

The cross sections that are obtained by solving the scattering equation numerically for the potential $V_{\text{opt}} = V_{\text{st}} + V_{\text{pol}} + iV_{\text{abs}}$ are shown by the OP curves of Fig. 1-2 and 5-8. How well these calculated cross sections agree with the experimental ones depends on the element and projectile energy, but the general conclusion is nevertheless that

this simple optical potential gives a marked improvement over the static model. One could of course obtain a much better agreement with the experimental data by using the radius parameter α_1 and excitation energy Δ as free rather than pre-determined quantities.

6.4. The total cross section

By means of the optical theorem we can express the total scattering cross section σ_{tot} (including inelastic processes) in terms of the imaginary part of the forward scattering amplitude, and it is interesting to compare the theoretical values obtained from the optical potential of Sect. 6.3 with the experimental ones quoted in [1]. This is done in Table II, where we have used the fits (38)-(39) for the absorption and polarization potentials. The table also shows the corresponding total Born cross sections; in this case σ_{tot} of course depends only on V_{abs} , since the real and imaginary parts of the Born amplitude are additive. In terms of the functions ϕ_j of Sect. 4 the total Born cross section, expressed in the usual unit πa_0^2 , is

$$\sigma'_{\text{Btot}} = \sigma_{\text{Btot}} / (\pi a_0^2) = 16\eta_1 \eta (a_0 k)^{-2} \sum_{j=1}^N a_j \beta_j^{-2} \times \int_0^\infty t_j dt_j \phi_j(\delta_j, t_j), \quad (40)$$

and we mention that for the complicated expression (27), as opposed to the fitted function (31), this is actually reduced to

$$\sigma'_{\text{Btot}} = 16\eta_1\eta(a_0k)^{-2} \sum_{j=1}^N a_j \beta_j^{-2} [-\ln(\delta_j/2) - \frac{1}{4}]. \quad (41)$$

We see from Table II that the agreement between theory (PW) and experiment (EXP) is satisfactory for Ne and Ar at 0.5 and 1keV. For Kr and Xe the agreement improves with increasing energy, but even at 3keV there is still quite a difference between the two. This is actually not too surprising; we have derived an optical potential by what is basically a high-energy approach, and according to the discussion in Sect. 6.2 the relevant quantity in this respect is actually not the projectile momentum $\underline{k}$ itself, but the ratio $\underline{k}/Z$.

6.5. Concluding remarks

The energy-dependent optical potential which is presented in Sect. 6.3 is quite simple to use and immediately applicable to any atom for which the magnetic susceptibility and electric polarizability are known. In order to arrive at this potential it has been necessary to treat the atomic structure effects in a rather cavalier fashion, i.e. by using the common-density version of the Glauber approximation and a one-term density function and static potential. We actually do not feel too badly about this, since the basic method that has been used for deriving the optical potential is in itself of a very approximate nature, as is indeed the very concept of a local optical potential.

It should, in conclusion, be emphasized that our

optical potential takes no account of exchange effects between the projectile and target electrons. Such effects will become increasingly important as the projectile energy gets lower. Exchange effects within the target have been taken care of implicitly by relating the electron density function to the experimental susceptibility.

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Table I. The potential parameter α_1 and
average excitation energy Δ for
rare gases

Element	α_1	Δ (eV)
Ne	1.09	58.0
Ar	0.706	40.4
Kr	0.654	39.5
Xe	0.566	36.8

Table II. Total cross sections (in units πa_0^2) for electron scattering on rare gases. PW: Partial-wave solution for the optical potential $V_{\text{opt}} = V_{\text{st}} + V_{\text{pol}} + iV_{\text{abs}}$. B: The Born approximation applied to the same potential. EXP: Experimental values quoted in [1]

Element	Energy (keV)	PW	B	EXP
Ne	0.5	1.42	0.76	1.14
	1	0.92	0.47	0.86
	2	0.56	0.28	
	3	0.41	0.20	
Ar	0.5	3.88	2.37	3.50
	1	2.67	1.45	2.16
	2	1.75	0.84	
	3	1.30	0.58	
Kr	0.5	5.19	3.88	15.3
	1	3.70	2.34	8.7
	2	2.53	1.34	
	3	1.95	0.92	3.8
Xe	0.5	7.23	6.15	17.7
	1	5.22	3.68	11.6
	2	3.59	2.09	
	3	2.79	1.41	4.8

Fig. 1. e^- scattering on Ne at 0.8 keV. Experimental results from [23]. The cross sections have been divided by the Rutherford cross section for scattering on the nucleus. The theoretical models are SP (static potential, exact), B1 (first Born), B12 (first and second Born), G (Glauber), GA (Glauber angle), SE (second-order eikonal), EB (eikonal-Born series), MG (modified Glauber), GSEP (Glauber with separate scatterers) and OP (optical potential). The curve SP_{TH-F} corresponds to the fit (3) to the Thomas-Fermi function, the other curves to the parameters α_1 and Δ given in Table I.

Fig. 2. e^- scattering on Ne at 3 keV. Experimental results from [24]. For the theoretical results see the legend of Fig. 1.

Fig. 3. The function $\tilde{\phi}_{abs}$ which determines the absorption potential ($V_{abs} = Z_1 Z_2 r^{-1} \phi_{abs}$, $\phi_{abs} = -2\eta_1 \tilde{\phi}_{abs}$) for e^- scattering on Ne at 0.8 keV. The unmarked curve corresponds to the average excitation energy Δ given in Table 1, and the curve marked G is derived from the Glauber model. The fitted curve is based on the asymptotic forms of $\tilde{\phi}_{abs}$ at small and large r , see eq. (31).

Fig. 4. The static potential V_{st} , polarization potential V_{pol} and absorption potential V_{abs} for e^- scattering on Ne at 0.2 keV.

Fig. 1

Fig. 2

Fig. 3

Fig 4

Fig. 5

Fig. 6

Fig. 7

Fig. 8