Collisions of charged particles with atoms

Author: Marc Barroso Mancha
Facultat de Física, Universitat de Barcelona, Diagonal 645, 08028 Barcelona, Spain

Advisor: Dr. Francesc Salvat

Abstract: Elastic collisions of charged particles with atoms are studied by using the classical and quantum theories for the scattering of particles in central potentials. A simple calculation scheme has been adopted and implemented in a Fortran program. Numerical results illustrate some characteristic features of the classical and quantum differential cross sections, and allow verifying the Bohr condition for the validity of the classical theory.

I. INTRODUCTION

Elastic collisions of fast charged particles with atoms cause large angular deflections of the trajectories of these particles. An accurate description of elastic collisions is required for Monte Carlo simulation of radiation transport, which finds applications in electron microscopy, medical physics, dosimetry, and in the design and quantification of radiation detection devices. Except for projectiles with low energies, elastic collisions can be described by means of the static-field approximation, that is, as the scattering of the projectile by the electrostatic field of the target atom. In this report we briefly formulate the classical and quantum theories of scattering by central potentials, and their implementation in a Fortran program for the case of electron scattering by an atomic potential model. Numerical results are used to reveal some characteristic features of the classical and quantum DCSs, and to analyse the applicability of Bohr’s condition for the validity of the classical scattering theory.

A. The interaction potential

We consider elastic collisions of charged particles of mass $M$ and charge $Z\alpha$ with neutral atoms of atomic number $Z$. For simplicity, the target atom is assumed to have a point nucleus much heavier than the projectile and fixed at the origin of coordinates, and a spherical electron cloud. The interaction with the projectile is considered to be purely electrostatic (static-field approximation),

$$V(r) = \frac{Z\alpha e^2}{r}\Phi(r). \quad (1)$$

The screening function $\Phi(r)$ represents the shielding of the nuclear charge by the atomic electrons, it equals unity at $r = 0$ and decreases monotonously with $r$ tending to zero at large radii.

To ease the calculations we use analytical screening functions of the form

$$\Phi(r) = \sum_{i=1}^{3} A_i \exp(-a_ir) \quad (2)$$

with parameters $A_i$ and $a_i$ determined by Salvat et al. [1], which approximate closely the atomic potentials obtained from self-consistent Dirac-Hartree-Fock-Slater calculations, and lead to an analytical expressions for the scattering amplitude and the phase shifts in the first Born approximation.

II. CLASSICAL COLLISION THEORY

We briefly review here the classical theory of scattering by central potentials. We assume that the projectile starts its motion very far from the target, with linear momentum $\vec{p}_i$ parallel to the polar axis and kinetic energy $E = p_i^2/2M$. The angular momentum $L$ and the impact parameter $b$ are related by

$$L = bp_i. \quad (3)$$

After the interaction, the particle moves in a direction that makes an angle $\theta$ with the polar axis. Using polar coordinates $(r, \phi)$ in the scattering plane, we have $\phi(t = -\infty) = \pi$ and $\phi(t = \infty) = \theta$. Notice that the scattering angle $\theta$ is the angle between the initial and final directions of the projectile, and it can only take values in the range $[0, \pi]$. A small detector at an angle $\theta$ may receive particles which have circled the centre of force and emerge with angles $\vartheta = \pm\theta$ plus integer multiples of $2\pi$.

To obtain the geometrical equation of the trajectory, we consider the constants of motion

$$L = Mr^2 \dot{\phi} \quad \text{and} \quad E = \frac{p^2}{2M} + V(r) = p_i^2. \quad (4)$$

Combining these equalities with the expression of the velocity in polar coordinates we obtain

$$\dot{r} = \pm \frac{1}{M} \sqrt{p^2 - \frac{L^2}{r^2}}. \quad (5)$$

The condition $\dot{r} = 0$ determines the distance $r_0$ of closest approach, i.e., the turning point of the radial motion.

*Electronic address: mbarroma8@alumnes.ub.edu
The sign on the right-hand side of Eq. (5) is \(-\) when the projectile is approaching the scattering centre, and \(+\) when the particle has passed the point of closest approach. Using the identity \(\dot{\phi} = L/(Mr^2)\), we can write

\[
\frac{d\phi}{dr} = \pm \frac{L/r^2}{\sqrt{p^2(r) - L^2/r^2}} dr.
\]  

(6)

Considering that the trajectory is symmetric with respect to the point of closes approach, we obtain [2]

\[
\vartheta(L) = \pi - 2 \int_{r_0}^{\infty} \frac{L/r^2}{\sqrt{p^2(r) - L^2/r^2}} dr. \tag{7}
\]

Although the deflection angle \(\vartheta(L)\) varies continuously with \(L\), the “inverse” function \(L(\vartheta)\) may be multivalued, see Fig. 4.

Considering that the number of projectile particles scattered per unit time to directions with polar angle \(\vartheta\) between \(b\) and \(b + db\) is equal to the number of inciding particles with impact parameters between \(b\) and \(b + db\) per unit time, we can conclude that scattering differential cross section (DCS) is given by [2]

\[
\frac{d\sigma}{d\Omega} = \frac{1}{2p_i^2 \sin \theta} \sum_j \left| \frac{dL_j^2}{d\vartheta} \right|_{L=L_j},
\]  

(8)

where the summation is over the angular momenta \(L\) that yield deflection angles \(\vartheta\) corresponding to the scattering angle \(\theta\).

A. Scattering by a screened Coulomb potential

In the case of the atomic potential \([1]\) we have

\[
\vartheta(L) = \pi - 2 \int_{r_0}^{\infty} \frac{L/r^2}{\sqrt{p^2 - 2MZ_iZe^2\Phi(r)/r - L^2/r^2}} dr. \tag{9}
\]

To facilitate the numerical calculations, we change the integration variable to \(u = (1 - r_0/r)^{1/2}\) and write

\[
\vartheta(L) = 2 \arctan \left( \frac{MZ_iZe^2\Phi(r_0)}{Lp_i} \right) +
\]

\[
+ 4 \int_0^1 \left\{ \frac{1}{\sqrt{C\Phi(r_0) + 2 - u^2}} - \frac{1}{\sqrt{C\Phi(r_0) + 2 - u^2 - Cy(u)}} \right\} \]  

(10)

with

\[
C = \frac{2MZ_iZe^2r_0}{L^2}, \quad g(u) = r_0 \frac{\Phi(r) - \Phi(r_0)}{r - r_0}. \tag{11}
\]

My Fortran program computes this integral for a dense grid of \(L\) values by using a 20-point adaptive Gauss-Legendre quadrature \([3]\), and represents the function \(\vartheta(L)\) by means of the natural cubic spline that interpolates the numerical table. The derivatives in Eq. (8) are obtained by computing \(d\vartheta/dL\) using the interpolating spline.

B. A second look at \(\vartheta(L)\)

The scattering characteristics are embedded in the function \(\vartheta(L)\) \([4]\). Interesting phenomena arise when the function has either maxima or minima, and when \(L(\vartheta)\) is multivalued. A maximum or minimum of \(\vartheta(L)\) causes a sharp peak in the DCS, a feature called rainbow scattering. When \(\vartheta(L)\) passes smoothly through a point where \(\sin \vartheta = 0\) (that is, through \(\vartheta = 0\), or \(\pm n\pi\)) the DCS becomes infinite and the situation is called glory scattering. If the energy of the projectile is close to a maximum of the effective radial potential, the radial component of the velocity is small and we may have orbiting trajectories. All these effects are related to each other, and some of them imply the existence of others. We will see examples of them in the Results section.

![FIG. 1: Classical deflection angle as a function of the angular momentum for scattering of electrons of the indicated energies by gold atoms.](image)

C. Validity of the classical theory

It is pertinent to ask when the classical theory is valid, that is, under what circumstances the classical DCSs agree with the predictions of the quantum formulation? Bohr \([5]\) considered this question on the basis of a simple argument. He regarded the incident beam of projectiles as an incoming wave that diffracts through a small circular hole with permeable edges. Then he estimated the minimal angular aperture of the transmitted beam by adding the apertures caused by diffraction and by the lateral variation of the potential within the hole, and
found that
\[
(\Delta \theta)_{\text{min}} = \sqrt{\frac{\hbar}{\partial \theta}}.
\] (12)

Consequently, the classical method should be valid as long as \((\Delta \theta)_{\text{min}}\) is much less than the deflection \(\theta\) of the particles due to the field. In the case of atomic potentials, Bohr’s argument implies that the classical calculation is valid for angles larger than
\[
\theta_{\text{class}} = \frac{\hbar}{p_i a_0 Z^{1/3}},
\] (13)

where \(a_0 Z^{1/3}\) is an estimate of the “atomic radius”. The correctness of Bohr’s condition will be confirmed numerically below in the Results Section.

III. QUANTUM COLLISION THEORY

In the quantum theory the scattering of particles by central potentials is described by the solution of the time-independent Schrödinger equation
\[
\left( -\frac{\hbar^2}{2M} \nabla^2 + V(r) \right) \psi(\vec{r}) = E \psi(\vec{r}) = \frac{p_i^2}{2M} \psi(\vec{r})
\] (14)

with the following asymptotic behaviour [6],
\[
\psi_E(\vec{r}) \sim e^{i\vec{k}_i \cdot \vec{r}} + e^{i\vec{k}_f \cdot \vec{r}} f(\theta, \phi).
\] (15)

The first term on the right-hand side is a plane wave with wave vector \(\vec{k}_i \equiv \vec{p}_i / \hbar\), which describes the incident electron beam, and the second term is a spherical wave modulated by the scattering amplitude \(f(\theta, \phi)\). The results from this stationary-state solution are equivalent to those from a more rigorous formulation that considers the time evolution of wave packets. The potentials considered in the present work are of finite range, that is, \(V(r)\) vanishes faster than \(r^{-1}\) as \(r \to \infty\).

Without losing generality, we choose a reference frame with its origin at the centre of force and the \(z\) axis in the direction of the initial momentum, so that \(\vec{k} = k \hat{z}\) and \(\vec{r} \cdot \vec{k}_i = rk, \cos \theta\), where \(\theta\) is the polar scattering angle. It is important to notice that, for central potentials, the scattering wave \(15\) is independent of the azimuthal angle \(\phi\), and the same holds for the scattering amplitude, \(f(\theta, \phi) = f(\theta)\). It can be shown that, under these conditions, the DCS is given by
\[
\frac{d\sigma}{d\Omega} = |f(\theta)|^2.
\] (16)

A. Partial-wave expansion

The scattering wave \(15\) can be expanded as
\[
\psi_E(\vec{r}) = (2\pi)^{-3/2} \frac{1}{kr} \sum_{\ell} (2\ell + 1) i^\ell \exp(i\delta_\ell) P_{E\ell}(r) P_\ell(\cos \theta),
\] (17)

where \(P_\ell(\cos \theta)\) are the Legendre polynomials, and \(P_{E\ell}(r)\) are the solutions of the radial equation with the asymptotic boundary condition
\[
P_{E\ell}(r) \sim k r - \frac{\ell \pi}{2} + \delta_\ell.
\] (18)

The quantities \(\delta_\ell\) are the phase shifts, which represent the effect of the potential on the large-\(r\) behaviour of the radial wave function. Notice that the expansion \(17\) is also valid for the plane waves, which are solutions of Eq. \(14\) with \(V \equiv 0\), in which case \(\delta_\ell = 0\) for all \(\ell\).

From the analysis of the asymptotic behaviour of the series \(17\) we obtain the following partial-wave series for the scattering amplitude
\[
f(\theta) = \frac{1}{k_i} \sum_{\ell} (2\ell + 1) \exp(i\delta_\ell) \sin(\delta_\ell) P_\ell(\cos \theta).
\] (19)

Inserting this expansion into Eq. \(16\), with the aid of the orthogonality of the Legendre polynomials, we have
\[
\sigma = \frac{4\pi}{k_i^2} \sum_{\ell} (2\ell + 1) \sin^2(\delta_\ell).
\] (20)

From the partial-wave expansion we see that
\[
\sigma = \frac{4\pi}{k_i} \text{Im} f(0).
\] (21)

This equality is known as the optical theorem, it expresses the fact that the scattering process conserves the number of particles.

Because the calculation of each phase shifts requires solving the corresponding radial equation, which is a delicate and lengthy work, we consider approximate methods to compute the phase shifts.

B. The plane-wave Born approximation

In the plane-wave Born approximation, the states of the projectile before and after the interaction are represented as plane waves with respective linear momenta \(\vec{p} = h k \hat{z}\) and \(\vec{p}' = h \vec{k}'\), and the interaction is treated as a perturbation to first order. The DCS can then be calculated by means of the Fermi golden rule. This approach gives the following scattering amplitude
\[
f^{(B)}(\theta) \equiv -\frac{M}{2\pi \hbar^2} \int d\vec{r} \exp(iq \cdot \vec{r}) V(r),
\] (22)
of the potential (19), the Born phase shifts provide a good approximation to the numerical phase shifts when |δ| ≪ 1. To ensure continuity of the phase shifts with ℓ, we set

\[ \delta_\ell = \begin{cases} \delta_\ell^{(WKB)} & \text{if } \ell < L, \\ C_\ell \delta_\ell^{(B)} & \text{otherwise} \end{cases} \tag{29} \]

with

\[ C_\ell \equiv 1 + \left( \frac{\delta_\ell^{(WKB)}}{\delta_\ell^{(B)}} - 1 \right) \exp \left( -\frac{\ell - L}{L} \right) \tag{30} \]

In my Fortran program, all the Born phase shifts larger than about 10^{-10} are calculated first, then the cut-off L is determined, and finally the WKB phase shifts with ℓ ≤ L are calculated.

Generally, the convergence of the partial-wave series above has been implemented in a Fortran program that calculates the classical and quantum DCSs for collisions of electrons with neutral atoms. The samples presented here correspond to target gold atoms (Z = 79). Because the program only computes the classical DCS for angles satisfying the Bohr condition (13), we plot the classical DCS only for angles larger than 45°.

Figure 2 displays the calculated classical DCS for electrons with various kinetic energies (the same energies for which θ is represented at Fig. 1). The four examples show a backward glory, with the DCS diverging at an angle that increases with the energy of the projectile.

Results from the quantum theory are shown in Figure 3 for the same set of kinetic energies as in Fig. 2 for the sake of comparison. It is worth mentioning that the present quantum calculations are in fairly good agreement with elaborate Dirac partial-wave calculations and with available experimental data [8].

C. Wentzel-Kramers-Brillouin approximation

Fairly accurate phase shifts can be calculated by using the Wentzel-Kramers-Brillouin (WKB) semi-classical approximation, together with the Langer correction, that yields the following formula [7]

\[ \delta_\ell^{(WKB)} = \frac{1}{2} \left( \ell + \frac{1}{2} \right) \pi - kr_0 + \int_{r_0}^{\infty} \left[ \sqrt{F_\ell(r)} - k \right] dr, \tag{27} \]

where

\[ F_\ell(r) = k^2 - \frac{2M}{\hbar^2} V(r) - \frac{r^2}{2} \left( \ell + \frac{1}{2} \right)^2, \tag{28} \]

and \( r_0 \) is the largest zero of \( F_\ell(r) \).

To simplify the calculation, in my program the integration variable is changed to \( x = 1/r \), and the resulting integral is computed by using the adaptive 20-point Gauss-Legendre quadrature method, which yields the phase shifts to very high accuracy.

D. Practical partial-wave expansion method

The scattering amplitude is calculated from its partial-wave expansion using the WKB phase shifts for orders \( \ell \leq L \) and the Born phase shifts for \( \ell > L \), with the cutoff value \( L \) equal to the lowest angular momentum for which \( |\delta_\ell^{(B)}| < 0.001 \). To ensure continuity of the phase shifts with \( \ell \), we set

\[ \delta_\ell = \begin{cases} \delta_\ell^{(WKB)} & \text{if } \ell < L, \\ C_\ell \delta_\ell^{(B)} & \text{otherwise} \end{cases} \tag{29} \]

with

\[ C_\ell \equiv 1 + \left( \frac{\delta_\ell^{(WKB)}}{\delta_\ell^{(B)}} - 1 \right) \exp \left( -\frac{\ell - L}{L} \right) \tag{30} \]

In my Fortran program, all the Born phase shifts larger than about 10^{-10} are calculated first, then the cut-off \( L \) is determined, and finally the WKB phase shifts with \( \ell \leq L \) are calculated.

Generally, the convergence of the partial-wave series [19] is slow. It can be accelerated by adding the Born scattering amplitude and subtracting its partial-wave expansion. Thus, we have

\[ f(\theta) = f(\theta)^{(B)} + \sum_\ell F_\ell P_\ell(\cos \theta), \tag{31} \]

with

\[ F_\ell = \frac{1}{2ik} (2\ell + 1) \left[ \exp(2i\delta_\ell) - 1 - 2i\delta_\ell^{(B)} \right]. \tag{32} \]
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1.0e-19
1.0e-18
1.0e-17
1.0e-16
1.0e-15
60 80 100 120 140 160 180
dσ/dΩ (cm$^2$/sr)
θ (deg)
E = 500 eV
E = 1000 eV
E = 2000 eV
E = 5000 eV

FIG. 2: Classical DCS for collisions of electrons with the indicated energies and gold atoms.

FIG. 4: Classical and quantum DCSs for collisions of 5 keV electrons with gold atoms.

Despite the evident differences between the classical and quantum results, the classical theory still gives DCS with the correct order of magnitude. Of course, the diffraction-like structures of the quantum DCS cannot be reproduced by the classical theory. At higher energies, however, the quantum DCS varies monotonously with the scattering angle and we may expect a closer agreement between the two theories. This is confirmed by the results for 5 keV electrons shown in Fig. 4, where the classical and quantum predictions are seen to agree pretty well at intermediate angles.

V. CONCLUSIONS

In this work we have studied the classical and quantum theories for the scattering of charged particles by neutral atoms. We have considered relatively simple calculation schemes, which allow rapid computations, and I have written a Fortran program that gives the DCS for collisions of electrons with arbitrary kinetic energies colliding with atoms of any element. From the numerical results I have understood the various features of the classical DCS. I have also verified the correctness of Bohr’s condition, by verifying that the classical and quantum theories yield similar results when the condition holds.

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[3] Course notes of Computational Physics, 2016, UB.