

# Study of atomic collisions by charged particles

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## Abstract

The Present study of collision processes involving positive ions provides a sensitive test of the approximate method to develop positron and electron scattering and yields useful information about the role of different works in collision dynamics. This study of laser assisted collision process involves an accurate description of the projectile and the target states in the presence of laser field.

**Keywords:** Electron-Atom Collisions, Laser Field Scattering, Electron Positron scattering

## INTRODUCTION

The study of charged particle scattering by atoms and molecules has been of great interest since the early days of modern physics [1-4]. Recently extensive studies have been carried out in the field of atomic and molecular collision processes in the absence and presence of electro-magnetic field due to its importance in laser induced chemistry working of different type of lasers, lasers induced gas-breakdown, plasma heating by laser etc. [5-10]. The understanding of the laser plasma interaction related to the laser fusion reactions requires a knowledge of the collision process in the presence of EM field occurring under various conditions among atoms, molecules, neutrals and charged particles.

If matter is exposed to intense ( $\geq 10^{14}$  w/cm<sup>2</sup>) electromagnetic radiation, besides well known perturbative linear process strong non-linear optical effects are becoming important. An ionization effect is called non-linear if the exciting photon energy  $\hbar\omega$  of the laser field is smaller than the binding energy of the system and therefore ionization in the context of Einstein explanation of the photo effect is forbidden. Nevertheless, the strong laser field allows for multi-photon ionization and direct optical field ionization by tunneling effects.

## Classical scattering and quantum formulation

Let a steady beam of mono energetic point particles incident upon a fixed scattering center, with a known potential energy function representing the interaction between incident particles and the scattering center. The incident flux density  $j_0$  is the number of beam particles crossing a unit area normal to the beam per unit time. Assuming there is no interaction between particles in the beam each

particle will traverse a trajectory which is completely determined by Newton's equation of motion and the "initial conditions", as specified by the incident energy,  $E$ , and impact parameter,  $\rho$ .

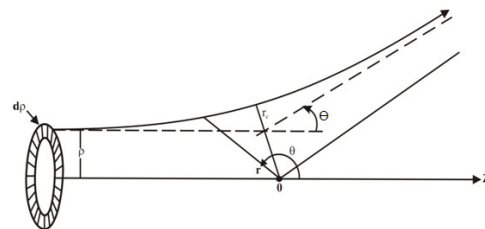


Fig 1. A classical trajectory of a particle in a central force field;  $r$ ,  $\theta$  are the instantaneous coordinates of the particle,  $\rho$  is the impact parameter,  $r_c$  is the distance of closest approach, and  $\Theta$  is the scattering angle.

The scattering angle  $\Theta$ , or angle between the asymptotic trajectories before and after the collision, is given by

$$\Theta = \pi - 2 \int_{r_c}^{\infty} \frac{dr}{r^2 \left[ \frac{1}{\rho^2} \left( 1 - \frac{V}{E} \right) - \frac{1}{r^2} \right]^{1/2}} \quad (1.1)$$

Here  $V(r)$  is the potential energy (assumed spherically symmetric) of the particle at distance  $r$  from the scattering center and  $r_c$  is the distance of closest approach, which is given by the largest positive root of

$$1 - \frac{V(r_c)}{E} - \frac{\rho^2}{r_c^2} = 0 \quad (1.2)$$

The differential cross section for elastic scattering  $d\sigma/d\Omega$  is destined by the relation

$$d\sigma(\Theta) = 2\pi \quad d\sigma/d\Omega \sin \Theta d\Theta$$

$$= \frac{\text{number of particles scattered into solid angle } d\Omega \text{ per unit time}}{\text{incident flux density}} \quad (1.3)$$

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After, the number of particles per unit time scattered into the element of solid angle  $2\pi \sin\Theta \, d\Theta$  is  $j_0 [2\pi \, d\sigma/d\Omega \sin\Theta \, d\Theta]$ . Equating these gives

$$\frac{d\sigma}{d\Omega} = \frac{\rho}{\sin\Theta} \left| \frac{d\rho}{d\Theta} \right| \quad (1.4)$$

Where both  $d\rho$  and  $d\Theta$  are taken to be positive differentials.

The total elastic scattering cross section is the integral of the differential cross section over all scattering angle

$$\sigma_e = 2\pi \int_0^\pi d\Theta \sin\Theta \, \frac{d\sigma}{d\Omega} \quad (1.5)$$

The classical total elastic scattering cross section diverges for all forces which do not have upper bounds on their ranges. This arises from the infinitesimal scattering angles corresponding to infinitely large impact parameters. These infinitesimal scatterings will not contribute to such transport processes as diffusion or conduction, where the relevant quantity is the momentum transport cross section.

$$\sigma_m = 2\pi \int_0^\pi d\Theta \sin\Theta (1 - \cos\Theta) \, \frac{d\sigma}{d\Omega} \quad (1.6)$$

In an attempt to describe the trajectory of a single particle in quantum mechanics we find that the uncertainty principle prevents us from exactly specifying the position and velocity at some initial time.

The equation of motion is now the time dependent Schrödinger equation

$$H\psi(r, t) = i\hbar \frac{\partial \psi(r, t)}{\partial t}, \quad (1.7)$$

where  $H$  is the Hamiltonian operator,

$$H = -(\hbar^2/2m) \nabla^2 + V(r). \quad (1.8)$$

In a field-free region the most general solution to (1.7) may be constructed from plane waves as

$$\psi(r, t) = \int dp' \, \alpha_{p'} e^{(i/\hbar)[p' \cdot r - E' t]}, \quad (1.9)$$

where the energy  $E' = p'^2/2m$ . The complementarity of the position and momentum as well as of the energy and time is apparent from this construction of the solution.

Having constructed an initial wave packet at  $t_i$  before the collision one can solve the Schrödinger equation of motion to obtain the evolution of the wave packet in time and thus find  $\psi(r, t)$ , where  $t_i$  is a time after the collision.

The use of wave packets is not appropriate in the quantum treatment of the scattering of a mono energetic beam of particles. This is because the requirement of being mono energetic (or having a completely well defined momentum) is incompatible with the localization in space which is required to study the motion of the packet in time. The mono energetic limit of the wave packet is obtained by setting  $\delta(P' - P)$ , or

$$\psi(r, t) \rightarrow \psi_p(r, t) = e^{(i/\hbar)[p \cdot r - E t]}, \quad (1.10)$$

A form of the wave function at large distances which will represent the time independent flow of the incident beam and the scattered beam is

$$\psi_k(r) \xrightarrow{r \rightarrow \infty} e^{ik \cdot r} + \frac{e^{ikr}}{r} f(\Theta, \Phi) \quad (1.11)$$

Where  $\Theta$  and  $\Phi$  are the polar and azimuthal angles of scattering relative to the direction of incidence,  $k$  and  $f(\Theta, \Phi)$  is the scattering amplitude.

From the definition of differential elastic scattering cross section (1.3), and the incident and scattered fluxes

$$d\sigma/d\Omega = |f(\Theta, \Phi)|^2 \quad (1.12)$$

So far in the quantum treatment we have not assumed a central scattering field, so the possible  $\Phi$  dependence in  $f$  is retained. The total elastic scattering cross section is

$$\sigma_e = \int d\Omega |f(\Theta, \Phi)|^2, \quad (1.13)$$

and unlike its infinite value for all long range potential fields in classical scattering, it remains finite in the quantum treatment for most such potentials. The above remarks apply to long range potentials which asymptotically go to zero more rapidly than  $1/r^2$ . As the peculiarities of the Coulomb potential will lead to an infinite total scattering cross section even in the quantum treatment.

## ELECTRON-ATOM COLLISIONS

In the treatment of the scattering of electrons by atoms the following three complications arise, which make the problem very much more difficult than that of scattering by a static force field.

1. The equation of motion for the system of incoming electron and target atom in both the classical and quantum description is a many body equation of motion. As such it will not be subject to exact solution, which was in principle possible for the central static field scattering problem.
2. The incident electron is identical to the target atom electrons, requiring that the total wave function satisfy the Pauli Exclusion Principle.
3. Inelastic processes may take place if the incident energy is high enough to cause transitions of the target atom to any of its excited states.

The time independent Schrödinger equation for the total system of target atom and incident electron is

$$[H_0(r_i) + H_a(r_j) + V(r_i, r_j) - E] \psi(r_i, S_i) = 0, \quad (1.14)$$

Where  $H_a$  is the atomic Hamiltonian,  $H_0$  is that of the incident electron,  $V$  is the interaction,  $r_i$  is the position coordinate of the  $i^{\text{th}}$  electron relative to the fixed nucleus, and  $S_i$  is its spin coordinate.

Although spin operators in the present approximation do not appear in the Hamiltonian, it is essential to retain the electron spin coordinates in the wave function in order to satisfy the Pauli Exclusion Principle.

If the target atom is initially in state  $\Psi_0(r_j, s_j)$  the asymptotic scattering wave function analogous to (1.11) is

$$\Psi(r_i, s_i) \xrightarrow{r_i \rightarrow \infty} \chi_{\alpha_0}(S_i) e^{ik_0 r_i} \Psi_0(r_j, s_j) + \sum_{\gamma \neq \alpha} \chi_{\alpha}(S_i) \frac{e^{ik_{\gamma} r_i}}{r_i} f_{0\gamma}(\hat{k}_0, \hat{k}_{\gamma}) \Psi_{\gamma}(r_j, s_j) \quad (1.15)$$

The subscripts 0 are used here in place of  $\gamma_0$  for the initial atomic state, which need not be the ground state of the target atom. The requirement of the Pauli principle that  $\Psi$  be anti symmetric in the interchange of any pair of  $r_j, s_j$  will lead to the validity of the above asymptotic form (to within  $\pm$  sign) as any  $r_i \rightarrow \infty$ . The spin functions  $\chi_{\alpha}(S_i)$  are the familiar  $\alpha$  and  $\beta$  representing spin up and down, and they are normalized such that

$\int ds_i \alpha^2(S_i) = \int ds_i \beta^2(S_i) = 1$  and  $\int ds_i \alpha(S_i) \beta(S_i) = 0$ . The expression (1.14) is seen to represent the particle flux density  $(\hbar/m)k_0$  in spin state  $\chi_{\alpha_0}$  incident upon the target atom in state  $\Psi_0$  and radially outgoing scattered electrons in spin state  $\chi_{\alpha}$  having flux densities  $(\hbar k_{\gamma}/m) |f_{0\gamma}|^2 / r_i^2$ , each scattered flux being associated with the excitation (or de-excitation) of the atom to state  $\Psi_{\gamma}$ . As many excited states will be included in the sum in (1.14) as are energetically accessible.

The differential cross section for excitation of the target state  $\gamma$  is obtained from the definition (1.3) as

$$I_{\sigma_{0\gamma}}(\hat{k}_0, \hat{k}_{\gamma}) = \frac{\frac{\hbar k_{\gamma}}{m} |f_{0\gamma}(\hat{k}_0, \hat{k}_{\gamma})|^2}{\frac{\hbar k_0}{m} r_i^2} \frac{r_i^2 d\Omega}{r_i^2} = \frac{k_{\gamma}}{k_0} |f_{0\gamma}(k_0, k_{\gamma})|^2 d\hat{k}_{\gamma} \quad (1.16)$$

where  $\hat{k}_{\gamma}$  represents the direction of scattering. This expression contains the result for elastic scattering if we let  $\gamma = 0$ . The total excitation cross sections are obtained again by integrating over scattering angle,

$$\sigma_{0\gamma}(r_0) = (k_{\gamma}/k_0) \int d\hat{k}_{\gamma} |f_{0\gamma}(\hat{k}_0, \hat{k}_{\gamma})|^2 \quad (1.17)$$

In general, if the initial state of the target atom is not spherically symmetric, the above cross section is still a function of the direction of incidence,  $\hat{k}_0$ . The cross section averaged over all possible directions of incidence upon an atom in an initial state of particular orientation,

$$\sigma_{0\gamma} = (1/4\pi) \int d\hat{k}_0 \sigma_{0\gamma}(\hat{k}_0) \quad (1.18)$$

is the same thing physically as the cross section for a given direction of incidence suitably averaged over all possible orientations of the target atom. The latter quantity is indeed what is measured in the laboratory when the target is volume of gas atoms or an unpolarized atomic beam.

## CONCLUDING REMARKS

The analysis of collision phenomenon plays a central role in almost all investigation of the microscopic structure of matter. Most of our knowledge about the forces and interactions between charged particles colliding with atomic molecular and ionic systems is derived through the scattering experiments.

The information associated with the electron impact excitation is useful in the understanding by the observed characteristic of spectral lines of aurora, solar corona and hot gaseous plasmas. Atomic and molecular collision process control the composition of upper and lower atmosphere; such studies are helpful to understand the fact behind the ozone layer depletion by simple series of atom-molecule collisions.

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