Nuclear Instruments and Methods in Physics Research B 279 (2012) 44–48

Contents lists available at SciVerse ScienceDirect

Nuclear Instruments and Methods in Physics Research B

journal homepage: www.elsevier.com/locate/nimb

# Classical theory of atomic collisions – The first hundred years

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ARTICLE INFO

*Article history:*
Received 9 August 2011
Received in revised form 4 September 2011
Available online 6 December 2011

*Keywords:*
Atoms
Collisions
Classical
Calculations

ABSTRACT

Classical calculations of the atomic processes started in 1911 with famous Rutherford's evaluation of the differential cross section for $\alpha$ particles scattered on foil atoms [1]. The success of these calculations was soon overshadowed by the rise of Quantum Mechanics in 1925 and its triumphal success in describing processes at the atomic and subatomic levels. It was generally recognized that the classical approach should be inadequate and it was neglected until 1953, when the famous paper by Gregory Wannier appeared, in which the threshold law for the single ionization cross section behaviour by electron impact was derived. All later calculations and experimental studies confirmed the law derived by purely classical theory. The next step was taken by Ian Percival and collaborators in 60s, who developed a general classical three-body computer code, which was used by many researchers in evaluating various atomic processes like ionization, excitation, detachment, dissociation, etc. Another approach was pursued by Michal Gryzinski from Warsaw, who started a far reaching programme for treating atomic particles and processes as purely classical objects [2]. Though often criticized for overestimating the domain of the classical theory, results of his group were able to match many experimental data. Belgrade group was pursuing the classical approach using both analytical and numerical calculations, studying a number of atomic collisions, in particular near-threshold processes. Riga group, lead by Modris Gailitis [3], contributed considerably to the field, as it was done by Valentin Ostrovsky and coworkers from Sanct Petersbourg, who developed powerful analytical methods within purely classical mechanics [4].

We shall make an overview of these approaches and show some of the remarkable results, which were subsequently confirmed by semiclassical and quantum mechanical calculations, as well as by the experimental evidence. Finally we discuss the theoretical and epistemological background of the classical calculations and explain why these turned out so successful, despite the essentially quantum nature of the atomic and subatomic systems.



## 1. Introduction

The term "atomic system" appears a paradigm of *contradictio in adjecto*. The original Greek meaning "indivisible" implies nonexistence of the internal structure. Strictly speaking, from epistemological point of view, *structure* and *indivisibility* need not be in contradiction. An electron is structureless (according to out present day inference) and indivisible (though not indestructible), but a proton, for example, is considered a system with internal structure, but yet indivisible. Its constituents, quarks, cannot be extracted from proton, though a host of various "elementary particles" may be extracted in the high-energy processes. In this respect quarks resemble more Anaxagoras' concept of $\mu o \iota \rho \alpha \iota$, which designated probably *share* rather than *part* [5].

In modern Greek, to mention this too, atom means an individual in everyday life, since the Latin term *individuum* means exactly the same "indivisible" (in-dividuum).

Year 1911 marked two important advances in our understanding the microscopic world: (i) Ernest Rutherford (1871–1937) and Johannes (Hans) Geiger (1882–1945), by shooting a metal foil by $\alpha$ particles [19], discovered the fact that atoms possessed the structure and (ii) Rutherford evaluated the angle-differential cross section for this collisional processes [1], which demonstrated that atoms have planetary structure, with nucleus and electrons moving around. Rutherford formula was obtained by evaluating trajectories of the impinging $\alpha$ particles and reads [6]:

$$\frac{d\sigma}{d\Omega} = \left(\frac{Z_1 Z_2 e^2}{4E \sin^2 \vartheta/2}\right)^2, \quad (1)$$

In the case of identical particles, the formula becomes

$$\frac{d\sigma}{d\Omega} = \left(\frac{Z_1 Z_2 e^2}{4E}\right)^2 [\csc^4 \vartheta/2 + \sec^4 \vartheta/2 + \lambda 8 \csc^2 \vartheta \cos(\kappa \ln \tan^2 \vartheta/2)], \quad (2)$$

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doi:10.1016/j.nimb.2011.10.055

$$\kappa = \frac{2\pi Z^2 e^2}{h\nu}, \quad \lambda = \begin{cases} 0, & \text{classical theory,} \\ 1, & \text{quantum mech. theory,} \end{cases} \tag{3}$$

where $h$ is Planck constant, $\nu$ is the mutual velocity, and $\lambda = 1$ introduces the *exchange* term. The latter appears peculiar to the quantum mechanics and cannot be obtained within the classical theory. It is important here to notice that it vanishes in the limit of small velocity, due to the rapid oscillations. This appears contrary to the standard passing from the quantum mechanical effects to the classical ones. As we shall see later on, Coulomb interaction appears unique in this context, since it is essentially the long-range force. Generally one may divide all potentials into three main classes:

$$V(r) = \beta/r, \quad \text{long-range potential,} \tag{4}$$

$$V(r) = \beta/r^n, \quad n > 1, \quad \text{medium-range pot.} \tag{5}$$

$$V(r) = \gamma r^{\eta} e^{-\alpha r}, \quad \alpha > 0, \quad \text{short-range pot.} \tag{6}$$

Power-law potentials are based on the concept of flux (of force lines) and are considered classical interactions, whereas exponential interactions are typically quantum mechanical and are based on the notion of exchange of intermediatory (boson) particles, as the case with strong interaction appears. Potentials with $n = 2$ in (5) acquire a special status among the medium-range interaction. The same holds for the linear harmonic oscillator potential ($n = -2$), which belongs also to the class of "classical interaction", as we shall see later on. As pointed out by many authors, one may only surmise to what extent the discovery of the nucleus might have been delayed, had it not been for the coincidence of the classical and Quantum mechanical cross sections. On the other hand the very appearance of the Quantum Mechanics might have been speeded up, for the success of the Old quantum theory relied heavily on the special properties of the $n = 1, -2$ potentials, as we shall discuss later on.

## 2. Classical vs. quantum mechanical

### 2.1. The classical approximation

With the advent of Quantum Mechanics (QM) it became clear when classical approach may be justified [7]. At the same time theoreticians learned why the previous calculations, like those in celestial mechanics, for instance, were successful. Since the invention of QM the physical theory separated into two branches: Classical Mechanics (CM) and QM. Based on the underlying physical ontology of the Wave mechanics, the criterion for applying CM was formulated in terms of the rate of change of the relevant de Broglie wavelength (we use atomic unites $\hbar, e, m_e = 1$):

$$\frac{d\lambda}{dr} \ll 2\pi, \tag{7}$$

In the case of binary encounters, the most frequent case in atomic collisions, with the reduced mass $\mu$, for the potentials from (4), (5), we have:

(i) Coulomb interaction of charges $Z_1$, $Z_2$

$$r \gg\gg \frac{1}{8\mu|Z_1 Z_2|}, \quad Z_1 Z_2 < 0, \tag{8}$$

(ii) $n = 2$ (monopole-dipole interaction)

$$\beta \gg\gg \frac{1}{2\mu}, \quad \beta < 0, \tag{9}$$

(iii) $n > 2$

$$r^{n-2} \ll\ll \frac{8\mu|\beta|}{n}, \quad \beta < 0, \tag{10}$$

Exponential interaction potentials turn out essentially beyond the classical approach [20].

### 2.2. Correspondence identities

Bohr's *Correspondence principle* defined the bridge, both ontological and epistemological, between the semiclassical and quantum mechanical domains. It states that for the large quantum numbers semiclassical and quantum mechanical results should merge as one goes to the infinite number limit. For the large principal quantum number $n$ and reasonably large angular momentum quantum number $l$ one may speak of electron trajectory and it was on this assumption de Broglie postulated the wave nature of microparticles, notably electrons. But is there situation where semiclassical and quantum mechanical results coincide for all values of quantum numbers? The answer is positive: for two interaction potentials $r^{\nu}, \nu = -1, 2$, Coulombic and harmonic oscillator cases, ignoring the spin variable (which is essentially a quantum mechanical quantity), energy spectra coincide [8]. Considering that these potentials describe arguably two the most important interactions in physics, this coincidence can not be overestimated, both from the methodological and historical points of view. It explains why Planck's quantum physics and Bohr's quantum theory were so successful, before Quantum Mechanics was invented. Correspondence identities appear thus a remarkable contribution due to Ian Percival and coworkers to the classical versus quantum mechanical physics issue. It explains albeit implicitly, why the classical methods turn out so successful in many physical situations, in particular in describing near threshold processes, as we shall see below.

## 3. Classical methods

In the classical approach all variables of a system appear continuous. Therefore, strictly speaking, *ab initio* classical calculations in atomic physics are not possible. Atomic parameters are taken either from the experimental data or from the quantum mechanical calculations. Never-the-less it is legitimate to calculate differential cross sections over the continuous variables [9]. If two subsystems $A$ and $B$ collide, and interaction between their constituent may be described by pairwise potential terms, Newton's equations of motion may be written as:

$$m_i \frac{d^2 \mathbf{r}_i}{dt^2} = -\sum_{i \neq j} \nabla_i V_{ij}(r_{ij}), \tag{11}$$

Eq. (11) is not amenable to exact solution, except in the most simple cases, and one usually makes various approximations. One of the most employed is the so-called *binary encounter approximation*, when the target electrons are treated as free particles, with nucleus and other electrons as spectators. The most popular method is statistical one, with relevant system parameters chosen at random, within the so-called Monte Carlo method, whose name speaks for itself [9]. Orbit integrations combined with Monte Carlo method, have been employed for a number of processes, like ionization, charge transfer, breakup processes etc. Particularly fertile calculations have been carried out in physical chemistry what is to be expected, since chemical molecules stand somewhere between atoms and macroscopic particles, belonging to the mesoscopic realm. With the advent of powerful digital computers Monte Carlo calculations have become very popular. Random number are generated by various algorithms, but in fact they are not random in he strict sense, but quasi-random, since it is quantum processes, with their intrinsic indeterminacy which can generate truly random numbers.