2 Characteristic Times in One-Dimensional Scattering

J. Gonzalo Muga

Departamento de Química-Física, Universidad del País Vasco, Apdo 644. Bilbao, Spain

2.1 Introduction

Quantum scattering theory deals with collisions, namely, interactions which are essentially localized in time and space. This means that the interaction potential must vanish rapidly enough in coordinate space, so that the wave packet tends to free-motion incoming and outgoing asymptotic states before and after the interaction is effective. The scope of scattering theory also includes “half-collisions” or “decay processes” where the stage before the collision is ignored, i.e., the evolution of the system is only considered from the interaction region.

This chapter reviews various quantities that have been proposed in scattering theory to characterize the temporal aspects of the collision. A quantum wave packet collision with a potential barrier in one dimension (1D) is fully described by the evolution of the wave function $\psi(x, t)$ from the incoming to the outgoing asymptotic states. However, the whole information contained in $\psi(x, t)$ is hardly required. A few well chosen quantities are often enough to provide a fair picture of the dynamics. In particular, one of these elementary parameters is the transmission probability $P_T$, but to describe the time dependence we also need to quantify the duration of the collision, the arrival time at a detector, the decay time of an unstable state, the asymptotic behaviour at short and large times, or response times, such as the time required to “charge” a well or achieve stationary conditions when a source is turned on.

In spite of the inherent time dependence of collisions, the treatises on quantum mechanics or scattering theory concentrate on solutions of the time-independent Schrödinger equation. This is in part because many scattering experiments to obtain cross sections are performed in quasi-stationary conditions, and also because the stationary scattering states form a basis to analyze the actual time dependent collision. In many cases wave packet scattering is relegated to justify the cavalier obtention by stationary methods of cross section expressions, and occasionally to discuss resonance lifetimes. Another widespread limitation of textbooks is the exclusive interest in the final results of the collision at asymptotic distances and times, which has been generally justified because “the midst of the collision cannot be observed”. However, while it is true that in many collision experiments only the asymptotic re-
sults are observed, modern experiments with femtosecond laser pulses or other techniques known as “spectroscopy of the transition state” do probe the structure and the evolution of the collision complex [1]. Also, in quantum kinetic theory of gases, accurate treatments must abandon the “completed collision” approximation and use a non-asymptotic description, e.g. in terms of Möller wave operators instead of $S$ matrices, as in the Waldmann–Snider equation and its generalizations for moderately dense gases [2].

The theory has to adapt to these new trends by paying more attention to the temporal description of the collisions. Even if we restrict ourselves to asymptotic aspects, the cross section does not contain the whole information available in a scattering process, since it is only proportional to the modulus of the $S$-matrix elements. Information on the phase is available from delay times with respect to free motion. In fact, the full collision and not just the asymptotic regimes should be understood to control or modify the products. This has motivated a recent trend of theoretical and experimental work to investigate the details of the interaction region and transient phenomena.

In this chapter we restrict ourselves to one dimensional scattering. Many physical systems can be described in one dimension: the application of the effective mass approximation to layered semiconductor structures leads to effective one dimensional systems [3]; some surface phenomena are described by 1D models [4]; and chemical reactions can in certain conditions be modeled by effective one dimensional potentials [5]. Moreover, the simplicity of 1D models has made them valuable as pedagogical and research tools. They facilitate testing hypotheses, new ideas, approximation methods and theories without unnecessary and costly complications. For the same reasons they are frequently used to examine fundamental questions of quantum mechanics. In particular, the time quantities treated in this book, such as tunneling or arrival times, have in most cases been examined in one dimensional models. Many results for 1D are inspired by results previously obtained in 3D, although the direct translation is not always trivial or possible. This is because 3D collisions with spherically symmetric potentials are described on the half line, by decomposition into partial waves, whereas 1D collisions involve the full line and a doubly degenerate spectrum.

The chapter is organized as follows: Section 2.2 provides a minimal overview of formal 1D scattering theory. The treatment is “formal” because no mathematically rigorous proofs are given. Instead, we summarize the operator structure of the theory and the results needed to define characteristic times later on. For a more rigorous mathematical presentation see e.g. [6]. Sections 2.3, 2.4 and 2.5 are devoted, respectively, to the dwell time, the delay time, and decay times (the exponential decay and its deviations). Quantities related to the tunneling time conundrum are scattered in several parts of the book. In this chapter 2.4.1 and 2.4.4 discuss the Hartman effect and negative delays, while Sect. 2.6 discusses the role of the Büttiker–Landauer “traversal