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Cross section versus time delay and trapping probability

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ABSTRACT

We study the behavior of the *s*-wave partial cross section $\sigma(k)$, the Wigner–Smith time delay $\tau(k)$, and the trapping probability $P(k)$ as function of the wave number k. The *s*-wave central square well is used for concreteness, simplicity, and to elucidate the controversy whether it shows true resonances. It is shown that, except for very sharp structures, the resonance part of the cross section, the trapping probability, and the time delay, reach their local maxima at different values of k. We show numerically that $\tau(k) > 0$ at its local maxima, occurring just before the resonant part of the cross section reaches its local maxima. These results are discussed in the light of the standard definition of resonance.

1. Introduction

By far, the most widely used scattering function is the cross section $\sigma(k)$. Its analysis provides essential information about all kinds of scattering phenomena in physics and it is specially important in the study of resonances. For sharp resonances, the *resonance part* of the cross section is generally assumed to be described by the famous Breit–Wigner resonance formula. Its importance cannot be overestimated since this formula is given in terms of the parameters that characterize the resonance; namely, the width and position of the (cross section) resonance (see e.g. [1] and references therein). This is perhaps the reason why, quite often, the term resonance is taken to mean a resonance in the cross section. In fact, it is sometimes explicitly stated that the resonance energy is defined as that which corresponds to the value of $\pi/2$ of the resonant part of the phase shift, see e.g. [2]. Furthermore, these parameters can be related to some fundamental quantities. For example, in nuclear physics, the width (position) corresponds to the decay width (mass) of a meta-stable particle [3]. Just as knowledge of individual resonances is important, so is the understanding of their statistical properties, such as the distribution of their widths or spacings, specially in the field of quantum chaos [4].

Since the cross section is defined in terms of the phase shift $\theta(k)$ and this is composed of a background part and a resonance part, to unveil the sought after resonance parameters from the data a complicated fitting procedure must be applied [1]. Thus, study of other scattering functions can yield important and complementary information about the system.

The Wigner–Smith delay time $\tau(k)$ [5] is such a quantity. Actually, knowledge of $\tau(k)$ may be considered necessary in order to comply with the most generally accepted definition of resonance [6–8]. Namely, a rapid increase in the phase shift through $\pi/2$ (modulo π). How fast? Fast enough so that there is time delay since a time delay implies the existence of a meta-stable state and vice versa [8].

In the literature resonances are sometimes defined as the poles of the scattering matrix S [6,8–10] (for a more mathematical definition see [11]). We shall refer to these as resonance *poles* to distinguish from the *scattering* resonances discussed above. Certainly, the two definitions are connected and the scattering resonances may be viewed as the manifestation of the resonances poles (occurring near the real axis). However, while the definition of resonance poles is unambiguous, the definition of scattering resonances seems to lack certain consistency that we shall try to point out in the remainder of this paper.

In this paper we shall focus on comparing the behavior of three scattering functions: The *s*-wave partial cross section $\sigma(k)$, the Wigner–Smith time delay $\tau(k)$, and the trapping probability $P(k)$ (to be defined in the next section). We will show that the "speed of the phase shift" $l(k) \equiv 2(\partial\phi/\partial k)$, see Eq. (13) below, can be considered itself a scattering function and it is the link between the other three functions.

One of the objectives of this work is to show that different closely related scattering functions do not in general peak at the same k values as the resonant part of the cross section and hence their study offers complementary information about the resonance

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properties of the system under study. Although the differences in the peak positions of the various scattering functions may be small there are underlying conceptual differences that may lead to a deeper understanding of resonance phenomena. We shall see that the centers of the resonances of $l(k)$ and $\tau(k)$ can be identified with the real part of the S-matrix poles in k-space, whereas those of $\sigma_\phi(k)$ with the absolute value of the pole.

To be able to get exact results for these quantities we shall use the s-wave central square well potential. Despite the simplicity of this potential, it has served not only as a textbook example to display basic features of quantum resonance scattering [12,13] but also as a model for some nuclear systems, see e.g. [2,14–16]. Paradoxically, some authors have pointed out that the square well does not give rise to "true" non-zero energy resonances [6,17]. The reason being that precisely at resonances of the cross section, the time delay is at most equal to zero. Others maintain that in spite of this the square well does produce Breit–Wigner resonances, thus advocating the "less restrictive definition of a resonance as an enhancement in the cross section due to a pole in the scattering amplitude" [12]. It appears then that the study of other scattering functions may elucidate the controversy and perhaps induce some polishing in the definition of resonance.

The speed of the phase shift $l(k)$ certainly plays a fundamental role. For the central square well, characterized by the "strength" α (given in Eq. (20)), we demonstrate that the local maxima of $l(k)$ occur just before the resonant part of the cross section reaches its local maxima. Further, we show that $\tau(k) > 0$ at all the local maxima of $l(k)$ except for very large values of α, where $\tau(k) \to 0$.

2. Scattering functions and resonances

In this brief presentation of the basic scattering quantities, we consider non-relativistic spinless scattering off finite-range potentials. Specifically, potentials decaying as $1/r$ or slower and short range potentials plus a Coulomb-like potentials are not considered here. For central finite-range scattering potentials with free-particle asymptotics, the asymptotic radial wave function ψ_ℓ for the orbital angular momentum l is (see e.g., p. 437 in [8] or p. 6 in [18])

$$\psi_\ell(k;r) = e^{-i\delta_\ell} + S_\ell(k) e^{i\delta_\ell}, \quad r > a_\ell \,, \tag{1}$$

where a_ℓ, is the interaction radius for the ℓ-wave, $\delta_\ell = kr - \ell\pi/2$, $S_\ell(k) = -e^{2i\theta_\ell(k)}$ is the ℓ-wave element of the S-matrix, and $\theta_\ell(k)$ is the ℓ-wave phase shift. S_ℓ can be written in terms of ψ_ℓ and its space derivative, evaluated at some $r \geq a_\ell$:

$$S_\ell = -e^{-2i\delta_\ell} \frac{1 + ik\psi_\ell/\psi_\ell'}{1 - ik\psi_\ell/\psi_\ell'} \tag{2}$$

$$= -e^{2i\theta_\ell} \,, \tag{3}$$

where

$$\theta_\ell = -(kr - \ell\pi/2) + \phi_\ell \tag{4}$$

and

$$\phi_\ell = \tan^{-1}[k\psi_\ell(k;r)/\psi_\ell'(k;r)] \tag{5}$$

is the so-called resonant part of the phase shift. Clearly, the phase shift $\theta_\ell(k)$ is independent of the radius r as long as it is in the asymptotic regime ($r \geq a$, where a is the interaction radius), whereas the resonant part $\phi_\ell(k)$ depends on the radius $r \geq a$ where it is calculated. For well defined radius of interaction a the natural choice for the evaluation of ϕ is $r = a_\ell$, see also Ref. [15].

2.1. Cross section

As shown in most books on quantum mechanics, for central potentials the s-wave partial cross section is given by

$$\sigma_\ell(k) = \frac{4\pi(2\ell+1)}{k^2} \sin^2(\theta_\ell) \,. \tag{6}$$

In this work we shall consider only the case $\ell = 0$; s wave scattering. Dropping the subscript $\ell = 0$ in all quantities, the s partial wave cross section is then written as

$$\sigma(k) = \frac{4\pi}{k^2} \sin^2(\theta) = \frac{\pi}{k^2} \mid 1 + S \mid^2, \tag{7}$$

where $S = -\exp(2i\theta)$, k is the wave number in the asymptotic region, and $\theta(k) = -kr + \phi$. Clearly, the phase shift $\theta(k)$ is independent of the radius r as long as it is in the asymptotic regime ($r \geq a$, where a is the interaction radius), whereas the resonant part ϕ depends on the radius $r \geq a$ where it is calculated. For s-waves, if $r = a$, the phase $-ka$ is the so-called hard sphere shift. As is customary [19] and convenient for our purposes, we shall be considering the scaled version of the cross section (or scattering amplitude):

$$\sigma_\theta(k) = \frac{k^2}{\pi} \sigma(k) = |1 + S|^2 = 4\sin^2(\theta) \tag{8}$$

and its resonance part

$$\sigma_\phi(k) = 4\sin^2(\phi) \,. \tag{9}$$

An important reason to separate the phase shift into resonant and non-resonant parts is that the resonance formula of Breit–Wigner refers exactly to the resonant part of the phase shift. Since this is not the usual case, there are formulas, like that of Fano's resonance shape [20] that can be used to fit and extract the so-called Breit–Wigner parameters defining the center and the width of the resonance [18,21]. These parameters, in the relativistic case, provide the (Breit–Wigner) mass and life time of the unstable particles. As far as we know [1] this requires fitting procedures with often several fitting parameters. The point is that in many practical applications, the splitting of the phase shift is needed to make sense of the data.

2.2. Time delay and effective traversal distance

The time delay is a commonly used quantity to characterize resonances, see e.g. [6,7,18,22]. In one dimension it is known also as the Wigner–Smith time delay and for a particle of mass μ with incident momentum $\hbar k$, it is defined as [23,24]

$$\tau(k) = -i\hbar S^* \frac{\partial S}{\partial E} = 2\hbar \frac{\partial \theta}{\partial E} \tag{10}$$

$$= \frac{\mu}{\hbar k} 2 \frac{\partial \theta}{\partial k} \,. \tag{11}$$

It is the difference between the time that a particle spends in the internal region in the presence of a scattering potential minus the time the particle would spend if there were no scattering potential [25]. $\tau(k)$ is directly connected with the existence of meta-stable states or the temporary capture of the projectile in the interaction region [8]. As mentioned in the Introduction, the established definition of resonance requires that $\tau(k)$ be greater than zero. The quantity $2(\partial\theta/\partial k)$ was called the "retardation stretch" by Wigner [23]. He used it to derive his causality condition, discussed in most books on scattering theory (see e.g. page 103 in [22] or page 466 in [8]). By splitting the phase shift into resonant and non-resonant parts (10) becomes