

Illustration of resonances and the law of exponential decay in a simple quantummechanical problem

Herbert Massmann

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of the so-called "four-wave mixing" problems being studied in the field of quantum optics. They would also be related to the study of wave-front catastrophes¹⁰ which were mentioned in the Introduction.²

ACKNOWLEDGMENT

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¹In Halliday and Resnik, for example, the only mention of this sort of interference is in two problems which involve SWR calculations.

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Illustration of resonances and the law of exponential decay in a simple quantum-mechanical problem

Herbert Massmann

Universidad de Chile, Casilla 653, Santiago, Chile

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The exact quantum-mechanical solution of a particle moving in a one-dimensional well formed by a delta barrier in front of an impenetrable well is used to illustrate the relation between scattering resonances and exponential decay from the well.

I, INTRODUCTION

The purpose of this contribution is to illustrate the resonance phenomena and the law of exponential decay in a very simple one-dimensional quantum-mechanical problem: a mass μ moving in a potential given by (see also Fig. 1)

$$V(x) = \begin{cases} \infty & x < 0 \\ W_0 \delta(x - x_0) & x \ge 0 \end{cases}$$
 (1)

The δ function in the potential can be considered as a square barrier of height h and width l in the limit $l \rightarrow 0$, $h \rightarrow \infty$ such that the product $hl = W_0$ remains constant. Without changing the essential features of the problem, the use of the δ function considerably reduces the algebra in the process of solving the Schrödinger equation, since one will effectively have to consider only two regions (region I and II) instead of three which would be the case if a finite barrier is considered. This simplification introduced by δ functions has been exploited in numerous occasions mainly in problems used for pedagogical purposes. A few cases, published recently in this journal, applied to bound state problems and scattering situations and are given in Refs. 2 and 3, respectively.

In Sec. II the time-independent Schrödinger equation with the potential given by Eq. (1) will be solved for a scattering type situation, that is, for the case in which a particle of energy E and mass μ will be incident from the right onto the δ barrier. Resonance phenomena are readily found; for certain energies the probability that the particle penetrates into region I will increase enormously. These resonances,

in the limit in which the transmission through the δ barrier is small, have the familiar Breit-Wigner shape⁴ (Sec. III). In this way, a simple expression for the width Γ_n of the resonance (or quasistationary state) is found.

In Sec. IV it is assumed that for t=0 the particle is trapped inside the well (region I) in a specific state, and the time evolution of this state will be considered. In particular, it is shown that the probability of finding the particle in region I decays according to the exponential law $P(t) = \exp(-t/\tau_n)$. It turns out, as expected, that the mean life τ_n is related to the width Γ_n of the quasistationary state

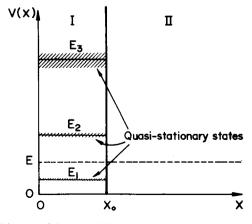


Fig. 1. Diagram of the potential.

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considered, by the relation $\Gamma_n = \hbar/\tau_n$. The relation between Γ_n and τ_n is further analyzed in Sec. V, using a semiclassical argumentation.

For the case of a finite barrier (instead of a δ barrier), some of the questions here considered have been worked out in a collection of quantum-mechanical problems by Flügge⁵ (see also references given therein).

II. STATIONARY STATES

Let us consider the time-independent Schrödinger equation

$$\left(-\frac{\hbar^2}{2\mu}\frac{d^2}{dx^2} + W_0\delta(x - x_0) - E\right)\psi(x) = 0$$
 (2)

and find the solution which satisfies the boundary condition $\psi(0) = 0$.

If $W_0 = 0$, the solution of Eq. (2) is given by

$$\psi_k^{(0)}(x) = \left(\frac{2}{\pi}\right)^{1/2} \sin(kx)$$

$$= \frac{i}{(2\pi)^{1/2}} \left(e^{-ikx} - e^{+ikx}\right), \tag{3}$$

where $k = +(2\mu E)^{1/2}$. Since the spectrum is continuous and nondegenerate, all the states of the system will be normalized to the δ function, that is,

$$\int_{0}^{\infty} \psi_{k}^{(0)*}(x)\psi_{k}^{(0)}(x)dx = \delta(k-k'). \tag{4}$$

The first term on the right-hand side of Eq. (3) represents an ingoing wave (that is, a wave which moves from $+\infty$ towards the origin), while the second term corresponds to an outgoing wave.

If $W_0 \neq 0$, or in other words, if a δ barrier is present at $x = x_0$, the solution of the Schrödinger equation (2) which satisfies the boundary condition is given by

$$\psi_k(x) = \left(\frac{2}{\pi}\right)^{1/2} e^{i\delta_k} \begin{cases} \sin(kx + \delta_k) & x \geqslant x_0 \\ A_k \sin(kx) & 0 \leqslant x \leqslant x_0 \end{cases}, \tag{5}$$

where, for phase δ_k and the amplitude A_k , one finds the expressions

$$\delta_k = -kx_0 + \arctan\left(\frac{\tan(kx_0)}{1 + (\alpha/kx_0)\tan(kx_0)}\right) \tag{6}$$

and

$$A_k = \{\sin^2(kx_0) + [\cos(kx_0) + (\alpha/kx_0)\sin(kx_0)]^2\}^{-1/2}.$$
 (7)

In Eqs. (6) and (7) we introduced the dimensionless constant α defined by

$$\alpha = :2\mu x_0 W_0 / \hbar^2 \,. \tag{8}$$

Note that δ_k is the phase by which, for $x > x_0$, the stationary wave is shifted due to the δ barrier at $x = x_0$, while A_k is the amplitude the stationary wave acquires inside the well formed by the wall at x = 0 and the δ barrier. As will be seen in Sec. V, α is related to the "penetrability" of the δ barrier. For $\alpha = 0$ the barrier is not present and as expected one has in that case $\delta_k = 0$ and $A_k = 1$ [that is, $\psi(x) = \psi^{(0)}(x)$]; while for $\alpha = \infty$ the barrier is impenetrable and therefore $\delta_k = -kx_0$ and $A_k = 0$ [that is, $\psi(x) = \psi^{(0)}(x - x_0)$].

Figure 2 shows the phase shift δ_k as a function of kx_0 for $\alpha = 20$. It may be seen from Fig. 2 that in the vicinity of

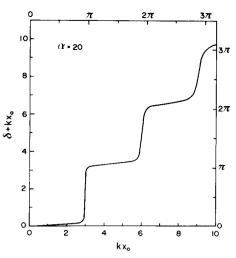


Fig. 2. Graph of the phase shift δ as a function of kx_0 for $\alpha = 20$. For $kx_0 = n\pi$ $(n \in \mathbb{N})$, the phase increases rapidly by π giving rise to resonances

 $kx_0 = n\pi$ (n being a positive integer), the phase shift δ_k increases by π . This is a typical characteristic of resonances.

Let R be the ratio between the probability of finding the particle in region I and the probability of finding it in region II in an interval of size x_0 (that is, the same size of region I). For R one finds

$$R = A_k^2 \left(1 - \frac{\sin(2kx_0)}{2kx_0} \right). \tag{9}$$

In Fig. 3, R is plotted as a function of the energy E for $\alpha = 20$. Resonances, which become broader as the energy increases, are readily observed. These resonances are related to the quasistationary states which exist in region I. If $\alpha = \infty$, then, in the well formed by the wall at x = 0 and

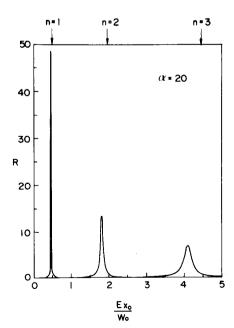


Fig. 3. Graph of R (which is related to the probability of finding the particle in region I) as a function of the energy E for $\alpha = 20$. The arrows on the top of the figure indicate the position the resonances would have if $\alpha \to \infty$ (that is, if the δ barrier becomes impenetrable).

the barrier at $x = x_0$, there exist stationary states when $k_n x_0 = n\pi$. If α is finite, these states are shifted to somewhat lower energies $[\bar{k}_n x_0 \approx n\pi(1 - 1/\alpha)]$ and will acquire a certain width Γ_n . For a very illuminating discussion of resonances and antibound states, see Ref. 6.

III. BREIT-WIGNER LINE SHAPE

For $x > x_0$, the wave function $\psi_k(x)$ [Eq. (5)] can be written as

$$\psi_k(x) = [i/(2\pi)^{1/2}](e^{-ikx} - e^{2i\delta_k}e^{+ikx}). \tag{10}$$

Comparing it with $\psi_k^{(0)}(x)$ it is found that the outgoing wave has been modified due to the δ barrier, by a factor

$$S = e^{2i\delta_k} \,. \tag{11}$$

This is the so called S-matrix, which for this problem is just a complex number. Using Eq. (6) it is found that the S-matrix can be written in the form

$$S = S^{(0)} \cdot e^{2i \arctan(2/\beta)} = S^{(0)} \left(1 - \frac{i}{i/2 - \beta} \right), \tag{12}$$

where $S^{(0)}$ (a slowly varying function of k) and β are, respectively, given by

$$S^{(0)} = :e^{-2ikx_0} \tag{13}$$

and

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$$\beta = : \frac{1 + (\alpha/kx_0)\tan(kx_0)}{2\tan(kx_0)}. \tag{14}$$

Let us evaluate β in the vicinity of a resonance. Resonances occur [see Eq. (6)] whenever

$$\tan(\bar{k}_n x_0) = -\bar{k}_n x_0 / \alpha . \tag{15}$$

If k is close to a resonant value \bar{k}_n , then

$$\tan(kx_0) \approx \tan(\bar{k}_n x_0) + x_0(k - \bar{k}_n)$$

$$= -(\bar{k}_n x_0/\alpha) + x_0 \Delta k \ . \tag{16}$$

Substituting Eq. (16) into (14), and keeping only terms in lowest order in $\Delta k = k - k_n$,

$$\beta \approx \frac{\alpha(\alpha+1)\Delta k}{2\bar{k}_n^2 x_0} \approx \frac{\alpha(\alpha+1)\mu(E-\bar{E}_n)}{2\hbar^2 \bar{k}_n^3 x_0} = \frac{E-\bar{E}_n}{\Gamma_n}, \quad (17)$$

where Γ_n is defined by

$$\Gamma_n = \frac{2\hbar^2 \bar{k}_n^3 x_0}{\mu \alpha (\alpha + 1)} \approx \frac{2\hbar^2 \pi^3 n^3}{x_0^2 \mu \alpha^2}.$$
 (18)

In order to obtain Eq. (17) it was assumed that $\alpha \cdot \Delta k \leqslant \overline{k}_n$. Replacing Eq. (17) into the expression for the S-matrix [Eq. (12)], one obtains the so-called Breit-Wigner formula for an isolated resonance⁴:

$$S = S^{(0)} \left(1 - \frac{i\Gamma_n}{(E - \overline{E}_n) + (i/2)\Gamma_n} \right). \tag{19}$$

The meaning of Γ_n is now clear: it is the width of the resonance located at $E = \overline{E}_n = \hbar^2 \hat{k}_n^2/(2\mu)$.

In order to see how well the expression (19) fits the resonance, we plot, in Figs. 4 and 5, $|S - S^{(0)}|^2$ as a function of E for the first and third resonances, respectively. The full line shows the results obtained using the exact expression [Eq. (12)] and the broken line the results found using the Breit-Wigner formula [Eq. (19)]. As the resonance gets wider, the agreement between the Breit-Wigner line shape (which is symmetric with respect to \overline{E}_n) and the actual shape of the

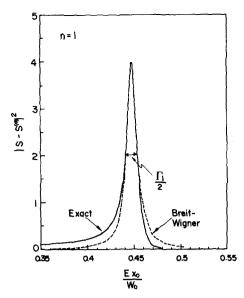


Fig. 4. Graph of $|S - S^{(0)}|^2$ as a function of energy for the first resonance.

resonance becomes less satisfactory. Actually the condition $\alpha \Delta k < \overline{k}_n$ used in deriving Eq. (19) is equivalent to

$$E - E_n \leqslant (\alpha/n\pi)\Gamma_n = \Gamma_n/(p_n)^{1/2}, \qquad (20)$$

where p_n [defined by Eq. (38)] is the probability that a particle of mass μ and energy $\hbar^2 k_n^2/(2\mu)$ impinging upon an isolated δ barrier $W_0\delta(x)$ will be able to penetrate it.

IV. EXPONENTIAL DECAY

Let us now consider the problem which is met with if the strength of the δ barrier depends on time:

$$W_0(t) = \begin{cases} \infty & t < 0 \\ W_0 = \text{finite constant} > 0 & t \ge 0 \end{cases}$$
 (21)

For t < 0, the barrier at $x = x_0$ is impenetrable and in region

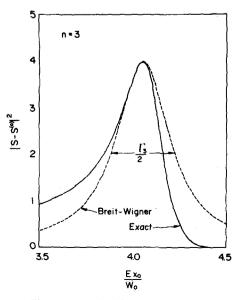


Fig. 5. Same as Fig. 4, but for the third resonance.

I one has discrete states for the energy values

$$E_n = \frac{\hbar^2 k_n^2}{2\mu} = \frac{\hbar^2}{2\mu} \cdot \frac{n^2 \pi^2}{x_0^2}, \quad n \in \mathbb{N} ,$$

with the corresponding wave function given by

$$\varphi_n(x,t) = \begin{cases} \left(\frac{2}{x_0}\right)^{1/2} \sin\left(\frac{n\pi}{x_0}x\right) e^{-iE_nt/\hbar} & 0 \leqslant x \leqslant x_0 \\ 0 & x \leqslant 0, x \geqslant x_0 \end{cases}$$
(22)

We assume that for t < 0 the system is in particular state n. Of course, in that case one has 100% probability of finding the particle in region I for t < 0.

At t = 0, the barrier becomes permeable and as time goes on, the probability of finding the particle in region I decreases. In order to find the time evolution of this probability, we have to study the time dependence of the state $\varphi_n(x,t)$ for t > 0.

For t > 0, the potential is again time independent and

$$\{\tilde{\psi}_k(x)\}_{k>0} = \{\exp(-i\delta_k)\cdot\psi_k(x)\}_{k>0}$$

[where $\psi_k(x)$ is given by Eq. (5)] is a complete and orthogonal set of normalized eigenfunctions for the problem. [Note that $\tilde{\psi}_k(x)$ are real functions and for $0 \leqslant x \leqslant x_0$ are given by $\psi_k(x) = A_k(2/\pi)^{1/2} \sin(kx)$.]

Expanding $\varphi_n(x,0)$ in terms of this complete set

$$\varphi_n(x,0) = \int_0^\infty \gamma_k \, \tilde{\psi}_k(x) dk \,, \tag{23}$$

the expansion coefficients are found to be given by the expression

$$\gamma_k = \int_0^{x_0} \varphi_n(x,0) \, \tilde{\psi}_k(x) dx$$

$$= \frac{2A_k}{(\pi x_0)^{1/2}} \int_0^{x_0} \sin(kx) \sin\left(\frac{n\pi}{x_0}x\right) dx . \tag{24}$$

The factor A_k is a rapidly varying function of k and is significantly different from zero only in the vicinity of a resonance (that is, in the vicinity of $k=k_m=m\pi/x_0, m\in\mathbb{N}$). On the other hand, the integral that appears in Eq. (24) varies slowly as a function of k, has its largest value for $k=m\pi/x_0$, and is zero for $k=m\pi/x_0$, $m\in\mathbb{N}$, $m\neq n$. These considerations show γ_k to be significantly different from zero only in the vicinity of $k_n=n\pi/x_0$ and therefore

$$\gamma_k \underset{\text{of } k_n}{\approx} (x_0/\pi)^{1/2} A_k$$
 (25)

Once the expansion coefficients are known, the time evolution of φ_n can be readily obtained:

$$\varphi_n(x,t) = \int_0^\infty \gamma_k \, \tilde{\psi}_k(x) e^{i(\pi k^2/2\mu)t} \, dk \,. \tag{26}$$

From this time dependence, the probability P(t) of finding the particle in region I can be approximately evaluated:

$$P(t) = \int_{0}^{x_{0}} |\varphi_{n}(x,t)|^{2} dx$$

$$= \int_{0}^{x_{0}} dx \left| \int_{0}^{\infty} \gamma_{k} \tilde{\psi}_{k}(x) e^{i(\hbar k^{2}/2\mu)t} dk \right|^{2}$$

$$\approx \int_{0}^{x_{0}} dx \left| \int_{\text{vicinity}}^{\text{vicinity}} \left(\frac{x_{0}}{\pi}\right)^{1/2} A_{k} \left[A_{k} \left(\frac{2}{\pi}\right)^{1/2} \sin(kx) \right] \right|$$

$$\times e^{i(\hbar k^{2}/2\mu)t} dk \right|^{2}$$

$$\approx \frac{2x_{0}}{\pi^{2}} \int_{0}^{x_{0}} dx \sin^{2}(k_{n} x)$$

$$\times \left| \int_{\text{vicinity}}^{\text{vicinity}} A_{k}^{2} e^{i(\hbar k^{2}/2\mu)t} dk \right|^{2}$$

$$\approx \left(\frac{x_{0}}{\pi}\right)^{2} \left| \int_{\text{vicinity}}^{\text{vicinity}} A_{k}^{2} e^{i(\hbar k^{2}/2\mu)t} \right|^{2}. \tag{27}$$

The amplitude A_k and the phase shift δ_k are closely related due to the continuity of the wave function at $x = x_0$. This has been used previously to relate, in the general case, scattering resonances with decay times. See, for example, Ref. 7. It is found from Eq. (5) that

$$A_k = \sin(kx_0 + \delta_k)/\sin(kx_0). \tag{28}$$

We now evaluate A_k^2 in the vicinity of the resonance located at $k_n = n\pi/x_0$ ($n \in \mathbb{N}$) under the same assumptions used in the previous section to find the Breit-Wigner shape for the S-matrix, that is $\alpha \gg n\pi$ and $\alpha \Delta k \ll k_n$.

From Eqs. (11) and (12):

$$\sin(kx_0 + \delta_k) = \sin[\arctan(2/\beta)] = (1 + \beta^2/4)^{-1/2}.$$
 (29)

Also, by analogy with Eq. (16),

$$\sin(kx_0) \approx -\frac{\overline{k}_n x_0}{\alpha} + x_0 \Delta k \underset{\alpha \Delta k < k_n}{\approx} -\frac{k_n x_0}{\alpha} \approx -\frac{n\pi}{\alpha}.$$
(30)

Replacing Eqs. (29) and (30) into (28),

$$A_{k}^{2} \approx \frac{(\alpha/n\pi)^{2}}{1+\beta^{2}/4} = \frac{\xi}{1+\xi^{2}x_{0}^{2}(k-\bar{k}_{x})^{2}},$$
 (31)

where \overline{k}_n gives the position of the resonances, and ξ is given by

$$\xi = : (\alpha/n\pi)^2 \,. \tag{32}$$

Substituting Eq. (31) into Eq. (27)

$$P(t) \approx \left(\frac{x_0}{\pi}\right)^2 \left| \int_{\substack{\text{vicinity} \\ \text{of } \bar{k}_n}} \frac{\xi e^{i(\hbar k^2/2\mu)t}}{1 + \xi^2 x_0^2 (k - \bar{k}_n)^2} dk \right|^2$$

$$\approx \left(\frac{x_0 \xi}{\pi}\right)^2 \left| \int_{-\infty}^{+\infty} \frac{e^{i(\hbar k^2/2\mu)t}}{1 + \xi^2 x_0^2 (k - \bar{k}_n)^2} dk \right|^2$$

$$= e^{-t/\tau_n} \quad t \geqslant 0 , \tag{33}$$

with τ_n given by

$$\tau_n = \hbar (\mu x_0^2 \alpha^2 / 2n^3 \pi^3 \hbar^2). \tag{34}$$

From Eq. (33) it is seen that the probability of finding the particle in region I decays according to the exponential law, with a mean lifetime τ_n . Comparing Eq. (34) with the definition of Γ_n [Eq. (18)] one gets the familiar relation

between the lifetime τ_n and the energy width of the resonance Γ_n :

$$\tau_n = \hbar/\Gamma_n \ . \tag{35}$$

Two references which complement the material presented in this paper, as they discuss similar problems from very different points of view, are the following: Ref. 8, where a time-dependent wave packet approach together with the analytic properties of the general scattering solution is used; and Ref. 9, which obtains interesting results using methods based on Feynman path integrals.

V. SEMICLASSICAL CONSIDERATIONS

In the following, a semiclassical argumentation will be used in order to find the mean lifetime τ_n which a particle placed inside the well (region I) requires to penetrate through the barrier and so "decay" into the region II.

If a particle of mass μ and energy $E_n = \hbar^2 k_n^2 / 2\mu$ is trapped in region I, the time T between two collisions with the δ barrier is given by

$$T = 2x_0/(\hbar k_n/\mu). \tag{36}$$

A simple calculation shows that the penetration probability p_n of a particle, through an isolated δ barrier $W_0 \cdot \delta(x - x_0)$, is given by

$$p_n = \frac{1}{1 + \left(\frac{\alpha}{2k_n x_0}\right)^2} \underset{\alpha > n\pi}{\longrightarrow} \left(\frac{2k_n x_0}{\alpha}\right)^2. \tag{37}$$

The mean lifetime τ is defined as the time for which the probability that the particle still remains in region I has decreased to 1/e. If $p_n \leqslant 1$ (which is the case if $\alpha \geqslant n\pi$), the number of collisions N of the particle against the barrier necessary for this to happen is implicitly defined by the relation

$$(1 - p_n)^N = 1/e . (38)$$

Taking the natural logarithm of this last expression and using the assumption $p_n \le 1$,

$$N = 1/p_n . (39)$$

Multiplying Eq. (39) by T, noting that $\tau_n = NT$ and using equations (36) and (37) in the limit $p_n \le 1$, one obtains for the mean lifetime the expression

$$\tau_n = T/p_n = \hbar (\mu \alpha^2/2\hbar^2 k_n^3 x_0). \tag{40}$$

This result coincides with the one found in the previous section [Eq. (34)].

This second way of obtaining the mean lifetime is much simpler than the approach used in Sec. IV and therefore seems more appealing, but on the other hand, relies strongly on Eq. (36). Can this classical relation be justified in some way? If one tries to do so, one gets into serious difficulties. In order to talk about a particle which hits the barrier with a period T, one would need to construct wave packets which are localized in space within a region Δx much smaller than the size of the well (that is, $\Delta x \ll x_0$). Furthermore one would require the center of mass of this wave packet to be moving with a velocity $\hbar k_n / \mu$ without spreading significantly over a time period T. A simple analysis shows that these requirements cannot be fulfilled for energies corresponding to small n values. For these cases, therefore, one has to renounce trying to construct such a classical picture. If, however, one ignores this difficulty and goes ahead with the classical relation Eq. (36), even for small n values, one surprisingly finds the right answer.

VI. CONCLUSIONS

For a very simple and pedagogically interesting case, the relationship between the width of scattering resonances and the decay times of the corresponding quasistationary states was obtained in a direct and explicit way.

The exact shape of the resonances was found, and from it the Breit-Wigner line shape was obtained illustrating in this way the conditions for which this approximate expression is valid.

Finally it may also be noted that most of the results presented in this article suffer only minor modifications when the sign of W_0 is reversed, that is, if instead of a δ barrier one has a δ well at $x = x_0$.

ACKNOWLEDGMENT

I would like to thank C. Infante for helpful comments.

¹For a standard textbook with easy δ-function and other related problems, see, for example, *Quantum Mechanics*, by C. Cohen-Tannaudji, B. Din, and F. Laloe (English translation published by Wiley, New York, 1977).

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