Paths of Discovery
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TRANSIENT PHENOMENA IN QUANTUM MECHANICS: DIFFRACTION IN TIME

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1. *Introduction*

Transient terms [1] are to be expected in a dynamical description of resonance scattering, from the analogy that this description has with the theory of resonant electric circuits [2]. As is well-known, in circuit theory the appearance of resonances in the stationary current is closely related with the transients of the circuit, as the same parameters (resonant frequencies and damping factors) appear in both [3].

The transient terms in a scattering process contain, besides those that could be considered analogous to the electric circuit theory, terms that are related to the time-energy uncertainty relation [4] as quantum mechanics is used in the description of the scattering.

To understand the physical meaning of the transient terms in the resonance scattering process, it seemed of interest to analyze first the transient effects that appear when the propagation of a beam of particles is interrupted. The more complicated phenomenon, where an actual scatterer (represented by a potential or by boundary conditions [5]) is introduced into the beam of incident particles, is briefly discussed in the papers mentioned.

We deal here with the transient terms in the wave function that appear when a shutter is opened. It will be shown in the next section, that when the state of the beam of particles is represented by a wave function satisfying the time-dependent Schroedinger equation, the transient current has a remarkable mathematical similarity with the intensity of light in the Fresnel diffraction by a straight edge [6]. The transient phenomena have therefore been given the name of diffraction in time.

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The form of the transient terms of ψ that appear when the shutter is opened, is strongly dependent on the type of wave equation satisfied by ψ. In the present paper, we analyze the transient terms that appear when the ψs satisfy the Schroedinger equation. Only for this equation is there an analogy with the phenomena of optical diffraction, which has to do with the resemblance that the solutions have with those that appear in Sommerfeld's [7] theory of diffraction.

2. *The shutter problem*

The problem we shall discuss in this note is the following: a monochromatic beam of particles of mass $m=1, \hbar=1$, energy $(k^2/2)$, moving parallel to the x-axis is interrupted at $x=0$ by a shutter perpendicular to the beam, as illustrated in Fig. 1. If at $t=0$ the shutter is opened, *what will be the transient particle current observed at a distance x from the shutter?*

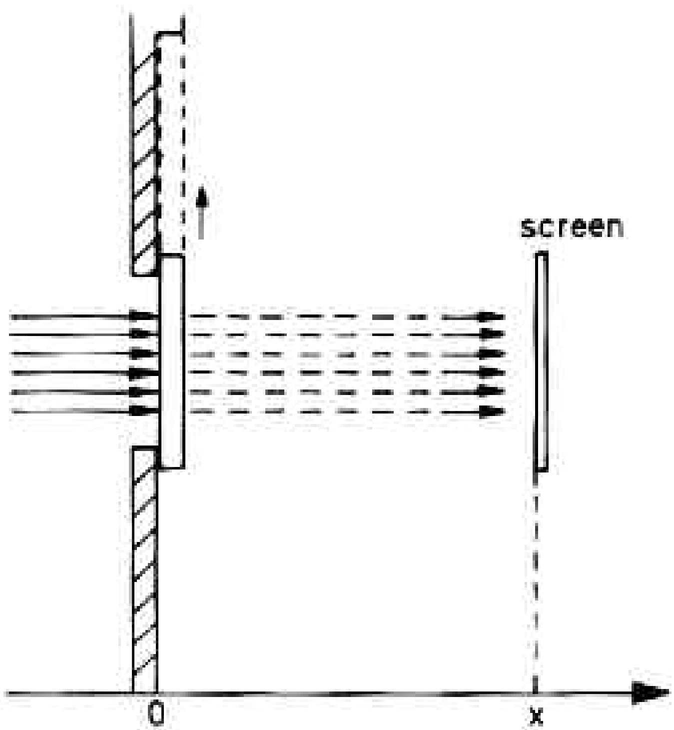

Fig. 1. The shutter problem.

To set the mathematical problem, we must first give the behaviour of the shutter, i.e., if it acts as a perfect absorber (no reflected wave), or a perfect reflector (an infinite potential barrier), or something between the two. For simplicity we will assume that the shutter acts as a perfect absorber, though it can easily be shown that for $x \gg \lambda$ (where λ is the wavelength $\lambda = (2\pi/k)$), the transient current obtained below holds for any type of shutter, so long as it acts as a device that, when closed, keeps the beam of particles on only one side of it.

For non-relativistic particles, the wave function $\psi(x, t)$ that represents the state of the beam of particles for $t > 0$, satisfies the time-dependent Schroedinger equation:

$$-i(\delta\psi/\delta t) = (1/2)(\delta^2\psi/\delta x^2), \tag{1}$$

and the initial conditions:

$$\psi(x, 0) = \begin{cases} \exp(ikx), & \text{if } x \leq 0; \\ 0, & \text{if } x > 0. \end{cases} \tag{2}$$

The solution of (1,2) can be given immediately with the help of the onedimensional Schroedinger Green function

$$G(x-x', t) = (2\pi t)^{-1/2} \exp(-i\pi/4) \exp[i(x-x')^2/2t]. \tag{3}$$

We have then

$$\begin{aligned} \psi(x, t) &= \int_{-\infty}^{0} G(x-x', t) \exp(ikx')dx' \\ &= \frac{1}{\sqrt{2}} \exp\left(-i\,\frac{\pi}{4}\right) \exp\left[i\left(kx - \frac{1}{2}k^2 t\right)\right] \\ &\times \int_{-\infty}^{\xi} \exp\left[i\left(\frac{1}{2}\right)u^2\right] du. \end{aligned} \tag{4}$$

where in the last equation we have made the change of variables

$$u = (x'-x)(\pi t)^{-1/2} + k\,(t/\pi)^{1/2}, \tag{5}$$

$$\xi = (\pi t)^{-1/2}(kt - x). \tag{6}$$

Introducing the Fresnel integrals

$$C(\xi) = \int_0^{\xi} \cos\left(\frac{\pi u^2}{2}\right) du.$$
$$S(\xi) = \int_0^{\xi} \sin\left(\frac{\pi u^2}{2}\right) du. \tag{7}$$

and making use of

$$\int_{-\infty}^{\xi} \exp\left(\frac{i\pi u^2}{2}\right) du = \frac{1}{2}(1+i). \tag{8}$$

we immediately arrive at the result

$$|\psi(x,t)|^2 = \left\{\left[C(\xi)+1/2\right]^2 + \left[S(\xi)+1/2\right]^2\right\}/2. \tag{9}$$

which has the familiar form of the diffraction of a light beam by a semiplane but with the difference that here ξ is the function (6) of position and time.

If we want to have snapshots of the probability density $|\psi(x,t)|^2$ at given instants of time we can make use of the Cornu spiral [8] diagram of Fig. 2.

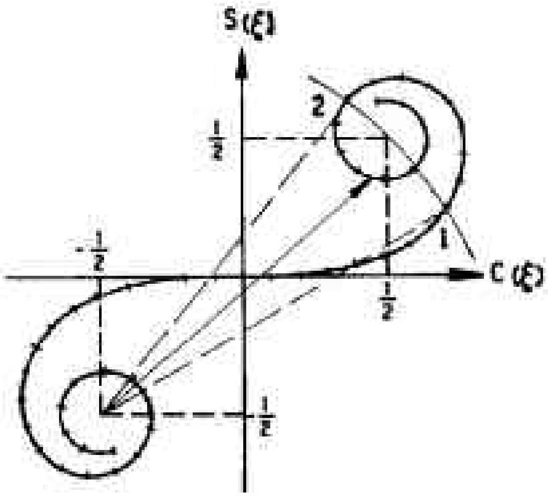

Fig. 2. Cornu spiral [8]. The value of ξ is marked along the curve while the values of the Fresnel integrals $C(\xi)$ and $S(\xi)$ are given along the abscissa and ordinate, respectively. One-half of the square of the magnitude of the vector from the point $(-\frac{1}{2},-\frac{1}{2})$ to a point on the curve with given ξ gives the probability density for that value of ξ.

The values of $C(\xi)$, $S(\xi)$ are given along abscissa and ordinate while ξ is marked along the curve itself. The value of $|\psi(x,t)|^2$ is one half the square of the distance from the point $(-1/2, -1/2)$ in the plane of Fig. 2 to the given point on the curve corresponding to the value ξ. For t fixed and x going from $-\infty$ to ∞ we see from (6) that ξ goes from $-\infty$ to ∞ passing through $\xi=0$ when $x=x_0=kt$. With the help of the Cornu spiral we then obtain that $|\psi(x,t)|^2$ has the form of the full line in Fig. 3. The classical distribution of particles at time t is indicated by the dashed line terminating abruptly at $x_0=kt$. We indicate in Fig. 3, marking it also with dashes, the probability density at $t=0$ which, from (2), is given by 1 for $x\leq 0$ and 0 for $x>0$.

We see from Fig. 3 that an initial sharp-edged wave packet will move with the classical velocity showing rapid oscillations near the edge. The width of these oscillations can be estimated through the distance $\Delta=x_1-x_2$ marked in the figure between the first two values of x, starting from the edge, in which the probability density takes the classical value 1. The values ξ_1, ξ_2 corresponding to x_1, x_2 are marked in the Cornu spiral of Fig. 2 and from (6) we have

$$\xi_1-\xi_2=0.85 = (\pi t)^{-1/2}\Big[(kt-x_2)-(kt-x_1)\Big] = (\pi t)^{-1/2}\,\Delta x. \tag{10}$$

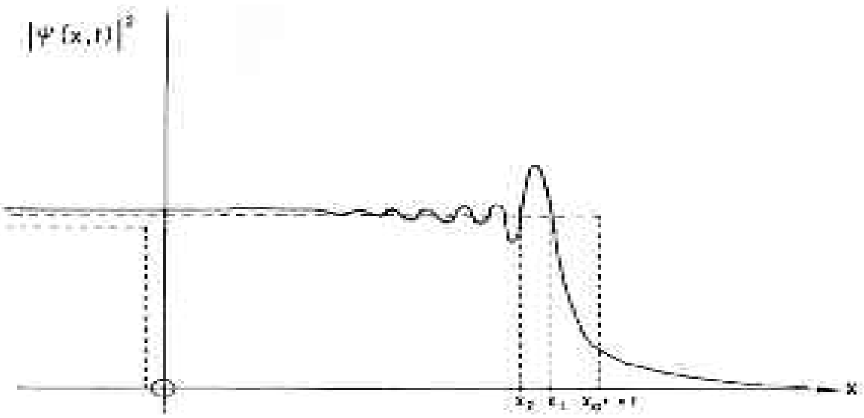

Fig. 3. Probability density of observing a particle at a given time t as a function of distance from the shutter. The dashed line extending to $x=x_0$ represents the classical result at a time t after the opening of the shutter. The dashed line extending to $x=0$ is the probability density before opening the shutter. The values x_1, x_2 are the first positions, starting from x_0, in which the probability density takes its stationary value. In the units we are using $x_0=vt=kt$, where v is the initial velocity of the particle.

Introducing $x_0 = kt$ we obtain finally

$$\Delta x = 0.85\ (\pi x_0/k)^{1/2} = 0.85\,(\lambda x_0/2)^{1/2}, \tag{11}$$

where $\lambda = (2\pi/k)$ is the wavelength of the particle. For particles of wave length $\lambda = 10^{-8}$cm at a distance $x_0 = 10^2$cm from the shutter, the width of the diffraction effect is of the order of 10^{-3}cm.

In Fig. 4 we graph $|\psi(x,t)|^2$ as function of t for fixed x and the width of the resonance in time can be estimated from the difference of the first two times $t_2 - t_1$ at which $|\psi(x,t)|^2$ takes its classical value. This difference can be determined with the help of the Cornu spiral as $\xi_2 - \xi_1$ of Eq. (10) continues to be 0.85 and the time width of diffraction in time is, from Eq. (11) given by,

$$\Delta t \equiv \frac{\Delta x}{v} = 0.85\ (\pi x_0/kv^2)^{1/2} \tag{12}$$

where v is the velocity of the particle. If we multiply numerator and denominator by $\hbar$, and use the fact that $\hbar k$ is the momentum of the particle i.e.

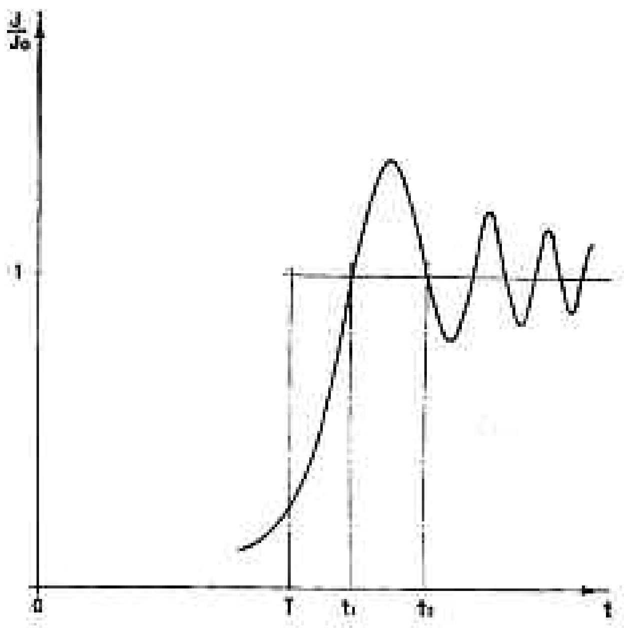

Fig. 4. Width of diffraction in time.

$\hbar k = mv$, with m its mass, we finally have that the width of the diffraction in time is in standard units

$$\Delta t = 0.85\ (\pi x_0 \hbar / m v^3)^{1/2} \tag{13}$$

For $x_0 = 1m$ and neutrons with a velocity corresponding to 300°K the diffraction width is

$$\Delta t = 0.27 \times 10^{-8} \text{sec} \tag{14}$$

If we graph the current as a function of time for a fixed x_0 as shown in Fig. 4 we note that the transient current increases monotically from the very moment in which the shutter is opened and therefore, in principle, an observer at a distance x_0 from the shutter could detect particles before a time x_0/c where c is the velocity of light. This would imply that some of the particles travel with velocities larger than c, and the error is due, of course, to employing the non-relativistic Schroedinger equation in the analysis.

In another publication we employed the ordinary and the Klein-Gordon equation and in both cases there is, at the point x_0, no current observed before the time (x_0/c).

The transient effects associated with the sudden opening of the shutter problem was done originally by the author (*Phys. Rev.* 85, 626, 1952) shortly after he got his Ph.D., and probably was the first analysis of transient effects in quantum mechanics. The field has developed enormously in the last 50 years and he would like to mention the work of M. Kleber 'Exact solutions for time dependent phenomena in quantum mechanics', *Physics Reports* 236 (6) 331 (1994), with 150 references and which presents a very complete review of the progress of the field until 1994.

He would like only to mention the fact that in the original discussion the shutter is opened suddenly. This is not physically possible and Kleber considers a case in which it can be opened slowly using the wave equation

$$\left[i \frac{\delta}{\delta t} + \frac{1}{2} \frac{\delta^2}{\delta x^2} + \frac{k}{\varepsilon t} \delta\,(x) \right] \psi\,(x, t) = 0 \tag{15}$$

The current is in units $(\hbar k/m)$ as function of time t in units $(m/\hbar k^2)$ for both slow $(\varepsilon = 10)$ and fast $(\varepsilon = 0.5)$ lowering of the short-range tunnelling barriers and is given in Fig. 5 at $x = 0$. The exact results (full lines) are compared with the sudden opening of the shutter with dashed dotted lines, which closely agree when $\varepsilon = 0.5$, but are quite different in the case when $\varepsilon = 10$.

3. *Analogues with Sommerfeld's diffraction theory*

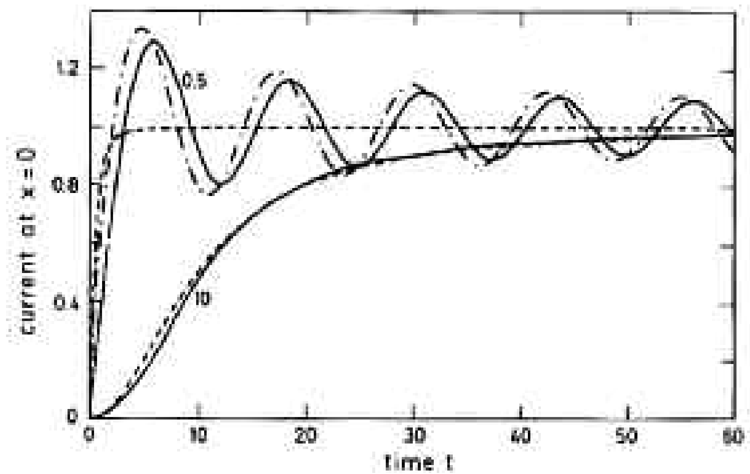

Fig. 5. Tunnelling current (in units of $\hbar k/m$) as a function of time (in units of $\hbar m/(\hbar k)^2$) for slow ($\varepsilon = 10$) and fast ($\varepsilon = 0.5$) lowering of the zero-range tunnelling barrier. The exact results (full lines) are compared with the current derived from the sudden limit (dash-dotted line). M. Kleber, *Physics Report* 236 (6) 1994 p. 384[9].

In the previous sections, the shutter problem for the Schroedinger wave equation was analyzed, and we obtain the corresponding wave functions. Rather than comparing the related transient currents with the intensity of light in optical diffraction [as suggested by the form of the non-relativistic probability density (9)], we shall look into the analogies between the wave functions themselves, and a family of solutions in Sommerfeld's theory of diffraction.

For electromagnetic diffraction problems in the plane, we need appropriate solutions of the two-dimensional Kirchhoff equation, which in polar coordinates has the form

$$(\nabla^2+k^2)\phi \equiv (\delta^2\phi/\delta r^2)+r^{-1}(\delta\phi/\delta r) + r^{-2}(\delta^2\phi/\delta\theta^2)+k^2\phi=0, \tag{16}$$

where $k=(2\pi/\lambda)$ and λ is the wavelength of the radiation.

The well-known family of solutions of (16) that is obtained with the help of the Riemann surface analysis of Sommerfeld [7], can be written in the form:

$$M'(r, \theta, \theta_0) = \exp(ikr)\exp(y'^2)\,\mathrm{erfc}(y'), \tag{17}$$

where:

$$y' = \exp(-i\pi/4)(2kr)^{\frac{1}{2}} \sin\left[\frac{1}{2}(\theta-\theta_0)\right], \tag{18}$$

and θ_0 is a parameter.

The M' satisfy (16) as can be seen from the fact that:

$$\left[\nabla^2 + k^2\right]\phi \equiv k^2(2ikr)^{-1}\exp(ikr) \times\left[d^2/dy'^2 - 2y'd/dy' - 2\right]\exp(y'^2)\,\mathrm{erfc}(y'), \tag{19}$$

and the right hand side of (19) vanishes.

Despite the fact that the time-dependent Schroedinger equation is of the parabolic type, while the Kirchhoff equation is of the elliptic type, they have solutions of the form (17) though of different arguments.

When a semi-infinite perfectly reflecting plane is introduced at $\theta = -(\pi/2)$, in the path of an electromagnetic wave polarized in the plane and propagating in the direction $\theta = 0$, the wave function $\phi(\mathrm{r}, \theta)$ that satisfies [7] the boundary conditions at $\theta = -(\pi/2)$, $(3\pi/2)$ and the asymptotic behaviour at $r \to \infty$ becomes:

$$\phi(\mathrm{r}, 0) = \frac{1}{2}\left[M'(\mathrm{r}, \theta, 0) - M'(\mathrm{r}, \theta, \pi)\right]. \tag{20}$$

From (20) and assuming $x \gg \lambda$ we obtain the characteristic Fresnel diffraction effect [6] for the intensity of the electromagnetic wave in the vicinity of $\theta = 0$.

A corresponding problem for the transient current appears when the shutter is represented as a perfect reflector, i.e., an infinite potential barrier.

In this case we note that in reference [10] corresponding to the initial condition [2] the $\psi(x, t)$ of (4) is replaced by

$$\frac{1}{2} M(x, k, t) \equiv \frac{1}{2}\exp(ix^2/2t)\exp(y^2)\,\mathrm{erfc}(y) \tag{21}$$

with

$$y=(-i\pi/4)(2t)^{-1/2}(x-kt). \tag{22}$$

If (2) is replaced $\exp(ikx)-\exp(-ikx)$ we immediately obtain that

$$\psi(x,t)=\frac{1}{2}\left[M(x,k,t)-M(x,-k,t)\right]. \tag{23}$$

From (9) and (23) and assuming also that $kx \geqslant 1$ we obtain the transient probability density of Fig. 4 which also shows a Fresnel diffraction effect for $t=T$, where T is the time of flight (x/k) in our units $\hbar=m=1$.

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