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General Formulation of the Scattered Matter Waves by a Quantum Shutter

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Abstract

The scattering process of matter waves by a quantum shutter is investigated by using the spectrum integral representation. The scattered fields are expressed in terms of the Fresnel function. It is shown that the obtained equation gives the Moshinsky function for a one dimensional problem of the plane wave. Also a general integral representation is derived for two dimensional problems. The scattering of matter waves for some special wave-packets are examined analytically and numerically.

Key Words: Edge diffraction, Schrödinger equation, Diffraction in time.

1. Introduction

The scattering of matter waves by a quantum shutter was first investigated by Moshinsky [1]. The problem consists of an aperture in a black screen, which is closed by a shutter. The shutter divides the space into two parts. In the first part the matter waves exist and they are separated from the second volume by the screen. The shutter is opened at time t_0 and the behavior of the transmitted waves to the second region is examined by the solution of the Schrödinger equation. The incident field is considered as a plane wave and the scattered waves are expressed in terms of the Fresnel function. It is put forward that the propagating waves, in the second region, shows interference characteristic, which is the result of diffraction, on the time axis. In a later study, Moshinsky examined the same problem in the context of the time-energy uncertainty relation [2]. Brukner *et al* studied the diffraction of matter waves in space and in time by taking into account more general geometries for the scatterers [3]. They used the Kirchhoff integral, derived as the solution of the Schrödinger equation, for the expression of the scattered waves. The scattering patterns for the single and double slits are studied numerically for finite open times of the shutter. Xiao investigated the scattering of evanescent waves by the quantum shutter by using the solution of Moshinsky in the context of tunneling [4, 5]. Later

Kalbermann studied the diffraction problem for a more general case of the incident wave, which is a Gaussian beam [6]. Godoy investigated the scattering problem of the shutter for Frunhofer and Fresnel regions by using the solution of Moshinsky for the plane wave incidence [7]. He also mentioned the similarity between optics and quantum mechanics.

It is the aim of this study to put forward a general solution of the shutter problem for arbitrary wave-packet incidence. The wave-packet will be expressed as a general solution of the Schrödinger equation by the Fourier integral transform [8]. As a second step, we will solve the quantum shutter problem for this general wave and express the result in terms of the Fresnel integral. The scattered wave will be decomposed into its sub-components, which are the geometrical optics (GO) and diffracted waves [9]. To our knowledge, such an approach does not exist in the literature for the shutter problem. The solution will be examined for plane wave and Gaussian beam incidences, analytically and numerically. Note that the scattered field is the sum of the diffracted and GO waves.

2. Theory

The general solution of the Schrödinger equation, which can be defined as

$$\nabla^2 \psi - j2\frac{k}{v_g}\frac{\partial \psi}{\partial t} = 0 \tag{1}$$

for a free particle, can be given by the equation of

$$\psi(x,t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} A(\alpha)\, e^{j\frac{\alpha^2}{2k}v_g t} e^{-j\alpha x} d\alpha \tag{2}$$

in terms of a one dimensional Fourier transform for a two dimensional case [8]. k and v_g are the wave-number and the group velocity of the particle. ψ is the wave function. Equation (2) represents a general expression of the wave-packets. $A(\alpha)$ is a function of α, in the spectral domain. The scattered wave-packets can be evaluated by using the integral of

$$\psi_s(x,t) = \int_{-\infty}^{\infty} \psi_0(x')\, g(x-x',t)\, dx' \tag{3}$$

where the Green's function of g can be defined as

$$g(x,t) = e^{j\frac{\pi}{4}}\sqrt{\frac{k}{2\pi v_g t}}\, e^{-jk\frac{x^2}{2v_g t}} \tag{4}$$

for $\psi_0(x)$ is the initial value of the wave-function. It can be determined by the equation of

$$\psi_0(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} A(\alpha)\, e^{-j\alpha x} d\alpha \tag{5}$$

which is the inverse Fourier transform of $A(\alpha)$. Now we consider the problem of the quantum shutter, the geometry of which is given in Figure 1. The black screen does not transmit or reflect the incident waves.

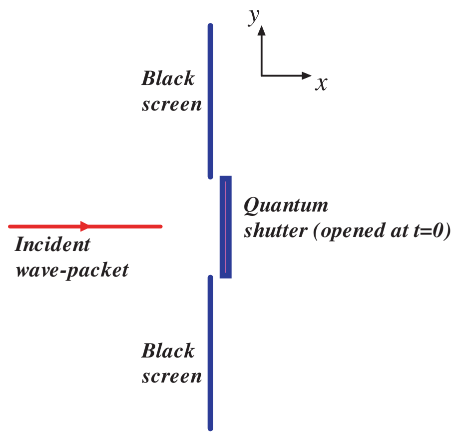

Figure 1. Geometry of the quantum shutter.

The shutter is opened at $t = 0$. The initial condition can be represented as

$$\psi_0(x') = \psi(x', 0)\, U(-x) \tag{6}$$

for $U(x)$ is the unit step function, which is equal to one for x $>$ 0 and zero otherwise [2]. Thus the scattering integral can be written as

$$\psi_s(x,t) = e^{j\frac{\pi}{4}} \sqrt{\frac{k}{2\pi v_g t}} \int_{-\infty}^{0} \psi(x', 0)\, e^{-jk\frac{(x-x')^2}{2v_g t}} dx' \tag{7}$$

which can be further arranged as

$$\psi_s(x,t) = \frac{e^{j\frac{\pi}{4}}}{2\pi} \sqrt{\frac{k}{2\pi v_g t}} \int_{-\infty}^{\infty} A(\alpha) \int_{-\infty}^{0} e^{-j\alpha x'} e^{-jk\frac{(x-x')^2}{2v_g t}} dx' d\alpha \tag{8}$$

by using Equation (5) in Equation (7). The variable transform of

$$x - x' = u \tag{9}$$

can be defined for the x' part of the integral, in Equation (8). Equation (8) reads

$$\psi_s(x,t) = \frac{e^{j\frac{\pi}{4}}}{2\pi} \sqrt{\frac{k}{2\pi v_g t}} \int_{-\infty}^{\infty} A(\alpha)\, e^{-j\alpha x} \int_{x}^{\infty} e^{-j\left(k\frac{u^2}{2v_g t} - \alpha u\right)} du d\alpha \tag{10}$$

when Equation (9) is considered. The integral of

$$\psi_s(x,t) = \frac{e^{j\frac{\pi}{4}}}{2\pi} \sqrt{\frac{k}{2\pi v_g t}} \int_{-\infty}^{\infty} A(\alpha)\, e^{-j\alpha x} e^{j\frac{\alpha^2}{2k} v_g t} \int_{x}^{\infty} e^{-j\left(\sqrt{\frac{k}{2v_g t}} u - \sqrt{\frac{v_g t}{2k}} \alpha\right)^2} du d\alpha \tag{11}$$

can be obtained by adding and subtracting the term of

$$C^2 = \frac{v_g t}{2k}\alpha^2 \tag{12}$$

to the phase function of the integral in Equation (10). Now we will take into account the variable transform of

$$\xi = u\sqrt{\frac{k}{2v_g t}} - \alpha\sqrt{\frac{v_g t}{2k}}. \tag{13}$$

As a result the scattering integral can be written as

$$\psi_s(x,t) = \frac{1}{2\pi}\int\limits_{-\infty}^{\infty} A(\alpha)\, F[\xi_e]\, e^{-j\alpha x} e^{j\frac{\alpha^2}{2k}v_g t} d\alpha, \tag{14}$$

where $F[x]$ is the Fresnel function and can be defined as

$$F[x] = \frac{e^{j\frac{\pi}{4}}}{\sqrt{\pi}}\int\limits_{x}^{\infty} e^{-jt^2} dt. \tag{15}$$

t_e is equal to

$$\xi_e = \sqrt{\frac{k}{2v_g t}}\left(x - \frac{\alpha}{k}v_g t\right). \tag{16}$$

An important property of the Fresnel function, which is used widely in optics and electromagnetics [9], is its decomposition to two sub-functions as

$$F[x] = U(-x) + sign(x)\, F[|x|]. \tag{17}$$

The unit step function, in Equation (17), represents a function with constant amplitude that has a discontinuity at $x = 0$. The second function has a phase shift of 180^0 at $x = 0$ and compensates the discontinuity of the unit step function. Thus the total function is continuous everywhere. The plot of the functions is given in Figure 2. The unit step function represents the GO field which propagates without being affected by the scatterer. The second function is related with the diffracted waves that compensates the discontinuity of the GO field on the transition boundary and is responsible for the field intensity at the shadow region.

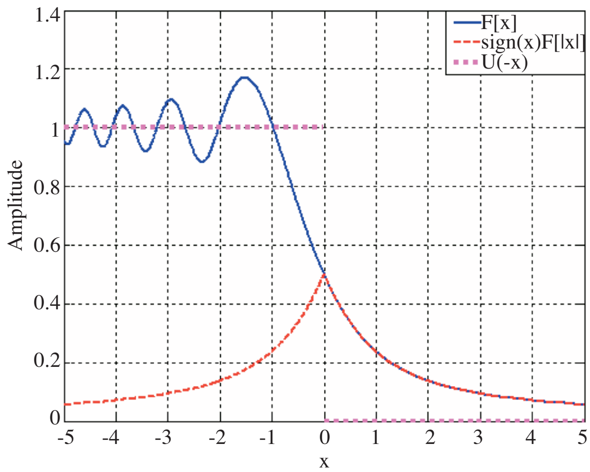

Figure 2. Plot of the Fresnel function and its sub-functions.

The scattered matter wave, given by Equation (14), can be rewritten as

$$\psi_s(x,t) = \psi_{GO}(x,t) + \psi_d(x,t) \tag{18}$$

where $\psi_{GO}(x,t)$ and $\psi_d(x,t)$ are equal to

$$\psi_{GO}(x,t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} A(\alpha)\, U(-\xi_e)\, e^{-j\alpha x} e^{j\frac{\alpha^2}{2k} v_g t} d\alpha \tag{19}$$

and

$$\psi_d(x,t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} A(\alpha)\, sign(\xi_e)\, F[|\xi_e|]\, e^{-j\alpha x} e^{j\frac{\alpha^2}{2k} v_g t} d\alpha \tag{20}$$

respectively. $\psi_{GO}(x,t)$ is the GO wave, which arrives an observation, at the right-hand side of the shutter, after an interval of time t_0. Before t_0, zero field will be observed at the observation point according to Equation (19). $\psi_d(x,t)$ is responsible from the diffraction in time. The existence of the probability wave at the observation point for $0 < t < t_0$ is the result of this component.

An interesting future of Equation (14) is the integrand of the integral. The incident wave is the inverse Fourier transform of

$$\psi_i(x,t) = \Im^{-1}\left[A(\alpha)\, e^{j\frac{\alpha^2}{2k} v_g t}\right], \tag{21}$$

where as the scattered field can be represented as

$$\psi_s(x,t) = \Im^{-1}\left[A(\alpha)\, F[\xi_e]\, e^{j\frac{\alpha^2}{2k} v_g t}\right]. \tag{22}$$

The scattered field can be directly found by multiplying the Fourier transform of the incident field by the Fresnel function.

3. Scattering of Pane Waves

In this section we will examine the problem, solved by Moshinsky [1, 2]. $A(\alpha)$ is equal to

$$A(\alpha) = 2\pi\delta(\alpha - k) \tag{23}$$

for a plane wave. $\delta(x)$ is the Dirac delta function. The incident field reads

$$\psi_i(x,t) = e^{-j\left(x - \frac{v_g}{2}t\right)} \tag{24}$$

when Equation (23) is used in Equation (2). The scattered field is directly found to be

$$\psi_s(x,t) = e^{-jk\left(x - \frac{v_g}{2}t\right)} F[\xi_e] \tag{25}$$

where ξ_e is equal to

$$\xi_e = \sqrt{\frac{k}{2v_g t}}\,(x - v_g t)\,. \tag{26}$$

$\psi_{GO}(x,t)$ and $\psi_d(x,t)$ can be written as

$$\psi_{GO}(x,t) = e^{-jk\left(x - \frac{v_g}{2}t\right)} U(-\xi_e) \tag{27}$$

and

$$\psi_d(x,t) = e^{-jk\left(x - \frac{v_g}{2}t\right)} sign(\xi_e)\, F[|\xi_e|] \tag{28}$$

according to Equations (19) and (20). The plot of the waves is given in Figure 3. x is equal to 6λ for λ is the de Broglie wave-length of the particle. The plane wave arrives x at a time of x/v_g. This portion of the scattered wave is the GO component as can be seen from Figure 3. The amplitude of the GO wave discontinuously increases to one from zero at $t_0 = x/v_g$. This discontinuity is compensated by the existence of the diffracted wave, which is represented by Eq. (28). Thus the total wave is continuous for all values of t at x. The two sub-components of the scattered wave interferes with each other and the total field has an interference characteristic after $t = t_0$. According to Figure 3, there is also a possibility for the particle to be observed at x just after the quantum shutter is opened.

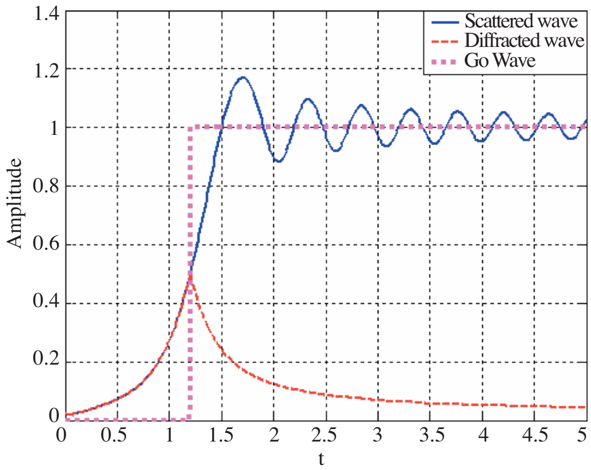

Figure 3. Scattered in time waves for plane wave incidence.

4. Scattering of a Gaussian Wave

The incident wave is a Gaussian wave packet, which can be defined as

$$\psi_i(x,t) = \frac{e^{-jk\frac{x^2}{2(v_g t + jb)}}}{\sqrt{2(v_g t + jb)}} e^{-jk\left(x - \frac{v_g}{2} t\right)} \tag{29}$$

where b is equal to $\pi/4k$ according to the normalization of the wave function. The formula, given in Equation (7), will be used for the evaluation of the scattered fields. The scattered Gaussian wave can be written by the integral of

$$\psi_s(x,t) = \sqrt{\frac{k}{4\pi b v_g t}} \int_{-\infty}^{0} e^{-k\frac{(x')^2}{2b}} e^{-jkx'} e^{-jk\frac{(x-x')^2}{2v_g t}} dx' \tag{30}$$

according to Equation (7). Equation (30) can be rewritten as

$$\psi_s(x,t) = \sqrt{\frac{k}{4\pi b v_g t}} \int_{0}^{\infty} e^{-k\frac{(x')^2}{2b}} e^{jkx'} e^{-jk\frac{(x+x')^2}{2v_g t}} dx' \tag{31}$$

by putting $-x'$ instead of x'. Equation (31) yields the expression of

$$\psi_s(x,t) = \sqrt{\frac{k}{4\pi b v_g t}} e^{-jk\frac{x^2}{2v_g t}} e^{jk\frac{b}{2}\frac{(x-v_g t)^2}{v_g t(b-jv_g t)}} \int_{0}^{\infty} e^{-jkg(x')} dx' \tag{32}$$

when the term of

$$C^2 = \frac{b}{2}\frac{(x-v_g t)^2}{v_g t(b-jv_g t)} \tag{33}$$

is added and subtracted to the phase function. $g(x')$ is equal to

$$g(x') = \left[x'\sqrt{\frac{b-jv_g t}{2v_g t b}} + \sqrt{\frac{b}{2}}\frac{x-v_g t}{\sqrt{v_g t(b-jv_g t)}}\right]^2. \tag{34}$$

We will define the variable transform of

$$\xi = x'\sqrt{\frac{b-jv_g t}{2v_g t b}} + \sqrt{\frac{b}{2}}\frac{x-v_g t}{\sqrt{v_g t(b-jv_g t)}} \tag{35}$$

as the next step. The scattered wave is found to be

$$\psi_s(x,t) = \frac{e^{-jk\frac{x^2}{2(v_g t + jb)}}}{\sqrt{2(v_g t + jb)}} e^{-jk\left(x - \frac{v_g}{2} t\right)} F[\xi_e] \tag{36}$$

for ξ_e is equal to

$$\xi_e = \sqrt{\frac{b}{2}} \frac{x - v_g t}{\sqrt{v_g t \left(b - j v_g t\right)}}. \tag{37}$$

The Fresnel function, in Equation (36), can not be separated to its sub-components directly as in Equation (17) since the argument of the function is complex in this case. Instead we will use the method, introduced in Reference [9]. A Fresnel function can be decomposed as

$$F\left[z\right] = U\left(y - x\right) + sign\left(x - y\right) F\left[\left|x - y\right| + sign\left(x - y\right)\sqrt{2} y e^{j\frac{\pi}{4}}\right] \tag{38}$$

where z is a complex function, which is equal to $x + jy$. Thus the time scattered wave function can be rewritten as

$$\psi_s\left(x,t\right) = \psi_{GO}\left(x,t\right) + \psi_d\left(x,t\right) \tag{39}$$

where $\psi_{GO}\left(x,t\right)$ and $\psi_d\left(x,t\right)$ are equal to

$$\psi_{GO}\left(x,t\right) = \frac{e^{-jk\frac{x^2}{2\left(v_g t + jb\right)}}}{\sqrt{2\left(v_g t + jb\right)}} e^{-jk\left(x - \frac{v_g}{2}t\right)} U\left[\zeta - \eta\right] \tag{40}$$

and

$$\psi_s\left(x,t\right) = \frac{e^{-jk\frac{x^2}{2\left(v_g t + jb\right)}}}{\sqrt{2\left(v_g t + jb\right)}} e^{-jk\left(x - \frac{v_g}{2}t\right)} sign\left[\eta - \zeta\right] F\left[\left|\eta - \zeta\right| + sign\left(\eta - \zeta\right)\sqrt{2}\zeta e^{j\frac{\pi}{4}}\right] \tag{41}$$

respectively. η and ζ represent the real and imaginary parts of ξ_e.

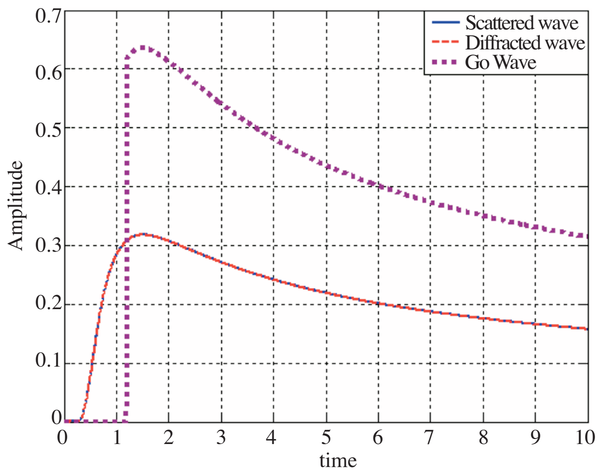

Figure 4. Scattered waves for a Gaussian beam.

Figure 4 shows the variation of the scattered waves versus time. The observation point is at 6λ. The GO wave increases discontinuously from zero to 0.6 at $t = 1.2$. This behavior is normal since the field arrives at the point of observation with a delay according to its velocity. The interesting feature of the plot is the structures of the diffracted and scattered waves. They have the same plot, which is rather different from that of a plane wave. The diffracted wave has a shift of 180^0 at the transition boundary. Its amplitude has an opposite sign with the amplitude of the GO wave. For this reason the amplitude of the total field (scattered wave) decreases. For this reason the diffracted and scattered waves have the same plot.

5. Conclusion

In this study the scattering in time of matter waves is investigated by expressing the Fourier transform of the wave function in terms of the Fresnel integral. The decomposition property of the Fresnel functions to its sub-components enabled us to express the scattered waves in terms of the interpretation of Young [11]. He proposed that the scattered field by an edge is composed of two sub-fields, which are the edge diffracted wave and the GO field. It is observed that this interpretation also holds for the scattering of matter waves. The transition region of the scattered wave is the arrival time of the GO wave to the observation point. The scattering of plane and Gaussian were beams also investigated analytically and numerically.

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