Diffraction in time: Fraunhofer and Fresnel dispersion by a slit

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Moshinsky's work on diffraction in time is recognized as a particular case of monoenergetic, quantum dispersion process. Diffraction in time is extended to include new initial conditions, which under free evolution exhibit temporal quantum interference patterns in close analogy to spatial diffraction patterns found in optics. We show that free propagation of states, which initially are stationary states of infinite potential wells, diffract in time similarly as a plane wave by a double slit. We introduce the concepts of mass transport by transient Fraunhofer and Fresnel dispersion currents.

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I. DIFFRACTION IN TIME

Similarities between optics and quantum mechanics have long been recognized [1]. In particular, time evolution of the quantum wave function $\psi(\mathbf{r},t)$ may be written in an analogous way to Huygens' principle in optics. This approach, called the Lagrangian formulation of quantum mechanics [2], proves that we can always find a Green's function $G(\mathbf{r},t;\mathbf{r}',t')$ such that for $t>t'$,

$$\psi(\mathbf{r},t)=\int d\mathbf{r}'\,G(\mathbf{r},t;\mathbf{r}',t')\,\psi(\mathbf{r}',t'). \tag{1}$$

One example of this equation is the three-dimensional (3D) time evolution of a free particle [3]

$$\psi(\mathbf{r},t)=\left[\frac{m}{2\pi i\hbar(t-t')}\right]^{3/2}\times\int d\mathbf{r}'\exp\left[\frac{im}{2\hbar}\,\frac{(\mathbf{r}-\mathbf{r}')^2}{t-t'}\right]\psi(\mathbf{r}',t'). \tag{2}$$

On the other hand, in the theory of image formation in optics, using the Fresnel-Kirchoff equation for light propagating in the direction of the $+z$ axis, if we know the monochromatic electric field $E(x',y',z')$ in an arbitrary z' plane, considered to be the source of Huygens wavelets, then the field in an arbitrary z plane is given by

$$E(x,y,z)=\frac{ie^{-ik(z-z')}}{\lambda(z-z')}\int\int dx'dy'\times\exp\left\{\frac{-ik}{2}\,\frac{[(x-x')^2+(y-y')^2]}{z-z'}\right\}\times E(x',y',z'). \tag{3}$$

In optics Eq. (3) is called a *Fresnel transformation* [4]. Comparing Eqs. (2) and (3) it is clear that quantum free propagation can also be considered a Fresnel transformation, with one important distinction: the quantum transformation is in *time*, not in space. It is not surprising then that some optical results in space coordinates are similarly obtained in quantum mechanics in the *time domain*.

One clear example of this symmetry was obtained a long time ago by Moshinsky [5], who addressed the following quantum one-dimensional (1D) shutter problem: consider a monoenergetic beam of free particles, $\varepsilon=p^2/2m$, moving parallel to the x axis. For negative times, the beam is interrupted at $x=0$ by a perfectly absorbing shutter perpendicular to the beam. Suddenly, at time $t=0$, the shutter is opened, allowing for $t>0$ the free time evolution of the beam of particles. What is the transient density observed at a distance x from the shutter? The problem implies the following initial condition:

$$\psi(x,0)=\exp(ipx/\hbar)\quad\text{for}\quad x\leqslant 0$$
$$=0\quad\text{for}\quad x>0. \tag{4}$$

Moshinsky proved that the free propagation of the beam had an exact, analytic solution. For $t>0$, the wave function becomes $\psi(x,t)\equiv M(x,t)$, where

$$M(x,t)=\frac{e^{-i\pi/4}}{\sqrt{2}}e^{(i/\hbar)(px-\varepsilon t)}\left[\left\{C(\xi(x,t))+\frac{1}{2}\right\}+i\left\{S(\xi(x,t))+\frac{1}{2}\right\}\right]. \tag{5}$$

$C(\xi)$ and $S(\xi)$ denote the real and imaginary parts of the complex Fresnel integral, $C(\xi)+iS(\xi)\equiv\int_0^{\xi}\exp(i\pi u^2/2)du$, and the Fresnel integral's argument ξ is a function of position and time

$$\xi(x,t)\equiv\sqrt{\frac{m}{\pi\hbar t}}\left(\frac{p}{m}t-x\right). \tag{6}$$

The function $M(x,t)$ has been called Moshinsky's function by Nussenzveigh [6,7] and other authors, and it has had many applications [8–12].

For the beam in the shutter problem, the probability density is then

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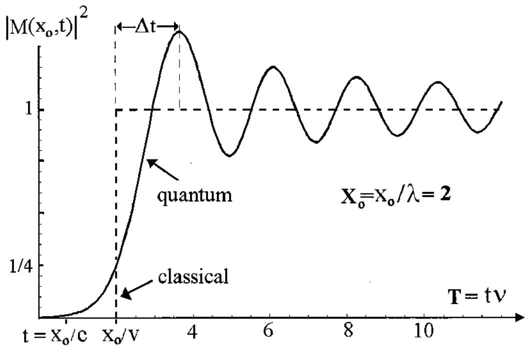

FIG. 1. Moshinsky's quantum diffraction in time. $X\equiv x/\lambda$ and $T\equiv t\nu$ are dimensionless quantities. Observation point $X_0=2$.

$$|M(x,t)|^2=\frac{1}{2}\left\{C(\xi(x,t))+\frac{1}{2}\right\}^2+\frac{1}{2}\left\{S(\xi(x,t))+\frac{1}{2}\right\}^2. \qquad (7)$$

This result is similar to the expression for the intensity of light in the Fresnel diffraction by an infinite straight edge in optics [13]. To plot Eq. (7) we define dimensionless quantities: $X\equiv x/\lambda = xp/2\pi\hbar$ and $T\equiv t\nu = t\varepsilon/2\pi\hbar$, such that the Fresnel argument in Eq. (6) becomes $\xi(X,T)=2\sqrt{T}-X/\sqrt{T}$. For a fixed position x_0, the plot of the probability density $|M(x_0,t)|^2$ as a function of time is shown in Fig. 1. For this peculiar time evolution, Moshinsky coined the name "diffraction in time." Discontinuity of the plane wave in the initial condition in Eq. (4) is the source of the analogy with Fresnel diffraction by a straight edge in optics. We stress the fact that diffraction in time is only similar to the optical one, for in optics the Fresnel integral's argument is linear in the distance to the edge, while in quantum theory the argument is nonlinear in time: $\xi\sim\sqrt{t}-1/\sqrt{t}$. Clearly, in Eq. (6) there is a singular point at $t=0$, and for very short times the similarity breaks down completely. Even worst, from Fig. 1 we see that for $x_0>0$ quantum theory predicts a density different from zero for times $0<t\leqslant x_0/c$, where c is the speed of light. Obviously this is an unphysical result. The nonrelativistic character of the Schrödinger's equation is the cause of this erroneous prediction. So for very short times, all time-dependent Schrödinger's results have to be disregarded. For $x_0/c<t<x_0/v$ instead of a front wave, as in the classical ballistic motion, we have a monotonous increasing behavior of the density. This is an expected consequence of the parabolic Schrödinger's equation. As for the Fresnel oscillations, the consequences are far reaching. For instance, at an arbitrary fixed position $(x_0>0)$, quantum theory predicts that the intensity of particles reaches its maximum value at a time Δt later than the classical "flight time" x_0/v. The delay Δt is of the order of $(\pi\hbar x_0/v^3)^{1/2}$ which for thermal neutrons with $v=2200$ m/s and $x_0=1$ m is of the order of 10^{-6} sec. The difficult experimental evidence of this quantum prediction has been confirmed until very recently by Szriftigiser *et al.* [14].

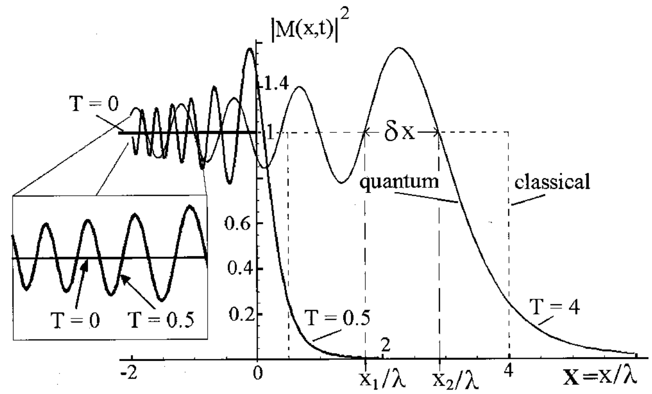

FIG. 2. Fresnel dispersion by an infinite straight edge. $X=x\nu$ and $T=t/\lambda$ are dimensionless variables. Inset: shows how the probabilty's oscillations cause compression and expansion density zones.

II. FRESNEL CURRENTS BY A STRAIGHT EDGE

The free particle time-evolution propagator $G(x,t;x',t')$ in Eq. (2) is dispersive. For any initial wave packet with finite size, $(\Delta x_0)^2\equiv\langle x^2\rangle_0-\langle x\rangle_0^2=$finite, the free spreading in space as a function of time is unavoidable, $(\Delta x)^2=(\Delta p_0 t/m)^2+(\Delta x_0)^2$. After a sufficiently long time, $(\Delta x)^2$ becomes as large as desired; the free wave packet spreads in space indefinitely, leading toward uniformity. This dispersion mechanism provides a means by which mass is microtransported in space. In fact, even if the center of the wave packet is at rest $\langle p\rangle=0$, dispersion induces a mass probability current in space $j(x,t)$. And what is more important, under appropriate initial conditions, the time evolution of the packet can generate intense transient probability currents. One particular example of this is the diffraction in time process given in Eq. (5). Its exact probability current is given by

$$j(x,t)=\frac{p}{m}|M(x,t)|^2+\left(\frac{\hbar}{4\pi mt}\right)^{1/2}\times\left[[S(\xi(x,t))+\tfrac{1}{2}]\cos\left(\frac{\pi}{2}\xi^2\right)-\left(C(\xi(x,t))+\frac{1}{2}\right)\sin\left(\frac{\pi}{2}\xi^2\right)\right]. \qquad (8)$$

The total current becomes the superposition of a convective and a dispersive currents.

The convective current

$$j_{con}(x,t)\equiv\frac{p}{m}|M(x,t)|^2, \qquad (9)$$

occurs only because the wave function $M(x,t)$ has a well-defined momentum, and the center $\langle x\rangle$ of the packet moves. For a fixed time t_0, since $\xi(x,t_0)\sim -x$, then $j_{con}(x,t_0)$ has in space a similar (but inverted) Fresnel diffraction pattern as $|M(x_0,t)|^2$ has in time. In Fig. 2 we show at different fixed times, $t_0\nu=(0,0.5,4)$, the quantum free evolution of density $|M(x,t_0)|^2$ plotted against coordinates x. We call this particular probability current density a Fresnel convective current by a straight edge. Notice from Fig. 2 that for short times, the Fresnel convective current has very strong transient fluctuations ($\sim 50\%$) about the initial value. A good measure of the "width" of this Fresnel convective current in position can be obtained from the difference between the first two positions at which $|M(x,t_0)|^2$ takes the classical value 1, i.e., $\delta x \equiv x_2 - x_1$, as shown in Fig. 2. The two positions at which the curve $|M(x,t_0)|^2$ of Fig. 2 intersects with the straight line 1 correspond to the values of ξ_1 and ξ_2 that can be obtained from the Cornu spiral [15], giving $\delta\xi \equiv \xi_2 - \xi_1 = 0.85$. For fixed time t_0 in Eq. (6) we have for neutrons ($m = 1.67\times 10^{-24}$ g),

$$\delta x = (\delta\xi)^2 \left(\frac{\pi\hbar\, t_0}{m}\right)^{1/2} = 3.2\times 10^{-2} t_0^{1/2}\ \mathrm{cm\,s}^{-1/2}, \quad (10)$$

which shows that the oscillations spread without bound in time. For neutrons, Fresnel convective current's space oscillations, after 1 s, give a spread of $\sim 10^{-2}$ cm. This is easier to measure than the Fresnel oscillations in time (10^{-6} s for $x_0 = 1$ m).

Notice that the Moshinsky's wave function given in Eq. (5) is a valid solution for $-\infty \leqslant x \leqslant +\infty$. This is a remarkable result because it implies that for any fixed positive time $t_0 > 0$ no matter how small, the very fact of a sudden removal of an absorbing wall at $x=0$, causes the initial constant probability density in space $|e^{ikx}|^2 = 1$ to be replaced by Fresnel's oscillations $|M(x,t_0)|^2$ all the way from $x=0$ down to $x = -\infty$ (a violation of relativity theory). Since the probability density oscillates up and down about the initial constant value, the oscillations's maxima and minima correspond to compressions and expansions of the initial density. In this sense, the whole negative space becomes interlaced with bunching and antibunching probability density zones. The amplitude of these oscillations decrease monotonically as we move back into negative x's. For big enough negative x's, bunching and antibunching zones become indistinguishable, giving eventually the appearance again of a uniform density.

Figure 2 shows how, as time develops, the density's compressions and expansions regions disperse in the forward direction. An observer fixed in space, let say at $x_0 = 2\lambda$, describes the temporal changes of probability density passing through his position as $|M(x_0,t)|^2$. This temporal change is precisely the one plotted in Fig. 1 and recognized as Fresnel diffraction in time by a straight edge. The observer describes the successive regions of probability density's compression and expansion passing him by, as Fresnel diffraction in time.

The dispersive current

$$j_{disp}(x,t) \equiv \left(\frac{\hbar}{4\pi m t}\right)^{1/2} \left[\left(S(\xi)+\frac{1}{2}\right)\cos\left(\frac{\pi}{2}\xi^2\right) - \left(C(\xi)+\frac{1}{2}\right)\sin\left(\frac{\pi}{2}\xi^2\right)\right], \quad (11)$$

which is independent of $\langle p\rangle$ is a pure transient dispersive current (the current goes to zero as $t^{-1/2}$). For a fixed time, for all negative x's, the current oscillates about the zero value, giving zones of positive and negative currents in space. The oscillating positive and negative currents are consequence of the interlaced compressions and expansion density zones in space. The current moves from any compression zone toward the adjacent right and left expansion zones. This explains the dispersive current's oscillations. For long times since $j_{disp}(x,t) \to 0$, the transport of mass, by diffraction in time, is effective only as a convective transport process $j_{con}(x,t)$.

We obtained the optical Fresnel diffraction pattern only because the initial wave function gives the same mathematical condition for diffraction by an infinite straight edge in optics, i.e., discontinuity of a monochromatic plane wave. However, it must be clear that other discontinuous, monoenergetic wave functions with different boundaries can be considered as initial conditions. If in free propagation we do so, due to the discontinuity and monochromaticity, quantum mechanics may have solutions with similar diffraction patterns as those found in optics.

The purpose of the present work is to search for new quantum monoenergetic dispersive processes that show corresponding diffraction patterns in optics. Next, we show an example of free time evolution leading to Fraunhofer and Fresnel diffraction patterns by a slit.

III. DIFFRACTION IN TIME FOR INITIALLY STATIONARY STATES

The previous 1D shutter problem had no restriction on the width of the initial wave function; consequently, the momentum (and energy) could have any value. Most of the time, however, we want to consider free time evolution of monoenergetic particles which, in agreement with the uncertainty principle, have some initial finite width in space. Next we show how diffraction in time considers a time-evolution process of this kind.

Let us consider the 1D stationary states of a free particle that is restrained by impenetrable, reflecting walls at the points $x=0$ and $x=a$. For simplicity, we consider an infinite square-well potential such that $V(x)=0$ for $(0<x<a)$ and $V(x)=+\infty$ for $(0<x$ and $x>a)$. The stationary wave functions are given by

$$\varphi_n(x) = [\exp(ik_n x) - \exp(-ik_n x)]/\sqrt{2ai^2} \quad \text{for} \quad 0 \leqslant x \leqslant a$$
$$= 0 \quad \text{for} \quad x<0 \ \text{and}\ a<x, \quad (12)$$

with $k_n \equiv n\pi/a$, $(n=1,2,3,\ldots)$.

Now, following Moshinsky, we address the following problem: if at time $t=0$ the above reflecting walls are suddenly removed, allowing for positive times the free propagation of the particle initially described by the wave function $\varphi_n(x)$. What is the transient density observed at a distance $x>a$ (or $x<0$)?

Clearly from Eq. (12) the stationary wave function $\varphi_n(x)$ is a superposition of two monochromatic, discontinuous, opposite-moving plane waves. Since each plane wave has a double discontinuity (at $x=0$ and $x=a$), we expect that each plane wave will contribute a double Fresnel diffraction in time. Indeed, next we will show that each individual discontinuous plane wave will have a free time evolution, giving a probability density equivalent to an optical diffraction pattern by a slit of width *a*. After substituting the initial condition $\psi_n(x,0)=\varphi_n(x)$ into the 1D version of Eq. (2), we get

$$\psi_n(x,t)=\left[\frac{m}{2\pi i\hbar t}\right]^{1/2}\int_0^a dx'\exp\left[\frac{im}{2\hbar}\frac{(x-x')^2}{t}\right]\varphi_n(x'). \tag{13}$$

The integral is straightforward, and we get for the exact free time evolution a superposition of a right- and left-moving diffracted in time plane waves

$$\psi_n(x,t)=\psi_{n,+}(x,t)+\psi_{n,-}(x,t). \tag{14}$$

Here, each function $\psi_{n,+}(x,t)$ and $\psi_{n,-}(x,t)$ denotes a diffraction in the time process

$$\psi_{n,+}(x,t)\equiv\frac{1}{(4i^3a)^{1/2}}[F_n(t,x-a)-F_n(t,x)]\times e^{(i/\hbar)(p_nx-\varepsilon_nt)}, \tag{15}$$

$$\psi_{n,-}(x,t)\equiv\frac{1}{(4i^3a)^{1/2}}[F_n(t,a-x)-F_n(t,-x)]\times e^{(i/\hbar)(-p_nx-\varepsilon_nt)}, \tag{16}$$

where $F_n(t,x)$ is the complex Fresnel integral given by

$$F_n(t,x)\equiv\int_0^{\xi_n(x,t)}\exp(i\pi u^2/2)du, \tag{17}$$

with the Fresnel's upper limit $\xi_n(x,t)$, depending on the quantum number *n*, given by

$$\xi_n(t,x)\equiv\sqrt{\frac{m}{\pi\hbar t}}\left(\frac{\hbar k_n}{m}t-x\right). \tag{18}$$

Hence, the total probability density becomes a coherent superposition of two processes,

$$|\psi_n(x,t)|^2=\frac{1}{4a}|\exp(ik_nx)[F_n(t,x-a)-F_n(t,x)]+\exp(-ik_nx)[F_n(t,a-x)-F_n(t,-x)]|^2. \tag{19}$$

To understand this total density, consider the right-moving wave contribution $\psi_{n,+}(x,t)$ alone. We have

$$|\psi_{n,+}(x,t)|^2=\frac{1}{4a}|F_n(t,x-a)-F_n(t,x)|^2, \tag{20}$$

which is identical in optics to the expression for the intensity of light in the Fresnel diffraction by a slit of width *a* [13]. We have in Eq. (20) the superposition of two Fresnel amplitudes generated by the corresponding edges of the slit. Two limit cases are important: diffraction by a narrow and by a wide slit.

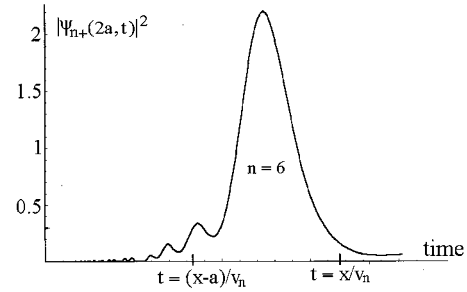

FIG. 3. Fraunhofer diffraction in time by a narrow slit for state $n=6$. Observation point $x=2a$.

(1) Diffraction in a narrow slit occurs when $a\sim\lambda_n$ or $n\sim2$. This happens for particles in the ground- and low-energy excited states. Both Fresnel functions $F_n(t,x-a)$ and $F_n(t,x)$ are separated in space by a distance *a*, and if $a\sim\lambda_n$, then each Fresnel function superpose each other with only a few oscillations of low frequency in the same space interval *a*. In this case, the superposition of the two Fresnel functions induce very strong interference effects. This strong-interference limit gives a diffraction in time pattern which in optics is called *Fraunhofer* diffraction by a slit. See Fig. 3 for an exact quantum diffracting in time case.

(2) On the other hand, diffraction in a wide slit occurs when $a\gg\lambda_n$ or $n\gg2$. This happens for particles in high-energy excited states. Now, in the space interval *a*, both Fresnel functions superpose each other with many high-frequency oscillations. Approximately, each Fresnel function is interfered by the asymptotic contribution, $(1+i)/2$, from the other. We have here a weak interference pattern, which in optics is called *Fresnel* diffraction by a slit; in this case a fixed observer detects diffraction in time of two, approximately independent, straight-edge Fresnel patterns, that is, two Moshinsky solutions. See Fig. 4 for the exact quantum case.

Clearly, as the quantum number *n* goes from 1 to ∞, the diffraction pattern by a slit evolves continuously from Fraunhofer to Fresnel, with all possible intermediate cases in between.

IV. YOUNG DISPERSION

For an arbitrary size *a* of the potential well, the exact quantum monoenergetic free time evolution of any initial

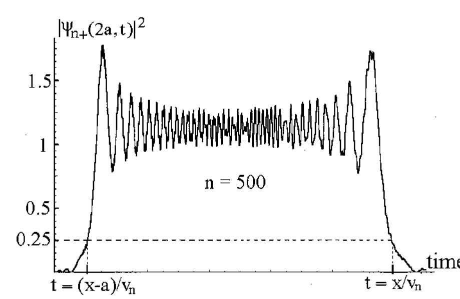

FIG. 4. Fresnel diffraction in time by a wide slit for state $n=500$. Observation point $x=2a$.

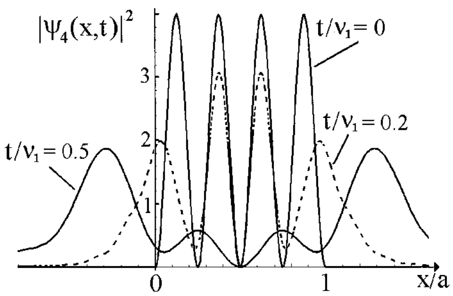

FIG. 5. Young dispersion for state $n=4$. x/a and $t\nu_1$ are dimensionless variables. $\nu_1=\pi\hbar/(4ma^2)$ is the zero point frequency.

stationary wave function $\varphi_n(x)$ is, according to Eq. (19), a coherent superposition of two opposite moving single-slits diffraction amplitudes. The equivalent optical diffraction pattern corresponds, approximately, to having two identical slits facing each other and having a light detector in the middle. In this sense, since we have the interference of two slits, the quantum dispersion pattern resembles roughly a Young interference experiment. We call the diffraction in time pattern given by Eq. (19) a Young dispersion process. In Fig. 5 we show the time evolution of this dispersive process for $n=4$. Since the present process has zero momentum, $\langle p\rangle=0$, the mass transport is not convective but a pure dispersive process, just what we wanted to show.

V. CONCLUSION

Finally, let us consider an initial wave packet $\psi(x,0)$ such that (i) it has an arbitrary shape for $0<x<a$, (ii) $\psi(x,0)=0$ for $x\leqslant 0$ and $x\geqslant a$, and (iii) it has an initial zero mean momentum, $\langle p\rangle_0=0$. Under free time evolution, since the wave packet $\psi(x,t)$ has its center $\langle x\rangle$ at rest, we expect from $\psi(x,t)$ to have a pure dispersive mass transport. Indeed, since the stationary wave functions $\varphi_n(x)$ given in Eq. (12) form a complete set of orthonormal eigenfunctions in the range $(0\leqslant x\leqslant a)$, and they also have a zero mean momentum, we can expand the initial wave packet in terms of the eigenfunctions

$$\psi(x,0)=\sum_{n=0}^{\infty} a_n\varphi_n(x), \tag{21}$$

where $a_n=\int_0^a\varphi_n^*(x)\psi(x,0)dx$. Now, we have already proved that under free time evolution, the eigenfunctions $\varphi_n(x)$ develop in time into a pure dispersive process; therefore, $\psi(x,0)$ will also develop into a pure dispersive mass transport process. In fact, according to Eq. (21), the free time evolution of $\psi(x,0)$ is obtained from the corresponding time evolution of $\varphi_n(x)$, already given in Eq. (14)

$$\psi(x,t)=\sum_{n=0}^{\infty} a_n\psi_n(x,t)$$

$$=\sum_{n=0}^{\infty} a_n[\psi_{n,+}(x,t)+\psi_{n,-}(x,t)]. \tag{22}$$

Here, we see how the arbitrary wave packet develops in time according to a coherent superposition of diffraction in time functions $\psi_{n,\pm}(x,t)$. The time-dependent probability density $|\psi(x,t)|^2$ is a complicated linear combination of Fresnel or Fraunhofer dispersions by a slit $|\psi_{n,\pm}|^2$, and the corresponding interferences amplitudes $\psi_{n,\pm}\psi^*_{n',\pm}$. The final density usually has no resemblance at all with any optical diffraction pattern. It becomes clear that diffraction in time functions $\psi_{n,\pm}(x,t)$ may play an important role in the description of some dispersive mass transport processes.

The classical transport theory (Boltzmann equation), which explains the mass transport at incoherent ballistic regimes (classical mesoscopic), misses completely the description of transport having microscopic times and quantum interference. Since diffraction in time describes a microscopic mass transport, with fast transient density currents and strong quantum interference, this quantum transport phenomenon should be added, as a theoretical complement, to the classical transport theory [16].

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