ON THE (NON)EXISTENCE OF QUANTUM PARTICLES’ TRAJECTORIES BEHIND AN INTERFEROMETRIC GRATING

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Abstract

Single particle interference experiments have documented the existence of trajectory of particles’ during the accumulation of an interference pattern. The expression for probability of particle’s arrivals to the screen was derived previously [22] by approximating the trajectories with straight lines, which start at various points of the slits, and using wave function of the transverse motion in the momentum representation. We use this expression to determine particle distribution at various distances along the lines parallel to a multiple slit grating. The agreement with usual probability density given by the modulus square of the wave function in coordinate representation is very good in the far field. In the near field the agreement is poor. This result supports the view that the trajectories of the particles do exist and that they are straight lines in the far fields, but further study on the form of the trajectories of particles’ in the near field is necessary.
1 Introduction

The flourishing of new techniques and ideas in quantum interferometry with photons, electrons, neutrons, atoms and molecules have caused an essential revision of argumentation in the controversies about foundations of quantum mechanics: i) non-reality versus objective reality of matter and photon waves, ii) complementarity versus compatibility of particle and wave properties of quantons, iii) completeness versus incompleteness of quantum mechanics, iv) non-existence versus existence of particle’s trajectories in an interferometer.

In Section 2 we review shortly the history of these controversies, and recent conclusions drawn from small $N$ interference experiments. We then apply new form of stationary solutions of the Schrödinger equation for a particle behind a grating (Sections 3,4,5) to describe quantum interference as a process of accumulation of many individual events – particles’ moving along the trajectories and arrivals to the screen (Section 6).

In this way we are accomplishing the task that Barut assigned [1] to theoretical physicists by writing: “It now becomes a task of theoretical physics to build models and theories of single events, and a task of experimental physics to record more of single events.”

2 Conclusions from interference experiments with small number $N$ of particles

Before the appearance of interference experiments with a small number $N$ of particles, Bohr’s principle of complementarity, claiming incompatibility of particle and wave aspects of quantum objects in the same experiment, was widely, although not unanimously, accepted. Bohr argued that this principle “allows us to escape from the paradoxical necessity of concluding that the behaviour of an electron or a photon should depend on the presence of a slit in the diaphragm through which it could be proved not to pass” [2]. For de Broglie, the dependence of the behaviour of particles on their environment (boundary conditions) was not paradoxical. Taking this nonclassical behaviour as a fact of nature, de Broglie [3] explained it by concluding that with a material particle is associated a matter wave.
In the new generation of interference experiments with beams of one per one particle, the particle aspect has been demonstrated, in addition to the wave aspect. Time evolution of the electron [4] and photon interference pattern [5, 6, 7], the measurement of the time of arrival of particles to the detector [8], the sizes of particles larger than their de Broglie wavelengths [9], the sizes of particles approaching the widths of the slits [10], are essential features of recent electron, neutron, atomic and molecular interference experiments.

From experiments involving atoms Cohen-Tannoudji [11] concludes: “The impact of the atoms on a detection plate is then observed giving a clear evidence of the wave-particle duality. Each atom gives rise to a localized impact on the detection plate. This is the particle aspect. But, at the same time, the spatial distribution of the impacts is not uniform (see Fig. 1 in [3]). It exhibits dark and bright fringes that are nothing but the Young fringes of the de Broglie waves associated with the atoms. Each atom is therefore at the same time a particle and a wave, the wave allowing one to get the probability to observe the particle at a given place.”

An important feature of quantum mechanics, namely the wave particle duality, can be shown in the Young’s double slit experiment for a single photon [5, 7] that is emphasized in the citation [5]. “The interference pattern which is observed at a screen placed behind two narrow slits is a proof that light can be described as an electromagnetic wave. But as the intensity of the incident light is lowered so that only one photon at the time strikes the screen, only localized impacts of individual photons are observed. After a long exposure time an interference pattern, build up from these localized impacts, slowly appears again. From this phenomena, one concludes that light behaves simultaneously like a wave and like particles.”

The results of these experiments strongly support Born’s [12], Einstein’s [13] and Barut’s [1] view on the necessity to complete quantum mechanics: “Born [12] in his first paper on the statistical interpretation of quantum mechanics has already emphasized the problematic situation between a single event and the probabilistic statements in repeated events. Einstein [13] repeatedly argued for the incompleteness of quantum mechanics because it did not describe single events. If the standard interpretation of quantum theory can only make predictions about repeated events, any assumption, tacit or explicit,
that we make on how a single event behaves or looks, must go beyond quantum mechanics,” wrote Barut [1]. He then continued by underlining [14–16] that quantum mechanics describes only the regularities of the interference pattern when enough dots (events) are collected. It does not explain the appearance of single dots on the screen in the Young experiment, neither it explains the patterns for small $N$ (stopped experiments, as Barut liked to say) [17].

Božić [18] applied Barut’s type of argumentation to oppose the conclusion of Badurek, Rauch and Tuppinger [19] about the equivalence of two interpretations of quantum beats in the double-resonance neutron experiment. One is based on de Broglie-Einstein description of quantum objects (quantons), where they are represented by waves and real particle aspect simultaneously. The other is due to Bohr and Heisenberg, where micro-objects correspond to probabilistic $\Psi(\vec{r},t)$ waves or observed particles, never the two simultaneously. Božić opposes their conclusion by: “It is true that the predictions of oscillations in intensity for large $N$ are the same in both interpretations. But what about experiments with small $N$? Quantum mechanics of Bohr and Heisenberg does not explain the patterns for small $N$, nor the time dependence of intensity which Badurek, Rauch and Tuppinger would plot if they would stop the experiment when the number of neutrons is small” [18]. Recently, the “stopping” of the analogous experiment with photons was done [6]. Measurements of the number of photons at the exit of Mach Zender interferometer as a function of phase difference, for various values of the total number of photons [6], definitely show that “in the standard quantum mechanics there is no theoretical curve to be compared with the results of small $N$ interference experiments,” as Barut emphasized many times [14, 16].

3 Wave function of a particle behind an $n$-slit grating

Clauser [20] noted that given the many discussions on the Young’s interference experiment, it was surprising that even the one-slit problem in quantum theory had not been provided with a rigorous solution. We agree with Clauser that the rigorous solution of the Schrödinger equation for one-slit and many-slits problem is an important task that is right at the heart of both, the measurement
problem and the conceptual foundations of quantum theory. In our previous papers we determined a new form of a rigorous solution of the Schrödinger equation for a particle behind a grating [22–24]. We then applied this solution in order to understand quantum interference as a recoil effect and to explain the process of accumulation of single events in a double slit experiment [22]. In this paper we shall apply this general form of a solution to a grating with larger number of slits ($n=40$, for example).

We consider a multiple slit grating situated in the $xz$ plane at $y=0$ and assume that the initial monochromatic matter wave of wave number $k = 2\pi/\lambda$ is spreading along $y$ axis from the source point $P_0 = (0, y_0, 0)$, which is very far from the grating. The initial stationary monochromatic wave

$$\Psi(x, y, z, t) = e^{-i\omega t} \psi_i(x, y, z) = Be^{-i\omega t}e^{iky} \quad y < 0 \quad (1)$$

satisfies the free particle Schrödinger’s equation and the corresponding Helmholtz equation for $y < 0$. $B$ is a constant and $\hbar \omega = \hbar^2 k^2 / 2m$.

At the right hand side of the grating we have to find the solution $\varphi(x, y, z)$ of the Helmholtz equation that satisfies the boundary conditions at the grating. The latter function is the coordinate part of the stationary solution $\Psi(x, y, z, t) = e^{-i\omega t} \varphi(x, y, z)$ of the Schrödinger equation. We derive the solution in two steps. At first, we find by direct substitution that the following function satisfies the Helmholtz equation for any values of $x, y, z$

$$\varphi(x, y, z) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} dk_x \int_{-\infty}^{+\infty} dk_z c(k_x, k_z)e^{ik_xx}e^{ik_zz}e^{iy\sqrt{k_x^2 - k_z^2 - k_x^2}} \quad (2)$$

where the function $c(k_x, k_z)$ is assumed to have non negligible values only for $k^2 \gg k_x^2 + k_z^2$. This implies that to a very good approximation $\varphi(x, y, z)$ is given by:

$$\varphi(x, y, z) =$$

$$= \frac{e^{iky}}{2\pi} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} dk_x dk_z c(k_x, k_z)e^{ik_xx}e^{ik_zz}e^{-ik^2 y/2k_x}e^{-ik^2 y/2k} \quad (3)$$

In the next step we determine $c(k_x, k_z)$ using boundary conditions. Since we are looking for the solution behind a grating (situated at $y =$
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0), which is completely transparent inside the slits and completely absorbing outside the slits, we require that \( \varphi(x, 0, z) = 0 \) for points outside the slits and \( \varphi(x, 0, z) = \psi^i(x, 0, z) \) for points inside the slits. This implies that the function \( c(k_x, k_z) \) is determined by

\[
c(k_x, k_z) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} dx' \int_{-\infty}^{+\infty} dz' \varphi(x', 0, z') e^{-ik_xx'} e^{-ik_zz'} = \]

\[
= \frac{1}{2\pi} \int \int_A dx' dz' \psi^i(x', 0, z') e^{-ik_xx'} e^{-ik_zz'}, \tag{4}
\]

where symbol \( A \) denotes the union of points at the slits.

It is important that the form (3) is equivalent to the Fresnel-Kirchhoff form of the solution of the Helmholtz equation, if the function \( c(k_x, k_z) \) is determined from the same boundary conditions at the grating as are the ones used in deriving the Fresnel-Kirchhoff integral.

By looking to the form (3) of the solution one is tempted to define a time dependent wave function of the transverse motion by substituting \( y \) under the integral sign in (3) by \( vt \) [21, 22]. Here, \( v \) denotes the initial velocity of the particle, assumed to be along the \( y \)-axis. The usual justification for such a substitution is that in reality the motion of the particle along the longitudinal axis looks like the motion of a classical particle, whereas the transverse motion is quantum [8]. With this substitution, and using the de Broglie relation \( mv = \hbar k \), two exponents of two \( y \)-dependent exponentials in the integral are transformed into the following time-dependent expressions

\[
k_x^2 \frac{y}{2k} = k_x^2 \frac{\hbar}{2m} t \quad \text{and} \quad k_z^2 \frac{y}{2k} = k_z^2 \frac{\hbar}{2m} t. \tag{5}
\]

With the aid of the latter substitution the wave function \( \Psi(x, y, z, t) \) takes the form of a product of two time dependent functions. The first function is a stationary plane wave along the \( y \)-axis with the initial energy \( \hbar \omega = mv^2/2 \). The second function has the form of a non-stationary solution of the two dimensional Schrödinger
equation in the $xz$ plane,

$$\Psi(x, y, z, t) =$$

$$= e^{ik_y} e^{-i\omega t} \int \int dk_x dk_z c(k_x, k_z) e^{ik_x x} e^{ik_z z} e^{\frac{-ik_x^2 \hbar t}{2m}} e^{\frac{-ik_z^2 \hbar t}{2m}}. \quad (6)$$

The latter function is denoted by $\psi(x, z, t)$ and is called the transverse wave function or the time dependent wave function of the transverse motion,

$$\psi(x, z, t) = \frac{1}{2\pi} \int \int dk_x dk_z c(k_x, k_z) e^{ik_x x} e^{ik_z z} e^{-i\omega_x t} e^{-i\omega_z t}, \quad (7)$$

where $\omega_x = \hbar k_x^2 / 2m$, $\omega_z = \hbar k_z^2 / 2m$. We see from Eq. (7) that the transverse wave function is independent of particle’s initial momentum, as correctly assumed by Kurtsiefer et al. [8].

The function (6) has an important property. One can directly verify that it satisfies exactly the time-dependent free particle Schrödinger equation. This is an interesting and unexpected result since the expression (6) was obtained by substituting the relation $y = vt$ into the approximate solution of the stationary Schrödinger equation. It could be an exact wave function of a particle behind a grating, provided that it satisfies the boundary conditions at the grating. However, it satisfies the boundary conditions at $y = 0$ only for $t = 0$. This problem could be resolved by substituting the plane wave along the $y$-axis (in the initial wave function as well as in the wave function behind a grating) by a wave packet with a well-defined wave front. Gottfried [25] has constructed the wave packet that satisfied above condition.

Transverse wave function in the momentum representation, $c(k_x, k_z)$, is determined by the boundary conditions at the grating. It is also independent of the initial longitudinal momentum. In addition, it is independent of time. Its modulus square determines the distribution of particles’ momentum. So, one is forced to conclude that particles with zero component of the transverse momentum acquire a small component of transverse momentum in passing through the grating. The distribution of momentum acquired at the grating does not change during the free evolution behind the grating.
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4 Transverse momentum distribution

For most commonly used boundary conditions at the one dimensional grating with \( n \) slits having equal widths \( \delta \) (\( \varphi(x, y = 0) = 1/\sqrt{n\delta} \) for \( x \) at the openings, \( \varphi(x, y = 0) = 0 \) for \( x \) outside the openings) one easily performs the integration in the following equation:

\[
c(k_x) = \frac{1}{\sqrt{2\pi}} \int_A dx' \psi_i(x', 0)e^{-ik_xx'}
\]

and obtains

\[
c_1(k_x) = \frac{\sqrt{2}}{\sqrt{\pi\delta}} \frac{\sin \frac{k_x\delta}{2}}{k_x} e^{-ik_xx_{cj}}
\]

and

\[
c_n(k_x) = \frac{\sqrt{2}}{\sqrt{\pi\delta}} \frac{\sin \frac{k_x\delta}{2}}{k_x} \sum_{j=1}^{n} e^{ik_xx_{cj}} = \frac{\sqrt{2}}{\sqrt{\pi n\delta}} \frac{\sin \frac{k_x\delta}{2}}{k_x} \sin \frac{k_x dn}{2},
\]

where \( x_{cj} \) denotes the coordinate of the center of the \( j^{th} \) slit. In order to understand how one-slit wave function changes with the increase of the width of the second slit and how the size of particles might influence the interference patterns it was proposed recently to study interference behind an asymmetric double slit interferometer [24]. The transverse wave function in momentum representation behind a grating with two slits of widths \( \delta_1 \) and \( \delta_2 \) is

\[
c_2^a = \frac{1}{\sqrt{2\pi(\delta_1 + \delta_2)}} \frac{2}{k_x} \left[ e^{ik_x d/2} \sin \frac{k_x\delta_1}{2} + e^{-ik_x d/2} \sin \frac{k_x\delta_2}{2} \right].
\]

Momentum distributions behind gratings with \( n = 1 \) slit, \( n = 2 \) equal slits, \( n = 2 \) unequal slits and \( n = 40 \) slits are represented in Figs. 1 and 2 for chosen sets of parameters. By comparing curves on Fig. 1 we see that the presence of the second slit induces oscillations of the one-slit curve. The mutual distance of slits \( d \) determines the period of oscillations. When number of slits is large, momentum distribution consists of three narrow maxima (Fig. 2).
5 Time evolution of particle’s space distribution in the near and far field behind a one-dimensional multiple slits grating

In our previous papers [21–23] we presented the plots of the function $|\psi(x,t)|^2$ behind a single slit, and behind one-dimensional gratings with two equal slits and two unequal slits. In the one-dimensional case the wave function of the transverse motion reads

$$\psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} dk_x c(k_x) e^{ik_x x} e^{-i\omega_x t}. \quad (12)$$

On the plots of $|\psi(x,t)|^2$ one recognizes Fresnel and Fraunhofer regime, in agreement with measurements of Kurtsiefer et al. [8] of the space distribution of atoms behind a symmetric double-slit grating.

Figure 3 shows the function $|\psi(x,t)|^2$ behind a one-dimensional grating having $n = 40$ slits at various characteristic distances $y$ from the grating. We see that very far from the slits, in the Fraunhofer regime, the function $|\psi(x,t)|^2$ consists of three narrow maxima. In the next section we are going to show that maxima in space distribution are a direct consequence of maxima in the transverse momentum distribution.

Talbot effect is clearly seen at the plots of $|\psi(x,t)|^2$ in the near field. At the Talbot distance $L_T = 2d^2/\lambda$ one finds the self image of the grating, as well as on distances that are integral multiples of $L_T$. At the distances $L_T/2 = d^2/\lambda$, $3d^2/\lambda$, $5d^2/\lambda$, ... this self images also appear, but they are shifted by $d/2$. Therefore, the transverse wave function, Eq. (12), contains the Talbot effect.

6 Screen arrival probability

Development of the interference pattern was explained [22] by using the transverse momentum distribution $|c(k_x)|^2$, applying the classical law of the addition of probabilities and assuming that particles move behind a grating along straight trajectories. The probability of particles’ arrival to a certain point $(x, y - vt)$ at time $t$, $\tilde{P}(x,t)$, is written as a sum of $n$ terms, $\tilde{P}_i(x,t)$, where $\tilde{P}_i(x,t)$ is the probability
that a quanton reaches \((x, y = vt)\) at time \(t\) after passing through the 
i-th slit of the grating, when all \(n\) slits are open.

The probability is derived using the following arguments. We 
assume that a particle with transverse momentum \(p_x = \hbar k_x\), which 
was at point \((x' = x - \hbar k_x t/m, y = 0)\), at time \(t = 0\) arrives at point 
\((x, y - vt)\) at time \(t\). We have to integrate over all possible \(k_x\) and 
\(x'\). Thus, the probability of particle’s arrival at point \(x\) at time \(t\) is

\[
\tilde{P}(x, t) = \int_{-\infty}^{+\infty} dk_x \int_{-\infty}^{+\infty} dx' |c(k_x)|^2 |\psi(x', 0)|^2 \delta(x - x' - \hbar k_x t/m). \tag{13}
\]

Substituting the boundary values of the function \(\psi\): \(\psi(x, 0) = 1/\sqrt{n\delta}\) 
for \(x \in A\) and \(\psi(x, 0) = 0\) for \(x \notin A\) in Eq. (13) and after integration 
over \(x'\) we obtain

\[
\tilde{P}(x, t) = \frac{1}{n\delta} \sum_{i=1}^{n} \int_{(m/\hbar t)(x-x_i^l)}^{(m/\hbar t)(x-x_i^r)} |c(k_x)|^2 dk_x. \tag{14}
\]

where \(x_i^l\) and \(x_i^r\) are the coordinates of the left and right edges of the 
i-th slit. The probability \(\tilde{P}(x, t)\) is the sum of \(n\) terms

\[
\tilde{P}_i(x, t) = \frac{1}{n\delta} \int_{(m/\hbar t)(x-x_i^l)}^{(m/\hbar t)(x-x_i^r)} |c(k_x)|^2 dk_x. \tag{15}
\]

The term \(\tilde{P}_i(x, t)\) is the probability for a particle reaching \((x, y)\) 
at time \(t\) after passing through the \(i\)-th slit of the \(n\)-slit grating. It is 
derived by assuming that particle and wave properties are compatible.

Numerical calculation for \(n = 2\) has shown \([22, 24]\) that in the far 
field the sum of probabilities \(\tilde{P}_1(x, t)\) and \(\tilde{P}_2(x, t)\) is nearly equal to 
the probability density \(|\Psi(x, y, t)|^2 = |\psi(x, t)|^2\). In the near field the 
agreement is not so good.

The results of numerical evaluation of \(\tilde{P}(x, t)\) for \(n = 40\) are pre-
sented in Fig. 4. We clearly see, by comparing plots at Figs. 3 and 
4 that in the far field the values of \(|\Psi(x, y, t)|^2 = |\psi(x, t)|^2\) and of 
\(\tilde{P}(x, t)\) are almost identical. This justifies the assumptions used in 
writing the expression (13) for probability \(\tilde{P}(x, t)\).
In the near field, however, the plots of probabilities of particles arrivals $\tilde{P}(x,t)$ give only partly correct the time (and space) development of the particle distribution. Self-images of the grating are correctly obtained at the Talbot distance $L_T = 2d^2/\lambda$ and at distances that are integral multiples of $L_T$. However, at the distances $L_T/2 = d^2/\lambda$, $3d^2/\lambda$, $5d^2/\lambda$ self images are not shifted by $d/2$. Instead they are obtained at the same place as the image at the distance $L_T = 2d^2/\lambda$.

In addition to explaining the distribution after theoretically infinite number of events has been accumulated in the far field, with this approach, we may obtain also a distribution of a smaller number of events. For that, we do not integrate over all momenta and slit points at the grating, as in Eq. (13), but over a randomly chosen ones. It is clear that the resulting curves do not show the regularity of curves obtained by integrating over all possible transverse momenta and slit points. Instead, one obtains a random distribution of points.

7 Conclusion

Single particle interference experiments brought new arguments supporting: objective reality of matter and photon waves, compatibility of particle and wave properties of quantons, the evidence of existence of particle’s trajectories during the accumulation of an interference pattern, and the necessity to complete quantum mechanics by the description of single events.

By integrating the probability density of transverse momenta multiplied by the probability density of particle’ distribution at the slits over all transverse momenta and over all slits points, we have derived the expression for the probability density for the particle’s arrival at time $t$ to a point behind a grating [22, 24]. The agreement with usual probability density given by the modulus square of the wave function in coordinate representation is very good in the far field. In the near field the agreement is poor. This was demonstrated previously [22, 24] for gratings with small number of slits. For a many slits grating, where Talbot Laue effect exists, this is demonstrated in this paper. This indicates that further study of the form of particle’s trajectories in the near field is necessary.
In addition to obtaining agreement with the distribution after many events have been accumulated in the far field, with this approach one might obtain also a distribution of a smaller number of events. For that, we do not integrate over all momenta and slit points at the grating but over a randomly chosen ones. This result will be reported in a forthcoming paper.

References


Figure 1: Particles’ transverse momentum distribution behind: (a) one-slit grating, (b) double-slit symmetric grating, (c) asymmetric double-slit grating. Parameters $\delta_1 = 1 \mu m$, $\delta_2 = 0.25 \mu m$, $d = 8 \mu m$, $c(p_x) = c(\hbar k_x) \equiv c(k_x)/\sqrt{\hbar}$.
Figure 2: Particles’ transverse momentum distribution behind a grating having $n = 40$ slits. Slit width $\delta = 0.5 \mu m$ and period of the grating $d = 1 \mu m$, $c(p_x) = c(\hbar k_x) \equiv c(k_x)/\sqrt{\hbar}$. 

\[ |c(p_x)|^2 \left[ \frac{10^{-6} m}{\hbar} \right] \]
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\[ |\psi(x, t)|^2 \left[ \frac{1}{\mu m} \right] \]

\[ y = 3 \frac{d^2}{\lambda} \]

\[ |\psi(x, t)|^2 \left[ \frac{1}{m} \right] \]

\[ y = 500 \frac{a^2}{\lambda} \]
Figure 3: The function $|\psi(x, t)|^2$ behind a $n = 40$ grating for $t = \frac{y}{v}$, where the distance $y$ is equal to $\text{(a)} \ L_T/2$, $\text{(b)} \ L_T$, $\text{(c)} \ 3L_T/2$, $\text{(d)} \ 500L_T/2$, $\text{(e)} \ 2000L_T/2$, $L_T = 2d^2/\lambda$ is the Talbot length. The parameters $\lambda = 5 \cdot 10^{-12}$ m and $d = 10^{-6}$ m
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Figure 4: The function $\tilde{P}(x,t)$ behind a $n = 40$ grating for $t = y/v$, where the distance $y$ is equal to (a) $L_T/2$, (b) $L_T$, (c) $3L_T/2$, (d) $500L_T/2$, (e) $2000L_T/2$, $L_T = 2d^2/\lambda$ is the Talbot length. The parameters $\lambda = 5 \cdot 10^{-12}$ m and $d = 10^{-6}$ m.