An asymmetric double-slit interferometer for small and large quantum particles

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Abstract

Quantum theory of interference phenomena does not take the diameter of the particle into account, since particles were much smaller than the width of the slits in early observations. In recent experiments with large molecules, the diameter of the particle has approached the width of the slits. Therefore, analytical description of these cases should include a finite particle size. The generic quantum interference setup is an asymmetric double slit interferometer. We evaluate the wave function of the particle transverse motion using two forms of the solution of Schrödinger’s equation in an asymmetric interferometer: the Fresnel-Kirchhoff form and the form derived from the transverse wave function in the momentum representation. The transverse momentum distribution is independent of the distance from the slits, while the space distribution strongly depends on this distance. Based on the transverse momentum distribution we determined the space distribution of particles behind the slits. We will present two cases: a) when the diameter of the particle may be neglected with respect to the width of both slits, and b) when the diameter of the particle is larger than the width of the smaller slit.
1 Introduction

Until recently various quantum interference experiments were conducted with objects (photons, electrons, neutrons,...) of the size much smaller than the characteristic dimensions of the diffraction structure [1]. The first single slit experiment with Rydberg atoms, objects of non negligible size with respect to the width of the slit was performed by Fabre et al. [2]. By measuring transmission through micrometer size slits, these authors determined the size of Rydberg atoms. Later, Hunter and Wadlinger [3] proposed the single-slit diffraction experiment in order to measure the diameter of the photon.

In order to investigate the reasons of unobservability of quantum effects in the classical world Arndt et al. [4], Nairz et al. [5], Brezger et al. [6] performed quantum interference experiments with objects of large mass and diameter, including macromolecules. The experiments raise various questions about theoretical concepts. The following three are obvious:

1) Are there new effects applying to particles bigger than their de Broglie wavelength?
2) Does internal structure have influence on interference?

Arndt et. al. emphasized the task [4]: “Here we report the observation of de Broglie wave interference of C\textsubscript{60} molecules by diffraction at a material absorption grating. This molecule is the most massive and complex object in which wave behavior has been observed. Of particular interest is the fact that C\textsubscript{60} is almost a classical body, because of its many excited internal degrees of freedom...”.

3) What happened with an ensemble of incoming particles if slits are smaller than the diameter of the particles?

In the experiment of Arndt et. al. the de Broglie wavelength of the interfering fullerenes is already smaller than their diameter by a factor of almost 400 and authors pointed out that “it would be certainly interesting to investigate the interference of objects the size of which is equal or even bigger than the diffracting structure” [4].

These experiments could shed more light on a long standing dilemma whether each quanton consists of a particle and accompanied wave (as two different compatible entities) [7], or quantons sometimes behave like a wave and sometimes behave like a particle (obeying principle of complementarity) [8]? The following citations illustrate the present situation.
“We performed an experiment which was proposed by Ghose, Home and Agarwal showing both classical wave-like and particle-like behaviors of single photon states of light in a single experiment, in conformity with quantum optics.” [9]. “Here we give a detailed justification of our claim that this experimental results contradict the tenet of mutual exclusiveness of classical wave and particle pictures assumed in Bohr’s complementarity principle.” [10]. “Simultaneous observations of wave and particle behavior is prohibited” [11].

“Although interference patterns were once thought of as evidence for wave motion, when looked at in detail it can be seen that the electron arrive in individual lumps. ... We must therefore conclude that electrons show wave-like interference in their arrival pattern despite the fact that they arrive in lumps just like bullets”. [12]

“It is frequently said or implied that the wave-particle duality of matter embodies the notion that a particle – the electron, for example – propagates like a wave, but registers at a detector like a particle. Here one must again exercise care in expression so that what is already intrinsically difficult to understand is not made more so by semantic confusion. The manifestations of wave-like behavior are statistical in nature and always emerge from the collective outcome of many electron events... That electrons behave singly as particles and collectively as waves is indeed mysterious, ... ” [13]

“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.” [14]

“...Ever since then the two sides of the same quantum object appeared together: on the one hand the non-local wave nature needed to describe the unperturbed propagation and on the other hand the local aspect of the object when it is registered by the detector” [4]

In this paper we present the theoretical study of the dependence of the quantum interference pattern on the diameter of the particle, assuming that the characteristic sizes of the diffraction structure are of the order of the diameter of the particle. We argue that an asymmetric double-slit interferometer (an interferometer whose slits have different widths $\delta_1$ and $\delta_2$) is the generic case for this study.
2 The particle wave function behind an asymmetric grating

We shall now determine, the wave function of a quanton which travels with velocity, \( \vec{v} = v\hat{i} \) through the region I, towards the slits and is then sent through the slits to the region II (Fig. 1). Results in this section are valid for arbitrary slits. This wave function is a stationary solution of the time-dependent two dimensional Schrödinger equation

\[
-\frac{\hbar^2}{2m} \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) \Psi(x, y, t) = i\hbar \frac{\partial}{\partial t} \Psi(x, y, t). \tag{1}
\]

The solution of (1) has the form

\[
\Psi(x, y, t) = e^{-i\omega t} \varphi(x, y), \tag{2}
\]

where \( \hbar \omega = \frac{mv^2}{2} \) and \( p = mv = \hbar k \). Space dependent function \( \varphi(x, y) \) satisfies the Helmholtz equation

\[
-\frac{\hbar^2}{2m} \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) \varphi(x, y) = \hbar \omega \varphi(x, y). \tag{3}
\]

The solution of this equation in the region I is a spherical wave

\[
\varphi(P') = \varphi(x', y') = A e^{i kr'}, \tag{4}
\]

where \( A \) is a constant and \( r' \) is a distance (Fig. 1) from the source \( (P_0) \) to the point \( P' = (x', y') \) in the region I. The distance \( a \) of the double-slit screen from the source \( P_0 \) being very large compared to the width of the slits, this spherical wave at the slit points \( (x' = x'', y' = 0) \) may be approximated by the plane wave. In the region II the equation (3) is as simple as before but initial condition makes the solution more difficult.

Solution known as Fresnel-Kirchhoff diffraction formula \cite{15} reads:

\[
\varphi(x, y) = -\frac{iA e^{ikx}}{2\lambda a} \int_A dx'' e^{iks} [1 + \cos \chi], \tag{5}
\]
where \( s = \sqrt{y^2 + (x'' - x)^2} \), \( \cos \chi = y/s \), \( \lambda = 2\pi/k \). The region \( \mathcal{A} \) is the union of all intervals along the \( x \)-axis where slits are open. From now on \( x'' \) represents a variable of integration along the line of the slits.

Far enough from the slits wave function resembles the Fourier transform of the wave field across the aperture. This can be verified from the Fresnel-Kirchhoff solution. In the far region it follows:

\[
\varphi(x, y) \approx -\frac{iA}{\lambda} \frac{e^{ika} e^{iky}}{a y} \int_{\mathcal{A}} dx'' \varphi(x'', 0) e^{-i k x x'' / y}. \tag{6}
\]

Wave function is now separable into two functions, one depending on \( y \) and the other depending on \( K_x \equiv k x / y [16] \):

\[
\varphi(x, y) = D(y) \mathcal{F}(K_x)
\]

\[
D(y) = -\sqrt{2\pi} \frac{i A e^{ika} e^{iky}}{\lambda a} y
\]

\[
\mathcal{F}(K_x) = \frac{1}{\sqrt{2\pi}} \int_{\mathcal{A}} dx'' \varphi(x'', 0) e^{-i K_x x''}. \tag{7}
\]

The solution of equation (3) in region II can be written in another form [17, 18, 19]. This form is more convenient for our analysis than the form (5). With approximation valid for small diffraction angles \( \chi \) we have:

\[
\varphi(x, y) = e^{iky} \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} dk_x c(k_x) e^{i k_x x} e^{-k^2 y^2 / 4y} \equiv e^{iky} \phi(x, y). \tag{8}
\]

where \( c(k_x) \) is the Fourier transform of the function \( \varphi(x, y) \) on the aperture \( \varphi(x, y = 0) \):

\[
c(k_x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} dx'' \varphi(x'', 0) e^{-i k x x''}. \tag{9}
\]

Inserting (9) into (8), after integration over \( k_x \) one finds

\[
\varphi(x, y) = e^{-i \pi / 4} e^{iky} \sqrt{\frac{k}{2\pi}} \frac{1}{\sqrt{y}} \int_{\mathcal{A}} \varphi(x'', 0) e^{\frac{i k (x - x'')^2}{2y}} dx''. \tag{10}
\]

This function is normalized \( \int_{-\infty}^{+\infty} |\varphi(x'', y)|^2 dx'' = 1 \), provided \( \int_{\mathcal{A}} |\varphi(x'', 0)|^2 dx'' = 1 \). The form (10) clearly expresses wave function’s dependence on the boundary condition and it is appropriate for numerical computation.
For large values of \( y \) the function \( \varphi(x, y) \) in (10) is approximated by

\[
\varphi(x,y) = \sqrt{\frac{k}{2\pi y}} e^{-i\pi/4} e^{ikx^2/2y} \int_A \varphi(x'',0)e^{-ikxx''/y}dx''.
\] (11)

Taking Eq. (9) into account, Eq. (11) takes the form

\[
\varphi(x,y) = e^{iky} \sqrt{\frac{k}{y}} e^{-i\pi/4} e^{ikx^2/2y} c(kx/y).
\] (12)

We see that the variable \( K_x = \frac{kx}{y} = \frac{mx}{ht} \) plays the role of \( k_x \).

Since \( K_x \) is proportional to \( x/y \) functions \( |\varphi(x,y) = \text{const}| \) are family of functions of \( x \) spreading along the \( x- \) axis as \( y \) increases. In fact, for each value of \( |\varphi| \), in the far field there exists the straight line with origin at the center of the grating along which this particular value of \( |\varphi| \) propagates.

3 The understanding of the space distribution using transverse momentum distribution

By assuming that the motion of an atom along the \( y \)-axis may be treated classically and that the transverse motion is quantum, one is tempted to use the relation \( y = vt \) and to determine the time dependent function of the transverse motion \( \psi(x,t) \) from the function \( \phi(x,y) \), by the following definition:

\[
\psi(x,t) \equiv \phi(x,vt) = \frac{1}{\sqrt{2\pi}} \int dk_x c(k_x)e^{ikx}e^{-i\omega_x t}
\] (13)

where \( \omega_x = \frac{\hbar k_x^2}{2m} \). We see that the function \( \psi(x,t) \) has the form of a general solution of the one-dimensional Schrödinger equation. The wave function \( c(k_x) \) is then seen as a wave function of this one-dimensional (transverse) motion in the momentum representation. Its modulus square, \( |c(k_x)|^2 \), determines the distribution of transverse momenta. The wave function \( \Psi(x,y,t) \) from Eq. (2) is expressed through \( \psi(x,t) \) as

\[
\Psi(x,y,t) = e^{iky}e^{-i\omega t}\psi(x,t).
\] (14)
By taking Eq. (12) into account one concludes that in the far field the relation (13) between the wave functions $\psi(x, t)$ and $c(k_x)$ reduces to the simpler form:

$$\psi\left(x, t = \frac{ym}{hk}\right) = \sqrt{\frac{k}{y}} e^{-i\frac{\pi}{4}} e^{ikx^2/2y} c(kx/y).$$

(15)

Based on the above factorization of the wave function $\Psi(x, y, t)$ and the properties of its factors summarized above, we proposed [18] the new expression for the probability density $\tilde{P}(x, t)$ for the particle’s arrival to a certain point $(x, y = vt)$ at time $t$:

$$\tilde{P}\left(x, \frac{y}{v}\right) = \tilde{P}(x, t) \equiv \int_{-\infty}^{+\infty} dk_x \int_{-\infty}^{+\infty} dx'' |c_n(k_x)|^2 |\phi(x'', 0)|^2 \delta\left(x - x'' - \frac{hk_x t}{m}\right).$$

(16)

Particles emerge from different points $(x'', 0)$ at the aperture. That is the reason for integration over $x''$. The contribution of each point at the aperture is proportional to $|\phi(x'', 0)|^2$. The integration over $dk_x$ and the function $|c_n(k_x)|^2$ reflect the contribution of various angles/moments in diffraction. Finally, $\delta$-function assumes straight trajectory from a point $(x'', 0)$ at the slits to the point $(x, y)$ and leads to the simplified form

$$\tilde{P}(x, t) = \int_{-\infty}^{+\infty} dk_x |c_n(k_x)|^2 \left|\phi\left(x - \frac{hk_x t}{m}, 0\right)\right|^2.$$  

(17)

By assuming that the function $\phi(x'', 0) = 0$ for $x'' \notin A$ and $\phi(x'', 0) = const$ such that $\int_A |\phi(x'', 0)|^2 = 1$, for $x'' \in A$, the Eq. (17) is transformed to the following useful form

$$\tilde{P}(x, t) = \frac{1}{\sqrt{\sum_{i=1}^{n} \delta_i}} \sum_{i=1}^{n} \int_{A_i} \tilde{P}_i(x-x_i) \, dk_x |c(k_x)|^2 \equiv \sum_{i=1}^{n} \tilde{P}_i(x, t).$$

(18)

Here $x_i^l$ and $x_i^r$ are the coordinates of the left and right edge of the $i$-th slit.

The total probability density $\tilde{P}(x, t)$ is a sum of $n$ terms, $\tilde{P}_i(x, t)$. $\tilde{P}_i(x, t)$ is interpreted to be the probability that a quanton reaches $(x, y = vt)$ at time $t$ after passing through the $i$-th slit of the $n$-slits grating.
Numerical calculation shows that far from the slits the function $\tilde{P}(x, t)$ (Fig. 4) is very nearly equal to the exact probability density $|\Psi(x, y, t)|^2 = |\psi(x, t)|^2$ (Fig. 2). Near the slits $\tilde{P}(x, t)$ and $|\psi(x, t)|^2$ qualitatively look similarly but they differ numerically.

4 On the possible influence of particle’s diameter on the interference pattern

We outline an approach to investigate how the widths of the slits influence the interference pattern in the double-slit experiment with quantons - photons, electrons, neutrons, atoms, molecules.

Interference effects are visible when the wavelength of quantons is of the order of the distance between the slits. In practice, this distance is $d = (2 - 50) \lambda$. The slit width is often equal or up to ten times smaller than the distance between the slits. In quantum interference experiments with electrons and neutrons the diameter of the particle is smaller than the wavelength. Consequently, in classical experiments the width $\delta$ of the slits is much greater than $D$. But, depending on the velocity, atoms may have de Broglie wavelength which is smaller than the diameter of the atom. With macromolecules such a situation encounters more often, as shown in the experiment of Arndt et. al. and discussed by Arndt et al. [4] and Nairz et al. [5]. So, interference experiments with such quantum particles could have the slit widths smaller than the particle diameter.

This requires a theoretical approach to quantum interference which takes the diameter of the particle into account [20]. A study of a quantum particle in an asymmetric double-slit interferometer ($\delta_1 > \delta_2$) seems to be useful for this purpose because we identify two characteristic cases for the ratio of slit widths $\delta_1$ and $\delta_2$ and the diameter of the particle $D$:

a) The diameter $D$ is negligible with respect to the widths $\delta_1$ and $\delta_2$.

b) The diameter $D$ is greater than the width $\delta_2$, where $\delta_2 < \delta_1$.

In the case a), which was until recently the only case of physical interest, there is no need to consider or take into account the diameter of the particle. The particle momentum $|c(k_x)|^2$ and space distribution $|\psi(x, t)|^2$ behind the grating are determined by the wave function

$$\psi(x, t) = \phi(x, vt) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} c(k_x)e^{i(k_xx-\omega_xt)}dk_x$$

(19)
where
\[ \phi(x, 0) = \psi(x, 0) = \begin{cases} \frac{1}{\sqrt{\delta_1 + \delta_2}} & x \in A, \quad A = \left( \frac{-d-\delta_1}{2}, \frac{-d+\delta_1}{2} \right) \cup \left( \frac{d-\delta_2}{2}, \frac{d+\delta_2}{2} \right) \\ 0 & x \notin A \end{cases} \] (20)

and
\[ c(k_x) = \frac{1}{\sqrt{2\pi(\delta_1 + \delta_2) k_x}} \left[ e^{ik_x d/2} \sin \frac{k_x \delta_1}{2} + e^{-ik_x d/2} \sin \frac{k_x \delta_2}{2} \right]. \] (21)

The functions \(|\psi(x, t)|^2\) and \(|c(k_x)|^2\) are graphically represented at Fig. 2 and Fig. 3, for the chosen set of parameters.

In the case \(b\), we are faced with the question how and where to take the diameter of the particle into account. We know that the diameter of the particle is not incorporated anywhere in the Schrödinger equation. But, we expect that a particle with diameter \(D\), such that \(\delta_1 > D > \delta_2\) could not pass through the second slit.

So, it seems to us that we are forced to assume that wave functions in the coordinate and momentum representation in the case \(b\) is also given by expressions (19)-(21).

The momentum distribution \(|c(k_x)|^2\) of particles is given also by (21), because it is determined by the values of the wave function at the boundary.

But the space distribution of particles in case \(b\) is different from the space distribution in case \(a\), because the particles arriving to the smaller slit can not go through. We conclude that particle distribution in case \(b\) is given by \(\tilde{P}_1(x, t)\) from the expression (18) of \(\tilde{P}(x, t)\).

\[ \tilde{P}(x, t) \approx \tilde{P}_1(x, t) = \frac{1}{\sqrt{\sum_{i=1}^n \delta_i}} \int \frac{\pi(x-x_i)}{\pi(x-x_i)} |c(k_x)|^2 dk_x. \] (22)

The probability \(\tilde{P}_1(x, t)\) is graphically represented in Fig. 5.

5 Conclusion

Inspired by current efforts to perform diffraction and interference experiments with objects of size that is equal or even larger than the diffraction structure, we outline an approach to investigate how the particle diameter influences the interference pattern in an asymmetric double slit interferometer.
We identify two characteristic cases for the ratio of slit widths $\delta_1$ and $\delta_2$ and the diameter $D$ of the particle: a) $D \ll \delta_1$ and $D \ll \delta_2$, b) $\delta_1 > D > \delta_2$. The wave function behind the grating has the same form in both cases because it is the solution of the Schrödinger equation which is not sensitive to the diameter of the particle.

The space distribution of particles in case a) is given as usual by the modulus square of this function. Using the same wave function and assuming that a particle with diameter $D$, such that $\delta_1 > D > \delta_2$ could not pass through the second slit, we determine the space distribution in case b). We conclude that the momentum distribution of particles behind the grating is the same in cases a) and b).

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Figure captions

Fig. 1. Illustration of a grating with \( n \) slits of various widths.

Fig. 2. The particle distribution function \(|\psi(x, t)|^2\) behind the asymmetric double slit grating \((\delta_1 = 1 \mu m, \delta_2 = 0.25 \mu m, d = 8 \mu m)\) close to the slits \((a, b)\) and far from the slits \((c, d)\). It is evaluated from the form (19) of the wave function. The initial longitudinal wave vector is \( k = 4\pi \cdot 10^{10} \text{ m}^{-1} \), the particle mass is \( m = 3.8189 \cdot 10^{-26} \text{ kg} \).

Fig. 3. The particle transverse momentum distribution \(|c(k_x)|^2\) behind the asymmetric double-slit grating \((\delta_1 = 1 \mu m, \delta_2 = 0.25 \mu m, d = 8 \mu m)\).

Fig. 4. The probability density \( \tilde{P}(x, t) \) of particles arrival to the point \( x \) at time \( t \) \((y = vt)\) behind the asymmetric double slit grating \((\delta_1 = 1 \mu m, \delta_2 = 0.25 \mu m, d = 8 \mu m)\) close to the slits \((a, b)\) and far from the slits \((c, d)\). It is evaluated from Eq. (18). Particles’ diameter \( D \) is negligible with respect to the widths of the slits. The initial longitudinal wave vector is \( k = 4\pi \cdot 10^{10} \text{ m}^{-1} \), the particle mass is \( m = 3.8189 \cdot 10^{-26} \text{ kg} \).

Fig. 5. The probability density \( \tilde{P}_1(x, t) \) of particles reaching \((x, y)\) at time \( t \) after passing through the larger slit, near the slits \((a, b)\) and far from the slits \((c, d)\). It is evaluated from Eq. (22). \( D \) is assumed to be larger than \( \delta_2 \) and smaller than \( \delta_1 \). The values of parameters are the same as in captions of Figs. 2,3,4.
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