



On the quantum theory of diffraction by an aperture and the Fraunhofer diffraction at large angles

Bernard Fabbro

► To cite this version:

Bernard Fabbro. On the quantum theory of diffraction by an aperture and the Fraunhofer diffraction at large angles. 2018. cea-01823747v1

HAL Id: cea-01823747

<https://cea.hal.science/cea-01823747v1>

Preprint submitted on 26 Jun 2018 (v1), last revised 5 Apr 2019 (v2)

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

On the quantum theory of diffraction by an aperture and the Fraunhofer diffraction at large angles

Bernard Fabbro

IRFU,CEA, Université Paris-Saclay, F-91191 Gif-sur-Yvette, France

E-mail: bernard.fabbro@cea.fr

June 21, 2018

Abstract. A theoretical model of diffraction based on the concept of quantum measurement is presented. It provides a general expression of the state vector of a particle after its passage through an aperture of any shape in a plane screen (diaphragm). In this model, the diaphragm is considered as a measurement device of the position of the particle and the postulate of wave function reduction is applied to describe the change of state of the particle during the measurement. It is shown that this change of state is more complex than a single projection because of the kinematics of the particle-diaphragm interaction. In the case of the diffraction at infinity (Fraunhofer diffraction), the model makes it possible to predict the intensity of the diffracted wave over the whole diffraction angle range (0° - 90°). The predictions of the quantum model and of the classical theories based on the Huygens-Fresnel principle (Fresnel-Kirchhoff (FK) and Rayleigh-Sommerfeld (RS1 and RS2)) are close at small diffraction angles but significantly different at large angles, a region for which specific experimental studies are lacking. A measurement of the intensity of the particle flow in this region should allow to test the classical theories and the presented quantum model.

Keywords: Quantum measurement, kinematics, Huygens-Fresnel principle, Fraunhofer diffraction, large diffraction angles

1 Introduction

Diffraction has been the subject of numerous studies that have led to significant progress in the knowledge of this phenomenon. However, this knowledge can be further improved because there is still research to be done both on the theoretical and experimental levels. Let us examine the situation by considering the example of diffraction by a screen edge or by an aperture in a plane screen (diaphragm) in the case where the diffracted wave is observed far enough beyond the screen.

Theoretical aspect. The intensity of the diffracted wave is obtained most often by calculations based on the Huygens-Fresnel principle or on the resolution of the wave equation with boundary conditions [1–9]. In these theories, the amplitude of the diffracted wave as well as its intensity (modulus squared of the amplitude) are functions of the spatial coordinates. Therefore, in the context of quantum mechanics, the amplitude of the diffracted wave can be

identified with a function proportional to the position wave function of the particle after its passage through the aperture of the diaphragm. However, this position wave function is necessarily that of the quantum state of the particle. So, in the above-mentioned theories, *the calculation of the diffracted wave amplitude is equivalent to a direct calculation of a wave function without prior calculation of the quantum state from which this wave function should be derived*. In principle, the quantum state of the particle after passing through the aperture should be calculable in the framework of a "purely quantum" theory of diffraction (i.e. a theory in which the calculations are made with state vectors in a Hilbert space). There are already theories of diffraction involving quantum mechanics but most of them do not provide the expression of a quantum state. The first theory of this type dates back to the beginnings of the history of quantum mechanics and treats the Fraunhofer diffraction by a grating by combining the concept of light quantum with Bohr's principle of correspondence [10]. Then, theories involving quantum mechanics to calculate diffraction are mostly those using path integrals [11–15]. Other models combine the resolution of the Schrödinger equation (or of the wave equation for photons) with the Huygens-Fresnel principle [16–18]. Only one calculation based explicitly on the concept of quantum measurement - therefore involving state vectors in a Hilbert space - seems to have been done until now. It is due to Marcella [19] and will be described and discussed in more detail below. Apart from this attempt - and that of the present paper - it seems that there is no other diffraction theory that gives the expression of the quantum state of the particle associated with a wave diffracted by an aperture.

Experimental aspect. The area of observation of the wave diffracted by an aperture is the entire half-space beyond the diaphragm. In the case of diffraction at infinity (Fraunhofer diffraction), this corresponds to the whole diffraction angular range (0° - 90°). However, it is known that the Fresnel-Kirchhoff (FK) and Rayleigh-Sommerfeld (RS1 and RS2) theories - based on the Huygens-Fresnel principle and hereafter called *classical diffraction theories* - disagree in the region of large diffraction angles [1]. This means that at least two of these three theories do not describe correctly the diffraction at large angles. However, from a survey of the literature, *it seems that no accurate experimental study of the diffraction at large angles has been carried out so far*. It is not surprising that these measurements were not made when the classical theories appeared (late nineteenth century) because such experiments were not feasible at the time. However, since then, the technologies in optics have made considerable progress (especially with the quasi-monochromatic laser sources and the accurate measurements of intensity using charge-coupled devices) so that it is now possible to reconsider this question and achieve an experimental study (note that the issue of large angles has quite recently attracted interest and gave rise to a theoretical model that uses the classical theory of diffraction to calculate the non-paraxial propagation in optical systems [20]). Moreover, if the aperture is in a non-reflective plane screen, we can assume that the intensity of the diffracted wave decreases continuously to zero when reaching the transverse direction. The RS1 theory proves to be the only one that predicts this decrease to zero and would therefore be the only valid classical theory over the whole diffraction angle range. Measurements in the region of large angles would therefore allow to confirm or refute this conjecture.

In response to the situation described above, we present a quantum model of diffraction giving the general expression of the quantum state of the particle associated with the diffracted wave. It explicitly uses the postulate of wave function reduction [21] by considering the diaphragm as a device for measuring the position of the incident particle. In this model, the intensity of the diffracted wave is calculated from the wave functions of the state of the particle after the measurement (hereafter called *final state*). The Huygens-Fresnel principle is not explicitly used as in the FK and RS1-2 theories but we will see that it is underlying in the model. The approach is inspired by that of Marcella [19] whose model allows to recover the well-known formula in $(\sin X/X)^2$ of the Fraunhofer diffraction by a slit. However, this result only applies to the small angles and some authors have further considered that the used method implicitly refers to classical optics [22]. In the present paper, we consider that these drawbacks do not call into question the validity of the "purely quantum" approach adopted by Marcella but that they instead come from the way in which the postulate of wave function reduction has been applied in the framework of this approach. In [19], the state of the particle after its passage through the aperture is supposed to result from a filtering of the position wave function of the incident particle, according to the hypothesis usually made in the case of a quantum measurement of position. Moreover, this "position filtering" is applied to a single coordinate in the plane of the diaphragm and it is implicitly assumed that the energy of the particle is conserved. Resuming the analysis of this question, we have been led to assume that the position filtering must correspond to a measurement of the three spatial coordinates and that it must be explicitly completed by an "energy-momentum filtering" in order to obtain a final state compatible with the kinematics of the particle-diaphragm interaction and with the presence of a diffracted wave beyond the diaphragm. Thanks to these modifications in the use of the postulate of the wave function reduction, it is possible to perform a calculation of the final state associated with the diffracted wave. In the case of the Fraunhofer diffraction, the quantum model allows to calculate the intensity over the whole diffraction angle range (0° - 90°). It leads to a prediction close to the classical predictions (FK and RS1-2) for small angles. In the region of large angles, the four predictions are different. Nevertheless, the quantum and RS1 models both predict a decrease in intensity to zero at 90° but, despite this, these two predictions are significantly different beyond 60° . The situation is therefore as follows: there is an unexplored angular range in which the diffraction has never been measured and several theories have different predictions for this range. Moreover, an accurate measurement of the particle flow (which is proportional to the intensity of the diffracted wave) in the region of large angles is now possible in the context of current technologies in optics. Such an experimental test would therefore improve our knowledge of diffraction.

The paper is organized as follows. In section 2, we express the amplitude of the diffracted wave in Fraunhofer diffraction predicted by the classical theories. Then, we introduce the appropriate diffraction angles for the calculation of the intensity up to the large angles. In section 3, we present the quantum model. We calculate the final state associated with the diffracted wave in the case of an incident monochromatic plane wave. Then, we establish

the quantum expression of the intensity in Fraunhofer diffraction. In section 4, we compare the classical and quantum predictions. We perform the calculation for a rectangular slit and we emphasize the interest of an experimental test for the large diffraction angles. Finally, we conclude and suggest some developments in section 5.

2 Fraunhofer diffraction for the 0° - 90° angular range in classical theories of diffraction

2.1 Experimental context

Consider an experimental setup which contains a source of particles and a diaphragm of zero thickness forming a plane with an aperture A . We suppose that the aperture can be of any shape and possibly formed of non-connected parts (e.g. a system of slits). It is only assumed that its area is finite. We then define the center of the aperture in the most convenient way according to the shape (symmetry center or appropriate center for a complicated shape). The device is in a coordinate system $(O; x, y, z)$ which origin O is located at the center of the aperture and which (Ox, Oy) plane is that of the diaphragm (figure 1). The source is located on the z axis (normal incidence) and the source-diaphragm distance is denoted s and is assumed to be large enough, so that the waves arriving at the aperture can be considered as plane waves. The observation point is located at a distance d from the aperture, beyond the diaphragm. Its position is denoted by the radius-vector $\mathbf{d}$.

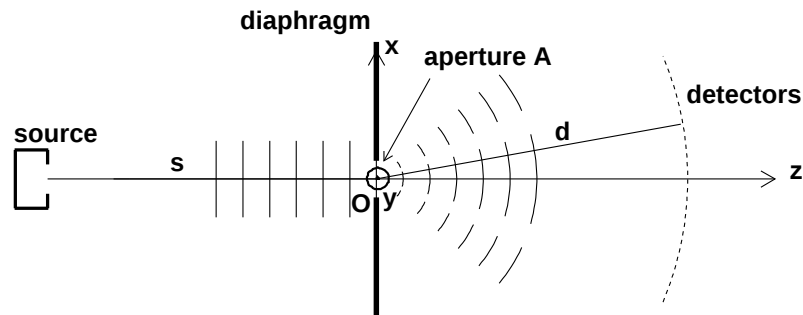


Figure 1. Section of the experimental setup in the horizontal plane (Ox, Oz) and schematic representation of the initial and final wave packets in the case of a slit.

It is assumed that the wavelength λ of the wave associated with the particles is smaller than the size of the aperture and that the Fraunhofer diffraction is obtained at distance d . In that case, the size of the aperture is negligible compared to d , so that detectors can be arranged on a hemisphere of center O and radius d in order to measure the angular distribution of the particles that passed through the aperture ¹.

¹ The criterion for the Fraunhofer diffraction is [1, 3]: $\Delta^2/(\lambda d) \ll 1$ (ditto for s), where $\Delta \equiv \max_{(x,y) \in A} \sqrt{x^2 + y^2}$ represents the size of the aperture. The assumption $\lambda \leq \Delta$ and this criterion imply that $\Delta \ll d$ (ditto for s). This relation and the criterion are satisfied if $d \rightarrow \infty$ and $s \rightarrow \infty$ (diffraction at infinity). These latter conditions are sometimes used as criteria [2].

2.2 Diffracted wave in the classical theories

According to the Huygens-Fresnel principle, the amplitude of the diffracted wave is equal to the sum of the amplitudes of spherical waves emitted from the wavefront located at the diaphragm aperture. This sum (hereafter called *classical amplitude*) is most often calculated by means of the Fresnel-Kirchhoff (FK) or Rayleigh-Sommerfeld (RS1 and RS2) theories which differ by their assumed boundary conditions. According to these theories, for a monochromatic plane wave of wavelength λ in normal incidence, the classical amplitude in Fraunhofer diffraction at a point of radius vector $\mathbf{d}$ beyond the diaphragm is expressed by [1, 2]:

$$\mathcal{U}_{\text{Cl.}}^{k,A}(\mathbf{d}) \simeq -C_0 \frac{i}{\lambda} \frac{\exp[ik(s+d)]}{sd} \Omega(\chi) \iint_A dx dy \exp \left[-ik \left(\frac{d_x}{d} x + \frac{d_y}{d} y \right) \right], \quad (1)$$

where $k = 2\pi/\lambda$ is the wave number, C_0 is a constant, χ is the angle:

$$\chi \equiv \chi(\mathbf{d}) \equiv (\mathbf{Oz}, \mathbf{d}), \quad (2)$$

hereafter called *deflection angle*, and $\Omega(\chi)$ is the *obliquity factor* which depends on the theory:

$$\Omega(\chi) \equiv \begin{cases} (1 + \cos \chi)/2 & \text{(FK)} \\ \cos \chi & \text{(RS1)} \\ 1 & \text{(RS2)} \end{cases}. \quad (3)$$

From (1) and (3), the values of the amplitudes in the three theories are close when the deflection angle χ is small. However, these values diverge from each other when χ increases, which means that the three classical diffraction theories have different predictions at large angles. If the diaphragm is assumed to be non-reflective, we can surmise that the amplitude must decrease continuously to zero at $\chi = \pi/2$. From (3), the right-hand side of (1) is in general non-zero when $\chi = \pi/2$, except for the RS1 theory. The latter would then be the most plausible classical theory for the large angles.

Since the distance d is large compared to the size of the aperture, the directions of the wave vectors $\mathbf{k}$ of all the waves arriving at point of radius-vector $\mathbf{d}$ are close to that of this radius-vector. It is the same for the momenta $\mathbf{p}$ of the associated particles, since $\mathbf{p} = \hbar \mathbf{k}$. Hence:

$$\mathbf{d} \simeq d \frac{\mathbf{p}}{p}. \quad (4)$$

From (4), the deflection angle given by (2) is such that $\cos \chi \simeq \cos(\mathbf{Oz}, \mathbf{p}) = p_z/p$ and we also have: $d_x/d \simeq p_x/p$ and $d_y/d \simeq p_y/p$. Then, substituting into (1) and given (3), we can express the classical amplitude in Fraunhofer diffraction as a function of the distance d and of the momentum direction $\mathbf{p}/p$:

$$\begin{aligned} \mathcal{U}_{\text{Class.}}^{p,A} \left(d, \frac{\mathbf{p}}{p} \right) &\simeq -C_0 \frac{i}{2\pi} \frac{p}{\hbar} \frac{\exp[i(p/\hbar)(s+d)]}{sd} \\ &\times \Omega \left(\arccos \frac{p_z}{p} \right) \iint_A dx dy \exp \left[-i \frac{p}{\hbar} \left(\frac{p_x}{p} x + \frac{p_y}{p} y \right) \right], \end{aligned} \quad (5)$$

where the modulus p of the momentum is a parameter (as k in (1)).

2.3 Diffraction angles in the half-space $z > 0$

To perform the calculation of the Fraunhofer diffraction up to the large angles, it is necessary to bring out the direction of $\mathbf{p}$ by replacing the Cartesian variables (p_x, p_y, p_z) by a system of variables including the momentum modulus and two appropriate angles. Equation (5) suggests what these angles could be. If the deflection angle χ is small, we have $p_z/p \simeq 1$, $p_x/p \simeq \theta_x$ and $p_y/p \simeq \theta_y$ where θ_x and θ_y are the *diffraction angles* defined in [3]. With the notations used here, these angles are given by: $\theta_x = (\mathbf{p}_z, \mathbf{p}_{xz})$ and $\theta_y = (\mathbf{p}_z, \mathbf{p}_{yz})$, where $\mathbf{p}_z$, $\mathbf{p}_{xz}$ and $\mathbf{p}_{yz}$ denote respectively the projections of the vector $\mathbf{p}$ on the z axis and on the planes (x, z) and (y, z) (figure 2).

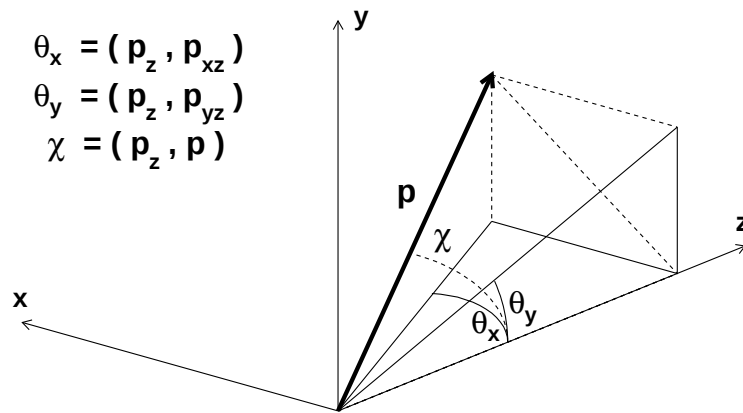


Figure 2. Variables (p, θ_x, θ_y) in the case of a momentum such that $p_z > 0$. θ_x and θ_y are the diffraction angles and χ is the deflection angle. $\mathbf{p}_z$, $\mathbf{p}_{xz}$ and $\mathbf{p}_{yz}$ are respectively the projections of the vector $\mathbf{p}$ on the z axis and on the planes (x, z) and (y, z) .

It can be assumed that the momentum of the particle associated with the diffracted wave is always such that $p_z > 0$. It turns out that the three variables (p, θ_x, θ_y) can replace the Cartesian variables over the whole half-space $p_z > 0$. In this half-space, we have: $p \in]0, \infty[$, $\theta_x \in]-\pi/2, +\pi/2[$, $\theta_y \in]-\pi/2, +\pi/2[$. So, the change of the variables (p_x, p_y, p_z) into the variables (p, θ_x, θ_y) is made by the following one-to-one transformation $\mathcal{H}$:

$$\mathcal{H}(p_x, p_y, p_z) \equiv \begin{cases} p = \sqrt{p_x^2 + p_y^2 + p_z^2} \\ \theta_x = \arctg(p_x/p_z) \\ \theta_y = \arctg(p_y/p_z) \end{cases}, \quad (6)$$

$$\mathcal{H}^{-1}(p, \theta_x, \theta_y) = \mathbf{p}(p, \theta_x, \theta_y) = \begin{cases} p_x = p \cos \chi \operatorname{tg} \theta_x \\ p_y = p \cos \chi \operatorname{tg} \theta_y \\ p_z = p \cos \chi \end{cases}, \quad (7)$$

where the deflection angle χ can be expressed as a function of θ_x and θ_y :

$$\chi \equiv \chi(\theta_x, \theta_y) = \arccos \left[(1 + \operatorname{tg}^2 \theta_x + \operatorname{tg}^2 \theta_y)^{-1/2} \right] \quad (8)$$

and is such that $0 \leq \chi < \pi/2$. For the small angles, we have from (7): $p_x \simeq p \theta_x$, $p_y \simeq p \theta_y$ and $p_z \simeq p$ so that we recover the diffraction angles θ_x and θ_y defined in [3].

2.4 Predictions of the classical theories for the relative intensity

From the experimental point of view, the quantity to be measured is the *directional intensity* $I(\theta_x, \theta_y)$ which is defined as the number of particles emitted from the origin O in the direction (θ_x, θ_y) per unit time and per unit solid angle (for simplicity, we assume that the rate of particle emission by the source is stable so that the intensity is time independent). Then, we obtain the *relative directional intensity* $I(\theta_x, \theta_y)/I(0,0)$ (hereafter called *relative intensity*) between the direction (θ_x, θ_y) and the forward direction $(0,0)$, used as the reference direction.

In the classical theory, the squared modulus of the amplitude at the observation point of radius-vector $\mathbf{d}$ is equal to the *local intensity* at that point. In the present case, where the size of the aperture is negligible compared to the distance d , this local intensity is defined as the number of particles coming from the origin O and arriving at point $\mathbf{d}$ per unit time and per unit area orthogonal to the radius vector $\mathbf{d}$. Since $\mathbf{d}$ and $\mathbf{p}$ have the same direction (see (4)), the local intensity at point $\mathbf{d}$ is proportional to the directional intensity $I_{\text{Class.}}^{p,A}(\theta_x, \theta_y)$ where θ_x and θ_y correspond to the direction of $\mathbf{p}$ and thus are given by (6). Therefore:

$$\left[\frac{I(\theta_x, \theta_y)}{I(0,0)} \right]_{\text{Class.}}^{p,A} = \frac{\left| \mathcal{U}_{\text{Class.}}^{p,A} \left(d, \frac{\mathbf{p}(p, \theta_x, \theta_y)}{p} \right) \right|^2}{\left| \mathcal{U}_{\text{Class.}}^{p,A} \left(d, \frac{\mathbf{p}(p, 0, 0)}{p} \right) \right|^2}. \quad (9)$$

Expressing $\mathbf{p}(p, \theta_x, \theta_y)$ and $\mathbf{p}(p, 0, 0)$ from (7) and substituting into (5) and then into (9), we see that d is eliminated and, denoting $S(A)$ the area of A , we get:

$$\left[\frac{I(\theta_x, \theta_y)}{I(0,0)} \right]_{\text{Class.}}^{p,A} \simeq \frac{\Omega(\chi)^2}{S(A)^2} \left| \iint_A dx dy \exp[-(i/\hbar)(p \cos \chi)(x \text{tg } \theta_x + y \text{tg } \theta_y)] \right|^2, \quad (10)$$

which is the prediction of the classical theories for the relative intensity over the whole angular range $\theta_x \in]-\pi/2, +\pi/2[$, $\theta_y \in]-\pi/2, +\pi/2[$.

3 Quantum model of diffraction by an aperture

3.1 Initial state

In order to compare the predictions of the quantum model with those of the classical theories presented in section 2, we choose as initial state the one associated with the monochromatic plane wave in normal incidence. This state is close to a momentum and energy eigenstate (therefore a stationary state) of the form:

$$\left| \psi_{\mathbf{p}_0}^{\text{in}}(t) \right\rangle = \exp[-(i/\hbar)E(p_0)t] \left| \mathbf{p}_0 \right\rangle, \quad (11)$$

where $\mathbf{p}_0 = (p_{0x}, p_{0y}, p_{0z}) = (0, 0, p_0)$ is the momentum of the incident particle and $E(p_0) = c\sqrt{m^2c^2 + p_0^2}$ is its energy. Since $\mathbf{p}_0 \cdot \mathbf{r} = p_0 z$, the position wave function of this initial state is the plane wave: $(2\pi\hbar)^{-3/2} \exp\{(i/\hbar)[p_0 z - E(p_0)t]\}$.

3.2 Position quantum measurement by a diaphragm

In the quantum theory, the diaphragm is considered as an apparatus for measuring the position of the incident particle [19, 23]. It is assumed that the process involving this position *quantum measurement* takes place in two stages:

(1) The actual quantum measurement, involving an interaction between the diaphragm and the particle passing through the aperture [24]. This interaction is assumed to be instantaneous and occur at some time t_1 . At this time, the initial state is projected on the final state and the initial position wave function undergoes a filtering so that the final position wave function is non-zero only in the region of the aperture (postulate of wave function reduction).

(2) The detection of the particle beyond the diaphragm, *after* the quantum measurement, at time $t_2 > t_1$. At that time t_2 , the final state of the particle has evolved since the time t_1 and corresponds to the diffracted wave propagating beyond the diaphragm. The detection of the particle at time t_2 can be considered as proof that a quantum measurement has occurred on it at a time t_1 prior to t_2 .

The aperture is located in the transverse plane and is bounded by an edge which clearly separates the "empty" part (i.e. the aperture itself) from the opaque part of the diaphragm. So, the initial position wave function undergoes a *transverse filtering* which corresponds to the measurement of the transverse coordinates (x, y) of the particle. However, two reasons lead us to assume that there exists a *longitudinal filtering*, so that the longitudinal coordinate z is also measured:

(a) At the time t_1 of the quantum measurement, the transverse coordinates (x, y) of the particle are experimentally determined with an accuracy corresponding to the size of the diaphragm aperture. However, at that time, the particle "is passing through the aperture", so that it cannot be too far from the plane of the diaphragm. Therefore, we can assume that its longitudinal coordinate z is also determined experimentally with some accuracy. Moreover, according to the Huygens-Fresnel principle, the particle detected beyond the diaphragm is associated with spherical waves emitted from the wavefront at the aperture. We can assume that the emission of these spherical waves begins at the time t_1 of the change of state caused by the quantum measurement and consequently that the particle is, at that time, on the wavefront at the aperture or at least in its proximity, hence in a region limited not only in (x, y) but also in z .

(b) During its passage through the aperture, the incident particle exchanges energy and momentum with the diaphragm [24]. However, in the kinematic conditions of the experiment (microscopic object interacting with a macroscopic device), the particle transfers a very small part of its energy to the diaphragm, so that the momentum modulus of the particle is almost conserved. So, denoting $\mathbf{p}$ the final momentum, we have the kinematic constraint:

$$\mathbf{p} \neq \mathbf{p}_0 \text{ in general, however: } p \simeq p_0. \quad (12)$$

Therefore, a change of p_{0x} and p_{0y} during the particle-diaphragm interaction must imply a change of p_{0z} , so that the relation $\sqrt{p_x^2 + p_y^2 + p_z^2} \simeq \sqrt{p_{0x}^2 + p_{0y}^2 + p_{0z}^2} = p_0$ is satisfied.

Since the changes of p_{0x} and p_{0y} result from filterings in x and y , we can assume that the change of p_{0z} results from a filtering in z . Conversely, if we consider that z is not measured, then it can be assumed that p_{0z} does not change. However, the measurement of x and y changes p_{0x} and p_{0y} . Therefore the modulus p_0 changes, which is not compatible with kinematics.

Remark. It is possible to show the non-conservation of the momentum modulus if z is not measured in the case of the initial state $|\psi_{\mathbf{p}_0}^{\text{in}}(t_1)\rangle$ defined by (11). If z is not measured, the projection to the final state is made by the operator $\iint_A dx dy |xy\rangle\langle xy| \otimes \int_{\mathbb{R}} dz |z\rangle\langle z|$. Applying this operator to $|\psi_{\mathbf{p}_0}^{\text{in}}(t_1)\rangle$, we obtain a final state which momentum wave function is equal to $(2\pi\hbar)^{-2} \exp[-(i/\hbar)E(p_0)t_1] \delta(p_0 - p_z) \iint_A dx dy \exp[-(i/\hbar)(p_x x + p_y y)]$. This wave function is non-zero only if $p_z = p_0$ whatever p_x and p_y . Therefore, we have most often: $p > p_0$, so that the modulus of the momentum is not conserved.

It therefore appears necessary to apply the postulate of wave function reduction to the *three* observables $\hat{X}, \hat{Y}, \hat{Z}$. This is the first assumption of the quantum model. It can be reformulated as follows:

Assumption 1. *A diaphragm is a device for measuring the three spatial coordinates of any particle passing through its aperture.*

Two issues then arise:

(i) Since the aperture is limited by an edge in the transverse plane whereas there are no edges along the longitudinal direction, the transverse filtering is not of the same type as that of the longitudinal filtering. This will lead to generalize the notion of projector (question treated in subsection 3.3 hereafter).

(ii) Since the three spatial coordinates are measured, the projection of the initial state causes, at time t_1 , a strong localization of the position wave function at the aperture, both in the transverse and longitudinal directions. However, due to the kinematic constraint (12), the final state of the particle after its interaction with the diaphragm must be very close to an energy eigenstate associated with the eigenvalue $E(p_0)$. Consequently, the spreading of the final wave packet in the radial directions from the origin O must be almost as large as that of the initial wave packet in the longitudinal direction (figure 1). The quantum model must therefore describe the transition from a very localized wave function at time t_1 towards a wave function whose extension is comparable to that of the initial wave packet as soon as $t > t_1$. This will lead to add an energy-momentum filtering to the position filtering (question treated in subsections 3.4 - 3.7 hereafter).

3.3 Position filtering with a reduction operator

We can consider that the transverse filtering is uniform on the whole area of the aperture so that the initial position wave function is simply transversely truncated. For the longitudinal coordinate, the absence of edges makes it difficult to assume a similar truncation and consequently to justify a uniform filtering. It seems preferable to consider a possibly non-

uniform longitudinal filtering, such that the transmission would be maximum in the plane of the diaphragm ($z = 0$) and would decrease to zero continuously on each side of this plane. According to the Huygens-Fresnel principle, this decrease should be "infinitely" rapid, so that the transmission function would be equal to the Dirac function $\delta(z)$. However, it is interesting to consider the more general case of a finite function forming a peak with a non-zero width. The Dirac function then corresponds to the limit case where the width tends to zero. Taking into account such a filtering with this type of transmission function requires to generalize the notion of projector.

Let us first consider an observable $\hat{X}$ having a non-degenerate 1D continuous spectrum and suppose that the measurement of $\hat{X}$ on a system in the initial state $|\psi^{\text{in}}\rangle$ gives a result within the interval $[x_0 - \Delta x/2, x_0 + \Delta x/2]$. Such a measurement projects the initial state on the following final state (see [21], §III.E.2.d.β, p.265):

$$|\psi^{x_0, \Delta x}\rangle = \frac{\hat{P}^{x_0, \Delta x} |\psi^{\text{in}}\rangle}{\sqrt{\langle \psi^{\text{in}} | \hat{P}^{x_0, \Delta x} | \psi^{\text{in}} \rangle}}, \quad (13)$$

where $\hat{P}^{x_0, \Delta x}$ is the projector:

$$\hat{P}^{x_0, \Delta x} \equiv \int_{x_0 - \Delta x/2}^{x_0 + \Delta x/2} dx |x\rangle \langle x|. \quad (14)$$

Since $\hat{P}^{x_0, \Delta x} = (\hat{P}^{x_0, \Delta x})^\dagger \hat{P}^{x_0, \Delta x}$, the denominator of the right-hand side of (13) is a normalization term which ensures that the state $|\psi^{x_0, \Delta x}\rangle$ is normalized to 1. Substituting (14) into (13) and multiplying by $\langle x|$, we can check that the action of the projector consists in filtering the initial position wave function, so that $\langle x | \psi^{x_0, \Delta x} \rangle$ is proportional to $\langle x | \psi^{\text{in}} \rangle$ for $x \in [x_0 - \Delta x/2, x_0 + \Delta x/2]$ and zero elsewhere. We can rewrite (14) in the form:

$$\hat{P}^{x_0, \Delta x} = \int_{\mathbb{R}} dx f_1^{x_0, \Delta x}(x) |x\rangle \langle x|, \quad (15)$$

where $f_1^{x_0, \Delta x}(x)$ is a *transmission function* equal to 1 if $x \in [x_0 - \Delta x/2, x_0 + \Delta x/2]$ or 0 otherwise. The projector defined by (14) is therefore associated with a *uniform* filtering on the interval $[x_0 - \Delta x/2, x_0 + \Delta x/2]$.

In order to take into account more general filterings, we replace (13) by

$$|\psi^{x_0, \Delta x}\rangle = \frac{\hat{R}^{x_0, \Delta x} |\psi^{\text{in}}\rangle}{\sqrt{\langle \psi^{\text{in}} | (\hat{R}^{x_0, \Delta x})^\dagger \hat{R}^{x_0, \Delta x} | \psi^{\text{in}} \rangle}}, \quad (16)$$

where $\hat{R}^{x_0, \Delta x}$ is a "generalized projector" called *reduction operator* and defined, by analogy with (15), as

$$\hat{R}^{x_0, \Delta x} \equiv \int_{\mathbb{R}} dx f^{x_0, \Delta x}(x) |x\rangle \langle x|, \quad (17)$$

where the transmission function $f^{x_0, \Delta x}(x)$ is this time not necessarily constant in the interval $[x_0 - \Delta x/2, x_0 + \Delta x/2]$ and zero elsewhere. For example, $f^{x_0, \Delta x}(x)$ can be a Gaussian centered at x_0 and of width Δx . The formulation (16) ensures that the state $|\psi^{x_0, \Delta x}\rangle$ is automatically

normalized to 1. Substituting (17) into (16) and expressing the probability density function (p.d.f.), we find:

$$\left| \langle x | \psi^{x_0, \Delta x} \rangle \right|^2 = \frac{f^{x_0, \Delta x}(x)^2 \left| \langle x | \psi^{\text{in}} \rangle \right|^2}{\int_{\mathbb{R}} dx' f^{x_0, \Delta x}(x')^2 \left| \langle x' | \psi^{\text{in}} \rangle \right|^2}. \quad (18)$$

For equation (18) to make sense at the limit $\Delta x \rightarrow 0$, it is necessary that $f^{x_0, 0}(x)^2 = C \delta(x - x_0)$ where C is a constant of arbitrary value and dimension. The easiest way is to choose $C = 1$, dimensionless. Thus, $f^{x_0, 0}(x)^2$ has the same dimension as that of $\delta(x - x_0)$ and therefore is a p.d.f.. Then, since the passage to the limit is continuous, it is logical to assume that $f^{x_0, \Delta x}(x)^2$ is a p.d.f. whatever $(x_0, \Delta x)$. Hence, by defining: $F_X^{x_0, \Delta x}(x) \equiv f^{x_0, \Delta x}(x)^2$, we see, from (17), that $\hat{R}^{x_0, \Delta x}$ is of the form:

$$\hat{R}^{x_0, \Delta x} \equiv \int_{\mathbb{R}} dx \sqrt{F_X^{x_0, \Delta x}(x)} |x\rangle \langle x|, \quad (19)$$

where $F_X^{x_0, \Delta x}(x)$ is a p.d.f. called *filtering p.d.f.*, where the subscript X represents the random variable associated with the measurement of the observable $\hat{X}$.

In principle, Δx cannot be strictly equal to zero because $F_X^{x_0, 0}(x) = \delta(x - x_0)$ so that we would get the square root of a Dirac function in (19). Nevertheless, we can treat this case by performing the calculations with a Gaussian distribution, and then calculating the limit when its width tends to zero.

From (19), we have: $(\hat{R}^{x_0, \Delta x})^2 \neq \hat{R}^{x_0, \Delta x}$, contrary to the case of a projector. However, for the uniform distribution: $F_X^{x_0, \Delta x}(x) = 1/\Delta x$ if $x \in [x_0 - \Delta x/2, x_0 + \Delta x/2]$ or 0 otherwise, the equations (14) and (19) lead to: $\hat{R}^{x_0, \Delta x} = (1/\sqrt{\Delta x}) \hat{P}^{x_0, \Delta x}$. Substituting into (16), we see that the factor $1/\sqrt{\Delta x}$ is eliminated and, since $(\hat{P}^{x_0, \Delta x})^\dagger \hat{P}^{x_0, \Delta x} = \hat{P}^{x_0, \Delta x}$, we finally obtain the *same state* $|\psi^{x_0, \Delta x}\rangle$ as that of equation (13). Therefore, the reduction operator is suitable for processing the change of state in the case of the measurement of an observable having a continuous spectrum: it allows to treat any type of filtering and it can be used in place of the usual projector in the particular case of a uniform filtering.

We now come to the three-dimensional generalization of (16) and (19). Since there are no edges in the longitudinal direction, the 3D equivalent of $F_X^{x_0, \Delta x}(x)$ for a diaphragm with an aperture A can be denoted $F_{\mathbf{R}}^{\mathcal{A}}(\mathbf{r})$ where the subscript $\mathcal{A}$ represents the volume in which $F_{\mathbf{R}}^{\mathcal{A}}(\mathbf{r})$ is not negligible. This volume includes the 2D aperture A and its width in the longitudinal direction is determined by the transmission function in this direction. It will be called "3D aperture $\mathcal{A}$ " in the following. The postulate of wave function reduction applied to the initial state $|\psi_{\mathbf{p}_0}^{\text{in}}(t_1)\rangle$ can then be formulated as follows:

Postulate of wave function reduction under the assumption 1. *The final state of the particle outgoing from the 3D aperture $\mathcal{A}$ immediately after interacting at time t_1 with the diaphragm is expressed by*

$$|\psi^{\mathcal{A}}(t_1)\rangle = \frac{\hat{R}^{\mathcal{A}} |\psi_{\mathbf{p}_0}^{\text{in}}(t_1)\rangle}{\sqrt{\langle \psi_{\mathbf{p}_0}^{\text{in}}(t_1) | (\hat{R}^{\mathcal{A}})^\dagger \hat{R}^{\mathcal{A}} | \psi_{\mathbf{p}_0}^{\text{in}}(t_1) \rangle}}, \quad (20)$$

where $\hat{\mathbf{R}}^{\mathcal{A}}$ is a "position reduction operator" defined as

$$\hat{\mathbf{R}}^{\mathcal{A}} \equiv \iiint_{\mathbb{R}^3} d^3r \sqrt{F_{\mathbf{R}}^{\mathcal{A}}(\mathbf{r})} |\mathbf{r}\rangle \langle \mathbf{r}|, \quad (21)$$

where $F_{\mathbf{R}}^{\mathcal{A}}(\mathbf{r})$ is a "position filtering p.d.f." defined on the 3D space and non-negligible only in the 3D aperture $\mathcal{A}$.

The expression of the p.d.f. $F_{\mathbf{R}}^{\mathcal{A}}(\mathbf{r})$ will be given later in subsection 3.8.

3.4 Inadequacy of the only-position filtering

The equation (20) expresses the final state only at time t_1 . It is therefore necessary to express the final state for $t > t_1$. Two observations allow to express two properties that the final state after time t_1 must have. First, due to the kinematic constraint (12), the final energy of the particle is very close to its initial energy $E(p_0)$. Secondly, experiment shows that there is no diffracted wave returning to the region where the source is located. This implies that the particle associated with the diffracted wave is always such that $p_z > 0$. Therefore, the final state must have the two following properties:

(P1) Compatibility with kinematics: the final state for $t > t_1$ is very close to an energy eigenstate associated with the eigenvalue $E(p_0)$.

(P2) Compatibility with the presence of the diffracted wave only beyond the diaphragm: the final state for $t > t_1$ is such that its momentum wave function is zero for $p_z \leq 0$.

Let us verify whether the state $|\psi^{\mathcal{A}}(t_1)\rangle$ given by (20) can evolve towards a state having the properties (P1) and (P2). Expressing $\hat{\mathbf{R}}^{\mathcal{A}} |\psi_{\mathbf{p}_0}^{\text{in}}(t_1)\rangle$ from (11) and (21) and substituting into (20), we get

$$|\psi^{\mathcal{A}}(t_1)\rangle = \exp[-(i/\hbar)E(p_0)t_1] \iiint_{\mathbb{R}^3} d^3r \sqrt{F_{\mathbf{R}}^{\mathcal{A}}(\mathbf{r})} \exp[(i/\hbar)p_0 z] |\mathbf{r}\rangle. \quad (22)$$

Hence: $|\langle \mathbf{r} | \psi^{\mathcal{A}}(t_1) \rangle|^2 = F_{\mathbf{R}}^{\mathcal{A}}(\mathbf{r})$ which is non-negligible only in the 3D aperture $\mathcal{A}$, due to the postulate of wave function reduction. Therefore:

$$\left| \langle \mathbf{r} | \psi^{\mathcal{A}}(t_1) \rangle \right|^2 \simeq 0 \text{ everywhere except in the 3D aperture } \mathcal{A}. \quad (23)$$

The position wave function of the state $|\psi^{\mathcal{A}}(t_1)\rangle$ is therefore strongly localized at the aperture. This results in a large spreading of the distributions of the three momentum components. It is therefore very likely that the distribution of the momentum modulus is also spread out and, consequently, that the state in question is not an energy eigenstate. Suppose, however, that this state is an energy eigenstate. In that case, it is a stationary state and it makes sense to consider it as the starting state of the temporal evolution of a state $|\psi^{\mathcal{A}}(t)\rangle$ having the property (P1). Therefore, $\forall t \geq t_1 : |\psi^{\mathcal{A}}(t)\rangle = \exp[-(i/\hbar)E(p_0)(t - t_1)] |\psi^{\mathcal{A}}(t_1)\rangle$ and, consequently, equation (23) is satisfied whatever $t \geq t_1$. As a result, the particle remains indefinitely trapped inside the 3D aperture $\mathcal{A}$, so that the average value of p_z is zero. Thus, the state has not the property

(P2). So, either the state $|\psi^{\mathcal{A}}(t_1)\rangle$ cannot evolve towards a state having the property (P1) or it can evolve towards a state having the property (P1) but then it has not the property (P2). This implies that the state $|\psi^{\mathcal{A}}(t_1)\rangle$ cannot evolve towards the state that must be that of the particle after its passage through the aperture of the diaphragm. We are thus led to the following conclusion: *at time t_1 , the state $|\psi^{\mathcal{A}}(t_1)\rangle$ must be immediately transformed by means of a new projection to a state having the properties (P1) and (P2).*

In summary: for any position filtering p.d.f. $F_{\mathbf{R}}^{\mathcal{A}}(\mathbf{r})$ non-negligible only in the 3D aperture $\mathcal{A}$, the state obtained from a position filtering only (see (20)-(21)) is necessarily a transitional state. This state must immediately undergo the action of an appropriate operator in order to become a final state close to an energy eigenstate associated with the eigenvalue $E(p_0)$ and such that its momentum wave function is zero for $p_z \leq 0$.

3.5 Position and energy-momentum filtering

From the above conclusion, the appropriate final state would be of the form:

$$|\psi^{p_0, \mathcal{A}}(t_1)\rangle = \frac{\hat{R}^{p_0} |\psi^{\mathcal{A}}(t_1)\rangle}{\sqrt{\langle \psi^{\mathcal{A}}(t_1) | (\hat{R}^{p_0})^\dagger \hat{R}^{p_0} | \psi^{\mathcal{A}}(t_1) \rangle}}, \quad (24)$$

where $\hat{R}^{p_0}$ would be an energy-momentum reduction operator projecting on a state such that the momentum modulus p.d.f. is close to $\delta(p - p_0)$ (hence the need for this operator to depend on p_0) and such that the momentum p.d.f. is zero for $p_z \leq 0$. Then, to obtain the expression of $|\psi^{p_0, \mathcal{A}}(t_1)\rangle$ as a function of the initial state $|\psi_{\mathbf{p}_0}^{\text{in}}(t_1)\rangle$, we substitute (20) into (24). The result is the expression (25) below, which is the second assumption of the quantum model.

Assumption 2. *Contrary to (20), the final state of the particle outgoing from the 3D aperture $\mathcal{A}$ immediately after interacting at time t_1 with the diaphragm is*

$$|\psi^{p_0, \mathcal{A}}(t_1)\rangle = \frac{\hat{R}^{p_0} \hat{R}^{\mathcal{A}} |\psi_{\mathbf{p}_0}^{\text{in}}(t_1)\rangle}{\sqrt{\langle \psi_{\mathbf{p}_0}^{\text{in}}(t_1) | (\hat{R}^{p_0} \hat{R}^{\mathcal{A}})^\dagger \hat{R}^{p_0} \hat{R}^{\mathcal{A}} | \psi_{\mathbf{p}_0}^{\text{in}}(t_1) \rangle}}, \quad (25)$$

where $\hat{R}^{\mathcal{A}}$ is the position reduction operator defined by (21) and $\hat{R}^{p_0}$ is an "energy-momentum reduction operator" defined, by analogy with (21), as

$$\hat{R}^{p_0} \equiv \iiint_{\mathbb{R}^3} d^3p \sqrt{F_{\mathbf{p}}^{p_0}(\mathbf{p})} |\mathbf{p}\rangle \langle \mathbf{p}|, \quad (26)$$

where $F_{\mathbf{p}}^{p_0}(\mathbf{p})$ is an "energy-momentum filtering p.d.f." defined as

$$F_{\mathbf{p}}^{p_0}(\mathbf{p}) \equiv \delta_{1 \text{sgn}[p_z]} \tilde{\delta}_p^{\Delta p}(|\mathbf{p}| - p_0), \quad (27)$$

where $\tilde{\delta}_p^{\Delta p}(|\mathbf{p}| - p_0)$ is a function forming a peak centered at $|\mathbf{p}| = p_0$, of width Δp close to zero but non-zero.

The width Δp is non-zero because the particle energy is not strictly conserved. Consequently $\sqrt{\tilde{\delta}_p^{\Delta p}(|\mathbf{p}| - p_0)}$ is well-defined and therefore (26) makes sense. The interpretation of (27) is therefore as follows: the filtering p.d.f. $F_{\mathbf{p}}^{p_0}(\mathbf{p})$ selects all the possible values of the momentum components such that the momentum modulus is close to p_0 (term $\tilde{\delta}_p^{\Delta p}(|\mathbf{p}| - p_0)$, property (P1)) and such that $p_z > 0$ (term $\delta_{1\text{sgn}[p_z]}$, property (P2)).

3.6 Quantum state associated with the diffracted wave

We now have all the ingredients to express the final state and to check if this state has the properties (P1) and (P2) mentioned in subsection 3.4. Substituting (21) and (26) into (25), and given (11) and (27), we are led to the following expression of the final state at time t_1 :

$$\begin{aligned} \left| \psi^{p_0, \mathcal{A}}(t_1) \right\rangle &= \frac{\exp[-(i/\hbar)E(p_0)t_1]}{\sqrt{N^{\mathcal{A}}(\mathbf{p}_0, \Delta p)}} \\ &\times \iiint_{\mathbb{R}^3} d^3 p \, \delta_{1\text{sgn}[p_z]} \sqrt{\tilde{\delta}_p^{\Delta p}(|\mathbf{p}| - p_0)} \mathcal{F}_{\mathbf{p}}^{\mathcal{A}}(\mathbf{p} - \mathbf{p}_0) |\mathbf{p}\rangle, \end{aligned} \quad (28)$$

where $\mathcal{F}_{\mathbf{p}}^{\mathcal{A}}(\mathbf{p} - \mathbf{p}_0)$ is the Fourier transform of the square root of the position filtering p.d.f.:

$$\mathcal{F}_{\mathbf{p}}^{\mathcal{A}}(\mathbf{p} - \mathbf{p}_0) \equiv \frac{1}{(2\pi\hbar)^{3/2}} \iiint_{\mathbb{R}^3} d^3 r \sqrt{F_{\mathbf{R}}^{\mathcal{A}}(\mathbf{r})} \exp[-(i/\hbar)(\mathbf{p} - \mathbf{p}_0) \cdot \mathbf{r}] \quad (29)$$

and $N^{\mathcal{A}}(\mathbf{p}_0, \Delta p)$ is the normalization term:

$$N^{\mathcal{A}}(\mathbf{p}_0, \Delta p) \equiv \iiint_{\mathbb{R}^3} d^3 p \, \delta_{1\text{sgn}[p_z]} \tilde{\delta}_p^{\Delta p}(|\mathbf{p}| - p_0) \left| \mathcal{F}_{\mathbf{p}}^{\mathcal{A}}(\mathbf{p} - \mathbf{p}_0) \right|^2. \quad (30)$$

From (28), the final momentum p.d.f. is independent of t_1 . So this p.d.f. can be written in the form:

$$\forall t_1 : \left| \langle \mathbf{p} | \psi^{p_0, \mathcal{A}}(t_1) \rangle \right|^2 \equiv f_{\mathbf{p}}^{p_0, \mathcal{A}}(\mathbf{p}). \quad (31)$$

From (28) and (31), we have:

$$f_{\mathbf{p}}^{p_0, \mathcal{A}}(\mathbf{p}) = \frac{1}{N^{\mathcal{A}}(\mathbf{p}_0, \Delta p)} \delta_{1\text{sgn}[p_z]} \tilde{\delta}_p^{\Delta p}(|\mathbf{p}| - p_0) \left| \mathcal{F}_{\mathbf{p}}^{\mathcal{A}}(\mathbf{p} - \mathbf{p}_0) \right|^2, \quad (32)$$

which can be considered as a p.d.f. defined in the half-space $p_z > 0$, due to the factor $\delta_{1\text{sgn}[p_z]}$. Such a p.d.f. can be transformed into a p.d.f. of the variables (p, θ_x, θ_y) by using the change of variables formula associated with the one-to-one transformation $\mathcal{H}$ (see (6)-(7)):

$$f_{P, \Theta_x, \Theta_y}^{p_0, \mathcal{A}}(p, \theta_x, \theta_y) = p^2 \Gamma(\theta_x, \theta_y) f_{\mathbf{p}}^{p_0, \mathcal{A}}(\mathbf{p}(p, \theta_x, \theta_y)), \quad (33)$$

where $\mathbf{p}(p, \theta_x, \theta_y)$ is given by (7) and

$$\Gamma(\theta_x, \theta_y) \equiv \frac{1}{p^2} \left| \det \left(\frac{\partial [p_x, p_y, p_z]}{\partial [p, \theta_x, \theta_y]} \right) \right| = \frac{\cos^3 \chi}{\cos^2 \theta_x \cos^2 \theta_y} \quad (34)$$

is the *angular factor* (absolute value of the jacobian of $\mathcal{H}^{-1}$ divided by p^2) which has been calculated from (7) and (8). From (32) and using the fact that $\text{sgn}[p_z(p, \theta_x, \theta_y)] = 1$ in the

half-space $z > 0$ and that $\mathbf{p}_0 = (0, 0, p_0) = \mathbf{p}(p_0, 0, 0)$, we can express $f_{\mathbf{p}}^{p_0, \mathcal{A}}(\mathbf{p}(p, \theta_x, \theta_y))$ and then apply the change of variables formula (33) to get the p.d.f. $f_{P, \Theta_x, \Theta_y}^{p_0, \mathcal{A}}(p, \theta_x, \theta_y)$. The result can be expressed in the form:

$$f_{P, \Theta_x, \Theta_y}^{p_0, \mathcal{A}}(p, \theta_x, \theta_y) = \frac{p^2 \tilde{\delta}_p^{\Delta p}(p - p_0)}{N^{\mathcal{A}}(\mathbf{p}_0, \Delta p)} \Gamma(\theta_x, \theta_y) \left| \mathcal{F}_{\mathbf{p}}^{\mathcal{A}}(\mathbf{p}(p, \theta_x, \theta_y) - \mathbf{p}(p_0, 0, 0)) \right|^2. \quad (35)$$

Then, to express $N^{\mathcal{A}}(\mathbf{p}_0, \Delta p)$, we apply the change of variables $(p_x, p_y, p_z) \rightarrow (p, \theta_x, \theta_y)$ in the integral of the right-hand side of (30). We obtain:

$$\begin{aligned} N^{\mathcal{A}}(\mathbf{p}_0, \Delta p) &= \int_0^\infty dp \, p^2 \tilde{\delta}_p^{\Delta p}(p - p_0) \\ &\quad \times \int_{-\pi/2}^{+\pi/2} d\theta_x \int_{-\pi/2}^{+\pi/2} d\theta_y \, \Gamma(\theta_x, \theta_y) \left| \mathcal{F}_{\mathbf{p}}^{\mathcal{A}}(\mathbf{p}(p, \theta_x, \theta_y) - \mathbf{p}(p_0, 0, 0)) \right|^2. \end{aligned} \quad (36)$$

Since Δp is close to zero and the p.d.f. $\tilde{\delta}_p^{\Delta p}(p - p_0)$ is not under a square root in (35) and (36), we can replace it by the Dirac distribution $\delta(p - p_0)$. Given the property: $f(x)\delta(x - x_0) = f(x_0)\delta(x - x_0)$, this leads to:

$$f_{P, \Theta_x, \Theta_y}^{p_0, \mathcal{A}}(p, \theta_x, \theta_y) \simeq \frac{p_0^2 \delta(p - p_0)}{N^{\mathcal{A}}(\mathbf{p}_0, 0)} \Gamma(\theta_x, \theta_y) \left| \mathcal{F}_{\mathbf{p}}^{\mathcal{A}}(\mathbf{p}(p_0, \theta_x, \theta_y) - \mathbf{p}(p_0, 0, 0)) \right|^2. \quad (37)$$

Then the marginal p.d.f. $f_P^{p_0, \mathcal{A}}(p)$ is obtained by integrating (37) over θ_x and θ_y . Expressing $N^{\mathcal{A}}(\mathbf{p}_0, 0)$ from (36) applied to $\Delta p = 0$, we see that this integration of (37) leads to an expression where $N^{\mathcal{A}}(\mathbf{p}_0, 0)$ is eliminated. What remains is

$$f_P^{p_0, \mathcal{A}}(p) \simeq \delta(p - p_0). \quad (38)$$

Therefore we have $p \simeq p_0$ in the final state which is exactly the kinematic constraint expressed by (12).

The equation (38) confirms that the final state at time t_1 given by (28) is close to an energy eigenstate associated with the eigenvalue $E(p_0)$. Therefore, this final state is close to a stationary state, so that its temporal evolution can be expressed by

$$\forall t \geq t_1 : \quad \left| \psi^{p_0, \mathcal{A}}(t) \right\rangle \simeq \exp[-(i/\hbar) E(p_0)(t - t_1)] \left| \psi^{p_0, \mathcal{A}}(t_1) \right\rangle. \quad (39)$$

So, from (31), (32) and (39), we see that:

$$\forall t \geq t_1, \forall p_z \leq 0 : \quad \left\langle \mathbf{p} \left| \psi^{p_0, \mathcal{A}}(t) \right\rangle = 0. \quad (40)$$

Finally, from (39) and (40), the final state $\left| \psi^{p_0, \mathcal{A}}(t) \right\rangle$ has the properties (P1) and (P2) mentioned in subsection 3.4 and is therefore the appropriate final state that we can associate with the diffracted wave beyond the diaphragm.

3.7 Discussion

The assumption 2 suggests to apply the postulate of wave function reduction by using (25) which involves the product of operators $\hat{R}^{p_0}\hat{R}^{\mathcal{A}}$. From (21) and (26), this product has two important features: (1) it is not commutative and (2) it depends on the momentum modulus p_0 of the incident particle.

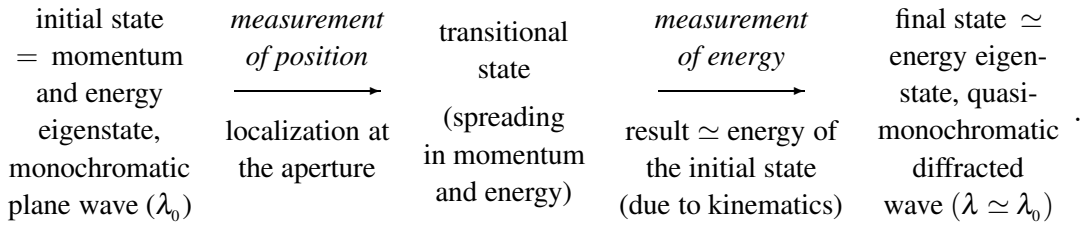
(1) The action of $\hat{R}^{p_0}\hat{R}^{\mathcal{A}}$ corresponds to two projections in a given order. First, the operator $\hat{R}^{\mathcal{A}}$ projects the initial state $|\psi_{\mathbf{p}_0}^{\text{in}}(t_1)\rangle$ on the transitional state $|\psi^{\mathcal{A}}(t_1)\rangle$ (see (20)). Secondly, the operator $\hat{R}^{p_0}$ projects this transitional state on the state $|\psi^{p_0,\mathcal{A}}(t_1)\rangle$ (see (24)) which is close to an energy eigenstate associated with the initial energy $E(p_0)$ (see (38)-(39)) and such that its momentum wave function is zero for $p_z \leq 0$ (see (40)). These two successive projections are equivalent to a direct transformation of the initial state $|\psi_{\mathbf{p}_0}^{\text{in}}(t_1)\rangle$ to the final state $|\psi^{p_0,\mathcal{A}}(t_1)\rangle$ (see (25)). Although $\hat{R}^{\mathcal{A}}$ and $\hat{R}^{p_0}$ do not commute, they do not correspond to two incompatible observables. The operator $\hat{R}^{\mathcal{A}}$ corresponds effectively to the three position observables $\hat{X}, \hat{Y}, \hat{Z}$ but the operator $\hat{R}^{p_0}$ does not correspond to the three observables associated with the momentum components. It corresponds to the *modulus* of the momentum. Due to kinematics, the measurement of the position of the particle causes a perturbation only on the *direction* of its momentum and not on the modulus. We can then admit that, although non-commutative, the product $\hat{R}^{p_0}\hat{R}^{\mathcal{A}}$ corresponds to two simultaneous measurements according to the following interpretation. The first measurement, associated with $\hat{R}^{\mathcal{A}}$, is the measurement of the position of the particle in the initial state $|\psi_{\mathbf{p}_0}^{\text{in}}(t_1)\rangle$. The second measurement, associated with $\hat{R}^{p_0}$, can be interpreted as a measurement of the energy of the particle in the transitional state $|\psi^{\mathcal{A}}(t_1)\rangle$ created by the position measurement, in the sense that the result $E(p_0)$ is obtained with near certainty after the interaction with the experimental device (in accordance with (38)). Although the process consists in two successive changes of state, we can consider that the two measurements are simultaneous because the particle occupies the transitional state $|\psi^{\mathcal{A}}(t_1)\rangle$ only at time t_1 .

Remark. If the order of the operators is inverted, the obtained state is the same as in the case of a position filtering only. Indeed, replacing $\hat{R}^{p_0}\hat{R}^{\mathcal{A}}$ by $\hat{R}^{\mathcal{A}}\hat{R}^{p_0}$ in (25) is equivalent to replace $|\psi_{\mathbf{p}_0}^{\text{in}}(t_1)\rangle$ by $\hat{R}^{p_0}|\psi_{\mathbf{p}_0}^{\text{in}}(t_1)\rangle$ in (20). From (11) and (26), we have: $\hat{R}^{p_0}|\psi_{\mathbf{p}_0}^{\text{in}}(t_1)\rangle = \sqrt{F_{\mathbf{P}}^{p_0}(\mathbf{p}_0)}|\psi_{\mathbf{p}_0}^{\text{in}}(t_1)\rangle$, which is expected since the initial state is an energy eigenstate associated with the eigenvalue $E(p_0)$. Hence, substituting into the right-hand side of (20) in place of $|\psi_{\mathbf{p}_0}^{\text{in}}(t_1)\rangle$, we see that $\sqrt{F_{\mathbf{P}}^{p_0}(\mathbf{p}_0)}$ is eliminated and we recover $|\psi^{\mathcal{A}}(t_1)\rangle$.

(2) In (20), the initial state $|\psi_{\mathbf{p}_0}^{\text{in}}(t_1)\rangle$ and the reduction operator $\hat{R}^{\mathcal{A}}$ can be respectively considered as representations of the incident particle and of the measurement device. Thus a sort of separation is established between the particle and the measurement device in the sense that, whatever the value of p_0 , the initial state is always projected by the same operator $\hat{R}^{\mathcal{A}}$ which then represents the "measurement device only". On the other hand, in (25), the initial state $|\psi_{\mathbf{p}_0}^{\text{in}}(t_1)\rangle$ still represents the incident particle but the operator $\hat{R}^{p_0}\hat{R}^{\mathcal{A}}$ depends on p_0 and consequently includes a piece of information on the incident particle. Therefore, the

operator $\hat{R}^{p_0}\hat{R}^{\mathcal{A}}$ is no longer a representation of the "measurement device only" but rather a representation of the system "particle + measurement device in interaction", so that there is no longer clear separation between the particle and the measurement device. The initial state is transformed by an operator which depends on this initial state itself (via $\hat{R}^{p_0}$). From this point of view, (25) seems more appropriate than (20) because it better reflects the fact that the measurement device and the particle form an inseparable system at the time of their interaction.

In summary, the order of the operators in the product $\hat{R}^{p_0}\hat{R}^{\mathcal{A}}$ and the fact that $\hat{R}^{p_0}$ depends on p_0 are two essential features of assumption 2. This assumption suggests to consider that the change of state of a particle - initially in a momentum eigenstate - at the time of a quantum measurement of position by a diaphragm is not a single projection but proceeds according to the following sequence:



The order of the measurements cannot be inverted because the associated operators do not commute. In spite of this non-commutativity, both measurements can be considered simultaneous if we admit that the transitional state is occupied for a period of time which tends to zero.

3.8 Quantum model prediction for the relative intensity in Fraunhofer diffraction

The marginal p.d.f. $f_{\Theta_x, \Theta_y}^{p_0, \mathcal{A}}(\theta_x, \theta_y)$ is the p.d.f. that the particle comes out of the aperture in the direction (θ_x, θ_y) . In Fraunhofer diffraction and if the wavelength is smaller than the size of the aperture, the latter, seen from the detectors, can be considered pointlike (see subsection 2.1). In this case, $f_{\Theta_x, \Theta_y}^{p_0, \mathcal{A}}(\theta_x, \theta_y)$ is equal to the directional intensity $I_{QM}^{p_0, \mathcal{A}}(\theta_x, \theta_y)$ normalized to 1:

$$\begin{aligned}
 \frac{I_{QM}^{p_0, \mathcal{A}}(\theta_x, \theta_y)}{\int_{-\pi/2}^{+\pi/2} d\theta'_x \int_{-\pi/2}^{+\pi/2} d\theta'_y I_{QM}^{p_0, \mathcal{A}}(\theta'_x, \theta'_y)} &= f_{\Theta_x, \Theta_y}^{p_0, \mathcal{A}}(\theta_x, \theta_y) \\
 &\equiv \int_0^\infty dp f_{P, \Theta_x, \Theta_y}^{p_0, \mathcal{A}}(p, \theta_x, \theta_y).
 \end{aligned} \tag{41}$$

From (41) (first equality), the relative intensity is given by

$$\left[\frac{I(\theta_x, \theta_y)}{I(0, 0)} \right]_{QM}^{p_0, \mathcal{A}} = \frac{f_{\Theta_x, \Theta_y}^{p_0, \mathcal{A}}(\theta_x, \theta_y)}{f_{\Theta_x, \Theta_y}^{p_0, \mathcal{A}}(0, 0)} \tag{42}$$

and can also be expressed in a form explicitly involving the final state ². From (41) (second equality), we calculate $f_{\Theta_x, \Theta_y}^{p_0, \mathcal{A}}(\theta_x, \theta_y)$ and $f_{\Theta_x, \Theta_y}^{p_0, \mathcal{A}}(0, 0)$ by integrating (37) over p . After this integration, given (12), it is convenient to replace p_0 with p , this latter notation henceforth indicating the modulus of both the initial momentum and the final momentum, as in section 2 where the conservation of the momentum modulus is implicitly assumed. Then, substituting the expressions of $f_{\Theta_x, \Theta_y}^{p, \mathcal{A}}(\theta_x, \theta_y)$ and $f_{\Theta_x, \Theta_y}^{p, \mathcal{A}}(0, 0)$ into (42) modified with the substitution $p_0 \rightarrow p$, we find:

$$\left[\frac{I(\theta_x, \theta_y)}{I(0, 0)} \right]_{\text{QM}}^{p, \mathcal{A}} \simeq \Gamma(\theta_x, \theta_y) \frac{|\mathcal{F}_{\mathbf{P}}^{\mathcal{A}}(\mathbf{p}(p, \theta_x, \theta_y) - \mathbf{p}(p, 0, 0))|^2}{|\mathcal{F}_{\mathbf{P}}^{\mathcal{A}}(0)|^2}. \quad (43)$$

To calculate the final state (see (28) and (30)) and the relative intensity (see (43)), it is necessary to calculate the Fourier transform of the square root of the position filtering p.d.f. $F_{\mathbf{R}}^{\mathcal{A}}(\mathbf{r})$ (see (29)). Therefore, we must express this p.d.f., which leads us to add a third assumption to the quantum model. The best possible assumption for $F_{\mathbf{R}}^{\mathcal{A}}(\mathbf{r})$ is that which would make it possible to express the "exact" theoretical final state from which it would in principle be possible to calculate any type of diffraction (Fresnel diffraction, Fraunhofer diffraction and intermediate case, according to the distance between the aperture and the detectors). It seems difficult to suggest such an assumption directly from general considerations. However, as a first test, we can use a simplified position filtering p.d.f. leading to an approximate state which allows to obtain a prediction for a given diffraction type. This is possible in the case of the Fraunhofer diffraction by using the following assumption:

Assumption 3. *In the case of the Fraunhofer diffraction, the 3D aperture $\mathcal{A}$ can be represented in the form $\mathcal{A} \equiv \{A, \Delta z\}$ where A is the 2D aperture in the diaphragm plane and Δz represents the transmission width of the longitudinal filtering. The position filtering p.d.f. is expressed by*

$$F_{\mathbf{R}}^{\mathcal{A}}(\mathbf{r}) = F_{X,Y}^A(x, y) F_Z^{\Delta z}(z), \quad (44)$$

where

$$F_{X,Y}^A(x, y) = \begin{cases} 1/S(A) & \text{if } (x, y) \in A \\ 0 & \text{if } (x, y) \notin A \end{cases}, \quad (45)$$

where $S(A)$ is the area of A , and

$$F_Z^{\Delta z}(z) = \tilde{\delta}_Z^{\Delta z}(z), \quad (46)$$

where $\tilde{\delta}_Z^{\Delta z}(z)$ is a p.d.f. forming a peak centered at $z = 0$ and of width Δz .

In Fraunhofer diffraction, all of the wavefront at the aperture contributes to the diffraction whereas in Fresnel diffraction only the part of the wavefront close to the edge of the aperture

² Expressing the right-hand side of (42) from (41) (second equality) and given (33) and (31), we obtain:

$$\left[\frac{I(\theta_x, \theta_y)}{I(0, 0)} \right]_{\text{QM}}^{p_0, \mathcal{A}} = \Gamma(\theta_x, \theta_y) \frac{\int_0^\infty dp p^2 \left| \langle \mathbf{p}(p, \theta_x, \theta_y) | \psi^{p_0, \mathcal{A}}(t_1) \rangle \right|^2}{\int_0^\infty dp p^2 \left| \langle \mathbf{p}(p, 0, 0) | \psi^{p_0, \mathcal{A}}(t_1) \rangle \right|^2}$$

(to be compared with (9) applied to $p = p_0$).

contributes [3]. This leads to assume that, in the case of the Fraunhofer diffraction, the filtering in z has the same characteristics whatever $(x, y) \in A$, and that consequently the random variable Z is independent from the random variables (X, Y) . Hence the equation (44) where $F_{X,Y}^A(x, y)$ and $F_Z^{\Delta z}(z)$ are the marginal p.d.f.s of $F_{\mathbf{R}}^{\mathcal{A}}(\mathbf{r})$, respectively called *transverse* and *longitudinal* filtering p.d.f.s.. On the other hand, in Fresnel diffraction, the filtering in z depends a priori on the distance between the point (x, y) and the edge so that Δz depends on (x, y) . Therefore, it is expected that $\mathcal{A}$ cannot be represented in the form $\{A, \Delta z\}$ (with Δz constant) and that $F_{\mathbf{R}}^{\mathcal{A}}(\mathbf{r})$ cannot be expressed in the form (44). This is the reason why the assumption 3 is restricted to the case of the Fraunhofer diffraction.

Since the transverse filtering is uniform, $F_{X,Y}^A(x, y)$ must be a uniform p.d.f.. Hence the equation (45).

From the Huygens-Fresnel principle, we can assume that the filtering p.d.f. $F_{\mathbf{R}}^{\mathcal{A}}(\mathbf{r})$ is concentrated on the wavefront at the aperture so that $F_Z^{\Delta z}(z)$ should in principle be equal to $\delta(z)$. However, given (44), $F_Z^{\Delta z}(z)$ is under a square root in (21). Therefore, $F_Z^{\Delta z}(z)$ cannot be strickly equal to $\delta(z)$. Hence the equation (46). If $\Delta z > 0$, the spherical waves forming the diffracted wave are emitted from several wavefronts contributing with different weights whose distribution is $F_Z^{\Delta z}(z)$ (which is negligible outside the volume $\mathcal{A}$ containing the 2D aperture A). In order to recover the case of the emission from only one wavefront, we have to perform the calculations with $\Delta z > 0$ and then calculate the limit for $\Delta z \rightarrow 0$ (note that calculations using the Huygens-Fresnel principle with 3D Fourier transforms have already been performed [25, 26]). Finally, Δz is a parameter of the quantum model in the case of the Fraunhofer diffraction. From the Huygens-Fresnel principle, its value should correspond to the limit $\Delta z \rightarrow 0$.

Thanks to the assumption 3 (see (44)) and bearing in mind that $p_0 \simeq p$ (see (12)), the Fourier transform (29) can be expressed in the form:

$$\mathcal{F}_{\mathbf{P}}^{\mathcal{A}}(\mathbf{p} - \mathbf{p}_0) \simeq \mathcal{F}_{P_x, P_y}^A(p_x, p_y) \mathcal{F}_{P_z}^{\Delta z}(p_z - p), \quad (47)$$

where:

$$\mathcal{F}_{P_x, P_y}^A(p_x, p_y) \equiv \frac{1}{2\pi\hbar} \iint_{\mathbb{R}^2} dx dy \sqrt{F_{X,Y}^A(x, y)} \exp[-(i/\hbar)(p_x x + p_y y)], \quad (48)$$

$$\mathcal{F}_{P_z}^{\Delta z}(p_z - p) \equiv \frac{1}{\sqrt{2\pi\hbar}} \int_{\mathbb{R}} dz \sqrt{F_Z^{\Delta z}(z)} \exp[(i/\hbar)(p - p_z)z]. \quad (49)$$

Substituting (47) into (43) and expressing $\mathbf{p}(p, \theta_x, \theta_y)$ and $\mathbf{p}(p, 0, 0)$ from (7), we obtain the *quantum formula of the relative intensity in Fraunhofer diffraction for a monochromatic plane wave* ($\lambda = 2\pi\hbar/p$) in normal incidence on a 3D aperture $\mathcal{A} \equiv \{A, \Delta z\}$:

$$\left[\frac{I(\theta_x, \theta_y)}{I(0, 0)} \right]_{\text{QM}}^{p, \mathcal{A}} \simeq \Gamma(\theta_x, \theta_y) T^A(p, \theta_x, \theta_y) L^{\Delta z}(p, \theta_x, \theta_y), \quad (50)$$

where $\Gamma(\theta_x, \theta_y)$ is given by (34) and

$$T^A(p, \theta_x, \theta_y) \equiv \frac{\left| \mathcal{F}_{P_x, P_y}^A(p \cos \chi \operatorname{tg} \theta_x, p \cos \chi \operatorname{tg} \theta_y) \right|^2}{\left| \mathcal{F}_{P_x, P_y}^A(0, 0) \right|^2} \quad (51)$$

is the "*transverse diffraction*" term and

$$L^{\Delta z}(p, \theta_x, \theta_y) \equiv \frac{\left| \mathcal{F}_{P_z}^{\Delta z}(p(\cos \chi - 1)) \right|^2}{\left| \mathcal{F}_{P_z}^{\Delta z}(0) \right|^2} \quad (52)$$

is the "*longitudinal diffraction*" term.

4 Interest and possibility of an experimental test

4.1 Comparison between quantum and classical formulae

Let us compare the quantum formula (50) to the classical one (see (10)). From (45), (48) and (51), we can rewrite (10) in the form:

$$\left[\frac{I(\theta_x, \theta_y)}{I(0, 0)} \right]_{\text{Class.}}^{p, A} \simeq \Omega(\chi)^2 T^A(p, \theta_x, \theta_y). \quad (53)$$

The comparison between the quantum formula (50) and the classical formula (53) shows the following features:

- (i) The transverse diffraction term $T^A(p, \theta_x, \theta_y)$ is the same in the two formulae.
- (ii) The angular factors are different and have not the same origin. The factor $\Gamma(\theta_x, \theta_y)$ of the quantum formula is equal to $\cos^3 \chi / (\cos^2 \theta_x \cos^2 \theta_y)$ (where χ is given by (8)) and is related to the Jacobian of the change of variables of the momentum p.d.f. (see (34)) whereas the factor $\Omega(\chi)^2$ of the classical formula is equal to the square of the obliquity factor involved in the expression of the classical amplitude (see (3)).
- (iii) The longitudinal diffraction term $L^{\Delta z}(p, \theta_x, \theta_y)$ is present only in the quantum formula and is not predicted by the classical theories.

When the angles θ_x and θ_y are small, the angular factors and the longitudinal diffraction term are all close to 1 so that the two formulae give similar results close to $T^A(p, \theta_x, \theta_y)$. On the other hand, the results differ when the angles increase. The difference can be significant at large angles and therefore observable experimentally as we shall see below.

4.2 Comparison of the predictions in the case of a slit

Let us consider a 3D aperture $\mathcal{R} \equiv \{\mathbf{R}, \sigma_z\}$ where $\mathbf{R}$ is a rectangular slit with width $2a$ and height $2b$, centered at $(x, y) = (0, 0)$ and σ_z is the standard deviation of a Gaussian longitudinal filtering p.d.f.. Equations (45) and (46) become:

$$F_{X,Y}^{\mathbf{R}}(x, y) = \begin{cases} 1/(4ab) & \text{if } (x, y) \in \mathbf{R} \\ 0 & \text{if } (x, y) \notin \mathbf{R} \end{cases}, \quad (54)$$

$$F_Z^{\sigma_z}(z) = (\sigma_z \sqrt{2\pi})^{-1} \exp \left\{ -\frac{z^2}{2\sigma_z^2} \right\}. \quad (55)$$

From (48) and (54), the Fourier transform of the square root of the transverse filtering p.d.f. $F_{X,Y}^R(x,y)$ is

$$\mathcal{F}_{P_x,P_y}^R(p_x,p_y) = \sqrt{\frac{a}{\pi\hbar}} \frac{\sin ak_x}{ak_x} \sqrt{\frac{b}{\pi\hbar}} \frac{\sin bk_y}{bk_y} \quad (56)$$

and from (49) and (55), the Fourier transform of the square root of the longitudinal filtering p.d.f. $F_Z^{\sigma_z}(z)$ is found to be [27]

$$\mathcal{F}_{P_z}^{\sigma_z}(p_z - p) = \left(\frac{2}{\pi} \right)^{1/4} \sqrt{\frac{\sigma_z}{\hbar}} \exp \{ -\sigma_z^2 (k - k_z)^2 \}. \quad (57)$$

We consider the intensity variation in the plane (Ox, Oz) corresponding to $\theta_y = 0$ and we set $\theta \equiv \theta_x$ for brevity. Then (8) and (34) imply respectively: $\chi = \theta$ and $\Gamma(\theta, 0) = \cos \theta$. Hence, substituting (56) into (51) and (57) into (52), we obtain the expressions of $T^R(p, \theta, 0)$ and $L^{\sigma_z}(p, \theta, 0)$ respectively. Finally, substituting these expressions into (50) and (53) (and expressing $\Omega(\theta)$ from (3)), we get:

$$\left[\frac{I(\theta, 0)}{I(0, 0)} \right]_{\text{QM}}^{p, \mathcal{R}} \simeq \cos \theta \left(\frac{\sin(ak \sin \theta)}{ak \sin \theta} \right)^2 \exp \{ -2\sigma_z^2 k^2 (1 - \cos \theta)^2 \}, \quad (58)$$

$$\left[\frac{I(\theta, 0)}{I(0, 0)} \right]_{\text{Class.}}^{p, R} \simeq \left\{ \begin{array}{c} (1 + \cos \theta)^2 / 4 \\ \cos^2 \theta \\ 1 \end{array} \right\} \left(\frac{\sin(ak \sin \theta)}{ak \sin \theta} \right)^2, \quad \left\{ \begin{array}{c} \text{(FK)} \\ \text{(RS1)} \\ \text{(RS2)} \end{array} \right\}. \quad (59)$$

An example of curves corresponding to the quantum and classical formulae (58) and (59) for a realistic experimental case is shown in figure 3. The curves are very close for small angles and become more and more different when θ increases.

If $\sigma_z = 0$, we are in the case where the particles associated with the diffracted wave come from the wavefront located at the aperture, in accordance with the Huygens-Fresnel principle. The longitudinal diffraction term (the exponential in (58)) is equal to 1. The quantum values are then as large as possible. They are smaller than the values of the FK and RS2 theories and larger than the values of the RS1 theory. The difference is small for the FK theory (and is significant only for the very large angles) whereas it is larger for the RS1 and RS2 theories. The only difference between the classical predictions and the quantum prediction is due to the angular factors³. In the case of the comparison between the quantum model and the RS1-2 theories, it is not necessary for the angle to be very large to obtain a significant gap. From (58) and (59), the ratios of the relative intensities QM/RS1 and RS2/QM are equal to $1/\cos \theta$ (note that they

³ There exists another formula, from classical optics, with the term $\cos \theta$ not squared, as in (58). This formula includes two terms: the right-hand side of (58) in the case $\sigma_z = 0$ plus a small additional term equal to $[2ak \cos(\chi/2)]^{-2}$ (see [8], §75, problem 1). Its calculation is based on the result of the first rigorous calculation of the diffraction by an edge, due to Sommerfeld [2, 4] and completed by Pauli [5]. In [8], this result is applied to the case of two edges of zero angle placed opposite one another to form a slit. However, the small additional term is non-zero in the whole angular range $0^\circ - 90^\circ$, so the intensity is not zero at the minima (see also [9]).

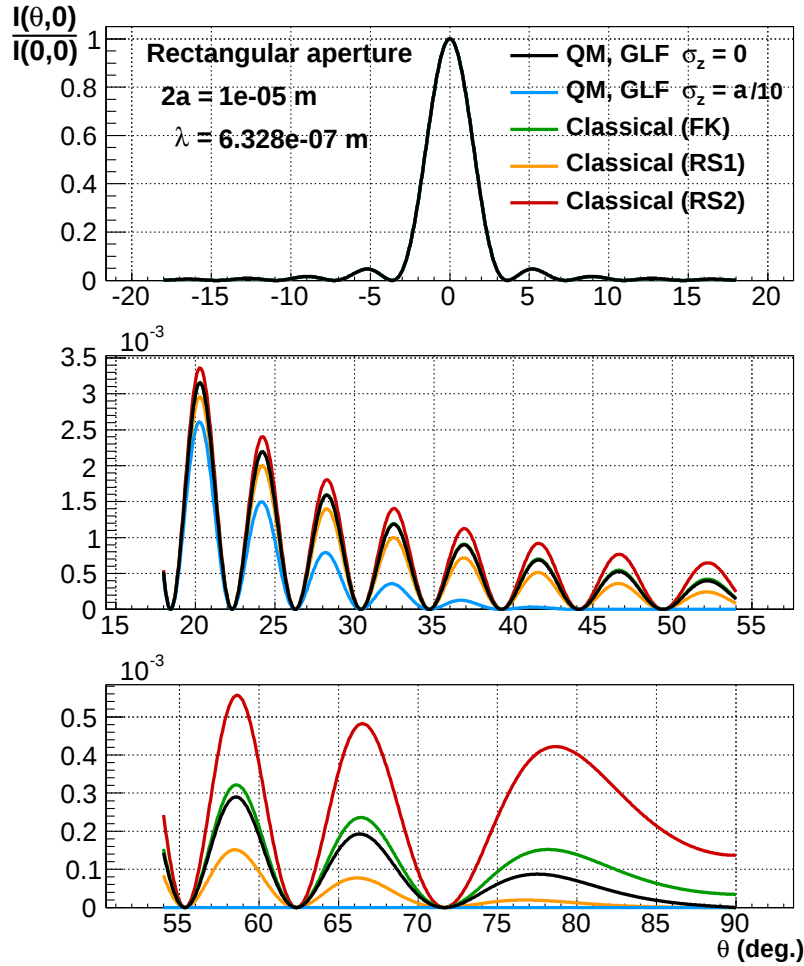


Figure 3. Comparison of the relative intensities in Fraunhofer diffraction as a function of the diffraction angle in the horizontal plane for a rectangular slit of width $2a = 10 \mu\text{m}$ and a monochromatic incident wave corresponding to photons of wavelength $\lambda = 632.8 \text{ nm}$ (Helium-Neon Laser). Five theoretical predictions are presented: three classical predictions corresponding to the theories of Fresnel-Kirchhoff (FK) and Rayleigh-Sommerfeld (RS1 and RS2) and two quantum predictions corresponding to two values of the standard deviation σ_z associated with a Gaussian longitudinal filtering (GLF, $\sigma_z = 0$ and $\sigma_z > 0$). The value $\sigma_z = 0$ corresponds to the case where the particles associated with the diffracted wave come from the wavefront at the aperture (Huygens-Fresnel principle) whereas a non-zero value corresponds to the case where several wavefronts contribute with different weights and this generates a damping.

are independent from a and k). They already reach the value 2 for $\theta = 60^\circ$. In the case of the comparison between the quantum model and the FK theory, the situation is less favorable. The ratio FK/QM is equal to $(1 + \cos \theta)^2 / (4 \cos \theta)$, which is $9/8$ for $\theta = 60^\circ$ and 2 for $\theta \simeq 80^\circ$ (figure 3).

If $\sigma_z > 0$, the particles associated with the diffracted wave come from several wavefronts which contribute with different weights given by the distribution $F_Z^{\sigma_z}(z)$. The longitudinal diffraction term is strictly less than 1. So the quantum relative intensity, maximum for $\sigma_z = 0$, undergoes a damping which increases as a function of σ_z . When σ_z is increasing from zero,

the quantum values eventually pass below the values of the RS1 theory. Coincidentally, the curves QM and RS1 can be very close but they cannot be exactly the same everywhere because the factors $\cos \theta$ and $\cos^2 \theta$ are different. If σ_z is large enough, the quantum curve decreases globally much more rapidly than the classical curves and a significant gap can be obtained at not too large angles (the non-zero value of σ_z chosen for figure 3 corresponds to this case).

In summary, the quantum formula leads to different predictions according to the value of σ_z and these predictions are different from that of the classical theories. Therefore, a measurement of the relative intensity in the region of large diffraction angles - where the gaps between the different predictions are significant - would be an appropriate experimental test of both the classical theories and the quantum model.

5 Summary and outlooks

The diffraction of the wave associated with a particle arriving on a diaphragm has been calculated by means of a theoretical model based exclusively on quantum mechanics. This model considers the diffraction as the consequence of a quantum measurement of the position of the particle passing through the diaphragm aperture. It has two main features which allow to ensure its compatibility with the Huygens-Fresnel principle and with the kinematics of the particle-diaphragm interaction. First, the diaphragm is considered as a measurement device not only of the transverse coordinates but also of the longitudinal coordinate of the particle. Secondly, the change of state during the measurement results from two successive projections involving a transitional state corresponding to the state of the particle when it is localized inside the aperture. The quantum model provides a general expression of the quantum state associated with the diffracted wave, leading in particular to a new formula of the relative intensity in Fraunhofer diffraction in the case of an incident monochromatic plane wave. This quantum formula is applicable to the whole angular range (0° - 90°). Comparison with the classical theories of diffraction based on the Huygens-Fresnel principle (Fresnel-Kirchhoff and Rayleigh-Sommerfeld theories) shows that the predictions are close for small diffraction angles but significantly different for large angles. Moreover, the quantum calculation predicts a "longitudinal diffraction" which can lead to a damping of the intensity at large angles. The absence of damping corresponds to the case where the particles associated with the diffracted wave come from a surface which could be identified with the wavefront emitting the spherical waves involved in the Huygens-Fresnel principle. On the other hand, the presence of a damping means that these particles would come from a volume including several wavefronts. A quantitative study performed in the case of the diffraction by a rectangular slit shows that a measurement of the relative intensity in the region of large angles should permit to compare these predictions to experimental data.

The quantum model presented here provides the expression of the quantum state of the particle associated with the diffracted wave in the case of the diffraction of a monochromatic plane wave in normal incidence by an aperture of finite area. If the observation point is distant so that the aperture can be considered pointlike and if the size of the aperture is larger

than the wavelength, this allows to calculate the relative directional intensity in Fraunhofer diffraction. Other applications of this model can be considered. In the case of a close observation point, where the aperture cannot be considered pointlike, the model should in principle provide the possibility of calculating the Fresnel diffraction. This requires to use a position filtering different from that used for the Fraunhofer diffraction. Moreover, the quantum model is a natural framework to treat the case of a non-monochromatic incident wave. This requires applying the model by replacing the initial state used in the present paper (momentum eigenstate) with a state corresponding to a wave packet.

Acknowledgements

I would like to thank M. Besançon, F. Charra and P. Roussel for helpful suggestions and comments on the manuscript. I am also thankful to the team of the IRAMIS-CEA/SPEC/LEPO for useful discussions on the feasibility of an experiment to measure the diffraction at large angles. This work was supported by the CEA. The figures were carried out using the ROOT software (<https://root.cern.ch/>).

References

- [1] Born M, Wolf E 1980 *Principles of Optics* (Cambridge University Press, 6th edition) chapter 8 sections 8.1-3,11
- [2] Sommerfeld A 1954 *Optics, Lectures on Theoretical Physics Vol IV* (Academic Press inc., NewYork) chapter 5 sections 34,38
- [3] Landau L D and Lifshitz E M 1962 *The Classical Theory of Fields* (Pergamon Press) chapter 7, §59-61.
- [4] Sommerfeld A 1896 Mathematische Theorie der Diffraction *Math. Ann.* **47** 317
- [5] Pauli W 1938 On Asymptotic Series for Functions in the Theory of Diffraction of Light *Phys. Rev.* **54** 924-31
- [6] Levine H and Schwinger J 1948 On the Theory of Diffraction by an Aperture in an Infinite Plane Screen I *Phys. Rev.* **74** number 8 958-74
- [7] Levine H and Schwinger J 1949 On the Theory of Diffraction by an Aperture in an Infinite Plane Screen II *Phys. Rev.* **75**, number 9 1423-32
- [8] Landau L D and Lifshitz E M 1960 *Electrodynamics of Continuous Media.* (Pergamon Press) chapter 10, §74-5.
- [9] Keller J B 1962 Geometrical Theory of Diffraction *J. Opt. Soc. Am.* **52** number 2 116-30
- [10] Epstein P S and Ehrenfest P 1924 The quantum theory of the Fraunhofer diffraction *Proc. Nat. Acad. Sci.* **10** 133-9
- [11] Feynman R P and Hibbs A R 1965 *Quantum Mechanics and Path Integrals* (McGraw-Hill, New York) sections 3.2-3
- [12] Barut A O and Basri S 1992 Path integrals and quantum interference *Am. J. Phys.* **60** 896-9
- [13] Field J H 2006 Quantum mechanics in space-time: The Feynman path amplitude description of physical optics, de Broglie matter waves and quark and neutrino flavour oscillations *Ann. Phys.* **321** 627-707
- [14] Beau M 2012 Feynman path integral approach to electron diffraction for one and two slits: analytical results *Eur. J. Phys.* **33** 1023-39
- [15] Field J H 2013 Description of diffraction grating experiments for photons and electrons in Feynman's space-time formulation of quantum mechanics: The quantum origins of classical wave theories of light and massive particles *Eur. J. Phys.* **34** 1507-31
- [16] Wu X Y, Zhang B J, Liu X J, Liu B, Zhang C L and Li J W 2009 Quantum Theory of Neutron Diffraction *Int. J. Mod. Phys. B* **23** number 15 3255-64

- [17] Wang L, Zhang B J, Hua Z, Li J, Liu X J and Wu X Y 2009 Quantum Theory of Electronic Multiple-Slit Diffraction *Prog. Theor. Phys.* **121** number 4 685-93
- [18] Wu X Y, Zhang B J, Yang J H, Chi L X, Liu X J, Wu Y H, Wang Q C, Wang Y, Li J W and Guo Y Q 2010 Quantum Theory of Light Diffraction *J. Mod. Opt.* **57** number 20 2082-91
- [19] Marcella T V 2002 Quantum interference with slits *Eur. J. Phys.* **23** 615-21
- [20] Shaoulov V, Satya R V, Schiavone G, Clarkson E and Rolland J 2004 Model of wide-angle optical field propagation using scalar diffraction theory *Opt. Eng.* **43** number 7 1561-7
- [21] Cohen-Tannoudji C, Diu B and Laloë F 1977 *Quantum Mechanics* (Wiley, New York and Paris) chapter 3
- [22] Rothman T and Boughn S 2011 'Quantum interference with slits' revisited *Eur. J. Phys.* **32** 107-13
- [23] Heisenberg W 1949 *The Physical Principles of the Quantum Theory* (Dover publications, New York, first publication: University of Chicago Press, 1930) section II.2.a;
- [24] Bohr N 1935 Can Quantum-Mechanical Description of Physical Reality be Considered Complete? *Phys. Rev.* **48** 696-702
- [25] McCutchen C W 1964 Generalized Aperture and the Three-Dimensional Diffraction Image *J. Opt. Soc. Am.* **54** number 2 240-4
- [26] Lin J, Yuan X C, Kou S S, Sheppard C J R, Rodríguez-Herrera O G and Dainty J C 2011 Direct calculation of a three-dimensional diffracted field *Opt. Lett.* **36** number 8 1341-3
- [27] Gradshteyn I S and Ryzhik I M 1994 *Tables of Integrals, Series, and Products. Fifth edition* (Alan Jeffrey, Editor) item 3.896.4 p 514