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

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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). This model meets the double requirement of compatibility with the Huygens-Fresnel principle and with the kinematics of the particle-diaphragm interaction. This led to assume that the diaphragm is a device for measuring the three spatial coordinates of the particle and that the transition from the initial state (incident wave) to the final state (diffracted wave) consists of two specific projections which occur successively in a sequence involving a transitional state. In the case of the diffraction at infinity (Fraunhofer diffraction), the model predicts the intensity of the diffracted wave over the whole angular range of diffraction (0° - 90°). The predictions of the quantum model and of the theories of 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 particle flow intensity in this region should make it possible to test the FK and RS1-2 theories and the suggested quantum model.

Keywords: Quantum measurement, particle-diaphragm interaction, Huygens-Fresnel principle, Fraunhofer diffraction, large diffraction angles

I. 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, models involving quantum mechanics to calculate diffraction are mostly those based on the formalism of path integrals [11–14] and those predicting quantum trajectories in the framework of hidden variables theories [15–17]. Other models combine the resolution of the Schrödinger equation (or of the wave equation for photons) with the Huygens-Fresnel principle [18–20]. 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 [21] 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 well known that the Fresnel-Kirchhoff (FK)

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and Rayleigh-Sommerfeld (RS1 and RS2) theories - based on the Huygens-Fresnel principle and hereafter called *classical* theories of diffraction - 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 due to the impossibility of having a sufficiently expanded dynamic range. Since then, technologies in optics have made considerable progress (especially thanks to quasi-monochromatic laser sources and accurate mesurements of intensity using charge-coupled devices), so that it is now possible to reconsider this question and achieve an experimental study (note however that the question of large angles has been the subject of experimental studies in the case of diffraction by two conductive strips [22] and of theoretical studies using classical diffraction theory to calculate non-paraxial propagation in optical systems [23]). 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 angular range of diffraction. 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 and making it possible to calculate the intensity in Fraunhofer diffraction over the whole angular range. It explicitly uses the postulate of wave function reduction [24] by considering the diaphragm as a device for measuring the position of the particle passing through the aperture. In this model, the intensity of the diffracted wave in Fraunhofer diffraction is calculated from the momentum wave function 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 [21] whose model predicts 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 other authors have furthermore concluded that the used method implicitly refers to classical optics [25]. In the present paper, we consider that these drawbacks do not come from the "purely quantum" aspect of the approach adopted by Marcella but from the way in which the postulate of wave function reduction has been applied in the framework of this approach. According to this postulate, the quantum measurement of the position results in a filtering of the position wave function of the initial state. In Ref. [21], this "position filtering" is applied to a single coordinate in the plane of the diaphragm and it is moreover 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 in order to make possible compatibility with the Huygens-Fresnel principle. We then show that the position measurement projects the initial state on a state whose momentum wave function is not compatible with the kinematics of the particle-diaphragm interaction. This led us to assume that this state is necessarily transitional and undergoes a specific projection which corresponds to a measurement involving an "energy-momentum filtering" of the momentum wave function. This makes it possible to obtain a final state that is compatible with kinematics and that can be associated with the diffracted wave. Finally, a general expression of the final state is obtained for any shape of aperture. For the intensity in Fraunhofer diffraction, we obtain an expression applicable to the whole diffraction angle range (0°- 90°). The predictions of the quantum model are in good agreement with those of the FK and RS1-2 theories in the region of small angles. For the 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 Sec. II, we describe the experimental context and the theoretical conditions for which the presented model is applicable. In Sec. III, we express the amplitude of the diffracted wave in Fraunhofer diffraction predicted by the classical theories in the case of an incident monochromatic plane wave. Then, we introduce the appropriate diffraction angles for the calculation of the intensity up to the large angles. In Sec. IV, we present the quantum model. We calculate the final state associated with the diffracted wave and establish the quantum expression of the intensity in Fraunhofer diffraction. In Sec. V, we compare the classical and quantum predictions. We perform the calculation for a rectangular slit and a circular aperture and then we emphasize the interest of an experimental test for the large diffraction angles. Finally, we conclude and suggest some developments in Sec. VI.

II. EXPERIMENTAL AND THEORETICAL CONTEXT

We consider an experimental setup which contains a source of particles and a diaphragm of zero thickness, forming a perfectly opaque 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 (Fig. 1).

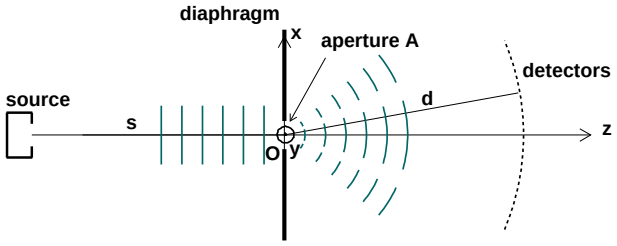


FIG. 1. Schematic representation of experimental setup (section in the horizontal plane (Ox, Oz)).

The source is located on the z axis (normal incidence) and the source-diaphragm distance, denoted s, is assumed to be large enough, so that the wave associated with any incident particle can be considered as a plane wave at the level of the aperture. The observation point is located at some distance d from the aperture, beyond the diaphragm. Its position is denoted by the radius-vector $\mathbf{d}$.

The present study is limited to the case where the incident wave is monochromatic. It is assumed that the wavelength λ is smaller than the size of the aperture and that the Fraunhofer diffraction is obtained at distance d. In this 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].

The case where the size of the aperture is not negligible compared to the distance d corresponds to the Fresnel diffraction and is not addressed in this study (the reason for this will be explained in Sec. VI).

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

In the quantum model presented hereafter, the spin is ignored. The predictions of the quantum model will therefore be compared with those of the *scalar theory of diffraction* according to which the Huygens-Fresnel principle can be deduced from the integral Helmholtz-Kirchhoff theorem [1]. There are several versions of this scalar theory which differ by their assumed boundary conditions. The best known are the theories of Fresnel-Kirchhoff (FK) and Rayleigh-Sommerfeld (RS1 and RS2). These theories are prior to quantum mechanics. So, for simplicity, they will be called hereafter *classical* scalar theories of diffraction.

III. PREDICTIONS OF THE CLASSICAL SCALAR THEORIES OF DIFFRACTION FOR THE 0°-90° ANGULAR RANGE

A. Amplitude of the diffracted wave

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. In the FK and RS1-2 theories, this sum is an integral whose approximate expression can be calculated according to the type of diffraction. Thus, in Fraunhofer diffraction, for a monochromatic plane wave of wavelength λ in normal incidence, the amplitude at a point of radius vector $\mathbf{d}$ beyond the diaphragm is expressed by [1, 2]:

$$\mathcal{U}^{k,\mathrm{A}}_{\mathrm{Cl.}}(\mathbf{d}) \simeq -C_0 \frac{\mathrm{i}}{\lambda} \frac{\exp\left[\mathrm{i}k\left(s+d\right)\right]}{sd} \times \Omega(\chi) \iint_{\mathrm{A}} \mathrm{d}x\mathrm{d}y \ \exp\left[-\mathrm{i}k\left(\frac{d_x}{d}x + \frac{d_y}{d}y\right)\right], \tag{1}$$

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

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

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

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

Substituting (3) into (1), we see that the values of the amplitudes predicted by the three theories are close when the deflection angle χ is small and gradually diverge from each other when χ increases. This is a reason for limiting the application of these theories to the area of small angles. However, it seems that there is no specific criterion giving a quantitative determination of a limit angle (e.g. a criterion similar to that involving the size of the aperture, the diaphragm-detector distance and the wavelength - see footnote 1 -). The classical theories actually predict the value of the amplitude for the whole angular range.

Moreover, if the diaphragm is assumed to be non-reflective, we can surmise that the amplitude must decrease continuously to zero at $\chi = 90°$. From (3), the right-hand side of (1) is in general non-zero when $\chi = 90°$, 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:

$$\mathbf{d} \simeq d\,\frac{\mathbf{p}}{p}. \tag{4}$$

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

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

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

B. 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 Ref. [3]. 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) (Fig. 2).

We can assume that there is no diffracted wave returning to the half-space $z \leq 0$. Therefore, 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 $\mathcal{H}$:

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

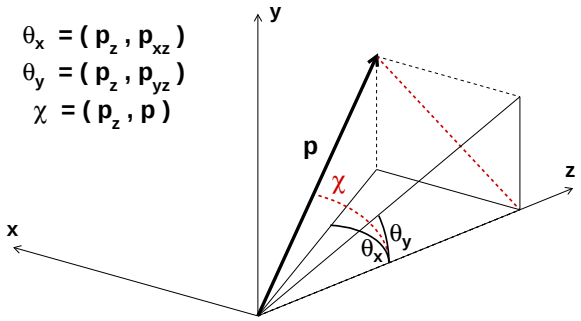


FIG. 2. Variables (p, θ_x, θ_y) in the case of a momentum such that $p_z > 0$. θ_x and θ_y are the diffraction angles and χ is the deflection angle. $\mathbf{p}_z$, $\mathbf{p}_{xz}$ and $\mathbf{p}_{yz}$ are respectively the projections of the vector $\mathbf{p}$ on the z axis and on the planes (x,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

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

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

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

and is such that $0 \leq \chi < \pi/2$. For the small angles, we have from (7) and (8): $p_x \simeq p\,\theta_x$, $p_y \simeq p\,\theta_y$ and $p_z \simeq p$ so that we recover the diffraction angles θ_x and θ_y defined in Ref. [3].

C. Relative intensity

From the experimental point of vue, 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 aperture 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 theories, the squared modulus of the amplitude at point of radius-vector $\mathbf{d}$ is equal to the *local* intensity at that point. This local intensity is defined as follows. Since the size of the aperture is negligible compared to the distance d, we can consider that all the particles arriving at point $\mathbf{d}$ come from the origin O (center of the aperture). In this context, we can therefore define the local intensity as the number of particles arriving at point $\mathbf{d}$ per unit time and per unit area orthogonal to the radius vector $\mathbf{d}$. Now, $\mathbf{d}$ and $\mathbf{p}$ have the same direction (see (4)). So, the local intensity at point $\mathbf{d}$ is proportional to the directional intensity $I^{\,p,\mathrm{A}}_{\mathrm{Class.}}(\theta_x, \theta_y)$ where θ_x

and θ_y correspond to the direction of $\mathbf{p}$ and therefore are given by (6). Hence:

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

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 $S(\mathrm{A})$ the area of A, we get:

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

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

IV. QUANTUM MODEL OF DIFFRACTION BY AN APERTURE

A. Introduction. Position measurement by a diaphragm

In the analysis presented below, we rely on the "standard" interpretation of quantum mechanics (Copenhagen interpretation, originally presented in [26] and then in most textbooks of quantum mechanics). According to this interpretation, the diaphragm can be considered as an apparatus for measuring the position of the particle passing through the aperture. This measurement, hereafter called *quantum measurement*, has the main characteristic of causing a momentum exchange that cannot be made infinitely small between the particle and the diaphragm [27]. This results in an irreversible change of the state of the particle during the measurement. We assume that this change of state is instantaneous and occurs at some time t_1 that separates the process into two periods to which we can associate an *initial state* (state before time t_1) and a *final state* (state after time t_1). We assume that we can specify these states as follows:

- Initial state: free particle state corresponding to the incident wave propagating towards the diaphragm.

- Final state: free particle state corresponding to the diffracted wave propagating beyond the diaphragm.

The evolution of the final state after time t_1 continues indefinitely if there are no detectors beyond the diaphragm. On the other hand, if the particle is detected, this evolution is broken by the detection at some time t_2 such that $t_2>t_1$ and a new change of state occurs.

In the next subsections, we study the change of state that occurs at time t_1 and then the evolution of the final state before any detection ($t_1\leq t<t_2$). We first describe the operator involved in the projection of the initial state (subsection IV B). Then, we show that the state resulting from this projection is necessarily a transitional state and we introduce a new operator that projects, just after time t_1, this transitional state on the appropriate final state (subsections IV C and IV D). We calculate the expression of the final state for $t\geq t_1$ and suggest a description of the process of measurement of position by a diaphragm (subsections IV E and IV F). Finally, the expression of the relative intensity in Fraunhofer diffraction is deduced (subsection IV G).

B. Projection of the initial state. Position filtering.

At time t_1, the initial state is projected on a new state and the initial position wave function undergoes a *filtering* so that the new position wave function is non-zero only if the transverse coordinates (x,y) correspond to the aperture of the diaphragm (postulate of wave function reduction). It can be considered that the transmission of the incident wave is the same over the entire area of the aperture so that the initial position wave function is simply transversely truncated. This type of filtering is both a *transverse* filtering and a *uniform* filtering. It is obtained by making the following projector:

$$\hat{\mathrm{P}}^{\mathrm{A}}_{\mathrm{T}} \equiv \iint_{\mathrm{A}}\mathrm{d}x\mathrm{d}y\,|\,xy\,\rangle\langle\,xy\,| \quad (11)$$

- called "transverse filtering projector" - act on the initial state. However, this projector is defined in the Hilbert subspace associated with the transverse motion of the particle. Therefore, the wave functions of the states of this subspace are partial wave functions only depending on the transverse coordinates or momentum transverse components. Now, the particle moves in the three-dimensional space and, consequently, *the appropriate Hilbert space is that of the states whose wave functions depend on the three coordinates or on the three momentum components*. We must therefore define, in this Hilbert space corresponding to the 3D motion of the particle, an operator acting like $\hat{\mathrm{P}}^{\mathrm{A}}_{\mathrm{T}}$ in the subspace corresponding to the 2D transverse motion. The simplest operator with this property is the projector:

$$\hat{\mathrm{P}}^{\mathrm{A},\Delta z} \equiv \hat{\mathrm{P}}^{\mathrm{A}}_{\mathrm{T}}\otimes\hat{\mathrm{P}}^{\Delta z}_{\mathrm{L}}, \quad (12)$$

where:

$$\hat{\mathrm{P}}^{\Delta z}_{\mathrm{L}} \equiv \int_{-\Delta z/2}^{+\Delta z/2}\mathrm{d}z\,|\,z\,\rangle\langle\,z\,| \quad (13)$$

is a "longitudinal filtering projector" whose action can be interpreted as a projection corresponding to a measurement of z giving a result inside the interval $[-\Delta z/2,+\Delta z/2]$ centered at $z=0$ which is the longitudinal coordinate of the diaphragm (Fig. 1). This measurement is then associated with a *longitudinal filtering* of the initial position wave function.

In summary, the action of $\hat{\mathrm{P}}^{\mathrm{A},\Delta z}$ corresponds to a measurement of the three coordinates (x, y, z) with an accuracy of the order of the size of the aperture A for the transverse coordinates and an accuracy of the order of Δz for the longitudinal coordinate. In this context, Δz is a parameter. Besides the case where Δz is finite, there are the following limit cases corresponding to two opposite situations:

- if $\Delta z \to \infty$, the partial projector $\hat{\mathrm{P}}_{\mathrm{L}}^{\Delta z}$ tends to the identity operator. The action of the projector $\hat{\mathrm{P}}^{\mathrm{A},\Delta z}$ then corresponds to a measurement of (x, y) (transverse filtering, accuracy given by the size of the aperture A) without measurement of z (no longitudinal filtering, no accuracy).

- if $\Delta z \to 0$ ($\Delta z \neq 0$), the action of $\hat{\mathrm{P}}^{\mathrm{A},\Delta z}$ concentrates the probability of presence of the particle in the region of the wavefront at the aperture and, consequently, its longitudinal coordinate is $z = 0$ with almost infinite accuracy. So, at the time t_1 of the change of state, the diffracted wave corresponding to the final state of the particle is about to be emitted from a volume including the wavefront at the aperture and its close vicinity. We are then close to a situation consistent with the Huygens-Fresnel principle. This case seems more plausible than the case $\Delta z \to \infty$ for which such compatibility does not appear. However, no value of Δz should be rejected a priori.

At the limit $\Delta z = 0$, a perfect compatibility with the Huygens-Fresnel principle would be obtained provided that the probability density function (p.d.f.) of the longitudinal coordinate of the particle at time t_1 is equal to $\delta(z)$, where $\delta(z)$ is the Dirac distribution. However, it is not possible to obtain this result using (13) because the integral of the right-hand side is zero if $\Delta z = 0$. Nevertheless, given the good agreement between the measurements performed so far and the predictions of the classical theories based on the Huygens-Fresnel principle, this is worth looking for a way to treat this limit case. Fortunately, it turns out that this is possible provided, however, that the notion of projector is generalized.

Consider a particle having a one-dimensional motion on the z-axis and suppose that the measurement of the observable $\hat{Z}$ on this particle in the initial state $\left| \psi_z^{\mathrm{in}} \right\rangle$ gives a result within the interval $[-\Delta z/2, +\Delta z/2]$. Such a measurement projects the initial state on the following final state [24]:

$$\left| \psi_z^{\Delta z} \right\rangle = \frac{\hat{\mathrm{P}}_{\mathrm{L}}^{\Delta z} \left| \psi_z^{\mathrm{in}} \right\rangle}{\sqrt{\left\langle \psi_z^{\mathrm{in}} \right| \hat{\mathrm{P}}_{\mathrm{L}}^{\Delta z} \left| \psi_z^{\mathrm{in}} \right\rangle}}, \tag{14}$$

where $\hat{\mathrm{P}}_{\mathrm{L}}^{\Delta z}$ is the projector defined in (13). From (13) and (14), the p.d.f. corresponding to the probability to obtain a result within the interval $[z, z + \mathrm{d}z]$ is:

$$\left| \left\langle z \right| \psi_z^{\Delta z} \right\rangle \Big|^2 = \left(\int_{-\Delta z/2}^{+\Delta z/2} \mathrm{d}z' \, \left| \left\langle z' \right| \psi_z^{\mathrm{in}} \right\rangle \right|^2 \right)^{-1} \times \begin{cases} \left| \left\langle z \right| \psi_z^{\mathrm{in}} \right\rangle \Big|^2 & \text{if } z \in [-\Delta z/2, +\Delta z/2] \\ 0 & \text{if } z \notin [-\Delta z/2, +\Delta z/2] \end{cases} \tag{15}$$

and we see that this leads to an undetermined value when $\Delta z = 0$. We could then replace (13) by $\hat{\mathrm{P}}_{\mathrm{L}}^{0} = |\, 0 \,\rangle\langle\, 0 \,|$ but substituting into (14) and then expressing the wave function, we get: $\left\langle z \right| \psi_z^0 \left\rangle \right. = \delta(z) \exp\left[\mathrm{i} \arg\left(\left\langle z \right| \psi_z^{\mathrm{in}} \left\rangle \right. \right) \right]$, which implies that the p.d.f. $\left| \left\langle z \right| \psi_z^0 \left\rangle \right. \right|^2$ is not defined.

However, it is possible to obtain an expression of the p.d.f. at the limit $\Delta z = 0$ by using the following method. First, we replace the projector $\hat{\mathrm{P}}_{\mathrm{L}}^{\Delta z}$ by a "generalized projector" $\hat{\mathrm{R}}_{\mathrm{L}}^{\Delta z}$ called *reduction operator* and defined as:

$$\hat{\mathrm{R}}_{\mathrm{L}}^{\Delta z} \equiv \int_{\mathbb{R}} \mathrm{d}z \, \sqrt{F_{\mathrm{L}}^{\Delta z}(z)} \; |\, z \,\rangle\langle\, z \,|, \tag{16}$$

where $F_{\mathrm{L}}^{\Delta z}(z)$ is a positive function whose properties will be described below. Secondly, we replace (14) by:

$$\left| \psi_z^{\Delta z} \right\rangle = \frac{\hat{\mathrm{R}}_{\mathrm{L}}^{\Delta z} \left| \psi_z^{\mathrm{in}} \right\rangle}{\sqrt{\left\langle \psi_z^{\mathrm{in}} \right| \left(\hat{\mathrm{R}}_{\mathrm{L}}^{\Delta z} \right)^{\dagger} \hat{\mathrm{R}}_{\mathrm{L}}^{\Delta z} \left| \psi_z^{\mathrm{in}} \right\rangle}}. \tag{17}$$

The formulation (17) ensures that the state $\left| \psi_z^{\Delta z} \right\rangle$ is automatically normalized to 1. Substituting (16) into (17) and expressing the p.d.f., we find:

$$\left| \left\langle z \right| \psi_z^{\Delta z} \right\rangle \Big|^2 = \frac{F_{\mathrm{L}}^{\Delta z}(z) \, \left| \left\langle z \right| \psi_z^{\mathrm{in}} \right\rangle \Big|^2}{\displaystyle\int_{\mathbb{R}} \mathrm{d}z' \, F_{\mathrm{L}}^{\Delta z}(z') \left| \left\langle z' \right| \psi_z^{\mathrm{in}} \right\rangle \Big|^2}. \tag{18}$$

Contrary to (15), the equation (18) makes sense at the limit $\Delta z = 0$, provided that $F_{\mathrm{L}}^{0}(z) = C(z)\,\delta(z)$ where $C(z)$ is any function of arbitrary dimension. Indeed, in this case (18) implies: $\lim_{\Delta z \to 0} \left| \left\langle z \right| \psi_z^{\Delta z} \left\rangle \right. \right|^2 = \delta(z)$, whatever $C(z)$. The easiest way is to choose $C(z) = 1$, dimensionless so that $F_{\mathrm{L}}^{0}(z) = \delta(z)$ and therefore is positive and normalized to 1. Then, since the passage to the limit $\Delta z = 0$ is continuous, it is logical to assume that $F_{\mathrm{L}}^{\Delta z}(z)$ is positive and normalized to 1 whatever Δz. We can therefore interpret $F_{\mathrm{L}}^{\Delta z}(z)$ as the weight with which the filtering selects the value $\left| \left\langle z \right| \psi_z^{\mathrm{in}} \left\rangle \right. \right|^2$ of the initial p.d.f. at z. This function $F_{\mathrm{L}}^{\Delta z}(z)$ will be called *longitudinal position filtering function.*

Since $F_{\mathrm{L}}^{0}(z) = \delta(z)$, the square root in the right-hand side of (16) is not defined and consequently (16) and (17) are not applicable when $\Delta z = 0$. The passage to the limit can only be done for the p.d.f., by using (18) [2].

From (16), we have: $\left(\hat{\mathrm{R}}_{\mathrm{L}}^{\Delta z} \right)^2 \neq \hat{\mathrm{R}}_{\mathrm{L}}^{\Delta z}$, contrary to the case of a projector. However, for the filtering function: $F_{\mathrm{L}}^{\Delta z}(z) = 1/\Delta z$ if $z \in [-\Delta z/2, +\Delta z/2]$ or 0 otherwise

[2] More generally, the case of a filtering function equal to the Dirac distribution can be treated by performing the calculations with a Gaussian of standard deviation σ_z and then passing to the limit $\sigma_z = 0$ if it is possible. This is the case not only for the p.d.f. of Eq. (18) but also for the relative intensity whose expression will be calculated later (subsection V B).

(uniform filtering), the equations (13) and (16) lead to: $\hat{\mathrm{R}}_{\mathrm{L}}^{\Delta z} = \Delta z^{-1/2}\,\hat{\mathrm{P}}_{\mathrm{L}}^{\Delta z}$. So, substituting into (17), we see that the factor $\Delta z^{-1/2}$ is eliminated. Then, since $\left(\hat{\mathrm{P}}_{\mathrm{L}}^{\Delta z}\right)^{\dagger}\,\hat{\mathrm{P}}_{\mathrm{L}}^{\Delta z} = \hat{\mathrm{P}}_{\mathrm{L}}^{\Delta z}$, the right-hand side of (17) is equal to the right-hand side of (14) and we finally obtain the same state $\left|\,\psi_z^{\Delta z}\,\right\rangle$ as that of Eq. (14). Therefore, the reduction operator can be used in place of the usual projector in the particular case of a uniform filtering. We assume that this type of operator is appropriate for the more general case of a non-uniform filtering.

In particular, the longitudinal filtering could be non-uniform for the following reason. The truncation made by the projector $\hat{\mathrm{P}}_{\mathrm{L}}^{\Delta z}$ is similar to that made by the projector $\hat{\mathrm{P}}_{\mathrm{T}}^{\mathrm{A}}$ involved in the transverse filtering. However, the two filterings are probably not of the same type because the aperture is limited by a material edge in the transverse plane whereas there are no edges along the longitudinal direction. The longitudinal filtering could then be a non-uniform filtering associated with a continuous filtering function forming a peak centered at $z = 0$ and of width Δz. This peak is not necessarily symmetric with respect to $z = 0$. The precise shape of the filtering function is part of the assumptions of the model. This shape can be important if Δz is large but probably does not matter if Δz is close to zero because the p.d.f. is then close to the Dirac distribution (for simplicity, we will consider symmetric filtering functions centered at $z = 0$ in the following).

The interval $[-\Delta z/2, +\Delta z/2]$ is a transmission interval that can be considered as an "aperture". In the case of a uniform filtering, it represents the region where the filtering function is non-zero. In the case of a non-uniform filtering, the filtering function can be non-zero everywhere (for example if it is a Gaussian). We are then led to define more generally the aperture as the interval outside of which the integral of the filtering function is negligible.

In summary, for the longitudinal coordinate, it is assumed that the projector $\hat{\mathrm{P}}_{\mathrm{L}}^{\Delta z}$ defined by (13) can be replaced by a reduction operator $\hat{\mathrm{R}}_{\mathrm{L}}^{\Delta z}$ of the form (16).

Using a similar generalization for the transverse coordinates, we assume that the projector $\hat{\mathrm{P}}_{\mathrm{T}}^{\mathrm{A}}$ given by (11) can be replaced by a reduction operator of the form:

$$\hat{\mathrm{R}}_{\mathrm{T}}^{\mathrm{A}} \equiv \iint_{\mathbb{R}^2} \mathrm{d}x\mathrm{d}y\, \sqrt{F_{\mathrm{T}}^{\mathrm{A}}(x,y)}\ \left|\,xy\,\right\rangle\left\langle\,xy\,\right|, \qquad (19)$$

where $F_{\mathrm{T}}^{\mathrm{A}}(x,y)$ is the transverse position filtering function. Since the transverse filtering is assumed to be uniform, this function is given by:

$$F_{\mathrm{T}}^{\mathrm{A}}(x,y) \;=\; \begin{cases} S(\mathrm{A})^{-1} & \text{if} \quad (x,y) \in \mathrm{A} \\ 0 & \text{if} \quad (x,y) \notin \mathrm{A} \end{cases}, \qquad (20)$$

where $S(\mathrm{A})$ is the area of A.

Finally, we assume that the projector $\hat{\mathrm{P}}^{\mathrm{A},\Delta z}$ defined by (12) can be replaced by the reduction operator:

$$\hat{\mathrm{R}}^{\mathcal{A}} \;\equiv\; \hat{\mathrm{R}}_{\mathrm{T}}^{\mathrm{A}} \otimes \hat{\mathrm{R}}_{\mathrm{L}}^{\Delta z}, \qquad (21)$$

where:

$$\mathcal{A} \;\equiv\; \mathrm{A} \times [-\Delta z/2, +\Delta z/2] \qquad (22)$$

is the volume of transverse section A, of length Δz, centered at the origin O. The aperture A and the interval $[-\Delta z/2, +\Delta z/2]$ are respectively called *transverse aperture* and *longitudinal aperture* and the volume $\mathcal{A}$ is called *generalized 3D aperture* (Fig. 3) (note that there exist calculations of diffraction based on the Huygens-Fresnel principle and involving another type of generalized aperture [28, 29]).

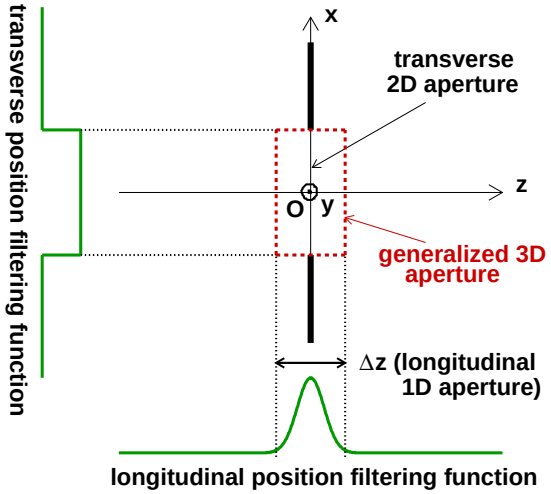


FIG. 3. Example of generalized 3D aperture (section in the (Ox, Oz) plane) and corresponding transverse and longitudinal position filtering functions, whose product is the (joint) position filtering function.

From (16), (19) and (21), we can express the reduction operator in the form:

$$\hat{\mathrm{R}}^{\mathcal{A}} \;\equiv\; \iiint_{\mathbb{R}^3} \mathrm{d}^3 r\, \sqrt{F^{\mathcal{A}}(\mathbf{r})}\ \left|\,\mathbf{r}\,\right\rangle\left\langle\,\mathbf{r}\,\right|, \qquad (23)$$

where $F^{\mathcal{A}}(\mathbf{r})$ is the joint position filtering function (hereafter called *position filtering function*) given by:

$$F^{\mathcal{A}}(\mathbf{r}) \;\equiv\; F_{\mathrm{T}}^{\mathrm{A}}(x,y)\; F_{\mathrm{L}}^{\Delta z}(z). \qquad (24)$$

The function $F_{\mathrm{T}}^{\mathrm{A}}(x,y)$ is given by (20) and the function $F_{\mathrm{L}}^{\Delta z}(z)$ forms a peak whose integral outside the interval $[-\Delta z/2, +\Delta z/2]$ is negligible. From this and (24), it follows that the integral of $F^{\mathcal{A}}(\mathbf{r})$ is negligible outside the volume $\mathcal{A}$ defined by (22).

According to the Huygens-Fresnel principle, the diffracted wave is emitted from the wavefront at the aperture, which corresponds to the case $\Delta z = 0$. Then, the case $\Delta z > 0$ can be interpreted as follows: the Huygens-Fresnel principle applies to several wavefronts contributing with different weights whose distribution is the longitudinal position filtering function $F_{\mathrm{L}}^{\Delta z}(z)$.

Following the analysis developed so far, we can formulate the first assumption of the quantum model as follows:

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

- Before the measurement, the initial state of the particle corresponds to the incident wave propagating towards the diaphragm.

- After the measurement, the final state corresponds to the diffracted wave propagating beyond the diaphragm.

- During the measurement, the initial state undergoes the action of the position reduction operator $\hat{\mathrm{R}}^{\mathcal{A}}$ *defined by (23).*

The assumption 1 does not specify the characteristics of the state resulting from the action of the operator $\hat{\mathrm{R}}^{\mathcal{A}}$ on the initial state. In fact, this state is not the final state associated with the diffracted wave. This question will soon be examined (subsection IV D). This requires a second assumption that applies only in the case where the incident wave is monochromatic.

C. Initial state associated with a monochromatic incident wave.

To compare the predictions of the quantum model with those of the classical scalar theories of diffraction presented in Sec. III, the appropriate initial state must correspond to a scalar monochromatic plane wave in normal incidence. Such a state is a momentum and energy eigenstate (therefore a stationary state) of the form:

$$\left| \psi^{\mathrm{in}}_{\mathbf{p}_0}(t) \right\rangle \;=\; \exp\left[-(\mathrm{i}/\hbar)\, E(p_0)\, t\right] \left| \mathbf{p}_0 \right\rangle, \qquad (25)$$

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. The position wave function of this initial state is the plane wave: $(2\pi\hbar)^{-3/2} \exp\{(\mathrm{i}/\hbar)\,[\,\mathbf{p}_0.\mathbf{r} - E(p_0)\,t\,]\}$ (where $\mathbf{p}_0.\mathbf{r} = p_0 z$ in the coordinate system of Fig. 1).

We assume that the state $\left| \psi^{\mathrm{in}}_{\mathbf{p}_0}(t) \right\rangle$ given by (25) can be used to describe the state of any free particle of momentum $\mathbf{p}_0$ if the spin is not taken into account. In particular, we admit that this use is valid for the photon in spite of the issues raised by the interpretation of the position wave function of a particle of zero mass [30–32]. In the following, the calculation of the relative intensity in Fraunhofer diffraction will require only *momentum* wave functions, so this problem of interpretation will not arise.

D. Transitional state. Energy-momentum filtering

According to the postulate of wave function reduction applied to the initial state $\left| \psi^{\mathrm{in}}_{\mathbf{p}_0}(t_1) \right\rangle$ and given the assumption 1, the state of the particle immediately after the position quantum measurement by the diaphragm provided with the "generalized 3D aperture" $\mathcal{A}$ is:

$$\left| \psi^{\mathcal{A}}(t_1) \right\rangle = \frac{\hat{\mathrm{R}}^{\mathcal{A}} \left| \psi^{\mathrm{in}}_{\mathbf{p}_0}(t_1) \right\rangle}{\sqrt{\left\langle \psi^{\mathrm{in}}_{\mathbf{p}_0}(t_1) \left| \left(\hat{\mathrm{R}}^{\mathcal{A}}\right)^{\dagger} \hat{\mathrm{R}}^{\mathcal{A}} \right| \psi^{\mathrm{in}}_{\mathbf{p}_0}(t_1) \right\rangle}}, \qquad (26)$$

where $\hat{\mathrm{R}}^{\mathcal{A}}$ is the position reduction operator defined by (23). Equation (26) expresses the final state only at time t_1. It is therefore necessary to express this state for $t > t_1$. Two observations allow to formulate two properties that the final state after time t_1 must have.

First, no significant difference between the wavelength of the diffracted wave and that of the incident wave is observed in diffraction experiments with a diaphragm. Hence, denoting λ and $\mathbf{p}$ the wavelength and the momentum in the final state, we have: $\lambda \simeq \lambda_0$ and consequently, given the de Broglie relation:

$$p \;\simeq\; p_0. \qquad (27)$$

This is consistent with kinematics. In the conditions of the experiment (microscopic object interacting with a macroscopic device), the particule transfers a very small part of its energy to the diaphragm, so that the momentum modulus of the particle is almost conserved. Therefore, the final state after time t_1 must have the following property:

(P1) *The final state for* $t > t_1$ *is close to an energy eigenstate associated with the eigenvalue* $E(p_0)$.

Secondly, we can assume that there is no diffracted wave returning from the aperture of the diaphragm to the region where the source is located. This implies that the particle associated with the diffracted wave is always such that:

$$p_z \;>\; 0. \qquad (28)$$

Hence the property:

(P2) *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 $\left| \psi^{\mathcal{A}}(t_1) \right\rangle$ given by (26) can evolve towards a state having the properties (P1) and (P2). Substituting (24) into (23), then the obtained result and (25) into (26) and given (20), we get the expression of $\left| \psi^{\mathcal{A}}(t_1) \right\rangle$. Then, we calculate the modulus squared of the momentum wave function, that is the momentum p.d.f. in the final state just after time t_1. The result is independent of t_1 and can be written in the form:

$$\left| \left\langle \mathbf{p} \left| \psi^{\mathcal{A}}(t_1) \right\rangle \right|^2 \;=\; f^{\mathrm{A}}_{P_x,P_y}(p_x,p_y)\; f^{p_0,\Delta z}_{P_z}(p_z), \qquad (29)$$

where:

$$f^{\mathrm{A}}_{P_x,P_y}(p_x,p_y) \;\equiv\; (2\pi\hbar)^{-2} S(\mathrm{A})^{-1} \times \left| \iint_{\mathrm{A}} \mathrm{d}x\mathrm{d}y\ \exp\left[-(\mathrm{i}/\hbar)(p_x x + p_y y)\right] \right|^2, \qquad (30)$$

$$f_{P_z}^{p_0,\Delta z}(p_z) \equiv (2\pi\hbar)^{-1} \times \left| \int_{\mathbb{R}} \mathrm{d}z \, \sqrt{F_{\mathrm{L}}^{\Delta z}(z)} \, \exp\left[(\mathrm{i}/\hbar)(p_0 - p_z)z\right] \right|^2 . \quad (31)$$

We can verify that $f_{P_x,P_y}^{\mathrm{A}}(p_x,p_y)$ and $f_{P_z}^{p_0,\Delta z}(p_z)$ are positive and normalized to 1. So, they are respectively the marginal p.d.f.s of the random variables (P_x,P_y) and P_z associated with the possible results of measurements of the observables $(\hat{P}_x,\hat{P}_y)$ and $\hat{P}_z$. Therefore, Eq. (29) expresses the fact that the random variables P_x and P_y are independent of the random variable P_z. However, this is incompatible with the relation (27) which involves on the contrary a strong dependence between the three components of the momentum since p_0 is a fixed value. Thus, the spreading of the momentum components caused by the measurement of the spatial coordinates generally results in a spreading of the momentum modulus. So, the state $\left|\, \psi^{\mathcal{A}}(t_1) \,\right\rangle$ is not an energy eigenstate and, consequently, has not the property (P1).

Moreover, from (31), the distribution $f_{P_z}^{p_0,\Delta z}(p_z)$ is none other than the modulus squared of the Fourier transform of $\sqrt{F_{\mathrm{L}}^{\Delta z}(z)}$. Therefore, if Δz is small enough, the width Δp_z of $f_{P_z}^{p_0,\Delta z}(p_z)$ can be larger than p_0 and the probability for p_z to be negative is then non-negligible. In this case, (28) is not satisfied and consequently the state $\left|\, \psi^{\mathcal{A}}(t_1) \,\right\rangle$ has not the property (P2). However, this state can have the property (P2) if Δz is large enough but, anyway, it has not the property (P1) because the probabilistic independence, mentioned above, between (P_x,P_y) and P_z is effective whatever Δz.

We are thus led to the following conclusion: *the state $\left|\, \psi^{\mathcal{A}}(t_1) \,\right\rangle$ cannot evolve towards the final state associated with the diffracted wave. It is a transitional state that must be transformed, just after time t_1, by means of a new projection to a state having the properties (P1) and (P2).*

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

$$\left|\, \psi^{p_0,\mathcal{A}}(t_1) \,\right\rangle = \frac{\hat{\mathrm{R}}^{p_0} \left|\, \psi^{\mathcal{A}}(t_1) \,\right\rangle}{\sqrt{\left\langle \psi^{\mathcal{A}}(t_1) \left| \left(\hat{\mathrm{R}}^{p_0}\right)^{\dagger} \hat{\mathrm{R}}^{p_0} \right| \psi^{\mathcal{A}}(t_1) \right\rangle}}, \quad (32)$$

where $\hat{\mathrm{R}}^{p_0}$ is 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, this point will be discussed hereafter in subsection IV F) and such that the momentum p.d.f. is zero for $p_z \leq 0$. The expression of this reduction operator must have a form similar to (23). We assume that the appropriate operator is:

$$\hat{\mathrm{R}}^{p_0} \equiv \iiint_{\mathbb{R}^3} \mathrm{d}^3p \, \sqrt{F^{p_0}(\mathbf{p})} \, \left|\, \mathbf{p} \,\right\rangle\!\left\langle\, \mathbf{p} \,\right|, \quad (33)$$

where $F^{p_0}(\mathbf{p})$ is an "energy-momentum filtering function" normalized to 1 and defined as:

$$F^{p_0}(\mathbf{p}) \equiv \frac{\delta_{1\,\mathrm{sgn}[p_z]} \, \widetilde{\delta}^{\,\Delta p}\left(|\mathbf{p}| - p_0\right)}{\iiint_{\mathbb{R}^3} \mathrm{d}^3p' \, \delta_{1\,\mathrm{sgn}[p_z']} \, \widetilde{\delta}^{\,\Delta p}\left(|\mathbf{p}'| - p_0\right)}, \quad (34)$$

where $\delta_{1\,\mathrm{sgn}[p_z]}$ is the Kroenecker delta and $\widetilde{\delta}^{\,\Delta p}\left(|\mathbf{p}| - p_0\right)$ is a function determined by kinematics and therefore 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 $\sqrt{\widetilde{\delta}^{\,\Delta p}\left(|\mathbf{p}| - p_0\right)}$ is well-defined and therefore (33) makes sense. The interpretation of (34) is therefore as follows: the filtering function $F^{p_0}(\mathbf{p})$ selects all the possible values of the momentum components such that the momentum modulus is close to p_0 (term $\widetilde{\delta}^{\,\Delta p}\left(|\mathbf{p}| - p_0\right)$, Eq. (27), property (P1)) and such that $p_z > 0$ (term $\delta_{1\,\mathrm{sgn}[p_z]}$, Eq. (28), property (P2)).

Then, to obtain the expression of $\left|\, \psi^{p_0,\mathcal{A}}(t_1) \,\right\rangle$ as a function of the initial state $\left|\, \psi_{\mathbf{p}_0}^{\mathrm{in}}(t_1) \,\right\rangle$, we substitute (26) into (32). The result is the expression (35) below, which is the second assumption of the quantum model.

Assumption 2. *In the case of a monochromatic plane wave in normal incidence (wavelength: $\lambda_0 = 2\pi\hbar/p_0$), the final state of the particle outgoing from the generalized 3D aperture $\mathcal{A}$ immediately after interacting at time t_1 with the diaphragm is:*

$$\left|\, \psi^{p_0,\mathcal{A}}(t_1) \,\right\rangle = \frac{\hat{\mathrm{R}}^{p_0}\hat{\mathrm{R}}^{\mathcal{A}} \left|\, \psi_{\mathbf{p}_0}^{\mathrm{in}}(t_1) \,\right\rangle}{\sqrt{\left\langle \psi_{\mathbf{p}_0}^{\mathrm{in}}(t_1) \left| \left(\hat{\mathrm{R}}^{p_0}\hat{\mathrm{R}}^{\mathcal{A}}\right)^{\dagger} \hat{\mathrm{R}}^{p_0}\hat{\mathrm{R}}^{\mathcal{A}} \right| \psi_{\mathbf{p}_0}^{\mathrm{in}}(t_1) \right\rangle}}, \quad (35)$$

where $\hat{\mathrm{R}}^{\mathcal{A}}$ is the position reduction operator defined by (23) and $\hat{\mathrm{R}}^{p_0}$ is the energy-momentum reduction operator defined by (33).

E. Final state associated with the diffracted wave

We now have all the ingredients to express the final state and to check if this state actually has the properties (P1) and (P2) mentioned in subsection IV D. Substituting (23) and (33) into (35), and given (25) and (34), we see that the denominator of the right-hand side of (34) is eliminated and we are led to the following expression of the final state at time t_1:

$$\left|\, \psi^{p_0,\mathcal{A}}(t_1) \,\right\rangle = N^{\mathcal{A}}(\Delta p)^{-1/2} \, \exp\left[-(\mathrm{i}/\hbar)E(p_0)\, t_1\right] \times \iiint_{\mathbb{R}^3} \mathrm{d}^3p \, \delta_{1\mathrm{sgn}[p_z]} \sqrt{\widetilde{\delta}^{\,\Delta p}(|\mathbf{p}|-p_0)} \, \mathcal{F}^{\mathcal{A}}(\mathbf{p}-\mathbf{p}_0) \left|\, \mathbf{p} \,\right\rangle, \quad (36)$$

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

$$\mathcal{F}^{\mathcal{A}}(\mathbf{p}-\mathbf{p}_0) \equiv (2\pi\hbar)^{-3/2} \times \iiint_{\mathbb{R}^3} \mathrm{d}^3r \, \sqrt{F^{\mathcal{A}}(\mathbf{r})} \, \exp\left[-(\mathrm{i}/\hbar)(\mathbf{p}-\mathbf{p}_0).\mathbf{r}\right] \quad (37)$$

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

$$N^{\mathcal{A}}(\Delta p) \equiv \iiint_{\mathbb{R}^3} \mathrm{d}^3p \ \delta_{1\,\mathrm{sgn}[p_z]}\ \widetilde{\delta}^{\,\Delta p}\left(|\mathbf{p}|-p_0\right) \times \left|\,\mathcal{F}^{\mathcal{A}}(\mathbf{p}-\mathbf{p}_0)\,\right|^2. \tag{38}$$

From (36), the final momentum p.d.f. is independent of t_1. So this p.d.f. can be written in the form:

$$\forall t_1: \quad \left|\left\langle\,\mathbf{p}\,\middle|\,\psi^{p_0,\mathcal{A}}(t_1)\,\right\rangle\right|^2 \equiv f_{\mathbf{P}}^{p_0,\mathcal{A}}(\mathbf{p}), \tag{39}$$

where $\mathbf{P}$ is the random vector $(P_x\ P_y\ P_z)$. From (36) and (39), we have:

$$f_{\mathbf{P}}^{p_0,\mathcal{A}}(\mathbf{p}) = N^{\mathcal{A}}(\Delta p)^{-1}\ \delta_{1\,\mathrm{sgn}[p_z]}\ \widetilde{\delta}^{\,\Delta p}\left(|\mathbf{p}|-p_0\right) \times \left|\,\mathcal{F}^{\mathcal{A}}(\mathbf{p}-\mathbf{p}_0)\,\right|^2, \tag{40}$$

which can be considered as a p.d.f. defined in the half-space $p_z>0$, due to the factor $\delta_{1\,\mathrm{sgn}[p_z]}$. Now, 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 $\mathcal{H}$ defined by (6)-(7):

$$f_{P,\Theta_x,\Theta_y}^{p_0,\mathcal{A}}(p,\theta_x,\theta_y) = p^2\ \Gamma(\theta_x,\theta_y)\ f_{\mathbf{P}}^{p_0,\mathcal{A}}(\,\mathbf{p}(p,\theta_x,\theta_y)\,), \tag{41}$$

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

$$\Gamma\left(\theta_x,\theta_y\right) \equiv \frac{1}{p^2}\left|\,\det\!\left(\frac{\partial\left[p_x,p_y,p_z\right]}{\partial\left[p,\theta_x,\theta_y\right]}\right)\,\right| = \frac{\cos\chi}{1-\sin^2\!\theta_x\,\sin^2\!\theta_y} \tag{42}$$

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 (40) and using the fact that $\mathrm{sgn}[p_z(p,\theta_x,\theta_y)]=1$ in the half-space $z>0$ and that $\mathbf{p}_0=(0\ \ 0\ \ p_0)=\mathbf{p}(p_0,0,0)$, we can express $f_{\mathbf{P}}^{p_0,\mathcal{A}}\left(\mathbf{p}(p,\theta_x,\theta_y)\right)$ and then apply the change of variables formula (41) 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:

$$f_{P,\Theta_x,\Theta_y}^{p_0,\mathcal{A}}(p,\theta_x,\theta_y) = N^{\mathcal{A}}(\Delta p)^{-1}\,p^2\,\widetilde{\delta}^{\,\Delta p}\left(p-p_0\right) \times \Gamma(\theta_x,\theta_y)\ \left|\,\mathcal{F}^{\mathcal{A}}\left(\,\mathbf{p}(p,\theta_x,\theta_y)-\mathbf{p}(p_0,0,0)\,\right)\right|^2. \tag{43}$$

Then, to express $N^{\mathcal{A}}(\Delta p)$, we apply the change of variables $(p_x,p_y,p_z)\to(p,\theta_x,\theta_y)$ in the integral of the right-hand side of (38). We obtain:

$$N^{\mathcal{A}}(\Delta p) = \int_0^{\infty}\mathrm{d}p\ p^2\ \widetilde{\delta}^{\,\Delta p}\left(p-p_0\right) \times \int_{-\pi/2}^{+\pi/2}\mathrm{d}\theta_x\int_{-\pi/2}^{+\pi/2}\mathrm{d}\theta_y\ \Gamma(\theta_x,\theta_y) \times \left|\,\mathcal{F}^{\mathcal{A}}\left(\,\mathbf{p}(p,\theta_x,\theta_y)-\mathbf{p}(p_0,0,0)\,\right)\right|^2. \tag{44}$$

Since Δp is close to zero and the function $\widetilde{\delta}^{\,\Delta p}\left(p-p_0\right)$ is not under a square root in (43) and (44), we can replace it by the Dirac distribution $\delta(p-p_0)$ and thus obtain an approximate expression of the p.d.f.. Given the property: $\delta(x-x_0)f(x)=\delta(x-x_0)f(x_0)$, this leads to:

$$f_{P,\Theta_x,\Theta_y}^{p_0,\mathcal{A}}(p,\theta_x,\theta_y) \simeq N^{\mathcal{A}}(0)^{-1}\,{p_0}^2\,\delta(p-p_0) \times \Gamma(\theta_x,\theta_y)\ \left|\,\mathcal{F}^{\mathcal{A}}\left(\,\mathbf{p}(p_0,\theta_x,\theta_y)-\mathbf{p}(p_0,0,0)\,\right)\right|^2. \tag{45}$$

Then the marginal p.d.f. $f_P^{p_0,\mathcal{A}}(p)$ is obtained by integrating (45) over θ_x and θ_y. Expressing $N^{\mathcal{A}}(0)$ from (44) applied to $\Delta p=0$, we see that this integration of (45) leads to an expression where $N^{\mathcal{A}}(0)$ is eliminated. What remains is

$$f_P^{p_0,\mathcal{A}}(p) \simeq \delta(p-p_0). \tag{46}$$

Therefore we have $p\simeq p_0$ in the final state which is exactly the kinematic constraint expressed by (27). The equation (46) confirms that the final state at time t_1, given by (36), 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:

$$\forall t\geq t_1: \ \left|\,\psi^{p_0,\mathcal{A}}(t)\,\right\rangle \simeq \exp\left[-(\mathrm{i}/\hbar)\,E(p_0)\,(t-t_1)\right]\left|\,\psi^{p_0,\mathcal{A}}(t_1)\,\right\rangle. \tag{47}$$

So, from (39), (40) and (47), we see that:

$$\forall t\geq t_1,\ \forall p_z\leq 0: \quad \left\langle\,\mathbf{p}\,\middle|\,\psi^{p_0,\mathcal{A}}(t)\,\right\rangle = 0. \tag{48}$$

Finally, from (47) and (48), the final state $\left|\,\psi^{p_0,\mathcal{A}}(t)\,\right\rangle$ has the properties (P1) and (P2) mentioned in subsection IV D and is therefore the appropriate final state that we can associate with the diffracted wave beyond the diaphragm.

F. Discussion

The assumption 2 suggests to apply the postulate of wave function reduction by using (35) which involves the product of operators $\hat{\mathrm{R}}^{p_0}\hat{\mathrm{R}}^{\mathcal{A}}$. From (23) and (33), 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) Although $\hat{\mathrm{R}}^{\mathcal{A}}$ and $\hat{\mathrm{R}}^{p_0}$ do not commute, they do not correspond to two incompatible observables. The operator $\hat{\mathrm{R}}^{\mathcal{A}}$ corresponds effectively to the three position observables $\hat{X},\hat{Y},\hat{Z}$ but the operator $\hat{\mathrm{R}}^{p_0}$ 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 $\hat{\mathrm{R}}^{p_0}\hat{\mathrm{R}}^{\mathcal{A}}$ corresponds to two simultaneous measurements according to the following interpretation. The first measurement, associated with $\hat{\mathrm{R}}^{\mathcal{A}}$, is the measurement of the position of the particle in the initial state $\left|\,\psi^{\mathrm{in}}_{\mathbf{p}_0}(t_1)\,\right\rangle$ (see (26)). The second measurement, associated with $\hat{\mathrm{R}}^{p_0}$, can be interpreted as a measurement of the energy and the momentum longitudinal component of the particle in the transitional state $\left|\,\psi^{\mathcal{A}}(t_1)\,\right\rangle$ created by the position measurement (see (32)). This measurement gives the result $E(p_0)$ with near certainty for the energy (property (P1), Eq. (46)-(47)) and the result $p_z > 0$ for the momentum (property (P2), Eq. (48)). 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 $\left|\,\psi^{\mathcal{A}}(t_1)\,\right\rangle$ only at time t_1.

(2) In (26), the initial state $\left|\,\psi^{\mathrm{in}}_{\mathbf{p}_0}(t_1)\,\right\rangle$ and the reduction operator $\hat{\mathrm{R}}^{\mathcal{A}}$ 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 $\hat{\mathrm{R}}^{\mathcal{A}}$ which then represents the "measurement device only". On the other hand, in (35), the initial state $\left|\,\psi^{\mathrm{in}}_{\mathbf{p}_0}(t_1)\,\right\rangle$ still represents the incident particle but the operator $\hat{\mathrm{R}}^{p_0}\hat{\mathrm{R}}^{\mathcal{A}}$ depends on p_0 and consequently includes a piece of information on the incident particle. Therefore, the operator $\hat{\mathrm{R}}^{p_0}\hat{\mathrm{R}}^{\mathcal{A}}$ 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 $\hat{\mathrm{R}}^{p_0}$). From this point of vue, (35) seems more appropriate than (26) 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 $\hat{\mathrm{R}}^{p_0}\hat{\mathrm{R}}^{\mathcal{A}}$ and the fact that $\hat{\mathrm{R}}^{p_0}$ 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:

initial state	*measurement of position*	transitional state	*measurement of energy and longitudinal component of momentum*	final state
= energy and momentum eigenstate, monochromatic plane wave (λ_0) propagating in z axis direction	⟶ result: $(x, y, z) \in$ generalized 3D aperture	wave function localized at the generalized 3D aperture, spreading in energy and momentum	⟶ results: $E \simeq$ energy of the initial state (due to kinematics) and $p_z > 0$ (particle exiting towards the half-space $z > 0$)	≃ energy eigenstate, quasi-monochromatic diffracted wave propagating beyond the diaphragm and such that $\lambda \simeq \lambda_0$.

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 particle occupies the transitional state for a period of time which tends to zero.

Remark. If the order of the measurements is inverted, the obtained state is the same as in the case of a position filtering only. Indeed, replacing $\hat{\mathrm{R}}^{p_0}\hat{\mathrm{R}}^{\mathcal{A}}$ by $\hat{\mathrm{R}}^{\mathcal{A}}\hat{\mathrm{R}}^{p_0}$ in (35) is equivalent to replace $\left|\,\psi^{\mathrm{in}}_{\mathbf{p}_0}(t_1)\,\right\rangle$ by $\hat{\mathrm{R}}^{p_0}\left|\,\psi^{\mathrm{in}}_{\mathbf{p}_0}(t_1)\,\right\rangle$ in (26). From (25) and (33), we have: $\hat{\mathrm{R}}^{p_0}\left|\,\psi^{\mathrm{in}}_{\mathbf{p}_0}(t_1)\,\right\rangle = \sqrt{F^{p_0}(\mathbf{p}_0)}\left|\,\psi^{\mathrm{in}}_{\mathbf{p}_0}(t_1)\,\right\rangle$, 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 (26) in place of $\left|\,\psi^{\mathrm{in}}_{\mathbf{p}_0}(t_1)\,\right\rangle$, we see that $\sqrt{F^{p_0}(\mathbf{p}_0)}$ is eliminated and we recover $\left|\,\psi^{\mathcal{A}}(t_1)\,\right\rangle$.

G. Quantum model predictions for the Fraunhofer diffraction

We now come to the expression of the relative intensity. The marginal p.d.f. $f^{p_0,\mathcal{A}}_{\Theta_x,\Theta_y}(\theta_x,\theta_y)$ 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 Sec. II). In this case, $f^{p_0,\mathcal{A}}_{\Theta_x,\Theta_y}(\theta_x,\theta_y)$ is none other than the directional intensity normalized to 1:

$$\frac{I^{p_0,\mathcal{A}}_{\mathrm{QM}}(\theta_x,\theta_y)}{\displaystyle\int_{-\pi/2}^{+\pi/2}\mathrm{d}\theta'_x\int_{-\pi/2}^{+\pi/2}\mathrm{d}\theta'_y\;I^{p_0,\mathcal{A}}_{\mathrm{QM}}(\theta'_x,\theta'_y)} = f^{p_0,\mathcal{A}}_{\Theta_x,\Theta_y}(\theta_x,\theta_y) \equiv \int_0^\infty \mathrm{d}p\;\; f^{p_0,\mathcal{A}}_{P,\Theta_x,\Theta_y}(p,\theta_x,\theta_y). \tag{49}$$

From (49) (first equality), the relative intensity is:

$$\left[\frac{I(\theta_x,\theta_y)}{I(0,0)}\right]^{p_0,\mathcal{A}}_{\rm QM} = \frac{f^{p_0,\mathcal{A}}_{\Theta_x,\Theta_y}(\theta_x,\theta_y)}{f^{p_0,\mathcal{A}}_{\Theta_x,\Theta_y}(0,0)}. \quad (50)$$

From (49) (second equality), we calculate $f^{p_0,\mathcal{A}}_{\Theta_x,\Theta_y}(\theta_x,\theta_y)$ and $f^{p_0,\mathcal{A}}_{\Theta_x,\Theta_y}(0,0)$ by integrating (45) over p. After this integration, given (27), it is convenient to replace p_0 by p, this latter notation henceforth indicating the modulus of both the initial momentum and the final momentum, as in Sec. III where the conservation of the momentum modulus is implicitly assumed. Then, substituting the expressions of $f^{p,\mathcal{A}}_{\Theta_x,\Theta_y}(\theta_x,\theta_y)$ and $f^{p,\mathcal{A}}_{\Theta_x,\Theta_y}(0,0)$ into (50) modified with the substitution $p_0 \to p$, we find:

$$\left[\frac{I(\theta_x,\theta_y)}{I(0,0)}\right]^{p,\mathcal{A}}_{\rm QM} \simeq \Gamma(\theta_x,\theta_y) \times \frac{\left|\mathcal{F}^{\mathcal{A}}\left(\mathbf{p}(p,\theta_x,\theta_y)-\mathbf{p}(p,0,0)\right)\right|^2}{\left|\mathcal{F}^{\mathcal{A}}(0)\right|^2}. \quad (51)$$

From (24) and since $p_0 \simeq p$ (see (27)), the Fourier transform (37) can be expressed in the form:

$$\mathcal{F}^{\mathcal{A}}(\mathbf{p}-\mathbf{p}_0) \simeq \mathcal{F}^{\rm A}_{\rm T}(p_x,p_y)\,\mathcal{F}^{\Delta z}_{\rm L}(p_z-p), \quad (52)$$

where:

$$\mathcal{F}^{\rm A}_{\rm T}(p_x,p_y) \equiv (2\pi\hbar)^{-1} \times \iint_{\mathbb{R}^2} {\rm d}x{\rm d}y\,\sqrt{F^{\rm A}_{\rm T}(x,y)}\,\exp[-({\rm i}/\hbar)(p_x x+p_y y)], \quad (53)$$

$$\mathcal{F}^{\Delta z}_{\rm L}(p_z-p) \equiv (2\pi\hbar)^{-1/2} \times \int_{\mathbb{R}} {\rm d}z\,\sqrt{F^{\Delta z}_{\rm L}(z)}\,\exp\left[({\rm i}/\hbar)(p-p_z)z\right]. \quad (54)$$

Quantum formula of the relative intensity in Fraunhofer diffraction. Substituting (52) into (51) 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 generalized 3D aperture $\mathcal{A} \equiv {\rm A}\times[-\Delta z/2,+\Delta z/2]$:

$$\left[\frac{I(\theta_x,\theta_y)}{I(0,0)}\right]^{p,\mathcal{A}}_{\rm QM} \simeq \Gamma(\theta_x,\theta_y)\,T^{\rm A}(p,\theta_x,\theta_y)\,L^{\Delta z}(p,\chi), \quad (55)$$

where χ and $\Gamma(\theta_x,\theta_y)$ are respectively given by (8) and (42), and

$$T^{\rm A}(p,\theta_x,\theta_y) \equiv \frac{\left|\mathcal{F}^{\rm A}_{\rm T}(p\cos\chi\,{\rm tg}\,\theta_x\,,\,p\cos\chi\,{\rm tg}\,\theta_y)\right|^2}{\left|\mathcal{F}^{\rm A}_{\rm T}(0,0)\right|^2} \quad (56)$$

is the *transverse diffraction term* and

$$L^{\Delta z}(p,\chi) \equiv \frac{\left|\mathcal{F}^{\Delta z}_{\rm L}(p(\cos\chi-1))\right|^2}{\left|\mathcal{F}^{\Delta z}_{\rm L}(0)\right|^2} \quad (57)$$

is the *longitudinal diffraction term*. The rigth-hand sides of (56) and (57) can be calculated using (53) and (54), where $F^{\rm A}_{\rm T}(x,y)$ is given by (20) and the function $F^{\Delta z}_{\rm L}(z)$ is part of the assumptions of the model.

V. INTEREST AND POSSIBILITY OF AN EXPERIMENTAL TEST

A. Comparison between quantum and classical formulae

Let us compare the quantum formula (55) to the classical one (see (10)). From (20), (53) and (56), we can rewrite (10) in the form:

$$\left[\frac{I(\theta_x,\theta_y)}{I(0,0)}\right]^{p,{\rm A}}_{\rm Class.} \simeq \Omega(\chi)^2\;T^{\rm A}(p,\theta_x,\theta_y). \quad (58)$$

The comparison between the quantum formula (55) and the classical formula (58) shows the following features:

(i) The transverse diffraction term $T^{\rm A}(p,\theta_x,\theta_y)$ 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 $(\cos\chi)/(1-\sin^2\theta_x\sin^2\theta_y)$ (where χ is given by (8)) and is related to the Jacobian of the change of variables of the momentum p.d.f. (see (41) and (42)) whereas the factor $\Omega(\chi)^2$ of the classical formula is equal to the square of the obliquity factor involved in the classical expression of the amplitude (see (1) and (3)).

(iii) The longitudinal diffraction term $L^{\Delta z}(p,\chi)$ 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 $T^{\rm A}(p,\theta_x,\theta_y)$. However, the results differ when the angles increase. The difference can be significant at large angles and therefore observable experimentally as we shall see below.

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 (42) imply respectively: $\chi = \theta$ and $\Gamma(\theta,0) = \cos\theta$. Hence, (55) and (58) lead to (after expressing $\Omega(\theta)$ from (3)):

$$\left[\frac{I(\theta,0)}{I(0,0)}\right]^{p,\mathcal{A}}_{\rm QM} \simeq \cos\theta\;T^{\rm A}(p,\theta,0)\;L^{\Delta z}(p,\theta), \quad (59)$$

$$\left[\frac{I(\theta,0)}{I(0,0)}\right]^{p,{\rm A}}_{\rm Class.} \simeq \left\{\begin{matrix}(1+\cos\theta)^2/4\\ \cos^2\theta\\ 1\end{matrix}\right\} T^{\rm A}(p,\theta,0) \quad , \quad \left\{\begin{matrix}({\rm FK})\\ ({\rm RS1})\\ ({\rm RS2})\end{matrix}\right\}, \quad (60)$$

where, from (20), (53) and (56):

$$T^{\rm A}(p,\theta,0) = \frac{1}{S({\rm A})^2}\left|\iint_{\rm A}{\rm d}x{\rm d}y\,\exp\left[-{\rm i}(k\sin\theta)x\right]\right|^2. \quad (61)$$

B. Predictions for a slit and a circular aperture

Let us apply the formulae (59), (60) and (61) to the cases of a rectangular slit and a circular aperture and to the case of a Gaussian longitudinal filtering.

a. Slit. Consider a rectangular slit R centered at $(x, y) = (0, 0)$, such that its medians correspond to the axis Ox (width $= 2a$) and Oy (height $= 2b$). In this case, we have: $S(\mathrm{R}) = 4ab$ and the integral of the right-hand side of (61) is given by:

$$\iint_{\mathrm{R}} \mathrm{d}x\mathrm{d}y\ \exp\left[-\mathrm{i}(k\sin\theta)x\right] = \int_{-a}^{+a} \mathrm{d}x\ \exp\left[-\mathrm{i}(k\sin\theta)x\right] \int_{-b}^{+b} \mathrm{d}y. \tag{62}$$

Integrating and then substituting into (61), we get:

$$T^{\mathrm{R}}(p,\theta,0) \ = \ \left(\frac{\sin(ak\sin\theta)}{ak\sin\theta}\right)^2. \tag{63}$$

b. Circular aperture. Consider a circular aperture C of radius r and centered at $(x, y) = (0, 0)$. We have: $S(\mathrm{C}) = \pi r^2$ and the integral of the right-hand side of (61) is given by:

$$\begin{aligned}\iint_{\mathrm{C}} \mathrm{d}x\mathrm{d}y\ \exp\left[-\mathrm{i}(k\sin\theta)x\right] &= \int_{-r}^{+r} \mathrm{d}x\ \exp\left[-\mathrm{i}(k\sin\theta)x\right] \int_{-\sqrt{r^2-x^2}}^{+\sqrt{r^2-x^2}} \mathrm{d}y \\ &= 4\int_0^r \mathrm{d}x\ \sqrt{r^2-x^2}\ \cos\left[(k\sin\theta)x\right].\end{aligned} \tag{64}$$

This integral is known [33] (3.771.8, p.464). Hence, substituting into (61) after the integration, we obtain:

$$T^{\mathrm{C}}(p,\theta,0) \ = \ \left(\frac{2J_1\left(rk\sin\theta\right)}{rk\sin\theta}\right)^2, \tag{65}$$

where $J_1(x)$ is the Bessel function of order 1.

c. Gaussian longitudinal filtering. The width Δz of the longitudinal aperture can be deduced from the standard deviation σ_z of the Gaussian filtering function and from the threshold α under which it is considered that a quantity is negligible. For example, if the integral of the Gaussian outside the interval is $\alpha = 10^{-2}$, we have [34]: $\Delta z(\sigma_z, \alpha) \simeq 5.16\,\sigma_z$. It is convenient to choose σ_z as parameter (instead of Δz) and use the following notations: the subscript $\Delta z(\sigma_z, \alpha)$ will be replaced by σ_z and the generalized 3D aperture $\mathcal{A} = \mathrm{A} \times [-\Delta z(\sigma_z, \alpha)/2, +\Delta z(\sigma_z, \alpha)/2]$ will be denoted $\{\mathrm{A}, \sigma_z\}$. So, let us assume that the longitudinal filtering function is Gaussian:

$$F_{\mathrm{L}}^{\sigma_z}(z) \ = \ (\sigma_z\sqrt{2\pi})^{-1}\ \exp\left[-z^2/\left(2{\sigma_z}^2\right)\right]. \tag{66}$$

Substituting (66) into (54), we get [33](3.896.4, p. 514):

$$\mathcal{F}_{\mathrm{L}}^{\sigma_z}(p_z - p) = \left(\frac{2}{\pi}\right)^{1/4}\left(\frac{\sigma_z}{\hbar}\right)^{1/2}\exp\left[-{\sigma_z}^2(k-k_z)^2\right]. \tag{67}$$

The longitudinal diffraction term is expressed by substituting (67) into (57). The factor $(2/\pi)^{1/4}(\sigma_z/\hbar)^{1/2}$ is then eliminated and we get:

$$L^{\sigma_z}(p,\theta) \ = \ \exp\left[-2{\sigma_z}^2k^2\left(1-\cos\theta\right)^2\right], \tag{68}$$

which makes sense if $\sigma_z = 0$ (see footnote 2).

Two examples of curves obtained from the formulae (59) and (60) for two different realistic experimental cases are shown in Figs. 4 and 5 respectively corresponding to the generalized 3D apertures $\mathcal{R} \equiv \{\mathrm{R}, \sigma_z\}$ and $\mathcal{C} \equiv \{\mathrm{C}, \sigma_z\}$:

- Fig. 4: rectangular slit, (59) and (60) are applied for $\mathcal{A} = \mathcal{R} = \{\mathrm{R}, \sigma_z\}$ and $T^{\mathrm{R}}(p, \theta, 0)$ is given by (63).

- Fig. 5: circular aperture, (59) and (60) are applied for $\mathcal{A} = \mathcal{C} = \{\mathrm{C}, \sigma_z\}$ and $T^{\mathrm{C}}(p, \theta, 0)$ is given by (65).

- In the two cases, $L^{\sigma_z}(p, \theta)$ is given by (68).

The main characteristic of these results is that the curves are very close for small angles and diverge more and more when θ increases until significant gaps are reached, whatever the experimental parameters (shape and size of the aperture, wavelength).

If $\sigma_z = 0$, the diffracted wave associated with the particle is emitted from the wavefront located at the aperture, in accordance with the Huygens-Fresnel principle. The longitudinal diffraction term given by (68) is equal to 1. Then, the quantum values are as large as possible and the difference between classical predictions and quantum prediction is due exclusively to the angular factors [3]. The QM values are smaller than the values of the FK and RS2 theories and larger than the values of the RS1 theory. From (59) and (60), the ratios of the relative intensities QM/RS1 and RS2/QM are equal to $1/\cos\theta$. They already reach the value 2 for $\theta = 60°$. Therefore, it is not necessary for the angle to be very large to obtain a significant gap between the predictions of the quantum model and those of the RS1-2 theories. On the other hand, the ratio FK/QM is equal to $(1 + \cos\theta)^2/(4\cos\theta)$ which is worth 9/8 for $\theta = 60°$ and 2 for $\theta \simeq 80°$. The difference is significant

[3] Note that there is a formula, from classical optics, with the same angular factor as that of the quantum formula (59) ($\cos\theta$ not squared). This classical formula is based on the result of the first rigorous calculation of the diffraction by a wedge, due to Sommerfeld [2, 4] and completed by Pauli [5]. This result has been applied to the case of two wedges of zero angle placed opposite one another to form a slit (see [8], §75, problem 1). The obtained formula includes two terms: the right-hand side of (59) (with $T^{\mathrm{A}}(p, \theta, 0) = T^{\mathrm{R}}(p, \theta, 0)$ given by (63) and $L^{\Delta z}(p, \theta) = 1$) plus a small additional term equal to $[2ak\cos(\theta/2)]^{-2}$. However, this small additional term is non-zero in the whole angular range $0° - 90°$, so the intensity is not zero at the minima (see also [9]).

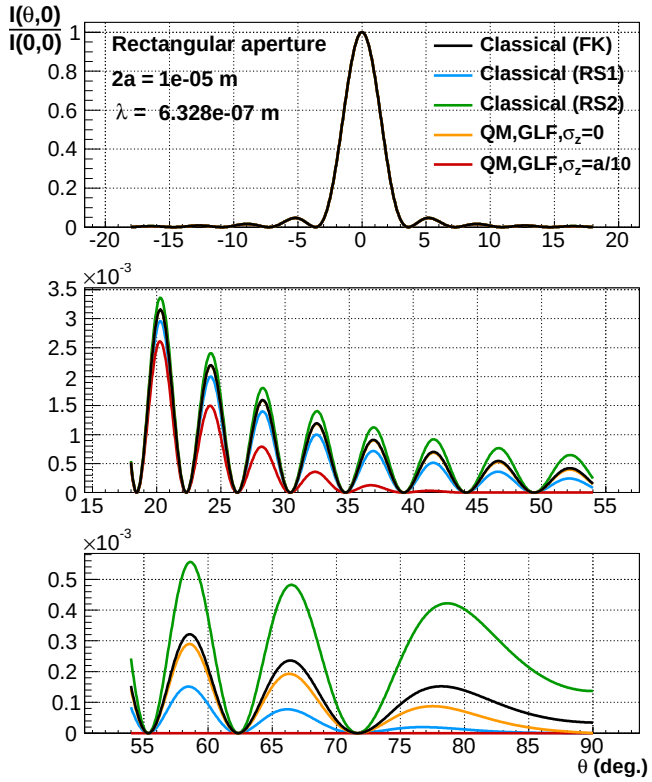


FIG. 4. Comparison of the relative intensities in Fraunhofer diffraction as a function of the diffraction angle in the horizontal plane for a rectangular slit of width $2a = 10$ μm and a monochromatic incident wave corresponding to photons of wavelength $\lambda = 632.8$ nm (Helium-Neon Laser). Five 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 $\sigma_z = a/10$). The value $\sigma_z = 0$ corresponds to the case where the diffracted wave associated with the particle is emitted from the wavefront at the aperture whereas a non-zero value corresponds to the case where several wavefronts contribute with different weights and this generates a damping increasing with θ and σ_z.

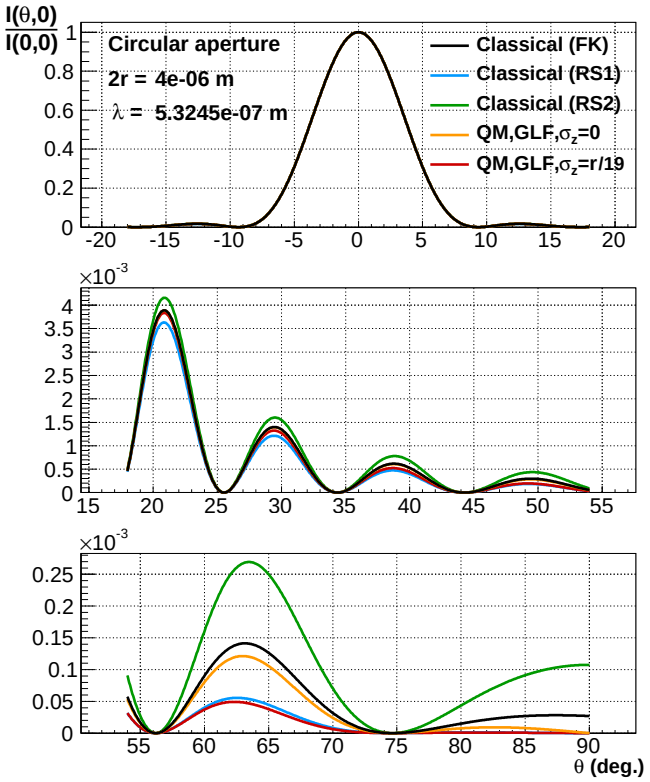


FIG. 5. Comparison of the relative intensities in Fraunhofer diffraction as a function of the diffraction angle in the horizontal plane for a circular aperture of diameter $2r = 4$ μm and a monochromatic incident wave corresponding to photons of wavelength $\lambda = 532.45$ nm (KTP Laser). The curves are different from those of Fig. 4 because the experimental parameters are different (shape and size of the aperture, wavelength). However, the gaps between them are the same (except for $\sigma_z = r/19$) because they depend only on the diffraction angle. The value $\sigma_z = r/19$ was chosen so that the quantum curve is close to the RS1 curve. Moreover, for this value, the damping is less important than that of Fig. 4 because the value $r/19$ is closer to zero than the value $a/10$.

only for the very large angles. So, the quantum model and the FK theory are in good agreement over a wide angular range.

If $\sigma_z > 0$, the diffracted wave associated with the particle is emitted from several wavefronts which contribute with different weights given by the distribution $F_{\mathrm{L}}^{\sigma_z}(z)$. 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 θ and σ_z. When σ_z is increasing from zero, the quantum values eventually pass below the values of the RS1 theory. 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 (Fig. 4). 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 (Fig. 5). Moreover, applying (68) to the case $\sigma_z \to \infty$ and then substituting into (59), we see that the intensity tends to a peak of zero width at $\theta = 0$. So, the quantum model predicts no diffraction at all in 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.

VI. CONCLUSION

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 is based on two main assumptions.

According to the first assumption, the diaphragm is considered as a measurement device not only of the transverse coordinates but also of the longitudinal coordinate of the particle, so that the initial state is projected on a state whose position wave function is localized in a "generalized 3D aperture" including the 2D aperture of the diaphragm. The longitudinal size Δz of this 3D aperture can be considered as the width of a "longitudinal aperture". It is a parameter whose value is between zero and infinity. If $\Delta z = 0$, the diffracted wave is emitted from the wavefront at the aperture, which is consistent with the Huygens-Fresnel principle. If $\Delta z > 0$, it can be assumed that the Huygens-Fresnel principle applies to several wavefronts which contribute with different weights according to some distribution whose integral outside the longitudinal aperture is negligible and whose shape is part of the assumptions of the model. Due to the position measurement, the momentum wave function of the state resulting from the projection of the initial state is incompatible with the kinematics of the particle-diaphragm interaction, so that this state is necessarily a transitional state. This is the reason of the second assumption which suggests, in the case of a monochromatic incident wave, that a specific operator projects the transitional state on the final state corresponding to the diffracted wave propagating beyond the diaphragm. Thus, the quantum model describes the change of state by two quasi-simultaneous successive projections.

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 theories of Fresnel-Kirchhoff and Rayleigh-Sommerfeld shows that the predictions are close for small diffraction angles but significantly different for large angles. Moreover, the quantum model predicts a damping of the intensity, increasing with angle and parameter Δz. If $\Delta z = 0$, there is no damping and the prediction of the quantum model is very close to that of the Fresnel-Kirchhoff theory over a wide angular range. As Δz increases, the damping reduces the diffraction at smaller and smaller angles and even removes it completely if $\Delta z \to \infty$. A study performed in the case of the diffraction by a rectangular slit and by a circular aperture shows that a measurement of the relative intensity in the region of large angles should make it possible to compare these predictions to experimental data and consequently to discriminate between the different theories.

The quantum model presented here provides an expression of the quantum state of the particle associated with the wave diffracted by an aperture of finite area. It is then possible to calculate the Fraunhofer diffraction, from the momentum wave function of this state, in the case of a monochromatic plane wave in normal incidence. Another application can be considered. The quantum model is a natural framework for treating 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) by a state corresponding to a wave packet. It will then be necessary to modify the second assumption of the model that currently applies only to the monochromatic case.

Finally, the question of calculating Fresnel diffraction from the suggested quantum model arises. For a particle whose quantum state is represented by a state vector of the Hilbert space, the momentum wave function is the Fourier transform of the position wave function. Now, when the Huygens-Fresnel principle is applied in the framework of the classical theory to calculate the amplitude of the diffracted wave, this Fourier transform is obtained only in the particular case of Fraunhofer diffraction, when it is possible to neglect the terms that must be taken into account in the case of Fresnel diffraction. These characteristic terms of Fresnel diffraction are therefore totally absent from the formalism of the state vectors and their associated wave functions. So, the suggested quantum model, based on this formalism, is not applicable in principle to the case of Fresnel diffraction.

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