Double Slit Diffraction Pattern of Gaussian Wave Packet Interacting with the Wall

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Abstract

The diffraction pattern by double slit is studied by incoming Gaussian wave packet subjected to scattering interaction with the wall and a truncation assumption when crossing the slits. Explicit results are valid for sufficiently smooth scattering amplitude. They concern large and narrow aperture of the incoming wave packet. For wave packet localized in spatial region smaller then the aperture of the slits there is no diffraction and the particle behaves classically. For wave packet peaked in the momentum probability distribution there are maxima, superimposed to the canonical diffraction pattern, in correspondence to the edges of the slits. Previous similar results are generalized and improved.

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1 Introduction

The two slit interference of particles, that originally was a pure thought experiment, represents a central point in the conceptual foundations of quantum mechanics [8]. As known, a beam of particles of well defined energy can be represented, after the slits, by a wave of the form $\psi = \psi_1 + \psi_2$, $\psi_1$, $\psi_2$ being the waves diffracted by the slit 1,2 respectively. The diffraction pattern is then a consequence of the statistical interpretation of $|\psi_1 + \psi_2|^2$ and of the quantum superposition of states. According to the principle, pure superpositions of pure states exist in quantum mechanics, in contrast to classical mechanics where the only superpositions of pure states are the statistical mixtures of them (e.g. [14]). Diffraction in time and diffraction both in space and time can
also be defined theoretically. Diffraction in time exists for Schrödinger waves, but not for light in vacuum [4]. The two slit electron pattern has been obtained experimentally (e.g. Ref. [10]), it has been reconstructed by computer simulated experiments (see e.g. Ref. [2]) and finally it has been reconstructed experimentally also by single incoming electron [13].

Due to the rapid and sophisticated technological development, a theoretical treatment of the experience in terms of wave packet would be more satisfactory. This also for a comparison with the previsions of other physical theories.

In the present paper the problem is formulated in the (sufficiently general) two dimensional Schrödinger formalism. As sketched in [7] a complete study is possible in abstract. For the purposes of the present paper it is better to represent the particle by a Gaussian wave packet that is free when far from the slits and that interacts with the wall when approaching the slits. The interaction is described in terms of potential scattering that acts on the wave packet before and after the slits. After the slits there is again a Schrödinger-like motion with initial condition the entering wave packet “truncated” by the wall. The treatment is specialized to the cases of a wave packet well defined in the momentum probability distribution or narrow with respect to the slits. In the first case the usual diffraction pattern is obtained with maxima superimposed in correspondence to the edges of the slits. In the second case one obtains a Gaussian spot on the screen, only for entering particle in correspondence of the slit regions, and therefore there is no diffraction. The results are valid for a potential interaction whose scattering amplitude has a smooth momentum dependence. In the calculations, components of the wave function that behave like $1/r$ after the slits and terms quadratic in the scattering amplitude are neglected.

The present study is an improvement and a generalization of two previous results [15, 16]. In Ref. [15] the deformation, due to the scattering-like interaction, of the wave packet when approaching the slits was neglected thus introducing a discontinuity in the description of the motion of the particle when passing the slits. In Ref. [16] instead the study was limited to a single slit and many results were proved to be essentially valid only for the Yukawa potential. Finally here the velocity of the particle has, contrarily to what assumed in [15, 16], a non trivial velocity component also in the direction of the slits.

2 Assumptions and general developments.

The coordinate system can be choosen, without loss of generality, so that the slits lie on the $y$–axis in the regions $S_1 = [a, b]$, $S_2 = [-c, -a]$, ($b > a$, $c > a > 0$). We denote the region of the slits $S = S_1 \cup S_2$, and the aperture of the slits by $d_1 = b - a$, $d_2 = c - a$. The particle, of mass $m$ and charge $q$,
is represented by a wave packet, solution of the Schrödinger equation, that comes from the negative regions. When far from the slits, the particle is given by a Gaussian wave packet centered at a point \( P \equiv (x(t), y(t)) \) freely moving with velocity \( v_{0k} = p_{0k}/m : x_k(t) = x_{0k} + v_{0k}t, k = x, y \). When approaching the slits the particle interacts with the charges induced on the wall of the slits. The induced charges are assumed to be constant in time, proportional to \( q \) and located at the edges of the slits. From the theory of Quantum potential scattering [12] the incident particle is then described by the wave function

\[
\psi(x, y, t) = \int \int dp_x dp_y c(p_x, p_y) u_{p_x p_y}(x, y) \exp\left(-\frac{i}{\hbar} \frac{p^2}{2m} t\right) \quad (1)
\]

\[
u_{p_x p_y}(x, y) = \frac{1}{2\pi\hbar}\left(e^{i\frac{2\pi}{\hbar}(p_x x + p_y y)} + \sum_{j=1}^4 f_j \frac{e^{ipr_j/\hbar}}{r_j}\right) \quad (2)
\]

where \( f_j(\theta_{p r_j}, \beta) \), \( j = 1, 2, 3, 4 \) is the scattering amplitudes relative to the center \( j \); \( r_j^2 = x^2 + (y - a_j)^2 \), \( a_1 = a, a_2 = b, a_3 = -\alpha, a_4 = -c \) and \( p = (p_x^2 + p_y^2)^{1/2} \). The solution (1) represents the particle at every time and for \( t \to -\infty \) represents an incoming free particle. According to the Gaussian-like description it is assumed [11, 5]

\[
c(P) = \frac{1}{\hbar \sqrt{\alpha \beta \pi}} \exp\left[ -\frac{(p_x - p_{0x})^2}{2 \alpha^2 \hbar^2} - \frac{(p_y - p_{0y})^2}{2 \beta^2 \hbar^2} - \frac{i}{\hbar} P \cdot X_0\right] \quad (3)
\]

The corresponding momentum probability distribution are such that \( \Delta p_x = \alpha \hbar / \sqrt{2} \) and \( \Delta p_y = \beta \hbar / \sqrt{2} \). The incident particle is then sum of a free Gaussian and of spherical wave packets the last representing the multi center scattering interaction. When passing the slits the wave packet is highly modified because part of it is reflected by the wall. Therefore we assume that, after the slits, the wave packet \( \psi_{\text{out}} \) propagates again as in equation (1) but with a new coefficient \( \widetilde{c}(p_x, p_y) \) re-defined by the “truncation” produced by the presence of the wall of the slits. Precisely we assume

\[
\psi_{\text{out}}(x, y, t) = \int_{\mathbb{R}^3} dp_x dp_y d\xi \int_{\mathbb{S}} d\eta \ u_{p_x p_y}^*(\xi, \eta) \psi_0(\xi, \eta) u_{p_x p_y}(x, y) \exp\left[-\frac{i}{\hbar} \frac{p^2}{2m} t\right] \quad (4)
\]

where \( \psi_0(x, y) \) is given by the expression (1) at a time \( t_0 \), considered as the initial time, in which the packet passes the slits.

The calculation of the integral (4) can be reduced by meaningful approximations. The expression (4) of \( \psi_{\text{out}} \) consists of the sum of 125 integrals as it appears from the expressions (1-2). Of these integrals, 100 behave like \( 1/r \) and can be neglected for a screen sufficiently far from the slits. The 16 integrals containing terms quadratic in \( f^2 \), and so proportional to the fourth power of the charge, can be neglected. By setting \( \psi_0 = \psi_{\text{diff}}^0 + \psi_{\text{scatt}}^0 \) (with \( \psi_{\text{scatt}}^0 \) the
four centers scattering part and $\psi_{\text{diff}}^0$ the free Gaussian part of $\psi(x, y, t)$ in eq. (1) at the mentioned time $t_0$), one is left with

$$\psi_{\text{out}} = \psi_{\text{diff}}(x, y, t) + \psi_{\text{scatt}}(x, y, t) + \psi_{\text{scatt}}^1(x, y, t)$$  \hspace{1cm} (5)$$

$$\psi_{\text{diff}} = \int_{R^3} dp_x dp_y d\xi \int_S d\eta \ e^{i[p_x(x-\xi)+p_y(y-\eta)-p^2 t/2m]} \frac{\psi_{\text{diff}}^0(\xi, \eta)}{(2\pi \hbar)^2}$$  \hspace{1cm} (6)$$

$$\psi_{\text{scatt}} = \int_{R^3} dp_x dp_y d\xi \int_S d\eta \ e^{i[p_x(x-\xi)+p_y(y-\eta)-p^2 t/2m]} \frac{\psi_{\text{scatt}}^0(\xi, \eta)}{(2\pi \hbar)^2}$$  \hspace{1cm} (7)$$

$$\psi_{\text{scatt}}^1 = \int_{R^3} dp_x dp_y d\xi \int_S d\eta \ e^{i[p_x(x+y-\xi-\eta)-\xi^2/2m]} \sum_{j=1}^4 f^j_p(\theta_{p r_j^\xi}) \frac{e^{i p r_j^\xi}}{r_j^2} \frac{\psi_{\text{diff}}^0(\xi, \eta)}{(2\pi \hbar)^2}$$  \hspace{1cm} (8)$$

($r_j^\xi \equiv (\xi, \eta - a_j), \ j = 1, 2, 3, 4$). It is a fact that also $\psi_{\text{scatt}}^1$ can be neglected for the screen sufficiently far from the slits. Indeed, meaningful contributions to the integral (8) for large $x$ comes from small values of $p_x$. One can then put $p_x^2 \cong 0, \ p \cong |p_y|$. So the integral (8) is proportional to $\int_{-\infty}^{\infty} \exp(\frac{1}{4} p_x x) dp_x = 2\pi \hbar \delta(x)$ that vanishes for $x \neq 0$ so that $\psi_{\text{scatt}}^1 = 0$.

Even with the last simplifications, the expression of $\psi_{\text{out}} = \psi_{\text{diff}} + \psi_{\text{scatt}}$ and the initial state $\psi_0(x, y)$ seem difficult to be determined in general. In the following Sections the limiting cases of narrow momentum or position probability distributions are studied.

### 3 Spatially large wave packet.

Suppose the uncertainty in the momentum probability distribution satisfies

$$\Delta p_x = \frac{\hbar \alpha}{\sqrt{2}} \ll 1, \quad \Delta p_y = \frac{\hbar \beta}{\sqrt{2}} \ll 1.$$  \hspace{1cm} (9)$$

From this assumption, by taking into account the expression (3), $c(p)$ results to be a peaked function for $p = p_0$. By then approximating $pr_j \cong p \cdot r_j^0$ ($r_j^0$ the projection of $r_j$ over $p_0$), after the integrations over $p_x, p_y$, the scattering part of $\psi$ in (1) has the form $\sum_{j=1}^4 f^j_p(\theta_{p r_j^0}) \psi_j(r_j^0 - \frac{p_0 t}{m} + x_0)/r_j$. By defining the initial time to be the time for which $\frac{p_0 t}{m} + x_0 = 0$, one can assume as initial state in (4) the expression

$$\psi_0 = \left(\frac{\alpha \beta \pi}{\pi}\right)^{\frac{1}{4}} e^{-\frac{x^2}{2}(x-x_0)^2 - \frac{y^2}{2}(y-y_0)^2 + \frac{m}{2}p_0(x-x_0)} + \sum_{j=1}^4 f^j_p(\theta_{p r_j^0}) \psi_j(r_j^0)$$  \hspace{1cm} (10)$$

$$= \psi_{\text{diff}}^0(x, y) + \psi_{\text{scatt}}^0(x, y)$$  \hspace{1cm} (11)$$

where $\psi_j(r_j^0)$ is a Gaussian packet centered in $r_j^0 = 0$ and practically constant in $x, y$, on account of the assumption (9). It is possible now to obtain $\psi_{\text{out}}$. 

We first calculate the expression \( \psi_{\text{diff}} \) in (6). The factorized form of the above \( \psi_{\text{diff}}^0 \) gives rise, when inserted into eq. (6), to a factorized form of \( \psi_{\text{diff}}(x, y, t) \). All integrals can be exploited exactly and one finally obtains

\[
\psi_{\text{diff}} = \phi(x, t) \phi_S(y, t) \tag{12}
\]

\[
\phi = \frac{\alpha^{1/2} \pi^{-1/4}}{(1 + i \hbar \alpha^2 t/m)^{1/2}} \exp \left[ - \frac{\alpha^2(x - x_0 - \frac{p_{oy}}{m} t)^2}{2(1 + i \hbar \alpha^2 t/m)} + i \frac{p_{ox}(x - x_0) - \frac{p_{ox}^2}{2m}}{\hbar} \right] \tag{13}
\]

\[
\phi_S = A_S \left\{ \text{erf} \left[ \frac{i \eta (y - b) - \beta^2 \hbar t (y_0 - b) - i \eta p_{oy}}{(2 \hbar \eta (\beta^2 t - i m))(1/2) - \text{erf}[b \to a] + \text{erf}[b \to -a] - \text{erf}[b \to -c] \right] } \right. \tag{14}
\]

\[
A_S = \frac{1}{2} \left[ \frac{m \beta \pi^{-1/2}}{m + i \beta^2 t} \right]^{1/2} \exp \left[ \frac{i m \beta^2 (y - y_0)^2 + \frac{m^2 p_{oy}(y - y_0) - \frac{p_{oy}^2}{2m}}{\beta^2 \hbar t - i m}}{\beta^2 \hbar t - i m} \right] \tag{15}
\]

where \( \text{erf} z = 2 \pi^{-1/2} \int_0^z \exp(-t^2) dt \) is the error function \([1]\). As expected, the expression (13) is the Gaussian-like one dimensional wave packet that is the time evolution of the initial Gaussian-like one dimensional wave packet. Instead the expression \( \phi_S \phi_S^\star \) gives the \( y \)-diffraction pattern that, in absence of scattering, is proportional to

\[
A_S A_S^\star = \frac{m \beta \pi^{-1/2}}{4(m^2 + \hbar \beta^2 t^2)^{1/2}} \exp \left[ - m^2 \beta^2 (y - y_0 - \frac{p_{oy} t}{m})^2 \right] \tag{16}
\]

and it is therefore centered in \( y = y_0 + \frac{p_{oy}}{m} t \). So far the approximation \( \beta \ll 1 \) has not been used. By setting \( \beta^2 = 0 \) into the expressions (14-15) one would have the approximated diffraction pattern. However, due to the presence of the \( \text{erf} \) function, it is better to put \( \beta^2 = 0 \) directly into the integral (6). After an integration over \( p_y \), by neglecting the term \( \eta \hbar \text{im}/(\hbar \hbar) \), one obtains

\[
\phi_S = \left[ \frac{2 \beta m}{i \hbar \pi^3/2} \right]^{1/2} \exp \left\{ \frac{i m}{\hbar} (y^2 - p_{oy} y_0) \right\} \left\{ e^{i (a+b)/ \eta} \sin \frac{(p_{oy} t - my_1) d_1}{2 \hbar \eta} \cos \frac{p_{oy} t - my_1}{2 \hbar \eta} + e^{i (a+b)/ \eta} \sin \frac{(p_{oy} t - my_2) d_2}{2 \hbar \eta} \cos \frac{p_{oy} t - my_2}{2 \hbar \eta} \right\} \tag{17}
\]

Two special situations seem of interest. In case of equal slits, \( b = c \), and for an incident particle with \( p_{oy} = 0 \) one obtains from eq (17)

\[
\phi_S = 2 \left[ \frac{2 \beta m}{i \hbar \pi^3/2} \right]^{1/2} \exp \left\{ \frac{i m}{2 \hbar} y^2 \right\} \sin \frac{my_1}{\hbar} \cos \frac{my_1}{\hbar} (b + a) \tag{18}
\]

that corresponds to the usual elementary treatment \([7]\).
Instead, for one of the slits much smaller than the other, \( c = a + \epsilon \), \( (\epsilon > 0, \epsilon^2 \ll 0) \) one finds

\[
\phi_S \phi_S^\ast \approx \frac{2 \beta m}{\hbar \tau} \left[ \sin \frac{2 \rho_0 y t - my}{2 \hbar} + \epsilon \frac{\sin (p_0 y t - my)}{p_0 y t - my} \cos \frac{p_0 y t - my}{2 \hbar} (b + 3a) \right]
\]  

(19)

In this case, in absence of scattering, the diffraction pattern corresponds to that of a single slit, obtained by an elementary treatment, plus periodic modulations, and results essentially centered on the screen at \( y = v_0 t \).

- For what concerns \( \psi_{\text{scatt}} \), we make the drastic approximation of considering it, for the time of interest, practically equal to its initial value \( \psi_{\text{scatt}}^0(x, y) \). This is motivated by the following consideration. From eq. (7), after an integration over \( p_x, p_y \), one has

\[
\psi_{\text{scatt}} = -\frac{im}{t \hbar} \int d\xi \int d\eta \exp \left\{ \frac{im}{2 \hbar} [(x - \xi)^2 + (y - \eta)^2] \right\} \psi_{\text{scatt}}^0(\xi, \eta)
\]  

(20)

The integrations over \( \xi, \eta \) can be performed by taking into account that \( \exp \left\{ \frac{im}{2 \hbar} (x - \xi)^2 \right\} \approx (1 + i \sqrt{\frac{\pi \hbar}{m}} \delta(x - \xi) \) for \( t \ll m/(2 \hbar) \) (e.g. \( t \ll 1 \) sec. for electrons, \( t \ll 700 \) sec. for protons). Hence \( \psi_{\text{scatt}} = 0 \) for \( y \) essentially not belonging to the region \( S \) of the slits and

\[
\psi_{\text{scatt}} \cong \psi_{\text{scatt}}^0 = \sum_{j=1}^{4} \frac{f_j}{r_j} \psi_j(\mathbf{r}_j^0)
\]  

(21)

for \( y \in S \). Since \( r_j = (x^2 + (y - a_j)^2)^{1/2} \) the scattering term \( \psi_{\text{scatt}} \) produces superimposed maxima, in correspondence, to \( y = a_j \), to the pure diffraction pattern previously calculated. This effect may be very small because, in principle, the scattering amplitude should be proportional to the square of the charge of the particle (and hence it is absent for uncharged particle). On the other hand it can be amplified in correspondence to particular scattering amplitude, namely for special interactions between particle and wall.

4 Narrow wave packet.

A second special case for which the general scheme of Sec. 2 can be further developed is that of sufficiently narrow incoming wave packet:

\[
(\Delta x)_0 = \frac{1}{\alpha \sqrt{2}} \ll 1, \quad (\Delta y)_0 = \frac{1}{\beta \sqrt{2}} \ll 1
\]  

(22)

To obtain \( \psi_{\text{out}} \) one has to preliminary give \( \psi_0 = \psi_{\text{diff}}^0 + \psi_{\text{scatt}}^0 \). For what concerns \( \psi_{\text{scatt}}^0 \), it can be achieved by considering the scattering part \( \psi_{\text{scatt}}^0 \) of
the incoming wave packet. According to eqs. (1-2) and choosing \( x_0 = 0 \), \( \alpha = \beta \) such part can be written

\[
\psi_{\text{scatt}}^{\text{in}} = \sum_{j=1}^{4} \frac{1}{r_j} \int_{R^2} \frac{dp_x dp_y}{2\pi \hbar} f_{p_x p_y} \exp \left[ \frac{i}{\hbar} (pr_j - \frac{p^2}{2m}) - \frac{(p - p_0)^2}{2\alpha^2 \hbar^2} \right] \tag{23}
\]

\[
\approx \sum_{j=1}^{4} \frac{1}{r_j} \int_{0}^{\infty} \frac{dp}{2\pi \hbar} \exp \left[ \frac{i}{\hbar} (pr_j - \frac{p^2}{2m}) - \frac{(p - p_0)^2}{2\alpha^2 \hbar^2} \right] \int_{0}^{2\pi} f_{p_x} d\varphi \tag{24}
\]

\[
\approx \sum_{j=1}^{4} \frac{1}{r_j} \phi_j(r_j - \frac{p_0}{m} t) \tag{25}
\]

(The equation (25) follows by the assumption that \( \int_{0}^{2\pi} f_{p_x} d\varphi \) is a sufficiently smooth function of \( p \)). On account of the assumption (22), the expression of \( \phi_j \) in eq. (25) is a spherical wave packet, moving radially, peaked in \( r_j = \frac{p_0}{m} t \). By choosing \( t = 0 \) as the initial time, the initial state for \( \psi_{\text{scatt}} \) can be assumed to be

\[
\psi_{\text{scatt}}^{0} = \sum_{j=1}^{4} \frac{1}{r_j} \phi_j(r_j) \tag{26}
\]

with now \( \phi_j(r_j) \) sufficiently peaked in \( r_j = 0 \) or, equivalently, in \( x = 0 \), \( y = a_j \). From eq. (26) and after integrations over \( \xi \), \( \eta \) the term \( \psi_{\text{scatt}} \) in eq. (7) results proportional to \( \int dp_x \exp \left[ \frac{i}{\hbar} p_x x \right] \). Therefore \( \psi_{\text{scatt}} \propto \delta(x) \) that vanishes on the screen localized at \( x \neq 0 \). Hence \( \psi_{\text{out}} \equiv \psi_{\text{diff}} \) under condition (22).

To obtain \( \psi_{\text{diff}} \) one has to give \( \psi_{\text{diff}}^{0} \) that, in all generality, it is again the one given in the previous case (see eqs. (10-11)) whose corresponding time evolution has been calculated in eqs. (12-15). Under the approximation (22), it holds then \( \psi_{\text{out}} = \psi_{\text{diff}} = \phi(x, t) \phi_S(y, t) \) with \( \phi(x, t) \) given in eq. (13) and with \( \phi_S(y, t) \) having the expression of eqs. (14-15) for large \( \beta \). One obtains

\[
\phi_S \phi_S^* = \frac{e^{-2m^2 \beta^2 (y-y_0 - \frac{p_0}{m} t)^2}}{2\hbar \beta \pi m^{-1}} \left\{ \left[ \int \frac{1}{\sqrt{\beta(y-b)-\frac{p_0}{m}}} \right] + \left[ \int \frac{1}{\sqrt{\beta(y+a)-\frac{p_0}{m}}} \right] \right\} dt \tag{27}
\]

that represents a non trivial Gaussian spot on the screen, narrower than the slit apertures, centered at \( y = y_0 + \frac{p_0}{m} t \) only in case \( y_0 \) is such that \( \frac{p_0}{m} - c < y_0 < \frac{p_0}{m} + a \) or \( \frac{p_0}{m} - a < y_0 < \frac{p_0}{m} + b \), approximately. The case \( p_{oy} = 0 \) was obtained in Ref. [16] for the single slit. Therefore, in case of narrow wave packet there is no diffraction and the particle passes the slits in a classical way.

5 Comments and Remarks.

According to the results of the previous Sections, superimposed maxima in correspondence to the edges of the slits appear in the two slit diffraction pattern
for particle with narrow momentum probability distribution. For wave packet narrow with respect to the slits there is no diffraction and the scattering effect is negligible. The results are valid for sufficiently smooth scattering amplitude.

A scheme very similar to the present one can be found in Ref. [9]. There, the diffraction of atoms by transmission gratings is interpreted by long-range van der Waals interaction. By using the results of Ref. [9] there is therefore the possibility of evaluating the relevance of the maxima in the context of the present scheme (A numerical calculation of that effect is currently under study).

The conclusions here obtained have interest also in relation to the predictions of Stochastic Electrodynamics (SED) with spin. Actually, SED with spin predicts spots in correspondence to the edges of the slits also in case of a narrow beam [7]. It predicts also different forms of the diffraction pattern in case the wall is made of metal or of dielectric [6]. It is possible that, to have a better confrontations of Quantum Mechanics and SED with spin, some of the approximation done here should be relaxed. In any case, it seems that a direct experimental verification of the predictions should be of interest.

As to the theoretical treatment, qualitative improvements could be obtained by considering the spin of the particle. With reference to Coulomb-like scattering one has however that the corresponding cross section has the same leading coefficient that in absence of spin [3]. Modifications are possibly expected for ultrarelativistic velocity with not too small scattering angle [3].

A sensible improvement of the study should come from a better determination of the charges induced on the wall. This seems a difficult problem to be solved because, in principle, the charges depend on $y$ and $t$ and on the consistency of the beam of particles.

References


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