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Single Slit Diffraction Pattern of Schrödinger Particle with Interaction with the Wall

Antonio Zecca

Dipartimento di Fisica dell' Universita' - Milano, Italy (Retired)
GNFM, *Gruppo Nazionale per la Fisica Matematica- Italy*
Address: Dipartimento di Fisica, Universita' di Milano, Via Celoria, 16 - Milano, Italy

Abstract

Diffraction of Schrödinger particle by single slit is considered in the two dimensional space. Mathematically, the problem amounts to the solution of Schrödinger equation with boundary. Due to the difficulty of giving exact analytical solution, the study is developed by the method of Gaussian wave packets that far from the barrier can be considered to be exact solutions. By including also a possible interaction of the particle with the wall, the diffraction pattern is determined by a truncation, a confinement and a scattering assumption. The results are coherent with previous ones and are now obtained in a form suitable for physical application.

Keywords: Foundation of Schrödinger QM; Gaussian states; Single slit; Confinement, truncation, scattering; Massive particle diffraction.

1 Introduction

Diffraction by slit is possible also for massive particle. This was originally seen experimentally [4, 9, 7]; it has been verified to be highly coherent with the theoretical prediction [19] and more recently again verified (e., g., [5]). The diffraction pattern has been also reconstructed by computer simulation experiment [1] and, experimentally, by single incoming electron [10]. Diffraction in time and both in space and time can also be defined theoretically [2, 8].

Diffraction of massive particles by slits is not explainable within ordinary classical mechanics (CM) while in Quantum Mehanics (QM) it is not unexpected, the Schrödinger equation been interpretable as describing motion in dispersive medium [3].

From a theoretical point of view, in standard QM, two points are of relevance: the statistical interpretation of the wave function and the superposition principle of the solutions. Accordingly, wave function solution of the Schrödinger equation must be of class L^2, and solutions that are not of class L^2 (e., g, plane wave in confined space) are not physical solutions but, by their superposition, one can represent the particle by wave packet solution that are of class L^2.

From a mathematical point of view the study of the diffraction pattern problem of Schrödinger particle by slit would require the definition of (essentially) selfadjoint Schrödinger operator. This can indeed be done, but it involves the formulation of the boundary conditions in the week sense [11] thus preventing a simple treatment.

A study of the diffraction pattern for 1, 2, many slits was done by using Gaussian wave packet and by confinement and truncation and scattering assumptions [14, 15, 12, 13, 18].

In the present paper the diffraction of particle by single slit with scattering is considered by using Gaussian wave packet. Those solutions represent a sufficiently general tool that includes both the limit of plane waves and peaked wave packet.

The problem is formulated in a unified way by the mentioned conditions that refer to the initial state for the time evolution after the slit. For what concerns the effect of truncation and confinement assumptions, the results previously obtained are reported. Instead the scattering assumption is studied more extensively and with a different approach of the previous ones. This allows to put in evidence further qualitative aspects that are also quantitatively put into evidence by suitable approximations. The final results are given a form suitable for evaluation and application to a wide class of central interaction with the wall.

2 Assumptions and Formulation of the Problem

The diffraction by slits of Schrödinger particle is considered here in the two Cartesian coordinate system $O(x, y)$. The slit region S and the region S^c not accessible to the particle are defined by

$$S = \{(x, y) : |x| < a,\ |y| < b\} \tag{1}$$

$$S^c = \{(x, y) : |x| \le a, |y| \ge b > 0\} \tag{2}$$

where a is supposed to be very small so that in the calculations it is supposed to vanish. Within this geometry the motion of a particle of mass m in the given geometry is then governed by the Schrödinger equation with Schrödinger operator

$$\hat{H} = -\frac{\hbar^2}{2m}\Big(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\Big) + V(x, y) = \hat{H}_0 + V(x, y) \tag{3}$$

where $V(x, y)$ is an infinite barrier on ∂S^c, the boundary of S^c. By extending the usual consideration of Quantum Mechanics, the eigenfunctions of $\hat{H}$ are required to vanish on the boundary ∂S^c. As outlined in [11] this is in fact possible in the weak sense. That seems a very complicated way. Here, we proceed in the following way. Far from the slit, the description of the free particle motion is done according to $\hat{H}_o$. Near the slit, special heuristic assumptions are required to hold.

Accordingly, the diffraction problem is schematized as follows. The free wave solution $\psi(x, y, t)$ at $t \to -\infty$ freely comes from remote x region. It passes the slit being subjected to a "truncation", a confinement in the y direction and to a central scattering interaction at one only extreme point of the slit:

$$\psi(x, y, t) \overset{t\to-\infty}{\longrightarrow} \psi_{in} = \frac{1}{2\pi\hbar}\int dp_x dp_y\, u_{p_x p_y}(x, y)\, c(\mathbf{p})\, e^{-\frac{i}{\hbar}(\frac{p^2}{2m})t} \tag{4}$$

$$\psi(x, y, t) \overset{t\to\infty}{\longrightarrow} \psi_{out} = \psi_{tr}(x, y) + \psi_{conf}(x, y) + \psi_{scatt}(x, y) \tag{5}$$

The choice of ψ_{in} to be a Gaussian wave packet allows to develop the calculations and to cover a wide class of situations.

Accordingly we assume:

$$u_{p_x p_y}(x, y) = (2\pi\hbar)^{-1} \exp\left[\tfrac{i}{\hbar}(p_x x) + p_y y)\right] \tag{6}$$

$$c(\mathbf{p}) = (\hbar\sqrt{\alpha\beta\pi})^{-1} \times$$

$$\times \exp\Big[-\frac{(p_x - p_{0x})^2}{2\alpha^2\hbar^2} - \frac{(p_y - p_{0y})^2}{2\beta^2\hbar^2} - \frac{i}{\hbar}\mathbf{p}\cdot\mathbf{x}_0\Big] = c_x(p_x)\, c_y(p_y) \tag{7}$$

$$\psi_{in}(x, y, t) = \psi(x, t)\cdot\phi(y, t) \tag{8}$$

$$\psi(x, t) = \alpha^{1/4}\pi^{-1/2}(1 + i\hbar\alpha^2\frac{t}{m})^{-1/2} \times$$

$$\times \exp\Big[-\frac{\alpha^2}{2}\frac{(x - x_0 - \frac{p_{ox}}{m}t)^2}{1 + i\hbar\alpha^2\frac{t}{m}} + \frac{i}{\hbar}p_{ox}(x - x_0) - \frac{i}{\hbar}\frac{p_{ox}^2}{2m}t\Big] \tag{9}$$

$$\phi(y, t) = \beta^{1/4}\pi^{-1/2}(1 + i\hbar\beta^2\frac{t}{m})^{-1/2} \times$$

$$\times \exp\Big[-\frac{\beta^2}{2}\frac{(y - y_0 - \frac{p_{oy}}{m}t)^2}{1 + i\hbar\beta^2\frac{t}{m}} + \frac{i}{\hbar}p_{oy}(y - y_0) - \frac{i}{\hbar}\frac{p_{oy}^2}{2m}t\Big] \tag{10}$$

As to ψ_{out} we assume $\psi_{tr}(x,y)$, $\psi_{conf}(x,y)$ to be of the form

$$\int\int dp_x dp_y \, v_{p_x p_y} (v_{p_x p_y}|\psi_o) \, e^{-\frac{i}{\hbar}(\frac{p^2}{2m})t} \tag{11}$$

$v_{p_x p_y}$ suitable eigenfunctions of $\hat{H}$.

As to ψ_{scatt}, it is supposed the particle to have central interaction with one only (for the sake of simplicity) edge of the slit:

$$\psi_{scatt}(x,y) = \frac{1}{r_1}\frac{1}{2\pi\hbar}\int\int dp_x dp_y \, (v_{p_x p_y}|\psi_o) \, f(p,\theta_{\widehat{pr_1}}) \; e^{\frac{i}{\hbar}(pr_1 - \frac{p^2}{2m_0}t)} \tag{12}$$

were $r_1^2 = x^2 + (y-b)^2$ and $f(p,\theta_{\widehat{pr_1}})$ is the 3-dimensional scattering amplitude (restricted to 2 dimensions) were $\theta_{\widehat{pr_1}})$ is the angle between $\mathbf{p}$ and $\mathbf{r_1}$, $(\mathbf{r_1} \equiv (x, y-b))$. In every case $\psi_0 = \psi_{in}(x,y,0)\chi_{[-b,b]}(y)$, $\chi_{[-b,b]}$ being the characteristic function of the interval $[-b,b]$.

2.1 Truncation assumption

For what concerns ψ_{tr}, it is assumed $v_{p_x p_y} = u_{p_x p_y}(x,y)$ plus the truncation assumption

$$\psi_0 = \chi_{[-b,b]}(y)\psi(x,y,0) \equiv \chi_{[-b,b]}(y)\psi(x,0)\phi(y,0) \tag{13}$$

Therefore by exploiting the calculation, one has

$$\psi_{tr} = \psi(x,t)\phi(y,t) \tag{14}$$

where $\psi(x,t)$ is exactly the one given in (9).

In the limit of $\Delta p_y = \hbar\beta/\sqrt{2}$, $\beta << 1$, and $p_{0y} = 0$ one has

$$|\phi_{tr}(y,t)|^2 = \frac{2m\beta b^2}{t\hbar\pi^{3/2}} \, \frac{\sin^2 \frac{bm}{\hbar t} y}{(\frac{bm}{\hbar t} y)^2} \tag{15}$$

that is the standard interference pattern with the central maximum.

In the limit, $\Delta y \le b$, $\Delta y = 1/(\beta\sqrt{2}) << 1$, $p_{0y} = 0$, the expression $(u_{p_x p_y}|\psi_0)$ can be calculated by extending the integral to R^2 thus obtaining $\psi(x,y,t) \equiv \psi(x)\phi(y)$ and the particle passes the slit in an undisturbed way [17].

2.2 Confinement assumption

Passing the slit the particle moves in the y direction being confined in $-b \le y \le b$ by an infinite barriers in $y = \pm b$. According to standard Qantum Mechanics this give rise to discrete energy spectrum of $\hat{H}_y$ of eigenvalues $W_n = p_n^2/(2m_0)$ and normalized eigenfunctions

$$v_{p_n}(y) = \chi_{[-b,b]}(y)\frac{1}{\sqrt{b}}\sin\frac{p_n}{\hbar}(y-b), \quad p_n = \frac{n\hbar\pi}{2b}, \; n = 1, 2, 3, .. \tag{16}$$

On account of the very small value of $\hbar$ the substitution $v_{p_n} \to v_{p_y}(y) = b^{-1/2}\sin p_y(y-b)/\hbar, \; p_y \in R$ represents a very good approximation. Therefore, in the present case, the calculation of (11) can be exploited by assuming

$$v_{p_xp_y} = 2\chi_{[-b,b]}(y)\frac{1}{\sqrt{2\pi\hbar b}}e^{\frac{i}{\hbar}p_xx}(e^{\frac{i}{\hbar}p_yy} - e^{-\frac{i}{\hbar}p_yy}), \quad p_x, p_y \in R \tag{17}$$

Accordingly [17], one has again the form $\psi_{conf}(x,y) \equiv \phi_C(y)\psi(x)$, with ψ as in (9).

In the limit of $\Delta p_y = \hbar\beta/\sqrt{2}, \; \beta << 1$ of entering y-plane wave one gets [17]:

$$|\phi_C(y,t)|^2 = 16\frac{m^3b^4\beta}{\hbar^3t^3\pi^{3/2}}\,y^2\,\frac{\sin^4\frac{bm}{\hbar t}y}{(\frac{bm}{\hbar t}y)^4} \tag{18}$$

that is still an interference pattern different from (15).

In the limit of $\Delta y = \sqrt{2}/\beta$, $\beta >> 1$, the entering wave packet is narrower with respect to the slit aperture. With $p_0 = 0 = y_0$ one obtains

$$\phi_C\phi_C^*(y,t) = \frac{2m\pi^{-1/2}}{\hbar t\beta}\exp\left[-\frac{m^2}{\beta^2t^2\hbar^2}(y^2+b^2)\right]\sin^2\frac{mb}{t\hbar}y \tag{19}$$

In order the Gaussian modulation to be visible it must be $\beta > 2^{3/2}/b$.

2.3 Scattering assumption

For what concerns ψ_{scatt}, some basic qualitative considerations may done. The expression (12), by identifying $v_{p_xp_y}$ with the eigenfunctions $u_{p_xp_y}$ in (6), reads:

$$\psi_{scatt} = \frac{1}{r_1}\frac{1}{2\pi\hbar}\int_0^\infty dp\;\tilde{c}(p)\,e^{\frac{i}{\hbar}(pr_1-\frac{p^2}{2m}t)} \tag{20}$$

$$\tilde{c}(p) = \int_0^\pi d\theta\,\sin\theta\;c(p,\theta)\,pf(p,\theta) \tag{21}$$

($\theta \equiv \theta_{\widehat{pr_1}}$) that represents a circular wave packet moving along the r_1 axis. If instead one identifies $v_{p_xp_y}$ with the expression (17) one has a circular wave packet moving as in the previous case and a second one moving along r_1, in the opposite sense with no physical meaning because it would reach negative region of r_1 for $t \to +\infty$. Accordingly, ψ_{scatt} produces two spot on the screen at distance x, symmetric with respect to $y = b$.

It is possible to develop the situation in limiting cases.

i) Suppose first the incident wave packet to be narrower then the slit aperture $\Delta y_{t_0} = \frac{1}{\beta\sqrt{2}} \leq 2b$ $(\beta \geq \frac{1}{2b})$ and has still a narrow probability distribution of the momentum $\Delta p_y \equiv \hbar\beta/\sqrt{2} \ll 1$ $(\beta \ll \sqrt{2}/\hbar)$. By choosing $v = u$ in (12), to a good approximation, the η integral can be extended to R so that $(u_{p_x p_y}|\psi_o) \equiv c(\mathbf{p})$. Therefore the equation (12) reads:

$$\psi_{scatt} = \frac{1}{r_1}\frac{1}{2\pi\hbar}\int_R\int_R dp_x dp_y\ c(\mathbf{p})\, f(p, \theta_{\widehat{pr_1}})\ e^{\frac{i}{\hbar}(pr_1 - \frac{p^2}{2m}t)} \tag{22}$$

with $c(\mathbf{p})$ as in (7). Moreover one can perform the substitution

$$\exp\,[-\frac{(p_y - p_{0y})^2}{2\beta^2\hbar^2} \quad \rightarrow \quad \sqrt{\pi}\ \delta(\frac{p_y - p_{oy}}{\hbar\sqrt{2}}) = \hbar\sqrt{2\pi}\,\delta(p_y - p_{oy}) \tag{23}$$

and similarly for α, p_x. Therefore from (7):

$$c(p) = \frac{2\hbar\sqrt{\pi}}{\sqrt{\alpha\beta}}\,\delta(\mathbf{p} - \mathbf{p_0})e^{-\frac{i}{\hbar}\mathbf{p_o x_0}} \tag{24}$$

$$\psi_{scatt} = \frac{1}{\sqrt{\pi\alpha\beta}}\,\frac{1}{r_1} f(p_o, \theta_{\widehat{p_0 r_1}})\ e^{\frac{i}{\hbar}(p_o r_1 - \frac{p_0^2}{2m}t)}e^{-\frac{i}{\hbar}\mathbf{p_o x_0}} \tag{25}$$

$$|\psi_{scatt}|^2 = \frac{C_1}{r_1^2}\ |f(p_o, \theta_{\widehat{p_0 r_1}})|^2, \qquad C_1 = \frac{1}{\pi\alpha\beta} \tag{26}$$

The last results are valid for sufficiently wide range of β values, that is by choosing $\hbar \ll 1/\beta \ll 2b$.

ii) Suppose now $\beta \ll 1$, $\beta^2 \simeq 0$. Choosing $v = u$ in (12) one has by (9), (10), (13):

$$\begin{aligned}
\Big(u_{\mathbf{p}}\Big|\psi_0\Big) \quad &= \Big(u_{p_x}\Big|\psi(x,0)\Big)\Big(u_{p_y}\Big|\phi(y,0)\chi(y)\Big) &(27)\\
&= c_x(p_x)\int_{-b}^{b} d\eta\ e^{-\frac{i}{\hbar}p_y\eta}\,\phi(\eta, 0) &(28)\\
&= \frac{\beta^{1/4}}{\pi}\sqrt{\frac{2}{\hbar}}\ c(p_x)\,e^{-\frac{i}{\hbar}p_{y0}y_0}\frac{\sin\frac{(p_y - p_{y0})}{\hbar}b}{\frac{(p_y - p_{y0})}{\hbar}} &(29)
\end{aligned}$$

By further choosing $\alpha \ll 1$, so that again $c_x(p_x) \sim \sqrt{\frac{\hbar 2\pi^{1/2}}{\alpha}}\ \delta(p_x - p_{0x})$, one obtains from (12), (29):

$$\psi_{scatt} = C\frac{e^{-\frac{i}{\hbar}p_{y0}y_0}}{r_1}\int_R dp_y\, f(p, \theta_{\widehat{pr_1}})\ e^{\frac{i}{\hbar}(pr_1 - \frac{p^2}{2m}t)}\ \frac{\sin\frac{(p_y - p_{y0})}{\hbar}b}{\frac{(p_y - p_{y0})}{\hbar}} \tag{30}$$

where now $\mathbf{p} \equiv (p_{0x}, p_y)$, $C = \frac{\pi^{1/4}}{\pi^2\hbar}\Big(\frac{\beta^{1/2}}{\alpha}\Big)^{1/2}$. To perform the calculation we further suppose the initial momentum of the incoming wave packet to vanish

$p_{y0} = 0$. The main contribution to the last integral comes then from very small values of p_y. Therefore under the approximations $p_y \ll 1$, $p_y^2 \simeq 0$, $p = \sqrt{p_{x0}^2 + p_y^2} \simeq |p_{x0}| = p_{x0}$ one has:

$$\psi_{scatt} = \frac{C}{r_1}\frac{\hbar}{b}\, e^{\frac{i}{\hbar}(p_{x0}r_1 - \frac{p_{x0}^2}{2m}t} f(p_{x0}, \theta_{\widehat{xr_1}}) \int_R dz \frac{\sin z}{z} \tag{31}$$

$$|\psi_{scatt}|^2 = \frac{C_2}{r_1^2}\, \Big|f(p_{x0}, \theta_{\widehat{xr_1}})\Big|^2, \qquad C_2 = \Big|\frac{C\hbar\pi}{b}\Big|^2 \tag{32}$$

The last result essentially describes a scattered wave packet in the limit of incoming plane wave. According to the approximations done, it differs from the case (26) of wave packet, narrower than the slit aperture, only for the in front coefficient.

[Note that if one chooses, in the calculations of (28) the expression of the confined eigen functions (17), then one obtains the result (31) doubled].

It seems useful to note that the coefficient C_1, C_2 have been obtained for two different sets of values of the parameters α, β, say $C_1 = C_1(\alpha_1, \beta_1)$, $C_2 = C_2(\alpha_2, \beta_2)$. The previous evaluations essentially hold for $\alpha_1 \simeq \alpha_2$, but $\beta_1 \ll \hbar^{-1}$, $\beta_2^2 \simeq 0$. One has

$$\frac{C_2}{C_1} = \frac{\hbar^2}{\pi^{1/2}}\frac{1}{b^2}\, \beta_2^{1/2}\beta_1 \quad \ll \frac{\hbar}{\pi^{1/2}\, b^2}\, \beta_2^{1/2} \ll\; 1 \tag{33}$$

Therefore the spot on the screen in case ii) results, as expected, smaller than in case i).

The above result is now made explicit in a simple situation. Suppose the wall is made of conducting or isolating material. Suppose the potential interaction and the corresponding scattering amplitude in the Born approximation be given by

$$V = -\frac{kq^2}{r_1}, \qquad f = k\frac{mq^2}{2p^2 \sin^2 \theta/2} \tag{34}$$

(the calculation is done in the 3-dimensional case and the result restricted to the 2-dimensional case). Then, for small angle $\theta = \theta_{\widehat{xr_1}}$ such that $\sin\theta \simeq y/x$, the result (32) reads

$$|\psi_{scatt}|^2 = \frac{C_2}{x^2 + (y-b)^2}\, \frac{4m^2\, q^4 k^2\, x^4}{p_{x0}^4\; (y-b)^4} \tag{35}$$

Therefore the scattering pattern at distance x has a maximum value in correspondence to $y = b$ and decreasing lateral values. Similar results can be easily obtained for the interaction potentials reported in [16]. As there mentioned in case of van der Waals-like interactions (see the similar treatment [6]) the results are coherent with the experimental data.

3 Comments

The complete diffraction pattern on the screen at a fixed distance from the slit is given by $|\psi_{out}|^2$. Up to interference terms, it is given by $|\psi_{tr}|^2 + |\psi_{conf}|^2 + |\psi_{scatt}|^2$. In the limit $\Delta y \leq b$, the wave packet passes undisturbed being subjected to an ordinary potential scattering. Instead for Δy sufficiently large, the pattern results meaningful and consists of the sum of a standard interference pattern (15), another interference pattern (18) and a scattering like spot term, e., g. (35), centered in $y = b$. The contributions of the interference terms seem in general difficult to be evaluated quantitatively.

For what concerns the role of the truncation, confinement and scattering assumptions they have been introduced on account of the difficulty of giving complete explicit analytical solution of the mathematical problem, as sketched in Section 1. A consequence is that by them it has implicitly assumed that the time evolution of the wave packet after the slit remains factorized in the coordinate dependence, a condition not so evident.

The final results have been obtained by analytical approximation assumptions, mainly in view of a qualitative description of the problem. They are however suitable for an experimental verification, in order to test the validity of the truncation, confinement and scattering assumptions. They could be quantitatively refined by relaxing the approximations done, or by a numerical evaluation.

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