Eur. Phys. J. Plus (2011) **126**: 18
DOI 10.1140/epjp/i2011-11018-8

THE EUROPEAN
PHYSICAL JOURNAL PLUS

Regular Article

Diffraction of Gaussian wave packets by a single slit

A. Zecca[a]

Dipartimento di Fisica dell'Università - Via Celoria, 16, 20133 Milano, Italy
GNFM, Gruppo Nazionale per la Fisica Matematica, Sesto Fiorentino (FI), Italy

Received: 22 October 2010
Published online: 18 February 2011 –

Abstract. A two-dimensional formulation of particle diffraction by a single slit is proposed within Schrödinger QM. The study is done in terms of Gaussian wave packets. A "confinement" assumption is considered together with a previous "truncation" assumption when the wave packet passes the slit. In the limiting situation of entering Gaussian wave packet peaked in the transverse-momentum probability distribution, the diffraction pattern results in an unaltered central maximum with lateral maxima narrower and higher than in the absence of the confinement assumption. For entering wave packets peaked in the transverse position probability distribution, the diffraction pattern consists of a central Gaussian spot with lateral diffraction maxima, not present in the absence of the "confinement" assumption, whose visibility depends on the configuration of the parameters. With a different analysis, a similar effect was obtained also in G. Kalbermann (J. Phys. A: Math. Gen. **35**, 4599 (2002)). Its experimental verification seems of interest to discriminate between Schrödinger QM and stochastic electrodynamics with spin.

1 Introduction

The diffraction pattern of particles by slits is, even with well-known problematic aspects [1], a distinguishing point between classical mechanics (CM) and quantum mechanics (QM). Generally speaking, the interference of particles is explained within QM and not within CM. This follows from the statistical interpretation of the wave function and by the property that, in QM, non-trivial pure superpositions of pure states are possible, while this is not so in CM [2,3]. An explanation of the interference (or diffraction) pattern by proper solutions of the Schrödinger equation is possible as well. The use of Gaussian wave packets has the advantage of including not only the limiting cases of plane waves and of wave packets narrower than the slit aperture, but also all the intermediate situations. A treatment in terms of Gaussian wave packets has been proposed for one and two slits, with and without interaction with the wall and the results compared with experimental data [4–6]. From those studies it appears that the case of single slit is sufficiently clear to put into evidence the main features of the problem without involving heavy calculations. Moreover, there results that an entering Gaussian wave packet, sufficiently peaked in the y-position probability distribution, passes the slit practically undisturbed while it produces a diffraction pattern if it is peaked in the y-momentum probability distribution (plane wave). The treatment is done in two dimensions with a Schrödinger operator so defined that the generalized eigenfunctions vanish on the boundaries only in a weak sense (*e.g.* see [7]).

In this paper we consider the last mentioned schematization for the one-slit problem in order to give a more realistic sense to the "vanishing" of the eigenfunctions. To that end, a "confinement" assumption is added to the previous "truncation" assumption. After the slit, it is again assumed a Schrödinger-like time evolution having, as initial state, the Gaussian wave packet truncated by the slit. The confinement assumption consists in that the y-dependence of the wave packet, when passing the slit, is that of a one-dimensional free particle confined in the region of the slit by infinite barriers. This involves the use of a discrete set of eigenfunctions that vanish on the boundaries of the slit. In order to explicitly perform the calculations, the summation over the discrete index is substituted, with good approximation, by an integral over a continuous index. Finally, an overall approximation is assumed that results, at any time, in a factorization of the wave function on its dependence on the x, y variables.

The general formulation is then studied in two limiting cases whose main results are as follows. For entering wave packet, peaked in the transverse-momentum probability distribution, the diffraction pattern appears qualitatively the same that in the absence of the confinement assumption, but with higher and deformed lateral maxima. Instead

[a] e-mail: antonio.zecca@mi.infn.it

an entering wave packet peaked in the y-position probability distribution produces a Gaussian spot. The Gaussian spot transforms, once a suitable condition on the parameters is satisfied, into a diffraction pattern with oscillations that unexpectedly increase in number if the entering packet becomes thinner. The prevision of a similar effect was derived also in [6] by different theoretical method. The last result is a quantum effect of the "confinement" assumption that was not considered in previous comparison [7] between Schrödinger QM and stochastic electrodynamics with spin. It seems therefore that the experimental test proposed in [7] to discriminate between the two theories should be refined.

2 Assumptions and general formulation

The one-slit diffraction problem can be formulated in a sufficiently satisfactory way by confining in two dimensions. Accordingly we consider the region of the (x, y)-plane non accessible to the particle, by $S = \{(x, y) : |x| < a, |y| > b > 0\}$ in the limit of very small a. With this geometry, a Schrödinger operator $\hat{H}_0$ for a free particle of mass m can be defined on a subset of the functions of $L^2(D)$, $D \equiv \mathbf{R}^2 \setminus S$ that vanish on the boundaries ∂S. As sketched in [7], the general eigenfunctions are again $u_{p_x p_y}(x, y) = u_{p_x}(x)u_{p_y}(y)$, $u_{p_x}(x) = (2\pi\hbar)^{-1/2} \exp(ip_x x/\hbar)$, $u_{p_y}(y) = (2\pi\hbar)^{-1/2} \exp(ip_y y/\hbar)$, $-\infty < p_x, p_y < \infty$, with $p^2 = p_x^2 + p_y^2 = 2mW$, W the eigenvalue of $\hat{H}_0$, and that satisfy the boundary conditions in the weak sense [7]. With these assumptions the particle is represented by the usual Gaussian wave packet centered at $P \equiv (x(t), y(t))$ and freely moving with velocity $v_{0k} = p_{0k}/m$, $x_k(t) = x_{0k} + v_{0k}t$, $p_{0k} \geq 0$, $k \equiv x, y$. Explicitly

$$\psi(x, y, t) = \psi(x, t)\phi(y, t), \tag{1}$$

$$\psi(x, t) = \frac{\alpha^{1/4}\pi^{-1/2}}{(1 + i\hbar\alpha^2 \frac{t}{m})^{1/2}} \exp\left[-\frac{\alpha^2}{2} \frac{(x - x_0 - \frac{p_{0x}}{m}t)^2}{1 + i\hbar\alpha^2 \frac{t}{m}} + \frac{i}{\hbar} p_{0x}(x - x_0) - \frac{i}{\hbar} \frac{p_{0x}^2}{2m} t\right], \tag{2}$$

$$\phi(y, t) = \frac{\beta^{1/4}\pi^{-1/2}}{(1 + i\hbar\beta^2 \frac{t}{m})^{1/2}} \exp\left[-\frac{\beta^2}{2} \frac{(y - y_0 - \frac{p_{0y}}{m}t)^2}{1 + i\hbar\beta^2 \frac{t}{m}} + \frac{i}{\hbar} p_{0y}(y - y_0) - \frac{i}{\hbar} \frac{p_{0y}^2}{2m} t\right]. \tag{3}$$

When reaching the slit, the wave packet is highly modified by the presence of the wall. Part of it is reflected by the wall and part of it passes the slit. We make the assumption that, when passing the slit, the wave packet has the form corresponding to (1) with $t = 0$ and that it is truncated by the slit. After the slit a Schrödinger-like time evolution is again assumed

$$\psi_{out}(x, y, t) = \int_{\mathbf{R}^2} \mathrm{d}p_x \mathrm{d}p_y \, u_{p_x p_y}(x, y) e^{-\frac{i}{\hbar}\frac{p^2}{2m}t} \int_{\mathbf{R}} \mathrm{d}\xi \int_{-b}^{b} \mathrm{d}\eta \, u^*_{p_x p_y}(\xi\eta)\phi_0(\xi, \eta), \tag{4}$$

where $\phi_0(x, y) = \psi_0(x)\phi_0(y)$, the expression of $\psi_0(x)$, $\phi_0(y)$ being given, by possibly re-defining the initial time, by the expressions $\psi_0(x, 0)$, $\phi_0(y, 0)$ in (2), (3), respectively. Accordingly, after the slit, the wave packet remains factorized in the x-, y-dependence:

$$\psi_{out}(x, y, t) = \psi_{out}(x, t)\phi_{out}(y, t), \tag{5}$$

$$\phi_{out}(y, t) = \int_R \mathrm{d}p_y \, u_{p_y}(\eta) \, e^{-\frac{i}{\hbar}\frac{p_y^2}{2m}t} \int_{-b}^{b} \mathrm{d}\eta \, u^*_{p_y}(\eta)\phi_0(\eta), \tag{6}$$

with $\psi_{out}(x, t)$ again of the form (2).

3 Improvement of the scheme

The scheme of the previous section was the basis for further considerations and applications that have been developed in different papers [4,5,8]. The scheme, however, contains some implicit approximations. The fact that the wave function is assumed to be factorized in the x-, y-dependence when passing the slit is not so evident and should be considered as a further approximation. It seems difficult to have a complete understanding of the interaction of the wave packet with the slit. Another aspect of interest is that, when the particle is in the region of the slit, it can be considered, for what concers its y-dependence, as a free one-dimensional particle confined in $-b < y < b$ by an infinite positive potential barrier located in $y = \pm b$. Therefore, according to standard results in QM (*e.g.* [9,10]), the relative Schrödinger operator admits of a discrete system of eigenfunctions that vanish at $y = \pm b$:

$$v_{p_n}(y) = \frac{1}{\sqrt{b}} \sin \frac{p_n}{\hbar}(y - b), \qquad p_n = n\frac{\hbar\pi}{2b}, \quad n = 0, 1, 2, \ldots . \tag{7}$$

Correspondingly, to obtain $\phi_{out}(y,t)$ one could project the state $\phi_0(y)$ over $v_{p_n}(y)$ instead of over $u_{p_y}(\eta)$ as assumed in (6). In this way one introduces a discrete index n that is difficult to be treated exactly. However, to carry out the calculation, a good approximation is to perform the substitution $v_{p_n}(y) \to v_{p_y}(\eta) = (\pi\hbar)^{-1/2}\sin[p_y(\eta-b)/\hbar]$, $p_y \in \mathbf{R}$. The values of p_n are indeed very densely distributed on the real line as it follows from eq. (7). According to these considerations one is led to consider, after the slit, the y-, t-dependence of the wave function to be given by

$$\phi_C(y,t) = \frac{2i}{\sqrt{\pi\hbar}} \int_{\mathbf{R}} \mathrm{d}p_y\, u_{p_y}(y) e^{-\frac{i}{\hbar}\frac{p_y^2}{2m}t} \int_{-b}^{b} \mathrm{d}\eta \left[e^{-\frac{i}{\hbar}p_y(\eta-b)} - e^{\frac{i}{\hbar}p_y(\eta-b)}\right]\phi_0(\eta). \tag{8}$$

By assuming now that both expressions $\phi_{out}(y,t)$ and $\phi_C(y,t)$ contribute to the diffraction, the y-dependence to be considered after the slit is given by $\phi_I(y,t) = \phi_{out}(y,t) + \phi_C(y,t)$ and the diffraction pattern is represented by $\phi_I(y,t)\phi_I^*(y,t)$.

4 The limit case of plane wave diffraction

We now compare the diffraction patterns produced by the descriptions (6), (8) in limiting case of physical interest. Suppose first the momentum probability distribution of the entering wave packet has a very small uncertainty $\Delta p_{0y} = \hbar\beta/\sqrt{2}$, $\beta \ll 1$. The calculations of the integrals (6) and (8) can be performed by neglecting the term β^2 and, after a first integration over p_y, also the terms $(im/2t\hbar)\eta^2$, $(im/2t\hbar)(\eta-b)^2$, respectively, since $|\eta| \le b \ll 1$. One finally obtains

$$\phi_{out}(y,t) = b\left(\frac{2\beta m}{it\hbar\pi^{3/2}}\right)^{\frac{1}{2}} \exp\left[\frac{i}{\hbar}\left(\frac{m}{2t}y^2 - p_{0y}y_0\right)\right] \frac{\sin\frac{b}{\hbar}\left(p_{0y}-\frac{m}{t}y\right)}{\frac{b}{\hbar}\left(p_{0y}-\frac{m}{t}y\right)}\,, \tag{9}$$

$$\phi_C(y,t) = 2i\left(\frac{m\beta b^2}{i\hbar t\pi^{3/2}}\right)^{\frac{1}{2}} \exp\left[\frac{i}{\hbar}\left(\frac{m}{2t}y^2 - p_{0y}y_0\right)\right]\left\{e^{\frac{i}{\hbar}\frac{bm}{t}y}\frac{\sin\frac{b}{\hbar}\left(p_{0y}-\frac{m}{t}y\right)}{\frac{b}{\hbar}\left(p_{0y}-\frac{m}{t}y\right)} - e^{-\frac{i}{\hbar}\frac{bm}{t}y}\frac{\sin^2\frac{b}{\hbar}\left(p_{0y}+\frac{m}{t}y\right)}{\frac{b}{\hbar}\left(p_{0y}+\frac{m}{t}y\right)}\right\}, \tag{10}$$

whose corresponding interference patterns for $p_{0y}=0$ are, respectively

$$|\phi_{out}(y,t)|^2 = \frac{2m\beta b^2}{t\hbar\pi^{3/2}}\,\frac{\sin^2\frac{bm}{\hbar t}y}{\left(\frac{bm}{\hbar t}y\right)^2}\,, \tag{11}$$

$$|\phi_C(y,t)|^2 = 16\frac{m^3b^4\beta}{\hbar^3t^3\pi^{3/2}}\,y^2\,\frac{\sin^4\frac{bm}{\hbar t}y}{\left(\frac{bm}{\hbar t}y\right)^4}\,. \tag{12}$$

Note that $|\phi_{out}(y,t)|^2$ gives the usual interference pattern with a maximum value at $y=0$ and then decreasing lateral maxima. Instead, $|\phi_C(y,t)|^2$ vanishes in $y=0$ while the lateral maxima, located in the same positions, are narrower. One has

$$\frac{|\phi_C(y,t)|^2}{|\phi_{out}(y,t)|^2} \le 8\,\pi\,y^2. \tag{13}$$

Therefore, the contribution of (8) to the interference pattern is qualitatively different than that of (6). If both contributions are considered, the diffraction pattern given by $\phi_I(y,t)\phi_I^*(y,t)$ results (apart from smaller interference contributions due to rectangular terms), is similar to that of $|\phi_{out}(y,t)|^2$ in $y=0$, but with the lateral maxima modified and strengthened.

5 Wave packets narrow with respect to the slit

The situation has interest also for entering wave packets narrower, in the y-direction, than the slit aperture. We assume then $(\Delta x)_0 = 1/\beta\sqrt{2}$, $\beta \gg 1$. The integral (4) has been calculated exactly in [8] in the double-slit case. Here it gives

$$\phi_{out}(y,t) = \frac{1}{2}\left[\frac{\beta m\pi^{-1/2}}{m+i\hbar\beta^2 t}\right]^{\frac{1}{2}} \exp\frac{im\frac{\beta^2}{2}(y-y_0)^2 + \frac{m}{\hbar}p_{oy}(y-y_0) - \frac{p_{oy}^2}{2\hbar}}{\beta^2\hbar t - im}$$
$$\times\left\{\mathrm{erf}\left[\frac{im(y-b) - t\hbar\beta^2(y_0-b) - it}{\left(2\hbar t(\hbar\beta^2 t - im)\right)^{1/2}}\right] - \mathrm{erf}\left[b \to -b\right]\right\}, \tag{14}$$

where $\operatorname{erf} z = 2\pi^{-1/2}\int_0^z \exp(-t^2)\mathrm{d}t$ [11]. Therefore, for $\beta \gg 1$ and $p_{0y} = 0$

$$|\phi_{out}(y,t)|^2 = \frac{m\beta\pi^{-3/2}}{\sqrt{m^2+t^2\hbar^2\beta^4}} \exp\left[\frac{-m\beta^2(y-y_0)^2}{m^2+\hbar^2t^2\beta^4}\right]\left|\int_{(y_0-b)\beta/\sqrt{2}}^{(y_0+b)\beta/\sqrt{2}} \exp(-t^2)\mathrm{d}t\right|^2, \tag{15}$$

that represents a Gaussian spot that is essentially different from zero for $-b \leq y_0 \leq b$ (as it follows from the value of the integral as a function of y_0), while it is reflected by the wall for $|y_0| > b$.

For what concerns the calculation of (8), note that the function to be integrated is very peaked for $\beta \gg 1$. Therefore, one can perform in (8) the substitution $\int_{-b}^{b}\mathrm{d}\eta \to \int_{\mathbf{R}}\mathrm{d}\eta$ and then proceed exactly by first integrating over p_y. One finally obtains

$$\phi_C(y,t) = \frac{-i(m\beta)^{1/2}}{\sqrt{2i\sqrt{\pi}(\beta^2t\hbar - im)}} \exp\left(-\frac{\beta^2}{2}y_0 - \frac{i}{\hbar}p_{0y}\right)$$
$$\times\left\{\exp\left[i\frac{m}{2\hbar t}(y+b)^2 + \frac{t\hbar\left(\beta^2y_0+\frac{i}{\hbar}p_{0y}-\frac{im}{\hbar t}(y+b)\right)^2}{2\beta^2t\hbar - im}\right] - \exp\left[i\frac{m}{2\hbar t}(y-b)^2 + \frac{t\hbar\left(\beta^2y_0+\frac{i}{\hbar}p_{0y}+\frac{im}{\hbar t}(y-b)\right)^2}{2\beta^2t\hbar - im}\right]\right\}. \tag{16}$$

To compare the results, let us now choose $p_{0y} = y_0 = 0$ in (16) so that

$$\phi_C(y,t) = \frac{2(m\beta)^{1/2}}{\sqrt{2i\sqrt{\pi}(\beta^2t\hbar - im)}} \exp\left\{(y^2+b^2)\left[\frac{m^2}{t\hbar(im-2\beta^2t\hbar)} - \frac{im}{t\hbar}\right]\right\} \sin\left\{\frac{mb}{t\hbar}y\left[1+\frac{2m}{2\beta^2t\hbar - im}\right]\right\}, \tag{17}$$

and, for large β,

$$\phi_C\phi_C^*(y,t) = \frac{2m\pi^{-1/2}}{\hbar t\beta} \exp\left[-\frac{m^2}{\beta^2t^2\hbar^2}(y^2+b^2)\right] \sin^2\frac{mb}{t\hbar}y\,. \tag{18}$$

The result (18) represents an oscillating interference pattern of periodic length $2\pi\hbar t/mb$, modulated by a Gaussian profile centered at $y = 0$, of width $\beta t\hbar/\sqrt{2}m$. The condition of visibilty of the oscillations is then

$$2\pi\frac{t\hbar}{mb} < \frac{\beta\hbar t}{m\sqrt{2}} \Longrightarrow \beta > \frac{2\pi\sqrt{2}}{b}\,, \tag{19}$$

a condition that can be easily obtained. One has also, for not too small time t,

$$\frac{\phi_C(y,t)}{\phi_{out}(y,t)} \cong 2\pi \qquad (\beta \gg 1). \tag{20}$$

(The same result is valid for $t \ll 1$.) Therefore, once condition (19) is verified an interference pattern is visible also in the case of very narrow entering Gaussian wave packet. It seems interesting, in this case, that the number of the visible maxima increases as the wave packet becomes more peaked.

6 Comments and remarks

In the previous sections a two-dimensional study of particle diffraction by single slit has been developed in the context of ordinary Schrödinger QM. The Gaussian wave packet representing the entering particle is assumed, when passing the slit, to be subject to a "truncation" and a "confinement" condition. Accordingly, the diffraction problem is formulated in general and studied in two important limiting physical situations. The diffraction pattern relative to the general situation, $|\phi_{out}(y,t) + \phi_C(y,t)|^2$, is compared with the diffraction pattern $|\phi_{out}(y,t)|^2$ previously obtained in the absence of the "confinement" assumption. The results are as follows.

For entering plane waves (cf. sect. 4), one can see that the "confinement" assumption gives, modulo secondary corrections given by the interference terms, an increase of the lateral maxima while it leaves the central maximum essentially unaltered.

In case of entering Gaussian wave packet sufficiently peaked in the y-position probability distribution (cf. sect. 5), the "confinement" assumption produces, modulo interference of rectangular terms of $|\phi_{out}(y,t)+\phi_C(y,t)|^2$, an increase of the value of the central Gaussian spot. However, once the threshold (19) is fulfilled, a diffraction pattern becomes more visible by making the entering Gaussian wave packet more peaked. This effect, already noted in [6] by a different argument, is a quantum effect that was not considered in comparing the predictions of Schrödinger QM and stochastic electrodynamics with spin [12]. Therefore, the experiment proposed [7] to discriminate between the two theories should be refined.

Finally, the results, combined with those of [8], furnish also a qualitative picture of the two slit diffraction pattern of particles. Suppose indeed two equal slits are disposed on the y-axis, symmetrically with respect to the x-axis, as done in [8]. Suppose the entering wave packet has again the form (1) with the "truncation" and the "confinement" assumption for each one of the slits toghether with the factorization assumption of the wave function. By the quantum superposition principle, the wave packet emerging from the slits 1,2 can be written $\phi_S(y,t) = \phi_1(y,t) + \phi_2(y,t)$ with $\phi_i(y,t) = \phi_{iout}(y,t) + \phi_{iC}(y,t)$, $i = 1,2$. Then, in the limit of entering plane wave ($\beta \ll 1$), by combining the results of [8] and those of sect. 4, one has that $\phi_S\phi_S^*(y,t)$ gives the usual elementary two-slit diffraction pattern with possible deformation of the lateral maxima, modulo small interference terms. Similarly, an entering packet with y_0 in the region of the slit 1 and y uncertainty smaller than the slits aperture, produces a diffraction pattern that is the interference of the diffraction of a plane wave by slit 2 (sect. 4) and a diffraction of a peaked packet by slit 1 (sect. 5).

References

1. R.P. Feynman, A.R. Hibbs, *Quantum Mechanics and Path Integrals* (McGraw Hill book Company, New York, 1965).
2. V.S. Varadarajan, *Geometry of Quantum Mechanics* (D. Van Nostrand Company, Inc., Princeton, NJ, 1968).
3. C. Cohen-Tannoudji, B. Din, F. Laloë, *Mecanique Quantique* (Herman, Paris, 1977).
4. A. Zecca, Nuovo Cimento B **119**, 197 (2004).
5. A. Zecca, Adv. Studies Theor. Phys. **2**, 385 (2008).
6. G. Kalbermann, J. Phys. A: Math. Gen. **35**, 4599 (2002).
7. A. Zecca, G. Cavalleri, Nuovo Cimento B **112**, 1 (1997).
8. A. Zecca, Adv. Studies Theor. Phys. **1**, 539 (2007).
9. E. Merzbacher, *Quantum Mechanics* (John Wiley & Sons, Inc., New York, 1970).
10. M. Reed, B. Simon, *Methods of Modern Mathematical Physics*, Vols. I, II (Academic Press, New York, 1975).
11. W. Abramovitz, I.E. Stegun, *Handbook of Mathematical Functions* (Dover Publication, New York, 1960).
12. G. Cavalleri, F. Barbero, G. Bertazzi, E. Cesaroni, E. Tonni, L. Bosi, G. Spavieri, G.T. Gillies, Front. Phys. China **5**, 107 (2010).