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Two-Slit Diffraction Pattern for Gaussian Wave Packets

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The complete prediction of diffraction for electrons passing through one or two slits is obtained from the pure wave propagation governed by the Schrödinger equation. By the further assumption of electromagnetic interaction between electrons and slits it is shown that, as already predicted by stochastic electrodynamics with spin, there exist lateral maxima on the diffraction pattern corresponding to the edges of the slits.

1. INTRODUCTION

The two-slit diffraction problem is a point where the predictions of quantum mechanics (QM) differ from those of classical mechanics. The diffraction pattern of particles through two slits is explained in an elementary way in QM by taking the absolute square of the sum (superposition) of probability amplitudes (pure states) associated with the slits (Feynman and Hibbs, 1965). This distinguishing property of the superposition principle in QM makes it possible to have pure superpositions of pure states, while in classical mechanics the only superpositions of pure states are statistical mixtures of them (see, e.g., Varadarajan, 1968; Zecca, 1981).

It is of some interest to have a treatment of the diffraction problem also for wave packets. In this present paper the case of incoming Gaussian wave packets is considered in the two-dimensional case. The considerations are developed by assuming the general mathematical scheme defined in a previous paper in the case of a single slit (Zecca and Cavalleri, 1997). At a first stage electromagnetic and spin interactions between electrons and slits are neglected. The time evolution of the wave packet after the slits is determined

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by a "truncation" assumption on the wave packet when passing through the slits. This gives the correct results, as is evident from special limiting situations that are treated separately. The results are in a form that easily generalizes to the n-slit case.

Recently (Zecca and Cavalleri, 1997), the diffraction pattern through a slit has been explained also in the context of a new stochastic electrodynamics (SED) with spin (Cavalleri, 1997). In the case of a beam of electrons that is narrow with respect to the aperture of the slits it has been found that the theory predicts three spots. The central spot corresponds to no deviation and is the one that has a QM counterpart. The other two are a pure SED-plus-spin effect and cannot be explained by the mentioned quantum mechanical description without interaction.

The last part of the paper is developed according to the idea that the lateral spots found in the SED-plus-spin context indeed have an explanation also from the QM point of view. Under the assumption of a conducting barrier the effect of the interaction of the electron with its image charges is considered. It is assumed that the diffraction pattern is the result of a diffracted and of a scattered wave packet. The diffracted wave packet corresponds to the one given in the absence of interaction, while the other packet, which is scattered by the interaction, is treated in the Born approximation. The results show qualitatively the existence of the lateral spots. The inclusion of the spin of the electron in the evaluation of the scattering effect gives the same qualitative results. The quantitative relevance of the spots seems, however, to be not decidable in the context of the given approximations. Therefore an experimental verification of the mentioned effect is required.

2. TWO-SLIT DIFFRACTION FROM SCHRÖDINGER QM

The two-slit diffraction problem is considered in the two-dimensional case and the region S that is inaccessible to the particle is assumed to be the subset of the (x, y) plane given by

$$S = \{(x,y): |x| < a, y \in (-\infty, -d' - b'] \cup [-d', d] \cup [d + b, \infty)\} \quad (1)$$

where a, b, b', d, d' are positive real numbers. The apertures of the slits are therefore b and b' ($b, b' \ll 1$ in the case of diffraction) and both have depth $2a$. The motion of a Schrödinger particle moving in that context can be sketched [as for the one-slit diffraction (Zecca and Cavalleri 1997) or as for any other plane motion with an inaccessible region] as a motion which is free outside S and subjected to the boundary condition of an infinite potential barrier in the region S. Any other kind of interaction is neglected. A coherent mathematical formulation of the Schrödinger operator requires a treatment in terms of weak solutions. This has already been done (Zecca and Cavalleri,

1997) for the one-slit diffraction problem and the procedure and results extend to the present case without modifications. As a consequence, the solution of the Schrödinger equation, which in general could not be separated in terms of the x and y dependences, can be approximated by factorized solutions that can be chosen to reasonably develop the calculations. Accordingly, the diffraction pattern of a beam of particles can be studied in the following way. We consider a free-particle Gaussian wave packet coming from the remote x region and with probability distribution centered on a point moving with velocity $v_{0x} = \hbar k_{0x}/m$ on an axis parallel to the x axis ($y = y_0$):

$$\psi(x, y, t) = \psi(x, t)\phi(y, t) \tag{2}$$

with

$$\psi(x, t) = \alpha^{1/2}\left\{\exp\left[-\frac{\alpha^2}{2}\frac{(x - x_0 - \hbar k_{0x}t/m)^2}{1 + i\hbar\alpha^2 t/m} + ik_{0x}(x - x_0) - i\hbar k_{0x}^2 t/2m\right]\right\} \times [\pi^{1/2}(1 + i\hbar\alpha^2 t/m)]^{-1/2} \tag{3}$$

and

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

To describe the motion of the wave packet after the slit, we assume that the part of the wave function $\psi(x, y, t)$ relative to the points (x, y) such that $-d' < y < d$ or $y > d + b$ or $y < -d' - b'$ are reflected toward the negative x region by the barrier S because no tunneling effect is possible with an infinite potential barrier.

We therefore assume that the wave packet just after the slit, at a time taken as initial $t = 0$, is

$$\psi_I(x, y, 0) = \psi_a(x, 0)\chi_I(y)\phi(y, 0) \tag{5}$$

where $\psi_a(x, 0)$ is the function $\psi(x, 0)$ in Eq. (3) with $x_0 = a$, and $\chi_I(y)$ is the characteristic function of the two-interval set $I = [d, d + b] \cup [-d' - b', -d']$. [With respect to the normalization, it is worth noticing that the wave function having norm 1 consists of the part given by (5) and the part of the wave packet reflected by the barrier. Therefore, the "initial state" (5) is implicitly assumed to evolve after the slits with constant norm that is less than 1.] Since the initial wave function is separated in the x and y dependences and the particle moves freely after the slits, one has

$$\psi_I(x, y, t) = \psi_a(x, t)\phi_I(y, t) \tag{6}$$

where $\psi_a(x, t)$ is again the function in Eq. (3) with $x_0 = a$, while

$$\phi_I(y, t) = \frac{1}{2\hbar}\frac{\beta^{1/2}}{\pi^{5/4}}\int_{\mathcal{R}} \exp\left[\frac{i}{\hbar}\left(p_y y - \frac{p_y^2 t}{2m}\right)\right] dp_y \times \int_I \exp\left[-\frac{i}{\hbar} p_y \xi - \frac{\beta^2}{2}(\xi - y_0)^2\right] d\xi \tag{7}$$

[We remark that Eq. (7) is in a form which could be immediatly generalized to the n-slit case.] The double integral in (7) can be performed by first integrating over the variable p_y,

$$\phi_I = \left[\frac{m\beta}{2\pi^{3/2} i\hbar t}\right]^{1/2} \exp\left[y^2 \frac{im}{2\hbar t} - y_0^2 \frac{\beta^2}{2}\right] \times \int_I \exp\left[-\xi^2\left(\frac{\beta^2}{2} - \frac{im}{2\hbar t}\right) + \xi\left(y_0\beta^2 - \frac{imy}{2\hbar t}\right)\right] d\xi \tag{8}$$

and then over ξ so to obtain

$$\begin{aligned}\phi_I(y, t) = \frac{1}{2}\left[\frac{m\beta}{\pi^{1/2}(m + it\hbar\beta^2)}\right]^{1/2} \exp\left[-\frac{m\beta^2}{2(m + it\hbar\beta^2)}(y - y_0)^2\right] \\ \times \left\{\operatorname{erf}\left[\frac{im(y + d') - \beta^2\hbar t(y_0 + d')}{(2\hbar t(\hbar t\beta^2 - im))^{1/2}}\right]\right. \\ - \operatorname{erf}\left[\frac{im(y + d' + b') - \beta^2\hbar t(y_0 + d' + b')}{(2\hbar t(\hbar t\beta^2 - im))^{1/2}}\right] \\ + \operatorname{erf}\left[\frac{im(y - d - b) - \beta^2\hbar t(y_0 - d - b)}{(2\hbar t(\hbar t\beta^2 - im))^{1/2}}\right] \\ \left. - \operatorname{erf}\left[\frac{im(y - d) - \beta^2\hbar t(y_0 - d)}{(2\hbar t(\hbar t\beta^2 - im))^{1/2}}\right]\right\}\end{aligned} \tag{9}$$

where $\operatorname{erf} z = 2\pi^{-1/2} \int_0^z \exp(-t^2)\, dt$ is the error function (Abramovitz and Stegun 1960).

3. TWO-SLIT QM DIFFRACTION: LIMITING CASES

3.1. Suppose the incoming wave packet is narrow with respect to both slits:

$$\Delta y = \frac{1}{\beta\sqrt{2}} \ll b, b' \tag{10}$$

Then from the definition of the erf function and by considering the dominant term for β very large in the arguments of the erf function, one gets from Eq. (9)

$$\begin{aligned}\phi_I\phi_I^* \cong & \frac{\pi^{-3/2}\beta m}{(m^2 + \hbar^2 t^2\beta^4)^{1/2}} \exp\left[-\frac{m^2\beta^2(y - y_0)^2}{m^2 + \hbar^2 t^2\beta^4}\right] \\ & \times \left\{ \int_{(y_0+d')\beta/\sqrt{2}}^{(y_0+b'+d')\beta/\sqrt{2}} \exp(-t^2)\, dt \right. \\ & \left. + \int_{(y_0-d-b)\beta/\sqrt{2}}^{(y_0-d)\beta/\sqrt{2}} \exp(-t^2)\, dt \right\}^2 \end{aligned} \tag{11}$$

From this expression it is evident that, since β is large and $b, b' \ll 1$, the contribution of the sum of the integrals becomes rapidly negligible unless $y_0 \in I$. Thus, this situation essentially describes an incident wave packet that passes through the slits with its configuration undisturbed or is reflected toward the negative x axis according to whether the incoming y-probability distribution is centered with regard to one of the slits or not.

3.2. Suppose now the incoming wave packet is very undetermined in the y-position probability distribution

$$\Delta y = \frac{1}{\beta\sqrt{2}} \gg b, b' \tag{12}$$

By setting $\beta^2 = 0$ in Eq. (8) and neglecting for large y values the term $-im/2\hbar t$, we calculate the integral and find

$$\begin{aligned}\frac{2\hbar t}{my} & \left\{ \exp\left[-\frac{imy}{\hbar t}\left(d + \frac{b}{2}\right)\right] \sin\frac{bmy}{2t\hbar} \right. \\ & \left. + \exp\left[\frac{imy}{\hbar t}\left(d' + \frac{b'}{2}\right)\right] \sin\frac{b'my}{2t\hbar} \right\} \end{aligned} \tag{13}$$

By assuming the geometrical configuration to be such that

$$d = d', \qquad b = b' \tag{14}$$

from (8), (13), and the given approximations finds

$$\phi_I(y, t)\phi_I^*(y, t) = \frac{2b^2\beta m}{\pi^{3/2} t\hbar} \exp[-\beta^2 y_0^2] \frac{\sin^2(bmy/2t\hbar)}{(bmy/2t\hbar)^2} \times \cos^2\left[\frac{my}{t\hbar}\left(d + \frac{b}{2}\right)\right] \tag{15}$$

As expected, this probability has is maximum at $y_0 = 0$. If now the separation of the slits is of the order of the slit aperture ($d \cong b$), the factor containing the cosine is practically negligible and the expression (15) essentially gives the elementary diffraction pattern of a plane wave through a single slit. If the separation of the slits is much greater than the aperture of the slit ($d \gg b$), expression (15) represents high-frequency pattern modulated by the mentioned elementary diffraction pattern.

4. QM DIFFRACTION: CONSIDERING ELECTROMAGNETIC INTERACTIONS

The diffraction patterns of the previous section are evidence of the pure wave propagation description of the particle as implied by the Schrödinger equation with boundaries. A more detailed description can be done by taking into account the relevance of possible interactions of the particle with the slits.

In the case of a single slit located at $x = 0$ with edges at $y = \pm b/2$ and of a conducting wall, the interaction of the incoming particle with its image charges on the slit seems to be the more important one. At a first approximation one has a Coulomb scattering of the incident electron by two centers located at $x = 0$, $y = \pm b/2$. The outgoing wave, which can be approximated in our scheme as $f_k \exp(ikr)/r \cong f_k \exp(ikx)/x$ (for large, positive x) is characterized in the Born approximation by a scattering amplitude of the form (see, e.g., Merzbacher, 1970)

$$f_{k_x} \cong -\frac{me^2}{2\hbar^2 k_x^2}\left[\frac{1}{\sin^2(\theta/2)} + \frac{1}{\sin^2(\theta'/2)}\right] \tag{16}$$

$$\cong -\frac{me^2}{2\hbar^2 k_x^2}\left[\frac{4x^2}{(y - b/2)^2} + \frac{4x^2}{(y + b/2)^2}\right] \tag{17}$$

where x is the position of the screen and we have used the approximations $\sin \theta/2 \cong (y - b/2)/2x$ and $\sin \theta'/2 \cong (y + b/2)/2x$. In case of two slits with geometrical configuration given by Eqs. (1) and (14) the interaction is with four scattering centers so that the outgoing scattered spherical wave packet can be roughly approximated by (Metzbacher, 1970)

$$\psi_{\text{out}}(x, y, t) \cong -\frac{me^2}{2\hbar^2 k_{0x}^2}\left[\frac{4x^2}{(y-b-d)^2}+\frac{4x^2}{(y-b)^2}+\frac{4x^2}{(y+d)^2}+\frac{4x^2}{(y+b+d)^2}\right]$$
$$\times\frac{1}{x}\exp\left(i\frac{\hbar k_{0x}^2}{2m}t\right)\psi_a(x-v_{0x}t, 0)\phi(y, 0)\chi_I(y) \tag{18}$$

Accordingly, after the slits, we assume that the wave function is given by the superposition

$$\Psi(x, y, t) \cong \psi_I(x, y, t) + \psi_{\text{out}}(x, y, t) \tag{19}$$

with ψ_I and ψ_{out} given by (6) and (18), respectively. The assumption is that the wave function is partly scattered and partly diffracted by the slits (this last term substitutes the transmitted wave packet that would occur in the pure scattering case). By taking x, t constant in Eq. (19) the expression $|\Psi(x, y)|^2$ gives the diffraction pattern on the screen located at x. The effect of the considered interaction is that of adding maxima to the pure diffraction pattern of the spectrum corresponding to the edges of the slits. Such maxima, which take an infinite value due to the approximation method employed, always should be present, but are more evident in the case of a narrow incoming beam ($\Delta y \ll 1$). It is of interest to see the quantitative order of this effect. By comparing the leading coefficient of (18) with, e.g., that of (5) ($\Delta y \gg 1$) one has, for sufficiently large t,

$$\frac{|\psi_{\text{out}}|^2}{|\psi_I|^2} \cong \frac{e^4}{E^2}\frac{x^2y^2}{(y-b)^4}\frac{m}{\hbar}\frac{1}{t} \cong 10^{-14}\frac{x^2y^2}{(y-b)^4}\frac{1}{t} \tag{20}$$

where Gaussian units have been used for an energy E corresponding to 1 eV. The divergence $1/(y - b)^4$ can therefore compensate, in principle, the very small value of the ratio. On the other hand, as mentioned, such a divergence is a consequence of the assumed Born approximation and even one takes the scattering contribution to be not relevant to the final diffraction pattern, it is not possible to decide this exactly in the context of the previous treatment. [One reaches the same conclusion in the case $\Delta y \ll 1$, that is, by using (11) in estimating the ratio (20).] To be more precise, one should also consider the repulsive magnetic interaction of the current given by the electron beam with its "image" currents of opposite sign on the slits. At least qualitatively, this tends to depress the values, if relevant, of the mentioned maxima corresponding to the edges of the slits and to reinforce the diffraction pattern corresponding to the central position of the slits.

Finally, a treatment that consider the spin of the electron does not change the prevous qualitative results because also in that case one would have a differential cross section with the same leading coefficient and behavior as that derived from (16) and (17) (Bethe and Salpeter, 1977, Chapter 15). It would be of interest to decide experimentally the existence of the above effects.

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