Gaussian wave packets passing through a slit: a comparison between the predictions of the Schrödinger QM and of stochastic electrodynamics with spin

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(ricevuto il 12 Maggio 1995; approvato il 28 Agosto 1995)

Summary. — The quantum-mechanical (QM) study is based on weak solutions of the eigenvalue problem for a Schrödinger operator with boundary. The most difficult case of a Gaussian with arbitrary width is solved. The QM diffraction pattern turns out to be equal to the one obtainable by elementary treatment by using the associate de Broglie wave only when the width of the Gaussian is infinite (plane wave). When the width Δy is much smaller than the aperture $2b$ of the slit, there is no diffraction and this can discriminate between usual quantum mechanics and the new stochastic electrodynamics (SED) with spin. Actually, SED plus spin predicts three spots (including the central one corresponding to no deviation) for a narrow beam ($\Delta y \ll 2b$) of electrons. By displacing the narrow beam, the entity of the deviation and the intensity of the spots change so that summing all the successive spots the usual diffraction pattern of QM for $\Delta y \gg 2b$ is obtained. A relevant experiment performed by a transmission electron microscope can therefore discriminate between QM and SED plus spin.

PACS 03.65 – Quantum theory; quantum mechanics.
PACS 42.25.Fx – Diffraction and scattering.

1. – Introduction

According to Barut and Zanghì [1] the *Zitterbewegung* may be interpreted in a realistic sense as a motion at the speed of light c of an almost point-like electron whose orbital angular momentum represents the spin.

The intense, almost monocromatic radiation of the spin (or better gyration) motion and the Döppler-Fizeau effect due to the universe expansion produce a power spectral density given, if written in standard terms, by [2]

$$\varrho(\omega) = \hbar\omega^3 (2\pi c^3)^{-1}, \tag{1}$$

i.e. equal to the zero-point field (ZPF) of QED. The ZPF is considered as virtual in QED and real in the new approach called stochastic electrodynamics (SED).

The spectrum (1) is Lorentz invariant and therefore allows a motion with inertia (no friction force according to the Einstein-Hopf formula). The stochastic property of (1) together with the «rigid» (*i.e.* independent of external macroscopic forces) *Zitterbewegung* may lead to a Schrödinger-like equation with corrective terms [3] (which, for hydrogen, give results roughly 1% of the Lamb shift [4]).

However, in SED plus spin the Schrödinger equation is considered as a rough approximation of a stochastic process, which works well for the average of the trajectories of each state and in regime conditions (for example, for electrons bound in atoms) but not for single trajectories as occurs for scattering. The application of a strongly modified Schrödinger-like equation to the scattering of low-energy electrons with hydrogen molecules is under study in the hope of solving the long-standing hydrogen controversy (the theoretical values of the ro-vibrational cross-sections calculated by usual QM differ up to 60% with respect to the experimental values [5]).

A similar restriction holds for the diffraction of electrons passing through one or more slits. The diffraction is due to the standing e.m. waves of the ZPF that establishes itself across the slit(s) and to a property of the spin (or gyration) motion (*Zitterbewegung*) with constant speed c whose centre C (of the gyration orbit) does *not* accelerate if the external force $\mathbf{F}$ is parallel to the plane of the gyration orbit [2]. The equation of motion of C is therefore, neglecting the radiation reaction,

$$m\mathbf{a} = \mathbf{F}\cdot\hat{\mathbf{n}}\hat{\mathbf{n}}\,, \tag{2}$$

where $\hat{\mathbf{n}}$ is the unit vector perpendicular to the plane of the gyration orbit. If $\hat{\mathbf{n}}$ is fixed, *i.e.* if it does not rotate, the effect on it of the ZPF is very small. Actually, the ZPF consists of trains of sinusoidal oscillations so that the velocity acquired by an electron in a half-wave is lost in the subsequent opposite wave. However, if $\hat{\mathbf{n}}$ rotates with angular velocity ω_n equal to that of the acting e.m. wave, two subsequent half-waves act differently. The effect is maximum if $\hat{\mathbf{n}}$ is roughly parallel to $\mathbf{F}$ in the first half-wave and perpendicular in the subsequent half-wave. Now $\hat{\mathbf{n}}$ tends to point toward the nearest attractive centre such as the nucleus of an atom or the nearest edge of the slit so that, if r is the minimum distance from the attractive centre and v the speed of the electron, it is

$$\omega_n \simeq v/r\,. \tag{3}$$

Consequently, the electron receives random transversal impulses,

$$mv_y = \hbar\omega_n(2c)^{-1} \tag{4}$$

from the ZPF which are maximum when ω_n coincides with some peak of the ZPF spectrum inside the slit (hence conditioned by the boundary).

That is why using «pure» SED (*i.e.* without spin) it is not possible to explain the diffraction. Actually, the ZPF is smaller near the slit than far from it. Yet ω_n is maximum when the electron passes the slit and almost zero when it is very far from material objects. The more confined (small r) the more the random impulses undergone (hence more diffusion) explains the origin of the stochastic uncertainty principle.

We show in sect. **5** that the diffraction pattern predicted by SED plus spin is equal to Schrödinger's one when the electron beam is transversally uniform and much larger than the slit aperture $2b$. However, if the beam is transversally much narrower than $2b$, the diffraction is still present since the electron simply probes the e.m. standing waves across the slit and due to the boundary-constrained ZPF. On the contrary, at least two separate small regions are necessary to have interference with the de Broglie associate wave. But is the rigorous solution of QM (obtainable by solving the Schrödinger equation) just equal to the elementary treatment in terms of de Broglie waves and reported in any textbook of theoretical physics? We have not found the rigorous solution of this basic problem that is, therefore, one of the aim of this paper. In this connection we define a Schrödinger free-particle operator H_0 acting on functions defined outside the barrier and vanishing on the border of the barrier representing the slit. The Fourier basis is the complete set of eigenfunctionals of H_0 which satisfy the boundary conditions in weak sense. In sect. **3** a Gauss beam is described in terms of weak solutions. After the slit the wave function is considered as the time evolution of an initial Gaussian beam truncated in correspondence of the slit. In sect. **4** the general form of the diffraction pattern is made explicit in some limiting cases.

In sect. **5** we derive the predictions of SED plus spin in a more detailed form than the general theory expounded in ref. [2]. There is a clear-cut difference between the predictions of Schrödinger QM (no diffraction when the transversal width Δy of the electron beam is much smaller than $2b$) and those of SED plus spin (still diffraction with a single pair of diffraction maxima plus the central non-deviated one). It is therefore highly desirable to perform the relevant experiment which could discriminate between QM and SED with spin.

2. – Formulation of the problem

We consider the one-slit diffraction problem in the 2-dimensional case, assume the slit to have sizes $2a$, $2b$ in the (x, y)-plane, and denote by $S = \{x, y): |x| < a, |y| > b\}$ the region which is inaccessible to the particle. The Schrödinger operator for a particle moving in this situation is

$$H = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right) + V(x, y) = H_0 + V, \tag{5}$$

where $V(x, y)$ represents an infinite step potential which does not allow a particle of arbitrary energy to penetrate the region S. This situation can be considered as the limiting case of a finite step potential, where, according to the usual considerations in QM, both the eigenfunctions and their derivatives are continuous in the discontinuities of the potential. Only the limit of an infinite step potential implies the vanishing of the eigenfunctions on the discontinuities of the potential [6, 7].

We therefore sketch the problem by assuming that the particle moves freely in the region of the (x, y)-plane outside the barrier, while it is subjected to the boundary condition of an infinite potential barrier in the region S.

Mathematically, this amounts to identifying H with H_0 and to defining a new free-particle Schrödinger operator H_0 acting on functions defined in the region D outside the barrier, $D = R^2 \setminus S$, and vanishing on the boundary ∂S of S. This is done in the weak sense according to the following considerations. Let $C_0^\infty(D)$ be the set of all infinitely differentiable functions with compact support contained in D. Then $H_0 = -(\hbar^2/2m)(\partial^2/\partial x^2 + \partial^2/\partial y^2)$ is a symmetric positive linear operator in $C_0^\infty(D)$ with respect to the inner product $(\phi, \psi) = \int_D \overline{\phi}\psi \, \mathrm{d}x \, \mathrm{d}y$ and therefore it can be extended to a self-adjoint operator in the Hilbert space $L_2(D)$ [8, 9]. The domain of the extended H_0 is a subset of the functions of $L_2(D)$ vanishing on the boundary ∂S. According to general results [8], the generalized eigenfunctions of H_0

$$u = A \exp[i(k_x x + k_y y)] + B \exp[i(k_x x - k_y y)] + C \exp[i(-k_x x + k_y y)] + D \exp[-i(k_x x + k_y y)], \tag{6}$$

with $k_x \geqslant 0$, $k_y \geqslant 0$ such that $k_x^2 + k_y^2 = 2mW/\hbar^2$ (where W is the eigenvalue of H_0), satisfy the boundary conditions in the weak sense [8], namely

$$\int_D \overline{u}(H_0 \phi - W\phi) \, \mathrm{d}x \, \mathrm{d}y = 0 \tag{7}$$

for every infinitely differentiable function ϕ in the domain of H_0. By allowing negative values for k_x and k_y, *i.e.* $-\infty < k_x, k_y < +\infty$, the eigenfunctions (6) are the basis for the Fourier transform

3. – Gaussian wave packet.

By using the previous results we study now the diffraction pattern of a beam of particles. We consider a free-particle Gaussian wave packet coming from the remote x-region and with a probability distribution centred on a point moving with velocity $\hbar k_{0x}/m$ on the x-axis ($y = 0$):

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

with

$$\psi(x, t) = \frac{\alpha^{1/2} \exp\left[-\dfrac{\alpha^2}{2} \dfrac{(x - x_0 - \hbar k_{0x} t/m)^2}{1 + i\hbar\alpha^2 t/m} + ik_{0x}(x - x_0) - i\hbar k_{0x}^2 t/2m\right]}{[\pi^{1/2}(1 + i\hbar\alpha^2 t/m)]^{1/2}} \tag{9}$$

and

$$\phi(y, t) = \left(\frac{\beta}{\pi^{1/2}(1 + i\hbar\beta^2 t/m)}\right)^{1/2} \exp\left[-\frac{\beta^2}{2} \frac{y^2}{1 + i\hbar\beta^2 t/m}\right]. \tag{10}$$

If x_0 is sufficiently negative a very good approximation is that $\psi(x, y, t)$ can be constructed from the $\psi(x, y, 0)$ initial Gaussian distribution by the usual integration method of the Schrödinger equation.

In order 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 $|y| > b$ is reflected towards the negative x-regions by the barrier S because no tunnelling effect is possible with an infinite potential barrier.

The truncation of the wave function when passing through the slit is also supported by considering the elementary case of a plane wave before the slit which emerges, after the slit, as proportional to the characteristic function of the $(-b, b)$ interval. Indeed in this case the p_y probability distribution is given by $|c(p_y)|^2$ where

$$c(p_y) \simeq A \int_{-b}^{b} \exp[-ip_y y/\hbar]\, \mathrm{d}y\,. \tag{11}$$

After a sufficiently large time interval, the y-position probability distribution can be obtained by exploiting the integral in eq. (11) and then by setting $y = p_y t/m$ in the result. We get

$$\phi(y, t)\, \phi^*(y, t) \simeq |A|^2 \left(\frac{2\hbar t}{my}\right)^2 \sin^2(myb/\hbar t)\,, \tag{12}$$

which is the well-known result for diffraction of a plane wave through a single slit, thus justifying the special truncation assumption.

In order to describe in general the time evolution of the wave packet after the slit we therefore assume that the wave packet just after the slit at a time taken as initial $(t = 0)$ is

$$\psi_b(x, y, 0) = \psi_a(x, 0)\, \chi_{(-b, b)}(y)\,, \tag{13}$$

where $\chi_{(-b, b)}(y)$ is the characteristic function of the interval $(-b, b)$ and $\psi_a(x, 0)$ is the function $\psi(x, 0)$ in eq. (9) with $x_0 = a$.

Since the initial wave function is separated in the x- and in the y-dependence, one has

$$\psi_b(x, y, t) = \psi_a(x, t)\, \phi_b(y, t)\,, \tag{14}$$

where $\psi_a(x, t)$ is again the function in eq. (12) with $x_0 = a$, while

$$\phi_b(y, t) = \left[\frac{\beta}{\pi^{1/2}}\right]^{1/2} \int_{-\infty}^{+\infty} \exp[i(p_y y - p_y^2 t/2m)/\hbar]\, \mathrm{d}p_y \int_{-b}^{b} \exp[-ip_y \xi/\hbar - \beta^2 \xi^2/2]\, \mathrm{d}\xi\,. \tag{15}$$

The last double integral can be performed by first integrating over the variable p_y,

$$\phi_b(y, t) = [2\hbar m\beta/it\pi^{1/2})]^{1/2} \exp[imy^2/(\hbar t)] \cdot \int_{-b}^{b} \exp[-\xi^2(\beta^2/2 + im/4\hbar t) + im\xi y/\hbar t]\, \mathrm{d}\xi \tag{16}$$

and then immediately obtaining

$$\phi_b(y,t) = \left[\frac{\hbar\beta m\pi^{1/2}}{it(\beta^2+im/2\hbar t)}\right)^{1/2} \exp\left[-y^2\,\frac{2m(m-2it\hbar\beta^2)}{\hbar t(2\hbar t\beta^2+im)}\right]\cdot \tag{17}$$

$$\cdot\left\{\operatorname{erf}\left[\frac{im(y+b/2)+b\hbar\beta^2 t}{\hbar t(2\beta^2+im/2\hbar t)^{1/2}}\right]-\operatorname{erf}\left[\frac{im(y-b/2)+b\hbar\beta^2 t}{\hbar t(2\beta^2+im/2\hbar t)^{1/2}}\right]\right\},$$

where $\operatorname{erf} z = 2(\pi)^{-1/2}\int\limits_0^z \exp[-t^2]\,dt$ is the error function [10].

4. – Limiting cases

4·1. We note that if the incoming wave packet is narrow with respect to the slit:

$$\Delta y = \frac{1}{\beta\sqrt{2}} \ll 2b\,, \tag{18}$$

then eq. (17) implies that $\phi_b(y,t)\,\phi_b^*(y,t)$ is essentially a Gaussian-like distribution since the y-dependence of the erf can be considered constant for β^2 very large. One can also obtain the same result by considering that the ξ-integral in eq. (15), when β^2 satisfies eq. (18), coincides with the integration over all the real axis. Thus the situation described in this case corresponds to an incident wave packet which passes through the slit and remains, after the slit, essentially undisturbed in its configuration.

4·2. Suppose now the incoming wave packet is very undetermined in the y-position probability distribution

$$\Delta y = \frac{1}{\beta\sqrt{2}} \gg 2b\,. \tag{19}$$

Then, by setting $\beta^2 = 0$ in eq. (17) and expressing the erf in terms of the Fresnel integrals [10], $C(z) + iS(z) = ((1+i)/2)\operatorname{erf}((\sqrt{\pi}/2)(1-i)z)$, one gets

$$\phi_b(y,t)\,\phi_b^*(y,t) \simeq 4\beta\pi^{1/2}\hbar^2\left\{\left[C\left(\frac{m^{1/2}(y+b/2)}{(2\hbar\pi t)^{1/2}}\right)-C\left(\frac{m^{1/2}(y-b/2)}{(2\hbar\pi t)^{1/2}}\right)\right]^2+\right. \tag{20}$$

$$\left.+\left[S\left(\frac{m^{1/2}(y+b/2)}{(2\hbar\pi t)^{1/2}}\right)-S\left(\frac{m^{1/2}(y-b/2)}{(2\hbar\pi t)^{1/2}}\right)\right]^2\right\}.$$

Equation (20) represents the most general solution and can be visualized by the tabulated Fresnel integrals [10].

In general, for $y \simeq b$, eq. (20) gives the Fresnel diffraction pattern. For y sufficiently large, the second term inside the exponent of the integral of eq. (16), *i.e.* $im/(4\hbar t)$ is much smaller than the last exponent $im\xi/(\hbar t)$ since $y \propto t$. Neglecting

$im/(4\hbar t)$ in eq. (16) (Fraunhofer approximation) with $\beta \to 0$ we get

$$\phi_b(y, t)\, \phi_b^*(y, t) = \frac{8m\beta\hbar}{t\pi^{1/2}} \frac{\sin^2(mby/\hbar t)}{(my/\hbar t)^2} \tag{21}$$

which represents the usual diffraction pattern consistent with what obtainable by elementary considerations in the wave propagation theory.

5. – Prediction of the diffraction pattern according to SED plus spin

We have already said in sect. **1** that diffraction remains in SED plus spin even if the transversal width Δy of the electron beam is much smaller than the slit aperture $2b$ since any electron simply acts as a probe of the standing e.m. waves of the ZPF across the slit. On the contrary, as proved in sect. **4**, diffraction disappears in QM when $\Delta y \ll 2b$. This is the main difference in the predictions. However, SED plus spin is more predictive and able to lead to the detailed diffraction pattern (which depends on the distance r of the electron beam from the nearest edge of the slit).

The angle θ of deviation is obtained from $\sin\theta = \langle v_y^2 \rangle^{1/2}/v$, where v is the electron speed before and after crossing the slit since the transversal impulse due to the ZPF modifies $\mathbf{v}$ but not $|\mathbf{v}|$. Using eq. (4) we get

$$\sin\theta = \pm\hbar\omega_n (2mcv)^{-1}. \tag{22}$$

The *deviation* depends therefore on the energy (hence momentum) per normal modes of the ZPF. The *intensity* of the deviated beam (hence of the lines on the far screen) depends on the spatial density of modes allowed by the slit. The amplitudes of the ZPF e.m. waves are spatially uniform in space and zero on the wall of the slit (at least for frequencies less than the plasma frequency of the slit wall if made of metal). Consequently, the *spatial* Fourier transform of the ZPF *amplitude* is

$$\varrho_s(k_y) = \frac{1}{2b} \int_{-b}^{b} \mathrm{d}y \exp[ik_y y] = \frac{\sin(k_y b)}{k_y b}. \tag{23}$$

The corresponding spatial distribution of the energy modes allowed by the slit is proportional to

$$\varrho_E(k_y)^2 \propto [\sin(k_y b)/k_y b]^2, \tag{24}$$

which is the standard expression for e.m. waves and also equivalent with what obtainable from eq. (21) (valid for $\Delta y \gg 2b$).

The intensity maxima occur for

$$k_y = 0 \quad \text{and} \quad k_y b = \pi(n + 1/2), \qquad n = 1, 2, 3 \ldots. \tag{25}$$

Since $k_y = \omega/c$, we get the deviations θ_m corresponding to intensity maxima substituting eq. (25) in eq. (22):

$$\sin\theta_m = 0 \quad \text{and} \quad \sin\theta_m = \frac{\hbar\pi}{2bmv}\left(n + \frac{1}{2}\right). \tag{26}$$

The detailed prediction of SED plus spin for the diffraction of a narrow beam of electrons (with $\Delta y \ll 2b$) is therefore that for each position of the entering beam there are only two angles of deviation given by eq. (22) with $\omega = v/r$, where r is roughly the distance from the nearest edge of the slit. The average intensity of the two deviated beams is given by eq. (24). Obviously, being a statistical process, there is always the central, non-deviated beam.

By displacing gradually the position of the entering beam and registering the successive pairs of opposite spots, the complete diffraction pattern due to a large beam ($\Delta y \gg 2b$) should be obtained.

6. – Comparison of the predictions of QM and SED plus spin

The diffraction pattern for a Gaussian wave packet has been obtained by Schrödinger equation in the general case of a width $(\sqrt{2}\beta)^{-1}$ of the Gaussian comparable with the aperture of the slit. The particular case $(\sqrt{2}\beta)^{-1} \gg b$ gives the same maxima of the diffraction pattern as easily obtainable by the de Broglie associate wave. When $(\sqrt{2}\beta)^{-1} \ll b$ there is no diffraction, still in agreement with the elementary considerations.

The results are similar to those obtainable from electromagnetism for the diffraction of e.m. waves although a Gaussian wave packet of e.m. waves propagates without changing its shape (there is no dispersion for the speeds of the various harmonics). The difference with respect to the Schrödinger case is, however, not relevant to the considerations of the previous sections.

Moreover, with no external magnetic fields, the electron spin seems to play no role in the problem.

On the contrary, the spin motion (meant as a gyration due to the e.m. self-reaction) plays a fundamental role in the explanation of diffraction inside stochastic electrodynamics (SED) implemented by spin [2]. Actually, the radiation of the electron inside the horizon of the universe produces [2] a stochastic e.m. field whose spectral power density is just equal to the zero-point field (ZPF) of quantum electrodynamics (QED) [2]. Boundary conditions modify the ZPF as occurs in the Casimir effect [11]. Precisely, the Maxwell equations with $\mathbf{E} = 0$ on the slit walls imply a reduction of the ZPF so that its spectrum inside the slit is modulated with maxima at wavelength $\lambda = 2b/(n + 1/2)$, where n is an integer.

7. – Conclusions and proposal of a feasible experiment to discriminate between QM and SED plus spin

In spite of the reduction of the ZPF near the slit, an electron receives effective transversal impulse, according to SED plus spin, when it passes the slit, since the spin axis $\widehat{\mathbf{n}}$ practically rotates only when it crosses the slit plane. If ω is the angular velocity of $\widehat{\mathbf{n}}$ when the electron crosses the slit, the electron undergoes a transversal impulse (either up or down) given by eq. (4). The intensity of the deflected beam depends on the spatial mode density allowed by the slit and given by eq. (24). Since

$$k_y b = 2\pi b/\lambda = bmv_y/\hbar \,, \tag{27}$$

the intensity distribution (24) is proportional to that given by eq. (21) as can be seen by putting $y = v_y t$ (actually, $\phi_b \phi_b^* t$ is proportional to the total number of deflected electrons inside a given solid angle).

Consequently, any narrow beam of electrons ($\Delta y \ll 2b$) should be divided into three parts: the central one, corresponding to no deflection, and a pair of opposite beams having a deviation angle given by eq. (22) and intensity given by eq. (24) with $k_y = \omega_n / c$. By displacing gradually the beam, the sum of the successive spots should give the complete pattern due to a large beam ($\Delta y \gg 2b$).

With regard to diffraction, there would therefore be a fundamental difference between electrons and photons, at variance with the usual prediction of QM. In fact, the radiation pattern for electrons obtained in the present work, strictly inside QM, is equal to that obtained from electromagnetism for e.m. waves. There is therefore the possibility of performing the relevant experiment which is able to discriminate between QM and SED plus spin. A feasible experiment could be performed by a transmission electron microscope focalizing the beam in the so-called "diffraction zone" and using a byprism to convert the very small angles of deviation into small displacement on the "object" plane. If no diffraction is observed, then SED plus spin will be disproved. If a pair of opposite spots plus central spot are observed, then Schrödinger's equation will be limited to regime situations and to the average of the trajectories of a given state.

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