

NEUTRON INTERFEROMETRY AND STOCHASTIC MECHANICS

by

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SUMMARY:

Fenyés-Nelson's derivation of Schrödinger wave functions within the stochastic formalism allows to reintroduce the notion of (random) particle trajectory in quantum theory. We extend this argument to diffracting crystals used in the triple von Laue interferometric experiments, to reveal the particle aspects of interference phenomena.

For low intensity neutron beams two interference scenarios are possible: (1) neutron self-interference (conventional) implies the essentially non-local phenomenon extending on few centimeters within the macroscopic apparatus, (2) indirect neutron interaction through memory effects in the diffracting crystal (usually dismissed on the basis of the current paradigm) is the remaining part of the hypothesis due to Buonomano, not disproved in the recent experimental test. A decisive experiment is discussed.

Motivation

The departure point for our investigation is an interesting series of papers [1-11] on neutron interferometry experiments, which together with the studies of photon interference [12-15] seem to open new avenues towards an understanding of the wave-particle duality problem and the superposition principle. The orthodox approach to quantum mechanics denies a possibility of saying anything about the particle trajectory, except for the probability distribution of particle location in space, although it is a single particle [1-15] which excites the counter or hits the detecting film in the experiment, see also [16,17] and compare e.g. investigations of a possible meaning of individual Feynman paths in quantum mechanics [18]. The essence of neutron interferometry lies in performing a series of reproducible one-particle experiments with a binary yes-no outcome. Neutrons are to pass through either the appropriately cut monolithic silicon crystal (Vienna group) or through three parallel crystal slabs (Bonse-Hart interferometer). The geometry of the arrangement implies that each single neutron emitted by the source, everywhere within the interferometer and at the exit, has two possible (macroscopically separating or converging) paths to follow. The time of flight of neutrons through the interferometer is orders of magnitude smaller than the mean interval between two consecutively born in the crystal neutron. In fact [4] the time of flight is $\sim 35 \mu\text{s}$, the time interval between consecutive neutrons $\sim 780 \mu\text{s}$. The coincidence tests confirm that single neutrons come at random to always one of the two detectors. Quite analogous situ-

ation is known to arise in electron interferometry [19] where at a very low current density, the statistical process of fringe formation can be seen as the image of statistically distributed light flashes of individual electrons. The same situation occurs in case of very low intensity photon beams [12-15]. Statistically significant outcomes (frequencies) arise after sufficiently many repetitions of the generic single particle experiment, under constant physical conditions. In case of neutron interferometry one can never tell which neutron has gone along which path, but only that in the number N of neutrons the fraction of $N-k$ reached one detector, while the fraction of $N-k$ reached another. A totality of single particle flights through the apparatus under (roughly) the same experimental conditions, we identify with the beam of particles notion (statistical ensemble [16-17]). It is a beam to which probabilistic predictions of quantum mechanical wave functions do apply, although it is customary [1-11] to employ the plane waves in theoretical analyses. Beam splitting and recombination by silicon crystal slabs, if accompanied by phase shifting operations results in the experimentally measured phase modulation of frequencies. It thus reveals wave phenomena although consecutive single clicks of the counters are registered merely.

Remark: Although the beam separation in the interferometer may be of a macroscopic size, the underlying quantum mechanical description always refers to the unsharp separation (up to exponential tails), so avoiding the problem raised in [20]: quantum mechanics does not literally apply to macroscopically separated quantum systems.

Apart from the fact that all experimental results of [1-11] find a formal justification in the standard rules of the game based on the Schrödinger equation, some obscurities still remain while representing the physical notions (particle path, beam of particles) within the well settled mathematical formalism of quantum theory. Undoubtedly single neutrons travel along space-time paths between the source and the detector, although the details of their trajectories are not accessible to the experimenter. But [3,4]:

"The question whether the wave function describes a single neutron or a beam has to be answered such that it describes a single neutron out of a certain beam. Therefore the wave packet representation contains parameters of the particle and of the beam, which are defined by the constraints of the experimental arrangement" albeit certainly some confusion must come from the statement about a single neutron self-interference [3,21].

"The experimental results manifest that every neutron has at the place of superposition (i.e. beam recombination) information about a physical situation in both possible beam paths" although with probability one only one path was followed by the detected neutron and not (simultaneously) both. Moreover with probability one only a single neutron has accomplished its route through the crystal long before the next one was born.

Perhaps it is not useless to invoke at this point the quite justified criticism by Lande [22] which originally pertains to the two slit diffraction thought experiments with electrons: the single electron knows nothing it is the experimental arrangement as a whole which determines its destination.

Random paths in quantum mechanics

Fényes-Nelson's stochastic mechanics (23) is one of very few (23-7) attempts to reconcile the individual particle trajectory notion with the wave (Schrödinger) theory of quantum phenomena. According to the recipes of (23) to a given solution of the Schrödinger equation one can in principle attribute a stochastic diffusion process satisfying the Newton second law in the mean. The corresponding stochastic differential equation describes a propagation of a point particle through a non-dissipative random medium. Sample paths of the process can be approximately identified with the realistic configuration space paths of (perhaps) physical particles. For a quantum particle in the conservative force field we have:

$$i\hbar\partial_t\psi(\vec{x},t) = \frac{\hbar^2}{2m}\Delta\psi(\vec{x}) + V(\vec{x})\psi(\vec{x},t) \quad (1)$$

which implies the continuity equation for $\rho = |\psi|^2$

$$\partial_t\rho = -\text{div}\vec{j} \quad \vec{j} = \frac{\hbar}{2mi}(\bar{\psi}\nabla\psi - \psi\nabla\bar{\psi}) \quad (2)$$

In case of nowhere zero ψ (locally at least, there are existence proofs for singular diffusions), upon a standard substitution $\psi = \exp(R + iS)$, (2) goes over into:

$$\partial_t\rho = \text{div}\{-\frac{\hbar}{m}\nabla S\circ\rho\} = \frac{\hbar}{2m}\Delta\rho - \text{div}\rho\vec{B} \quad (3)$$

where:

$$\rho = \exp 2R, \quad \vec{B} = \vec{u} + \vec{v}, \quad \vec{u} = \frac{\hbar}{m}\nabla R, \quad \vec{v} = \frac{\hbar}{m}\nabla S, \quad \vec{B}_* = \vec{v} - \vec{u} \quad (4)$$

and one more equation

$$\partial_t\rho = -\frac{\hbar}{2m}\Delta\rho - \text{div}\rho\vec{B}_* \quad (5)$$

is obeyed by ρ . It is identifiable as the backward Fokker-Planck equation, while (3) is the forward one.

In the theory of stochastic processes such equations are known to determine the time development of the respectively forward and backward transition probability densities for the diffusion process.

Setting $\nu = \frac{\hbar}{2m}$, $\vec{B} = \frac{\hbar}{m}\nabla(R+S)$ in the forward case we have

$$\partial_t p(\vec{y},0,\vec{x},t) = \text{div}_x\{\nu\nabla_x p(\vec{y},0,\vec{x},t) - \vec{B}(\vec{x},t)p(\vec{y},0,\vec{x},t)\} \quad (6)$$

According to the rules of the Ito stochastic calculus, one can uniquely associate (6) with the stochastic differential equation

$$d\vec{X}(t) = \vec{B}(\vec{X}(t),t)dt + \sqrt{2\nu}d\vec{W}(t) \quad (7)$$

where $d\vec{W}(t)$ represents the normalized Wiener noise. $\vec{X}(t)$ takes values in R^3 as a continuous function of time, and with time passing draws a stochastic trajectory in the configuration space. Given $\rho_0(\vec{x}) = \rho(\vec{x},0)$ and $p(\vec{y},0,\vec{x},t)$ solving (6). Apparently $\int d^3\vec{y}p(\vec{y},0,\vec{x},t)\rho_0(\vec{y})$ provides a solution of (6) with the initial condition $\rho_0(\vec{x})$, hence by the uniqueness theorem for the parabolic (Kolmogorov) equation it equals $\rho(\vec{x},t)$.

The normalization $\int d^3\vec{x}\rho(\vec{x},t)=1$ is preserved by virtue of $\int d^3\vec{x}p(\vec{y},0,\vec{x},t)=1$. Let us emphasize that the knowledge of $p(\vec{y},0,\vec{x},t)$ does not determine $\rho(\vec{x},t)$ unless $\rho_0(\vec{x})$ is specified. Consequently, given (3) it is rather natural to

demand the validity of this equation not only for $\rho(\vec{x}, t)$ but also for the transition probability densities $p(\vec{y}, 0, \vec{x}, t)$ which automatically associates (7) with (1).

Remark 1: The existence and uniqueness of solution of the stochastic differential equation (7) with the initial condition $\vec{X}(t_0) = \vec{x}_0$ is discussed in (27-8). To have (7) solved in the interval: $[t_0, T]$ one usually imposes the smoothness (Lipschitz) condition: $|\vec{B}(\vec{x}, t) - \vec{B}(\vec{y}, t)| \leq K|\vec{x} - \vec{y}|$ for all \vec{x}, \vec{y} and $t \in [t_0, T]$, K being a constant, and the growth condition $2\nu + |\vec{B}(\vec{x}, t)|^2 \leq K'(1 + |\vec{x}|^2)$. The latter, if fulfilled guarantees that the solution will not explode for finite times.

As is well known (26,29) the Schrödinger equation (1) can be equivalently rewritten as a coupled system of equations, one of which is (3), while another has the familiar Hamilton-Jacobi form:

$$\partial_t S = \frac{\hbar}{2m} \{ |\nabla R|^2 - |\nabla S|^2 + \Delta R \} - \frac{V}{\hbar} \quad (8)$$

Let us define the conditional expectation for the stochastic process $\vec{X}(t)$ solving (7)

$$E_t [f(\vec{X}(t'))] = E[f(\vec{X}(t') | \vec{X}(t) = \vec{x})] = \int d^3\vec{y} p(\vec{x}, t, \vec{y}, t') f(\vec{y}) \quad (9)$$

In terms of (9) the mean forward and backward derivatives D_+ , D_- of the process can be introduced

$$(D_{\pm} f)(\vec{X}(t), t) = \lim_{\Delta t \downarrow 0} E_t \left\{ \pm \frac{1}{\Delta t} [f(\vec{X}(t \pm \Delta t), t \pm \Delta t) - f(\vec{X}(t), t)] \right\} = (\partial_t + \vec{B}_{\pm} \cdot \nabla \pm \frac{\hbar}{2m} \Delta) f(\vec{X}(t), t) \quad (10)$$

such that

$$D_+ \vec{X}(t) = \vec{B}_+ = \vec{B} \quad D_- \vec{X}(t) = \vec{B}_- = \vec{B}_* \quad (11)$$

and there holds

$$\frac{m}{2} (D_+ D_- + D_- D_+) \vec{X}(t) = \frac{m}{2} (D_+ b_- + D_- b_+) (\vec{X}(t), t) = \hbar \nabla \{ \partial_t S - \frac{\hbar}{2m} [|\nabla R|^2 - |\nabla S|^2 + \Delta R] \} (\vec{X}(t), t) \quad (12)$$

By equating (which is a restriction on the process making it time reversal invariant)

$$\frac{m}{2} (D_+ D_- + D_- D_+) \vec{X}(t) = -\nabla V \quad (13)$$

the second Newton law of motion is obeyed in the stochastic mean. Apparently we deal here with the gradient form on (9). Since the osmotic \vec{u} and current \vec{v} velocities are gradients, it is convenient to rewrite (3) and (8) in terms of them only. Then

$$\partial_t \vec{u} = \frac{\hbar}{2m} \Delta \vec{v} - \nabla(\vec{v} \cdot \vec{u}) \quad \partial_t \vec{v} = \frac{\hbar}{2m} \Delta \vec{u} + \frac{1}{2} \nabla(\vec{u}^2) - \frac{1}{2} \nabla(\vec{v}^2) - \frac{1}{m} \nabla V \quad (14)$$

may be considered as the starting point for the stochastic analysis, once the initial velocity fields $\vec{u}(\vec{x}, t_0)$, $\vec{v}(\vec{x}, t_0)$ are chosen and the Cauchy problem (14) is solvable.

Remark 2: Let us emphasize that the causal approach (2-4) exploits directly equations (3) and (8). It is precisely the Hamilton-Jacobi form of (8) which allows to associate certain deterministic motions with the wave equation (1). In the stochastic approach the situation is different. The paramount importance of the stochastic differential equation (7) makes here quite a substantial difference between the

deterministic and random implementation of (possibly particle) trajectories associated with solutions of (1).

Equations (3), (8) provide us merely with another form of (1), while the equivalence of (14) with (7),(13) is more intricate. On the other hand, by taking the gradients of (3), (8) we recover (14), hence *on the mathematical (at least) level a manifest link exists between Schrödinger wave functions and random (diffusive) motions of point particles.*

The major problem of stochastic mechanics is then to reveal to which extent wave functions are derivable on purely probabilistic (diffusion processes) grounds.

Apparently it amounts to recovering the potentials upon an assumption that $\vec{u}(\vec{x},t), \vec{v}(\vec{x},t)$ solving (14) are gradient fields. Let \vec{u}, \vec{v} solve (14) with the initial data $\vec{u}_0(\vec{x}) = \vec{u}(\vec{x}, t_0), \vec{v}_0(\vec{x})$. By introducing $\vec{B} = \vec{u} + \vec{v}$ we can pass to the stochastic differential equation (7) which in turn implies (6). Accordingly $\rho(\vec{x},t)$ is determined by the choice of $\rho(\vec{x}, t_0)$. Assuming that $\vec{u}_0(\vec{x})$ is the gradient field, we can locally reproduce the potential with the accuracy up to the additive constant (e.g. Poincaré lemma). The normalization condition $\int \rho(\vec{x}, t_0) d^3\vec{x} = 1, \exp 2R_0 = \rho_0$ removes the arbitrariness, hence $\vec{u}_0(\vec{x})$ determines $\rho_0(\vec{x})$ and by (6) $\rho(\vec{x},t)$.

With $\rho(\vec{x},t)$ established, we are finally left with the equation (13) whose integration amounts to solving the Cauchy problem

$$\partial_t s + H(\nabla s, \vec{x}, t) = 0$$

$$s(\vec{x}, t_0) = s_0(\vec{x}), \nabla s_0(\vec{x}) = m\vec{v}_0(\vec{x}), \vec{s} = \hbar \vec{S} \quad (15)$$

with

$$H(\vec{p}, \vec{x}, t) = \frac{\vec{p}^2}{2m} + U(\vec{x}, t)$$

$$U(\vec{x}, t) = V(\vec{x}, t) - \frac{\hbar^2}{2m} \frac{\Delta \rho^{1/2}}{\rho^{1/2}} \quad (16)$$

Indeed, if we have a solution $s(\vec{x},t)$ of (15), then $\nabla s(\vec{x},t)$ solves (13), hence (14). By the uniqueness argument for solutions of the Cauchy problem, $\nabla s(\vec{x},t) = m\vec{v}(\vec{x},t)$ provides a solution of (14) with $\vec{v}_0(\vec{x}) = \frac{1}{m}\nabla s_0(\vec{x})$. The only non-uniqueness pertains to the initial data $\nabla s_0(\vec{x}) = m\vec{v}_0(\vec{x})$ since in the contractible spatial area $\vec{v}_0(\vec{x})$ determines the corresponding potential up to the additive constant.

To see how this arbitrariness can be removed, let us consider the absolute expectation value of (15). Then $\langle \partial_t s \rangle = -\langle H \rangle$ where (integrate by parts (30))

$$\langle H \rangle = \int d^3\vec{x} \left[\frac{m}{2} (\vec{v}^2 - \vec{u}^2) + V(\vec{x}, t) - \frac{\hbar}{2} \text{div} \vec{u} \right] \rho(\vec{x}, t) =$$

$$\int d^3\vec{x} \left[\frac{m}{2} (\vec{u}^2 + \vec{v}^2) + V(\vec{x}, t) \right] \rho(\vec{x}, t) =$$

$$\int d^3\vec{x} \mathcal{E}(\vec{x}, t) \rho(\vec{x}, t) \quad (17)$$

and the assumption of the localizability (e.g. $\langle H \rangle < \infty$) of the total (mean) energy of the diffusion process is necessary to have (15) uniquely solved on the basis of (14). The term $\int d^3\vec{x} \frac{m}{2} (\vec{u}^2 + \vec{v}^2) \rho(\vec{x}, t)$ is known as the kinetic energy of the diffusion process.

By the continuity equation we have

$$\partial_t \langle s \rangle = \int d^3\vec{x} (\partial_t \rho) \cdot s + \langle \partial_t s \rangle = m \langle \vec{v}^2 \rangle + \langle \partial_t s \rangle \quad (18)$$

Hence (15) implies

$$\partial_t \langle s \rangle = m \langle \vec{v}^2 \rangle - \langle H \rangle \quad (19)$$

which admits a unique solution $\langle s \rangle(t)$ for given initial data

$$\langle s \rangle(t_0) = \langle s_0 \rangle.$$

By making the restriction

$$\langle s_0 \rangle = 0 \quad (20)$$

we have a guarantee that $\langle s \rangle(t)$ is determined in terms of \vec{u} and \vec{v} only

$$\langle s \rangle(t) = \int_{t_0}^t [m \langle \vec{v}^2 \rangle - \langle H \rangle] dt \quad (21)$$

Given an arbitrary integral $s'(\vec{x}, t)$, $\langle s'_0 \rangle \neq 0$ of (15).

Then, apparently

$$s(\vec{x}, t) = s'(\vec{x}, t) - \langle s'_0 \rangle \quad (22)$$

obeys both (20) and (15).

Accordingly *Schrödinger wave functions with phases obeying (15), (20) can be set in a one-to-one correspondence with the diffusion process (7), (13).*

The mapping $\{\vec{u}, \vec{v}\} \leftrightarrow \{\rho, S\}$ was investigated by us locally (in a contractible area). However, its extensions can be fruitfully studied by viewing the Schrödinger equation as the linearization of the coupled nonlinear system (14). Then, with all previous reservations concerning the uniqueness of the map, once $\rho(\vec{x}, t), S(\vec{x}, t)$ are in hands, we can introduce the diffusion processes for which $\{\rho, S\}$ is a pair of potentials implementing the gradient fields $\{\vec{u}, \vec{v}\}$.

Random trajectories of the conditioned Wiener process are known⁽³¹⁾ to provide a natural probabilistic background for the Feynman's path concept, which is condensed in the Feynman-Kac formula. Its particular case is the path integral expression for the heat equation kernel, whose stochastic mechanics implementation was discussed in⁽³²⁾.

Indeed, the simplest example of the smooth Markovian diffusion is the Wiener process with the transition probability density solving the heat equation:

$$\partial_t p(\vec{y}, 0, \vec{x}, t) = \nabla \Delta_x p(\vec{y}, 0, \vec{x}, t) \\ p(\vec{y}, 0, \vec{x}, t) = (4\pi \nu t)^{-3/2} \exp\left\{-\frac{|\vec{y} - \vec{x}|^2}{4\nu t}\right\} \quad (23)$$

The corresponding stochastic differential equation reads $d\vec{X}(t) = (2\nu)^{1/2} d\vec{W}(t)$.

The Wiener process can be used for the construction of more complicated diffusions, like these described by Eq.(6), (7). The general formula for the small time transition probability is available (Ref.35, Chap.4.7) and reads:

$$p(\vec{y}, s, \vec{x}, s+\Delta t) = (4\pi \nu \Delta t)^{-3/2} \\ \exp\left\{-\frac{|\vec{x} - \vec{y} - \vec{b}(\vec{y}, s)\Delta t|^2}{4\nu \Delta t}\right\} \quad (24)$$

The uses of this small time formula become apparent when passing to the finite difference (discrete) approximation of random paths. Consider the family $\{I_j \subset \mathbb{R}^3, j=1, 2, \dots, n\}$ of Borel sets, with $t = (n+1)\Delta t$. The random paths are approximated by broken trajectories:

$$\{\vec{X}(s): \vec{X}(0) = \vec{x}_0, \vec{X}(t) = \vec{x}_f, \vec{X}(j\Delta t) \in I_j, j=1, 2, \dots, n\}$$

with the initial \vec{x}_0 and final \vec{x}_f points fixed.

The cylinder sets are measurable i.e. the transition probability density conditioned to refer to the cylinder set reads:

$$\int_{I_1} d\vec{x}_1 \dots \int_{I_n} d\vec{x}_n p(\vec{x}_0, 0, \vec{x}_1, \Delta t) p(\vec{x}_1, \Delta t, \vec{x}_2, 2\Delta t) \dots \\ p(\vec{x}_n, n\Delta t, \vec{x}_f, t) = \quad (25)$$

$$\int_{I_1} d\vec{x}_1 \dots \int_{I_n} d\vec{x}_n \prod_{j=1}^{n+1} \left\{ \left[4\pi \nu (t_j - t_{j-1}) \right]^{-3/2} \exp \left[- \frac{|\vec{x}_j - \vec{x}_{j-1} - b(x_{j-1}, t_{j-1}) \Delta t|^2}{4\pi \nu (t_j - t_{j-1})} \right] \right\}$$

$$t_0 = 0, t_{n+1} = t, \vec{x}_{n+1} = \vec{x}_f$$

The so introduced conditional Wiener measure on the cylinder set does explicitly attribute the real positive probability weight to each discrete approximant $(\vec{x}_0, \vec{x}_1, \dots, \vec{x}_n, \vec{x}_f)$ of the random path. This measure is known to be countably additive on all cylinder subsets of the set of all continuous trajectories defined on $[0, t]$ and conditioned to connect fixed points \vec{x}_0 and \vec{x}_f .

A formal replacement of all I_j by R^3 followed by the $n \rightarrow \infty$ limit in the partition $\Delta t = t/(n+1)$ gives a path integral expression for the complete transition probability density $p(\vec{x}_0, 0, \vec{x}_f, t)$. One must however remember that neither of n -dependent factors in (25) taken separately admits the well defined $n \rightarrow \infty$ limit, albeit the whole expression does.

The above discussion well exemplifies the conclusions of (33,34) on the purely probabilistic origin of Feynman paths.

Remark : Numerous objections were raised against the physical relevance of stochastic mechanics, but most essential of them were found (36,37) to come from the misunderstanding of relationships between quantum and stochastic observables. The contribution to the present volume (38) appears not to account correctly for the principal feature of the stochastic mechanics which is time reversal invariance. The issue was discussed at length in (29) to indicate why it is not shared by irreversible stochastic processes of standard statistical physics.

According to the previous analysis we can view the wave functions as symbolic representations of collections of sample paths, and thus of the underlying random (stochastic) field, which we identify with the medium through which individual particles are to propagate.

It is the background (universal Brownian motion of [23]) random field hypothesis, which might involve objections against a physical reality of stochastic mechanics. However, its applicability is undoubtful whenever physical reasons of randomness can be explicitly identified, like in the specific problem studied in (39-42). Useful suggestions can here be also drawn from experimental reports on neutron flight times through the diffracting crystals (43). In neutron experiments the very fact of neutron propagation through monolithic crystals, leads to the natural notion of the random medium: apart from the ordered (lattice) structure crystal own excitations plus these born through interactions with the incident particle, allow to attribute the random medium role to the crystal. Neutrons effectively diffuse through the crystal and random fluctuations are necessarily superimposed on motions due to the periodic potential of the crystal lattice.

According to the above picture the ambiguous (albeit justified by tradition) assignment of wave functions to neutron beams can be understood in the framework of stochastic mechanics: wave functions govern the (statistical) dynamics of collections of individual, randomly perturbed single particle trajectories. Thus we are at the point where particle and wave aspects of quantum mechanics may consistently match.

Beam splitting and Recombination in Neutron Interferometry

1. Experimental setting

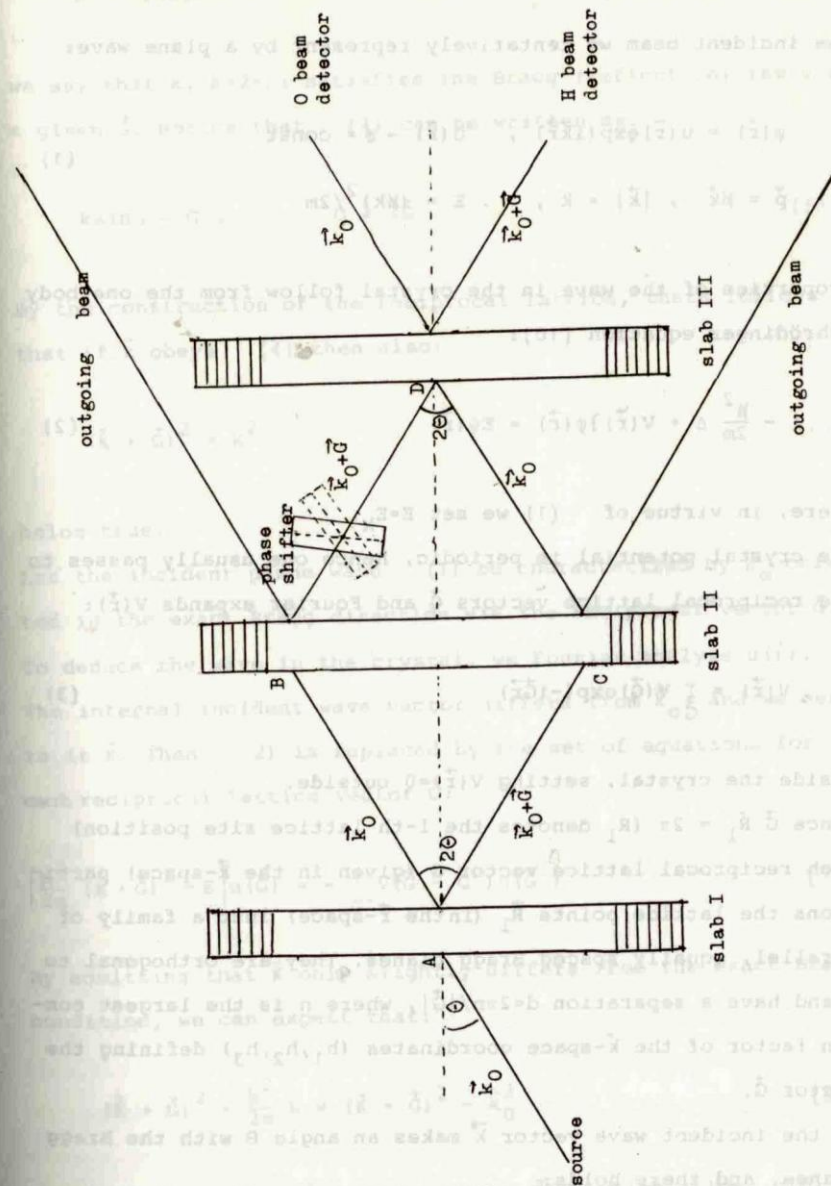
Neutron interferometry deals with fairly monochromatic neutrons [1-4] with the de Broglie wavelength of about $1-2 \text{ \AA}$ i.e. velocities of about 2000 m/s. A wavelength spread is less than one promille.

Traditionally monochromatic beams are represented in quantum mechanics by plane waves, and the dynamical theory of neutron reflection, refraction and diffraction amounts to analyzing solutions of the Schrödinger equation in the form of plane waves [4,9,-11]. Let us reproduce a schematic diagram of the interferometer (patterned after Fig.1 of [9] and Fig.16 of [10]):

(see the figure enclosed on the separate page)

The neutron beam is coherently split in slab I. Lattice planes are indicated to show our (a bit impractical) choice of the ideal geometry for the symmetric Laue case, which applies here. The two diverging beams are again coherently split in slab II, but only the reflected components are preserved to converge and get recombined, next split again in slab III. The slab III splitting induces the interference pattern visible in the modulation of counting rates at the detectors, provided we enforce a phase change of one beam against the other.

The two beam components which leave slab II outward, can in principle be separately registered. Their absence in the recombination area apparently results in what is sometimes called the wave packet reduction.



2. Beam splitting

The incident beam we tentatively represent by a plane wave:

$$\begin{aligned}\psi(\vec{r}) &= u(\vec{r})\exp(i\vec{k}\vec{r}), & u(\vec{r}) + \phi &= \text{const} \\ \vec{p} &= \hbar\vec{k}, & |\vec{k}| &= k, & E &= (\hbar k)^2/2m\end{aligned}\quad (1)$$

Properties of the wave in the crystal follow from the one-body Schrödinger equation [10]:

$$\left\{ -\frac{\hbar^2}{2m}\Delta + V(\vec{r}) \right\} \psi(\vec{r}) = E\psi(\vec{r}) \quad (2)$$

where, in virtue of (1) we set $E = E_k$.

The crystal potential is periodic, hence one usually passes to the reciprocal lattice vectors \vec{G} and Fourier expands $V(\vec{r})$:

$$V(\vec{r}) = \sum_{\vec{G}} V(\vec{G})\exp(-i\vec{G}\vec{r}) \quad (3)$$

inside the crystal, setting $V(\vec{r})=0$ outside.

Since $\vec{G}\vec{R}_1 = 2\pi$ (R_1 denotes the 1-th lattice site position) each reciprocal lattice vector G (given in the \vec{k} -space) partitions the lattice points \vec{R}_1 (in the \vec{r} -space) into a family of parallel, equally spaced Bragg planes. They are orthogonal to \vec{G} and have a separation $d=2\pi n/|\vec{G}|$, where n is the largest common factor of the \vec{k} -space coordinates (h_1, h_2, h_3) defining the vector \vec{G} .

If the incident wave vector \vec{k} makes an angle θ with the Bragg planes, and there holds:

$$n\lambda = 2d\sin\theta \quad (4)$$

we say that \vec{k} , $k=2\pi/\lambda$ satisfies the Bragg (reflection) law via a given \vec{G} . Notice that (4) can be written as:

$$k\sin\theta = G, \quad G = |\vec{G}| \quad (5)$$

By the construction of the reciprocal lattice, there follows that if \vec{k} obeys (4) then also:

$$(\vec{k} + \vec{G})^2 = k^2 \quad (6)$$

holds true.

Let the incident plane wave (1) be characterized by \vec{k}_0 oriented in the exact Bragg direction via the reciprocal vector \vec{G} .

To deduce the wave in the crystal, we Fourier analyze $u(\vec{r})$.

The internal incident wave vector differs from \vec{k}_0 , and we denote it \vec{k} . Then (2) is replaced by the set of equations for each reciprocal lattice vector \vec{G} :

$$\left[\frac{\hbar^2}{2m} (\vec{k} + \vec{G})^2 - E \right] u(\vec{G}) = - \sum_{\vec{G}'} V(\vec{G} - \vec{G}') u(\vec{G}') \quad (7)$$

By admitting that \vec{k} only slightly differs from the exact Bragg condition, we can expect that:

$$(\vec{k} + \vec{G})^2 - \frac{\hbar^2}{2m} E = (\vec{k} + \vec{G})^2 - k_0^2 \quad (8)$$

is small for either $\vec{G}=0$ or a certain $\vec{G}\neq 0$, which allows $u(0)$ and

$u(\vec{G})$ to be relatively large against the other Fourier coefficients. This two-plane-wave approximation ansatz replaces (7) by:

$$\left[\frac{\hbar^2}{2m} (K^2 - k_0^2) + V(0) \right] u(0) = -V(-\vec{G})u(\vec{G}) \quad (9)$$

$$\left\{ \frac{\hbar^2}{2m} \left[(K + G)^2 - k_0^2 \right] + V(0) \right\} u(\vec{G}) = -V(\vec{G})u(0)$$

Introducing:

$$K_0 = k_0 \left[1 - \frac{2m}{\hbar^2 k_0^2} V(0) \right]^{1/2}, \quad \vec{K}_G = \vec{k}_0 + \vec{G} \quad (10)$$

we can rewrite (9) as follows:

$$(K^2 - K_0^2)u(0) + \frac{2m}{\hbar^2} V(-\vec{G})u(\vec{G}) = 0 \quad (11)$$

$$(K_G^2 - K_0^2)u(\vec{G}) + \frac{2m}{\hbar^2} V(-\vec{G})u(0) = 0$$

which admits a non-trivial solution only if:

$$(K^2 - K_0^2)(K_G^2 - K_0^2) = \left(\frac{2m}{\hbar^2} \right)^2 V(\vec{G})V(-\vec{G}) \quad (12)$$

holds true. This secular equation determines the internal wave vector in terms of $\vec{k}_0, V(0), V(\pm\vec{G})$.

Remark: It is instructive to notice that \vec{K}_0 of (10) is the vector length proper to the case when Bragg reflection condition 4) is not satisfied. The corresponding Schrödinger equation refers then to refraction only: the crystal is practically transparent for neutrons.

Since \vec{K} and \vec{K}_0 are supposed to be slightly different, the boundary condition suggests that $\vec{K} - \vec{K}_0$ should differ from \vec{k}_0 by an increment in the normal direction:

$$\vec{K} = \vec{k}_0 + k_0 \epsilon \vec{n} \quad (13)$$

\vec{n} is a unit vector perpendicular to the surface of the crystal and thus to \vec{G} as well. Then:

$$\begin{aligned} \vec{K}^2 &\sim k_0^2 + 2k_0^2 \epsilon \cos\theta_B = k_0^2(1+2\gamma) \\ (\vec{K} + \vec{G})^2 &\sim K^2 + G^2 + 2\vec{K}\vec{G} = (k_0^2 + G^2 + 2\vec{k}_0\vec{G}) + \\ &+ 2k_0^2 \epsilon \cos\theta_B = k_0^2(1+2\gamma) \end{aligned} \quad (14)$$

and the solution of (12) immediately follows:

$$\gamma = \epsilon \cos\theta_B = \frac{m}{\hbar^2 k_0^2} \{-V(0) \pm [V(\vec{G})V(-\vec{G})]^{1/2}\} \quad (15)$$

$$\gamma = \gamma_{\pm}, \quad \epsilon = \epsilon_{\pm}$$

It implies that the \vec{k}_0 incident plane wave generates in the crystal two internal plane waves in the forward direction $\vec{K}^+ = \vec{K}(\gamma_+)$ and $\vec{K}^- = \vec{K}(\gamma_-)$ respectively, and two internal waves in the diffracted direction \vec{K}_G^+ and \vec{K}_G^- respectively. Hence a complete internal wave generated in the crystal reads:

$$\psi(\vec{r}) = \sum_{\alpha=\pm} [u^{\alpha} \exp(i\vec{K}^{\alpha}\vec{r}) + u_G^{\alpha} \exp(i\vec{K}_G^{\alpha}\vec{r})] \quad (16)$$

where u^+, u^-, u_G^+, u_G^- are to follow from (11) and the boundary conditions.

Along the entrant surface we must have:

$$u_G^+ + u_G^- = 0 \quad u^+ + u^- = \phi \quad (17)$$

where we use the (almost a constant in the area of interest) previous amplitude notion ϕ instead of $u(\vec{r})$, to implement a plane wave approximation. Notice, that the diffracted wave is entirely born within the crystal.

By using a guess [8] with C^+ and C^- being real numbers:

$$u^+ = [C^- / (C^- - C^+)] \phi, \quad u^- = -[C^+ / (C^- - C^+)] \phi \quad (18)$$

$$u_G^+ = [C^+ C^- / (C^- - C^+)] \phi = -u_G^-$$

we realize that (17) gets reduced to identities, while in virtue of (11) which determines the ratios of amplitudes, we obtain:

$$\left[\frac{u(0)}{u(\vec{G})} \right]^2 = \frac{V(-\vec{G})}{V(0)} \frac{K_G^2 - K_0^2}{K^2 - K_0^2} \quad (19)$$

which, by (12) implies:

$$C^\pm = \frac{2m}{\hbar^2} \frac{V(\vec{G})}{(K_G^\pm)^2 - K_0^2} = \frac{\hbar}{2m} \frac{(K^\pm)^2 - K_0^2}{V(-\vec{G})} = \pm [V(\vec{G})V(-\vec{G})]^{1/2} / V(-\vec{G}) \quad (20)$$

We then continue the internal waves up to the rear (exit) side

of the crystal at which a superposition:

$$\begin{aligned} \psi(\vec{r}) &= V_0 \psi_0(\vec{r}) + V_H \psi_G(\vec{r}) \\ \psi_0(\vec{r}) &= \phi \exp(i\vec{k}_0 \vec{r}) \\ \psi_G(\vec{r}) &= \phi \exp[i(\vec{k}_0 + \vec{G}) \vec{r}] \end{aligned} \quad (21)$$

is to come out.

For the crystal of thickness D , we can express positions on the rear side by these on the entrant side:

$$\vec{r}_{out} = \vec{r}_{in} + D \vec{n} \quad (22)$$

where (17) refers to $\vec{r} = \vec{r}_{in}$.

Since $\vec{k} = \vec{k}_{||} + \vec{n} k_{\perp}$, $\vec{k}_{||}$ denoting a component of \vec{k} parallel to the crystal surface, the boundary conditions:

$$\psi^+(\vec{r}_{out}) + \psi^-(\vec{r}_{out}) = V_0 \psi_0(\vec{r}_{out}) \quad (23)$$

$$\psi_G^+(\vec{r}_{out}) + \psi_G^-(\vec{r}_{out}) = V_H \psi_G(\vec{r}_{out})$$

imply (see (13) and remember that $\vec{G} \parallel \vec{r}_{||}$):

$$\begin{aligned} u^+ \exp(iDk_0 \epsilon^+) + u^- \exp(iDk_0 \epsilon^-) &= V_0 \phi \\ u_G^+ \exp(iDk_0 \epsilon^+) + u_G^- \exp(iDk_0 \epsilon^-) &= V_H \phi \\ \vec{k}^\pm &= \vec{k}_{0||} + k_0 (\cos \theta_B + \epsilon^\pm) = \vec{k}_0 + k_0 \epsilon^\pm \vec{n} \end{aligned} \quad (24)$$

After accounting for (15), we can introduce another notation in (24):

$$Dk_0 \epsilon^\pm = -\sigma^\pm \delta, \quad \epsilon^\pm = (-\sigma^\pm \delta) / Dk_0$$

$$\sigma = \frac{mDV(0)}{k_0^2 \cos \theta_B}, \quad \delta = \frac{mD}{k_0^2 \cos \theta_B} V(\vec{G}) V(-\vec{G})^{1/2} \quad (25)$$

so that:

$$u^+ \exp(i\delta) + u^- \exp(-i\delta) = V_0 \phi \exp(i\sigma) \quad (26)$$

$$u_G^+ \exp(i\delta) + u_G^- \exp(-i\delta) = V_H \phi \exp(i\sigma)$$

via (18) implies:

$$V_0 = \cos \delta + i \frac{c^- + c^+}{c^- - c^+} \sin \delta \exp(-i\sigma) \quad (27)$$

$$V_H = 2i \frac{c^+ c^-}{c^- - c^+} \sin \delta \exp(-i\sigma)$$

In virtue of (20) we have finally:

$$V_0 = \cos \delta \cdot \exp(-i\sigma) \quad (28)$$

$$V_H = i \sin \delta \frac{[V(\vec{G}) V(-\vec{G})]^{1/2}}{V(-\vec{G})} \exp(-i\sigma)$$

Since $V(\vec{G})$ and $V(-\vec{G})$ come from the Fourier expansions, by equating $V(\vec{G}) = |V(\vec{G})| \exp(i\alpha)$ we find $V(-\vec{G}) = |V(\vec{G})| \exp(-i\alpha)$, and so:

$$V_H = i \sin \delta \exp(i\alpha - \sigma) \quad (29)$$

which implies a normalization formula:

$$|V_0|^2 + |V_H|^2 = 1 \quad (30)$$

unavoidably necessary in case of the no-absorption map:

$$\phi \exp(i\vec{k}_0 \vec{r}) \rightarrow \phi [V_0 \exp(i\vec{k}_0 \vec{r}) + V_H \exp(i(\vec{k}_0 + \vec{G}) \vec{r})] \quad (31)$$

which is to represent the beam splitting induced by the diffracting crystal. Notice that (20) implies a surprisingly simple result:

$$u^+ = \frac{1}{2} \phi = u^-, \quad u_G^+ = -u_G^- = \frac{\phi}{2} \frac{[V(\vec{G}) V(-\vec{G})]^{1/2}}{V(-\vec{G})} = \frac{1}{2} \exp i\alpha \quad (32)$$

$$\psi_{\text{forw}}(\vec{r}) = \frac{\phi}{2} [\exp(i\vec{k}^+ \vec{r}) + \exp(i\vec{k}^- \vec{r})] =$$

$$= \frac{\phi}{2} [\exp(i\vec{k}_0 - \vec{n}_D^{\sigma} \vec{r}) \cdot [\exp(i\vec{n}_D^{\delta} \vec{r}) + \exp(-i\vec{n}_D^{\delta} \vec{r})]] =$$

$$= \phi [\exp(i\vec{k}_0 - \vec{n}_D^{\sigma} \vec{r}) \cdot \cos(\frac{\delta}{D} \vec{n} \vec{r})]$$

$$\psi_{\text{diff}}(\vec{r}) = i\phi \exp(i\alpha) [\exp(i\vec{k}_0 + \vec{G} - \vec{n}_D^{\sigma} \vec{r}) \sin(\frac{\delta}{D} \vec{n} \vec{r})]$$

$$\psi(\vec{r}) = \psi_{\text{forw}}(\vec{r}) + \psi_{\text{diff}}(\vec{r})$$

By computing the squared modulus of the above internal crystal wave field, we realize that the obtained intensity has a trivial nodal set (no true repelling surfaces for the stochastic diffusion). Hence a local representation of this wave-field in terms of the stochastic flow and its random paths is a priori possible within the diffracting crystal.

3. Plane waves and wave packets in quantum mechanics

As observed in (44) there is a fundamental difficulty linked to the physical interpretation of plane waves, which however is simply disregarded both in quantum mechanical text-books and in research papers (neutron interferometry is a good example). The plane wave ansatz (1) is not quite realistic if compared with the experimental situation, where [4] monochromatic neutrons are injected successively into the crystal. Such neutrons, if in a free flight, should pass a mean distance L during the transit time $T=L/v$, where a typical velocity value is about 2000 m/s. It implies that in statistical terms, we must describe a probability distribution which at time T is peaked (concentrated) about certain \vec{R}_0 , while at a later time $T+t$ is peaked about a new space location $\vec{R}=\vec{R}_0+\vec{v}t$.

Obviously such a picture has nothing to do with plane waves and their predicted everywhere the same probability density. We did not even mention their much more serious defect of not belonging to the Hilbert space, hence precluding their realistic probabilistic interpretation.

Obviously properly weighted superpositions of plane waves give rise to Hilbert space wave packets, and the wave packet which is quite appropriate for the experiments of interest is the minimum-uncertainty one. If in free propagation it reads

$$\psi_{\vec{q},\vec{p}}^+(\vec{r},t) = \frac{1}{(\pi\Delta^2)^{3/2}} \frac{1}{(1 + \frac{i\hbar t}{m\Delta^2})^{3/2}} \exp\left\{-\frac{1}{(2\Delta^2 + \frac{2i\hbar t}{m})} (\vec{r} - \vec{q} - \frac{\vec{p}}{m}t)^2\right\} \exp\left\{\frac{i}{\hbar} \vec{p} \cdot [\vec{x} - \vec{q}(t) + \frac{\vec{p}t}{2m}]\right\}$$

$$\vec{q}(t) = \vec{q} - \vec{p}t/m \quad (33)$$

The initial half-width of the packet is Δ , and it is initially peaked about phase space point (\vec{q},\vec{p}) . While evolving in time it spreads out, but at a later time it is still peaked about a point $\vec{q}(t)=\vec{q} - \frac{\vec{p}}{m}t$. It follows from [17] that in case of neutrons, the velocity dispersion equals $\Delta_v \sim 10\text{m/s}$, if the spatial dispersion is $\Delta \sim 10^{-2}\text{m}$. Experimentally produced beams are collimated to about such a size [8], hence the wave packet spreading can be safely disregarded on the time scale $T \leq 10^3\text{s}$. It implies that the "frozen" Gaussian is a proper fit instead of (32):

$$\psi_{\vec{q},\vec{p}}^+(\vec{r},t) = \frac{1}{(\pi\Delta^2)^{3/2}} \exp\left\{-\frac{1}{2\Delta^2} (\vec{x} - \vec{q} - \frac{\vec{p}}{m}t)^2\right\} \exp\left\{\frac{i}{\hbar} \vec{p} \cdot (\vec{x} - \vec{q} - \frac{\vec{p}t}{2m})\right\} = \phi_{\vec{q},\vec{p}}^+(\vec{x},t) \exp\left\{\frac{i}{\hbar} \vec{p} \cdot (\vec{x} - \vec{q} - \frac{\vec{p}t}{2m})\right\} \quad (34)$$

Since in our case $\vec{p}=\hbar\vec{k}$, $|\vec{k}|=k=2\pi/\lambda \sim 10^{10}\text{m}^{-1}$, and the typical slab thickness is [10] $D \sim 0,3\text{cm}$, when considering the situation in the slab area the space - dependent Gaussian factor can be safely replaced by a constant, at least if compared with the rapidly varying phase factor, whose oscillation interval equals λ .

It is thus a point at which we can replace the moving in space Gaussian wave packet by a plane wave: the packet gets entirely frozen at the time when the wave packet centroid enters the crystal. And this instantaneous freezing trick allows to save the standard belief that $\exp(-i\vec{k}\vec{r})$ plane wave "represents" a propagation in the positive or negative \vec{k} direction, because a wave packet attached to it does so.

One must however remember that the group velocity of the Gaussian wave $\vec{v} = \frac{\vec{E}}{m}$ which refers to the mean particle velocity is twice the phase velocity of the pertinent plane wave. The citation from (44) should clarify the issue: "in the quantum mechanical case... it is fundamentally misleading to look at $\exp(i\vec{k}\vec{r} - i\omega(k)t)$, $\omega(k) = \hbar k^2/2m$ as a travelling wave". Contrary to the classical theory where $\exp(\dots)$ would be replaced by $\cos(\vec{k}\vec{r} - \omega(k)t)$ i.e. a genuine travelling wave, in quantum theory plane waves refer to stationary (generalized) states, and as such have much more in common with standing waves.

4. Beam recombination

While employing "frozen" wave functions, and confining the analysis of diffraction by a crystal to $\Delta \sim 10^{-2}$ m beams, we can take advantage of the previous plane wave analysis.

Let $\psi_{\vec{q}, \vec{p}}^+(\vec{r}, 0)$ with the centroid coordinate $\vec{q} = 0$ be a representation of the neutron beam at the entrant side of slab I, at the time instant $t=0$. The mean passage time of neutrons through the slab is incomparably shorter than the transit time between neighboring slabs. Thus we shall keep the Gaussian probability, density time independent as well (in addition to neglecting its variability). Thus we begin with:

$$\phi \rightarrow \frac{1}{(\pi\Delta^2)^{3/2}} \exp\left(-\frac{\vec{r}^2}{2\Delta^2}\right) = \phi_{0,0}(\vec{r}, 0) \quad (35)$$

The neutron beam while on leave from slab I is represented by a superposition of two minimum-uncertainty wave packets, both initially peaked about $\vec{q} = 0$, but with diverging momenta: $\vec{p}_0 = \hbar\vec{k}_0$

and $\vec{p}_G = \hbar(\vec{k}_0 + \vec{G})$ respectively. They are next supposed to propagate freely until slab II is reached. Since $|\vec{k}_0| = |\vec{k}_G| = mv/\hbar$, after time $T = (\vec{r}_B - \vec{r}_A)/v = (\vec{r}_C - \vec{r}_A)/v$ the centroids of our wave functions reach slab II at positions \vec{r}_B, \vec{r}_C respectively. Their separation is of about $5 \cdot 10^{-2}$ m, hence definitely macroscopic. In this case, even for not very sharply peaked Gaussians, their overlap is negligible, and propagation through the crystal of the two diverging beams can be considered separately:

$$|\psi(\vec{r}, t)|^2 \sim |V_0|^2 |\phi_{\vec{r}_B, 0}(\vec{r}, 0)|^2 + |V_H|^2 |\phi_{\vec{r}_C, 0}(\vec{r}, 0)|^2 \quad (36)$$

The time dependence is here absorbed in the new positions of centroids, hence by using them as reference points of the new coordinate system (related to each wave separately) relative coordinates can be used, and thus all previous beam splitting discussion applies without any modifications.

Notice that integrating (36) over R^3 we recover the meaning of the normalization identity (23).

If instead of slab II, counters would be introduced in proper positions (i.e. about \vec{r}_B and \vec{r}_C respectively), the relative frequencies obtained should converge to counting probabilities:

$$p_0 = |V_0|^2 \int d^3r |\phi_{\vec{r}_B, 0}(\vec{r}, 0)|^2 = |V_0|^2 = \cos^2 \delta$$

$$p_H = 1 - p_0 = \sin^2 \delta$$

$$\delta = \frac{mD|V(\vec{G})|}{\hbar^2 k_0 \cos \theta_B} \quad (37)$$

Let us turn to the slab II diffraction of each beam separately.

After splitting, the forward fraction of the incident \vec{k}_0 beam is sent away (and eventually registered). The same pertains to the forward fraction of the $(\vec{k}_0 + \vec{G})$ beam. They get eliminated from further processing.

At the rear side of slab II we are thus left with widely separated (but now moving in convergent directions) partial beams, whose mathematical representation reads (we again disregard the transit time through the crystal):

$$\begin{aligned} \psi_{II}(\vec{r}, t) = & V_H V_0 |\phi_{\vec{r}_B, 0}(\vec{r}, 0)| \exp \frac{i}{\hbar} \vec{p}_G \cdot (\vec{r} + \frac{\vec{p}_G T}{2m}) + \\ & + V_{-H} V_H |\phi_{\vec{r}_C, 0}(\vec{r}, 0)| \exp \frac{i}{\hbar} \vec{p}_0 \cdot (\vec{r} + \frac{\vec{p}_0 T}{2m}) \end{aligned} \quad (38)$$

The coefficient V_{-H} indicates that we have split the beam incident with momentum \vec{p}_G , and preserved its (here diffracted) component \vec{p}_0 . Since it arises by referring to $-\vec{G}$ instead of \vec{G} , we have:

$$V_{-H} = i \sin \delta \exp -i(\alpha + \epsilon) \quad (39)$$

The sent away components correspond to intensities V_0^2 (\vec{p}_0 direction) and $V_H V_0$ (\vec{p}_G direction).

Would we allow the beam to propagate freely in time (take time interval $3T$ or $4T$ the arising wide separation of the four Gaussian components would allow to compute the counting probabilities

$$\begin{aligned} P_{II} + P_{lost} &= 1 \\ P_{II} &= |V_H V_0|^2 + |V_{-H} V_H|^2 = \sin^2 \delta \cos^2 \delta + \sin^4 \delta = \sin^2 \delta \\ P_{lost} &= P_{lost}^0 + P_{lost}^H = |V_0|^2 + |V_0 V_H|^2 = \cos^2 \delta \end{aligned} \quad (40)$$

Since we can in principle measure P_{lost}^0 and P_{lost}^H by introducing the additional counters, the previous analysis allows for the following conclusion: neutrons arriving at slab III come from two widely separated directions with probabilities $p(\vec{p}_G) = |V_H V_0|^2 = \sin^2 \delta \cos^2 \delta$ and $p(\vec{p}_0) = |V_H V_{-H}|^2 = \sin^4 \delta$ respectively, with $p(\vec{p}_G) + p(\vec{p}_0) = P_{II}$.

Let the incident wave function at slab III be given by:

$$\begin{aligned} \psi_{III}^{in}(\vec{r}, t) = & V_H V_0 |\phi_{\vec{r}_D, 0}(\vec{r}, 0)| \exp \frac{i}{\hbar} \vec{p}_G \cdot (\vec{r} + \frac{\vec{p}_G t}{m}) + \\ & + V_H V_{-H} |\phi_{\vec{r}_D, 0}(\vec{r}, 0)| \exp \frac{i}{\hbar} \vec{p}_0 \cdot (\vec{r} + \frac{\vec{p}_0 t}{m}) \end{aligned} \quad (41)$$

It is peaked about \vec{r}_D and the time interval $2T$ has passed to allow for neutron migration from \vec{r}_A to \vec{r}_D .

By linearity of the Schrödinger equation, we can still analyze beam splitting of each incoming beam separately.

But then the superposition must be formed:

$$\begin{aligned} \psi_{III}^{out}(\vec{r}, t) &= \psi_{III}(\vec{r}, t) = \psi_0(\vec{r}, t) + \psi_H(\vec{r}, t) \quad (42) \\ \psi_0(\vec{r}, t) &= 2V_{-H} V_H V_0 |\phi_{\vec{r}_D, 0}(\vec{r}, 0)| \exp \frac{i}{\hbar} \vec{p}_0 \cdot (\vec{r} + \frac{\vec{p}_0 t}{m}) \\ \psi_H(\vec{r}, t) &= (V_H^2 V_{-H} + V_0^2 V_H) |\phi_{\vec{r}_D, 0}(\vec{r}, 0)| \exp \frac{i}{\hbar} \vec{p}_G \cdot (\vec{r} + \frac{\vec{p}_G t}{m}) \end{aligned}$$

Letting the split wave to evolve freely, we get a spatial separation of the 0 and H beam due to which counting probabilities for each direction follow (one should be warned at this point that the use of plane waves in fact precludes any idea of spatial localisation of the subbeams in the above, and what one has on mind is the plane wave approximation of the realistic wave packets in not too extended spatial areas):

$$P_0 = \int d^3r |\psi_0(\vec{r}, t)|^2 = 4 |v_{-H} v_H v_0|^2 = 4 \cos^2 \delta \sin^4 \delta$$

$$P_H = \int d^3r |\psi_H(\vec{r}, t)|^2 = \sin^2 \delta (-\sin^2 \delta + \cos^2 \delta)^2 = \sin^2 \delta - p_0 \quad (43)$$

Remark : All our considerations in the present section are based on drastic simplifications, which cannot reveal the whole complexity of wave phenomena induced in the diffracting crystal. They might serve as local approximations of true wave fields only. As example, the misset Bragg angle leads to exciting the nontrivial wave field in the whole Borrmann fan⁽⁴⁵⁾ so that the plane wave formula (32) is essentially modified. We must insert to (16) the following functions:

$$\vec{K}^\pm = \vec{k}_0 - \vec{N}^\pm \quad \vec{K}_G^\pm = \vec{K}^\pm + \vec{G}$$

$$\vec{N}^\pm = \frac{1}{\cos \Theta_B} \left[\gamma_0 - \frac{1}{2} \beta \pm \frac{1}{2} (\beta^2 + 4\gamma^2)^{1/2} \right] \vec{n} \quad (44)$$

where $\gamma_0 = v_0/2k_0$ and $\gamma^2 = \gamma_G \gamma_{-G}$ while the crystal misset angle enters $\beta = k_0 \Delta \theta \sin 2\Theta_B$.

The wave amplitudes are:

$$u^+ = \frac{1}{2} \frac{\beta + (\beta^2 + 4\gamma^2)^{1/2}}{(\beta^2 + 4\gamma^2)^{1/2}} \phi \quad u^- = -\frac{1}{2} \frac{\beta - (\beta^2 + 4\gamma^2)^{1/2}}{(\beta^2 + 4\gamma^2)^{1/2}} \phi \quad (45)$$

$$u_G^+ = \frac{\gamma_G}{(\beta^2 + 4\gamma^2)^{1/2}} \phi \quad u_G^- = \frac{\gamma_{-G}}{(\beta^2 + 4\gamma^2)^{1/2}} \phi$$

These plane waves should next be integrated with a proper momentum space distribution to form the wave packet. Dynamical diffraction theory was formulated in⁽⁴⁶⁾ for Gaussian wave packets.

Beam recombination and interference phenomena: standard understanding

It is conventionally argued that the measurable interference phenomenon appears if a phase difference between the recombined beams is somehow produced, prior to superposing them in slab III. Since in the interferometer neutrons which follow routes ABD (I) or ACD (II) achieve a macroscopic separation of about 5 cm, different phase shift operations can be adopted with respect to e.g. beam I with either completely negligible or controllable effect on the other beam.

Let beam I be shifted in phase: in case of Gaussian packets their centroids suffer simultaneously spatial shifts [8] but this effect is negligible against the phase change. Then the formula for the incident wave at slab III should be modified:

$$v_H v_0 + v_H v_0 \exp(i\phi) \quad (1)$$

which in turn implies

$$2v_H v_{-H} v_0 + v_H v_{-H} v_0 (1 + \exp(i\phi))$$

$$v_H^2 v_{-H} + v_0^2 v_H + v_H^2 v_{-H} + v_0^2 v_H \exp(i\phi) \quad (2)$$

The corresponding probabilities attributed to the outgoing beams read then

$$P_0^\phi = 2(1 + \cos\phi) \cos^2 \delta \cdot \sin^4 \delta = \frac{1}{2}(1 + \cos\phi) P_0$$

$$P_H^\phi = \sin^2 \delta |-\sin^2 \delta + \cos^2 \delta \exp(i\phi)|^2 = \sin^2 \delta - P_0^\phi \quad (3)$$

thus showing a cosine modulation which is characteristic for wave interference: P_0^ϕ can take any value from the interval $[0, P_0]$.

It thus results in the definite destructive interference pattern: the mere phase change of beam I results either in a partial or even in a complete ($\phi=\pi$) reduction of a counting rate at the 0 - detector. In the latter case $p_0^\pi=0$ and all incoming neutrons are transmitted by slab III into the H - counter.

Remark: The experimental data show a full range cosine modulation of counting rates, but these oscillations occur about a relatively high treshold: the 0-channel is never completely closed for neutrons. This incongruency of observations with the theoretical predictions up to the author's knowledge was never under serious debate, except for mentioning [4] that the non-existence of the complete beam modulation (down to 0) may be perhaps attributed to various imperfections of the crystal, the phase shifting material or the neutron beam itself (which is never purely monochromatic).

Let us confine attention to the ideal case (3). A serious conceptual problem arises here from the experimental data:

- (1) Each single neutron accomplishes its route through the interferometer before the next one is born in the arrangement
- (2) Due to a macroscopic separation of routes I and II, we are allowed to implant phase shifting devices so that their effect on beam I neutrons reduces to zero on beam II route
- (3) Neutrons arriving at either 0 or H counter, in the absence of phase shift, come at random from either I or II channel. What does destroy this random pattern, when a phase shift is induced?

A difficulty with the understanding of (3) and generally of the interference phenomenon is still under debate [1-4,12-15] see also [21-23]. Rather typical argument [14,21,3] used in this context, tells us that in the double slit experiment, due to its particle character the photon (neutron, electron) always passes through one of the slits. However, in order to explain the interference pattern it seems necessary to assume that the photon (electron, neutron) or at least its (their) wave function has traveled along both paths. Anyway in the area of interference the particle must have an information ("know") about what has happened along both paths [3,4,21,23]. At this point it is reasonable to invoke again Lande's criticism. But we have much stronger argument in hands. Namely in the stochastic formulation of quantum mechanics, the dynamics is entirely due to a stochastic differential equation. In case of a Markov process (applicable to a wide class of phenomena) there is no memory of the past involved in the stochastic particle motion. In fact while following a sample path, at no space point a particle itself can "remember" of which direction it came from. Moreover, it is as likely to continue or to change abruptly its direction of motion due to a random influence of the environment. It thus appears that the realistic phenomena to be accounted for, are related to an interaction of the consecutively arriving single neutrons with the crystal lattice, in a reproducible series (sampling) of performances. But then instead asking "how does the neutron know" we are enforced to ask what in reality happens in the diffracting crystal.

Plane waves versus individual particles: Alternative interference scenario, or what can be saved from Buonomano's hypothesis?

According to our previous discussion the plane wave notion $\exp(i(\vec{k}_0 \vec{r} - \omega t))$ appears as a local approximation of the traveling wave function:

$$f(\vec{r} - \frac{\hbar}{m} \vec{k}_0 t) \exp(i(\vec{k}_0 \vec{r} - \omega t)) \quad \text{where} \quad |f(\vec{r} - \frac{\hbar}{m} \vec{k}_0 t)|^2$$

stands for a Gaussian probability density. Its variability with \vec{r}, t is considered negligible against rapid oscillations of the plane wave factor in the areas (crystal) of interest.

Since in all our manipulations it is $\int d^3r |f(\vec{r} - \frac{\hbar}{m} \vec{k}_0 t)|^2 = p_f$ which refers to the probability with which the f-beam excites the detector (counter), hence the Gaussian probability density informs us about a distribution of individual particle members of the f-beam in space. Thus the phase factor must definitely play another role.

It is rather customary to attribute a plane wave to a single particle in quantum mechanics, and we find it consistent with the previous analysis.

However a plane wave cannot describe a single dot on a photoplate or a single click in the counter. The relevant probabilistic information comes from the definite state preparation procedure and is thus given (if we confine attention to pure states) in $|f(\vec{r} - \frac{\hbar}{m} \vec{k}_0 t)|^2$.

Nelson's approach is unique in attributing a physical meaning to space-time variability of phase factors, and the role of such (usually plane wave) factors becomes really unquestionable when passing to a description of individual stochastic (sample) trajectories, see e.g. at the computer simulations (47).

Another computer simulation (48) links Wilson chamber tracks with the plane wave as a symbolic description of the corresponding random medium (call it a background field as Nelson does). It suggests that plane waves really apply to description of particle motion through a gas, liquid or another structureless (albeit perhaps not too dense) material body.

As mentioned before such understanding of quantum mechanical plane wave instead referring to a single particle, refers rather to random response of the environment on the presence of momentum \vec{p} particle in it.

Pursuing this line of thought, the wave field in the crystal (slab I, incident beam splitting) describes again a random response of (this time structured) the material body on being penetrated by the incident \vec{k}_0 neutron.

Slab II discussion essentially exploits the above feature, but we supplement it by the assumption that a macroscopic spatial separation, in virtue of crystal internal excitation noise is capable of destroying any communication (correlation interference) between random fields active in the beam splitting areas. Thus the random field response of the crystal to the incident neutron has definitely a localized character.

The situation at slab III is critical for the understanding of what a quantum mechanical superposition principle really means.

To implement interference theoretically, we have followed tradition with the wave function continued to the overlap area along path I and path II simultaneously. But this procedure is in fact a rather subtle ansatz, since we know very well what is a random response of the crystal to the \vec{k}_0 neutron.

We know as well how the $\vec{k}_0 + \vec{G}$ beam would be split by the crystal. The superposition of the phase shifted wave with unshifted bears features of the simultaneous presence of the \vec{k}_0 and $\vec{k}_0 + \vec{G}$ neutrons in the crystal, which is never the case during neutron interferometry experiments. Our possible explanation is based on the following hypothesis (Buonomano (49)):

each single neutron while travelling through a crystal apart from being randomly perturbed along its flight through lattice potentials leaves behind an imprint of its flight and perturbations.

One should not forget that we follow at this point the Wilson chamber intuitions. The life-time of the neutron imprint in the crystal is certainly finite but as show the experimental data of the size $\sim 10^{-7}$ s at least.

If a single neutron enters the crystal, its random guide through it is plane wave. If after sufficiently short time another member of the coherent beam penetrates the crystal, the random response of the crystal depends on what kind of field is still in existence and what kind of random response induces the newly born neutron itself.

It means that neutrons do not literally interfere with themselves. Rather random fields induced by migrating neutrons do interfere. It at least justifies the use of plane wave superpositions like this related to slab III.

The finite life-time of the neutron imprint in the crystal combined with the obvious probabilistic arguments allows to predict that:

there is always a non-zero probability of neutron transmission to both O- and H counters even if the ideal phase difference

($\phi = \pi$) is implemented. The interesting feature of interference experiments is the relatively high counting threshold about which the phase dependent oscillations are seen, and for which no convincing explanation exists in the literature: most people believe that low neutron fringe visibility comes from the difficulty of the experiments background counts and the partial coherence of neutrons.

Remark 1: The ideal case considered previously shows that neutrons come from the phase shifter with the probability (relative to the whole beam) $|V_H V_0|^2 = \sin^2 \delta \cos^2 \delta$, while these from the \vec{k}_0 direction with the probability $\sin^4 \delta$. Depending on the particular value of δ they may substantially differ.

As a result in any sequence of single neutron flights through the interferometer, there may arise a relatively long series of beam I neutrons which is intermitted by either single or relatively short series of beam II neutron arrivals to slab III. If the time intervals between single neutron emissions are comparable with the excitation (trail in the crystal) life-time, it is obvious that a significant fraction of $\vec{k}_0 + \vec{G}$ neutrons gets diffracted by the crystal slab III according to the $\vec{k}_0 + \vec{G}$ rule i.e. with the outgoing \vec{k}_0 and $\vec{k}_0 + \vec{G}$ neutrons, irrespective of what a phase shift is.

Remark 2: Investigations of the longitudinal coherence [8] show a significant reduction of the interference contrast (amplitude of cosine oscillations of the counting rates gets lowered) with the growth of the thickness of the phase shifting material. Since phase shift of the wave packet is always accompanied by a spatial shift of its centroid, it implies a delay of the phase shifted neutrons compared to the normal transit time. In statis-

tical terms this phenomenon can be interpreted in terms of the finite life-time of neutron trails in the crystal. The original explanation of the phenomenon [8] refers to the decreasing overlap of the interfering wave packets.

There is an isolated attempt (49) to understand particle aspects of interference in terms of crystal memory effects. However this non-ergodic approach to quantum mechanics allows the interference to happen only after a sufficient number of neutrons has travelled through the interferometer (memory accumulation). Recent experiment (50) provides a convincing dismissal of the memory accumulation ansatz. However the remaining part of the Buonomano's scenario is the emergence of the memory effect itself.

From purely mathematical viewpoint Nelson's stochastic mechanics shows an exact equivalence with the well established Schrödinger equation formalism. However stochastic mechanics is unique in allowing in a consistent way to study the individual particle propagation (stochastic sample paths) and so to address the particle aspects of quantal wave phenomena (e.g. interference and diffraction). Moreover as shows the analysis of [23,37] it adds to the standard quantum formalism new observables (like first hitting times) which could not be even imagined in the standard approach. Although it is consistent with the standard interference scenario (nice discussion of the issue is given in (51)) it allows as well for the alternative picture based on the still remaining piece of the Buonomano's hypothesis:

the neutron while travelling through the crystal picks up its stochastic behaviour from the crystal (via unknown in detail

interactions with crystal lattice centres) and also leaves a trail in the crystal that allows the crystal to "remember" the phase of the neutron wave function. Although the life-time of the trail is certainly finite, it is responsible for the observed interference of low intensity beams: neutrons passing the interference region cannot interact (interfere) directly, but only in the indirect way - via memory effects in this region.

The above scenario can be subject to an apparent experimental verification (much more conclusive than in case of the dismissal of the report [12] about a possible destruction of the interference pattern for very low intensity photon beams). Namely in the standard setting used by Vienna group, neutrons come to the apparatus with the interval of about 0,2s. Since quite efficient neutron beam shutters are available, it is enough to repeat standard neutron interferometry experiments under the condition that:

- (1) approximately the same number of neutrons is registered (2000 or 3000) during the single exposition time
- (2) each experiment is repeated for a sequence 0,2s, 0,4s, 0,6s, 0,8s... of controlled intervals between the single neutron emissions to the apparatus.

The expected outcome is the definite decrease of the interference contrast (call it a destruction of the interference pattern) with the growth of the emission interval.

Unrealizable in case of photon interferometry [12], such controlled lowering of the neutron beam intensity is a technically feasible, but missing (50), decisive test against or in favour of the memory effect scenario for low intensity beam interference. Albeit current paradigms view it as unnecessary.

Acknowledgment:

The paper was in large part completed during my stay in Genoa. I would like to express my warm thanks to Professor Gianni Cassinelli for an inspiring hospitality there. The financial assistance of Istituto Nazionale di Fisica Nucleare is gratefully acknowledged.

I would like to thank Professor Johann Summhammer for correspondence on the paper and providing me with his recent experimental data, prior to publication.

References:

1. J. Summhammer, The physical quantities in the random data of neutron interferometry, Delphi Conf. talk, Oct. 1987
2. H. Rauch, Phys. Blatter, 41(1985)190
3. H. Rauch, J. Physique C3 Suppl. 45(1984)197
4. H. Rauch, in: Open questions in quantum physics, ed. G. Tarozzi A. van der Merwe, Reidel 1985
5. G. Badurek et al., Phys. Rev. Lett. 51(1983)1015, see also J. Phys. A 16(1983)1188
6. H. Rauch, et al., Phys. Lett. A 54(1975)425
7. M. P. Silverman, Eur. J. Phys. 1(1980)116
8. H. Kaiser et al., Phys. Rev. Lett. 50(1983)560, see also M. Arif et al., Phys. Rev. A 35(1987)2810
9. J. L. Standemann et al., Phys. Rev. A 21(1980)1419
10. V. F. Sears, Can. J. Phys. 56(1978)1261
11. A. G. Klein, S. A. Werner, Rep. Progr. Phys. 46(1983)259
12. L. Janossy, in: Cooperative phenomena, ed. H. Haken, M. Wagner, Springer 1973, see also Yu. P. Dontsov, A. I. Baz. Sov. Phys. JETP 25(1967)1, and R. L. Pfleeger, L. Mandel, Phys. Rev. 159(1967)1084
13. P. Grangier et al., Europhys. Lett. 1(1986)173, see also J. D. Franson et al., Phys. Rev. A 37(1988)2511
14. T. Hellmuth et al., Phys. Rev. A 35(1987)2532
15. P. Mittelstaedt et al., Found. Phys. 17(1987)891
16. R. G. Newton, Am. J. Phys. 48(1980)1029
17. G. Patsakos, Am. J. Phys. 44(1976)158
18. L. F. Abbott, M. B. Wise, Am. J. Phys. 49(1981)37, see also Y. Aharonov, M. Vardi, Phys. Rev. D 21(1980)2235
19. P. G. Merli et al. Am. J. Phys. 44(1976)306
20. D. Aerts, Found. Phys. 12(1982)1131
21. C. Dewdney et al. Lett. Nuovo Cim. 40(1984)481; see also Ref. 25
22. A. Lande, Am. J. Phys. 43(1975)701
23. E. Nelson, Quantum Fluctuations, Princeton Univ. Press, Princeton, 1985
24. J. P. Vigiier, Physica B 151(1988)386
25. J. P. Vigiier, Ann. der Phys. 7(1988)61
26. D. Bohm, B. Hiley, Physics Reports 172(1989)94
27. I. Gikhman, A. Skorokhod, Theory of Random Processes, vol. 3, in Russian, Nauka, Moscow, 1972
28. W. Horsthemke, R. Lefever, Noise-induced Transitions, Springer, Berlin, 1984
29. F. Guerra, Physics Reports 77(1981)263
30. E. Nelson, Phys. Rev. 150(1966)1079
31. J. Glimm, A. Jaffe, Quantum Physics: A Functional Integral Point of View, Springer, Berlin, 1981
32. S. Albeverio, R. Hoegh-Krohn, J. Math. Phys. 15(1974)1745
33. H. Rafii-Tabar, Phys. Lett. A 138(1989)353
34. N. Cufaro-Petroni, Phys. Lett. A, to appear
35. H. Risken, The Fokker-Planck Equation, Springer, Berlin, 1989
36. Ph. Blanchard, S. Golin, M. Serva, Phys. Rev. D 34(1986)3732
37. Ph. Blanchard, Ph. Combe, W. Zheng, Mathematical and Physical Aspects of Stochastic Mechanics, Lecture Notes in Physics vol. 281, Springer, Berlin, 1987
38. A. Kypriandis, contribution to this volume
39. R. Durran, A. Truman, Planetsimal Diffusions, Swansea Mth. College, preprint 1987
40. P. Garbaczewski, Phys. Rev. D 33(1986)2916
41. P. Garbaczewski, D. Prorok, Fortschr. Phys. 35(1987)771
42. P. Garbaczewski, D. Prorok, in: Stochastic Methods in Mathematics and Physics, Karpacz 1988, ed. R. Gielerak, W. Karwowski, World Scientific, Singapore 1989

- 43. C.G. Shull et al. Phys.Rev.Lett. 44(1980)1715, see also C.G. Shull, Phys.Rev.Lett. 21(1968)1585
- 44. B. Diu, Eur.J.Phys. 1(1980)231
- 45. S.A. Werner, A.G. Klein, Neutron Optics, in: Methods of Exp.Phys. 23A(1986)259
- 46. D. Petrascheck, Phys.Rev. B36(1987)6549
- 47. M. McClendon, H. Rabitz, Phys.Rev. A37(1989)3479
- 48. K. Yasue, J-C. Zambrini, Ann.Phys.(NY) 159(1985)99
- 49. V. Buonomano, A.F. Prado de Andrade, Found.Phys. 18(1988)401
- 50. J. Summhammer, Nuovo Cim. 103B(1989)265
- 51. E. Wichman, Quantum Theory, Berkeley Course vol.4, MacGraw Hill Book Co.

THE VALUE OF QUANTUM MECHANICS

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ABSTRACT

We may summarize our work stating that Quantum Mechanics is a practical partly irrational creation of the human mind. Such a creation is not univogue to the physical world of the microcosmos; there could be quite different formulations of Quantum Mechanics. Present day Quantum Mechanics allows us to dominate the microcosmos but does not quite present an ontological objective description of the same.

1. SCIENCE AND HUMAN BEINGS

Science is often defined as the universal agreement of all human beings on experimentally obtained knowledge.

It is essential that such knowledge be obtained by means of experiments, i.e., using measuring instruments.

The observable qualities are defined by the proper measuring instruments that are always instruments submitted to Classical Mechanics since they belong to the macroscopic world.

Inspiration plays no less a role in Science than it does in the realm of Art. It is a childish notion to think that a mathematician attains any scientifically valuable result by sitting at his desk with a ruler, calculating machines or other mechanical means. Both kinds of work require "frenzy" (in the sense of Plato "mania") and inspiration.

In contrast with these preconditions which scientific work shares with Art, Science has a fate that profoundly distinguishes it from artistic