Journal of Physics: Conference Series **2883** (2024) 012004 doi:10.1088/1742-6596/2883/1/012004

Quantum Neutron Scattering — Feynman Paths Information, Weak Values and Intensity Deficit Effect

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Abstract. The conventional theory of non-relativistic neutron beam scattering from many-body systems treats the beam essentially as a classical system, because the neutron dynamical variables are captured in the main theoretical formulas (e.g. time-correlation functions) not as quantum mechanical operators but as c-numbers only. This simplification results in the full decoupling of the probe particles' dynamics from the quantum dynamics of the scatterer. Further, neutrons' wavefunctions are represented with plane waves, and thus the concept of neutron's finite coherence length in momentum space becomes irrelevant. Making contact with modern quantum theoretical approaches (e.g., quantum entanglement, Feynman paths, "which-path information" versus interference, Weak Values theory) new observable effects of non-relativistic quantum beam scattering may be exposed and/or predicted, such as a surprising intensity deficit in neutron Compton scattering (NCS) of epithermal neutrons from protons of H-containing materials. Here, the NCS-intensity deficit observed in scattering from liquid C_6H_6 is discussed and interpreted from first principles, in the general frame of Weak Values theory. Moreover, based on Feynman's didactical argument that there isn't any interference between distinguishable neutron paths, we show that this NCS-effect cannot be interpreted as being caused by destructive interference of neutron paths scattered from entangled (two or a few) protons, as was earlier proposed by some authors.

1 Introduction

The well established particle-wave dual nature of a quantum object, also known as complementarity, allows for various (often strange appearing) quantum correlation and interference phenomena, like e.g. the "bomb detection" method in a Mach-Zehnder interferometer (MZI) and the associated interaction-free measurement (IFM) method discovered by Elitzur and Vaidman [1]. A striking quantum phenomenon is *quantum entanglement* (QE) – the most debated aspect of quantum mechanics ever since the theory was formulated about 100 years ago. QE (see e.g. [2]) is the phenomenon that two or more particles can exist in a shared quantum state, regardless of how far apart they are. Einstein criticized QE as a "spooky action at a distance" and Schrödinger said it was quantum mechanics' most important trait; see e.g. [3, 4]. Nowadays QE is considered as the most important quantum resource [5] which quantum information science and the associated emerging new quantum technologies are based on; cf. [6, 7, 8].
In this paper, the focus is specifically on *non-relativistic* scattering of particles off many-body (or condensed matter) systems, with emphasis on *incoherent* (and inelastic) neutron scattering (INS) applying thermal or epithermal [9, 10] neutrons.

Here "incoherent" means that a neutron (or any other particle such as a photon, electron, or atom) collides and scatters from a single particle, such as a nucleus (or atom). When neutrons scatter from protons (often referred to as H-atoms), the scattering is predominantly incoherent due to the neutron-proton *spin-flip mechanism* involved in the collision process; see e.g. [9, 10, 11].
Importantly, this implies that the scattering process provides "which-path information" (see e.g. the textbook [12]), which identifies the scattering proton from all other potential scatterers in its environment. Consequently, this destroys any possible quantum interferences between different paths that the neutron could take in the scattering process.
For the purposes of the present paper, a very clear first-principles explanation of this effect — and of *coherent* versus *incoherent* scattering — can be found in the Feynman Lectures [13], in particular Sec. 3.3. For illustration, let us consider here the main point, which is as follows. Consider neutron scattering from a crystal consisting of atoms with nuclear spin 1/2, in particular the case that the neutron has spin-up and all the crystal nuclei have spin-down (before scattering). Due to the aforementioned spin-flip effect, this causes the *incoherent* part of the scattering process, which exhibits no sharp interference peaks in the scattered neutron beam — in contrast to the sharp peaks caused by coherent scattering (as e.g. in the well known case of Bragg scattering in X-ray crystallography). This spin-flip causes the aforementioned "which-path information", also called "which-way" or "welcher-Weg" information. Namely, the specific spin-flipped scattering nucleus (now having spin-up) is singled out from the other nuclei (still having spin-down). This is the generally valid quantum-mechanical cause that suppresses quantum interference phenomena. Feynman strongly emphasizes this phenomenon as follows ([13], p. 3-9):
"You may argue, "I don't care which atom is up." Perhaps you don't, but nature knows; and the probability is, in fact, what we gave above — there isn't any interference."
These considerations are clearly related to the intrinsic physical connections between the basic quantum-mechanical concepts of wave-particle duality, complementarity, uncertainty principle, and which-path knowledge versus interference. See e.g the discussions in Refs. [12, 14, 15, 16].
A few remarks regarding the paper's contents may be helpful.
Here, we emphasize the fact that conventional (neutron) scattering theory treats the neutron beam essentially as a classical (or semi-classical) system and usually as a plane wave [9, 10, 17, 18]. This limitation has certain severe theoretical and experimental consequences, which are examined here critically. In this context, the specific topics of impulsive (von Neumann, or strong) measurement and creation of QE caused by the scattering are considered, together with the more recent, basic concepts of Weak Value (WV) and Two-State Vector Formalism (TSCF). For associated references, the interested reader may be referred to [19, 20, 21, 22, 23, 24] and papers cited therein.
The experimental part concerns incoherent (and inelastic) neutron scattering (INS) with thermal and epithermal neutrons, which is a well established experimental technique, cf. [11]. In particular, we consider the experimental field of epithermal neutron scattering (i.e., in the energy transfer range 1-100 eV) which is commonly known as neutron Compton scattering (NCS) or deep-inelastic neutron scattering (DINS) [17, 18, 25, 26].
To show the experimental relevance of the theory, we consider in some detail a related concrete NCS-experiment (from liquid C_6H_6) that has no known interpretation within conventional theory, but which can be understood with the considered modern quantum theoretical approaches and concepts (here: QE, Feynman paths and which-path information versus quantum interference, neutron coherence length, and especially Weak Values). It will be shown that these concepts provide novel insights (i.e. beyond the limits of conventional theory) into the experimental topics under investigation.

2 Neutron beam as a classical system — Conventional theory

In the conventional (or standard) non-relativistic neutron scattering theory [9, 10, 11], quantum entanglement (QE) is nowhere explicitly mentioned, despite the fact that a neutron and the colliding nucleus are in general entangled after collision.
Namely, this always happens if the scattering interaction is strong enough, so that an initial not entangled two-body product state evolves into a linear superposition of final two-body states

$$|\psi_n\rangle \otimes |\phi_H\rangle \longrightarrow \sum_j c_j\, \psi_{n,j}\rangle \otimes |\phi_{H,j}\rangle \tag{1}$$

with amplitudes c_j $(j = 1, 2, ...)$ and $\sum |c_j|^2 = 1$. In general, this final state is entangled. This basic quantum-theoretical fact is not captured within conventional theory — which is consistent with the fact

that by definition there does not exist QE between a quantum object (the scatterer) and a classical one (neutron).
Moreover, the quantum degrees-of-freedom (DoF) of the neutron are not properly incorporated into the fundamental scattering formulas of the theory, such as the equation for the partial differential cross-section or the van Hove correlation functions. Instead, these formulas only involve classical quantities (c-numbers) referring to the neutron.
E.g. consider the basic formulas of the theory, e.g. the expression for the partial differential cross-section,

$$\frac{d^2\sigma_A}{d\Omega d\omega} = \frac{k_f}{k_i}\sigma_A S(\mathbf{Q},\omega) \tag{2}$$

$E = \hbar\omega$ is the energy transfer (from the neutron to the scatterer A); $d\Omega$ is the solid angle measured/covered by the detector; $\mathbf{k}_i$ and $\mathbf{k}_f$ are the initial and the final wave vectors of the scattered neutron; $\mathbf{Q}$ is the momentum transfer vector to the scatterer A due to the collision with the neutron, that is, $\mathbf{Q} = \mathbf{k}_i - \mathbf{k}_f$; and finally, σ_A is the scattering cross-section of A.

2.1 Some related physical considerations

$S(\mathbf{Q},\omega)$ is the so-called dynamic structure factor of the scattering system A, which contains dynamical variables of A only. I.e., the wave function of the neutron-A complete system contains dynamical variables referring to A only, but not to the neutron. Hence, here the neutron is essentially treated as a classical object, as no operator quantity appears here referring to any dynamical variable of the neutron. [Clearly, the scattering cross-section σ_A of the neutron-A collision process, and the initial (k_i) and final (k_i) wave vectors of the impinging and scattered neutron are *c*-numbers.]
It can be shown that the formal reason for this is related to properties of the first Born approximation and the so-called Fermi's Golden Rule which the conventional theory is based on [9, 10, 17, 18]. As a consequence, the two systems (neutron and scattering system) are decoupled by definition.
Another detail to point out here is that that the typical quantum concept of the particle's (or beam's) finite coherence length, l_{coh} (especially in momentum space, see below) is also absent in the formalism of conventional neutron scattering theory. Indeed, the main Eq. 2 contains the values of the initial and final wave vectors only, which are considered as *plane waves* — another simplification of conventional theory.
Thus, the scattering process describes the scattering probability from an infinitely well defined state $\mathbf{k}_i$ to an accordingly precise final state $\mathbf{k}_f$. Of course, the actually observed quantity is the (double) average over the finite distributions of $\mathbf{k}_i$ and $\mathbf{k}_f$ related with a real experimental setup.
Moreover, the following crucial point made by conventional theory should be considered: According to standard quantum mechanics, there are no quantum interference effects between incoming particles (here, neutrons) with different wave numbers. Thus it might be natural to assume that there is no experimentally detectable difference between
(a) a wave packet with a given finite coherence length (i.e., a coherent superposition of waves with different wave numbers) and
(b) an incoherent classical ensemble of plane waves, i.e. waves with zero coherence length in momentum space.
This assumption is because every observable scattering quantity is expected to only depend on the square $|a(\mathbf{k})|^2$ of the $\mathbf{k}$-component of the incoming beam, and not on products $|a(\mathbf{k_1})a^*(\mathbf{k_2})|$ of components with different wave numbers ($\mathbf{k}_1 \neq \mathbf{k}_2$), where the asterisk indicates complex conjugation. This consideration is consistent with Dirac's famous remark in his textbook:
"...Each photon then interferes only with itself. Interference between two different photons never occurs."; see [27], p. 9.
Summarizing, in the frame of standard scattering theory it holds that an experimental problem is completely characterized by the classical wave number distributions of the incoming and outgoing particle (or photon) beams; structural details of the wave functions of the beam-particles are irrelevant, and thus also the coherence properties of these wave functions. Impinging and scattered neutrons are described by plane waves; see e.g. [9, 10, 11].

2.2 Further theoretical details

Some additional remarks on the validity of Eq. 2 are in order. In conventional theory, it holds

$$S(\mathbf{Q},\omega) = \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} \exp(-i\omega\, t)F(\mathbf{Q},t)\, dt \tag{3}$$

where $F(\mathbf{Q},t)$ is the so-called intermediate correlation function [28]

$$F(\mathbf{Q},t) = \frac{1}{N}\sum_{j,k}^{N}\langle \exp(-i\mathbf{Q}\cdot\mathbf{r}_j(0))\exp(i\mathbf{Q}\cdot\mathbf{r}_k(t))\rangle \tag{4}$$

Here, the operators $\mathbf{r}_j(t)$, with $j = 1, ...N$, represent the spatial positions, *in the Heisenberg representation*, of the particles of the N-body scattering system A with Hamiltonian H_A. (For simplicity of presentation, here it is assumed that these particles are identical.) $\langle ... \rangle$ represents an appropriate average over all N particles of A.
The unitary time evolution operator

$$U_A(t) = \exp(-\frac{i}{\hbar}H_A t) \tag{5}$$

defines the Heisenberg operators

$$\mathbf{r}_j(t) = U_A^\dagger(t)\mathbf{r}_j\, U_A(t) \tag{6}$$

where $\mathbf{r}_j \equiv \mathbf{r}_j(0)$. Note that $(j = 1, ...N)$ refers to the N-body system A, but not to the neutron. More explicitly, the neutron-system interaction Hamiltonian H_{nA} and the Hamiltonian of the free neutron H_n play no role in the scattering formalism.
The Heisenberg operators $\mathbf{r}_j(t)$ in Eqs. (4) and (6) are sometimes intuitively understood to be the positions of the scattering particles. [This is often done in so-called molecular dynamics simulations of atomic and molecular systems.] However, this is a crude oversimplification, because the unitary operator $U_A(t)$ is an N-body operator depending on the N-body Hamiltonian H_A. Consequently, all $\mathbf{r}_j(t)$ are (for $t \neq t_0$) not one-body, but N-body quantities, too. (The pathological limiting case of A consisting on N non-interacting atoms is irrelevant for the present paper.)
Moreover, it is crucial that the exact Hamiltonian of the *complete* neutron-system is not H_A but

$$H = H_A + H_n + H_{nA} \tag{7}$$

with obvious notations (n: neutron). Of course H contains DoF of the neutron, too.

3 Impulsive von Neumann measurement and some results of Weak Values theory

In WV-TSVF theory, the measurement process is characterized by an impulsive von Neumann interaction Hamiltonian [29], see below. This incorporates an observable for a pointer or measuring apparatus, whose wave function is denoted by $|\Phi\rangle$. That is, the pointer itself is also a quantum object.
The implementation of the von Neumann model, which describes an ideal impulsive interaction, is modeled by the two-body interaction Hamiltonian

$$H_{int} = g(t)\,\hat{M}\otimes\hat{A} \quad \text{with} \quad g(t) = g\delta(t-t_0) \tag{8}$$

where $\hat{M}$ is a dynamical variable of the pointer and $\hat{A}$ is the system's operator representing the physical quantity to be measured. $g(t)$ is a (small and real) coupling function, and t_0 specifies the time of the impulsive two-body collision. In an ideal measurement, $g(t)$ is nonzero only during a very short time interval—formally captured with the delta function— and thus the free Hamiltonians of the participating systems during this time period can be neglected.
The von Neumann measurement, also known as strong measurement, provides the eigenvalues of the measured observable. However, it simultaneously disturbs the measured system, resulting in a change of its initial state. The final state corresponds to an eigenstate of the operator representing the observable. Alternatively, by weakly coupling a measuring device to the system, a technique known as Weak Measurement (WM), it becomes possible to extract specific information while limiting the disturbance on the system induced by the measurement. As initially proposed by Aharonov and collaborators (see references cited in the Introduction), additional physical insights are unveiled when one selectively post-selects a specific outcome (or final state of the system under i.
Let the initial system-apparatus state, i.e. for $t < t_0$ be $\psi_i \otimes \Phi_i$. Due to the interaction, this evolves as follows:

$$\psi_i \otimes \Phi_i \rightarrow e^{-ig\hat{A}\otimes\hat{M}}\psi_i \otimes \Phi_i \tag{9}$$

For convenience, and as often done in theoretical papers, in the following derivations we temporarily put $\hbar = 1$. We also may write g instead of $g(t)$.

Then one post-selects (with a strong measurement) a specific final state of the system, say ψ_f. The experimental result is associated with the corresponding apparatus' final state, Φ_f, from which the measurement's result is determined. Φ_f is obtained by tracing out the dynamical variables of the system, i.e.,

$$\Phi_f = \langle\psi_f|e^{-ig\hat{A}\otimes\hat{M}}|\psi_i\rangle\Phi_i \tag{10}$$

In the following one considers the weak interaction limit (i.e., small g) and obtains through power expansion of the exponent:

$$\Phi_f \approx \langle\psi_f|1 - ig\hat{A}\otimes\hat{M}|\psi_i\rangle\Phi_i = \langle\psi_f|\psi_i\rangle(1 - igA^w\hat{M})\Phi_i \approx \langle\psi_f|\psi_i\rangle e^{-igA^w\hat{M}}\,\Phi_i \tag{11}$$

A^w is the WV of the system's observable $\hat{A}$. It is assumed that $\langle\psi_f|\psi_i\rangle \neq 0$. Thus the state of the measuring device evolves with an effective *one-body* Hamiltonian $\hat{H}_M = gA^w\hat{M}$, i.e.,

$$\Phi_i \to e^{-igA^w\hat{M}}\Phi_i \tag{12}$$

Thus the following interesting result is obtained: The pointer's dynamics displays information about the system only through the single number A^w, which is in general complex.

3.1 Von Neumann Hamiltonian for neutron scattering and WV of the system variable

For the following theoretical derivations we will make the specific choice $\hat{M} = \hat{p}$, i.e., the pointer's variable in the interaction Hamiltonian will be the neutron's momentum $\hat{p}$.
We will also need the variance of $\hat{p}$ in its initial (e.g., before scattering) pointer state

$$Var_p = \langle\Phi_i|\hat{p}^2|\Phi_i\rangle - \langle\Phi_i|\hat{p}|\Phi_i\rangle^2 \tag{13}$$

In the theoretical treatment of the experimental neutron scattering results presented below, it will be shown that the imaginary part $Im[A^w]$ of A^w is of particular interest. According to the general WV-TSVF theory, the pointer momentum after the interaction changes from $\langle p\rangle_i$ (its initial value) to

$$\langle p\rangle_f = \langle p\rangle_i + 2\,g\,Im[A^w]\,Var_p \tag{14}$$

(its final value) Note that Var_p refers to the apparatus (or pointer), and not the scattering system. Moreover, the real part of the weak value, $Re[A^w]$, is determined by the shifted position (x-shift) of the pointer, i.e.

$$\langle x\rangle_f = \langle x\rangle_i + g\,Re[A^w] \tag{15}$$

For full derivations and further explanations see e.g. [23, 22].
It will be shown that, in our investigations, the relevant WV entering the scattering process is purely imaginary. The physical significance of an imaginary WV was analyzed by Dressel and Jordan [24].

3.2 Neutron-proton collisional dynamics in NCS or DINS

Let now the system be a proton (H atom) of a many-body specimen, which scatters the impinging neutron.
For the system's dynamical variable we choose $\hat{X}$, which denotes the position operator of the hit nucleus (or H atom)
To simplify notation, we take the direction of momentum-transfer vector Q to be parallel to the x-axis of the laboratory system. Now the von Neumann impulsive interaction Hamiltonian reads

$$H_{int} = g\,\hat{p}\otimes\hat{X} \tag{16}$$

The sign of g is not specified yet.
Now one has to calculate the WV of the system variable $\hat{X}$, according to

$$X^w \equiv \frac{\langle\psi_f|\hat{X}|\psi_i\rangle}{\langle\psi_f|\psi_i\rangle} \tag{17}$$

Clearly, the explicit forms of the state vectors in configuration space are very complicated (and time dependent over a short time interval around the time t_0 of collision). So we may be able to perform a part of the calculation in the momentum space—as done in our earlier works [30, 31]. To do so, one has the replacement

$$\hat{X} \to -\frac{1}{i}\frac{\partial}{\partial \hat{P}} \tag{18}$$

(using here temporarily the common convention $\hbar = 1$), where $\hat{P}$ is the associated momentum variable of the quantum system. (Note that the fundamental commutation relation $[\hat{P}, \hat{X}] = 1/i$ is fulfilled.)
Let us now calculate the WV X^w in the momentum representation, making the usual assumption of the wave functions of initial and final states to be approximated by Gaussians, i.e having the form $G(P) = \exp(-P^2/2\sigma_P^2)$. σ_P refers to the initial state of the proton (i.e. before collision). This gives for the nominator

$$\begin{aligned}\langle\psi_f|\hat{X}|\psi_i\rangle &= (-1/i)\langle\psi_f|\frac{\partial}{\partial\hat{P}}|\psi_i\rangle = (-1/i)\langle G(P-Q)|\frac{\partial}{\partial\hat{P}}|G(P)\rangle \\ &= (-1/i)\,(-1/\sigma_P^2)\langle G(P-Q)|\hat{P}|G(P)\rangle \\ &= -i\,1/\sigma_P^2\,\langle\psi_f|\hat{P}|\psi_i\rangle \end{aligned} \tag{19}$$

The integral $\langle\psi_f|\hat{P}|\psi_i\rangle$ is exactly the same as the one that appeared in the calculation of the WV of momentum P in our earlier exploration of incoherent neutron scattering (INS) using thermal neutrons [30, 31]. Those calculations showed that P^w is real and positive. Thus we immediately arrive at the crucial (see below) result that X^w is *purely imaginary.*
Here, let us repeat the short calculation of P^w, see [30, 31]:

$$\begin{aligned} P_w &= \frac{\langle G_f|\hat{P}|G_i\rangle}{\langle G_f|G_i\rangle} = \frac{\int dP\, G(P-Q)_f P G(P)_i}{\int dP\, G(P-Q)_f G(P)_i} \\ &= +\frac{Q}{2} \end{aligned} \tag{20}$$

The value of the integral in the numerator follows immediately from the following facts: (a) the two functions G are positioned symmetrically around the middle point $\bar{P} = Q/2$ — one function is centered at 0, the other at Q; and (b) in this integral P is a linear factor. Note also that this result is independent of the width of the Gaussian G.
It should be noted that this integral, and thus P^w, will change with variations of the assumed shape (and width) of the final state G_f. E.g. in the impulse approximation (IA) of NCS, the final state of H is assumed to be a plane wave (at least approximately), due to large impulse transfers (say, $30 - 80$ Å in the experiment of Section 5).
It is important to point out the physical nature of the post-selected protonic state in the context of a conventional, standard NCS (DINS) experiment. Here, this post-selection is not done by some fictitious instrumentation, but just by the environment of the struck proton which of course is not as specific as in the above WV-theoretical remarks. (I.e., variations of the microscopic environment of the struck proton imply variations of the measured WV.) More detailed discussion of these issues is given in [30].
Thus we obtain from Eqs. (19) and (20)

$$X^w = -i\,1/\sigma_P^2\frac{Q}{2} \tag{21}$$

which is a negative imaginary number, (if the smallness parameter g is choosen positive). It may be noted that an imaginary WV is associated with the *backaction* of one system on the second, due to their interaction [24]. Again, the aforementioned remarks about the protonic final state imply corresponding variations of the factor $Q/2$ in this result for X^w.
Now we may apply the main result (14) of the WV-TSVF theory [23, 22]. By re-introducing explicitly the factor $\hbar$ in the expression for momentum transfer, $Q \to \hbar Q$, we obtain for the WV-*correction* to the conventionally expected pointer momentum,

$$[\langle\hat{p}\rangle_f - \langle\hat{p}\rangle_i]_{\text{WV-correction}} = -2\,g/\sigma_P^2\frac{\hbar Q}{2}\,Var_p \;= -g\,\hbar Q\frac{Var_p}{Var_P} \tag{22}$$

using the definition $Var_P = \sigma_P^2$. Note that $Q > 0$ since the neutron impinges on the system (initially at rest) along the positive x-axis and thus the momentum transfer on the scatterer is positive, $\hbar Q > 0$.

Journal of Physics: Conference Series **2883** (2024) 012004 doi:10.1088/1742-6596/2883/1/012004

This result contains the variances of both quantum participants (i.e. neutron and scatterer) in the collisional process. Eq. (22) predicts an "anomalous" momentum transfer deficit in the neutron-nucleus collision; see e.g. [30, 31, 32].
Already here let us stress the following result. In the plane-wave approximation of conventional theory, $Var_p = 0$ and thus the last equation implies that the derived WV-correction (or any related "anomaly") vanishes identically [30, 31, 32].

4 Intensity deficit in neutron Compton scattering from H-containing materials

In this section we consider exclusively the experimental method of neutron Compton scattering (NCS), and in particular an effect known as intensity deficit in the scattering from protons of H containing materials. Here it will be of crucial importance to take into account the value of some NCS characteristic parameters, i.e. the collisional time window, and the energy and momentum transfers involved.

4.1 Characteristic parameters of NCS (DINS)

In the context of NCS, which applies to so-called *epithermal* neutrons, the achieved momentum and energy transfers are large, i.e.

$$\Delta E \approx 1 - 100 \text{ eV} \qquad \text{and} \qquad |\mathbf{Q}| \approx 20 - 200 \text{ Å}^{-1} \tag{23}$$

As a consequence, here the so-called Impulse Approximation (IA) applies [18, 17]. Moreover, the time scale — often called "scattering time", τ_{sc} — characterizing the neutron-proton scattering dynamics is very short [17], i.e. about

$$\tau_{sc} \sim 100 - 1000 \text{ as} \tag{24}$$

(as: attosecond, 10^{-18} s). These physical parameters are provided at eVS-Vesuvio, the electron-Volt instrument of the neutron spallation source ISIS, Rutherford Appleton Laboratory, UK. These parameters are related as described by the theoretical result of Sears [18, 17]

$$\tau_{sc}\, |\mathbf{Q}| \langle v_0 \rangle \approx 1 \tag{25}$$

In this formula, $\langle v_0 \rangle$ is the root-mean-square velocity of the nucleus (here: proton) before collision, which of course depends on the system (material) under investigation. $\hbar\mathbf{Q}$ is the momentum transfer as already defined in the previous sections. Furthermore, it holds that τ_{sc} equals the t-width of the intermediate correlation function $F(\mathbf{Q}, t)$, Eq. (4), [17, 18].
In the IA, the scattering is assumed to be essentially incoherent, essentially meaning that each neutron scatters from a *single* nucleus—a single proton, in our case. Indeed, experimental determination of the energy transfer associated with the measured H-recoil peak shows that the mass of the struck H atom of the benzene-sample (see below) is equal to 1 a.m.u.—i.e., the neutron collides with a single proton.
For these reasons, the NCS (or DINS) method is applied to explore *single-particle* properties, and especially the *momentum distribution* of an atom in its initial state. Furthermore, this is supposed to reflect structural details of the Born-Oppenheimer potential V_{BO} acting on the struck atom *before collision* [17].
It may be noted that the original motivation to establish the NCS experimental method was the proposal by Hohenberg and Platzman [25] to measure the momentum distributions $n(p)$ of He atoms in the normal or superfluid liquid state of helium [17, 18].

4.2 WV interpretation of the intensity deficit effect

A surprisingly straightforward consequence based on the preceding theoretical derivations predicts, from first principles, the so-called *intensity deficit* effect for hydrogen, earlier observed in several neutron Compton scattering (NCS) experiments from various H-containing materials; see e.g. [33, 34, 35, 36] and papers cited therein.
To show this, it suffices to refer to the preceding general WV-theoretical result, Eq. (12), stated here again for convenience:

$$\Phi_i \to \Phi_f = e^{-igA^w \hat{M}} \Phi_i \tag{26}$$

In our specific case of NCS we made the specific choice $\hat{A} = \hat{X}$. The above obtained WV result for A^w implies $X^w = -i|Im[X^w]|$, and thus we obtain the surprising result

$$\Phi_i \to \Phi_f = e^{-g|Im[X^w]|\hat{M}} \Phi_i \tag{27}$$

This result is clearly outside the frame of conventional theory, since this short-time evolution of the struck system (here: proton) is *non-unitary.*
Now *assume* that g is positive, $g > 0$. (In the experimental section below it is shown that this assumption is consistent with the presented experiment). Then the exponential factor in the last equation *reduces* the norm of the pointer-state wave function after scattering,

$$||\Phi_f|| < ||\Phi_i|| \tag{28}$$

As already noted, this time evolution is non-unitary.
Now, in our case (see below) we are interested in the scattering intensity from protons (or H). On physical grounds, it is obvious that $\langle\Phi_f|\Phi_f\rangle$ is proportional to the scattering intensity (I_H) as measured by the pointer:

$$\langle\Phi_f|\Phi_f\rangle \propto I_H \tag{29}$$

In physical terms, this reduction of scattering intensity (due to the WV-effect under consideration) also implies that the transmission component of the impinging neutron beam should be correspondingly increased, since the sum of scattered and transmitted intensities must be equal to the initial beam intensity.
Finding (28) is sometimes criticized as being an artifact of the post-selection process, and not a true quantum dynamical effect, due to the fact that here the pointer operator $\hat{p}$ commutes with the interaction Hamiltonian H_{int}. However, it must be emphasized that there is no arbitrariness, or any "improper approximation" involved in the preceding derivation of the imaginary weak value X^w and the associated non-unitary evolution Eq. (27). In this context, note also that the choice of the final state of the system (i.e. a displaced Gaussian in momentum space) is common in various theoretical investigations. Recall that in the IA, this final state is approximated with a delta-function in momentum space.
Some more physical insight may be provided by the following observation. The finding that here X^w has a vanishing real part implies that the associated pointer's position remains invariant, i.e.

$$\langle\hat{x}\rangle_f = \langle\hat{x}\rangle_i$$

This is fully consistent with the impulsive, δ-like, nature of H_{int}. In simple terms, the hit system has no time to change its position just after the δ-interaction is turned off.

5 Experiment: H-intensity deficit in NCS from liquid benzene and its interpretation with WV theory

In short, the experimental NCS procedure is as follows. From a measured time-of-flight (TOF) spectrum with an individual detector, the data analysis routine determines the relevant peak areas A_X, or intensities I_X, (with X=H, C, Nb) from the measured partial differential cross-section $d^2\sigma/d\omega d\Omega$; see Section 2. Thus one determines by standard numerical analysis the ratio

$$R_{exp} \equiv \frac{I_H}{I_X} \tag{30}$$

Standard NCS theory [17, 18, 10] predicts that the expected value R_{conv} of this ratio is

$$R_{conv} = \frac{N_H\sigma_H}{N_X\sigma_X} \tag{31}$$

N_X is the number density of atom X, and σ_X is the tabulated cross-section of the nucleus of X.
Here we are interested in the ratio I_H/I_C for benzene—which is achieved by the data analysis after subtraction of the "overlapping" Nb-peak of the metallic nyobium container; see Figure 1(A).
Surprisingly, the experimental results presented below (and many others, too) exhibit a striking intensity deviation, i.e.,

$$(I_H/I_C)_{exp} \approx 0.75\,(I_H/I_C)_{conv.theory} \tag{32}$$

This effect has found no conventional interpretation thus far.
Assuming approximately that the heavier C-atoms behave "conventionally", we may attribute this effect to the H atoms (i.e. the protons) and speak of the *H-intensity deficit* effect.
Parenthetically, some accompanying NCS measurements on deuterated benzene (C_6D_6) were made, which showed a considerably smaller (although still discernible) D-intensity deficit relative to the C-intensity (results not shown).

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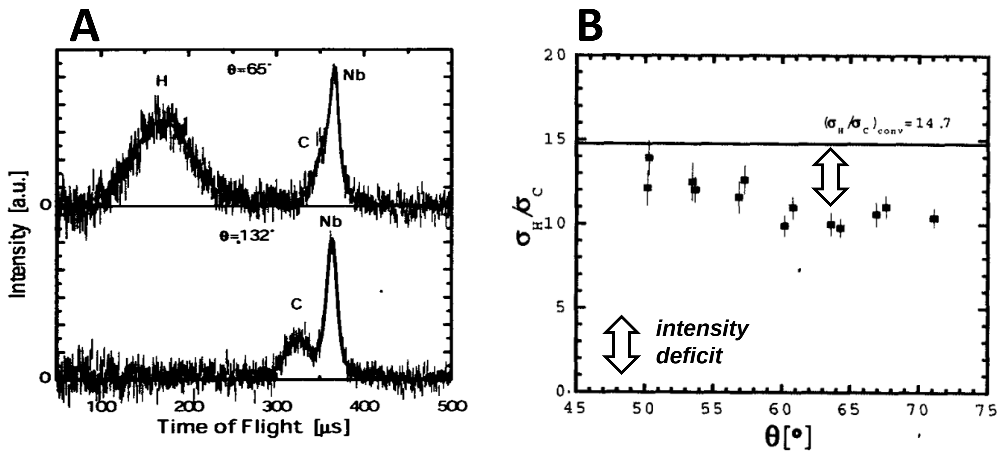

Figure 1: Experimental NCS results obtained from liquid benzene (C_6H_6). (**A**) Two time-of-flight (TOF) spectra measured on a liquid sample of C_6H_6 within a niobium (Nb) container, at a temperature of 295 K. The experiments were done with the spectrometer eVS-Vesuvion of ISIS spallation source, UK. The solid lines depict the fitted TOF spectra. The peaks' positions are calculated based on conventional theory. The C- and Nb-recoil peaks overlap at a scattering angle of $\theta = 65^o$. However, at $\theta = 132^o$, the maxima of these two peaks are clearly distinguishable, enabling accurate determination of their intensities. (**B**) Ratios of neutron cross-sections (equivalent to intensities' ratios) for H and C obtained experimentally at various scattering angles (detector positions). The error bars represent counting statistics only. The vertical line at 14.7 denotes the ratio σ_H/σ_C derived from the tabulated cross-section values for H and C. Surprisingly, the observed values of I_H/I_C are approximately 20-30% smaller than the predicted values based on conventional theory.

This finding can be understood as follows. In a given experimental setup (i.e, given neutron initial energy and geometry of the apparatus), the energy and momentum transfers (ΔE and $\hbar Q$) on D are smaller than those on H, due to simple classical kinematics of a two-body collision. This affects the aforementioned scattering time τ_{sc}, which, according to Eq. (25), increases. E.g., in the setup of the experiments on H- and D-benzene, the neutron-D scattering time is larger than 1 femtosecond, which is significantly longer than that in scattering from of H-benzene. Thus the neutron-D collision should be less good modeled with an impulsive von Neumann model Hamiltonian. Moreover, a longer τ_{sc} value physically implies that the highly excited physical system "neutron & struck D & environment", has more time to smear out (due to relaxation processes) the specific quantum phase relations which underlay the Weak Values dynamics, the latter being a specific quantum interference phenomenon [19, 20].

5.1 Which-path information and impossibility of neutron beam interferences in NCS from several entangled protons

Earlier [37], a theoretical interpretation of the NCS-intensity deficit effect from H containing materials was proposed, being based on the hypothesis that two (or more) entangled protons may exist in the characteristic coherence volume of the neutron beam—a few Å^3, in the short time-window of NCS, see relation (24). (This hypothesis also motivated our related original NCS experiment [38].)
The experimentally observed intensity deficit was interpreted to be the result of destructive interference when a neutron is scattered from two of more indistinguishable entangled protons. It was argued that this QE concerns spatial and spin degrees of freedom, due to the identity of the involved protons [37].

It was theoretically derived in [37] that the assumed QE should reduce the scattering intensity of the system. This reduction should be tantamount to a destructive quantum interference of the various participating, possible neutron paths scattered from the mentioned entangled protons. Clearly, this physical view goes beyond the standard one [17, 18], which considers NCS (or, equivalently, DINS) essentially as a two-body scattering process.

However, this theoretical proposal appears highly questionable in the light of modern quantum mechanics, in which the aforementioned phenomenon of impossibility of interference in the case of which-path information plays a central role. Indeed, the high energy transfer on a hit proton (say, e.g., 10-50 eV — which even breaks the chemical C-H bond) makes it clearly distinguishable from the other H atoms of the scattering system — independently of whether QE effects be present or not. In other terms, this large energy transfer is equivalent to a strong which-path information, which rules out the aforementioned proposed interpretation of the intensity deficit effect as caused by destructive interference. Namely, here there exists a significant which-path information for the scattered neutron, because the scattering proton is well distinguishable from all other non-hit protons being in the aforementioned coherence volume.

To put it differently, the NCS-intensity deficit effect can be attributed to the collision of a neutron with a single hydrogen atom (which interacts with its environment). Simply put, this effect is unrelated to any assumed quantum interference of several neutron paths originating from different protons. This is in line with the conventional viewpoint that the NCS scattering is incoherent [17, 18, 26].

The conceptual similarity to the common quantum two-slit experiment should be obvious: When we have information about which path a particle (such as a neutron, atom, or photon) takes, this cancels the interference pattern on the screen (i.e., the measurement device). Moreover, having partial knowledge about the path reduces the visibility of the interference fringes accordingly; see [12, 14, 15, 16].

We may emphasize that the preceding remarks fully agree with Feynman's statement stressed in the Introduction, which here may be rephrased as follows:

You may argue, "I don't care which specific proton has scattered the neutron". Perhaps you don't, but nature knows; and neutron's scattering amplitude behaves, in fact, as we just discussed —– there isn't any quantum interference.

6 Additional and concluding remarks

We summarize here some results and findings of particular importance. Most of them were presented and discussed above.

(A) The conventional neutron scattering theory contains quantum dynamical variables of the scattering material only, and not those of the impinging beam (neutrons), the latter being treated as classical.

(B) The average $\langle ... \rangle$ occurring in the correlation functions of conventional theory (see Section 2) is the *canonical ensemble* of thermal equilibrium, However, the NCS (DINS) process is clearly a "violent" *non-equilibrium* process (e.g., it breaks the C-H bonds in the experiment of Section 5), which highly disturbs the hit nuclei and their local environments. As a neutron beam usually contains a very small number of neutrons (as compared with the number of particles of the bulk system), one might argue that the system remains in equilibrium "on the average". However, the NCS (DINS) experiment explores the dynamics of the neutron interacting with one H and its (nanoscopic) local environment, rather than the bulk (macroscopic) system.

(C) The widely applied *plane wave approximation* of the conventional theory is inappropriate in the physical context of NCS (DINS), as the derivations of Sections 3 and 4 show. Especially, the derived momentum transfer deficit simply disappears in this approximation, because the derived WV-corrections become identical to zero. For detailed derivations see [30]. Further implications of both mentioned effects on the popular field of momentum-distribution measurement and the associated local Born-Oppenheimer potential of the struck proton are under investigation.

(D) The considered intensity deficit effect cannot be interpreted as being caused by destructive quantum interference of the beam (here: neutron) scattered from (a few) entangled protons, as we showed with the aid of Feynman's analysis based on the distinguishable neutron paths in the example of magnetic scattering [13]; see the Introduction.

(E) The preceding physical considerations and derivations strongly support the experimental relevance and predictive power of the new WV and TSVF theory originally proposed by Aharonov and collaborators; cf. [19, 20, 21, 22, 32].

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Acknowledgments
I am grateful to an anonymous reviewer for insightful comments, clarifying remarks and helpful suggestions.

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