

No case against scattering theory

Joachim Wuttke^{a,1}

^aJülich Centre for Neutron Science at MLZ, Forschungszentrum Jülich GmbH, Lichtenbergstraße 1, 85747 Garching, Germany

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In a series of papers (1–3), Frauenfelder *et al.* propose a radical reinterpretation of incoherent neutron scattering by complex systems, specifically by protein hydration water, drawing into doubt the “currently accepted model, used for > 50 y” (3). Under this model they subsume not only assumptions about the scattering target (*sample*) but also the theory that connects sample and scattering signal. Effectively, they attack the insight (4) that the *dynamic structure factor* $S(q, \omega)$ (which they incorrectly call “the scattering intensity”) abstracts from scattering kinematics and depends only on nuclear position operators acting on the sample. They claim that the established theory cannot account for the q dependence of elastic incoherent neutron scattering from isotropic samples. As a remedy, they suggest fits that account *ad hoc* for the recoil of the sample and the transit time of the neutron.

Frauenfelder *et al.* overlook that the isotropy of n - p scattering is broken by the setup of a scattering experiment: incoming beam direction and detector location define the scattering vector \mathbf{q} . Through $S(\mathbf{q}, \omega)$, the measured cross section depends on \mathbf{q} , or q for isotropic samples. The non-Gaussianity of $S(q, 0)$ is long known (5) and can have various reasons (6). Faulty Gaussian extrapolations $S(q \rightarrow 0, 0) < 1$ do not disprove scattering theory.

Recoil is inherent in the accepted scattering theory [see (7) for a particularly clear exposition] since $S(\mathbf{q}, \omega)$ only involves transition probabilities that change the sample momentum by $-\hbar\mathbf{q}$. The recoil energy is not linear in \mathbf{q} , as posited in (3), but quadratic. It is implicitly contained in $S(\mathbf{q}, \omega)$, clearly appears in the limiting cases of an unbound scatterer or of large q [see e. g. Appendix G in (8)], and gives rise to a distinct factor when $S(\mathbf{q}, \omega)$ is approximated for a classical system (9).

To account for transit times, Frauenfelder *et al.* request that neutrons be described as de Broglie wave packets (3). This is not explicitly done in standard texts because incident and scattered wave packet “share absolutely the same time

dependence” (10). There are no cross terms: the scattering intensity, given as the squared modulus of a superposition of wave amplitudes turns out to be the sum of squared moduli of monochromatic wave amplitudes. Therefore the established practice of accounting for finite energy resolution at the level of scattering intensities, not of wave functions, is perfectly adequate.

Thus there is nothing wrong with the accepted scattering theory. The “woes” of (3) are unfounded. The proposed heuristic injection of recoil and transit time only would make $S(q, \omega)$ inconsistent. With all this, nothing is said about the physical idea that quasielastic spectra might be explained by protein substate fluctuations. To make this idea verifiable, it needs to be cast into a mathematical model that yields $S(q, \omega)$ *within* the established correlation function formalism (4), without reversing scattering theory.

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¹E-mail: j.wuttkefz-juelich.de