Eur. Phys. J. H (2024)49:9
https://doi.org/10.1140/epjh/s13129-024-00072-9

THE EUROPEAN PHYSICAL JOURNAL H

Regular Article

Gian-Carlo Wick and neutron physics in the 1930s

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Received 2 December 2023 / Accepted 21 March 2024

Abstract The Italian theorist Gian-Carlo Wick is well known for his work in mathematical physics. Nevertheless, working with Fermi's group in Rome in the 1930s, he took on several behind-the-scenes roles that resulted in important papers in neutron physics. He clarified Fermi's methodology for calculating neutron slowing down probabilities; using transport theory, he provided a comprehensive general method for calculating the neutron scattering albedo; and with an insight into the way, neutron scattering could yield information about lattice dynamics, he formulated the first theory of inelastic thermal neutrons scattering in crystalline materials. This work and his contributions are not well known today. We discuss its physical essence, its relevance to neutron physics, and its subsequent impact in later work.

1 Introduction

The Italian theorist Gian-Carlo Wick is well known for a 1950 theorem that provided the basis for a systematic derivation of Feynman rules starting from second-quantized field equations. But from 1932 to 1937, when he was working in the Physics Institute of the University "La Sapienza" in Rome, he published several important papers related to experimental neutron physics. Fifty years later, in his reminiscences "Physics and Physicists in the Thirties" [38], he wrote (citation from the page 567): "When, in the fall of 1932 I was offered an assistantship by Fermi, I became Fermi's pupil and I worked in almost daily contact with him for about five years, and I have learned more from him than from anyone else." And further, on page 575, Wick added that his own work there was inspired "in a particular way by the experimental work in Rome that I could watch every day with my own eyes. As an example, the evaluation of the results of work with slow neutrons required the solution of diffusion problems; I found an extremely simple technique to solve some of these problems."

Arriving in Rome in 1933, after a year in Germany working on atomic and molecular physics, he quickly became an integral member of Fermi's group. He first solved a problem suggested by Fermi: how to extract the value of the then-unknown proton magnetic moment from a Stern–Gerlach measurement of the magnetic moment of a hydrogen molecule [29]. Simultaneously, he participated [26, 30] in the physical interpretation of a phenomenon discovered by Segre and Amaldi in atomic physics–anomalous displacement of high spectral lines of alkali atoms in the atmosphere of a foreign gas. Details of Fermi's explanation of this effect, and Wick's role, are discussed by us [15].

With the publication in 1934 of Fermi's theory of beta decay, Wick showed that this theory naturally described not only the emission of electrons but also the emission of positrons. And going further [31], he predicted the phenomenon of K-electron capture in radioactive nuclei, experimentally demonstrated later by Alvarez [1].

Following the 1932 discovery of the neutron, Fermi's efforts switched to neutron physics, leading to an extraordinarily creative period, well-documented in a series of papers by Guerra, Leone, and Robotti [16]. By the Spring of 1934, artificial radioactivity induced by fast neutrons (energy about 8 MeV) from the nuclear reaction ^{4}He + ^{9}Be = ^{12}C + n, had been discovered, and by Autumn 1934, the effect of a large amplification of the radioactivity, induced by thermal neutrons (energy of order 25 meV, wavelength 1.8 A), was discovered.

What role did Wick, not specifically an experimental physicist, but highly trained in mathematical physics, play in all of this? This cannot today be known with certainty. But from looking at his papers and Fermi's papers, we speculate that he played a crucial supporting function: thinking about the problems Fermi encountered in different ways, suggesting alternative methods, and in the case of the theory of inelastic thermal neutron scattering in condensed matter, initiating a new field of investigation with his realization that thermal neutrons, unlike X-rays,

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could both absorb from and release energy to the crystal lattice in a detectable fashion. We discuss three of his papers, in turn, the first relating to the neutron slowing down problem, the second relating to calculations of the neutron albedo in material, and the third, his paper on inelastic thermal neutron scattering in crystalline media.

2 Neutron slowing down problem ("Wick and Fermi")

In a 1984 symposium honoring Wick's retirement, T D Lee reminisced [[19]] that he had been in a 1947 class of Fermi's at the University of Chicago when Fermi, talking about the problem of neutrons slowing down, had said "this was solved by Wick," adding: "Gian-Carlo Wick is very good physicist." Having this in mind, we start this section with [32–35] paper [32].

The paper opens with a quotation from an earlier paper by Amaldi et al. [2] "It is easily shown that an impact of a neutron against a proton reduces, on the average, the neutron energy by a factor of *1/e,*" and continues "According to reports from several sides, the above passage in a paper by Professor Fermi is considered somewhat obscure. Since a more detailed explanation might be of interest also to others, it was thought advisable to make it generally known."

Wick goes on to write that the mean neutron energy after one collision, $<E'>$, is equal to one half of the neutron energy E before the collision $<E'> = (E/2)$, and since this is the case for all subsequent collisions, he can write after n collisions, $<E_n> = E/(2)^n$. He then introduces the now universally used logarithmic energy decrement variable $u = log\ (E/E')$, and defining $x = log(E/E_n)$, shows that $<x> = n$ with a probability distribution function given by $P(x) = [x^{n-1}/(n\text{-}1)!]e^{-x}$. Setting n = 1 confirms Fermi's statement.

Wick ascribes his use of the logarithmic energy decrement to Fermi, as later does Bethe [6] who also clarifies that there is a legitimate point of confusion concerning the appropriate mean—arithmetic or geometric. It is now agreed the latter is the right way to characterize the result of the collisions. Wick's paper is the first time the logarithmic energy decrement (now called the lethargy) is mentioned by any member of the Rome group.

Condon and Breit [10] followed soon with a detailed derivation of all the results, tracing the first work on a similar problem (the development of the probability density function for the sum of "n" uniformly distributed random variables) back to Laplace [21] in 1820. Intriguingly, Fermi cites Laplace in his thesis publication [11]. It is clear that he would have been very familiar with probability arguments from this work, as, we may assume, would Wick. Fermi's remark in that class with TD Lee supports the idea that Wick had much to do with developing those initial ideas.

Today, transport theory dominates theoretical discussions of neutron slowing down processes. But arguments that similar results can be obtained from probability calculations continued to appear decades later. In the 1970s, Barnett [5] argued that the first- and higher-order moments calculations were amenable to probabilistic arguments and gave fully correct results.[1] Transport theory proponents, Paveri-Fontana [22] countered with proofs showing that the results were the same. As recently as 2018, Ganapol et al. [14] discussed probabilistic neutron slowing down as a mathematical model for entropy.

3 Thermal neutrons, the albedo problem

"Albedo" is Latin for "whiteness." It was introduced into optics by Johann Heinrich Lambert in his 1760 work "Photometria" [20]. In its simplest form, it is a measure of diffuse light reflection from a surface. For a plane-parallel beam, it is the ratio of the flux reflected in all directions by unit area of the surface relative to the incident flux per unit area. More generally, albedo calculations will involve considerations of radiative transfer, a major topic in stellar and atmospheric physics. Chandrasekhar established the field in 1960 with his definitive textbook "Radiative Transfer" [9].

[1] For E_0 = 2 MeV and En = 1 eV, Barnett finds $< n >$ = 15.5 + -3.8, to be compared with $< n >$ = 20.9 using the arithmetic average, and n_{peak} = 14.5 from the Wick–Fermi distribution.

There are many similarities between radiative transfer of light and thermal neutron transport. For neutrons, there is the added complication of defining how "albedo" might be measured. Fermi and Wick worked extensively on these questions in 1936, using different approaches; Fermi in 1D and Wick in full 3D. Wick's work made an impression on Chandrasekhar, who stated [8] "More recently an important investigation by G. C. Wick has come to the author's notice in which an alternative method for solving equations ... has been developed. It is the object of this paper to describe Wick's method in its astrophysical context and to show its particular adaptability for solving the standard problems of radiative transfer in the theory of stellar atmospheres."

Both Fermi and Wick considered an infinite half-space of a hydrogenous material. Wick applied the Boltzmann transport equation of radiation to neutrons, known to be valid for the 3D geometry, while Fermi invented his own intuitive "one dimensional model" of neutron diffusion. Wick published his results first [33], followed by Fermi, several months later [12], who compared results. In 1943, Wick resumed work on the albedo problem and published [37] a more extensive discussion; this was the paper picked up by Chandrasekhar.

Wick's approach was to use the Boltzmann integrodifferential equation for the probability density function for the neutrons $f(\boldsymbol{r},\boldsymbol{v};\boldsymbol{t})$ diffusing in a hydrogenous medium; t is time, and the bold symbols for position $\boldsymbol{r}$ and velocity $\boldsymbol{v}$ are vectors. He greatly simplified the mathematics by using a specific physical model of diffusion, assuming, following Fermi, that thermal neutron scattering during collisions is spherically symmetric. He also assumed that neutrons all have the same constant speed corresponding to a thermal energy of about 30 meV. Physically this is valid, on average, because neutrons are in thermal equilibrium with hydrogen molecules. Diffusion is now a stationary process, and the transport equation is time independent. Choosing the x-axis to be the symmetry axis, the two variables are the x coordinate, and an angle coordinate $u = cos\theta$, where θ is the angle between the x-axis and the direction of the neutron velocity $\boldsymbol{v}$ (normalized to $v = 1$). With these assumptions, the Boltzmann transport equation has a simple form:

$$u\frac{\mathrm{d}f(x,\,u)}{\mathrm{d}x} + f(x,\,u) - \frac{N}{2(N+1)}\int_{-1}^{+1} f(x,\,u)\mathrm{d}u = 0. \tag{1}$$

When neutrons enter a paraffin medium occupying the half-space between $x = 0$ and $x = \infty$, some are reflected, returning through the boundary surface $x = 0$ after collisions with the nuclei in the paraffin. Others are lost due to capture within the paraffin. The probability density at the boundary is represented by $f(0,\,u)$ with positive u-values for ingoing and negative values for outgoing neutrons. The quantity $f(x,\,u)d\tau du$ has the physical meaning of the number of neutrons in the volume $\mathrm{d}\tau$ at position x with angle values from u to $u + du$. $N = \sigma_s/\sigma_c$ is a characteristic of the hydrogenous medium, the ratio of the thermal neutron cross-sections for scattering and capture. In these early papers, N is also thought of as representing the number of mean free paths between collisions.

We omitted a source term in the equation. When that is included, Wick can calculate the albedo, the angular distribution of thermal neutrons inside and outside of paraffin, and the radioactivity induced by neutrons in the paraffin media. Wick solved his integrodifferential equation by expressing the integral in Eq. (1) as the weighted *sum* of several terms: $\sum_i^{2n} p_i f(x_i,\,u)$, where the weights p_i and the optimal discrete coordinates x_i are calculated following Gauss's formula for numerical quadrature. In this way, the problem is converted to the solution of a system of several linear differential equations. The accuracy of the approximation depends on the number of terms in the sum. Three terms were enough for the albedo problem.

Wick pointed out [33] and later clarified in detail [37] that two kinds of albedo should be considered for describing the diffusion of thermal neutrons. The first albedo β, the *current albedo*, was introduced in accordance with the classical definition: the ratio of the number of reflected neutrons to the number of the incident neutrons. In terms of the probability density function, the albedo, β, is then the ratio of neutron currents:

$$\beta = -\int_{-1}^{0} uf(0,\,u)\mathrm{d}u \Big/ \int_{0}^{1} uf(0,\,u)\mathrm{d}u \tag{2}$$

The result of the β calculation depends on the initial function *f(0,u)* at the boundary surface for $0 < u < 1$, that is, on the angular distribution of the incident neutrons. For an isotropic flux density, Wick obtained the "strong" estimate $\beta = 1\text{–}4/(\sqrt{(3\mathrm{N})})$, to be compared with the Fermi's "approximate" result $\beta = 1\text{–}2/(\sqrt{(\mathrm{N})})$ [[12]]. At that time, neutron flux angular distribution measurements were not possible, and a comparison of these expressions with experiment could not be made.

To circumvent this measurement problem, a second definition had been introduced by Amaldi and Fermi [3] based on neutron densities measured with 1/v activation detectors and a thin absorber inside a paraffin cube, cut in two. Wick called this the measurable albedo β_m, (the index “m” in the β_m), which in his theory was given by:

$$\beta_m = \int_{-1}^{0} f(0, u)\mathrm{d}u / \int_{0}^{1} f(0, u)\mathrm{d}u \tag{3}$$

His theoretical approximation, reported in [12], gave $\beta_m = 1\text{–}2/(\sqrt{}(N + 1) + 1)$. The Fermi–Amaldi experimental values were $\beta_m = 0.82$ and $N = 125$. With the modern values 50 barn for the scattering cross-section and 0.33 barn for the capture cross-section, one obtains $\beta_m = 0.85$.

Wick's achievement in his “albedo” papers was the development of a systematic mathematical method for solution of the transport integrodifferential equation to arbitrary precision. His work formed the basis for development and clarification of the results obtained by the Fermi's group in their experiments on slow neutron diffusion in paraffin and served as a basis [13] for refuting a critique by Halpern et al. [18] of their albedo interpretation. Subsequently, during the development of nuclear reactors, many others worked on the problem of neutron albedo, with increasing generality. As an example, we mention Placzeck [23].

4 Wick's theory of neutron inelastic scattering by crystalline media

By 1937, all members of the Fermi group except Amaldi and Wick had left Rome and Wick himself had accepted an offer from Rossi and Bernardini to collaborate on analysis of cosmic-ray experiments. Nevertheless, continuing to think deeply about neutron physics, he published a series of short, single author papers [34–36], that laid the foundations of the theory of inelastic slow neutron scattering in condensed media.

Wick's insight was to realize that in crystalline media, thermal neutrons could exchange energy and momentum with phonons, the quanta of crystal lattice vibrations. The equations for the conservation of energy and the wave vectors are different from those for scattering by free nuclei, and the situation is interesting compared to X-ray scattering because the energy changes of the neutrons are detectable.

Wick begins the discussion with the case of a crystal lattice, spacing d, at zero temperature. Neutron inelastic scattering can only excite the acoustic phonons since there is nothing to absorb. As a result, the conservation equations for momentum and energy can be written as follows:

$$\boldsymbol{p}_1 - \boldsymbol{p} = h\boldsymbol{s}$$

$$\frac{\boldsymbol{p}_1^2}{2m} + h\nu = \boldsymbol{p}^2/2m$$

Here $\boldsymbol{p}$ and $\boldsymbol{p}_1$ are vectors of neutron momenta before and after scattering, respectively, $\boldsymbol{s}$ is the phonon wave vector with the magnitude $s = 1/\lambda$ (λ is the phonon wavelength), m is the neutron mass, ν is the phonon frequency, and $h\ \nu$ is the phonon energy.[2] It follows from these equations that, for inelastic scattering with phonon creation where the neutron loses energy, the initial neutron momentum must satisfy the condition:

$$\mathrm{p} > \mathrm{m}\nu\lambda + \mathrm{h}/2\lambda. \tag{4}$$

This condition is satisfied for many crystals in the thermal energy region, and Wick can use the Debye model and the known concept of Brillouin zones.

For inelastic scattering at finite temperature, the neutron can absorb energy from the acoustic phonons. He comments that this is expected to decrease as the crystal temperature goes down, and that eventually the crystal will become transparent for neutrons with the wavelength $\lambda_n > 2d$.

Finally, Wick calculates the total cross-section of slow neutron inelastic scattering in crystals. He follows the theory developed by Fermi for neutron scattering by protons bound in molecules, this time applying it for wave functions in crystals. His result is a cross-section containing an integral over the “eigen-frequencies” of the crystal vibrations (Eq. (14) in [36]). For a cold crystal, $\lambda_n < 2d$ and $p > \sim h/2d$, Wick estimates the partial inelastic cross-section with the neutron energy lost (phonons emitted) between ε and $\varepsilon + d\varepsilon$ as follows:

$$\mathrm{d}\sigma = \frac{\sigma_0 6\mathrm{d}}{\mathrm{MhV}^3}\varepsilon \mathrm{d}\varepsilon, \tag{5}$$

[2] Even though it is not used today. We keep the 1930s notation of Wick's paper.

here σ_0 is the neutron interaction cross-section with free nuclei of mass M, and $V = \nu\lambda$ is the phonon velocity, assumed to be constant. For the case of a crystal at finite temperature T, Debye lattice temperature θ, and $\lambda_n <$ 2d, he deduces an approximate expression for the inelastic neutron scattering cross-section with neutron energy gain:

$$\sigma = \sigma_0 \frac{3h^3}{16\pi \mathrm{Mp}^2 \mathrm{Vd}^3} T^3 \theta^{-3}. \tag{6}$$

Wick is careful to distinguish two possible parts of the neutron scattering cross-section: *coherent* (the interfering part) and *incoherent* (the noninterfering part). The expressions above are for fully incoherent cross-sections.

Later, as experimental capabilities developed, other theorists built on Wick's work and began investigating in more detail thermal and cold neutron scattering by nuclei bound in the crystal lattice. Extending Wick's approach, Pomeranchuk [25] calculated the influence of the temperature on scattering, now taking full account of the neutron spin. Halpern et al. [17] investigated scattering by ferro-magnetics, also including neutron polarization. A more complete theory of neutron inelastic scattering by a polycrystalline medium was presented later by Weinstock [28]. All papers cited Wick's pioneering studies.

The really new era in this field began in 1954 with the publication by Placzek and Van Hove of papers [24, 27] on crystal dynamics, dispersion relations, and correlation functions. After citing Wick's contributions, they stated that until then only the total inelastic scattering cross-sections had been studied due to the limitations of the simplified Debye model of lattice vibrations. They argued that differential cross-section measurements were needed to determine the actual vibrational spectrum of the crystal, i.e., the dispersion relations $\omega = \omega_j(\mathbf{q})$ between the frequency, ω, the wave vector **q,** and the polarization $j = 1,2,3$ of the plane-wave phonon vibration.

Van Hove [27] introduced the *scattering function* S(**κ**, ω) depending explicitly on the momentum and energy transferred in the scattering. Here, $\hbar\boldsymbol{\kappa} = \hbar(\mathbf{k_0} - \mathbf{k'})$ is the neutron momentum transfer ($\mathbf{k_0}, \mathbf{k'}$ are the wave vectors before and after scattering), and $\hbar\omega = E_0 - E'$ is the energy transfer. Many present authors call this function the "scattering law" or the "dynamic structure factor." The double differential cross-section for incoherent scattering into an element of solid angle Ω, with neutrons of final energies E', can then be written as follows:

$$\frac{d^2\sigma}{d\Omega dE'} = \frac{\sigma_{inc}}{4\pi} \frac{k'}{k_0} \mathrm{S}(\boldsymbol{\kappa}, \omega) \tag{7}$$

From the conservation laws, the neutron arguments **κ**, ω are directly related to the phonon arguments **q** and ω. As a result, the scattering function S(**κ**, ω) depends only on the crystal dynamics, and the dispersion relations are deduced from the analysis of the double differential cross-sections. Van Hove also introduced the dynamic correlation function G(**r**,t), the Fourier transform of S(**κ**, ω), as more useful for theoretical calculations with specific models of crystal dynamics.

At the end of the 1950s, intense neutron beams became widely available at nuclear research reactors, and innovative experimental work could take advantage of these theoretical developments. Half a century later, the pioneering efforts of Brockhouse and Shull were recognized with the Nobel Prize in Physics [7].

We conclude by quoting from Amaldi's review [4] of the history of nuclear and neutron physics in 1930s. Wick's papers, he wrote "paved the way for a very important and presently widely used technique for measuring the dispersion relations of the phonons in crystals and providing direct information on the dynamics of solid-state substances."

5 Summary

We have reviewed three single author papers written by Wick in the 1930s. The first was on a probabilistic derivation of the result for the energy distribution of neutrons slowing down as they scatter multiple times in a hydrogenous medium. Wick introduced into print for the first time the logarithmic energy decrement, known today as the lethargy variable. The second paper introduced a 3D transport theory formalism that allowed for arbitrary accuracy in the solution of the albedo problem in neutron physics: What fraction of neutrons incident on a surface get reflected vs absorbed. His formalism accommodated solution to two different ways of experimentally measuring the albedo and allowed for resolution of a controversy about which of these methods was the more valid. And in the third paper, he showed that slow neutrons could yield information that X-ray scattering in crystals could not because the neutrons had energies comparable to the energies of the lattice vibrations. He wrote specific equations for inelastic neutron scattering cross-sections, carefully distinguishing between coherent and incoherent inelastic scattering cross-sections.

All these papers are on aspects of slow neutron scattering, not an area of physics typically associated with him. But working closely with Fermi in Rome, interacting on an almost daily basis, following all the results from the research group, we can see that Wick absorbed much, immersed himself deeply in all that was happening, and proceeded to come up with creative and original ways of formulating solutions, laying the groundwork for new avenues of research. His contributions appear to be much more than simply "filling in the details" of existing bodies of knowledge.

Looking back at the output of Fermi and his colleagues, one is struck by the range of problems they explored and the group's extraordinary productivity. The output is a testament to Fermi's singular abilities as a physicist, and his managerial kills in attracting and retaining such a talented supporting cast. Wick is not talked about as a member of "I ragazzi di Via Panisperna" but it seems to us today that he has earned honorary posthumous appointment to that august group!

Acknowledgements The authors are grateful to Professors F.Guerra, N. Robotti, and R. Wilson for their help in locating documents that helped shape this report.

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