

#### ELEMENTS OF SLOW-NEUTRON SCATTERING

Basics, Techniques, and Applications

Providing a comprehensive and up-to-date introduction to the theory and applications of slow-neutron scattering, this detailed book equips readers with the fundamental principles of neutron studies, including the background and evolving development of neutron sources, facility design, neutron-scattering instrumentation and techniques, and applications in materials phenomena.

Drawing on the authors' extensive experience in this field, this text explores the implications of slow-neutron research in greater depth and breadth than ever before in an accessible yet rigorous manner suitable for both students and researchers in the fields of physics, biology, and materials engineering. Through pedagogical examples and in-depth discussion, readers will be able to grasp the full scope of the field of neutron scattering, from theoretical background through to practical, scientific applications.

JOHN M. CARPENTER was Professor of Nuclear Engineering at the University of Michigan from 1964–1975. He later became a Senior Physicist at Argonne National Laboratory where he originated and built the first accelerator-based pulsed neutron sources. He is now a Distinguished Scientist Emeritus at Argonne National Laboratory and was awarded the Clifford Shull Prize in Neutron Physics in 2006.

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If, in some cataclysm, all of scientific knowledge were to be destroyed, and only one sentence passed on to the next generation of creatures, what statement would contain the most information in the fewest words? I believe that it is the **atomic hypothesis** (or the atomic **fact**, or whatever you wish to call it) that **all things are made of atoms – little particles that move around in perpetual motion, attracting each other when they are a little distance apart and repelling upon being squeezed into one another.** In that one sentence, you will see, there is an **enormous** amount of information about the world, if just a little imagination and thinking are applied.

Richard P. Feynman Lectures on Physics, 1963. (Printed with permission from Pearson Education.)

Cover illustration: The curve is a semilogarithmic plot of the Ewald function describing the reflectivity of a perfect single crystal as a function of the deviation of the glancing angle from the nominal Bragg angle for a given wavelength. Original cover design by J. M. Carpenter.



We dedicate this book to Rhonda DeCardy Carpenter and Rosa Po Po Wong.



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#### **Preface**

With "a little imagination and thinking," scientists have learned to use parts of atoms - neutrons - as probes to glean enormous amounts of information about the world. We have neutrons in the first place inasmuch they are one of the basic constituents of nuclear matter. It also comes about that because neutrons interact strongly but locally with atomic nuclei and because neutrons equilibrated at everyday temperatures have wavelengths comparable to interatomic distances, neutrons are ideally suited as probes of the structure and motions of matter on the atomic length scale. Objects of neutron studies include not only molecules, but also larger assemblies of crystals, polymers, and membranes - fluid and solid, ordered and disordered. Because neutrons have no electric charge, they penetrate deeply into sample materials, providing a true volume average measure of their properties and making it possible to nondestructively define a fiducial volume deep within. And because neutrons carry a magnetic moment, they sense magnetic order and excitations. The wide range of topics that neutron scattering methods address are the business of neutron scattering, which concern substances important to daily living, from engineering materials and earth matter to the stuff of life itself – materials in a very broad sense.

The extent of applications of neutron scattering in science and technology has grown immensely since the beginnings: tentative probing and establishment of principles by the pioneers such as Enrico Fermi, Shyoji Nishikawa, and Lise Meitner in the 1930s; early developments of applications using neutron beams from the first reactors in the 1940s and 1950s; broadening of uses and enlargement of the community of researchers as high-flux research reactors came on the scene in the 1960s and 1970s; and a burgeoning of applications as instruments and techniques evolved for an ever-widening range of specific purposes in the 1980s and 1990s and beyond. Very importantly, starting in the early 1970s, a new basis for neutron scattering research emerged: accelerator-driven pulsed spallation neutron sources. Enabling technologies grew very rapidly – accelerator science, knowledge of



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spallation source engineering, development of applications-oriented time-of-flight neutron scattering techniques and instrumentation, and affordable computer power to support the new sources – first in the United States at Argonne National Laboratory in the early 1970s and spreading to the United Kingdom and Japan in the 1980s and 1990s. The new sources opened new horizons for neutron scattering in all traditional branches of science, engineering, and technology addressed by neutron methods; also, the prospects for more powerful versions foreshadow a flourishing of new uses of neutron scattering.

We realize that there are already a number of excellent books on the subject of neutron scattering and that more have been appearing in recent years. In this book we aim to provide an introduction to the subject suited to the needs of advanced undergraduates, graduate students, and their professors; those who, although not aspiring to true expertise in the techniques, require a general understanding of the subject; and also those who intend deeper study, for use as a first text. Furthermore, many of the existing texts predate the use of some of the time-of-flight techniques developed for use in pulsed neutron beams from pulsed spallation neutron sources. As facility designers and neutron researchers, we offer a broad range of information, a "how-to" book, to the ever-broadening community of interested people. We maintain a website, http://www.slowneutronscattering.com, to promote communication with readers and to extend coverage beyond the contents of this book. Cross-references to the web page will be cited as "CL 2015" (Carpenter and Loong 2015), with the individual topic indicated in square brackets – for example, "CL 2015 [large systems]."

#### About the authors

John M. Carpenter was Professor of Nuclear Engineering at the University of Michigan from 1964 until 1975. He moved to Argonne National Laboratory in 1975 to assume responsibility for development of pulsed spallation neutron sources. There, he and his colleagues built and operated the first-ever pulsed spallation neutron sources equipped for neutron scattering, ZING-P and ZING-P', and later IPNS. He retired in 2007 and now as Emeritus Scientist maintains his office at Argonne.

Chun-Keung Loong joined the Intense Pulsed Neutron Source (IPNS) division of Argonne National Laboratory in 1982, becoming a senior physicist in 1997. He worked on the development of pulsed-source neutron chopper spectrometers and conducted materials research with users at IPNS and collaborators elsewhere. Since retirement in 2007, he remains active in worldwide development of accelerator-driven neutron sources and scattering instrumentation through participation in international workshops, reviews, and lectureships at universities and laboratories in the Americas, Asia, and Europe.



## Acknowledgments

When nuclear reactors and particle accelerators were pioneered, no one anticipated the advent of neutron user facilities (likewise the synchrotron X-ray counterparts) equipped with assorted state-of-the-art scattering instruments tailored to materials research. Since then, developments have been continuous and demanding and proceed with intensity. We have had the privilege of many years at Argonne National Laboratory, which has borne witness to critical advances in the field, and have benefited through interactions with IPNS users, including eager students, who planted in our minds the ideas that should be elucidated in a textbook on neutron scattering. We are indebted to our colleagues at Argonne and at sister research institutions for their support of the work in slow-neutron scattering and, during the last several years, for their encouragement and help in the writing of this book. Many of them graciously shared with us figures and other materials that we have included in our book, for which we are grateful. Others have reviewed portions and commented on the contents. Any mistakes readers find are due to the authors.

We thank all the reviewers for their careful, vigilant scrutiny: Ken Anderson, Carla Andreani, Sow-Hsin Chen, Erik Iverson, Alexander Kolesnikov, Kim Lefmann, Michael Loewenhaupt, David Mildner, Steven Nagler, Raymond Osborn, David Price, Roger Pynn, Marie-Louise Saboungi, Eric Schooneveld, Arthur Schultz, Roberto Senesi, Sunil Sinha, and Pappanan Thiyagarajan, among many others. We received essential help from Wes Agresta, Kathryn Carpenter, Scott Cudrnak, Kelly Cunningham, Catherine Eyberger, and Renée Manning. We are much obliged to our ANL librarians for their assiduous, professional assistance. Above all, we are grateful to Rhonda Carpenter – our tireless editor and project manager – for her thorough readings, for her steadfast attention and careful guidance, and for her expert advice on the manuscript, without which this book could never have come to fruition.



## Symbols and notations

Following are definitions of symbols unique to this book or needing further explanation than in the text and symbols with multiple uses, mostly excluding conventional terminology.

Vectors: boldface with overbar arrow. Scalars: lowercase, not bold.

Symbols	Meaning	Section or equation number of first appearance
β	$1/k_BT$	1.11
$2\delta\theta_D$	Full width of the Darwin plateau	(5.18)
γ	Greuling-Goertzel parameter	(1.102)
$\mu$	Reduced neutron mass	(1.12)
$\frac{\mu}{\mu}$	Neutron magnetic moment	1.2
$\mu_N$	Time-decay constant for the Nth normal mode	(1.60)
ξ	Mean logarithmic energy loss per collision	1.10
$\mu_N \ oldsymbol{\xi} \ oldsymbol{ec{a}}_i$	Reciprocal lattice vector basis vector in the <i>i</i> th direction	5.3
D	Diffusion constant	(1.31)
h, k, l	Miller indices for crystal diffraction	5.3
$N_{\uparrow}$	Number of particles in a sample having spins in the "↑" direction	(5.11)
$P_{\uparrow}$	Polarization, i.e., the fraction of particles in a sample having spins in the "↑" direction	(5.11)
$r_{e}$	Classical electron radius	1.2
r <sub>e</sub> R	Surface reflectivity	(5.24)
T	Interpulse interval in a pulsed source, $T = 1/f_s$	(6.4)
$ar{v}$	Neutron speed	(1.53)
F	Fourier transform operator	(3.14)
H	Hamiltonian operator	(3.74)
L	Laplace transform operator	(1.55), (A3.1)