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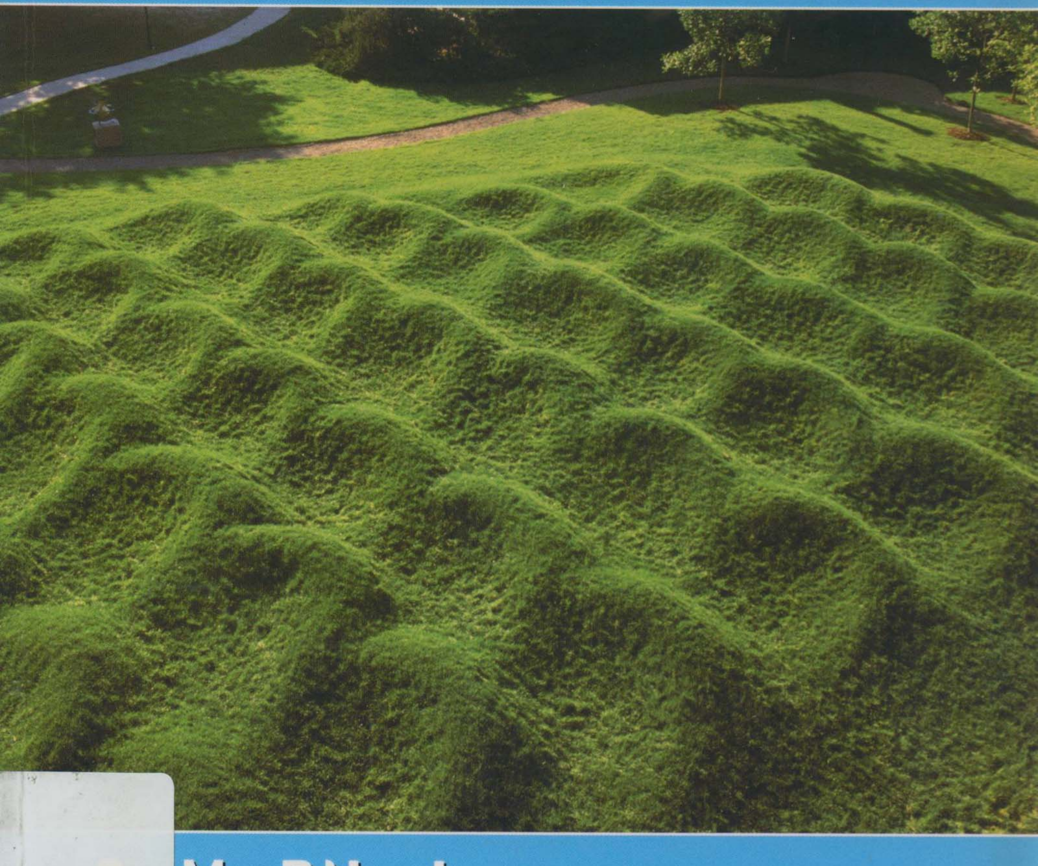
Introduction to Quantum Mechanics

IN CHEMISTRY, MATERIALS SCIENCE, AND BIOLOGY



S. M. Blinder

Introduction to Quantum Mechanics

in Chemistry, Materials Science and Biology

S. M. Blinder

University of Michigan

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Selected Physical Constants

Atomic mass constant $u = 1.66053873 \times 10^{-27}$ kg
Avogadro's constant $N_A = 6.02214199 \times 10^{23}$ mol^{-1}
Bohr magneton $\mu_B = 9.27400899 \times 10^{-24}$J T^{-1}
Bohr radius $a_0 = 0.5291772083 \times 10^{-10}$ m
Boltzmann constant $k = 1.3806503 \times 10^{-23}$J K^{-1}
Compton wavelength $h/m_e c = 2.426310215 \times 10^{-12}$ m
Electron mass $m_e = 9.10938188 \times 10^{-31}$ kg
Electron-volt $eV = 1.602176462 \times 10^{-19}$ J
$= 96.485$ kJ mol$^{-1} \simeq 8065.5$ cm^{-1}
Elementary charge $e = 1.602176462 \times 10^{-19}$ C
Fine-structure constant $\alpha = 7.297352533 \times 10^{-3}$, $\alpha^{-1} = 137.03599976$
Gravitational constant $G = 6.673 \times 10^{-11}$ m^3 kg^{-1} s^{-2}
Molar gas constant $R = 8.314472$ J mol^{-1} K^{-1}
Nuclear magneton $\mu_N = 5.05078317 \times 10^{-27}$ J T^{-1}
Permeability of vacuum $\mu_0 = 4\pi \times 10^{-7}$N A^{-2}
Permittivity of vacuum $\epsilon_0 = 8.854187817 \times 10^{-12}$ F m^{-1}
$1/4\pi\epsilon_0 = 8.98755 \times 10^9$ m F^{-1}
Planck's constant $h = 6.62606876 \times 10^{-34}$ J s
$\hbar = 1.054571596 \times 10^{-34}$ J s
Proton mass $m_p = 1.67262158 \times 10^{-27}$ kg
Proton-electron mass ratio $m_p/m_e = 1836.1526675$
Rydberg constant $\mathcal{R}_\infty = 10973731.568549$ m^{-1}
Second radiation constant $hc/k = 1.4387752 \times 10^{-2}$ m K
Speed of light in vacuum $c = 2.99792458 \times 10^8$ m s^{-1}

Greek Alphabet

A, α alpha	I, ι iota	P, ρ rho
B, β beta	K, κ kappa	Σ, σ sigma
Γ, γ gamma	Λ, λ lambda	T, τ tau
Δ, δ delta	M, μ mu	Υ, υ upsilon
E, ϵ epsilon	N, ν nu	Φ, ϕ phi
Z, ζ zeta	Ξ, ξ xi	X, χ chi
H, η eta	O, o omicron	Ψ, ψ psi
Θ, θ theta	Π, π pi	Ω, ω omega

Introduction to Quantum Mechanics

in Chemistry, Materials Science and Biology

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For our daughters, Amy Rebecca and Sarah Jane.

Preface

This book is the product of 40 years of distilled experience teaching quantum theory to juniors, seniors and graduate students. It is intended as a less weighty text for one semester of the physical chemistry sequence or for a stand-alone course in quantum mechanics for students of chemistry, materials science, molecular biology, earth science and possibly even physics.

The supplements appended to several chapters contain optional material for more adventurous students, but can be guiltlessly omitted without loss of continuity. Likewise, the more advanced topics in Chapters 12-16 can be omitted or lightly skimmed. I have purposely limited the number of problems after each chapter and geared them toward conceptual understanding rather than numerical drill. For those desiring a larger selection of problems and worked-out examples, we recommend the companion volume in the Academic Press Complementary Science Series, *Fundamentals of Quantum Chemistry* by James E. House.

It is a pleasure to acknowledge the expert advice and support of Jeremy Hayhurst, Senior Editor at Academic Press/Elsevier Science. My thanks also to the several reviewers who suggested numerous improvements and rooted out errors and obscurities, including Dr. James P. McTavish, Prof. Peter Lykos, Prof. Neil R. Kestner, Prof. Doug Doren, Prof. Lawrence S. Bartell and Prof. Paul Engelking.

Finally, I must gratefully acknowledge the years of inspiration and encouragement provided by my many teachers, students, colleagues and family members, too numerous and varied to be cited individually.

S.M. Blinder
Ann Arbor, Michigan
August 2003

About the Author

S. M. Blinder is professor emeritus of chemistry and physics at the University of Michigan, Ann Arbor. Born in New York City, he received his PhD in chemical physics from Harvard in 1958 under the direction of W. E. Moffitt and J. H. Van Vleck (Nobel Laureate in Physics, 1977). Professor Blinder has over 100 research publications in several areas of theoretical chemistry and mathematical physics. He was the first to derive the exact Coulomb (hydrogen atom) propagator in Feynman's path-integral formulation of quantum mechanics. He is the author of two earlier books: *Advanced Physical Chemistry* (Macmillan, 1969) and *Foundations of Quantum Dynamics* (Academic Press, 1974).

Professor Blinder has been at the University of Michigan since 1963. He has taught a multitude of courses in chemistry, physics, mathematics and philosophy, mostly, however, on the subject of quantum theory. In earlier incarnations he was a Junior Master in chess and an accomplished cellist. He is married to the classical scholar Frances Ellen Bryant with five children.

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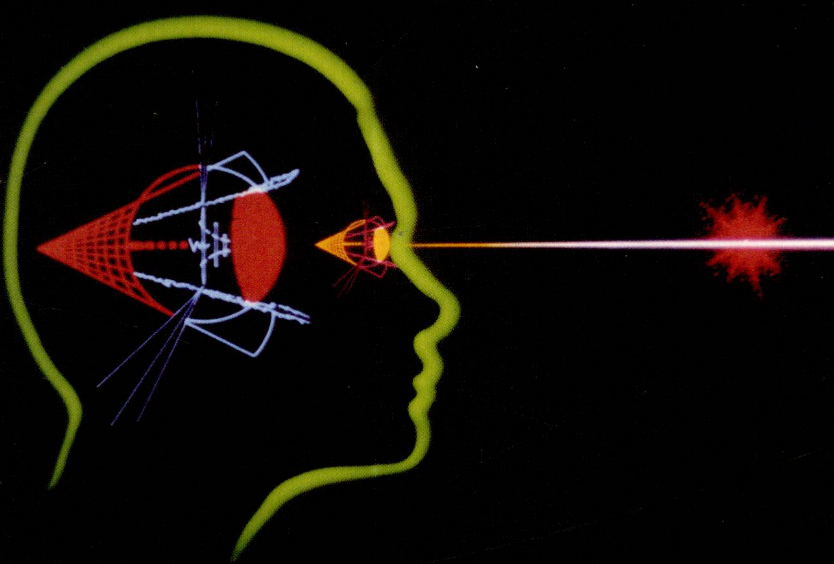

Paul Davidovits

Physics in Biology and Medicine

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Paul Davidovits *Boston College*

This is a book you should consider if you are teaching the one-semester premed course. This text could be used in two ways: 1) as a text for a one-term course in the physics of the body (without calculus) for non-physics majors in premed or allied health programs, or 2) as a supplementary text for the introductory physics course, particularly for premed students.

—RUSSELL HOBBIE
University of Minnesota, retired

There is certainly a viable market [for this book], if not as a stand-alone physics text, as a collection of problems, examples, and discussions at the boundary between physics and biology/medicine. It is very well written; it is certainly accurate; and it is pretty complete.

—DAVID CINABRO
Wayne State University

Paul Davidovits, Professor of Chemistry at Boston College, was co-awarded the prestigious year 2000 R.W. Wood prize from the Optical Society of America for his seminal work in optics. His contribution was foundational in the field of confocal microscopy (discussed herein), which allows engineers and biologists to produce optical sections through 3-D objects such as semiconductor circuits, living tissues, or a single cell. Dr. Davidovits earned his doctorate, masters, and undergraduate degrees from Columbia University. Prior to his appointment at Boston College, he was a faculty member at Yale University. He has published more than 100 papers in physical chemistry.

At one time scientists believed that a "vital force" governed the structure and organization of biological molecules. Today, most scientists realize that organisms are governed by the laws of physics on all levels.

While almost two centuries of research have found that physical laws fully apply to biology, work is far from complete. Basic questions at the atomic, molecular, and organismal levels remain unanswered. Even when typically complex molecular structure is known, function is not yet predictable. Nourishment, growth, reproduction, and communication distinguish biological matter from inorganic matter, yet these mechanisms are understood only qualitatively.

This book furthers our understanding by relating important concepts in physics to living systems. Applications of physics in biology and medicine are emphasized, with no previous knowledge of biology required. The analysis is largely quantitative, but only high-school physics and mathematics are assumed. Underlying basic physics appears in appendices. Biological systems are described in only enough detail for physical analysis.

The organization is similar to basic physics texts: solid mechanics, fluid mechanics, thermodynamics, sound, electricity, optics, and atomic and nuclear physics. A bibliography gives important sources for further reading.

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John B. Kogut

Introduction to Relativity

John B. Kogut *University of Illinois at Urbana-Champaign*

This is an excellent text that covers special relativity and a first time introduction to general relativity at an accessible level. The book achieves its goals by providing a pedagogical derivation of all the important concepts from first principles and using only elementary mathematical tools. It should fill an important gap in the literature.
—MIRJAM CVETIC
University of Pennsylvania

This book is an excellent introduction to special relativity in a manner that appropriately reflects the modern view of the subject. . . . With this text in hand, there is little excuse for any good undergraduate in any of the sciences to graduate without a pretty good understanding of the essentials.
—CHARLES C. DYER
University of Toronto

John Kogut is professor of physics at the University of Illinois at Urbana-Champaign. His specialty is high-energy theoretical physics, in particular, the physics of quarks and gluons. He has authored more than 200 articles and reviews, including pioneering papers on the light-cone approach to field theory, the Parton model, the statistical mechanics approach to field theory, and computational methods in high energy (lattice gauge) theory. Dr. Kogut was nominated for the 1987 Nobel Peace Prize (with M. Weissman, L. Gronlund, and D. Wright) by thirty members of the U. S. House of Representatives. A former Sloan Foundation and Guggenheim Fellow, he was educated at Princeton and Stanford Universities.

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This book is a unique, concise, and accessible foundation for the study of special and general relativity. It is written for anyone drawn to the rich intellectual and philosophical implications of relativity, especially undergraduate physics, engineering, and astronomy majors who may go on to study modern astrophysics, cosmology, and unified field theories.

Special relativity is developed from two basic notions: that force-free frames of reference are indistinguishable and that nature possesses a universal speed limit—the speed of light. Basic results are introduced with a minimum of algebra by constructing clocks and meter sticks so that time dilation, space contraction, and the relativity of simultaneity can be derived, explained, and illustrated. Minkowski diagrams are introduced to visualize these effects concretely. The Twin Paradox is resolved in detail. The roles of force, energy and momentum, and conservation laws in particle collisions are presented and illustrated through discussions and problems.

Although many topics of general relativity require some mathematical and physical background, Chapters 7 and 8 of the book successfully describe the core tenets at the basic level of the previous six chapters on special relativity. The Equivalence Principle is explained as the centerpiece of Einstein's theory of gravity. It states that a uniform gravitational field produces an environment that is physically indistinguishable from that in a uniformly accelerating reference frame. The gravitational red shift, the Twin Paradox as a problem of twins aging at different rates in different gravitational potentials, and the bending of light in a gravitational field are discussed and illustrated. The formulation of gravity as the theory of curved space-time is introduced at an elementary level.

The book contains a wealth of instructional and thought-provoking problems.

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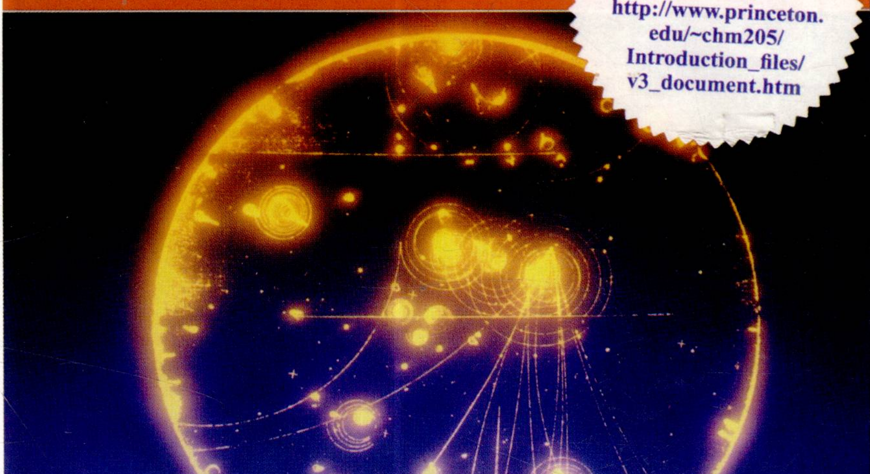

Warren S. Warren

The Physical Basis of Chemistry

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...is even more broadly applicable to the current generation of students...

"This is a great book to supplement either an advanced general chemistry course or a junior-level physical chemistry course. It would serve opposite functions in those two settings, but would work well in either. As a supplement to an introductory chemistry textbook, it would provide mathematically advanced students with additional challenge and rigor. As a supplement to a physical chemistry textbook, it would provide a bridge between the standard introductory material and the mathematically more sophisticated physical chemistry texts."
—DEBORAH HUNTLEY
Saginaw State University

Warren S. Warren, Professor of Chemistry at Princeton University, received his Ph.D. in Chemistry from U.C. Berkeley in 1980. His publications range from *Physical Review Letters* and invited papers in *Science* on his research in nuclear magnetic resonance and ultrafast laser spectroscopy to the *Journal of Chemical Education*. He received the 1982 Nobel Laureate Signature Award of the American Chemical Society and has held numerous fellowships.

Lord Ernest Rutherford, 1908 Nobel Laureate in Chemistry, put it bluntly:

Science is divided into two categories: physics and stamp collecting.

But he would have been astonished to see the transformation of biology from "stamp collecting" into molecular biology, genomics, biochemistry, and biophysics in this century. This transformation occurred only because, time and time again, fundamental advances in theoretical physics drove the development of useful new tools for chemistry. Chemists in turn learned how to synthesize and characterize ever more complex molecules, and eventually created a quantitative framework for understanding biology and medicine.

This book presents the physical, mathematical, and statistical concepts necessary for understanding the structure and function of molecules. The emphasis is placed on understanding the critical core material in quantum mechanics, thermodynamics, and spectroscopy that should be understood by any scientist or student of science. It is designed to enhance any general chemistry text by reintroducing concepts that require a little mathematical sophistication. It is also useful as a stand-alone background text for introductions to materials science, biophysics, and clinical imaging.

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