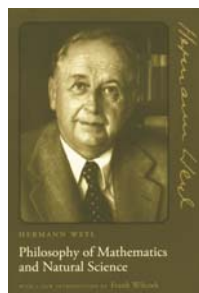


pioneered the application of group theory to quantum theory. He also initiated the gauge principle, in his unification of electromagnetism and gravity proposed in 1918 immediately after Albert Einstein's formulation of general relativity.

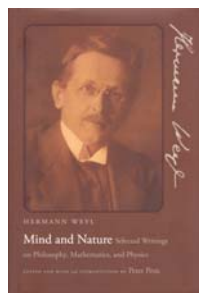
Weyl's genius had another aspect: his engagement with and writings on foundational, even philosophical, aspects of mathematics, physics, and the scientific worldview. His book *Philosophy of Mathematics and Natural Science* is a masterpiece. The original was written in German for the *Handbuch der Philosophie* and published in 1927. An authorized 1949 English translation by Olaf Helmer from Princeton University Press contained numerous corrections, additions, and six appendices spanning 80 pages. In view of the 20 years separating the German original and the American release, Weyl considered rewriting the book in English himself, but ultimately rejected the idea. In the preface, he writes, "How could I hope to recapture the faith and spirit of that epoch of my life when I first composed it ... after due literary preparations dashing off the manuscript in a few weeks?" The translation has long been out of print, so this recent republication, with a very fine introduction by Frank Wilczek, is to be highly valued.

Of course, every book, even one by a genius, is a creature of its time. So Weyl's discussions of some topics—especially in cosmology, molecular biology, and evolutionary theory, which have exploded since 1949—now seem either dated or too brief. But even in such cases, Weyl's grasp of the contemporary science is thorough and his awe at the intricacy and unity of nature and his open-mindedness about unsolved scientific problems make inspirational reading. Besides, when we consider foundational topics of mathematics or physics that were center stage in Weyl's time, his discussions are always both wise and thought-provoking. One example in the foundations of mathematics is Weyl's discussion of his doctoral adviser David Hilbert's formalism; to Hilbert's chagrin, Weyl was drawn to L. E. J. Brouwer's intuitionism. An example from physics is Weyl's discussion of quantum theory, which is full of expository detail from spectroscopy to noncommutativity and entanglement—Weyl admits that "the meaning of quantum physics ... is not yet clari-



fied as thoroughly as ... relativity theory" (p. 264). There are also wise yet very individual discussions of much more specific topics—for example, the nature of the continuum and why space is three-dimensional. Weyl's *Philosophy of Mathematics and Natural Science* should be on every mathematician's or physicist's bookshelf.

Weyl's *Mind and Nature: Selected Writings on Philosophy, Mathematics, and Physics* is of more interest to historians or to philosophers like me, but I still heartily recommend it to physicists and mathematicians. A selection of philosophical writings from the period 1921–55, it is beautifully edited with an introduction and scholarly endnotes by Peter Pesic. *Mind and Nature* includes several treasures: two lecture series, from 1932 and 1934; two letters from 1922—one by Weyl and the other by Einstein—about relativity theory's bearing on the idea of mechanism; and a touchingly personal essay from 1955 about "the part which philosophical reflection ... has played in my life" (p. 204). From that essay, it emerges—to the dismay of any philosopher trained in the analytic tradition!—that Weyl was profoundly influenced by Edmund Husserl's phenomenology and its roots in German idealism, a school of philosophy that tries to deduce



substantial conclusions about what we know and how we know it by analyzing experience.

There are other texts about Weyl's scientific legacy: His *Classical Groups* (1939), *Algebraic Theory of Numbers* (1940), and *Symmetry* (1952; all from Princeton University Press) and his *Theory of Groups and Quantum Mechanics* (Methuen, 1931; Dover, 1950) remain in print and are inspiring reads. Top-quality scientific and historical commemorations of his work and legacy continue to be published. Two examples are *Hermann Weyl's Raum-Zeit-Materie and a General Introduction to His Scientific Work*, edited by Erhard Scholz (Birkhauser, 2001), and *Groups and Analysis: The Legacy of Hermann Weyl*, edited by Katrin Tent (Cambridge University Press and London Mathematical Society, 2008).

Reading *Philosophy* and *Mind and Nature* was a poignant experience for me, since so many pages reminded me of how Nazism destroyed German science and philosophy. Taken together,

these books give a remarkably detailed and fascinating picture of Weyl's philosophical outlook in the last 30 years of his life. What a pleasure, what a privilege, to read and contemplate Hermann Weyl's monumental achievements.

Jeremy Butterfield
Trinity College
Cambridge, UK

Ab Initio Molecular Dynamics

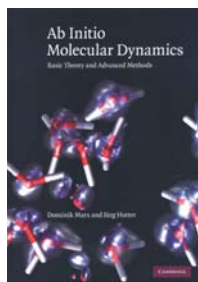
Basic Theory and Advanced Methods

Dominik Marx and Jürg Hutter
Cambridge U. Press, New York,
2009. \$80.00 (567 pp.).
ISBN 978-0-521-89863-8

The dynamics of molecules in a material or a chemical reaction can be simulated by calculating the time history of the internuclear coordinates according to the potential that governs internuclear motion. By the Born–Oppenheimer approximation, the potential is the electronic energy plus internuclear repulsion evaluated at a fixed internuclear configuration. Such simulations are useful in areas as diverse as nanoscale science, quantum photochemistry, combustion, biochemistry, catalysis, and atmospheric and environmental chemistry.

In the formative years of molecular dynamics simulations, the potential was represented by an analytic function, and only after hit-or-miss attempts to fit electronic-structure energy calculations or experimental data to potential functions could the dynamics be determined. However, about 35 years ago, a new approach began to replace that unsystematic, labor-intensive process. Direct dynamics, as it became known, does not require the fitting of the potential or force to an analytic function: The results of an electronic-structure calculation of the potential are used directly, without fitting, to advance the time step whenever the dynamics algorithm calls for energy or force. Direct dynamics began in the 1970s, and now a plethora of approaches are available in which either density functional theory or wavefunction theory is used to acquire the electronic energies. That this evolving field now has a pedagogical monograph in the form of Dominik Marx and Jürg Hutter's *Ab Initio Molecular Dynamics: Basic Theory and Advanced Methods* is a significant milestone.

The terms used in the book's title, and in the field in general, are often



the charge of an electron. However, many physicists and materials scientists—including Marx and Hutter—apply the *ab initio* label to density functional theory, even though the density functional approximations that are most frequently used have some empirical character. Also, Marx and Hutter's use of "molecular" in their title is too restrictive since the methods contained in their book can be applied to problems such as determining the structure of metallic nickel or of ceramic yttrium-doped strontium cerate—materials that do not contain molecules.

Even the term "quantum dynamics" is ambiguous. I use it to indicate that the dynamics, as opposed to the potential, is treated quantum mechanically. Some experts, though, use it even when the dynamics is classical, provided that the potential comes from explicitly quantal calculations. Marx and Hutter use the term "molecular dynamics" to denote any classical or semiclassical time-dependent method of propagating the coordinates of the nuclei in a system composed of atoms; for them, "*ab initio*" molecular dynamics means that the potential is obtained via an explicitly quantum treatment. Also, some experts refer to analytical potential functions as molecular mechanics, but Marx, Hutter, and others often call the same functions classical even if they were derived from fitting quantal electronic-structure calculations or from quantal experiments.

In most of *Ab Initio Molecular Dynamics*, the internuclear motion is treated as classical, but there is also an up-to-date 33-page section on path-integral approximations to quantal dynamics. Although direct dynamics can be applied with a variety of electronic-structure propagation algorithms, this book focuses squarely on Kohn-Sham density functional methods and the extended-Lagrangian-type propagation schemes introduced in 1985 by Roberto Car and Michele Parrinello. Furthermore, even within that restriction, the density functionals considered are largely restricted to the generalized gradient approximation, which no longer represents the state of the art in density functional approximations. However, I applaud the

authors for introducing the projector-augmented-wave method as an alternative to pseudopotentials for representing core electrons and for introducing the combined quantum mechanical and molecular mechanical method.

In a book replete with 1669 references, reviews of algorithmic developments, equations, flow charts, lines of code, and comments on software program organization, it is a mark of the field's maturity that not all widely used approaches are covered. For example, *Ab Initio Molecular Dynamics* introduces metadynamics as the method for sampling rare events in statistical ensem-

bles; the more standard approach of umbrella sampling is not mentioned. However, a student or newcomer to the field of molecular dynamics will find the approaches discussed in *Ab Initio Molecular Dynamics* a good place to start.

The section on excited electronic states is a useful overview of several approaches, but is disappointing in its treatment of dynamics. For example, the authors say that the Zhu-Nakamura approach cures the shortcomings of Landau-Zener-Stueckelberg theory, but neither captures the multidimensional nature of surface crossings and locally avoided crossings in polyatomic

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systems. Also missing is a discussion of decoherence.

Ab Initio Molecular Dynamics is not a self-contained work. In many cases the authors present equations without sufficient background to motivate the operations and without sufficient detail. Also, I found it hard to follow the book in places except by consulting its well-placed references. On the plus side, the text is written clearly and informed by the state-of-the-art research experiences of the authors themselves. Reading it is a valuable experience akin to spending time in their research groups.

Donald G. Truhlar
University of Minnesota
Minneapolis

Gamma-Ray Bursts

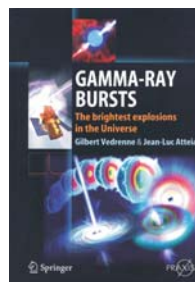
The Brightest Explosions in the Universe

Gilbert Vedrenne and Jean-Luc Atteia
Praxis/Springer, New York, 2009.
\$189.00 (571 pp.).
ISBN 978-3-540-39085-5

As one popular saying goes: "When you have seen one gamma-ray burst,

you have seen *one* gamma-ray burst." Since the discovery of GRBs in 1973, scientists have been mystified and enthralled by these astronomical phenomena, not only for their extreme energies, but also for the broad variations in their burst luminosities, peak fluxes, morphology, time structure, and spectral energy distributions. In-deed, GRBs have produced a rich field of study for more than 35 years.

In *Gamma-Ray Bursts: The Brightest Explosions in the Universe*, French gamma-ray astronomers Gilbert Vedrenne and Jean-Luc Atteia have summarized both the observational history and the theoretical understanding of GRBs through 2007. Vedrenne has been involved in gamma-ray astronomy since before the first GRB was reported, and experimentalist Atteia has been studying the gamma-ray sky since the early 1980s. Tapping into their wide and deep perspectives, the authors write an engaging account of the field, covering the accidental discovery of the first GRB by instruments designed to monitor atmospheric nuclear test ban violations and the years of early observations by an international armada of satellites.



For more than 20 years, the leading GRB progenitors were thought to be neutron stars in our own galaxy. The energies required to produce those titanic explosions at cosmological distances were unimaginable, and hints of cyclotron lines in early experiments were consistent with a neutron-star origin. In the 1990s that picture changed dramatically. Accurate x-ray positions determined by scientists using the Italian *BeppoSAX* satellite to study the burst afterglow phase enabled the identification of optical counterparts and the subsequent determination of distance using optical redshifts. It was also during that time that NASA's *Compton Gamma Ray Observatory* determined the isotropic distribution of GRBs in the sky, which led, in many observers' minds, to a cosmological origin for the bursts. We now know that GRBs are located at cosmological distances, that many of them are accompanied by afterglows at x-ray- to radio-wavelength energies, and that they appear to fall into two categories—long and short. Vedrenne and Atteia recount that history in the first four chapters of their text, describing the famous bursts of the *BeppoSAX* era and those observed with the MIT-based international *HETE* (*High Energy Transient Explorer*) 2 and NASA's *Swift* satellites.

Following the introductory chapters, the authors lay the theoretical framework for bursts and other related phenomena such as GRB afterglows, jet formation, fireballs, and blastwaves. Despite the complex physics, they do an admirable job of summarizing the wide range of theoretical models that are currently vying to explain GRB observations. This section functions more as a technical reference when compared to the more broadly accessible earlier chapters. Throughout the book, each chapter is packed with references to the original papers and offers concluding remarks that summarize the main points and the outstanding issues. This book will be appreciated by graduate students and practicing scientists, if they can afford the \$189 price tag. Govert Schilling and Naomi Greenberg-Slovin's *Flash! The Hunt for the Biggest Explosions in the Universe* (Cambridge University Press, 2002) is more accessible and affordable, and is the book I recommend to my undergraduate students.

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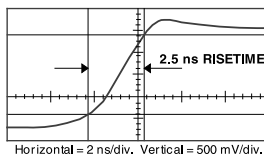
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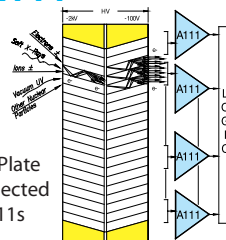
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Gain-Bandwidth f_T > 1.5 GHz
Power: 19 mW typical
Slew rate: >475 V/ μ s



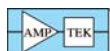
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