

BOOK REVIEWS | AUGUST 01 2017

## ***Interacting Electrons: Theory and Computational Approaches*** **FREE**

**Interacting Electrons: Theory and Computational Approaches.** Richard M. Martin Lucia Reining David M. Ceperley 842 pp. Cambridge U.P., New York, 2016. Price: \$89.99 (hardcover). ISBN 978-0-521-87150-1.

Justin C. Smith; Kieron Burke



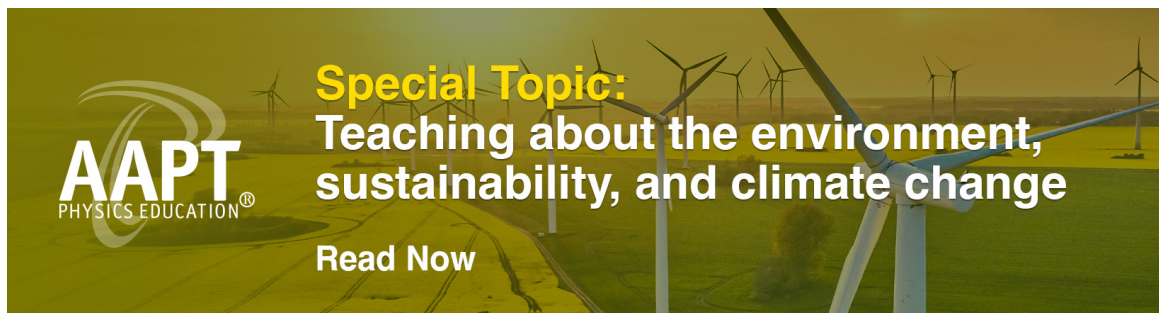
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**QBism: The Future of Quantum Physics.** Hans Christian von Baeyer. 265 pp. Harvard U.P., Cambridge, MA, 2016. Price: \$24.95 (hardcover). ISBN 978-0-674-50464-6. (Richard Healey, Reviewer.)

QBism is not a homophonic quantization of an early 20th century art movement but an increasingly influential set of ideas on how to understand quantum theory and its implications for science. This engaging book may serve as its popular manifesto.

What came to be known as quantum Bayesianism and later QBism began at the turn of the 21st century as a point of view on states and probabilities in quantum theory developed by physicists working in quantum information theory. More recently, the QBist vision of science has extended beyond quantum theory.

Applied to radioactive decay, the Born Rule of quantum theory successfully predicts such things as the half-life of the first excited state of the hydrogen atom. Most physicists regard this and other probabilities predicted by quantum theory as objective physical features of the world, typically identifying the probability of decay with the relative frequency of decay as measured in an experiment. But any probability between 0 and 1 inclusive is *logically* consistent with any actual relative frequency, however improbable, and appealing to the low probability of a radically deviant frequency renders a frequency account of probability circular.

QBists agree with De Finetti and some (though not all) statisticians who hold that there is no such thing as objective probability—there are only the various degrees of belief each of us has regarding matters of which he or she is currently ignorant. The quantum state yields probabilities of measurement outcomes, and QBists also adopt a subjectivist or personalist interpretation of quantum states. For them, a quantum state assignment does not represent the state of the physical world but the state of mind of the one who assigns it, and the Schrödinger equation does not describe the evolution of the system to which she assigns this state but tells her how to modify her beliefs about what she will find when measuring it (if she learns nothing new in the interim).

After a brief introduction, von Baeyer's book is in three parts. The first and longest part offers a general reader an almost equation-free historical introduction to quantum theory. Part II is a brief overview of probability, emphasizing its applications in daily life as well as quantum theory. The author presents criticisms of classical and frequentist interpretations of probability; he illustrates an application of Bayes' theorem to determine one's probability of having cancer given a positive test result; and he argues that its versatility, generality, and logical consistency recommend a subjective Bayesian interpretation as the primary interpretation of probability. While the medical example illustrates

Bayes' theorem, it does nothing to bolster this argument since a frequentist will identify the prior probability of cancer with the base rate in the population.

We finally meet QBism in the six short chapters of Part III. von Baeyer anticipates the shocked reaction against its subjectivity he expects from those (like him) for whom physics represented an ideal of objective scientific inquiry into the nature of reality. His prior defense of subjective Bayesianism may have softened the blow, but many will still be reluctant to abandon the view that a system's wave-function represents its objective physical state. To convince them to do so, he argues that QBism's subjective view of quantum states and probabilities naturally resolves "paradoxes" of wave-collapse, Wigner's friend, and Schrödinger's cat, while doing away with "spooky" action at a distance.

If a system's wave-function represents its objective physical state, then wave-collapse (von Neumann's projection postulate, Dirac's quantum jump) is a physical process whose occurrence is difficult or impossible to reconcile with Schrödinger evolution, relativistic spacetime structure, and local action. But for a QBist there is no problem since there is no such process. Any user of quantum theory should merely reassign her wave-function to update her personal degrees of belief on learning the outcome of a measurement. Wigner and his friend may assign different wave-functions, reflecting their different experiences about what happens inside the friend's isolated laboratory. The superposed entangled quantum state assigned to Schrödinger's cat represents not its physical state but the assigner's state of belief about what he will find when opening the box with the cat in it. There is no Einstein-Podolsky-Rosen paradox because their criterion of reality is false: no element of reality is required to ground a prediction with probability unity—merely the subjective certainty of the one who makes the prediction. Bell's theorem does not demonstrate instantaneous action at a distance because quantum correlations violating Bell inequalities concern not the outcomes of spatially separated measurements but a *localized* agent's expectations about such outcomes.

I believe such undoubted benefits of QBism may be purchased more cheaply, as I explain elsewhere.<sup>1</sup> Sometimes two agents should assign to a system different quantum states because their physical (not mental) situations give them access to different information. But physical conditions determine an objectively correct state assignment for each situation. The resulting Born probabilities represent neither frequencies nor any agent's actual degrees of belief, but the objectively correct degrees of belief for anyone who happened to be in that situation. They exemplify an *objective* Bayesian account of probability. In favorable circumstances, their correctness may be experimentally manifested by relative frequencies.

Just over a century ago, a reviewer of the cubist manifesto wrote “their theory of painting is founded upon a philosophic idealism. It is impossible to paint things ‘as they are,’ because it is impossible to know how and what they ‘really’ are;” and that the manifesto’s whole object is “to defend cubism as the liberator from systems, the means of expression of the one truth, which is the truth in the artist’s mind.” That’s all very well for art, you may say, but not for a hard science like physics, which aims to say how the objective world really is and what laws govern it.

Von Baeyer defends his QBist manifesto against such skepticism in the final, more philosophical, part of his book, which matches its subtitle *The Future of Quantum Physics*. He foresees not only the general acceptance of a QBist interpretation of quantum theory but also the extension of the QBist vision of science to the rest of physics and beyond. He views laws of nature as created by us to economically summarize what we have experienced and takes QBism to honor Wheeler’s vision of a participatory universe in which “particles” and agents jointly create a universe whose external reality is manifested by the unpredictable experiences that result from each agent’s interactions with it. According to QBists Chris Fuchs and David Mermin, each agent uses quantum theory not so much to predict the outcomes of experiments as to better anticipate his or her individual experiences of them as well as other people’s reports of their experiences. Von Baeyer seeks to secure the objectivity of QBist science by appeal to a large common core of shared experiences, but it is not clear what this comes to if all I know of your experiences is what I hear from your lips.

Von Baeyer’s understanding of QBism is reliably based not only on familiarity with QBist writings but also on many conversations with its proponents, whose views he quotes, especially in the last part of his book. Many physicists, including Einstein and Bell, aspired to create a perfect map or model of ultimate physical reality. QBism scotches that aspiration: for a QBist “science is not about ultimate reality but about what we can reasonably expect” (p. 221). Is this an admission of defeat? Not according to Marcus Appleby, for whom a world we could perfectly map would be too confining—as limited as ourselves.

Today, QBism offers just one of a wide variety of radically different takes on quantum theory, each with its supporters. Converts like von Baeyer make especially enthusiastic advocates, and this book is a simply and attractively written manifesto that fairly and concisely represents the view its author favors. Any physicist who skips or ploughs through its first part will then be rewarded by an elementary introduction to the main QBist ideas, which may or may not encourage a deeper study. A general reader should be warned that QBism is today a radical minority view among physicists. As a philosopher of physics, I found the treatment of probability overly brisk and remain unpersuaded by von Baeyer’s defense of the objectivity of QBist science.

<sup>1</sup>R. Healey, “Quantum states as objective informational bridges,” *Found. Phys.* **47**, 161–173 (2017); , “Quantum-Bayesian and pragmatist views of quantum theory,” in *The Stanford Encyclopedia of Philosophy* (Spring

2017 Edition), Edward N. Zalta (ed.), available at <<https://plato.stanford.edu/archives/spr2017/entries/quantum-bayesian/>>.

*Richard Healey is Professor of Philosophy at the University of Arizona. As a philosopher of physics, he has been trying to understand quantum theory for over 40 years while seeking to convince physicists and philosophers how much they stand to learn from each other by cooperating in this undertaking. His forthcoming book The Quantum Revolution in Philosophy represents his latest attempt to do both.*

### **Interacting Electrons: Theory and Computational Approaches.**

Richard M. Martin, Lucia Reining, and David M. Ceperley. 842 pp. Cambridge U.P., New York, 2016. Price: \$89.99 (hardcover). ISBN 978-0-521-87150-1. (Justin C. Smith and Kieron Burke, Reviewers.)

Condensed matter is the largest, most diverse field of physics, and perhaps the one with the most immediate impact on our everyday lives. Electronic structure theory is playing an ever increasing role in this field, as both our computers and our abilities to create complex materials are constantly improving.

For materials, there are two fairly distinct approaches. The more traditional is to write some model Hamiltonian that describes the most important physics, fit its parameters to experimental information, and find accurate (if not exact) solutions to this Hamiltonian. This remains the dominant paradigm in strongly correlated systems, where even a qualitative understanding of some exotic phenomena are missing such as for the cuprate and pnictide superconductors.

The other approach is to take the full electronic Hamiltonian, and attempt to accurately solve the quantum mechanics without empirical input. This is called first-principles, and often the primary aim is to find the ground-state energy extremely accurately, as very tiny energy differences determine, for example, where molecules will adsorb on a surface or how fast a chemical reaction will occur. This pursuit is shared by quantum chemists for molecules and computational scientists working on materials, and even some in geoscience.

The starting point of most such investigations is Kohn-Sham density functional theory (DFT), and Richard Martin’s book *Electronic Structure: Basic Theory and Practical Methods* (2004) is an indispensable guide to this subject. Density functional theory is a tremendous physics success story, but relatively underappreciated in its home community. For example, density functional theory calculations were behind the prediction<sup>1</sup> and subsequent finding<sup>2</sup> of the world’s highest temperature (203 K) superconductor, hydrogen sulfide under pressure. These calculations are now so widespread that John Perdew, the condensed matter theorist responsible for much of modern density functional theory development, is substantially more cited than Ed Witten, Phil Anderson, or Walter Kohn. (In fact, Perdew appears to be the most cited physicist ever.)

But most physicists, while they need to know where the atoms are and what reactions will occur, care more about the



response of a material to external stimuli (photons, electrons, etc.) than to, e.g., its cohesive energy. Basic density functional theory is designed to yield only ground-state properties. Moreover, the popular approximations in density functional theory tend to fail for strongly correlated systems, which include many of the oxide materials vital to energy technologies. There is an extreme need to both extract response properties and to develop more accurate, reliable alternatives to vanilla density functional theory. Moreover, density functional theory takes such a radically different approach from the outset that it is almost impossible to connect it with standard approaches to solving the Schrödinger equation. (The simple two-site Hubbard model can be a good starting point.<sup>3</sup>)

This is the great value of *Interacting Electrons: Theory and Computational Approaches*. It provides an overview of the interacting electron problem, but also lays a fairly complete introduction to density functional theory and Green's functions. The main purpose of this book is to go well beyond density functional methods and in doing so it provides the foundations of the GW approximation, the Bethe-Salpeter equation, Dynamical Mean Field Theory, quantum Monte Carlo, and much more. There is significant breadth in these topics, but *Interacting Electrons* does a noteworthy job of introducing them in a sensible order and paying homage to the influences and differing approaches from which they arose. This may be the only volume in which all these topics are simultaneously treated with sufficient depth and in a shared framework—laying the conceptual basis, showing the actual methods (often with handy flowcharts), and demonstrating various applications, including descriptions of areas within condensed matter that have benefited from these methods. The appendices are also of very high quality and are an indispensable tool for bringing readers up to speed.

We recommend this book strongly for at least three disparate audiences. Because of the excellent treatment of fundamentals, this should be required reading for a second or third year graduate student who runs materials calculations but also wants a deeper understanding of the underlying theory. It is also a must-read for anyone working in strongly-correlated systems who needs to understand the performance and limitations of these many approaches to electronic structure. And while this is certainly not a book about molecules, with only passing references at best, it does form an excellent self-contained starting point for quantum chemists who are working on materials problems and wish to learn the strengths and weaknesses of materials methods and codes.

Finally, this book provides a great reference for all those folks who are *not* running such calculations, but need to read and understand the papers of those who are.

<sup>1</sup>D. Duan, Y. Liu, F. Tian, D. Li, X. Huang, Z. Zhao, H. Yu, B. Liu, W. Tian, and T. Cui, "Pressure-induced metallization of dense (H<sub>2</sub>S)<sub>2</sub>H<sub>2</sub> with high-Tc superconductivity," *Sci. Rep.* **4**, 6968 (2014).

<sup>2</sup>A. P. Drozdov, M. I. Erements, I. A. Troyan, V. Ksenofontov, and S. I. Shylin, "Conventional superconductivity at 203 kelvin at high pressures in the sulfur hydride system," *Nature* **525**, 73–76 (2015).

<sup>3</sup>D. J. Carrascal, J. Ferrer, J. C. Smith, and K. Burke, "The Hubbard dimer: A density functional case study of a many-body problem," *J. Phys.: Condens. Matter* **27**, 393001 (2015).

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*Kieron Burke is a Chancellor's Professor of Chemistry and of Physics at University of California, Irvine, and has worked on electronic structure theory for about 25 years.*

**Void: The Strange Physics of Nothing.** James Owen Weatherall. 196 pp. Yale U.P., New Haven, CT, 2016. Price: \$26 (hardcover). ISBN 978-0-300-20998-3. (Peter W. Milonni, Reviewer.)

Fields are believed to be the fundamental constituents of the universe, particles being excitations, or quanta, of fields. There are quantum fluctuations of fields even in a space with no particles. The photon number, for example, can be zero while the electric and magnetic fields fluctuate about their zero averages. The most important effect, historically, of these vacuum field fluctuations was discovered in the spectrum of the hydrogen atom. The energy levels of an electron in a Coulomb potential can be calculated exactly, but they do not exactly reproduce the observed hydrogen spectrum because the Coulomb interaction is not the whole story: the electron also interacts with the vacuum field. Experiments in the late 1940s revealed that the 2s<sub>1/2</sub> and 2p<sub>1/2</sub> levels of the hydrogen atom, which should be equal according to the solution of the Dirac equation for the Coulomb potential alone, differ by about 1058 MHz, the famous Lamb shift.

Another effect attributable to vacuum fields was predicted at around the same time by Hendrik Casimir. In a vacuum, there is energy associated with the field fluctuations, much like the zero-point energy of the ground state of the simple harmonic oscillator in quantum mechanics. Casimir considered the change in this energy caused by two perfectly conducting, uncharged parallel plates. When the plates are separated by a finite distance only certain field modes are possible, unlike when the plates are infinitely far apart. The vacuum energy in both cases is infinite, but Casimir derived a finite value for the energy difference that implied an attractive force between the plates. Experiments many years later verified Casimir's prediction, and recently a "dynamical Casimir effect," in which photons are created when one of the plates is very rapidly displaced, has been observed.

The possibility of creating particles out of a vacuum has been known for a long time. It was shown by Sauter in 1931 that electron-positron pair production can occur in a uniform electric field. This "sparking of the vacuum," or Schwinger pair production, requires field strengths on the order of 10<sup>18</sup> V/m and for this reason has not yet been directly observed. But other phenomena in which particles are created by interactions with vacuum fields have been observed in high-intensity laser experiments, for instance. Feynman diagrams suggest that the fluctuating vacuum can be imagined to consist of virtual particle-antiparticle pairs that are continually created and annihilated. Schwinger pair production is often interpreted heuristically as a pulling apart by the

field of virtual electron-positron pairs. Hawking radiation has been described as a result of virtual particles near the event horizon of a black hole falling in before annihilation can occur, their antiparticles then being free to escape as radiation.

Weatherall writes very readably, and without any equations or mystifying jargon, about the different conceptions of empty space in Newtonian physics, relativity, and quantum field theory, especially as they relate to what it means for there to be something rather than nothing. He wastes few words on the recent, heated debates about whether “the physics of nothing” can answer the age-old question of *why* there is something rather than nothing. Although his book is primarily a very gentle introduction to the physics of the vacuum and how our understanding of it has evolved, he includes many interesting notes and references to the research literature, and in an epilogue he explains the difficulties involved in constructing a quantum theory of gravity and touches briefly on the string landscape and other speculations.

Newton broke with Aristotelian ideas that motion could only result from pushing and pulling by something, and therefore was not possible in a vacuum, and with ideas about the structure of space that led Descartes to imagine a “plenum” filling all of space. Newton’s laws of motion described absolute, not relative motion, and he believed that absolute motion implied absolute space (and time), independent of any observer or point of reference, and with no plenum. In his famous rotating bucket experiment, he interpreted the concave shape of the water surface when there was no relative motion between the water and the bucket as a consequence of motion with respect to absolute space. Leibniz disagreed. His metaphysics led him to regard all motion as relational and to believe that there could be no absolute space.

After revisiting these old ideas about the structure of space, Weatherall describes work by Howard Stein to the effect that Newton erred in thinking that his laws required absolute space, and that in his bucket experiment Newton only showed “that there are physical consequences to a body’s accelerating.” Lacking both first-hand knowledge of the *Principia* and familiarity with Stein’s work, I can say nothing further about that. But I was somewhat surprised that nothing was said about Mach’s rejection of Newtonian absolute space and his influential conjecture that the curvature of the water surface in the bucket experiment is due to rotation with respect to “the mass of the earth and the other celestial bodies.” (Mach’s principle, that local inertial frames are determined by such large-scale distributions of mass, was taken seriously by Einstein.)

The discussions of the aether, Maxwell’s electromagnetism, special relativity, and Minkowski space-time, though covering territory very familiar to readers of this journal, are brisk and entertaining. Here and throughout the book, there are anecdotes about some of the characters in the story, the main character here being, of course, Einstein. Most relevant to “the physics of nothing” are the discussions about vacuum solutions of Einstein’s field equation relating the curvature

of space-time to the energy-momentum tensor. De Sitter found that the equation allows space-time curvature even in the absence of any “stuff.” Weatherall explains why Einstein “hated” de Sitter’s solution, and how he “ultimately accepted the possibility of empty space-times with complex structure.” As for the gravitational waves he discovered with his field equation, Einstein had periodic misgivings. At one point, he and Nathan Rosen submitted a paper to the *Physical Review* in which they concluded that gravitational waves do not exist. When the paper was rejected after a negative report by a referee, Einstein wrote an angry letter to the editor, saying he and Rosen had submitted their paper “for publication, not for review.” Howard Robertson, evidently without divulging that he had been the referee, later convinced Einstein that the arguments in the paper were incorrect, and in a revised paper Einstein and Rosen argued that gravitational waves were possible. Weatherall writes that “It is not clear [Einstein] ever reached a stable view on the matter,” and concludes the chapter with a paragraph on the recent confirmation of the existence of gravitational waves.

Perhaps, as John Wheeler said, “No point is more central than this, that empty space is not empty.” Empty space is certainly not “empty” in quantum field theory, which is generally thought, with good reason, to be one of the most successful theories in the history of science. The third and last chapter of this book focuses mainly on the development of the most accurately tested quantum field theory, quantum electrodynamics, beginning with some of the most “non-classical” features of quantum theory itself. The contributions of Dirac, Jordan, Feynman, Schwinger, and others are described, along with remarks about their personalities and opinions about the mathematical foundations of quantum field theory and its handling of infinities, which Dirac felt was “just not sensible mathematics.” Feynman, however, is said to have “dismissed worries about the mathematical rigor” of the theory. (I have a copy of a letter from Feynman to Wheeler, dated 19 May 1966, that reads, in its entirety, “Dear John, I am not interested in what today’s mathematicians find interesting. Kind regards. Sincerely yours, Richard P. Feynman,” signed “Dick.”) The importance of the first accurate estimate of the Lamb shift by Hans Bethe is appropriately emphasized, but its characterization as the first calculation of an observable consequence of vacuum polarization is inaccurate. Bethe’s result could be interpreted as an effect of the fluctuating vacuum field on the atom, or the emission and absorption of virtual photons, but he did not account for vacuum polarization, which was later found by others to contribute only about 27 MHz to the Lamb shift in hydrogen. I was somewhat surprised by the absence in the text of any discussion of the Casimir effect, which is arguably the most palpable effect attributable to the vacuum electromagnetic field and one that has been of particular interest in recent years. (Actually, the Casimir force can be explained, like Bethe’s result for the Lamb shift, without explicit reference to the vacuum field. But I digress.)

The vacuum has recently been the subject of quite a few books. This one might be the most congenial to readers who

are interested in “the physics of nothing” as it has come to be understood, but not in any of its more mathematical aspects. Its main message is that the physics of the vacuum is strange but fundamental, and it makes a good case for that.

*Peter W. Milonni is a Fellow of the Los Alamos National Laboratory and a Research Professor of Physics at the University of Rochester. He has worked in areas relating to quantum fluctuations of electromagnetic fields.*

## BOOKS RECEIVED

**The Physics of Cancer.** Caterina A. M. La Porta and Stefano Zapperi. 186 pp. Cambridge U.P., New York, 2017. Price: \$59.99 (hardcover) ISBN 978-1-107-10959-9.

**Quantum Scaling in Many-Body Systems: An Approach to Quantum Phase Transitions (2nd ed.).** Mucio Continentino. 245 pp. Cambridge U.P., New York, 2017. Price: \$69.99 (hardcover) ISBN 978-1-107-15025-6.

**An Introduction to X-ray Physics, Optics, and Applications.** Carolyn A. MacDonald. 365 pp. Princeton U.P., Princeton, NJ, 2017. Price: \$80 (hardcover) ISBN 978-0-691-13965-4.

**Rays, Waves, and Scattering: Topics in Classical Mathematical Physics.** John A. Adam. 612 pp. Princeton U.P., Princeton, NJ, 2017. Price: \$80 (hardcover) ISBN 978-0-691-14837-3.

**The Physical World: An Inspirational Tour of Fundamental Physics.** Nicholas Manton and Nicholas Mee. 569 pp. Oxford U.P., New York, 2017. Price: \$38.95 (paper) ISBN 978-0-19-879611-4.

**Precision Cosmology: The First Half Million Years.** Bernard J. T. Jones. 775 pp. Cambridge U.P., New York, 2017. Price: \$94.99 (hardcover) ISBN 978-0-521-55433-6.

**Natural Complexity: A Modeling Handbook.** Paul Charbonneau. 369 pp. Princeton U.P., Princeton, NJ, 2017. Price: \$49.50 (paper) ISBN 978-0-691-17035-0.

**The Philosophy of Cosmology.** Khalil Chamcham, Joseph Silk, John D. Barrow, and Simon Saunders (eds.). 526 pp. Cambridge U.P., New York, 2017. Price: \$69.99 (hardcover) ISBN 978-1-107-14539-9.

**Quantum Theory from First Principles: An Informational Approach.** Giacomo Mauro D’Ariano, Giulio Chiribella, and Paolo Perinotti. 357 pp. Cambridge U.P., New York, 2017. Price: \$74.99 (hardcover) ISBN 978-1-107-043425-8.

**Finn’s Thermal Physics (3rd ed.).** Andrew Rex. 386 pp. CRC Press, Boca Raton, FL, 2017. Price: \$51.96 (paper) ISBN 978-1-4987-1887-5.

**Get Funded: An Insider’s Guide to Building an Academic Research Program.** Robert J. Trew. 293 pp. Cambridge U.P., New York, 2017. Price: \$32.99 (paper) ISBN 978-1-107-65719-9.

**Principles of Radiometric Dating.** Kunchithapadam Gopalan. 221 pp. Cambridge U.P., New York, 2017. Price: \$74.99 (hardcover) ISBN 978-1-107-19873-9.

**Classical Field Theory.** Joel Franklin. 217 pp. Cambridge U.P., New York, 2017. Price: \$69.99 (hardcover) ISBN 978-1-107-18961-4.

**Practical Bayesian Analysis.** Coryn A. L. Bailer-Jones. 303 pp. Cambridge U.P., New York, 2017. Price: \$37.99 (paper) ISBN 978-1-316-64221-4.

**Ultracondensed Matter by Dynamic Compression.** William J. Nellis. 167 pp. Cambridge U.P., New York, 2017. Price: \$140 (hardcover) ISBN 978-0-521-51957-5.

**Universal Themes of Bose-Einstein Condensation.** Nick P. Proukakis, David W. Snoke, and Peter W. Littlewood (eds.). 661 pp. Cambridge U.P., New York, 2017. Price: \$100 (hardcover) ISBN 978-1-107-08569-5.

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