ELLIOTT H. LIEB
AND
ROBERT SEIRINGER

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CAMBRIDGE
UNIVERSITY PRESS

CAMBRIDGE UNIVERSITY PRESS
Cambridge, New York, Melbourne, Madrid, Cape Town, Singapore, São Paulo, Delhi

Cambridge University Press
The Edinburgh Building, Cambridge CB2 8RU, UK

Published in the United States of America by Cambridge University Press, New York

www.cambridge.org
Information on this title: www.cambridge.org/9780521191180

First published 2010

Printed in the United Kingdom at the University Press, Cambridge

A catalog record for this publication is available from the British Library

Library of Congress Cataloging in Publication data
Lieb, Elliott H.
The stability of matter in quantum mechanics / Elliott H Lieb, Robert Seiringer.
p. cm.
Includes bibliographical references and index.
ISBN 978-0-521-19118-0 (hardback)
1. Thomas-Fermi theory. 2. Quantum theory. 3. Matter – Properties. 4. Structural stability.
I. Seiringer, Robert. II. Title.
QC173.4.T48L543 2010
530.12 – dc22 2009031810

ISBN 978-0-521-19118-0 Hardback

THE STABILITY OF MATTER IN QUANTUM MECHANICS

Research into the stability of matter has been one of the most successful chapters in mathematical physics, and is a prime example of how modern mathematics can be applied to problems in physics.

A unique account of the subject, this book provides a complete, self-contained description of research on the stability of matter problem. It introduces the necessary quantum mechanics to mathematicians, and aspects of functional analysis to physicists. The topics covered include electrodynamics of classical and quantized fields, Lieb–Thirring and other inequalities in spectral theory, inequalities in electrostatics, stability of large Coulomb systems, gravitational stability of stars, basics of equilibrium statistical mechanics, and the existence of the thermodynamic limit.

The book is an up-to-date account for researchers, and its pedagogical style makes it suitable for advanced undergraduate and graduate courses in mathematical physics.

ELLIOTT H. LIEB is a Professor of Mathematics and Higgins Professor of Physics at Princeton University. He has been a leader of research in mathematical physics for 45 years, and his achievements have earned him numerous prizes and awards, including the Heineman Prize in Mathematical Physics of the American Physical Society, the Max-Planck medal of the German Physical Society, the Boltzmann medal in statistical mechanics of the International Union of Pure and Applied Physics, the Schock prize in mathematics by the Swedish Academy of Sciences, the Birkhoff prize in applied mathematics of the American Mathematical Society, the Austrian Medal of Honor for Science and Art, and the Poincaré prize of the International Association of Mathematical Physics.

ROBERT SEIRINGER is an Assistant Professor of Physics at Princeton University. His research is centered largely on the quantum-mechanical many-body problem, and has been recognized by a Fellowship of the Sloan Foundation, by a U.S. National Science Foundation Early Career award, and by the 2009 Poincaré prize of the International Association of Mathematical Physics.

To

Christiane, Letizzia and Laura

Preface

The fundamental theory that underlies the physicist's description of the material world is quantum mechanics – specifically Erwin Schrödinger's 1926 formulation of the theory. This theory also brought with it an emphasis on certain fields of mathematical analysis, e.g., Hilbert space theory, spectral analysis, differential equations, etc., which, in turn, encouraged the development of parts of pure mathematics.

Despite the great success of quantum mechanics in explaining details of the structure of atoms, molecules (including the complicated molecules beloved of organic chemists and the pharmaceutical industry, and so essential to life) and macroscopic objects like transistors, it took 41 years before the most fundamental question of all was resolved: Why doesn't the collection of negatively charged electrons and positively charged nuclei, which are the basic constituents of the theory, implode into a minuscule mass of amorphous matter thousands of times denser than the material normally seen in our world? Even today hardly any physics textbook discusses, or even raises this question, even though the basic conclusion of stability is subtle and not easily derived using the elementary means available to the usual physics student. There is a tendency among many physicists to regard this type of question as uninteresting because it is not easily reducible to a quantitative one. Matter is either stable or it is not; since nature tells us that it is so, there is no question to be answered. Nevertheless, physicists firmly believe that quantum mechanics is a 'theory of everything' at the level of atoms and molecules, so the question whether quantum mechanics predicts stability cannot be ignored. The depth of the question is further revealed when it is realized that a world made of bosonic particles would be unstable. It is also revealed by the fact that the seemingly innocuous interaction of matter and electromagnetic radiation at ordinary, every-day energies – quantum electrodynamics – should be a settled, closed subject, but it is not and it can be understood only in the context of perturbation theory. Given these observations, it is clearly important to know that at least the quantum-mechanical part of the story is well understood.

It is this stability question that will occupy us in this book. After four decades of development of this subject, during which most of the basic questions have gradually been answered, it seems appropriate to present a thorough review of the material at this time.

Schrödinger's equation is not simple, so it is not surprising that some interesting mathematics had to be developed to understand the various aspects of the stability of matter. In particular, aspects of the spectral theory of Schrödinger operators and some new twists on classical potential theory resulted from this quest. Some of these theorems, which play an important role here, have proved useful in other areas of mathematics.

The book is directed towards researchers on various aspects of quantum mechanics, as well as towards students of mathematics and students of physics. We have tried to be pedagogical, recognizing that students with diverse backgrounds may not have all the basic facts at their finger tips. Physics students will come equipped with a basic course in quantum mechanics but perhaps will lack familiarity with modern mathematical techniques. These techniques will be introduced and explained as needed, and there are many mathematics texts which can be consulted for further information; among them is [118], which we will refer to often. Students of mathematics will have had a course in real analysis and probably even some basic functional analysis, although they might still benefit from glancing at [118]. They will find the necessary quantum-mechanical background self-contained here in chapters two and three, but if they need more help they can refer to a huge number of elementary quantum mechanics texts, some of which, like [77, 22], present the subject in a way that is congenial to mathematicians.

While we aim for a relaxed, leisurely style, the proofs of theorems are either completely rigorous or can easily be made so by the interested reader. It is our hope that this book, which illustrates the interplay between mathematical and physical ideas, will not only be useful to researchers but can also be a basis for a course in mathematical physics.

To keep things within bounds, we have purposely limited ourselves to the subject of stability of matter in its various aspects (non-relativistic and relativistic mechanics, inclusion of magnetic fields, Chandrasekhar's theory of stellar collapse and other topics). Related subjects, such as a study of Thomas–Fermi and Hartree–Fock theories, are left for another day.

Our thanks go, first of all, to Michael Loss for his invaluable help with some of this material, notably with the first draft of several chapters. We also thank László Erdős, Rupert Frank, Heinz Siedentop, Jan Philip Solovej and Jakob Yngvason for a critical reading of parts of this book.

Elliott Lieb and Robert Seiringer
Princeton, 2009

The reader is invited to consult the web page http://www.math.princeton.edu/books/ where a link to errata and other information about this book is available.

Contents

CHAPTER 1

Prologue

1.1 Introduction

The basic constituents of ordinary matter are electrons and atomic nuclei. These interact with each other with several kinds of forces – electric, magnetic and gravitational – the most important of which is the electric force. This force is attractive between oppositely charged particles and repulsive between like-charged particles. (The electrons have a negative electric charge $-e$ while the nuclei have a positive charge $+Ze$, with $Z = 1, 2, \ldots, 92$ in nature.) Thus, the strength of the attractive electrostatic interaction between electrons and nuclei is proportional to Ze^2, which equals $Z\alpha$ in appropriate units, where α is the dimensionless **fine-structure constant**, defined by

$$\alpha = \frac{e^2}{\hbar c} = 7.297\,352\,538 \times 10^{-3} = \frac{1}{137.035\,999\,68}, \tag{1.1.1}$$

and where c is the speed of light, $\hbar = h/2\pi$ and h is Planck's constant.

The basic question that has to be resolved in order to understand the existence of atoms and the stability of our world is:

Why don't the point-like electrons fall into the (nearly) point-like nuclei?

This problem of classical mechanics was nicely summarized by Jeans in 1915 [97]:

> "There would be a very real difficulty in supposing that the (force) law $1/r^2$ held down to zero values of r. For the force between two charges at zero distance would be infinite; we should have charges of opposite sign continually rushing together and, when once together, no force would be adequate to separate them ... Thus the matter in the universe would tend to shrink into nothing or to diminish indefinitely in size."

A sensitive reader might object to Jeans' conclusion on the grounds that the non-zero radius of nuclei would ameliorate the collapse. Such reasoning is beside the point, however, because the equilibrium separation of charges observed in nature is not the nuclear diameter (10^{-13} cm) but rather the atomic size (10^{-8} cm) predicted by Schrödinger's equation. Therefore, as concerns the problem of understanding stability, in which equilibrium lengths are of the order of 10^{-8} cm, there is no loss in supposing that all our particles are point particles.

To put it differently, why is the energy of an atom with a point-like *nucleus* not $-\infty$? The fact that it is not is known as **stability of the first kind**; a more precise definition will be given later. The question was successfully answered by quantum mechanics, whose exciting development in the beginning of the twentieth century we will not try to relate – except to note that the basic theory culminated in Schrödinger's famous equation of 1926 [156]. This equation explained the new, non-classical, fact that as an electron moves close to a nucleus its kinetic energy necessarily increases in such a way that the minimum total energy (kinetic plus potential) occurs at some positive separation rather than at zero separation.

This was one of the most important triumphs of quantum mechanics!

Thomson discovered the electron in 1897 [180, 148], and Rutherford [155] discovered the (essentially) point-like nature of the nucleus in 1911, so it took 15 years from the discovery of the problem to its full solution. But it took almost three times as long, 41 years from 1926 to 1967, before the second part of the stability story was solved by Dyson and Lenard [44].

The second part of the story, known as **stability of the second kind**, is, even now, rarely told in basic quantum mechanics textbooks and university courses, but it is just as important. Given the stability of atoms, is it obvious that bulk matter with a large number N of atoms (say, $N = 10^{23}$) is also stable in the sense that the energy and the volume occupied by $2N$ atoms are twice that of N atoms? Our everyday physical experience tells us that this additivity property, or linear law, holds but is it also necessarily a consequence of quantum mechanics? Without this property, the world of ordinary matter, as we know it, would not exist.

Although physicists largely take this property for granted, there were a few that thought otherwise. Onsager [145] was perhaps the first to consider this kind of question, and did so effectively for classical particles with Coulomb interactions but with the addition of hard cores that prevent particles from getting too close together. The full question (without hard cores) was addressed by Fisher and Ruelle in 1966 [66] and they generalized Onsager's results to smeared out charges. In 1967 Dyson and Lenard [44] finally succeeded in showing that stability of the second kind for truly point-like quantum particles with Coulomb forces holds but, surprisingly, that it need not do so. That is, the *Pauli exclusion principle*, which will be discussed in Chapter 3, and which has no classical counterpart, was essential. Although matter would not collapse without it, the linear law would *not* be satisfied, as Dyson showed in 1967 [43]. Consequently, stability of the second kind does *not* follow from stability of the first kind! If the electrons and nuclei were all bosons (which are particles that do not satisfy the exclusion principle), the energy would not satisfy a linear law but rather decrease like $-N^{7/5}$; we will return to this astonishing discovery later.

The Dyson–Lenard proof of stability of the second kind [44] was one of the most difficult, up to that time, in the mathematical physics literature. A challenge was to find an essential simplification, and this was done by Lieb and Thirring in 1975 [134]. They introduced new mathematical inequalities, now called Lieb–Thirring (LT) inequalities (discussed in Chapter 4), which showed that a suitably modified version of the 1927 approximate theory of Thomas and Fermi [179, 62] yielded, in fact, a lower bound to the exact quantum-mechanical answer. Since it had already been shown, by Lieb and Simon in 1973 [129, 130], that this Thomas–Fermi theory possessed a linear lower bound to the energy, the many-body stability of the second kind immediately followed.

The Dyson–Lenard stability result was one important ingredient in the solution to another, but related problem that had been raised many years earlier. Is it true that the 'thermodynamic limit' of the free energy per particle exists for an infinite system at fixed temperature and density? In other words, given that the energy per particle of some system is bounded above and below, independent of the size of the system, how do we know that it does not oscillate as the system's size increases? The existence of a limit was resolved affirmatively by Lebowitz and Lieb in 1969 [103, 116], and we shall give that proof in Chapter 14.

There were further surprises in store, however! The Dyson–Lenard result was not the end of the story, for it was later realized that there were other sources of instability that physicists had not seriously thought about. Two, in fact. The eventual solution of these two problems leads to the conclusion that, ultimately, stability requires more than the Pauli principle. It also requires an upper bound on both the physical constants α and $Z\alpha$.[1]

One of the two new questions considered was this. What effect does Einstein's relativistic kinematics have? In this theory the Newtonian kinetic energy of an electron with mass m and momentum $\boldsymbol{p}$, $\boldsymbol{p}^2/2m$, is replaced by the much weaker $\sqrt{\boldsymbol{p}^2c^2 + m^2c^4} - mc^2$. So much weaker, in fact, that the simple atom is stable only if the relevant coupling parameter $Z\alpha$ is not too large! This fact was known in one form or another for many years – from the introduction of Dirac's 1928 relativistic quantum mechanics [39], in fact. It was far from obvious, therefore, that many-body stability would continue to hold even if $Z\alpha$ is kept small (but fixed, independent of N). Not only was the linear N-dependence in doubt but also stability of the first kind was unclear. This was resolved by Conlon in 1984 [32], who showed that stability of the second kind holds if $\alpha < 10^{-200}$ and $Z = 1$.

Clearly, Conlon's result needed improvement and this led to the invention of interesting new inequalities to simplify and improve his result. We now know that stability of the second kind holds if and only if *both* α and $Z\alpha$ are not too large. The bound on α itself was the new reality, previously unknown in the physics literature.

Again new inequalities were needed when it was realized that magnetic fields could also cause instabilities, even for just one atom, if $Z\alpha^2$ is too large. The understanding of this strange, and totally unforeseen, fact requires the knowledge that the appropriate Schrödinger equation has '*zero-modes*', as discovered by Loss and Yau in 1986 [139] (that is, square integrable, time-independent solutions with zero kinetic energy). But stability of the second kind was still open until Fefferman showed in 1995 [57, 58] that stability of the second kind holds if $Z = 1$ and α is very small. This result was subsequently improved to robust values of $Z\alpha^2$ and α by Lieb, Loss and Solovej in 1995 [123].

The surprises, in summary, were that stability of the second kind requires bounds on the fine-structure constant and the nuclear charges. In the relativistic case, smallness of α and of $Z\alpha$ is necessary, whereas in the non-relativistic case with magnetic fields, smallness of α and of $Z\alpha^2$ is required.

[1] If $Z \geq 1$, which it always is in nature, a bound on $Z\alpha$ implies a bound on α, of course. The point here is that the necessary bound on α is independent of Z, even if Z is arbitrarily small. In this book we shall not restrict our attention to integer Z.