Springer Tracts in Modern Physics
172

D. Braun

Dissipative Quantum Chaos and Decoherence

Springer

Daniel Braun

Dissipative Quantum Chaos and Decoherence

With 22 Figures

Springer

Dr. Daniel Braun
University of Essen
Institute of Physics
Universitätsstrasse 5
45117 Essen, GERMANY
E-mail: daniel@indy1.theo-phys.uni-essen.de

Library of Congress Cataloging-in-Publication Data.

Die Deutsche Bibliothek - CIP-Einheitsaufnahme

Braun, Daniel:
Dissipative quantum chaos and decoherence/Daniel Braun. – Berlin;
Heidelberg ; New York ; Barcelona ; Hong Kong ; London ; Milan ; Paris;
Singapore; Tokyo: Springer, 2001
(Springer tracts in modern physics; Vol. 172)
(Physics and astronomy online library)
ISBN 3-540-41197-6

Physics and Astronomy Classification Scheme (PACS): 03.65.Sq, 03.67.Lx, 05.20.Gg

ISSN print edition: 0081-3869
ISSN electronic edition: 1615-0430
ISBN 3-540-41197-6 Springer-Verlag Berlin Heidelberg New York

Springer-Verlag Berlin Heidelberg New York
a member of BertelsmannSpringer Science+Business Media GmbH

Typesetting: Camera-ready copy from the author using a Springer LaTeX macro package
Cover design: *design & production* GmbH, Heidelberg

Printed on acid-free paper SPIN: 10777023 56/3141/tr 5 4 3 2 1 0

Springer Tracts in Modern Physics
Volume 172

Now also Available Online

Starting with Volume 163, Springer Tracts in Modern Physics is part of the Springer LINK service. For all customers with standing orders for Springer Tracts in Modern Physics we offer the full text in electronic form via LINK free of charge. Please contact your librarian who can receive a password for free access to the full articles by registration at:

http://link.springer.de/series/stmp/reg_form.htm

If you do not have a standing order you can nevertheless browse through the table of contents of the volumes and the abstracts of each article at:

http://link.springer.de/series/stmp/

There you will also find more information about the series.

Springer
Berlin
Heidelberg
New York
Barcelona
Hong Kong
London
Milan
Paris
Singapore
Tokyo

Physics and Astronomy ONLINE LIBRARY
http://www.springer.de/phys/

Springer Tracts in Modern Physics

Springer Tracts in Modern Physics provides comprehensive and critical reviews of topics of current interest in physics. The following fields are emphasized: elementary particle physics, solid-state physics, complex systems, and fundamental astrophysics.
Suitable reviews of other fields can also be accepted. The editors encourage prospective authors to correspond with them in advance of submitting an article. For reviews of topics belonging to the above mentioned fields, they should address the responsible editor, otherwise the managing editor.
See also http://www.springer.de/phys/books/stmp.html

Preface

One hundred years after the discovery of the first foundations of quantum mechanics, there are still many open and fascinating questions dealing with the relation between quantum mechanics and classical mechanics. Everyday life and three and a half centuries of successful application of classical mechanics have left us with the conviction that we can predict precisely the fate of an individual object if we know sufficiently precisely its initial conditions and the forces that act on it. Quantum mechanics gives us a very different picture of reality. It states that the information that we may gather about any object can never be as complete as in classical mechanics, and we can only predict statistical distributions for experimental data.

Shortly before the beginning of the twentieth century, Henri Poincaré discovered that even within classical mechanics the predictability of very simple classical systems might be very poor, and for sufficiently long times prediction might be just impossible owing to a very strong sensitivity to initial conditions. Such systems were later termed "chaotic". We know today that chaotic behavior is far more common in nature than the regular, integrable motion in, say, Kepler's problem or the harmonic oscillator. It is therefore natural to abandon the attempt to predict the fate of individual objects, for initial conditions are never precisely known. By going over to an ensemble description, as is also done in statistical mechanics, one allows space for uncertainties in the initial conditions. Furthermore, within an ensemble description classical mechanics uses a vocabulary that is much more similar to that of quantum mechanics. Both then predict an evolution of the probability distributions of observables, and we can study how the quantum mechanical evolution law goes over into the classical one.

Nevertheless, the transition from quantum mechanics to classical mechanics is still far from simple, as the classical limit is highly singular. An initial "blob" corresponding to a reasonably localized distribution in phase space is rapidly torn apart by a chaotic classical dynamics, which stretches and folds it to ever finer scales while covering rapidly the entire available phase space. Heisenberg's uncertainty relation, on the other hand, prevents the production of arbitrarily fine scales by quantum mechanical time evolution. And yet another difference between the quantum mechanical world and the classical world exists: probabilities add very differently in the cases of quantum

mechanics and classical mechanics. In quantum mechanics probability amplitudes that are squared to give probability distributions have to be added, and this can give rise to quantum mechanical interference effects. In classical mechanics we add probabilities directly and quantum mechanical interference is absent.

It has become obvious during the last twenty years that an important ingredient of the transition from quantum mechanics to classical mechanics is the interaction of a system with its environment. Such a coupling leads typically to dissipation of energy and to decoherence. While the former process is already present in classical mechanics, and by itself leads to a washing out of phase space structures (although on classical scales), decoherence is genuinely quantum mechanical and means that interference patterns are destroyed. Thus, decoherence is the process that allows us to recover classical probability theory from the quantum mechanical theory.

The relations and connections of the quantum mechanical time evolution to the classical evolution for systems that are coupled to an environment are the main subject of this book. The book deals mostly with systems with large quantum numbers, i.e. a semiclassical regime. A new formalism is developed that allows us to efficiently calculate the effects of dissipation and decoherence. It turns out that many of the concepts, such as periodic-orbit theory, trace formulae and zeta functions, that have been introduced to deal with the quantum mechanics of classically chaotic but isolated systems can be extended to situations where dissipation and decoherence are important. Furthermore, I shall deal in some detail with exceptional situations where decoherence is very weak in spite of a strong coupling to the environment. In the young theory of quantum computing, such situations have gained substantial interest in the last few years.

The present book would not have been possible without the help and support of many people. It is my pleasure to thank Prof. Fritz Haake for giving me the opportunity to work on this project in Essen and for his continuous interest, countless discussions and ideas. His enthusiasm and his warm and encouraging support made it a pleasure to work with him.

I would also like to thank Prof. Petr A. Braun, with whom I had the privilege to work closely. With pleasure I think back to his visits to Essen, and to his warm hospitality during my stay in St. Petersburg.

A big "thank you" also to Profs. Marek Kuś and Karol Życzkowksi, frequent visitors to Essen, with whom I have enjoyed working.

During my time in Essen and at numerous conferences and workshops and on visits, I had the pleasure to meet and have discussions with many physicists. Special thanks are owed to Alex Altland, Tobias Brandes, Andreas Buchleitner, Doron Cohen, Predrag Cvitanovic, David DiVincenzo, Bruno Eckhardt, Klaus Frahm, Yan Fyodorov, Pierre Gaspard, Theo Geisel, Nicolas Gisin, Sven Gnutzmann, Martin Gutzwiller, Peter Hänggi, Serge Haroche, Etienne Hofstetter, Martin Janssen, Maria José-Sanchez, Stefan Kettemann,

Roland Ketzmerick, Ilki Kim, Peter Knight, Bernhard Kramer, Wolfgang Lange, Angus MacKinnon, Günter Mahler, Gilles Montambaux, Michael Pascaud, Frédéric Piéchon, Sarben Sarkar, Rüdiger Schack, Ferdinand Schmidt-Kaler, Henning Schomerus, Petr Šeba, Pragya Shukla, Uzy Smilansky, Hans-Jürgen Sommers, Andrew Steane, Frank Steiner, Walter Strunz, Mikhail Titov, Imre Varga, Gábor Vattay, David Vitali, Jürgen Vollmer, Joachim Weber, Ulrich Weiß, Christoph Wunderlich, Hugo Zbinden, Isa Zharekeshev and Wojciech Zurek for the enrichment they brought to my knowledge of physics relevant to the topics of this book.

The numerical calculations were partly performed at the John von Neumann Center for Computing (the former Hochleistungsrechenzentrum Jülich) in Jülich. This work was supported by the Sonderforschungsbereich 237 "Unordnung und große Fluktuationen" (DFG special research program 237, "Disorder and large fluctuations").

Essen, October 2000 *Daniel Braun*

Springer Tracts in Modern Physics

155 **High-Temperature-Superconductor Thin Films at Microwave Frequencies**
By M. Hein 1999. 134 figs. XIV, 395 pages

156 **Growth Processes and Surface Phase Equilibria in Molecular Beam Epitaxy**
By N.N. Ledentsov 1999. 17 figs. VIII, 84 pages

157 **Deposition of Diamond-Like Superhard Materials**
By W. Kulisch 1999. 60 figs. X, 191 pages

158 **Nonlinear Optics of Random Media**
Fractal Composites and Metal-Dielectric Films
By V.M. Shalaev 2000. 51 figs. XII, 158 pages

159 **Magnetic Dichroism in Core-Level Photoemission**
By K. Starke 2000. 64 figs. X, 136 pages

160 **Physics with Tau Leptons**
By A. Stahl 2000. 236 figs. VIII, 315 pages

161 **Semiclassical Theory of Mesoscopic Quantum Systems**
By K. Richter 2000. 50 figs. IX, 221 pages

162 **Electroweak Precision Tests at LEP**
By W. Hollik and G. Duckeck 2000. 60 figs. VIII, 161 pages

163 **Symmetries in Intermediate and High Energy Physics**
Ed. by A. Faessler, T.S. Kosmas, and G.K. Leontaris 2000. 96 figs. XVI, 316 pages

164 **Pattern Formation in Granular Materials**
By G.H. Ristow 2000. 83 figs. XIII, 161 pages

165 **Path Integral Quantization and Stochastic Quantization**
By M. Masujima 2000. 0 figs. XII, 282 pages

166 **Probing the Quantum Vacuum**
Pertubative Effective Action Approach in Quantum Electrodynamics and its Application
By W. Dittrich and H. Gies 2000. 16 figs. XI, 241 pages

167 **Photoelectric Properties and Applications of Low-Mobility Semiconductors**
By R. Könenkamp 2000. 57 figs. VIII, 100 pages

168 **Deep Inelastic Positron-Proton Scattering in the High-Momentum-Transfer Regime of HERA**
By U.F. Katz 2000. 96 figs. VIII, 237 pages

169 **Semiconductor Cavity Quantum Electrodynamics**
By Y. Yamamoto, T. Tassone, H. Cao 2000. 67 figs. VIII, 154 pages

170 **d–d Excitations in Transition-Metal Oxides**
A Spin-Polarized Electron Energy-Loss Spectroscopy (SPEELS) Study
By B. Fromme 2001. 53 figs. XII, 143 pages

171 **High-T_c Superconductors for Magnet and Energy Technology**
By B. R. Lehndorff 2001. 139 figs. XII, 209 pages

172 **Dissipative Quantum Chaos and Decoherence**
By D. Braun 2001. 22 figs. XI, 132 pages

Contents

1. Introduction

The notion of "chaos" emerged in classical physics about a century ago with the pioneering work of Poincaré. After two and a half centuries of application of Newton's laws to more and more complicated astronomical problems, he was privileged to discover that even in very simple systems extremely complicated and unstable forms of motion are possible [1]. It seems that this first appeared a curiosity to his contemporaries. Moreover, quantum mechanics and relativistic mechanics were soon to be discovered and distracted most of the attention from classical problems. In any case, classical chaos interested mostly only mathematicians, from G. Birkhoff in the 1920s to Kolmogorov and his coworkers in the 1950s. Only Einstein, as early as 1917, i.e. even before Schrödinger's equation was invented, clearly saw that chaos in classical mechanics also posed a problem in quantum mechanics [2]. The rest of the world started to realize the importance of chaos only when computers allowed us to simulate simple physical systems. It then became obvious that integrable systems, with their predictable dynamics, that had been the backbone of physics for by then three centuries were an exception. Almost always there are at least some regions in phase space where the dynamics becomes irregular and very sensitive to the slightest changes in the initial conditions. The in principle perfect predictability of classical systems over arbitrary time intervals given a precise knowledge of all initial positions and momenta of all particles involved is entirely useless for such "chaotic" systems, as initial conditions are *never* precisely known.

The understanding of quantum mechanics naturally developed first of all with the solution of the same integrable systems known from classical mechanics, such as the hydrogen atom (as a variant of Kepler's problem) or the harmonic oscillator. With the growing conviction that integrable systems are a rare exception, it became natural to ask how the quantum mechanical behavior of systems whose classical counterpart is chaotic might look. Research in this direction was pioneered by Gutzwiller. In the early 1970s he published a "trace formula" which allows one to calculate the spectral density of chaotic systems [3, 4]. That work was extended later by various researchers to other quantities, such as transition matrix elements and correlation functions of observables. All of these theories are "semiclassical" theories. They make use of classical information, in particular classical periodic orbits, their actions

and their stabilities, in order to express quantum mechanical quantities. And they are (usually first-order) asymptotic expansions in $\hbar$ divided by a typical action.

The true era of quantum chaos started, however, with the discovery by Bohigas and Giannoni [5] and Berry [6] and their coworkers in the early 1980s that the quantum energy spectra of classically chaotic systems show universal spectral correlations, namely correlations that are described by random-matrix theory (RMT). The latter theory, developed by Wigner, Dyson, Mehta and others starting from the 1950s, assumes that the Hamilton operator of a complex system can be well represented by a random-matrix restricted only by general symmetry requirements. Since there are no physical parameters in the theory (other than the mean level density, which, however, has to be rescaled to unity for any physical system before it can be compared with RMT), the predicted spectral correlations are completely universal. Over the years, overwhelming experimental and numerical evidence has been accumulated for this so called "random-matrix conjecture" – but still no definitive proof is known.

With the help of Gutzwiller's semiclassical theory, Berry has shown that the spectral form factor (i.e. the Fourier transform of the autocorrelation function of spectral density fluctuations) should agree with the RMT prediction, at least for small times [7]. How small these times should be is arguable, but at most they can be the so-called Heisenberg time, $\hbar$ divided by the mean level spacing at the relevant energy. From the derivation itself, one would expect a much earlier breakdown, namely after the "Ehrenfest time" of order $h^{-1} \ln \hbar_{\mathrm{eff}}$, in which h means the Lyapunov exponent and $\hbar_{\mathrm{eff}}$ an "effective" $\hbar$. At that time the average distance between periodic orbits becomes so small that the saddle-point approximation underlying Gutzwiller's trace formula is expected to become unreliable.

In his derivation Berry uses a "diagonal approximation" which is effectively a classical approximation: the fluctuations of the density of states are expressed by Gutzwiller's trace formula as a sum over periodic orbits. Each orbit contributes a complex number with a phase given by the action of the orbit in units of $\hbar$. In the spectral form factor the product of two such sums enters, and in the diagonal approximation only the "diagonal" terms are kept, with the result that the corresponding phases cancel. The off-diagonal terms are assumed to vanish if an average over a small energy window is taken, since they oscillate rapidly. For times larger than the Heisenberg time the off-diagonal terms cannot be neglected, and so far it has only been possible to extract the long-time behavior of the form factor approximately and with additional assumptions by bootstrap methods that use the unitarity of the time evolution, relating the long-time behavior to the short-time behavior [8].

The question arose as to whether semiclassical methods might work better if a small amount of dissipation was present. Dissipation of energy introduces,

almost unavoidably, decoherence, i.e. it destroys quantum mechanical interference effects. Therefore dissipative systems are expected to behave more classically from the very beginning, and so one might indeed expect an improvement. To answer this question was a main motivation for the present work. As for most simple questions, the answer is not simple, though: in some aspects the semiclassical theories do work better, in others they do not.

First of all, there are aspects of the semiclassical theory that seem to work as well with dissipation as without. One of them is the existence of a Van Vleck propagator, an approximation of the exact quantum propagator to first order in the effective $\hbar$. Gutzwiller's theory is based on it in the case without dissipation. And a corresponding semiclassical approximation can be obtained for a pure relaxation process by means of the well-known WKB approximation.

Things become more complicated because of the fact that a density matrix, not a wave function, should be propagated if dissipation of energy is included (alternatively, one might resort to a quantum state diffusion approach, as was done numerically in [9], but then one has to average over many runs). If the wave function lives in a d-dimensional Hilbert space, the density matrix has d^2 elements, and its propagator P is a $d^2 \times d^2$ matrix, instead of a $d \times d$ matrix as for the propagator F of the wave function. This implies that many more traces (i.e. traces of powers of P) are needed if one wants to calculate all the eigenvalues of P.

Furthermore, the eigenvalues of P move into the unit circle when dissipation is turned on. For arbitrary small dissipation and small enough effective $\hbar$ their density increases exponentially towards the center of the unit circle. This has the unpleasant consequence that numerical routines that reliably recover eigenvalues of F *on* the unit circle from the traces of F become highly unstable. They fail even for rather modest dimensions, even if the numerically "exact" traces are supplied – not to mention semiclassically calculated ones that are approximated to lowest order in the effective $\hbar$. This must be contrasted with the case of energy-conserving systems, where it has been possible to calculate very many energy levels, e.g. for the helium atom [10] or for hydrogen in strong external electric and magnetic fields [11, 12], or even entire spectra for small Hilbert space dimensions [13].

But dissipation of energy does improve the status of semiclassical theories in various other respects. First of all, the diagonal approximation, which is not very well controlled for unitary time evolutions, can be rigorously *derived* if a small amount of dissipation is present. As a result one obtains an entirely *classical* trace formula, namely the traces of the Frobenius–Perron operator that propagates phase space density for the corresponding classical system. Periodic orbits of a *dissipative* classical map are now the decisive ingredients, and there is a much richer zoo of them compared with nondissipative systems. Fixed points can now be point attractors or repellers, and the overall phase space structure is usually a strange attractor. The traces are entirely real,

and no problems with rapidly oscillating terms arise, nor are Maslov indices needed. The absence of the latter in the classical trace formula cannot be appreciated enough, as their calculation can in practice be rather difficult. The ignorance of the Maslov phases seems to have prevented, for example, a semiclassical solution of the helium atom for more than 70 years, in spite of heroic efforts by many of the founding fathers of quantum mechanics before this was done correctly by Wintgen et al. [10] (see the historical remarks in [14]).

Despite the numerical difficulties in the calculation of eigenvalues, the semiclassically obtained traces can be used to reliably obtain the *leading* eigenvalues, i.e. the eigenvalues with the largest absolute values of the quantum mechanical propagator, from just a few classical periodic orbits. These eigenvalues become independent of the effective $\hbar$ if the latter is small enough, and they converge to the leading complex eigenvalues of the Frobenius–Perron operator $P_{\rm cl}$, the so-called Ruelle resonances. All time-dependent expectation values and correlation functions carry the signature of these resonances, as well as the decaying traces of P themselves. So a little bit of dissipation (an "amount" that vanishes in the classical limit is enough, as we shall see) ensures that the *classical* Ruelle resonances determine the *quantum mechanical* behavior.

As for the range of validity of the semiclassical results, there seems to be no improvement at first glance. The trace formula for the dissipative system is valid at most up to the Heisenberg time of the dissipation-free system, but is eventually limited to the Ehrenfest time for the same technical reasons as for the periodic-orbit theory for nondissipative systems. But this *is* in fact an enormous improvement: for small values of the effective $\hbar$ all correlation functions, traces etc. have long ago decayed to their stationary values before the Heisenberg time (which typically increases with decreasing effective $\hbar$) or, for exponentially small effective $\hbar$, even before the Ehrenfest time is reached, just because the decay happens on the classical and therefore $\hbar$-independent time-scales set by the Ruelle resonances. Only exponentially small corrections to the stationary value are left at the Heisenberg time. One may therefore say that the semiclassical analysis is valid over the entire *relevant* time regime – something one cannot so easily claim for unitary time evolutions.

The important aspect of dissipation that makes quantum mechanical systems look more classical is not dissipation of energy itself, but decoherence. It was long believed that decoherence is an inevitable fact if a system couples to its environment. In particular, it typically restricts the existence of superpositions of macroscopically distinct states, so-called Schrödinger cats, to extremely small times. That is one of the main reasons why these beasts are never observed! However, in the course of our investigations of dissipative quantum maps we have found that exceptions are possible. If the system couples to the environment in such a way that different states acquire exactly the same time-dependent phase factor owing to a symmetry in the coupling