Semiclassical approximations beyond the leading order in $\hbar$

Theoretical studies of higher-order $\hbar$ contributions and their influence on experimental transport properties of mesoscopic systems

Dissertation
zur Erlangung des Doktorgrades der Naturwissenschaften
(Dr. rer. nat.)
der naturwissenschaftlichen Fakultät II – Physik
der Universität Regensburg

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September 1999

Die Arbeit wurde von Prof. Dr. M. Brack angeleitet.
Das Promotionsgesuch wurde am 27. 9. 1999 eingereicht.
das Kolloquium fand am 12. 11. 1999 statt.

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Version 1.1 vom 26. 11. 1999
published under `http://www.joachim-blaschke.de`

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Chapter 1

Introduction

Mesoscopic systems, a rapidly progressing field of physical research in the last two decades, are of increasing technological and commercial interest. Semiclassical approximations, i. e. expansions of quantum mechanical equations to leading order in $\hbar$, are appropriate tools for the theoretical description of these systems in between the microscopic and the macroscopic regime. The validity of these approximations requires higher-order $\hbar$ corrections to be negligible. The influence of higher-order corrections is studied theoretically using model systems, and their contributions are traced down in experimental data on magnetoconductance.

Since the early days of quantum mechanics the question how the wave approach is related to the classical description has not been satisfactorily settled. For nearly one century now physicists work with either the classical or the quantum approach, 'well knowing' in which cases the one or the other theoretical description is appropriate. Although the general belief is that quantum mechanics is the basic theory and that classical behavior corresponds to the limit for large systems[1], this relation has not been rigorously established. The open questions concern on the one hand the properties of the transition region between quantum mechanical and classical behavior, the so-called *mesoscopic* regime. On the other hand the nature of the classical and the quantum measurement process is not completely clear by now.

In the present work, only the first question is considered. Readers interested in more fundamental questions concerning alternative interpretations of quantum mechanics [109], consistent formulations of the measurement process [116, 102], and the problems which arise when the interpretation of the Copenhagen School is applied to macroscopic systems [108, 115] are referred to the literature. In the context of this thesis the standard quantum mechanical description following the Copenhagen interpretation is assumed to be exact for arbitrary system sizes, even on classical length scales.

In recent years the rapid development in nanostructure technology has triggered increasing interests in mesoscopic systems. The most remarkable progress has been achieved in the technology of growing and processing semiconductor heterostructures. These build the basis of two-dimensional electron gases (2DEG). Using advanced lithographic techniques on high-mobility samples it has become feasible to laterally confine the 2DEG on size scales smaller than the phase coherence lengths. In these experiments, quantum interference

[1]Large means in this context large quantum numbers.

effects become relevant. For natural quantum systems like atoms, nuclei or clusters only a few (if any) parameters can be controlled experimentally. The semiconductor nanostructures, in contrast, can be tailored to very specific needs and prepared in virtually arbitrary shapes. This new experimental freedom led to the discovery of a variety of novel, often surprising effects emerging from quantum interference. Among the most prominent are weak localization [88, 94, 90], quantized conductance [99], universal conductance fluctuations [93] and commensurability oscillations [83, 55, 84, 63, 41]. The rapid development in this area and the continued interest from a large community of both theoretical and experimental research groups promises exciting new effects within the next years.

Mesoscopic systems, however, are not only challenging for people in basic research, but they also attract huge commercial interest. This is mainly evoked by the fact that the structures on today's highly integrated semiconductor devices have reached a scale where quantum interference effects are no longer negligible. Future development of memory components and logic devices – which includes further miniaturization – can be achieved following two strategies: The first approach is to choose a geometric design of circuits that strongly suppresses quantum interference effects. This approach allows the vast existing knowledge about conventional chip design to be transferred – at least partially – to the quantum regime. Another, more innovative strategy exploits quantum effects explicitly by the development of a new kind of electronics based on interference. The success of both strategies obviously relies on a detailed understanding of mesoscopic physics.

Therefore, an appropriate theoretical description of mesoscopic systems is strongly desired for basic research as well as for commercial applications. Mesoscopic systems generically include a large number of electrons, so that according to the Pauli principle a huge number of eigenstates of the system have to be determined in a quantum calculation. For this reason quantum calculations are often prohibitive due to the numerical effort involved. Much of the detailed interference information, however, is lost in the experimental realization. This is mainly due to finite temperature and impurity effects which broaden the line widths. Semiclassical methods provide an alternative approach. In the form applied in this dissertation, they naturally introduce a hierarchy of energy resolutions. This makes semiclassical approximations a well adapted tool for the description of systems which are subject to finite temperature and impurity effects (see Sec. 3 for details on this point). The semiclassical ansatz considerably reduces the numerical effort involved in the theoretical description of mesoscopic systems.

Formally, semiclassical approximations are approximations of quantum mechanical equations in leading order in $\hbar$. They yield asymptotically correct descriptions for states with high quantum numbers. In practice, however, even the ground state is usually well reproduced. For integrable systems the basic ideas for an expansion of quantum mechanics in orders of $\hbar$ were set up by Wetzel, Kramers and Brillouin [85, 51, 20] soon after the formulation of wave mechanics. Completely chaotic systems, in contrast, could not be treated with this approach. For those, it took until the late 60's to derive an appropriate formulation, the famous Gutzwiller *trace formula*. This Fourier-like sum has classical periodic orbits as individual Fourier components, so that this theory is also termed *periodic orbit theory* (POT). This new ansatz led to a revival of semiclassical approximations, which attracted more and more interest. The trace formula was extended to a large variety of systems, including systems with continuous symmetries or mixed phase space. Analogous formulae were developed for other observables than the level density, e. g. conductance and susceptibility.

An appealing feature of the trace formula is that it can be expressed in terms of the classical properties of the system. It establishes as such a connection between the quantum oscillations and the classical dynamics of the system. The POT is therefore not only a convenient tool calculating the properties of mesoscopic systems. It additionally opens up the possibility of an intuitive interpretation of the observed quantum interference effects in terms of classical periodic orbits. This often underestimated feature removes the 'black box' character of quantum calculations. An intuitive understanding of the origin of the interference effects provides a powerful guideline for designing devices with certain desired properties.

A central problem for all semiclassical approximations is the question of the range of applicability. Under which conditions does the leading order in $\hbar$ contain the essential physics, and when are higher-order contributions to be included? A possible approach to this question is to consider higher-order expansions in $\hbar$. There are attempts following this ansatz [30], but they are both analytically and numerically extremely involved. The aim of the present work is to examine higher-order $\hbar$ corrections without loosing the main advantages of semiclassical approximations, namely their numerical and conceptual simplicity. This work therefore considers some prominent corrections in higher order of $\hbar$, calculates their influence and gives an intuitive explanation of their origin and strength. The goal is to provide rules based on easily accessible data whether certain $\hbar$ corrections have to be taken into account. This knowledge is finally used to describe the experimentally observed features of the magnetoconductance of a mesoscopic device.

This thesis is structured as follows: The first part (chapter 4) is dedicated to the examination of a model system, the circular disk. Its simplicity will allow quite detailed investigations, since $\hbar$ corrections can be included analytically. The applicability to experiment is limited, so that the results are only compared to the corresponding quantum data. The second part of this work applies the semiclassical approach to experiments on magnetoconductance. First the free electron gas is considered as a simple example (chapter 6). Later in chapter 7 the channel with central antidots is treated exemplarily for realistic, and thus more complicated situations. The merits and limitations of the semiclassical approximation are considered, and higher order $\hbar$ effects are examined both theoretically and in the experimental data.

Each of these two parts is preceded by a chapter providing an overview of the applied methods. They give a summary of the relevant literature and present the techniques developed in this thesis.

The last chapter is both a summary and an outlook, collecting the main results and pointing out open questions which seem worth further investigations.

Please note that, apart from the short section on the integer hall effect in chapter 6 this thesis only contains information published[2] in refereed journals. Whenever possible, please cite the original publications instead of this work.

[2] Chapter 4 on the disk billiard, including the work on the correct implementation of smoothing presented in Sec. 3.4 and Sec. 3.2, is contained in Refs. [4, 5]. The relation between dislocations and bifurcations of the channel with antidots of chapter 7 is submitted and available as preprint [6], the remaining part of chapter 7 is presently prepared for publication [7].

Before starting out I want to apologize sincerely for all the errors on the following pages. They somehow found a way to escape my notice. All readers willing to contribute to the collection of misprints are invited to communicate their findings to `mail@joachim-blaschke.de`. Thanks for your kind cooperation.