Available online at www.sciencedirect.com
ScienceDirect
Annals of Physics 322 (2007) 315–340
ANNALS of PHYSICS
www.elsevier.com/locate/aop

$\hbar$ expansions in semiclassical theories for systems with smooth potentials and discrete symmetries

Holger Cartarius *, Jörg Main, Günter Wunner

1. Institut für Theoretische Physik, Universität Stuttgart, 70550 Stuttgart, Germany

Received 20 January 2006; accepted 25 January 2006
Available online 24 March 2006

Abstract

We extend a theory of first order $\hbar$ corrections to Gutzwiller's trace formula for systems with a smooth potential to systems with discrete symmetries and, as an example, apply the method to the two-dimensional hydrogen atom in a uniform magnetic field. We exploit the C_{4v}-symmetry of the system in the calculation of the correction terms. The numerical results for the semiclassical values will be compared with values extracted from exact quantum mechanical calculations. The comparison shows an excellent agreement and demonstrates the power of the $\hbar$ expansion method.

PACS: 03.65.Sq; 05.45.Mt

Keywords: Semiclassical theories; Gutzwiller's trace formula; $\hbar$ expansions; Discrete symmetries; Diamagnetic hydrogen atom

1. Introduction

Semiclassical theories have become very important for a deeper understanding of quantum systems, and Gutzwiller's trace formula [1] has become a powerful tool for classically chaotic systems. It provides a semiclassical approximation of the quantum level density in

* Corresponding author. Fax: +49 (0) 711 685 4909.
E-mail address: Holger.Cartarius@itp1.uni-stuttgart.de (H. Cartarius).

0003-4916/$ - see front matter
doi:10.1016/j.aop.2006.01.006

terms of classical periodic orbits. In a systematic expansion of the level density in powers of $\hbar$ it can be considered as the leading order. Higher orders of this asymptotic expansion have been developed in several studies [2–4], but for a long time were only tested for billiard systems, i.e., systems with hard walls instead of smooth potentials. By extending an expansion which was derived by Gaspard et al. [3,4], Grémaud [5] developed $\hbar$ corrections to Gutzwiller's trace formula for quantum systems with a smooth potential. He presented a first-order $\hbar$ correction term to Gutzwiller's trace formula and obtained numerical results for the diamagnetic hydrogen atom. Comparisons with values extracted from exact quantum calculations showed that the semiclassical results can be computed with very high accuracy.

However, in the theory presented in [5] some important topics have not yet been considered. For example, the $\hbar$ corrections cannot be calculated for classical orbits which have a turning point (i.e., the velocity vanishes completely at this point). Furthermore, discrete and continuous symmetries have not been included.

If there are discrete symmetries the eigenstates of the quantum system split up into several subspaces. In these subspaces, classical orbits which are not periodic without a symmetry transformation contribute to the level density. Preliminary results for the diamagnetic hydrogen atom, which is an example system with discrete symmetries, were published in [6] without explaining which modifications in the numerical calculations the introduction of discrete symmetries entails. In particular, an analysis of the differential equations which have to be solved to obtain the correction terms is not presented. In this paper, we want to give a transparent derivation of the modifications necessary for the calculation of the correction terms in systems with discrete symmetries. We will show in detail how such symmetries of the Hamiltonian have to be taken into account. It will be explained in which equations it is necessary to introduce symmetry operations and which transformations lead to the correct boundary conditions of the classical Greens function, which is an essential part of the correction terms. Furthermore, we want to give a deeper understanding of the significance of the symmetry of the system for the quantum spectrum and the connection to periodic orbits.

We will apply the method to the diamagnetic hydrogen atom. The three-dimensional hydrogen atom in a uniform magnetic field has a continuous symmetry, namely the rotational invariance around the magnetic field axis. Continuous symmetries have a substantial influence on the correction terms. Actually one cannot obtain the correct results for the first-order $\hbar$ correction for the three-dimensional hydrogen atom with the formulas presented because the rotational invariance leads to additional contributions to the first-order corrections. Therefore, we will consider the hydrogen atom as a pure two-dimensional system as it was done before in [5]. If one uses semiparabolic coordinates, the potential of the two-dimensional diamagnetic hydrogen atom exhibits a discrete C_{4v}-symmetry. The $\hbar$ corrections will be calculated for selected periodic orbits taking into account that discrete symmetry. The semiclassical results will be compared with the analysis of exact quantum calculations. The agreement between the results of both methods turns out to be very good.

The outline of the paper is as follows. In Section 2, we will first give a summary of the derivation of the $\hbar$ corrections without taking into account discrete symmetries. In Section 3, we will introduce the hydrogen atom in a uniform magnetic field with all aspects relevant for the calculation of the correction terms. We will also discuss the influence of the rotational invariance of the three-dimensional hydrogen atom. Then we will extend the