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SPECTRAL SUM RULES FOR THE CIRCULAR AHARONOV-BOHM QUANTUM BILLIARD

by

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A B S T R A C T

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1. Introduction

Recently I proposed a new method [illegible] for the calculation of bound state energies in quantum mechanics. Since the method is based on sum rules derived for the spectral zeta function of the Hamiltonian H,

$$\zeta_H(s) \equiv \mathrm{Tr}\, H^{-s} , \qquad (1.1)$$

the method has been called "sum rule method". Although the basic idea is extremely simple, to my knowledge, the method has not been used before in quantum mechanics. This is surprising in view of the following facts.

First of all, the sum rule method turns out to yield extremely accurate values for low-lying energy levels. This has been illustrated in Refs. 1, 2 in the case of one- and threedimensional confinement potentials where the computed energies agreed with the exact energies within an error of some [illegible] per cent.

Secondly, "zeta functions" of various kinds have been extensively studied by mathematicians, starting with Euler and, in particular, with Riemann in his basic work on the Riemann zeta function

$$\zeta(s) \equiv \sum_{n=1}^{\infty} \frac{1}{n^s} . \qquad (1.2)$$

Whereas in the last century* the main emphasis was on the connection to number theory, Jacobi theta functions and Dirichlet series, the importance of generalized zeta functions was realized around 1900 in the theory of integral equations. The spectral zeta function (1.1) was first studied in 1949 by Minakshisundaram following a remark of H. Weyl.

In recent years, the zeta function (1.1) has been used as a convenient method for the regularization of determinants arising in the path integral approach to quantum field theory.

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of a positive, non-degenerate ground state energy E_0

$$0 < E_0 < E_1 \leq E_2 \leq \cdots \tag{2.2}$$

and furthermore, it will increase indefinitely

$$\lim_{n\to\infty} E_n = \infty \; . \tag{2.3}$$

We are only interested in the properties of the energies E_n, not in the wave functions ψ_n. Generically, the energies are of the form

$$E_n = \varepsilon\, \sigma(n) \qquad , \; n \in \mathbb{N}_0 \; , \tag{2.4}$$

where ε has the dimension of an energy and $\sigma(n)$ is a dimensionless function of n. The spectral zeta function of H, Eq. (1.1), is then given by

$$\zeta_H(s) = \sum_{n=0}^{\infty} \frac{1}{E_n^s} = \varepsilon^{-s} \sum_{n=0}^{\infty} \frac{1}{[\sigma(n)]^s} \quad . \tag{2.5}$$

Using the relation

$$\frac{1}{\sigma^s} = \frac{1}{\Gamma(s)} \int_0^{\infty} d\tau\, \tau^{s-1}\, e^{-\sigma\tau} \tag{2.6}$$

one obtains the following integral representation

$$\varepsilon^s\, \Gamma(s)\, \zeta_H(s) = \int_0^{\infty} d\tau\, \tau^{s-1}\, Z_H(\tau) \tag{2.7}$$

which gives ζ_H as the Mellin transform of the partition function

$$Z_H(\tau) \equiv \sum_{n=0}^{\infty} q^{\sigma(n)} \quad , \; q \equiv e^{-\tau} \tag{2.8}$$

($\tau = \varepsilon\beta$, $\beta = 1/kT = t/\hbar$, T = temperature, k = Boltzmann constant, [illegible] euclidean time). Splitting the integral (2.7) in the form

$$\varepsilon^s \Gamma(s) \zeta_H(s) = \int_0^{1} d\tau\, \tau^{s-1} Z_H(\tau) + \int_1^{\infty} d\tau\, \tau^{s-1} Z_H(\tau) \tag{2.9}$$

it is easy to see that the second integral is an entire function of s (since $Z_H(\tau) \sim e^{-\sigma(0)\tau}$ for $\tau \to \infty$ with $\sigma(0) > 0$), whereas the first integral represents a meromorphic function of s with a leading simple pole at s = d/2 and residue

$$\left(\frac{m}{2\pi\hbar^2}\right)^{d/2} \frac{V(D)}{\Gamma(d/2)} \tag{2.10}$$

(m = mass of particle, V(D) = volume of D). This result follows from the fact that $Z_H(\tau)$ is nothing but the trace of the heat kernel (euclidean time evolution kernel)

$$Z_H(\tau) = \int_D dx\, \langle x |\, e^{-\beta H} | x \rangle \tag{2.11}$$

which for large temperatures or small times ($t \to 0+$) is dominated by the free particle kernel. In fact, the d-dimensional heat kernel can be expressed in the form

$$\langle x' |\, e^{-\frac{t}{\hbar}H} | x \rangle = \left(\frac{m}{2\pi\hbar t}\right)^{d/2} e^{-\frac{m}{2\hbar t}(x-x')^2} + g(t;x',x) \tag{2.12}$$

where the 'correction' g satisfies the following lemma[5] *): If $\ell(x)$ denotes the minimum distance between $x \in D$ and points on ∂D, then, in any finite interval of t,

$$|g(t;x',x)| < \frac{C}{t^{d/2}}\, e^{-\frac{m}{2\hbar t}\ell^2(x)} \tag{2.13}$$

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*) The first use of the heat kernel method seems to be due to Carleman[15]. Later, important work was done by Minakshisundaram and Pleijel[16], [illegible] and [illegible]. In the recent literature, the coefficients of the small t expansion of the trace of the heat kernel are sometimes called Seeley coefficients. [illegible]. These coefficients are topological invariants of the manifold D.

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1. - INTRODUCTION

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First of all, the sum rule method turns out to yield extremely accurate values for low-lying energy levels. This has been illustrated in Refs. 1), 2) in the case of one- and threedimensional confinement potentials where the computed energies agreed with the exact energies within an error of about 10^{-4} per cent!

Secondly, "zeta functions" of various kinds have been extensively studied by mathematicians, starting with Euler and, in particular, with Riemann in his basic work on the Riemann zeta function

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Whereas in the last century*) the main emphasis was on the connection to number theory, Jacobi theta functions and Dirichlet series, the importance of generalized zeta functions was realized around 1900 in the theory of integral equations[4)]. The spectral zeta function (1.1) was first studied in 1948 by Minakshisundaram[5)] following a remark of H. Weyl.

In recent years, the zeta function (1.1) has been used as a convenient method for the regularization of determinants arising in the path integral approach to quantum field theory[6)].

*) References to the work (following Riemann) up to 1903 can be found in the interesting paper by Epstein[3)].

Very interesting functional relations for the zeta function (1.1) have been obtained by Voros[7] for a class of one-dimensional potential models following earlier work of Parisi[8].

In the meantime, our sum rule method has been applied to a study of quantum billiards in two interesting papers[9), 10)]. In Ref. 9), Itzykson et al. consider a class of two-dimensional quantum billiards, in particular triangular billiards. In Ref. 10), Berry studies a class of Aharonov-Bohm quantum billiards, i.e. the "circular", "heart" and "Africa" billiard (the names refer to the shape of the billiard domains). In his study, Berry has concentrated on finding explicit formulae for the zeta function (1.1) at $s = 2$ as a function of the magnetic flux.

My purpose here is to present a detailed, quantitative discussion of the sum rule method for the circular Aharonov-Bohm quantum billiard. Working with the zeta function (1.1) for a given angular momentum, we are able to calculate the "partial wave zeta functions" for $s = 1, 2, \ldots, 10$. This allows the computation of the ground state energy to a very high precision.

Before we outline the plan of this paper, let us say a few words on the billiard problem in general. The classical billiard ball problem was introduced by Birkhoff[11] to investigate the ergodic properties of classical dynamical systems. In the generic example of a two-dimensional billiard, one considers a point particle which moves freely in a bounded domain D of the euclidean plane and is elastically reflected at the boundary ∂D. (For details see Refs. 12), 13).)

Recently, Berry[14] has extended these studies to quantum mechanics, i.e. quantum billiards. In the simplest case, one considers the free Schrödinger equation in a simply connected, bounded domain D with vanishing wave function on ∂D. Examples in two dimensions are the rectangular, triangular, circular and stadion billiard. Of course, the mathematical problem is rather old, being the eigenvalue problem of the Helmholtz equation describing a vibrating membrane with clamped edge*). Nevertheless, the problem turns out to be non-trivial in cases where the classical bouncing ball problem is not integrable since the classical motion may be chaotic. An example is the stadion

*) Indeed, several membrane problems have already been solved in the last century: rectangular membrane (Poisson, 1829), equilateral triangle (Lamé, 1852), circular membrane (Clebsch, 1862).

billiard whose classical trajectories are stochastic[15].

This paper is organized as follows. In Sec. 2 we discuss the general analytic properties of the zeta function (1.1) and related spectral functions. As an illustration, the zeta functions for a few simple quantum systems are explicitly given. In Sec. 3 we derive a closed integral expression for the zeta function at the integer values $s = N \in \mathbb{N}$. This integral expression allows, at least in principle, the calculation of the spectral zeta function for all N once the zero energy Green's function of the Hamiltonian is known. In Sec. 4 we outline the sum rule method as proposed in Ref. 1). Sec. 5 contains our exact results for the circular quantum billiard. In particular, we present in Sec. 5.2 exact expressions for the partial wave zeta function. Some remarks on the WKB approximation and its possible improvement are made in Sec. 5.3. Our main results are discussed in Sec. 6, where the circular Aharonov-Bohm quantum billiard is treated in detail. Using the exact expressions for the zeta function derived in Sec. 5, we are able to study the sum rule method up to a very high level of approximation. As an important result we observe a very fast convergence of the sum rule method to the exact ground state energy as a function of the magnetic flux ("precocious convergence"). Finally, Sec. 7 gives a summary of this work together with our conclusions. In Appendix A and B we discuss the mathematical properties of the circular zeta function. In Appendix C we collect some useful formulae for the "generalized Lerch's transcendent".

2. - THE ZETA FUNCTION OF THE HAMILTONIAN AND RELATED SPECTRAL FUNCTIONS

The quantum systems to be studied in this paper are determined by a Hamiltonian H defined in a bounded euclidean domain $D \subset \mathbb{R}^d$ ($d = 1, 2, \ldots$) with Dirichlet boundary conditions on ∂D:

$$\begin{aligned} H\psi_n(x) &= E_n\psi_n(x) \qquad && x \in D \\ \psi_n(x) &= 0 && x \in \partial D \qquad (2.1) \\ \int_D dx\, |\psi_n(x)|^2 &= 1 \, . \end{aligned}$$

For the systems to be considered, the energy spectrum $\{E_n\}$ will be discrete with a positive, non-degenerate ground state energy E_o

$$0 < E_o < E_1 \leq E_2 \leq \cdots \tag{2.2}$$

and furthermore, it will increase indefinitely

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for all x' in D, where c is a constant independent of x' and t. One thus obtains for $\tau \to 0$

$$Z_H(\tau) = \left(\frac{m\varepsilon}{2\pi\hbar^2\tau}\right)^{d/2} V(D) + \cdots \qquad (2.14)$$

which produces in the first integral in Eq. (2.9) a pole at $s = d/2$ with the residue (2.10). For example, for the two dimensional zeta function one has

$$\zeta_H^{d=2}(s) = \frac{mA}{2\pi\hbar^2} \cdot \frac{1}{s-1} + B + O(s-1), \ \mathrm{Re}\, s > \frac{1}{2} \qquad (2.15)$$

where $A \equiv V(D)$ is the area of D and B denotes the finite part. By mapping the simply connected two-dimensional euclidean domain D on the upper half complex plane, Itzykson et al.[9] expressed B by a single integral involving only the function which generates the conformal mapping.

Knowing the zeta function, one obtains the partition function and the spectral density $\rho_H(E)$ by an inverse Mellin transform ($c > 1$)

$$Z_H(\tau) = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} ds\ \tau^{-s} \varepsilon^{s}\, \Gamma(s) \zeta_H(s) \qquad (2.16)$$

$$\rho_H(E) \equiv \sum_{n=0}^{\infty} \delta(E - E_n) = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} ds\ E^{s-1} \zeta_H(s)\,. \qquad (2.17)$$

The last relation can be used to obtain the spectral staircase

$$N_H(E) \equiv \sum_{n=0}^{\infty} \Theta(E - E_n) = \int_0^E dE'\ \rho_H(E') \qquad (2.18)$$

which counts the number of eigenvalues $\leq E$. By application of a Tauberian theorem one obtains Weyl's famous asymptotic formula[21]

$$N_H(E) = \left(\frac{m}{2\pi\hbar^2}\right)^{d/2} \frac{V(D)}{\Gamma(d/2)}\, E^{d/2} + O\left(E^{\frac{d-1}{2}}\right), \quad E \to \infty \qquad (2.19)$$

which was conjectured by H.A. Lorentz in his Wolfskehl lecture at Göttingen (1910)*).

Another useful representation of the zeta function follows from the relation

$$\frac{1}{E_n^s} = \frac{1}{\pi} \sin \pi s \int_0^{\infty} dE\ \frac{E^{-s}}{E_n + E} \qquad (2.20)$$

and is given by

$$\zeta_H(s) = \frac{1}{\pi} \sin \pi s \int_0^{\infty} dE\ E^{-s} k_H(E) \qquad (2.21)$$

where $k_H(E)$ is the trace of the resolvent

$$k_H(E) \equiv \mathrm{Tr}\left(\frac{1}{H+E}\right) = \sum_{n=0}^{\infty} \frac{1}{E_n + E} = \int_0^{\infty} d\beta\ e^{-\beta E} Z_H(\varepsilon\beta)\,. \qquad (2.22)$$

As an illustration, we give in Table 1 the spectra and the corresponding zeta functions for a few simple quantum systems: the one-dimensional "box billiard" (a free particle in a box with length L), the one-dimensional harmonic oscillator, the "triangle billiard" (a free particle in an equilateral triangle) and the "square billiard" (a free particle moving in a two-dimensional box with equal side lengths). For these systems, the zeta function can be explicitly calculated in terms of the zeta function of Riemann, Eq. (1.2), and a Dirichlet L-function**)

$$L_k(s) \equiv \sum_{n=1}^{\infty} \frac{\chi_k(n)}{n^s}\ , \quad k = 1, 2, 3, \ldots \qquad (2.23)$$

with Dirichlet character $\chi_k(n) = \pm 1$ or 0, $\chi_k(n+k) = \chi_k(n)$. Notice that the one-dimensional harmonic oscillator is not a quantum billiard, and thus the leading pole of the zeta function has not to lie at $s = 1/2$.

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*) For a review on this subject, see Ref. 22).

**) Except for $k = 1$, where $L_1(s) = \zeta(s)$, $L_k(s)$ are entire functions of s.

The above listed examples show that even very simple quantum systems lead already to zeta functions which involve non-trivial number-theoretic functions. It is thus not surprising that for more complicated sytems one has not yet been able to derive a closed expression for the zeta function and related spectral functions.

From the well-known functional relation for the Riemann zeta function [23] one obtains the following functional relation for the zeta function of the one-dimensional box billiard ($\varepsilon = \hbar^2\pi^2/2m\,L^2$)

$$\zeta_{Box}(s) = \frac{\sqrt{\varepsilon}}{\pi}\left(\frac{2\pi}{\varepsilon}\right)^{2s} \sin \pi s \; \Gamma(1-2s)\, \zeta_{Box}\left(\tfrac{1}{2}-s\right) \quad . \tag{2.24}$$

Eq. (2.24) allows an analytic continuation of the zeta function to the region Res < 0, i.e. outside the original region of convergence. The original hope of Minakshisundaram-Pleijel and Weyl, that the spectral zeta function would satisfy in general a functional equation of the type (2.24), "is still unsubstantiated"[24]. A rare exception is the one-dimensional quartic oscillator where some functional equations have been found by Voros[7].

Up to now we have mainly concentrated on the leading pole of the zeta function (the Weyl term) which is determined by the high temperature behaviour of the partition function or, equivalently, by the asymptotic behaviour of the energy spectrum. The main emphasis in the present paper will be on the lower part of the spectrum, i.e. on the computation of the ground state energies. This part of the spectrum is governed by the large s behaviour of the zeta function and is much harder to control. It is thus a great surprise to discover that already a knowledge of the zeta function at the very low integer points s = 2, 3 or 4 is enough to obtain accurate values for the ground state energies. This observation is the basis for our "sum rule method"[1), 2)] which will be discussed in Sec. 4. But before let us show how the zeta function at integer points, $s = N \in \mathbb{N}$, can be calculated by means of a closed integral expression.

3. - CLOSED INTEGRAL EXPRESSION FOR THE ZETA FUNCTION AT s = N

Consider the zeta function (2.5) at the integer points*) $s = N_o$, $N_o + 1, \ldots$

$$\zeta_H(N) = \sum_{n=0}^{\infty} \frac{1}{E_n^N} \quad , N = N_o, N_o+1, \ldots \tag{3.1}$$

The negative energy moments (3.1) are given[1)] by the trace of a generalized Green's function $G_H^{(N)}$**)

$$\zeta_H(N) = \mathrm{Tr}\; G_H^{(N)} \equiv \int_D dx\; G_H^{(N)}(x,x) \tag{3.2}$$

$$\begin{aligned} G_H^{(N)}(x,x') &= \left[G_H^{(N)}(x',x)\right]^* \equiv \zeta_H(N;x,x') \\ &\equiv \langle x|\, H^{-N} \,|x'\rangle = \sum_{n=0}^{\infty} \frac{\psi_n(x)\psi_n^*(x')}{E_n^N} \end{aligned} \tag{3.3}$$

with

$$\begin{aligned} G_H^{(0)}(x,x') &= \delta^{(d)}(x-x') \\ H_x\, G_H^{(N)}(x,x') &= G_H^{(N-1)}(x,x') \quad . \end{aligned} \tag{3.4}$$

For quantum billiards it was shown in Ref. 5) that $\zeta_H(s;x,x')$ is an entire function of s, if x and x' are distinct points in D, with so-called "trivial zeros" at s = 0, -1, -2, ... For x' = x one obtains a meromorphic function of s with a leading simple pole at s = d/2 and the same trivial zeros as before.

*) For quantum billiards, $N_o = [d/2] + 1$, where $[x]$ denotes the largest integer less than or equal to x.

**) "Iterated kernels" of this type were first studied by Volterra in his famous papers on the theory of integral equations[4)]. The problem of the analytic continuation of $\zeta_H(s;x,x')$ for x' = x as a function of s was first investigated by Carleman[6)] in the case d = 2. The general investigation for x' ≠ x is due to Minakshisundaram[5)] who called these functions "generalized Epstein zeta functions".

Notice that a knowledge of all the energy moments (3.1) determines completely the trace of the resolvent in a disc with radius E_o in the complex energy plane*)

$$\mathrm{Tr}\left(\frac{1}{H-E}\right) = \sum_{N=0}^{\infty} \zeta_H(N+1)\, E^N \quad . \tag{3.5}$$

It is easy to see that the Green's functions $G_H^{(N)}$ can be recursively calculated form the integral relations[1)]

$$G_H^{(N)}(x,x') = \int_D dy\, G_H(x,y)\, G_H^{(N-1)}(y,x') \tag{3.6}$$

where $G_H \equiv G_H^{(1)}$ is the Green's function of H (the resolvent kernel of H evaluated at $E = 0$).

From (3.2) and (3.6) we obtain the following <u>closed integral expression for the zeta function</u> at $s = N$

$$\zeta_H(N) = \int_D \prod_{k=1}^{N} dx_k\, G_H(x_1,x_2)\, G_H(x_2,x_3) \cdots G_H(x_N,x_1) . \tag{3.7}$$

These relations yield for $N = N_o, N_o + 1, \ldots$ a hierarchy of <u>sum rules</u> for the negative power sums of the bound state energies. Once the zero-energy Green's function G_H has been determined, the problem is reduced to the evaluation of definite integrals which may be achieved by symbolic algebra. Notice that the even energy moments can be expressed as

$$\zeta_H(2N) = \int_D dx \int_D dx' \left| G_H^{(N)}(x,x')\right|^2 . \tag{3.8}$$

For three-dimensional confinement potentials of the form $V(r) = g\, r^p$, $g > 0$, $p > 0$ we have calculated the zeta function (3.1) for $N = 1, 2$ and for fixed angular momentum[1), 2)].

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*) Here we assume that the leading pole of the zeta function lies to the left of the line Re $s = 1$. This is true for $d = 1$ and for the partial wave zeta functions for $d = 2$.

4. - <u>THE SUM RULE METHOD</u>

The spectral zeta function can be rewritten as

$$\zeta_H(s) = E_o^{-s}\,(1 + \eta(s)) \quad . \tag{4.1}$$

Here we have introduced the (dimensionless) <u>spectral eta function</u>

$$\eta(s) \equiv \sum_{n=1}^{\infty} x_n^s \quad , \quad x_n \equiv \frac{E_o}{E_n} \tag{4.2}$$

which is a meromorphic function of s with the same poles (but different residua) as the zeta function. For systems with a non-degenerate spectrum we have

$$0 < x_{n+1} < x_n < 1 \qquad \forall n \in \mathbb{N} \tag{4.3}$$

and we thus infer that $\eta(s)$ is a strictly monotone decreasing, positive function of s with the limit

$$\lim_{s\to\infty} \eta(s) = 0 \quad . \tag{4.4}$$

Let us now define two new spectral functions (with dimension of energy) which are proportional to the ground state energy E_o (times an expression which depends only on the eta function)

$$L(s) \equiv [\zeta_H(s)]^{-\frac{1}{s}} = E_o\,[1+\eta(s)]^{-\frac{1}{s}} \tag{4.5}$$

$$R(s) \equiv \frac{\zeta_H(s)}{\zeta_H(s+1)} = E_o\, \frac{1+\eta(s)}{1+\eta(s+1)} \quad . \tag{4.6}$$

Then it follows from (4.4)

$$\lim_{s\to\infty} L(s) = \lim_{s\to\infty} R(s) = E_o \tag{4.7}$$

i.e. the spectral functions L(s) and R(s) approach in the limit $s \to \infty$ the ground state energy E_o. Furthermore, we infer from the monotony of $\eta(s)$ that L(s) is a lower bound to the ground state energy

$$L(s_1) < L(s_2) < E_o \quad , \quad s_1 < s_2 , \tag{4.8}$$

whereas R(s) is an upper bound

$$R(s_1) > R(s_2) > E_o \quad , \quad s_1 < s_2 . \tag{4.9}$$

Thus the spectral functions L(s), R(s) lead to the embracing relation $(s_1 < s_2)$

$$L(s_1) < L(s_2) < E_o < R(s_2) < R(s_1) \tag{4.10}$$

for the ground state energy E_o.

In Sec. 3 we showed that there exist sum rules for the zeta function at integer values, $s = N \geq N_o$, which are given by the closed integral expression (3.7). From these sum rules we can calculate the spectral functions L(s) and R(s) at s = N via. Eqs. (4.5) and (4.6), respectively, and thus evaluate the embracing relation (4.10) for $s_1 = N$, $s_2 = N + 1$. We are therefore led to a new method for the calculation of the ground state energy E_o, which we call "sum rule method"[1), 2)] since it is based on the sum rules (3.7). In contrast to most of the other well-known methods, the sum rule method simultaneously gives an upper and lower bound and thus provides an exact measure for the error of the approximation achieved at a given N. For a fixed N, we define the Nth approximant $E_o(N)$ to the ground state energy by the arithmetic mean of the upper and lower bound

$$E_o(N) \equiv \frac{1}{2}\left(R(N) + L(N)\right) \tag{4.11}$$

with an exact error

$$\delta(N) \equiv \frac{1}{2}\left(R(N) - L(N)\right) . \tag{4.12}$$

From (4.7) follows

$$\lim_{N\to\infty} E_o(N) = E_o$$
$$\lim_{N\to\infty} \delta(N) = 0 \quad . \tag{4.13}$$

For d-dimensional quantum billiards, the lowest possible N value to start with is $N_o = [d/2] + 1$. Since N_o is very close to the leading pole of the zeta function at s = d/2, we cannot hope that the embracing relation (4.10), evaluated at $s_1 = N_o$, gives a good upper and lower bound. If, however, the lower and upper bound deviate in a nearly symmetrical fashion from the exact energy E_o, the N_oth approximant $E_o(N_o)$, Eq. (4.11), should already give an useful estimate for the ground state energy. That this is indeed the case has been confirmed in Refs. 1), 2) by a numerical evaluation for various one- and three-dimensional confinement potentials. It is also true for the circular Aharonov-Bohm (AB) quantum billiard (see Sec. 6). The typical error of the lowest approximant is of the order of 10%.

Let us now turn to the crucial question of convergence of the sum rule method. The spectral eta function (4.2) behaves asymptotically as

$$\eta(s) \underset{(s\to\infty)}{\sim} e^{-as} \quad , \quad a \equiv \ln\left(1 + \frac{\Delta}{E_o}\right) \tag{4.14}$$

where $\Delta \equiv E_1 - E_o$ is the energy gap between the ground state and the first excited state. From (4.14) and Eqs. (4.5) and (4.6) one obtains the asymptotic behaviour

$$L(s) \underset{(s\to\infty)}{\sim} E_o\left[1 - \frac{1}{s}\, e^{-as}\right] \tag{4.15}$$

$$R(s) \underset{(s\to\infty)}{\sim} E_o\left[1 + e^{-as}\right] . \tag{4.16}$$

We therefore conclude that the sum rule method converges exponentially to the true ground state energy. The rate of convergence depends on the coefficient a, Eq. (4.14), and is the better the larger the energy gap Δ is.Eqs.

(4.15) and (4.16) show that the lower bound L(s) converges faster to E_o than the upper bound R(s). We thus expect that there exists an $\bar{s}$ such that for $s \geq \bar{s}$ the lower bound L(s) is much closer to the exact ground state energy than the upper bound R(s). For the same reason, the lower bound should yield for $s \geq \bar{s}$ an excellent estimate for E_o, which is even superior to the approximant (4.11). The surprsing result of our numerical study of confinement potentials[1), 2)] and of the circular AB quantum billiard (see Sec. 6) is, that the values obtained for $\bar{s}$ are rather small. In Tables 2 to 7 we display the numerical values of the functions L(s), R(s) and $E_o(s)$ for s = 1, 2, ..., 10 for the AB quantum billiard. For a given s, we have underlined the value which is closest to the exact ground state energy. It is seen that for $s \geq 4$ the lower bound L(s) indeed yields the best estimate. L(4) is only too low by 0.1%, at the worst (Table 7). With $\bar{s}$ having a value as small as 4, we can conclude that the sum rule method converges very fast, i.e. it shows "precocious convergence".

Up to now we have concentrated on the calculation of the ground state energy E_o. Let us briefly show how the sum rule method can be generalized to obtain simultaneously the energy E_1 of the first excited state. For that purpose we define the function

$$\bar{L}(s) \equiv x\left[1 - \frac{y^s}{s}\right] \tag{4.17}$$

depending on two parameters, $x > 0$, $0 < y < 1$. If we assume that the zeta function is given at the two points s = N and N + 1 with $N \geq \bar{s}$, we can calculate L(N) and L(N+1) from Eq. (4.5). By demanding $\bar{L}(N) = L(N)$, $\bar{L}(N+1) = L(N+1)$, we can determine the free parameters x and y. Comparing (4.17) with the asymptotic law (4.15) we infer the following extrapolated energies

$$(E_o)_{extrap.} \equiv x \quad , \quad (E_1)_{extrap.} \equiv \frac{x}{y} \quad . \tag{4.18}$$

Since the lower bound L(s) shows for $s \geq \bar{s}$ precocious convergence, we expect the function $\bar{L}(s)$ for $s \geq \bar{s}$ to be a very good approximation to L(s). Thus the values (4.18) should provide accurate estimates for E_o and E_1. As an example, we consider the one-dimensional box billiard, calculate L(5) and L(6) and determine the parameters x and y. We then obtain from (4.18)

$$(E_o)_{extrap.} = 1.000\ 000\ 74\ (E_o)_{exact} \ ,$$
$$(E_1)_{extrap.} = 0.995\ 731\ (E_1)_{exact} \ . \tag{4.19}$$

Clearly, not only the ground state energy, but also the energy of the first excited level, is obtained with high precision.

5. - THE CIRCULAR QUANTUM BILLIARD

5.1 General results for the circular zeta function

In the case of the circular quantum billiard, the domain D is a disc of radius R. Introducing polar coordinates r, θ , $0 \leq r \leq R$, $0 \leq \theta \leq 2\pi$, the wave function can be written as

$$\Psi_{n\ell}(r,\Theta) = \frac{u_{n\ell}(r)}{\sqrt{r}} \, \frac{e^{i\ell\Theta}}{\sqrt{2\pi}} \tag{5.1}$$

where $n \in \mathbb{N}_o$ is the radial quantum number and $\ell \in \mathbb{Z}$ is the angular momentum. $u_{n\ell}(r)$ denotes the reduced radial wave function with normalization

$$\int_0^R dr\, [u_{n\ell}(r)]^2 = 1 \tag{5.2}$$

and boundary conditions

$$u_{n\ell}(0) = u_{n\ell}(R) = 0 \ . \tag{5.3}$$

The normalized eigenfunctions are given by*)

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*) Since the Bessel operator (see Eq. (5.11)) depends on ℓ only quadratically, one gets the two solutions J_ℓ and $J_{-\ell}$. But $J_{-\ell} = (-1)^\ell J_\ell$, and we can restrict ourselves to $J_{|\ell|}$.

$$u_{n\ell}(r) = N_{n\ell}\sqrt{r}\; J_{|\ell|}\left(j_{n+1}(|\ell|)\frac{r}{R}\right),$$

$$N_{n\ell} = \frac{\sqrt{2}}{R}\left[J_{|\ell|+1}\left(j_{n+1}(|\ell|)\right)\right]^{-1} \tag{5.4}$$

where $j_n(\alpha)$ denotes the nth positive zero of the Bessel function $J_\alpha(z)$. The energy spectrum is given by

$$E_{n\ell} = \varepsilon\, \sigma_\ell(n) \quad ,$$

$$\varepsilon = \frac{\hbar^2}{2mR^2} \quad , \quad \sigma_\ell(n) = \left[j_{n+1}(|\ell|)\right]^2 . \tag{5.5}$$

Thus the circular zeta function has the following representation

$$\varepsilon^s \zeta_\odot(s) \equiv \sum_{\ell=-\infty}^{\infty} \zeta_{|\ell|}(s)$$

$$= \zeta_0(s) + 2\sum_{\ell=0}^{\infty} \zeta_{\ell+1}(s) \tag{5.6}$$

where the circular partial wave zeta function (with fixed "angular momentum" α) is defined by

$$\zeta_\alpha(s) \equiv \sum_{n=1}^{\infty} \frac{1}{\left[j_n(\alpha)\right]^{2s}} \quad . \tag{5.7}$$

From the general discussion of Sec. 2 we know that the zeta function (5.6) must be a meromorphic function of s with a dominant simple pole at $s = 1$ and residue $(m/2\pi\hbar^2) \cdot \pi R^2 = 1/4\,\varepsilon$. We shall see below that this pole is caused by a divergence of the ℓ-summation in Eq. (5.6). The problem is now reduced to a study of the partial wave zeta function (5.7). Before we discuss (5.7) in detail, let us summarize what was known up to now about the complete zeta function (5.6).

In Appendix A we shall derive a closed expression for the partial wave resolvent kernel. Taking the trace and rewriting the ℓ-summation as a Sommerfeld-Watson transform, one can infer the large energy-behaviour of the trace of the complete resolvent. This has already been done by Stewartson and Waechter[25] and will not be repeated here. These authors obtain the following small τ behaviour of the circular partition function ($\hbar = 2m = R = 1$, i.e. $\varepsilon = 1$)

$$Z_\odot(\tau) = \frac{A_\odot}{4\pi}\frac{1}{\tau} - \frac{L_\odot}{8\sqrt{\pi}}\frac{1}{\sqrt{\tau}} + \frac{1}{6} + \frac{\sqrt{\pi}}{128}\sqrt{\tau} + \frac{2}{315}\tau + \frac{37\sqrt{\pi}}{2^{14}}\tau^{3/2} + O(\tau^2) \tag{5.8}$$

where $A_\odot = \pi$ and $L_\odot = 2\pi$ are the area and circumference, respectively, of the unit disc. Using the asymptotic expansion (5.8), we derive for the circular zeta function*)

$$\zeta_\odot(s) = \frac{a_1}{s-1} + \frac{a_{1/2}}{s-1/2} + \frac{a_{-1/2}}{s+1/2} + \frac{a_{-3/2}}{s+3/2} + \varphi(s) \tag{5.9}$$

where $\varphi(s)$ is a regular function for $\mathrm{Re}\, s > -5/2$. Thus $\zeta_\odot(s)$ has a series of poles at $s = 1, 1/2, -1/2, -3/2, \ldots$ with residua

$$a_1 = -a_{1/2} = \frac{1}{4} \;,\; a_{-1/2} = -\frac{1}{256} \;,\; a_{-3/2} = \frac{111}{2^{16}} \quad . \tag{5.10}$$

5.2 Exact results for the circular partial wave zeta function at $s = N$

In this section we shall present exact results for the partial wave zeta function (5.7) at positive integer values. The zeta function (5.7) is nothing but the spectral zeta function of the Bessel operator

$$-\frac{d^2}{dr^2} + \frac{\alpha^2 - 1/4}{r^2} \tag{5.11}$$

acting on functions $f(r)$ defined in the interval $0 \leqslant r \leqslant 1$ with Dirichlet boundary conditions $f(0) = f(1) = 0$.

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*) Notice that the factor $\Gamma(s)$ in Eq. (2.7) kills the poles which one may have expected at $s = 0, -1, -2, \ldots$.

At first sight one may think that it is hopeless to obtain exact expressions for the zeta function (5.7), since it is well-known that there does not exist a closed expression for the zeros of Bessel functions (except the case $\alpha = 1/2$). One only knows the Mc Mahon expansion (5.20) which is an asymptotic expansion for $n \to \infty$. Since $j_n(\alpha)$ $(\alpha \neq 1/2)$ is not of the form $(an + b)^c$ [with a, b, c = constants, independent of n] or of a similar type involving products of this form, it is not clear from the beginning that the reciprocal power sums of zeros of Bessel functions can be given in a closed form. Surprisingly enough, it turns out that the zeta function (5.7) can be exactly calculated at the points $s = N$, $N \in \mathbb{N}$. In the course of the work summarized in Ref. 1), we have calculated the zeta function (5.7) at the points s = 1, 2, ..., 6 from the recursion relation (A.13) derived in Appendix A. We then became aware of the interesting history of these sum rules which is briefly sketched at the end of Appendix A.

From the general relations derived in Appendix A we can infer that $\zeta_\alpha(N)$ is a rational function of α which we shall write in the form

$$\zeta_\alpha(N) = \frac{P_N(\alpha)}{Q_N(\alpha)} \quad , \quad N \in \mathbb{N} . \tag{5.12}$$

Here $Q_N(\alpha)$ is a polynomial in α of degree

$$\delta_Q(N) = \sum_{n=1}^{N} \left[\frac{N}{n}\right] \tag{5.13}$$

and is explicitly given in the product form

$$Q_N(\alpha) = 2^{2N} \prod_{n=1}^{N} (\alpha+n)^{\left[\frac{N}{n}\right]} . \tag{5.14}$$

$P_N(\alpha)$ denotes a polynomial of degree

$$\delta_P(N) = \delta_Q(N) - (2N-1) \tag{5.15}$$

and may be written as

$$P_N(\alpha) = \sum_{n=0}^{\delta_P(N)} a_n(N)\, \alpha^n . \tag{5.16}$$

Using the recursion relation (A.13), I have calculated the coefficients $a_n(N)$ up to N = 10. I could not find a direct relation between the polynomials Q_N, P_N and the well-known classical polynomials. From (5.12), (5.13) and (5.15) one obtains the following asymptotic behaviour for $\alpha \to \infty$

$$\zeta_\alpha(N) = \frac{a_{\delta_P(N)}(N)}{2^{2N}}\, \alpha^{-(2N-1)} + O\left(\alpha^{-2N}\right) . \tag{5.17}$$

From (5.17) we infer that the ℓ-summation in Eq. (5.6) diverges for s = 1, but is convergent for s = 2, 3, ..., in agreement with the general results of Sec. 2.

Below we shall give the exact expressions for the partial wave zeta function (5.7) at the integer values s = 1, 2, ..., 10:

$$\zeta_\alpha(1) = \frac{1}{4(\alpha+1)} \quad , \quad \zeta_\alpha(2) = \frac{1}{16(\alpha+1)^2(\alpha+2)} ,$$

$$\zeta_\alpha(3) = \frac{1}{32(\alpha+1)^3(\alpha+2)(\alpha+3)} , \tag{5.18}$$

$$\zeta_\alpha(4) = \frac{5\alpha+11}{256(\alpha+1)^4(\alpha+2)^2(\alpha+3)(\alpha+4)} ,$$

$$\zeta_\alpha(5) = \frac{7\alpha+19}{512(\alpha+1)^5(\alpha+2)^2(\alpha+3)(\alpha+4)(\alpha+5)} ,$$

$$\zeta_\alpha(6)=\frac{21\alpha^3+181\alpha^2+513\alpha+473}{2048\,(\alpha+1)^6(\alpha+2)^3(\alpha+3)^2(\alpha+4)(\alpha+5)(\alpha+6)}\,,$$

$$\zeta_\alpha(7)=\frac{33\alpha^3+329\alpha^2+1081\alpha+1145}{4096\,(\alpha+1)^7(\alpha+2)^3(\alpha+3)^2(\alpha+4)(\alpha+5)(\alpha+6)(\alpha+7)}\,,$$

$$\zeta_\alpha(8)=\frac{429\alpha^5+7\,640\alpha^4+53\,752\alpha^3+185\,430\alpha^2+311\,387\alpha+202\,738}{65\,536\,(\alpha+1)^8(\alpha+2)^4(\alpha+3)^2(\alpha+4)^2(\alpha+5)(\alpha+6)(\alpha+7)(\alpha+8)}\,,$$

$$\zeta_\alpha(9)=\frac{715\alpha^6+16\,567\alpha^5+158\,568\alpha^4+798\,074\alpha^3+2\,217\,079\alpha^2+3\,212\,847\alpha+1\,893\,046}{131\,072\,(\alpha+1)^9(\alpha+2)^4(\alpha+3)^3(\alpha+4)^2(\alpha+5)(\alpha+6)(\alpha+7)(\alpha+8)(\alpha+9)}\,,$$

$$\zeta_\alpha(10)=\frac{P_{10}(\alpha)}{Q_{10}(\alpha)}\,, \qquad (5.18\text{ctd})$$

$$\begin{aligned}\tfrac{1}{2}P_{10}(\alpha)=\;&2431\,\alpha^8+80\,425\,\alpha^7+1\,152\,851\,\alpha^6\\&+9\,315\,667\,\alpha^5\\&+46\,240\,675\,\alpha^4+143\,917\,279\,\alpha^3\\&+273\,583\,653\,\alpha^2+289\,891\,557\,\alpha\\&+130\,934\,438\,,\end{aligned}$$

$$\begin{aligned}\tfrac{1}{2}Q_{10}(\alpha)=\;&524\,288\,(\alpha+1)^{10}(\alpha+2)^5(\alpha+3)^3(\alpha+4)^2\cdot\\&\cdot(\alpha+5)^2(\alpha+6)(\alpha+7)(\alpha+8)(\alpha+9)(\alpha+10)\,.\end{aligned}$$

For $\alpha = 1/2$ there exists a closed expression for all s values in terms of the zeta function of Riemann

$$\zeta_{\frac{1}{2}}(s)=\pi^{-2s}\,\zeta(2s)\,. \qquad (5.19)$$

5.3 The WKB approximation for the circular zeta function

As already mentioned, no closed expression is known for the zeros of Bessel functions. One has, however, Mc Mahon's asymptotic expansion[26] *)

$$j_n(\alpha)=\pi\nu\left[1-\frac{\mu-1}{8\pi^2\nu^2}-\frac{4(\mu-1)(7\mu-31)}{3\cdot 8^3\,\pi^4\nu^4}+O\!\left(\frac{1}{\nu^6}\right)\right] \qquad (5.20)$$

which is valid for $n \gg \alpha$, α fixed, $\nu = n + (2\alpha-1)/4$, $\mu = 4\alpha^2$. Substitution of the leading term of (5.20) in (5.5), yields exactly the WKB result for the energy eigenvalues. Using these WKB energies in Eq. (5.7), we obtain the WKB approximation

$$\pi^{2s}\varepsilon^s\,\zeta_\odot^{WKB}(s)=\zeta\!\left(2s,\tfrac{3}{4}\right)+2\sum_{\ell=0}^{\infty}\zeta\!\left(2s,\frac{2\ell+5}{2}\right) \qquad (5.21)$$

with the corresponding WKB approximation for the partial wave zeta function

$$\pi^{2s}\,\zeta_\alpha^{WKB}(s)=\zeta\!\left(2s,\frac{2\alpha+3}{4}\right). \qquad (5.22)$$

Here $\zeta(s,\alpha)$ is the generalized zeta function[27] which is a meromorphic function of s with a simple pole at $s = 1$. Thus the zeta function (5.22) and the first term in Eq. (5.21) are meromorphic functions of s with a simple pole at $s = 1/2$. With the help of the integral representation[27] ($\mathrm{Re}\,s > -1$, $\mathrm{Re}\,\alpha > 0$)

$$\zeta(s,\alpha)=\frac{\alpha^{1-s}}{s-1}+\frac{1}{2}\alpha^{-s}+\frac{1}{\Gamma(s)}\int_0^\infty dx\,x^{s-1}e^{-\alpha x}\left[\frac{1}{e^x-1}-\frac{1}{x}+\frac{1}{2}\right] \qquad (5.23)$$

we can carry out the ℓ-summation in Eq. (5.21) and obtain the result

$$\zeta_\odot^{WKB}(s)=\frac{2}{\pi^2\varepsilon}\cdot\frac{1}{s-1}+F(s) \qquad (5.24)$$

---

*) No explicit formula is available for the general term.

where $F(s)$ is regular for $s > 1/2$. This result agrees with our general formula (2.15) apart from the fact that the residue of the pole at $s = 1$ is too small by a factor $\pi^2/8 \approx 1.23$. The reason for this discrepancy is clear: although the WKB formula (5.22) has the correct power behaviour in α for $\alpha \to \infty$, the coefficient of the leading term is not correct as a consequence of the fact that the expansion (5.20) is only valid for $n \gg \alpha$. We thus conclude that the WKB approximation is not reliable for the complete zeta function which is very sensitive to the large α-behaviour.

At this point we may ask whether a modified WKB approximation improves the result. To study this question, let us take the next term in the expansion (5.20) into account which, after expanding in powers of ν, leads to the improved WKB energies

$$E_{n\alpha}^{\text{WKB-impr.}} = \varepsilon\pi^2 \left[\left(n + \frac{\alpha}{2} + \frac{3}{4} \right)^2 - \frac{\alpha^2 - 1/4}{\pi^2} \right] . \quad (5.25)$$

To (5.25) corresponds the zeta function

$$\pi^{2s} \zeta_\alpha^{\text{WKB-impr.}}(s) = \Phi\left(1, s, \frac{2\alpha+3}{4}, \frac{1}{\pi}(\alpha^2 - 1/4)^{1/2}\right) \quad (5.26)$$

where we have defined a "generalized Lerch's transcendent" $\phi(z, s, a, b)$ [see Appendix C]. The result (5.26) is really an improvement compared to (5.22). If one evaluates, for example, (5.26) at $s = 1$ and considers the limit $\alpha \to \infty$, one obtains the correct α-behaviour with a coefficient which deviates only by a factor $(2/\pi)\ln\left[(1+2/\pi)/(1-2/\pi)\right] \approx 0.96$ from the exact result [see Eq. (5.18)].

6. - THE CIRCULAR AHARONOV-BOHM QUANTUM BILLIARD

6.1 General results for the bound state Aharonov-Bohm effect*)

Consider a particle of mass m and charge e, confined to an infinite cylinder of radius R. Identify the cylinder axis with the z axis of a cylindrical coordinate system (r, θ, z), $0 \leq r \leq R$, $0 \leq \theta \leq 2\pi$, $-\infty < z < \infty$. Imagine, further, the idealized situation where an external constant magnetic field $\vec{B}$ is generated by an infinitely long solenoid of negligible radius along the z axis. While the magnetic field is non-vanishing only on the z axis, there is a constant magnetic flux

$$\Phi = \int_{\partial D_\odot} \vec{A} \cdot d\vec{s} \quad (6.1)$$

threading the domain $D_\odot$, where $\vec{A}$ is the vector potential, $\vec{B} = \vec{\nabla} \times \vec{A}$. Here $D_\odot$ is a disc of radius R, lying in the plane $z = 0$. The particle must not touch the solenoid, and thus its wave function has to vanish at $r = 0$. Since the wall of the cylinder is supposed to be impenetrable, the wave function also vanishes at $r = R$.

The Hamiltonian for the bound state Aharonov-Bohm effect is (in Gaussian units)

$$H = \frac{1}{2m}\left(\frac{\hbar}{i}\vec{\nabla} - \frac{e}{c}\vec{A}\right)^2 . \quad (6.2)$$

Choosing the gauge $\operatorname{div}\vec{A} = 0$, the vector potential $\vec{A}$ is given by

$$A_r = A_z = 0 \ , \quad A_\theta = \frac{\Phi}{2\pi r} . \quad (6.3)$$

Since the dependence on the variable z is irrelevant for our purpose, we disregard it from now on and consider only the two-dimensional motion in the domain

$$D_\odot = \{ (r, \theta) \mid 0 \leq r \leq R, \ 0 \leq \theta \leq 2\pi \} . \quad (6.4)$$

We are thus led to study the Hamiltonian

$$H_{AB} = -\frac{\hbar^2}{2m}\left[\frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\left(\frac{\partial}{\partial \theta} - i\alpha\right)^2\right] \quad (6.5)$$

*) The bound state Aharonov-Bohm effect has been discussed by Beyers and Yang[28] and Peshkin[29]. For a recent general review on the Aharonov-Bohm effect, see Ref. 30).

which defines the circular Aharonov-Bohm (AB) quantum billiard*). Here the reduced flux α is defined by

$$\alpha = \frac{\phi}{\phi_o} \quad , \quad \phi_o = 2\pi\hbar c/e \simeq 10^{-7}\ \mathrm{gauss}\cdot\mathrm{cm}^2 \tag{6.6}$$

where ϕ_o is London's unit of flux.

For the wave functions and energy eigenvalues one obtains the same results as for the circular (non-magnetic) quantum billiard, Eqs. (5.1) to (5.5), but with the replacement $|\ell| \to |\ell - \alpha|$ **). Thus the zeta function for the circular AB quantum billiard is given by

$$\varepsilon^s \zeta_{AB}(s;\alpha) \equiv \sum_{\ell=-\infty}^{\infty} \zeta_{|\ell-\alpha|}(s) \tag{6.7}$$

where the α-dependence is explicitly indicated and the partial wave zeta function is defined in Eq. (5.7). For vanishing magnetic flux, $\alpha = 0$, we have of course (see Eq. (5.6))

$$\zeta_{AB}(s;0) = \zeta_{\odot}(s) \quad . \tag{6.8}$$

The following properties of ζ_{AB} are a direct consequence of the representation (6.7):

i) ζ_{AB} is a periodic function of α with period 1, i.e. it is periodic in the magnetic flux ϕ with a period given by London's unit flux ϕ_o

$$\zeta_{AB}(s;\alpha+k) = \zeta_{AB}(s;\alpha) \quad \forall k \in \mathbb{Z} . \tag{6.9}$$

This allows us to consider only the interval $-1/2 < \alpha \leqslant 1/2$.

*) A very clear discussion of the scattering AB effect has been given by Kretzschmar in Ref. 31).

**) Here the solution $J_{-(\ell-\alpha)}$, $\ell-\alpha > 0$, is excluded because of its singularity at the origin for $\alpha \notin \mathbb{Z}$. - For a clarification of a recent controversy on the correct definition of the angular momentum operator, see Ref. 32).

ii) ζ_{AB} is an even function of α

$$\zeta_{AB}(s;-\alpha) = \zeta_{AB}(s;\alpha) . \tag{6.10}$$

From i) and ii) follows that the basic interval to be considered is the interval $0 \leqslant \alpha \leqslant 1/2$ to which we shall restrict ourselves in the following. From the Mellin transform (2.16) and the above properties we infer that the partition function of the circular AB quantum billiard is an even periodic function of ϕ with period ϕ_o. This result is in agreement with a general theorem of Beyers and Yang[28)].

6.2 Accurate estimate of the ground state energy as a function of the magnetic flux

The zeta function will now be used as an input in the sum rule method discussed in Sec. 4 to obtain a very accurate estimate of the ground state energy of the circular AB quantum billiard as a function of the magnetic flux. Since the ground state has $\ell = 0$, it is sufficient to consider the S-wave zeta function, which, according to (6.7), is given by the circular zeta function $\zeta_\alpha(s)$ $[0 \leqslant \alpha \leqslant 1/2]$, defined in (5.7).

The embracing relation (4.10) takes the following*) form

$$L(N;\alpha) < L(N+1;\alpha) < \cdots < E_o(\alpha) < \cdots < R(N+1;\alpha) < R(N;\alpha) \tag{6.11}$$

where the lower and upper bounds are defined as a function of s and α by

$$L(s;\alpha) \equiv [\zeta_\alpha(s)]^{-\frac{1}{s}} \quad , \quad R(s;\alpha) \equiv \frac{\zeta_\alpha(s)}{\zeta_\alpha(s+1)} \quad . \tag{6.12}$$

In Tables 2 to 7 we present a detailed numerical evaluation of the embracing relation (6.11) for N = 1 to 10 and for six different values of

*) From now on we set $\hbar = 2m = R = 1$, i.e. $\varepsilon = 1$. $E_o(\alpha)$ denotes the ground state energy, with quantum numbers $n = \ell = 0$, as a function of the reduced magnetic flux α .

the reduced magnetic flux, covering the basic interval $0 \leqslant \alpha \leqslant 1/2$ in steps of 0.1. In addition to the lower and upper bounds (6.12) we also give the Nth approximant to the ground state energy defined by

$$E_0(N;\alpha) \equiv \frac{1}{2}\left(L(N;\alpha) + R(N;\alpha)\right) . \qquad (6.13)$$

In Tables 2 to 7 we have underlined the result which is closest to the exact energy.

From Tables 2-7 we can draw the following conclusions. If the circular zeta function is known only at $s = 1$, one has only the lower bound $L(1;\alpha)$ which leads to a very bad estimate since this bound is too low by $\gtrsim$ 65 to 75% over the α range considered. The reason for the failure of the sum rule method in the case $s = 1$ becomes clear, if we remember that the circular partial wave zeta function has a pole at $s = 1/2$. $\zeta_\alpha(s)$ varies therefore appreciably near $s = 1$ and does not yet show a behaviour which resembles the asymptotic behaviour for $s \to \infty$.

If the zeta function is known at $s = 1$ and 2, one can form the upper bound $R(1;\alpha)$ and a new improved lower bound $L(2;\alpha)$. Although the upper bound is not very useful by itself, the first approximant $E_0(1;\alpha)$ gives already a good estimate which is only 10 - 15% too low. Even better, however, is the lower bound $L(2;\alpha)$ which agrees with the exact result within an error of 0.2% (for $\alpha = 0$) and 3.9% (for $\alpha = 1/2$).

In case the zeta function is known at $s = 2$ and 3, one may hope to see the asymptotic behaviour since one is far away from the pole at $s = 1/2$. Looking at the Tables 2 to 7 one sees that this is indeed the case. The second approximant $E_0(2;\alpha)$ agrees with the exact ground state energy within an error of 1%. A similar "precocious convergence" of the sum rule method has already been found in our previous papers[1), 2)] (see also Sec. 4).

If the zeta function is known at higher integer s values, the accuracy of the estimate improves very quickly. The third approximant has an error which is already as small as 0.2 to 0.4%. From the general discussion of Sec. 4 we know that the lower bound converges for $N \to \infty$ faster than the upper bound. This is clearly seen in Tables 2 to 7, which show that the lower bound indeed gives for $N \geqslant 4$ the best value. For zero magnetic flux,

the error decreases from 10^{-2}% for $N = 4$ to 10^{-5}% for $N = 8$. In the case of "maximal" magnetic flux, $\alpha = 1/2$, the error decreases similarly, but is larger roughly by a factor of 10. In both cases, $\alpha = 0$ and $\alpha = 1/2$, the lower bound agrees for $N = 10$ with the exact bound state energy in all six decimal places displayed in Tables 2 to 7. Notice that for $\alpha = 1/2$ the square root of the given values gives an approximation to π, since $E_0(1/2) = \pi^2$.

For the special value $\alpha = 1/2$, we can check the sum rule method up to much larger N values because of the exact relation (see Eq. (5.19))

$$L(s;\tfrac{1}{2}) = \pi^2 \left[\zeta(2s)\right]^{-\frac{1}{s}} , \ \mathrm{Re}\, s > \frac{1}{2} . \qquad (6.14)$$

Using the tabulated values[33)] of the Riemann zeta function up to $s = 42$, we obtained the following results for the relative error of the lower bound (6.14): $1 \cdot 10^{-7}$ (for $N = 10$), $3 \cdot 10^{-10}$ (for $N = 14$), $1 \cdot 10^{-14}$ (for $N = 21$).

The above discussion exemplifies in a quantitative fashion that the sum rule method provides indeed a very powerful method for the calculation of bound state energies. The circular AB quantum billiard represents one of the rare cases where the zeta function is known up to high s values, even though the energy eigenvalues are non-trivial since they are not given in a closed analytic form. Since a similar behaviour, in particular "precocious convergence", has also been found in a study of one- and three-dimensional quantum systems[1), 2)], it seems justified to expect that this is a general feature of the sum rule method.

6.3 The complete zeta function

To obtain the complete zeta function for the AB quantum billiard, we have to carry out the summation over the partial wave zeta function, see Eq. (6.7). If we introduce for $\mathrm{Re}\, s > 1$ the function

$$\lambda(s;\alpha) \equiv \sum_{\ell=0}^{\infty} \zeta_{\ell+\alpha}(s) \ , \ \alpha \neq -1,-2,\ldots \qquad (6.15)$$

we obtain for the complete zeta function the relation

$$\zeta_{AB}(s;\alpha) = \lambda(s;\alpha) + \lambda(s;1-\alpha), \quad 0 \leq \alpha < 1 . \tag{6.16}$$

From our general discussion in Sec. 2 we infer that $\lambda(s;\alpha)$ is a meromorphic function of s with a dominant simple pole at s = 1. Since the partial wave zeta function is explicitly known at the integers s = 1, 2, ..., 10, see Eq. (5.18), we can evaluate (6.15) and thus the complete zeta function (6.16) at these points. As a consequence of the asymptotic behaviour (5.17), the summation in Eq. (6.15) converges for $s \geqslant 2$.

Since the partial wave zeta function is a rational function of α, see Eq. (5.12), the ℓ-summation in Eq. (6.15) can be explicitly performed. The final result is a linear combination of the diagamma function and its derivatives

$$\lambda(N;\alpha) = \sum_{n=1}^{N} C_n(N)\psi(\alpha+n) + \sum_{n=1}^{[\frac{N}{2}]} \sum_{p=2}^{[\frac{N}{n}]} \frac{(-1)^p}{(p-1)!} D_n^p(N)\,\psi^{(p-1)}(\alpha+n) . \tag{6.17}$$

This result is derived in Appendix B.

As an example, let us consider the case N = 2. We then obtain the exact result (see Appendix B)

$$\zeta_{AB}(2;\alpha) = \frac{1}{16}\left[\frac{\pi^2}{\sin^2\pi\alpha} - \frac{1}{\alpha^2} - \frac{1}{(1-\alpha)^2} - \frac{3}{(1+\alpha)(2-\alpha)}\right], \tag{6.18}$$
$$0 \leq \alpha \leq 1/2 .$$

Notice that the expression (6.18) is much simpler than the expression given in Ref. 10) which still involves a summation over sine and cosine integrals.

From Eq. (6.18) we obtain the lower bound

$$L_{AB}(2;\alpha) \equiv \left[\zeta_{AB}(2;\alpha)\right]^{-\frac{1}{2}} < E_0(\alpha) . \tag{6.19}$$

In Table 8 we have evaluated (6.19). Since s = 2 is very close to the pole of the zeta function at s = 1, one does not expect the lower bound (6.19) to be a very accurate one. This is clearly seen in Table 8 which shows that the deviation from the exact result varies between - 22% and - 45% going from $\alpha = 0$ to $\alpha = 1/2$. We know, of course, that the estimate should considerably improve if one goes to higher s values. We have checked this by using Eq. (6.17). Here we do not, however, reproduce the details of this evaluation, since we have already discussed in Sec. 6.2 the sum rule method based on the partial wave zeta function. The main conclusion is, that one should use the partial wave zeta function for a determination of the ground state energy, since the results obtained are much better than those obtained from the complete zeta function. Indeed, the deviation of the lower bound at s = 2 is only - 4% at $\alpha = 1/2$ using the partial wave zeta function, whereas the corresponding figure is - 45% in the case of the complete zeta function.

7. - SUMMARY AND CONCLUSIONS

In this paper I have presented in detail the results of a quantitative study of the sum rule method. The circular Aharonov-Bohm quantum billiard was chosen because of the recent interest[10)] in this quantum system and because it is one of the few non-trivial systems where exact analytic results are still available thus allowing a check of the method up to high orders of approximation. In Secs. 1 and 2 I gave a rather general introduction to quantum billiards, zeta functions and related spectral functions. The basic tool, the sum rule method, was discussed in Secs. 3 and 4. The sum rule method is based on two crucial observations: i) the possibility to calculate the zeta function at integer values from a knowledge of the zero-energy Green's function by means of closed integral expressions (Sec. 3). ii) The embracing relation (4.10) which simultaneously gives a lower and upper bound to the ground state energy. The sum rule method offers a new method for estimating bound state energies with the nice property that the error of the estimate is exactly known at each order of approximation.

The zeta function for the circular Aharonov-Bohm quantum billiard was given in terms of the circular zeta function, the zeta function of the (non-magnetic) circular quantum billiard. Exact results for the circular zeta function were given in Sec. 5. Based on these results, we were able to study in great detail in Sec. 6 the sum rule method for the Aharonov-Bohm quantum billiard. The main conclusion to be drawn is that the sum rule method works extremely well yielding accurate estimates for the ground state energy as a function of the magnetic flux. As in our previous investigations [1), 2)], we observed a very rapid convergence of the sum rule method, i.e. "precocious convergence". It is almost sure that a further study of the sum rule method will be rewarding.

As a final observation let us draw attention to the relation of the spectral sum rules discussed in this paper to the famous QCD sum rules[34)]. Although, up to now, this relation has not been worked out in the field-theoretical case, the relation to the moments of Bell and Bertlmann[35)] can be explicitly stated. The work of Ref. 35) is devoted to a study of the following "QCD moments" ($N \geq N_o$, see Sec. 3)

$$M_N^{QCD}(E) \equiv \sum_{n=0}^{\infty} \frac{4\pi\,|\psi_{no}(0)|^2}{(E_{no}-E)^N} \quad . \tag{7.1}$$

Here $\psi_{no}(0)$ is the S-wave wavefunction at the origin, E_{no} are the S-wave energies and n denotes the radial quantum number. The moments (7.1) are the non-relativistic analogues of the QCD sum rules of Ref. 34). For $|E| < E_{oo}$ (7.1) can be expanded in a power series in the energy E

$$M_N^{QCD}(E) = 4\pi \sum_{\nu=0}^{\infty} \frac{(N-1+\nu)!}{(N-1)!\,\nu!}\, G_o^{(N+\nu)}(0,0)\, E^{\nu} \tag{7.2}$$

where the expansion coefficients are nothing but the S-wave partial waves of the generalized Green's functions (3.3) (generalized Epstein zeta functions) evaluated at x = x' = 0:

$$G_\ell^{(N)}(x,x') \equiv \sum_{n=0}^{\infty} \frac{\psi_{n\ell}(x)\,\psi_{n\ell}^*(x')}{E_{n\ell}^N} \quad . \tag{7.3}$$

Since the Green's functions (7.3) can be computed from a recursion relation [1)] identical in form to Eq. (3.6), the expansion coefficients of the series (7.2) can be explicitly calculated. Studies along these lines would be interesting.

Appendix A. The circular partial wave zeta function

Consider the trace of the circular partial wave resolvent [see Eq. (2.2)] defined by ($z \in \mathbb{C}$)

$$k_\alpha(z) \equiv \sum_{n=1}^{\infty} \frac{1}{[j_n(\alpha)]^2 - z} \tag{A.1}$$

where $j_n(\alpha)$ denotes the nth positive zero of the Bessel function $J_\alpha(z)$. Expanding in powers of z, one realizes that $zk_\alpha(z)$ is the generating function of the circular partial wave zeta function

$$\zeta_\alpha(s) \equiv \sum_{n=1}^{\infty} \frac{1}{[j_n(\alpha)]^{2s}} \tag{A.2}$$

evaluated at positive integer s values, i.e.

$$z\,k_\alpha(z) = \sum_{N=1}^{\infty} \zeta_\alpha(N)\, z^N \quad . \tag{A.3}$$

To compute the resolvent (A.1), we recall the infinite product representation[36)]

$$\Gamma(\alpha+1)\left(\frac{z}{2}\right)^{-\alpha} J_\alpha(z) = \prod_{n=1}^{\infty}\left(1 - \frac{z^2}{[j_n(\alpha)]^2}\right) , \tag{A.4}$$

$$\alpha \neq -1, -2, \cdots \quad .$$

Taking the logarithmic derivative of Eq. (A.4) and using

$$\frac{d}{dz}\left(z^{-\alpha} J_\alpha(z)\right) = -z^{-\alpha} J_{\alpha+1}(z)$$

we obtain an expression which is of the form of the r.h.s. of Eq. (A.1), and we therefore get the simple result

$$z^2 k_\alpha(z^2) = \frac{z}{2}\,\frac{J_{\alpha+1}(z)}{J_\alpha(z)} \quad . \tag{A.5}$$

After use of the recursion relation

$$J_{\alpha+1}(z) = \frac{2\alpha}{z} J_\alpha(z) - J_{\alpha-1}(z) \tag{A.6}$$

we can combine Eqs. (A.3) and (A.5) to arrive at the relation

$$\varphi_\alpha(z) \equiv \frac{z}{2} \frac{J_{\alpha-1}(z)}{J_\alpha(z)} = \alpha - \sum_{N=1}^{\infty} \zeta_\alpha(N)\, z^{2N} . \tag{A.7}$$

The function $\varphi_\alpha(z)$ fulfills the recursion relation

$$\varphi_\alpha(z) = \alpha + \frac{b z^2}{\varphi_{\alpha+1}(z)} \quad , \quad b = -\frac{1}{4} . \tag{A.8}$$

Iteration of (A.8) leads to the infinite continued fraction

$$\varphi_\alpha(z) = \alpha + \cfrac{b z^2}{(\alpha+1) + \cfrac{b z^2}{(\alpha+2) + \cfrac{b z^2}{(\alpha+3)+\cdots}}} \tag{A.9}$$

$$\equiv \alpha + \frac{b z^2}{(\alpha+1)+} \; \frac{b z^2}{(\alpha+2)+} \; \frac{b z^2}{(\alpha+3)+} \cdots .$$

A comparison of Eqs. (A.7) and (A.9) shows that the zeta functions $\zeta_\alpha(N)$ can be succesively obtained by truncating the continued fraction (A.9) after the Nth term and expanding the Nth convergent of $\varphi_\alpha(z)$ in a power series in z^2. This method is very convenient for small N. In fact, we have originally used this method to calculate the first five zeta functions. The results are given in Eq. (5.18). For higher N values, this method becomes very cumbersome. It is then more practical to work directly with a recursion relation for the zeta functions. This recursion relation can again be derived from (A.7) by expanding the Bessel functions in their well-known power series in z and then using the standard recursion relation for the coefficients of a power series defined by the quotient of two given power

series. Since the derivation is straightforward but rather lengthy, we do not reproduce it here but just give the final linear recursion relation for the circular partial wave zeta functions ($N \in \mathbb{N}$)

$$\zeta_\alpha(N) = A_\alpha(N) + \sum_{n=1}^{N-1} B_\alpha(n)\, \zeta_\alpha(N-n) \tag{A.10}$$

where the coefficients are given by

$$A_\alpha(1) = \zeta_\alpha(1) = \frac{1}{4\,(\alpha+1)} \quad , \tag{A.11}$$

$$A_\alpha(N) = (-1)^{N+1} \frac{(2\alpha+2N+1)(2\alpha+2N+3)\cdots(2\alpha+4N-5)(2\alpha+4N-3)}{2^{N+1}(2N-2)!\,(\alpha+1)(\alpha+2)\cdots(\alpha+N)} ,$$

$$(N=2,3,\ldots) \tag{A.12}$$

$$B_\alpha(n) = (-1)^{n+1} \frac{(2\alpha+2n+1)(2\alpha+2n+3)\cdots(2\alpha+4n-3)(2\alpha+4n-1)}{2^{n}(2n)!\,(\alpha+1)(\alpha+2)\cdots(\alpha+n)} ,$$

$$(n=1,2,\ldots) .$$

From Eqs. (A.10) to (A.12) follows immediately that $\zeta_\alpha(N)$ is a rational function of α which we shall write in the form given in Eq. (5.12). Inspection of the explicit results given in Eq. (5.18) led us to the ansatz (5.14) for the denominator-polynomial Q_N. Using the recursion relation (A.10), it is then not difficult to prove by complete induction that (5.14) holds for all $N \in \mathbb{N}$. In spite of its apparent simplicity, the recursion relation (A.10) is not yet optimal for a determination of the nominator-polynomial P_N. In fact, if one rewrites the r.h.s. of Eq. (A.10) as a single fraction with denominator Q_N, one obtains at first an expression for P_N, which contains much higher powers in α than one expects according to Eq. (5.15), i.e. the final result is only obtained after a lot of cancellations. (For example, in the case N = 3, there appears a polynomial of degree four, whereas after all possible cancellations one is left just with a constant, see Eq. (5.18).) Thus I was searching for a different recursion relation. Surprisingly enough, there exists the following non-linear recursion relation for the circular partial wave zeta functions ($N \in \mathbb{N}$)

$$(\alpha+N+1)\,\zeta_\alpha(N+1)=\varepsilon_N\left[\zeta_\alpha\left(\tfrac{N+1}{2}\right)\right]^2+2\sum_{n=0}^{[\frac{N-2}{2}]}\zeta_\alpha(n+1)\,\zeta_\alpha(N-n),$$

$$\varepsilon_N=\begin{cases}1 & N \text{ odd}\\ 0 & N \text{ even}\end{cases} \qquad (A.13)$$

I have used (A.13) for a calculation of the zeta functions up to N = 10, given in Eq. (5.18). From these results we came to the guess (5.15) for the true degree of the polynomial P_N and thus to the ansatz (5.16). In order to prove Eq. (5.15), it is enough to show that the zeta function has for $\alpha \to \infty$ the asymptotic behaviour (5.17) where the coefficients

$$C_N \equiv a_n(N)\Big|_{n=\delta_P(N)} \qquad (A.14)$$

are non-vanishing. With the help of Eq. (A.13) it is not difficult to derive the above statements. Furthermore, one obtains the following recursion relation for the coefficients (A.14)

$$C_{N+1}=\varepsilon_N\left[C_{\frac{N+1}{2}}\right]^2+2\sum_{n=0}^{[\frac{N-2}{2}]}C_{n+1}\,C_{N-n} \qquad (A.15)$$

which can be used to calculate the coefficients of the highest power of the polynomials $P_N(\alpha)$. Of course, there must exist analogous relations for the remaining coefficients in (5.16), but we have not pursued this further. We just mention one sum rule which follows from Eq. (5.12) by putting $\alpha = 1/2$, using the relation (5.19) and recalling that the Riemann zeta function $\zeta(2N)$ can be expressed in terms of the Bernoulli numbers B_{2N}

$$P_N\left(\tfrac{1}{2}\right)=\sum_{n=0}^{\delta_P(N)}\frac{a_n(N)}{2^n}=2^{4N-1-\delta_Q(N)}\frac{|B_{2N}|}{(2N)!}\prod_{n=1}^{N}(2n+1)^{[\frac{N}{n}]} \qquad (A.16)$$

As a last relation I state the following conjecture

$$\zeta_\alpha(0)=-\alpha \qquad (A.17)$$

which is suggested by Eq. (A.7). The conjecture (A.17) is correct for $\alpha = 1/2$ since in this case it agrees with Riemann's zeta function at s = 0.

Finally, let us add some historical remarks. For the special value $\alpha = 0$, the first few sum rules of Eq. (5.18) have been computed first by Euler[37] who assumed formula (A.4) when $\alpha = 0$. A continued fraction representation, similar to Eq. (A.9), was already known to Bessel[38] and has been used by Jacobi[39] to calculate the first three zeta functions. Explicit expressions for the zeta functions (5.18) up to N = 5 have been found by Rayleigh[40], and immediately afterwards Cayley[41] found the zeta function for N = 8. The relation to Bernoulli numbers in the case $\alpha = 1/2$ was observed by Gubler and Graf[42]. To my knowledge, the zeta functions for N = 6, 7, 9 and 10, given in Eq. (5.18), have been computed for the first time in our paper.

Appendix B. A general formula for the complete circular zeta function

The complete zeta function has been expressed in Eq. (6.16) in terms of the function λ defined in Eq. (6.15). At the points s = 2, 3, ... we obtain with the help of Eq. (5.12) the general result

$$\lambda(N;\alpha)=\sum_{\ell=0}^{\infty}\frac{P_N(\ell+\alpha)}{Q_N(\ell+\alpha)} \qquad (B.1)$$

Since the roots of the polynomials $Q_N(\alpha)$ together with their multiplicities are explicitly known (see Eq. (5.14)), we can decompose the expression in Eq. (B.1) into the following partial fractions (N = 2, 3, ...)

$$\zeta_\alpha(N)=\frac{P_N(\alpha)}{Q_N(\alpha)}=-\sum_{n=1}^{N}\frac{C_n(N)}{\alpha+n}+\sum_{n=1}^{[\frac{N}{2}]}\sum_{p=2}^{[\frac{N}{n}]}\frac{D_n^p(N)}{(\alpha+n)^p} \qquad (B.2)$$

Here we have isolated the sum over the simple poles since it requires a regularization if inserted in (B.1)

Since $\alpha\zeta_\alpha(N)$ behaves as $\alpha^{-(2N-2)}$ for $\alpha \to \infty$ (see Eq. (5.17)), we obtain from (B.2) the sum rules

$$\sum_{n=1}^{N}C_n(N)=0\ ,\quad N=2,3,\ldots \qquad (B.3)$$

With the help of these sum rules we can regularize the first term of (B.2) (written already in the form in which this term enters (B.1)) in the following way

$$-\sum_{n=1}^{N} \frac{C_n(N)}{(\ell+\alpha)+n} = + \sum_{n=1}^{N} C_n(N)\left[\frac{1}{\ell+1} - \frac{1}{\ell+(\alpha+n)}\right] . \tag{B.4}$$

We then obtain the final expression

$$\lambda(N;\alpha) = \sum_{n=1}^{N} C_n(N)\psi(\alpha+n) + \sum_{n=1}^{[\frac{N}{2}]} \sum_{p=2}^{[\frac{N}{n}]} \frac{(-1)^p}{(p-1)!} D_n^p(N)\psi^{(p-1)}(\alpha+n) \tag{B.5}$$

where $\psi(z)$ is the digamma function

$$\psi(z) \equiv \frac{d \ln\Gamma(z)}{dz} = -\gamma + \sum_{\ell=0}^{\infty}\left[\frac{1}{\ell+1} - \frac{1}{\ell+z}\right] \tag{B.6}$$

$$\psi(1) = -\gamma = -0.577\,215\ldots \quad .$$

Thus the problem is reduced to a determination of the coefficients C_n and D_n^p in Eq. (B.2). The final result (B.5) can be further simplified by using the following relations for $\psi(z)$[23)]

$$\psi(z+N) = \sum_{m=0}^{N-1} \frac{1}{z+m} + \psi(z) \quad , N\in\mathbb{N}, \tag{B.7}$$

$$\psi(1+z) - \psi(1-z) = \frac{1}{z} - \pi \cot \pi z \quad .$$

As an example, let us discuss the cases N = 2 and 3. For N = 2 we obtain from Eq. (5.18)

$$\zeta_\alpha(2) = \frac{1}{16}\left[-\frac{1}{\alpha+1} + \frac{1}{\alpha+2} + \frac{1}{(\alpha+1)^2}\right] \tag{B.8}$$

which according to (B.5) leads to

$$\lambda(2;\alpha) = \frac{1}{16}\left[\psi(\alpha+1) - \psi(\alpha+2) + \psi'(\alpha+1)\right] \quad . \tag{B.9}$$

Inserting this expression in Eq. (6.16) and using the relations (B.7) we obtain the final result

$$\zeta_{AB}(2;\alpha) = \frac{1}{16}\left[f(\alpha) - \frac{1}{(1-\alpha)^2} - \frac{3}{(1+\alpha)(2-\alpha)}\right] \tag{B.10}$$

where $f(\alpha)$ is defined by

$$f(\alpha) \equiv \frac{\pi^2}{\sin^2\pi\alpha} - \frac{1}{\alpha^2} = \sum_{n=0}^{\infty} \zeta(2n+2)\,\alpha^{2n} \quad . \tag{B.11}$$

For N = 3 one obtains

$$\lambda(3;\alpha) = \frac{1}{256}\left[-7\psi(\alpha+1) + 8\psi(\alpha+2) - \psi(\alpha+3) - 6\psi'(\alpha+1) - 2\psi''(\alpha+1)\right] \tag{B.12}$$

which can be further simplified as in the case N = 2.

Appendix C. Generalized Lerch's transcendent

We define the "generalized Lerch's transcendent" by

$$\Phi(z,s,a,b) \equiv \sum_{n=0}^{\infty} \frac{z^n}{[(a+n)^2 - b^2]^{s/2}} \tag{C.1}$$

which is an analytic function of z in the cut z-plane, the cut being from 1 to ∞ along the positive real z-axis. Special cases of the function (C.1) are:

$$\Phi(z,s,a,0) = \Phi(z,s,a) \quad , \tag{C.2}$$

$$\Phi(1,s,a,0) = \zeta(s,a) \,, \tag{C.3}$$

$$\Phi(1,s,1,0) = \zeta(s) \,. \tag{C.4}$$

Here the function on the r.h.s. of (C.2) is Lerch's transcendent[23]; relation (C.2) explains why we called the function (C.1) the generalized Lerch's transcendent. The function (C.1) possesses a lot of nice properties[43]. But here we mention only a few. One has the following integral representation

$$\Phi(z,s,a,b) = \frac{\sqrt{\pi}}{\Gamma(\frac{s}{2})} \int_0^\infty dx \, x^{\frac{s-1}{2}} \frac{e^{-ax}}{1-ze^{-x}} \frac{I_{(s-1)/2}(|b|x)}{(2|b|)^{(s-1)/2}} \tag{C.5}$$

where $I_\alpha(z)$ denotes the modified Bessel function. Eq. (C.5) can be used for an analytic continuation of the function (C.1). In Eq. (5.26) we require the function (C.1) at $z = 1$; for $s = N$ we obtain

$$\Phi(1,N+1,a,b) = \frac{(-1)^N (2N)!}{(N!)^2 (2b)^{2N+1}} \left[\psi(a+b) - \psi(a-b) \right] \tag{C.6}$$

$$+ \frac{1}{N!(2b)^{N+1}} \sum_{k=0}^{N-1} \frac{(N+k)!}{k!(N-k)!} \frac{1}{(2b)^k} \left[(-1)^{N+1} \psi^{(N-k)}(a-b) - (-1)^{N+1} \psi^{(N-k)}(a+b) \right].$$

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TABLES

Table 1

Energy spectra and spectral zeta functions for one-dimensional (box billiard, harmonic oscillator) and two-dimensional (triangle billiard, square billiard) quantum systems. The zeta functions have been expressed in terms of the Riemann zeta function (1.2) and a Dirichlet L-function (2.23).

Tables 2 - 7

Numerical evaluation of the embracing relation (6.11) for the circular Aharonov-Bohm quantum billiard for N = 1 to 10 as a function of the reduced magnetic flux α, Eq. (6.6), for α = 0, 0.1, 0.2, 0.3, 0.4, 0.5. Shown are the upper (R) and lower (L) bounds (6.12) together with the Nth approximant to the ground state energy, Eq. (6.13). Units $\hbar = 2m = R = 1$ are used, i.e. $\varepsilon = 1$. The numbers in parantheses give the same results but normalized to the exact ground state energy which is given in the last line. For each N, the value which is closest to the exact energy is underlined.

Table 8

Evaluation of the lower bound (6.19) for the circular Aharonov-Bohm quantum billiard as a function of the reduced magnetic flux α, Eq. (6.6), for α = 0, 0.1, 0.2, 0.3, 0.4, 0.5. For comparison, also the exact ground state energy is shown.

Table 1

quantum system	energy spectrum	spectral zeta function $\cdot \varepsilon^s$
box billiard (d=1)	$\varepsilon n^2, \; n \in \mathbb{N}$	$\zeta(2s)$
harmonic oscillator (d=1)	$\varepsilon(n+\frac{1}{2}), \; n \in \mathbb{N}_0$	$(2^s-1)\,\zeta(s)$
triangle billiard (d=2)	$\varepsilon(n_1^2+n_2^2+n_1 n_2), \; n_1, n_2 \in \mathbb{N}$	$\zeta(s)\,L_3(s) - \zeta(2s)$
square billiard (d=2)	$\varepsilon(n_1^2+n_2^2), \; n_1, n_2 \in \mathbb{N}$	$\zeta(s)\,L_4(s) - \zeta(2s)$

Table 2 (α = 0)

N	L(N;α)		E_0(N;α)		R(N;α)	
1	2	(0.35)	<u>5</u>	(0.87)	8	(1.38)
2	5.657	(0.978)	<u>5.828</u>	(1.008)	6	(1.038)
3	5.769	(0.998)	<u>5.794</u>	(1.002)	5.818	(1.006)
4	<u>5.781 255</u>		5.785 364		5.789 474	
5	<u>5.782 898</u>		5.783 627		5.784 355	
6	<u>5.783 141</u>		5.783 273		5.783 406	
7	<u>5.783 179</u>		5.783 203		5.783 228	
8	<u>5.783 184 745</u>		5.783 189 30		5.783 187 53	
9	<u>5.783 185 759</u>		5.783 186 61		5.783 187 46	
10	<u>5.783 185 928</u>		exact ground state energy: 5.783 186			

Table 3 (α = 0.1)

N	$L(N;\alpha)$	$E_o(N;\alpha)$	$R(N;\alpha)$
1	2.098 (0.32)	5.670 (0.87)	9.240 (1.41)
2	6.376 (0.975)	6.598 (1.009)	6.820 (1.043)
3	6.521 (0.997)	6.555 (1.002)	6.589 (1.008)
4	6.537 689	6.543 718	6.549 746
5	6.540 099	6.541 240	6.542 381
6	6.540 479	6.540 701	6.540 923
7	6.540 542	6.540 586	6.540 630
8	6.540 553	exact ground state energy:	
9	6.540 555 29	6.540 556	
10	6.540 555 63		

Table 4 (α = 0.2)

N	$L(N;\alpha)$	$E_o(N;\alpha)$	$R(N;\alpha)$
1	2.191 (0.30)	6.376 (0.87)	10.560 (1.44)
2	7.120 (0.972)	7.400 (1.010)	7.680 (1.048)
3	7.302 (0.996)	7.347 (1.003)	7.392 (1.009)
4	7.324 148	7.332 662	7.341 177
5	7.327 550	7.329 258	7.330 967
6	7.328 119	7.328 472	7.328 825
7	7.328 220	7.328 294	7.328 368
8	7.328 239	exact ground state energy:	
9	7.328 242 11	7.328 243	
10	7.328 242 77		

Table 5 (α = 0.3)

N	$L(N;\alpha)$	$E_o(N;\alpha)$	$R(N;\alpha)$
1	2.280 (0.28)	7.120 (0.87)	11.960 (1.47)
2	7.886 (0.968)	8.233 (1.011)	8.580 (1.053)
3	8.111 (0.996)	8.170 (1.003)	8.229 (1.010)
4	8.140 205	8.151 856	8.163 507
5	8.144 860	8.147 323	8.149 785
6	8.145 681	8.146 217	8.146 753
7	8.145 834	8.145 953	8.146 071
8	8.145 864	exact ground state energy	
9	8.145 869 48	8.145 871	
10	8.145 870 66		

Table 6 (α = 0.4)

N	$L(N;\alpha)$	$E_o(N;\alpha)$	$R(N;\alpha)$
1	2.366 (0.26)	7.903 (0.88)	13.440 (1.50)
2	8.676 (0.965)	9.098 (1.012)	9.520 (1.059)
3	8.948 (0.995)	9.023 (1.003)	9.098 (1.012)
4	8.985 468	9.000 991	9.016 514
5	8.991 669	8.995 107	8.998 546
6	8.992 815	8.993 600	8.994 385
7	8.993 039	8.993 221	8.993 403
8	8.993 084	exact ground state energy:	
9	8.993 093 81	8.993 096	
10	8.993 095 81		

Table 7 ($\alpha = 0.5$)

N	$L(N;\alpha)$		$E_o(N;\alpha)$		$R(N;\alpha)$	
1	2.450	(0.25)	8.725	(0.88)	15.000	(1.52)
2	9.487	(0.961)	9.993	(1.013)	10.500	(1.064)
3	9.813	(0.994)	9.907	(1.004)	10.000	(1.013)
4	9.859 570		9.879 785		9.900 000	
5	9.867 642		9.872 316		9.876 990	
6	9.869 200		9.870 314		9.871 429	
7	9.869 518		9.869 788		9.870 058	
8	9.869 586		exact ground state energy:			
9	9.869 600		$\pi^2 \approx 9.869\,604$			
10	9.869 603 46					

Table 8

α	$L_{AB}(2;\alpha)$	$E_o(\alpha)_{exact}$
0	4.50	5.78
0.1	4.83	6.54
0.2	5.10	7.33
0.3	5.30	8.15
0.4	5.42	8.99
0.5	5.46	$\pi^2 \approx 9.87$