THE BERRY-KEATING OPERATOR ON COMPACT QUANTUM GRAPHS WITH GENERAL SELF-ADJOINT REALIZATIONS

SEBASTIAN ENDRES AND FRANK STEINER

ABSTRACT. The Berry-Keating operator $H_{\mathrm{BK}} := -\mathrm{i}\hbar \left(x \frac{\mathrm{d}}{\mathrm{d}x} + \frac{1}{2} \right)$ [M. V. Berry and J. P. Keating, SIAM Rev. 41 (1999)] governing the Schrödinger dynamics is discussed in the Hilbert space $L^2\left(\mathbb{R}_>, \mathrm{d}x\right)$ and on compact quantum graphs. A complete classification of all self-adjoint extensions of H_{BK} acting on compact quantum graphs is given together with the corresponding secular equation in form of a determinant whose zeros determine the discrete spectrum of H_{BK}. In addition, an exact trace formula and the Weyl asymptotics of the eigenvalue counting function are derived. Furthermore, we introduce the "squared" Berry-Keating operator $H_{\mathrm{BK}}^2 := -x^2 \frac{\mathrm{d}^2}{\mathrm{d}x^2} - 2x \frac{\mathrm{d}}{\mathrm{d}x} - \frac{1}{4}$ which is a special case of the Black-Scholes operator. Again, all self-adjoint extensions, the corresponding secular equation, the trace formula and the Weyl asymptotics are derived for H_{BK}^2 on compact quantum graphs. Some simple examples are worked out in detail.

1. INTRODUCTION: THE HYPOTHETICAL HILBERT-POLYA OPERATOR

There is an old idea, usually attributed to Hilbert [1] and Polya [4] that the nontrivial (i.e. complex) zeros s_n of the Riemann zeta function $\zeta(s)$ have a spectral interpretation. Writing $s_n := \frac{1}{2} - \mathrm{i}\tau_n$, the Riemann hypothesis states that the nonimaginary solutions τ_n of $\zeta(\frac{1}{2} - \mathrm{i}\tau_n) = 0$ are real, that is the nontrivial zeros s_n lie on the critical line $\operatorname{Re} s = \frac{1}{2}$. The Hilbert-Polya approach towards a proof of the Riemann hypothesis consists in finding a Hilbert space $\mathcal{H}$ and a self-adjoint operator H in $\mathcal{H}$ whose discrete spectrum is exactly given by the nontrivial zeros $\tau_n = \mathrm{i}\left(s_n - \frac{1}{2}\right)$.

Around 1950, Selberg [5] introduced his zeta function $Z(s)$ in analogy with $\zeta(s)$ and with the intention to shed some light on the nontrivial Riemann zeros and the Riemann hypothesis. He noticed the striking similarity between his famous trace formula for the Laplace-Beltrami operator on e.g. compact Riemannian manifolds and the explicit formulae of number theory, whose most general form is Weil's explicit formula [3]. The nontrivial zeros of the Selberg zeta function $Z(s)$ fulfil the analogue of Riemann's hypothesis and appear in the spectral side of the trace formula being directly related to the spectrum of the Laplacian. The other side of the trace formula has a purely geometrical interpretation, since it is given by a sum over the length spectrum of the closed geodesics (periodic orbits) of the geodesic flow, i.e. the free motion of a point particle on a given hyperbolic manifold. This system was already studied by Hadamard [6, 7] in 1898 and has played an important role in the development of ergodic theory ever since. Hadamard proved that all trajectories in this system are unstable and that neighbouring trajectories diverge in time at an exponential rate, the most striking property of deterministic chaos.

In 1980, Gutzwiller [8] drew attention to this system as a prototype example of quantum chaos by identifying the Laplacian on hyperbolic manifolds with the Schrödinger operator in quantum mechanics. In this way he related the nontrivial zeros of the Selberg zeta function to the quantum energies of a dynamical system whose classical trajectories are chaotic. Furthermore, he realized that the Selberg trace formula is an exact version of his trace formula, the celebrated Gutzwiller trace formula [9], which holds for general quantum systems with a chaotic classical counterpart, but in this case only approximately, i.e. in the so-called semiclassical limit where Planck's constant $\hbar$ approaches zero.

In 1985, Berry [10] emphasized that the search for the hypothetical Hilbert-Polya operator in terms of a Schrödinger operator obtained from the quantization of a classically chaotic system might be a fruitful route to proving the Riemann hypothesis. He discussed in detail the properties of

this operator that are suggested by the quantum analogy. Prompted by a paper written by Connes [11] (see also [12]), who devised a self-adjoint operator (Perron-Frobenius) of a classical dynamical system together with a classical (Lefschetz) trace formula in noncommutative geometry, Berry and Keating [13, 14] speculated that the conjectured Hilbert-Polya operator might be some quantization of the extraordinarily simple classical Hamiltonian function $H_{\mathrm{cl}}(x, p)$ of a single coordinate x and its conjugate momentum p:

$$(1.1) \qquad\qquad H_{\mathrm{cl}}(x, p) := xp.$$

In this paper, we shall study the quantization of the classical Berry-Keating Hamiltonian (1.1) on compact quantum graphs and shall give a complete classification of the self-adjoint realizations of the corresponding Berry-Keating operator. In addition, we shall also study the quantization of the corresponding "squared" operator.

2. Classical dynamics and quantization of the Berry-Keating operator

Let us consider the classical dynamics of a particle moving on the real line $\mathbb{R}$ generated by the Berry-Keating Hamiltonian (1.1) with corresponding phase space $\mathcal{P} : (x, p) \in \mathbb{R} \times \mathbb{R}$. The classical time evolution (Hamiltonian flow) is governed by Hamilton's equations

$$(2.1) \qquad\qquad \dot{x}(t) = \frac{\partial H_{\mathrm{cl}}}{\partial p} = x(t) \quad \text{and} \quad \dot{p}(t) = -\frac{\partial H_{\mathrm{cl}}}{\partial x} = -p(t).$$

Starting at time $t = 0$ at an arbitrary point $(x_0, p_0) \in \mathcal{P}$ in phase space, the unique solutions are [13]

$$(2.2) \qquad\qquad x(t) = x_0 \mathrm{e}^t \quad \text{and} \quad p(t) = p_0 \mathrm{e}^{-t}.$$

Obviously, the point $(0, 0) \in \mathcal{P}$ is an unstable point. We note that the Hamiltonian (1.1) is time independent corresponding to the conserved "energy" $E := H_{\mathrm{cl}}(x(t), p(t)) = x_0 p_0 \in \mathbb{R}$, and thus the particle moves in $\mathcal{P}$ on the "energy surface" (hyperbola) $xp = E$. Obviously, the classical motion is unbounded. Therefore, Berry and Keating [13, 14] introduced some regularization procedures, leading to a truncation of phase space, which we shall discuss below, but first we would like to discuss quantum mechanics.

Quantization of the classical system requires to choose a Hilbert space $\mathcal{H}$ and to replace the classical Hamiltonian (1.1) by a self-adjoint operator H in $\mathcal{H}$. With the standard choice $\mathcal{H} := L^2(\mathbb{R}, \mathrm{d}x)$, the simplest operator corresponding to (1.1) is obtained by Weyl ordering of the coordinate operator x (acting by multiplication) and the momentum operator $p = -\mathrm{i}\hbar \dfrac{\mathrm{d}}{\mathrm{d}x}$ (acting by differentiation) leading to the Berry-Keating operator [13, 14]

$$(2.3) \qquad\qquad H_{\mathrm{BK}} := \frac{1}{2}(xp + px) = -\mathrm{i}\hbar \left(x\frac{\mathrm{d}}{\mathrm{d}x} + \frac{1}{2} \right),$$

and the Schrödinger equation

$$(2.4) \qquad\qquad \mathrm{i}\hbar \frac{\partial \Psi(x, t)}{\partial t} = H_{\mathrm{BK}} \Psi(x, t).$$

As was to be expected from our discussion of the classical motion, the operator H_{BK} is unbounded and does not have a discrete spectrum corresponding to bound states, but rather has a continuous spectrum $\lambda \in \mathbb{R}$ corresponding to scattering states obtained by solving the eigenvalue problem

$$(2.5) \qquad\qquad H_{\mathrm{BK}}\psi(x) = \lambda\psi(x).$$

Writing $\lambda = \hbar k$, $k \in \mathbb{R}$, Planck's constant drops out from (2.5), and the eigenvalue problem reads $(s := -\frac{1}{2} + \mathrm{i}k)$

$$(2.6) \qquad\qquad x\frac{\mathrm{d}\phi_s(x)}{\mathrm{d}x} = s\phi_s(x).$$

For $x \in \mathbb{R}$, (2.6) possesses the general solution

$$(2.7) \qquad\qquad \phi_s(x) = c_1 x_+^s + c_2 x_-^s,$$

where $x_{\pm}^s$ denote the generalized functions, see e.g. [15]

$$(2.8) \qquad x_+^s := \begin{cases} 0 & \text{for } x \leq 0 \\ x^s & \text{for } x > 0 \end{cases} \quad \text{and} \quad x_-^s := \begin{cases} |x|^s & \text{for } x < 0 \\ 0 & \text{for } x \geq 0 \end{cases},$$

which is well defined for $\operatorname{Re} s > -1$. In [13] , Berry and Keating studied as a special case the simplest choice for the continuation of the eigenfunctions across the singularity at $x = 0$ by considering the even eigenfunctions $(c_1 = c_2 = c)$ $\phi_s^{even}(x) = c|x|^s$.

Let us discuss in more detail the case that the quantum dynamics takes place on the positive half-line $x \in \mathbb{R}_>$. Then H_{BK} acting on $\mathcal{D}(\mathbb{R}_>)$, the set of infinitely continuous differentiable functions with compact support on $\mathbb{R}_>$, is essentially self-adjoint (see e.g. [16] [both deficiency indices are equal to zero]). Therefore, the closure of this operator is self-adjoint. The general solution of the time-independent Schrödinger equation (2.5) is given by

$$(2.9) \qquad \psi_k(x) := \frac{1}{\sqrt{2\pi}} x_+^{-\frac{1}{2}+ik} \quad \text{with} \quad k \in \mathbb{R},$$

which is obviously not in $L^2(\mathbb{R}_>, \mathrm{d}x)$ and satisfies the orthonormality relation

$$(2.10) \qquad \langle \psi_k \mid \psi_{k'} \rangle := \int_0^\infty \overline{\psi}_k(x)\psi_{k'}(x)\mathrm{d}x = \delta(k - k')$$

and the completeness relation

$$(2.11) \qquad \int_{-\infty}^\infty \psi_k(x)\overline{\psi}_k(x')\mathrm{d}k = \delta(x - x').$$

We thus have for any $\phi \in L^2(\mathbb{R}_>, \mathrm{d}x)$ the spectral decomposition

$$(2.12) \qquad \phi(x) = \int_{-\infty}^\infty A(k)\psi_k(x)\mathrm{d}k$$

with

$$(2.13) \qquad A(k) := < \psi_k|\phi > = \int_0^\infty \overline{\psi}_k(x)\phi(x)\mathrm{d}x$$

and (assuming $< \phi|\phi > = 1$)

$$(2.14) \qquad \int_{-\infty}^\infty |A(k)|^2\mathrm{d}k = 1.$$

Forming a general wave packet with a given amplitude $A(k)$ satisfying (2.12) and (2.14), one obtains $(x \in \mathbb{R}_>)$

$$(2.15) \qquad \phi(x) = \sqrt{\frac{2\pi}{x}} \hat{A}(\ln x),$$

where $\hat{A}$ denotes the Fourier transform of A

$$(2.16) \qquad \hat{A}(y) := \frac{1}{2\pi} \int_{-\infty}^\infty A(k)\mathrm{e}^{iky}\mathrm{d}k.$$

Let us also mention an alternative to the spectral decomposition (2.12) for the Berry-Keating operator. Defining the Mellin transform $\check{\phi}$ of ϕ by

$$(2.17) \qquad \check{\phi}(s) := \int_0^\infty x^{s-1}\phi(x)\mathrm{d}x,$$

we obtain for the wave number amplitude $A(k)$, see (2.13),

$$(2.18) \qquad A(k) = \frac{1}{\sqrt{2\pi}}\check{\phi}\left(\frac{1}{2} - \mathrm{i}k\right),$$

from which $\phi(x)$ can be recovered as the inverse Mellin transform

$$(2.19) \qquad \phi(x) = \frac{1}{2\pi\mathrm{i}}\int_{\frac{1}{2}-\mathrm{i}\infty}^{\frac{1}{2}+\mathrm{i}\infty}\check{\phi}(s)x^{-s}\mathrm{d}s = \frac{1}{2\pi}\int_{-\infty}^{\infty}\check{\phi}\left(\frac{1}{2} - \mathrm{i}k\right)x^{-\frac{1}{2}+\mathrm{i}k}\mathrm{d}k = \int_{-\infty}^{\infty} A(k)\psi_k(x)\mathrm{d}k$$

in agreement with (2.12).

The unitary group

$$(2.20) \qquad U(t) := \exp(-\frac{\mathrm{i}t}{\hbar}H_{\mathrm{BK}}) = \mathrm{e}^{-\frac{t}{2}}\mathrm{e}^{-tD}$$

generated by the Berry-Keating operator (2.3) acts on functions $\phi \in \mathcal{H}$ as

$$(2.21) \qquad (U(t)\phi)(x) = \mathrm{e}^{-\frac{t}{2}}\phi\left(\mathrm{e}^{-t}x\right).$$

Here we have used the relation $H_{\mathrm{BK}} = -\mathrm{i}\hbar\left(D + \frac{1}{2}\right)$, where $D := x\dfrac{\mathrm{d}}{\mathrm{d}x}$ is the generator of scaling transformations (dilations). Let us mention that the operator D has been discussed by Arendt [17, 18, 19], where $A_p := -D$ is considered as the generator of a semigroup on e.g. $L^p(\mathbb{R}_>, \mathrm{d}x)$ $(1 \le p < \infty)$ with Dirichlet and Neumann boundary conditions.

On the other hand, the action of the unitary operator $U(t)$ on eigenfunctions ψ of H_{BK} gives according to (2.5)

$$(2.22) \qquad (U(t)\psi)(x) = \mathrm{e}^{-\mathrm{i}\frac{\lambda}{\hbar}t}\psi(x),$$

which in turn leads with (2.21), $\lambda = \hbar k$, $s = -\frac{1}{2} + \mathrm{i}k$ and $\kappa := \mathrm{e}^{-t} > 0$ $(t < \infty)$ to

$$(2.23) \qquad \psi(\kappa x) = \kappa^s\psi(x).$$

This shows that an eigenfunction ψ of H_{BK} must be a homogeneous function with (complex) degree $s = -\frac{1}{2} + \mathrm{i}k$. Differentiation of (2.23) with respect to κ and then setting $\kappa = 1$ leads back to the eigenvalue problem (2.6) which possesses for $x \in \mathbb{R}_>$ the unique solution (2.9)

For the (retarded) integral kernel $K_{\mathrm{BK}}(x, x_0; t)$ of the time-evolution operator $U(t)$ one obtains $(x, x_0 \in \mathbb{R}_>; \Theta(t)$ is the Heaviside step function)

$$(2.24) \qquad K_{\mathrm{BK}}(x, x_0; t) = \mathrm{e}^t\sqrt{\frac{x_0}{x}}\delta\left(x - x_0\mathrm{e}^t\right)\Theta(t).$$

We observe that the quantum mechanical time evolution follows in the configuration space exactly the classical trajectory (2.2). Starting at time $t = 0$ with the initial wave function $\phi \in L^2(\mathbb{R}_>, \mathrm{d}x)$, one obtains with (2.24) the wave function $\psi(x, t)$ at a later time $t > 0$

$$(2.25) \qquad \begin{aligned} \psi(x, t) &= \int_0^\infty K_{\mathrm{BK}}(x, x_0; t)\phi(x_0)\mathrm{d}x_0 \\ &= \mathrm{e}^{-\frac{t}{2}}\phi\left(\mathrm{e}^{-t}x\right) \end{aligned}$$

in complete agreement with (2.21). We also give the result for the resolvent kernel (outgoing Green's function [a small positive imaginary part ($\epsilon > 0$) has been added to $\lambda = \hbar k$]), see e.g. [20, p.26],

$$
\begin{aligned}
G_{\mathrm{BK}}(x, x_0; \lambda) &:= \frac{\mathrm{i}}{\hbar} \int_0^\infty \mathrm{e}^{\frac{\mathrm{i}}{\hbar}(\lambda + \mathrm{i}\epsilon)t} K_{\mathrm{BK}}(x, x_0; t)\mathrm{d}t \\
&= \int_{-\infty}^\infty \frac{\psi_{k'}(x)\overline{\psi}_{k'}(x_0)}{\hbar k' - \lambda - \mathrm{i}\epsilon}\mathrm{d}k' \\
&= \frac{2\pi\mathrm{i}}{\hbar}\psi_k(x)\overline{\psi}_k(x_0)\Theta(x - x_0),
\end{aligned}
$$

(2.26)

which satisfies the inhomogeneous time-independent Schrödinger equation (see (2.5))

$$(2.27) \qquad (H_{BK,x} - \hbar k) \, G_{\mathrm{BK}}(x, x_0; \hbar k) = \delta(x - x_0).$$

Since the operator (2.3) acting in the Hilbert space $L^2(\mathbb{R}, \mathrm{d}x)$ respectively $L^2(\mathbb{R}_>, \mathrm{d}x)$ has only a continuous spectrum, it cannot be considered (with the above realization) as a candidate for the hypothetical Hilbert-Polya operator. Thus there remains the task to find another Hilbert space for which the quantization of the classical Hamiltonian (1.1) possesses a discrete spectrum. Perhaps the required space is a quantum graph, with xp acting on edges between vertices, a possibility already mentioned by Berry and Keating [13]. It is the purpose of our paper to discuss the self-adjoint realizations on compact quantum graphs and in a forthcoming paper [21] on noncompact quantum graphs.

3. Semiclassical regularization of the Berry-Keating operator

Before we come to an investigation of quantum graphs, we would like to discuss an alternative and very interesting approach also put forward by Berry and Keating [13] (see also Connes [11, 12]) which is based on semiclassical arguments. It is well known that the number of quantum levels with energy less than E, the counting function $N(E)$, is for any classical bounded Hamiltonian $H_{\mathrm{cl}}(x, p)$ in one dimension given by (see e.g. [22]))

$$(3.1) \qquad N(E) = \frac{1}{2\pi\hbar}\,\mathrm{area}(E)\,(1 + \mathrm{O}(\hbar)),$$

where

$$(3.2) \qquad \mathrm{area}(E) := \int_{\mathcal{P}} \mathrm{d}x\mathrm{d}p\,\Theta(E - H_{\mathrm{cl}}(x, p))$$

is the phase-space area under the contour $H_{\mathrm{cl}}(x, p) = E$. Obviously, there is a problem if this formula is applied to the Hamiltonian (1.1), since the classical motion is not bounded, so that $\mathrm{area}(E)$ is infinite. Therefore, Berry and Keating [13] proposed to regularize the system by a suitable truncation of phase space in such a way that $\mathrm{area}(E)$ becomes finite.

The regularization proposed by Berry and Keating [13] is to truncate x and p by considering the "regularized phase space" $\mathcal{P}_{reg} := (l_x, \infty) \times (l_p, \infty)$ together with the semiclassical condition $l_x l_p = 2\pi\hbar$. This truncation cuts off not only the "small" coordinate $x \le l_x$ respectively momentum values $p \le l_p$, but it leads for a given "energy" $E > 0$ also to a cut off at the "large" values $x = \frac{E}{l_p}$ respectively $p = \frac{E}{l_x}$ since $E = H_{\mathrm{cl}}(x, p)$ holds. Without specifying the behaviour of the classical motion at the end points of the trajectories, we follow Berry and Keating and obtain from (3.1) and

(3.2)

$$N(E) = \frac{1}{2\pi\hbar} \left(\int\limits_{l_x}^{\frac{E}{l_p}} \frac{E}{x} \mathrm{d}x - l_p \left(\frac{E}{l_p} - l_x \right) \right) (1 + \mathrm{O}(\hbar))$$

(3.3)

$$= \frac{1}{2\pi\hbar} E \left(\ln \left(\frac{E}{2\pi\hbar} \right) - 1 \right) + 1 + \dots.$$

Setting $\hbar = 1$ together with a modification of $N(E)$ by adding $-\frac{1}{8}$ to the right-hand side of (3.3) which was suggested by Berry and Keating [13, 14] in order to take into account the Maslov index, we arrive at the leading asymptotics of the counting function of the nontrivial zeros of the Riemann zeta function

(3.4)
$$N(E) = \frac{E}{2\pi} \ln \left(\frac{E}{2\pi} \right) - \frac{E}{2\pi} + \frac{7}{8} + \mathrm{O}\left(\ln E \right).$$

Following the argumentation of Berry and Keating [13, 14] for the modification of $N(E)$, we get for the corresponding Maslov index $\mu = -\frac{1}{2}$. This seems at first a little bit peculiar since there is no magnetic flux or spinning particle given and therefore, the Maslov index should be an integer number as it is for "normal" quantum systems like the harmonic oscillator. We want to mention that there is actually no rigorous argument for the choice of the Maslov index (correction) simply by the fact that so far we have not yet imposed any boundary conditions on the operator, and in the corresponding classical description there is therefore a lack of jump or scattering condition at the end points of the trajectories. The scattering conditions in section 16 (example 16.2) could provide a possible remedy for the above mentioned discrepancy of the Maslov index with respect to "normal" systems. Furthermore, there is only one possibility in the classical case for the behaviour of the particle at the end point of the trajectory if one wants to preserve the constancy of the Hamiltonian for all time: the particle must jump from the point $\left(\frac{E}{l_p}, l_p \right)$ to the point $\left(l_x, \frac{E}{l_x} \right)$ in phase space, which corresponds to a kind of ring-system (one-dimensional torus with the topology of S^1) in the configuration space.

4. Classical dynamics and quantization of the "squared" Berry-Keating operator

In order to allow some kind of reflection at the end points of the trajectories, we shall also consider the classical Hamiltonian

(4.1)
$$\widetilde{H}_{\mathrm{cl}}(x, p) := x^2 p^2,$$

which is the square of the Berry-Keating Hamiltonian (1.1). Note that (4.1) can be derived from the Lagrangian

(4.2)
$$L(x, \dot{x}) = \frac{1}{4} \left(\frac{\dot{x}}{x} \right)^2$$

and that Hamilton's equations do not decouple in this case as in (2.1). In fact, one obtains

(4.3)
$$\dot{x}(t) = \frac{\partial \widetilde{H}_{\mathrm{cl}}}{\partial p} = 2x^2 p(t) \quad \text{and} \quad \dot{p}(t) = -\frac{\partial \widetilde{H}_{\mathrm{cl}}}{\partial x} = -2xp^2(t),$$

and the solutions are

(4.4)
$$x(t) = x_0 \mathrm{e}^{2x_0 p_0 t} \quad \text{and} \quad p(t) = p_0 \mathrm{e}^{-2x_0 p_0 t}.$$

If one broadens the phase space to

(4.5)
$$\mathcal{P}_{reg,b} := (l_x, \infty) \times ((l_p, \infty) \cup (-l_p, -\infty))$$

one now has the possibility to scatter from the end point $\left(\frac{E}{l_p}, l_p \right)$ of a trajectory of the form (4.4) to the end point $\left(\frac{E}{l_p}, -l_p \right)$. This corresponds to a reflection on a wall like in a one-dimensional billiard system. This is one reason why we rather consider H_{cl} and accordingly H_{BK} as a momentum

(operator) and $\widetilde{H}_{\mathrm{cl}}$ and respectively H_{BK}^2 as an energy (operator). Further hints to this choice will follow in the sequel.

Before investigating the "squared" Berry-Keating operator (4.6) on quantum graphs, we would like to consider this operator in the framework of standard quantum mechanics restricting ourselves, however, to the positive half-line $\mathbb{R}_>$ as in the discussion of the original Berry-Keating operator in section 2. A formal calculation of $\widetilde{H} := H_{\mathrm{BK}}^2$ gives (setting from now on $\hbar = 1$):

$$(4.6) \qquad H_{\mathrm{BK}}^2 := \left(-\mathrm{i} \left(x \frac{\mathrm{d}}{\mathrm{d}x} + \frac{1}{2} \right) \right)^2 = -x^2 \frac{\mathrm{d}^2}{\mathrm{d}x^2} - 2x \frac{\mathrm{d}}{\mathrm{d}x} - \frac{1}{4}.$$

Again as in section 2, H_{BK}^2 acting on $\mathcal{D}(\mathbb{R}_>)$ is essentially self-adjoint, and in the following we always consider the self-adjoint closure of this operator. It is worthwhile to mention that the squared operator (4.6) is a special case of the famous Black-Scholes operator [23, 24] whose interesting mathematical properties have been discussed e.g. in [17, 18, 19].

It is easy to see that the functions $\psi_k(x)$ ($k \in \mathbb{R} \setminus \{0\}$) defined in (2.9) are the only eigenfunctions of H_{BK}^2 on $\mathbb{R}_>$ corresponding to the continuous spectrum $\lambda = k^2 > 0$. Here the eigenvalue $\lambda = 0$ (respectively $k = 0$) corresponds to the two eigenfunctions

$$(4.7) \qquad \psi_{0,1}(x) = \frac{1}{\sqrt{2\pi}} x_+^{-\frac{1}{2}} \quad \text{and} \quad \psi_{0,2}(x) = \frac{1}{\sqrt{2\pi}} x_+^{-\frac{1}{2}} \ln x.$$

An eigenvalue $\lambda = k^2 > 0$ possesses the two linearly independent eigenfunctions $\psi_k(x)$ and $\psi_{-k}(x)$.

Introducing the (retarded) integral kernel of the time-evolution operator (unitary group)

$$(4.8) \qquad \widetilde{U}(t) := \mathrm{e}^{-\mathrm{i}t H_{\mathrm{BK}}^2}$$

by

$$(4.9) \qquad \psi(x,t) := \left(\widetilde{U}(t)\phi \right)(x) =: \int_{\mathbb{R}_>} \widetilde{K}(x, x_0; t)\phi(x_0)\mathrm{d}x_0,$$

where $\phi(x) \in L^2(\mathbb{R}_>, \mathrm{d}x)$ is the initial wave function at $t = 0$, we obtain (cp. [20, p.27])

$$(4.10) \qquad \begin{aligned} \widetilde{K}(x, x_0; t) &= \int_{-\infty}^{\infty} \psi_k(x)\overline{\psi}_k(x_0)\mathrm{e}^{-\mathrm{i}k^2 t}\Theta(t)\mathrm{d}k \\ &= (4\pi\mathrm{i}t x x_0)^{-\frac{1}{2}} \mathrm{e}^{\mathrm{i}\frac{(\ln x - \ln x_0)^2}{4t}}\Theta(t). \end{aligned}$$

The kernel $\widetilde{K}$ satisfies the inhomogeneous time-dependent Schrödinger equation

$$(4.11) \qquad \left(\mathrm{i}\frac{\partial}{\partial t} - H_{BK,x}^2 \right) \widetilde{K}(x, x_0; t) = \mathrm{i}\delta(x - x_0)\delta(t - t'),$$

i.e. it is the retarded Green's function. With (4.9), the action of $\widetilde{U}(t)$ on $\phi \in L^2(\mathbb{R}_>, \mathrm{d}x)$ is given by ($t > 0$)

$$(4.12) \qquad \left(\widetilde{U}(t)\phi \right)(x) = (4\pi\mathrm{i}t)^{-\frac{1}{2}} \int_{-\infty}^{\infty} \mathrm{e}^{\mathrm{i}\frac{\tau^2}{4t}} \mathrm{e}^{-\frac{\tau}{2}} \phi\left(\mathrm{e}^{-\tau} x \right) \mathrm{d}\tau,$$

which expresses the fact that $\widetilde{U}(t)$ is a combination of the scaling transformation generated by the operator $D = x\frac{\mathrm{d}}{\mathrm{d}x}$ (see eq. (2.21)) and the transformation generated by the operator $T := x^2\frac{\mathrm{d}^2}{\mathrm{d}x^2}$, since $\widetilde{U}(t) = \mathrm{e}^{\mathrm{i}\frac{t}{4}}\mathrm{e}^{\mathrm{i}tT}\mathrm{e}^{2\mathrm{i}tD}$. Notice that the transformation generated by T reads

$$(4.13) \qquad \left(\mathrm{e}^{\mathrm{i}tT}\phi \right)(x) = \frac{\mathrm{e}^{-\mathrm{i}\frac{t}{4}}}{(4\pi\mathrm{i}t)^{\frac{1}{2}}} \int_{-\infty}^{\infty} \mathrm{e}^{\mathrm{i}\frac{\tau^2}{4t} + \frac{\tau}{2}} \phi\left(\mathrm{e}^{-\tau} x \right) \mathrm{d}\tau,$$

and that the operators D and T commute. The resolvent kernel (outgoing Green's function) of H_{BK}^2 is given by

$$
(4.14) \qquad \begin{aligned}
\widetilde{G}(x, x_0; \lambda) &:= \mathrm{i} \int_0^\infty \mathrm{e}^{\mathrm{i}(\lambda + \mathrm{i}\epsilon)t} \widetilde{K}(x, x_0; t)\, \mathrm{d}t \\
&= \left(4 x x_0 \left(-\lambda - \mathrm{i}\epsilon\right)\right)^{-\frac{1}{2}} \mathrm{e}^{-(-\lambda - \mathrm{i}\epsilon)^{\frac{1}{2}} |\ln x - \ln x_0|},
\end{aligned}
$$

which shows that $\widetilde{G}$ has a cut on the positive real axis in the complex λ-plane (if $\sqrt{z}$ is defined with a cut on the negative real axis in the z-plane). With $k := \sqrt{\lambda} > 0$ one obtains ($x, x_0 \in \mathbb{R}_>$)

$$
(4.15) \qquad \begin{aligned}
\widetilde{G}\left(x, x_0; k^2\right) &= \frac{\mathrm{i}}{2k\sqrt{xx_0}} \mathrm{e}^{\mathrm{i}k|\ln x - \ln x_0|} \\
&= \frac{\mathrm{i}\pi}{k} \begin{cases} \psi_k(x)\overline{\psi}_k(x_0) & \text{for} \quad x \geq x_0 \\ \overline{\psi}_k(x)\psi_k(x_0) & \text{for} \quad x < x_0 \end{cases}
\end{aligned}
$$

in agreement with the general form of the Green's function of a Sturm-Liouville operator (see e.g. [25, p.112]).

5. SEMICLASSICAL ESTIMATE FOR THE EIGENVALUE COUNTING FUNCTION OF THE "SQUARED" BERRY-KEATING OPERATOR

Using again the semiclassical formula (3.1), we obtain for the counting function in the quadratic case

$$
(5.1) \qquad \begin{aligned}
N(E) &= \frac{1}{2\pi\hbar} 2 \left(\int_{l_x}^{\frac{\sqrt{E}}{l_p}} \frac{\sqrt{E}}{x}\, \mathrm{d}x - l_p \left(\frac{\sqrt{E}}{l_p} - l_x \right) \right) (1 + \mathrm{O}(\hbar)) \\
&= 2 \left[\frac{k}{2\pi} \ln\left(\frac{k}{2\pi}\right) - \frac{k}{2\pi} + \frac{7}{8} \right] + \dots,
\end{aligned}
$$

where the reflection at the "wall" $x = \frac{\sqrt{E}}{l_p}$ has been accounted for in the second line by including the Maslov index correction. Furthermore, we have introduced the "wave number" k, $E =: \hbar^2 k^2$, and have used $l_x l_p = 2\pi\hbar$. We note that in this case we obtain twice the counting function of the Riemann zeros (for which only those with positive imaginary part are counted), since each energy value E comes with two values $\pm k$. Notice, that in this case the Riemann zeros are not interpreted as "energies" but rather as "momenta" $\hbar k$ respectively "wave numbers" k. Formula (5.1) agrees with the well-known universal law that $N(E)$ for a bounded system in d dimensions grows asymptotically as $N(E) = \mathrm{O}\left(E^{\frac{d}{2}}\right)$, and thus for a one-dimensional system one expects $N(E) = \mathrm{O}\left(\sqrt{E}\right) = \mathrm{O}(k)$, eventually modified by a factor $\ln\left(\sqrt{E}\right)$.

6. COMPACT GRAPHS

We shall present a short overview on compact graphs using the notations of [26] and [27].

A compact graph $\Gamma = (\mathcal{V}, \mathcal{E}, \mathbf{I})$ is a finite set of vertices $\mathcal{V} = (v_1, \dots, v_V)$ and a finite set of edges $\mathcal{E} = (e_1, \dots, e_E)$. Here we have defined $E := |\mathcal{E}|$ and $V := |\mathcal{V}|$ for the total number of edges and vertices, respectively. Each vertex $v \in \mathcal{V}$ is at least connected with one element $\tilde{v} \in \mathcal{V}$ by some edge $e \in \mathcal{E}$, where $v = \tilde{v}$ is allowed. Furthermore, each edge $e \in \mathcal{E}$ connects two vertices v and $\tilde{v}$ in $\mathcal{V}$, again $\tilde{v} = \tilde{v}$ is possible. The topology of the graph is given by these relations of the edges and the vertices. Each edge e is assigned an interval $I_e = [a_e, b_e]$ with $0 < a_e < b_e < \infty$. The set of all intervals is denoted by $\mathbf{I}$. We remark that the choice of the starting point a_e and the end point b_e of the edge e is arbitrary and there is no orientation of the graph assumed. We denote two edges as adjacent iff they share at least one vertex as endpoint. We need the notion of a path and of a

periodic orbit of the graph. We slightly differ from the definition in [27] for further convenience. A path $p(x_0, x) \coloneqq \left((e_i)_{i=0}^{n+1}, x_0, x\right)$ is a set of a finite sequence of edges $(e_i)_{i=1}^{n}$ where the points $x_0, x \in \mathbf{I}$ denote the starting and endpoints of the path. Furthermore, it is required that

- the edges e_i and e_{i+1} are adjacent,
- the point x_0 must be an element of I_0 and x must be an element of I_{n+1}.

The case $x_0 = x$ is admissible and corresponds to a closed path. In [27] or [28] only the first item is required for a closed path at which we set $e_1 = e_{n+1}$. We shall call this case a closed orbit. Especially a closed orbit is only characterized by a sequence of edges $(e_i)_{i=1}^{n}$. For the definition of a periodic orbit γ, we shall keep with the usual definition as in [27], then γ is an equivalence class of closed orbits and can be characterized by a representative $\gamma = (e_i)_{i=1}^{n}$. The set of all periodic orbits is denoted by $\mathfrak{P}$.

We could then equip the graph with a metric structure in an obvious way like in [27]. Especially this would mean that the length of the edge e_i will be $l_i = b_i - a_i$. However, here we take another choice for the lengths and the metric structure of the graph. We define the length $\mathfrak{l}_p(x_0, x)$ of the path $p(x_0, x) \coloneqq \left((e_i)_{i=0}^{n+1}, x_0, x\right)$ as follows. We denote by y_1 and y_n the endpoints of the intervals I_1 and I_n corresponding to the shared vertices of the edges e_1, e_2 and e_{n-1}, e_n. In particular this means that y_1 is identical with a_1 or b_1 and y_n is identical with a_n or b_n. Then the length $\mathfrak{l}_p(x_0, x)$ is defined as

$$(6.1) \qquad \mathfrak{l}_p(x_0, x) \coloneqq \left| \ln\left(\frac{y_1}{x_0}\right) \right| + \sum_{i=1}^{n} \ln\left(\frac{b_i}{a_i}\right) + \left| \ln\left(\frac{y_n}{x}\right) \right|.$$

Furthermore, we define in a natural way the length $\mathfrak{l}_\gamma$ of a periodic orbit γ

$$(6.2) \qquad \mathfrak{l}_\gamma \coloneqq \ln\left(\prod_{i=1}^{n} \frac{b_i}{a_i}\right).$$

In order to define a metric structure of the graph, we need the notion of connectedness. Given two points x_w and x_z on some intervals I_w and I_z, we denote the corresponding edges with e_w and e_z. We define x_w and x_z as connected iff there exists a path $p(x_0, x) \coloneqq \left((e_i)_{i=0}^{n+1}, x_w, x_z\right)$. The graph Γ is connected iff all points of the intervals $\mathbf{I}$ are connected. Not necessarily but for convenience, we assume in the following that the graph Γ is connected. The distance $d_{w,z}$ of two points w and z on the edges of the graph is defined by

$$(6.3) \qquad d_{w,z} \coloneqq \min\left\{\mathfrak{l}_p; \ p \text{ connects } x_w \text{ and } x_z\right\}.$$

We remark that this choice of the metric for the graph will correspond to a "hyperbolic" metric in one dimension. In this case the determinant of the metric tensor g at the point x is $(\det g)(x) = \dfrac{1}{x^2}$. The reason for our choice of the metric will be explained in section 14.

7. The Berry-Keating Operator on compact quantum graphs

We define, in accordance with [27]:

$$(7.1) \qquad \begin{aligned} C_0^\infty(\Gamma) &\coloneqq \bigoplus_{i=1}^{E} C_0^\infty[a_i, b_i] \quad \text{and} \\ \mathcal{H} &\coloneqq L^2(\Gamma) \coloneqq \bigoplus_{i=1}^{E} L^2\left([a_i, b_i], \mathrm{d}x\right) \quad \text{with} \quad 0 < a_i < b_i < \infty. \end{aligned}$$

This means that a function of the Hilbert space $\mathcal{H}$ is represented by an orthogonal sum of functions which are defined on the corresponding edges:

$$(7.2) \qquad \psi \in L^2(\Gamma) \quad \text{iff} \quad \psi = \bigoplus_{i=1}^{E} \psi_i \quad \text{with} \quad \psi_i \in L^2(I_i, \mathrm{d}x).$$

The first function space in (7.1) will be a possible operator core for the closed Berry-Keating operator with (7.5) as domain of definition. Therefore the self-adjoint extensions of H_{BK} are also with respect to $C_0^\infty(\Gamma)$. The space $\mathcal{H}$ is a Hilbert space if we equip it with the scalar product

$$(7.3) \qquad \langle \psi, \phi \rangle := \sum_{j=1}^{E} \int_{a_j}^{b_j} \overline{\psi_j(x_j)} \phi_j(x_j) \mathrm{d}x_j.$$

We then define the Berry-Keating operator on compact graphs (in the following we set $\hbar = 1$):

$$(7.4) \qquad H_{\mathrm{BK}}\psi := \left(-\mathrm{i}\left(x\frac{\mathrm{d}}{\mathrm{d}x} + \frac{1}{2} \right)\psi_1, \ldots, -\mathrm{i}\left(x\frac{\mathrm{d}}{\mathrm{d}x} + \frac{1}{2} \right)\psi_E \right),$$

for $\psi \in C_0^\infty(\Gamma)$. Since we have a compact graph Γ, multiplication by x is a bounded closable operation. Thus by perturbation arguments, see e.g. [29, p.183], we conclude that H_{BK} is closable since the standard momentum operator $p = -\mathrm{i}\dfrac{\mathrm{d}}{\mathrm{d}x}$ is closable. Furthermore, we note that multiplication by the argument is also a (bounded) bijection from

$$(7.5) \qquad D_0^1(\Gamma) := \bigoplus_{i=1}^{E} H_0^1[a_i, b_i]$$

to itself. $H_0^1[a_i, b_i]$ is the set of absolutely continuous functions on $[a_i, b_i]$ which vanish at the endpoints of the intervals. Again by perturbation arguments for the momentum operator, we therefore conclude that the domain of definition of the closure of H_{BK} is equal to (7.5). Furthermore, by similar arguments the adjoint operator of $(H_{\mathrm{BK}}, D_0^1(\Gamma))$ is given by $(H_{\mathrm{BK}}, H^1(\Gamma))$ in which

$$(7.6) \qquad H^1(\Gamma) := \bigoplus_{i=1}^{E} H^1[a_i, b_i]$$

is the set of absolutely continuous functions on the intervals of the graph Γ, c.p. [29, p.100].

We mention at this point that the projections of the spaces $D_0^1(\Gamma)$ and $H^1(\Gamma)$ on the intervals of the graph Γ coincide with the corresponding Sobolev spaces, see e.g. [30]. The operator $(H_{\mathrm{BK}}, D_0^1(\Gamma))$ is symmetric and it is possible to show that the deficiency indices are (E, E), compare e.g. [16, p.142]. By a proper Sobolev embedding theorem and the compactness of the graph Γ it follows that the differential operator on $D_0^1(\Gamma)$ possesses compact resolvent, see also [31]. Thus by the compact resolvent theorem, c.p. [32, p.245], and the relatively compact perturbation theorem, c.p. [32, p.113], the operator possesses a purely discrete spectrum.

8. Classification of the self-adjoint extensions of the Berry-Keating operator

In order to characterize the self-adjoint extensions we follow the ideas of [16, p.138] and [26], see also [33] for a comprehensive discussion. Therefore we define the complex symplectic form on $H^1(\Gamma) \times H^1(\Gamma)$, c.p. [16, p.138]:

$$(8.1) \qquad [\phi, \psi]_1 := \left\langle \phi, H_{\mathrm{BK}}^+ \psi \right\rangle_{L^2(\Gamma)} - \left\langle H_{\mathrm{BK}}^+ \phi, \psi \right\rangle_{L^2(\Gamma)} \quad \text{for} \quad \phi, \psi \in H^1(\Gamma).$$

We call a subspace $\mathcal{X}$ $[\cdot, \cdot]_1$-symmetric, iff $[\phi, \psi]_1 = 0$ for all $\phi, \psi \in \mathcal{X}$. Due to the von Neumann extension theory, see e.g. [16], the self-adjoint extensions are exactly the maximal $[\cdot, \cdot]_1$-subspaces of $H^1(\Gamma)$. We follow the approach by Kostrykin and Schrader [26] to classify these extensions. By a proper Sobolev embedding theorem we can define:

$$(8.2) \qquad \Psi_{\mathrm{bv}} := (\psi_1(a_1), \ldots, \psi_E(a_E), \psi_1(b_1), \ldots, \psi_E(b_E))^T \quad \text{for} \quad \psi \in H^1(\Gamma).$$

For convenience, we also define:

$$(8.3) \qquad I_\pm := \begin{pmatrix} \mathbb{1}_{E \times E} & 0 \\ 0 & -\mathbb{1}_{E \times E} \end{pmatrix}, \quad D_{(ab)} := \begin{pmatrix} \boldsymbol{a} & 0 \\ 0 & \boldsymbol{b} \end{pmatrix},$$

with

(8.4) $$\boldsymbol{a}_{ij} := \delta_{ij} a_i \quad \text{and} \quad \boldsymbol{b}_{ij} := \delta_{ij} b_i \quad \text{for} \quad 0 \leq i, j \leq E$$

and

(8.5) $$J := \begin{pmatrix} 0 & \mathbb{1}_{E \times E} \\ -\mathbb{1}_{E \times E} & 0 \end{pmatrix} \quad , \quad U := \frac{1}{\sqrt{2}} \begin{pmatrix} i\mathbb{1}_{E \times E} & \mathbb{1}_{E \times E} \\ -\mathbb{1}_{E \times E} & -i\mathbb{1}_{E \times E} \end{pmatrix}.$$

By a simple calculation we obtain the identity:

(8.6) $$U^{+} \left(i I_{\pm} \right) U = J.$$

Thus we obtain for (8.1) by integration by parts using the unitarity of U:

(8.7) $$\begin{aligned} [\psi, \phi]_1 &= \left\langle \Phi_{\mathrm{bv}}, i I_{\pm} D_{(\boldsymbol{ab})} \Psi_{\mathrm{bv}} \right\rangle_{\mathbb{C}^{2E}} \\ &= \left\langle D_{(\boldsymbol{ab})}^{\frac{1}{2}} \Phi_{\mathrm{bv}}, i I_{\pm} D_{(\boldsymbol{ab})}^{\frac{1}{2}} \Psi_{\mathrm{bv}} \right\rangle_{\mathbb{C}^{2E}} \\ &= \left\langle U D_{(\boldsymbol{ab})}^{\frac{1}{2}} \Phi_{\mathrm{bv}}, J U D_{(\boldsymbol{ab})}^{\frac{1}{2}} \Psi_{\mathrm{bv}} \right\rangle_{\mathbb{C}^{2E}} \quad \text{for all} \quad \psi, \phi \in H^1(\Gamma). \end{aligned}$$

To define the square root of $D_{(\boldsymbol{ab})}$ we have used the usual definition of a positive operator in [30, p.196], which in this case simply means to take the square root of the (diagonal) entries in $D_{(\boldsymbol{ab})}$. Note that

(8.8) $$\omega(\cdot, \cdot) := \langle \cdot, J \cdot \rangle_{\mathbb{C}^{2E}}$$

defines a nondegenerate complex symplectic form on $\mathbb{C}^{2E} \times \mathbb{C}^{2E}$. We call a subspace $\mathcal{L}$ of $\mathbb{C}^{2E}$ a Lagrangian subspace iff

(8.9)
- $a, b \in \mathcal{L} \quad \text{then} \quad \omega(a, b) = 0.$
- Whenever for a subspace $\tilde{\mathcal{L}} \supset \mathcal{L}$ the first item holds, it follows $\tilde{\mathcal{L}} = \mathcal{L}$.

For the Lagrangian subspaces of $\mathbb{C}^{2E}$ we apply the result of [26]. A subspace $\mathcal{L}$ is Lagrangian iff there exist two matrices $A, B \in \mathrm{Mat}(E \times E, \mathbb{C})$ with:

(8.10) $$\begin{aligned} AB^{+} &= BA^{+} \quad \text{and} \\ \mathrm{rank}(A, B) &= 2E, \end{aligned}$$

and, furthermore, it holds:

(8.11) $$\mathcal{L} = \left\{ \phi \in \mathbb{C}^{2E}; \ \phi := \begin{pmatrix} \phi_1 \\ \phi_2 \end{pmatrix} \quad \text{and} \quad A\phi_1 + B\phi_2 = 0 \right\}.$$

In (8.10) the matrix (A, B) is formed of the columns of A and B, and we have introduced two maps

(8.12) $$(\cdot)_i : \mathbb{C}^{2E} \to \mathbb{C}^E \quad \text{for} \quad 1 \leq i \leq 2$$

by

(8.13) $$\phi_i := \begin{cases} (\mathbb{1}, 0)\phi & \text{if} \quad i = 1, \\ (0, \mathbb{1})\phi & \text{if} \quad i = 2. \end{cases}$$

Furthermore, as mentioned in [34], these matrices are not uniquely defined. Two sets of matrices A, B and $\widetilde{A}, \widetilde{B}$ define the same Lagrangian subspace iff there exists an invertible matrix C with

(8.14) $$A = C\widetilde{A} \quad \text{and} \quad B = C\widetilde{B}.$$

$U D_{(\boldsymbol{ab})}^{\frac{1}{2}}$ is a bijection from $\mathbb{C}^{2E}$ onto itself. Therefore, with (8.1) and (8.7) we infer with the same arguments as in [26], that there is a one-to-one correspondence between the self-adjoint extensions of $\left(H_{\mathrm{BK}}, D_0^1(\Gamma) \right)$ and the Lagrangian subspaces of $\mathbb{C}^{2E}$. Each domain of definition of such a self-adjoint extension is exactly the preimage with respect to (8.2) of a subspace

(8.15) $$\mathcal{L} = \left\{ \Psi_{\mathrm{bv}} \in \mathbb{C}^{2E}; \ A \left(U D_{(\boldsymbol{ab})}^{\frac{1}{2}} \Psi_{\mathrm{bv}} \right)_1 + B \left(U D_{(\boldsymbol{ab})}^{\frac{1}{2}} \Psi_{\mathrm{bv}} \right)_2 = 0 \right\},$$

where A and B fulfil (8.10). The converse is also true.

9. Determination of the eigenvalues of H_{BK}

All possible eigenfunctions ψ_k to an eigenvalue k of H_{BK} are of the form:

$$(9.1) \qquad \psi_k(x) = \left(\alpha_1 \frac{1}{\sqrt{x}} \mathrm{e}^{ik \ln x}, \ldots, \alpha_E \frac{1}{\sqrt{x}} \mathrm{e}^{ik \ln x} \right).$$

We denote the column vector (8.2) corresponding to ψ_k by $\Psi_{bv,k}$. In order to apply (8.15) for determining the eigenvalues k and the corresponding eigenvectors ψ_k, we calculate $U D^{\frac{1}{2}}_{(\boldsymbol{ab})} \Psi_{bv,k}$ using (8.5).

$$
\begin{aligned}
(9.2) \qquad U D^{\frac{1}{2}}_{(\boldsymbol{ab})} \Psi_{bv,k} &= U \begin{pmatrix} \mathrm{e}^{ik \ln \boldsymbol{a}} & 0 \\ 0 & \mathrm{e}^{ik \ln \boldsymbol{b}} \end{pmatrix} \boldsymbol{\alpha} \\
&= \frac{1}{\sqrt{2}} \begin{pmatrix} \mathrm{i}\mathrm{e}^{ik \ln \boldsymbol{a}} & \mathrm{e}^{ik \ln \boldsymbol{b}} \\ -\mathrm{e}^{ik \ln \boldsymbol{a}} & -\mathrm{i}\mathrm{e}^{ik \ln \boldsymbol{b}} \end{pmatrix} \boldsymbol{\alpha} \\
&= \frac{1}{\sqrt{2}} \begin{pmatrix} \mathrm{i}\mathrm{e}^{ik \ln \boldsymbol{a}} + \mathrm{e}^{ik \ln \boldsymbol{b}} & 0 \\ 0 & -\mathrm{e}^{ik \ln \boldsymbol{a}} - \mathrm{i}\mathrm{e}^{ik \ln \boldsymbol{b}} \end{pmatrix} \boldsymbol{\alpha}.
\end{aligned}
$$

For convenience we have used the notations:

$$
\begin{aligned}
(9.3) \qquad \left(\mathrm{e}^{ik \ln \boldsymbol{a}} \right)_{ij} &:= \delta_{ij} \mathrm{e}^{ik \ln a_i} \quad \text{and} \\
\left(\mathrm{e}^{ik \ln \boldsymbol{b}} \right)_{ij} &:= \delta_{ij} \mathrm{e}^{ik \ln b_i} \quad \text{for} \quad 1 \le i, j \le E
\end{aligned}
$$

and

$$(9.4) \qquad \boldsymbol{\alpha} := (\alpha_1, \ldots, \alpha_E, \alpha_1, \ldots, \alpha_E)^T.$$

Therefore, we get:

$$
\begin{aligned}
(9.5) \qquad \sqrt{2} \left(U D^{\frac{1}{2}}_{(\boldsymbol{ab})} \Psi_{bv,k} \right)_1 &= \left(\mathrm{i}\mathrm{e}^{ik \ln \boldsymbol{a}} + \mathrm{e}^{ik \ln \boldsymbol{b}} \right) \boldsymbol{\alpha}_1 \\
\sqrt{2} \left(U D^{\frac{1}{2}}_{(\boldsymbol{ab})} \Psi_{bv,k} \right)_2 &= - \left(\mathrm{e}^{ik \ln \boldsymbol{a}} + \mathrm{i}\mathrm{e}^{ik \ln \boldsymbol{b}} \right) \boldsymbol{\alpha}_2.
\end{aligned}
$$

Taking into account that $\boldsymbol{\alpha}_1 = \boldsymbol{\alpha}_2 =: \tilde{\boldsymbol{\alpha}}$ we obtain for the expression in (8.15)

$$
\begin{aligned}
(9.6) \qquad \sqrt{2} &\left[A \left(U D^{\frac{1}{2}}_{(\boldsymbol{ab})} \Psi_{bv,k} \right)_1 + B \left(U D^{\frac{1}{2}}_{(\boldsymbol{ab})} \Psi_{bv,k} \right)_2 \right] \\
&= \left(A \left(\mathrm{i}\mathrm{e}^{ik \ln \boldsymbol{a}} + \mathrm{e}^{ik \ln \boldsymbol{b}} \right) - B \left(\mathrm{e}^{ik \ln \boldsymbol{a}} + \mathrm{i}\mathrm{e}^{ik \ln \boldsymbol{b}} \right) \right) \tilde{\boldsymbol{\alpha}} \\
&= \left(\mathrm{i} \left(A + \mathrm{i}B \right) \mathrm{e}^{ik \ln \boldsymbol{a}} + (A - \mathrm{i}B) \mathrm{e}^{ik \ln \boldsymbol{b}} \right) \tilde{\boldsymbol{\alpha}}.
\end{aligned}
$$

Kostrykin and Schrader have shown, see [26], that $A \pm \mathrm{i}B$ are invertible under the assumption (8.10). With the notation

$$(9.7) \qquad \boldsymbol{C}(k) := \mathrm{e}^{ik \ln \boldsymbol{a}} \tilde{\boldsymbol{\alpha}}$$

and, because $(A - \mathrm{i}B)$ and $(A + \mathrm{i}B)^{-1}$ commute, see [35], we get:

$$
\begin{aligned}
(9.8) \qquad & A \left(U D^{\frac{1}{2}}_{(\boldsymbol{ab})} \Psi_{bv,k} \right)_1 + B \left(U D^{\frac{1}{2}}_{(\boldsymbol{ab})} \Psi_{bv,k} \right)_2 = 0 \\
&\Leftrightarrow \left(\mathbb{1} - \mathrm{i} \frac{A - \mathrm{i}B}{A + \mathrm{i}B} \mathrm{e}^{ik \ln \frac{\boldsymbol{b}}{\boldsymbol{a}}} \right) \boldsymbol{C}(k) = 0,
\end{aligned}
$$

with $\mathrm{e}^{ik \ln \frac{\boldsymbol{b}}{\boldsymbol{a}}}$ similarly defined as in (9.3). Due to the similarity of (9.8) with the secular equation for the common Laplace operator on compact graphs, see [34], we denote:

$$(9.9) \qquad \mathcal{S}(A, B) := \mathrm{i} \frac{A - \mathrm{i}B}{A + \mathrm{i}B} \quad \text{and} \quad \mathcal{T}(\boldsymbol{a}, \boldsymbol{b}; k) := \mathrm{e}^{ik \ln \frac{\boldsymbol{b}}{\boldsymbol{a}}}.$$

It follows with exactly the same arguments as in [26] that $\mathcal{S}(A, B)$ is unitary, and we shall call it also the S-matrix of the quantum graph. The unitarity of $\mathcal{T}(\boldsymbol{a}, \boldsymbol{b}; k)$ iff $k \in \mathbb{R}$ is obvious. Since, for all $k \in \mathbb{C}$, $\boldsymbol{C}(k) = 0$ iff $\tilde{\boldsymbol{\alpha}} = 0$ it follows that equation (9.8) is fulfilled iff

$$(9.10) \qquad \mathcal{F}(k) := \det \left(\mathbb{1}_{E \times E} - \mathcal{S}(A, B) \mathcal{T}(\boldsymbol{a}, \boldsymbol{b}; k) \right) = 0.$$

Furthermore, the multiplicity of the eigenvalue one of $\mathcal{S}(A,B)\mathcal{T}(\boldsymbol{a},\boldsymbol{b};k)$ coincides with the multiplicity of the eigenvalue k of H_{BK}. We remark that the geometric multiplicities and the algebraic multiplicities of $\mathcal{S}(A,B)\mathcal{T}(\boldsymbol{a},\boldsymbol{b};k)$ coincide since this matrix is diagonalizable.

In contrast to the S-matrix of the generic negative Laplacian $-\Delta$ on graphs, the S-matrix $\mathcal{S}(A,B)$ is always independent of k. (The S-matrix of $-\Delta$ is independent of the wave number k iff $S^+ = S$, see [34].) But we remark that the independence of the S-matrix on the eigenvalue will also occur when we replace H_{BK} by the standard momentum operator (with $x \in \mathbb{R}$)

$$(9.11) \qquad p := -\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}x}.$$

The calculations are quite analogous. In fact every self-adjoint extension of p can be characterized by the same matrices A and B as in (8.10) and we would get the same S-matrix $\mathcal{S}(A,B)$. The only difference in the secular equation between the operators H_{BK} and p then is the form of the second matrix in (9.9) which in the case of p is given by

$$(9.12) \qquad T(\boldsymbol{a},\boldsymbol{b};k) := \mathrm{e}^{\mathrm{i}k(\boldsymbol{b}-\boldsymbol{a})}.$$

This is one reason why we rather relate H_{BK} with a momentum operator than an energy operator as indicated in section 2. A possible interpretation of the occurrence of the logarithm in $\mathcal{T}$ will be given in section 14. However, the analogy of $p^2 = -\Delta$ and H_{BK}^2 is not so obvious.

10. The "squared" Berry-Keating Operator

Our Hilbert space will be $\mathcal{H} = L^2(\Gamma)$, see (7.2) and (7.3). Now again we seek self-adjoint extensions of (4.6) with respect to $C_0^\infty(\Gamma)$. Of course in order to obtain a self-adjoint operator, the task is to specify an appropriate domain $D(H_{\mathrm{BK}}^2)$ for this operator with

$$(10.1) \qquad C_0^\infty(\Gamma) \subset D(H_{\mathrm{BK}}^2).$$

In fact one simple possibility is to define H_{BK}^2 as the "squared" Berry-Keating operator, which means:

$$(10.2) \qquad H_{\mathrm{BK}}^2\psi := H_{\mathrm{BK}}\left(H_{\mathrm{BK}}\psi\right), \quad \psi \in D(H_{\mathrm{BK}}^2) := \{\phi \in D(H_{\mathrm{BK}}); \ H_{\mathrm{BK}}\phi \in D(H_{\mathrm{BK}})\}.$$

It follows immediately that H_{BK}^2 is self-adjoint if H_{BK} is self-adjoint using Friedrichs' extension theorem [16, p.180]. But in fact there are many possible self-adjoint extensions which cannot be realized in such a way. We will give simple examples in section 16. We can generalize these constructions to consider non-self-adjoint but closed realizations of H_{BK} and then form

$$(10.3) \qquad H_{\mathrm{BK}}^+ H_{\mathrm{BK}} \quad \text{or} \quad H_{\mathrm{BK}} H_{\mathrm{BK}}^+.$$

This is an idea quite analogous to the concept of supersymmetry, see [36] and [37] (the technique of factorization was already introduced by Schrödinger [38] and reviewed in [39]). The second cited have used this technique but they don't explicitly mention it. However only a certain kind of self-adjoint extension can be attained in such a way. In [37] these are exactly the self-adjoint extensions which correspond to k-independent S-matrices corresponding to these extensions. This relation between the S-matrices and the self-adjoint extensions of the negative Laplace operator $-\Delta$ on metric graphs is explained in [34].

We would like to give an overview of the starting point of our considerations from a mathematical point of view. The proofs of these statements are similar as in section 7 using the same references as there. Therefore, we only summarize the results:

- The operator H_{BK}^2 acting on $C_0^\infty(\Gamma)$ or

$$(10.4) \qquad D_0^2(\Gamma) := \bigoplus_{i=1}^{E} H_0^2[a_i, b_i] \quad \text{with} \quad 0 < a_i < b_i < \infty$$

  is symmetric. $H_0^2[a_i, b_i]$ is the set of absolutely continuous functions which posses absolutely continuous derivative on $[a_i, b_i]$ and which together with their first derivatives vanish at the endpoints of the intervals.
- H_{BK}^2 acting on $D_0^2(\Gamma)$ is closed.

- The adjoint operator of $\left(H_{\mathrm{BK}}^2, D_0^2(\Gamma)\right)$ is $\left(H_{\mathrm{BK}}^2, H^2(\Gamma)\right)$. Here

$$(10.5) \qquad H^2(\Gamma) := \bigoplus_{i=1}^{E} H^2[a_i, b_i] \quad \text{with} \quad 0 < a_i < b_i < \infty$$

  is the space of functions being absolutely continuous on the intervals of the graph Γ and possesses absolutely continuous derivatives.
- The deficiency indices are $(2E, 2E)$, thus $\left(H_{\mathrm{BK}}^2, D_0^2(\Gamma)\right)$ possesses infinitely many self-adjoint extensions.
- The spectrum of every self-adjoint extension is purely discrete.

Again as in section 7 the projections of the spaces $D_0^2(\Gamma)$ and $H^2(\Gamma)$ on the intervals of the graph Γ coincide with the corresponding Sobolev spaces, see again e.g. [30]. We shall follow a general approach to find all these self-adjoint extensions, quite analogous as in section 8 and based on [26].

11. Classification of the self-adjoint extensions of the "squared" Berry-Keating operator

First, we define Ψ_{bv} as in (8.2) for $\psi \in H^2(\Gamma)$ and additionally

$$(11.1) \qquad \Psi_{\mathrm{bv}}' := \left(\psi_1'(a_1), \ldots, \psi_E'(a_E), -\psi_1'(b_1), \ldots, -\psi_E'(b_E)\right)^T \quad \text{for} \quad \psi \in H^2(\Gamma),$$

in which ψ_i' is the derivative of ψ_i on the interval I_i. Similarly as in (8.1), we define a symplectic form on $H^2(\Gamma) \times H^2(\Gamma)$

$$(11.2) \qquad [\phi, \psi]_2 := \left\langle \phi, {H_{\mathrm{BK}}^2}^+ \psi \right\rangle_{L^2(\Gamma)} - \left\langle {H_{\mathrm{BK}}^2}^+ \phi, \psi \right\rangle_{L^2(\Gamma)} \quad \text{for } \phi, \psi \in H^2(\Gamma).$$

With the same arguments as for H_{BK} in section 7 the task is to find all maximal $[\cdot, \cdot]_2$-symmetric subspaces of $H^2(\Gamma)$ in order to find all self-adjoint extensions to $\left(H_{\mathrm{BK}}^2, D_0^2(\Gamma)\right)$. We shall adapt the definition of J in (8.5) by

$$(11.3) \qquad J := \begin{pmatrix} 0 & \mathbb{1}_{2E \times 2E} \\ -\mathbb{1}_{2E \times 2E} & 0 \end{pmatrix}$$

and (see (8.3))

$$(11.4) \qquad \widetilde{D}_{(\boldsymbol{ab})} := \begin{pmatrix} D_{(\boldsymbol{ab})} & 0 \\ 0 & D_{(\boldsymbol{ab})} \end{pmatrix}, \quad [\boldsymbol{\psi}]_{\mathrm{bv}} := \begin{pmatrix} \Psi_{\mathrm{bv}} \\ \Psi_{\mathrm{bv}}' \end{pmatrix} \quad \text{for} \quad \psi \in D_0^2(\Gamma).$$

We obtain for $\phi, \psi \in H^2(\Gamma)$ using partial integration and the fact that J and $\widetilde{D}_{(\boldsymbol{ab})}$ commute:

$$(11.5) \qquad \begin{aligned} [\psi, \phi]_2 &= \sum_{i=1}^{E} \left\{ b_i^2 \left(\overline{\psi_i'(b_i)} \phi(b_i) - \overline{\psi_i(b_i)} \phi'(b_i) \right) - a_i^2 \left(\overline{\psi_i'(a_i)} \phi(a_i) - \overline{\psi_i(a_i)} \phi'(a_i) \right) \right\} \\ &= \left\langle [\psi]_{\mathrm{bv}}, J \widetilde{D}_{(\boldsymbol{ab})}^2 [\phi]_{\mathrm{bv}} \right\rangle_{\mathbb{C}^{4E}} \\ &= \left\langle \widetilde{D}_{(\boldsymbol{ab})} [\psi]_{\mathrm{bv}}, J \widetilde{D}_{(\boldsymbol{ab})} [\phi]_{\mathrm{bv}} \right\rangle_{\mathbb{C}^{4E}}. \end{aligned}$$

Taking the scalar product in the definition of $\omega(\cdot, \cdot)$ in (8.8) with respect to $\mathbb{C}^{4E}$, we infer as in section 8 that the self-adjoint extensions of $\left(H_{\mathrm{BK}}^2, D_0^2(\Gamma)\right)$ are exactly the preimages of

$$(11.6) \qquad \begin{aligned} \boldsymbol{\mathcal{L}} &= \left\{ [\phi]_{\mathrm{bv}} \in \mathbb{C}^{4E}; \; A \left(\widetilde{D}_{(\boldsymbol{ab})} [\phi]_{\mathrm{bv}} \right)_1 + B \left(\widetilde{D}_{(\boldsymbol{ab})} [\phi]_{\mathrm{bv}} \right)_2 = 0 \right\} \\ &= \left\{ [\phi]_{\mathrm{bv}} \in \mathbb{C}^{4E}; \; A D_{(\boldsymbol{ab})} \Phi_{\mathrm{bv}} + B D_{(\boldsymbol{ab})} \Phi_{\mathrm{bv}}' = 0 \right\} \end{aligned}$$

with respect to $[\cdot]_{\mathrm{bv}}$ in (11.4). In (11.6) we have used $\cdot_i$ defined in (8.13). The matrices A and B are now elements of $\mathrm{Mat}(2E \times 2E, \mathbb{C})$ with the adopted conditions

$$(11.7) \qquad \begin{aligned} AB^+ &= BA^+ \quad \text{and} \\ \mathrm{rank}(A, B) &= 4E. \end{aligned}$$

12. Determination of the eigenvalues of H_{BK}^2

We want to solve the eigenvalue problem

$$(12.1) \qquad H_{\mathrm{BK}}^2 \psi = \lambda \psi.$$

To tackle this problem, it will be convenient to consider the "wave number" k defined by $\lambda^{\frac{1}{2}} := k$. It is a trivial observation that $\pm k$ correspond to the same eigenvalue λ. This fact will be revealed in the symmetry of the secular equation for the "wave number".

Of course, additionally to (12.1) the eigenvector ψ must be in the domain of definition of the operator. However, the general form of the eigenvector to an eigenvalue $\lambda = k^2 \neq 0$ is

$$(12.2) \qquad \psi_k(x) = \left(\frac{1}{\sqrt{x}} \left(\alpha_1 e^{ik \ln x} + \beta_1 e^{-ik \ln x} \right), \ldots, \frac{1}{\sqrt{x}} \left(\alpha_E e^{ik \ln x} + \beta_E e^{-ik \ln x} \right) \right).$$

We can proceed as in [26]. Therefore we compute $\Psi_{bv,k}$ and $\Psi'_{bv,k}$ using the definitions in (8.3) and (9.3).

$$(12.3) \qquad \begin{aligned} \Psi_{bv,k} &= D_{(ab)}^{-\frac{1}{2}} \begin{pmatrix} e^{ik \ln a} & e^{-ik \ln a} \\ e^{ik \ln b} & e^{-ik \ln b} \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} \\ \Psi'_{bv,k} &= \left(-\frac{1}{2} D_{(ab)}^{-\frac{3}{2}} \begin{pmatrix} e^{ik \ln a} & e^{-ik \ln a} \\ -e^{ik \ln b} & -e^{-ik \ln b} \end{pmatrix} + ik D_{(ab)}^{-\frac{3}{2}} \begin{pmatrix} e^{ik \ln a} & e^{-ik \ln a} \\ -e^{ik \ln b} & -e^{-ik \ln b} \end{pmatrix} I_{\pm} \right) \begin{pmatrix} \alpha \\ \beta \end{pmatrix}. \end{aligned}$$

In order to be in the domain of definition of a self-adjoint realization, $\Psi_{bv,k}$ and $\Psi'_{bv,k}$ must be in some $\mathcal{L}$ of (11.6) defined by the two matrices A and B. We make the identification, c.p. [34],

$$(12.4) \qquad X(k; a, b) := \begin{pmatrix} e^{ik \ln a} & e^{-ik \ln a} \\ e^{ik \ln b} & e^{-ik \ln b} \end{pmatrix},$$

$$(12.5) \qquad Y(k; a, b) := \begin{pmatrix} e^{ik \ln a} & e^{-ik \ln a} \\ -e^{ik \ln b} & -e^{-ik \ln b} \end{pmatrix} \quad \text{and} \quad Y'(k; a, b) := \begin{pmatrix} e^{ik \ln a} & -e^{-ik \ln a} \\ -e^{ik \ln b} & e^{-ik \ln b} \end{pmatrix}.$$

Thus we conclude, with the definition for the bold symbols in accordance with (8.4):

$$(12.6) \qquad \begin{aligned} 0 &\overset{!}{=} A D_{(ab)} \Phi_{\mathrm{bv}} + B D_{(ab)} \Phi'_{\mathrm{bv}} \\ &= \left(A D_{(ab)}^{\frac{1}{2}} X(k; a, b) + B D_{(ab)}^{-\frac{1}{2}} Y(k; a, b) \begin{pmatrix} -\frac{1}{2} + ik & 0 \\ 0 & -\frac{1}{2} - ik \end{pmatrix} \right) \begin{pmatrix} \alpha \\ \beta \end{pmatrix} \\ &= \left(\left(A D_{(ab)}^{\frac{1}{2}} - \frac{1}{2} B D_{(ab)}^{-\frac{1}{2}} I_{\pm} \right) X(k; a, b) + ik B D_{(ab)}^{-\frac{1}{2}} Y'(k; a, b) \right) \begin{pmatrix} \alpha \\ \beta \end{pmatrix}. \end{aligned}$$

At this point we make two observations: Since $D_{(ab)}^{-\frac{1}{2}}$ is self-adjoint, we conclude

$$(12.7) \qquad A D_{(ab)}^{\frac{1}{2}} \left(B D_{(ab)}^{-\frac{1}{2}} \right)^{+} = AB^{+}.$$

Since $D_{(ab)}^{-\frac{1}{2}}$ and $D_{(ab)}^{\frac{1}{2}}$ are invertible and diagonal, it is easy to show that

$$(12.8) \qquad \mathrm{rank}(A D_{(ab)}^{\frac{1}{2}}, B D_{(ab)}^{-\frac{1}{2}}) = \mathrm{rank}(A, B) = 4E.$$

Therefore we define

$$(12.9) \qquad A D_{(ab)}^{\frac{1}{2}} =: A' \quad \text{and} \quad B D_{(ab)}^{-\frac{1}{2}} =: B'$$

and observe that A' and B' also fulfil the conditions (11.7). Therefore we can apply a theorem of Kuchment [31]. It states that two matrices A' and B' fulfil (11.7) iff there exists an invertible matrix C with:

$$(12.10) \qquad A' = C P_{\ker B'} + C P_{\ker B'}^{\perp} L' P_{\ker B'}^{\perp} \quad \text{and} \quad B' = C P_{\ker B'}^{\perp}.$$

In (12.10) we have defined $P_{\ker B'}$ as the projector onto the kernel of B' and $P^\perp_{\ker B'}$ as the corresponding orthogonal projector. The matrix L' is self-adjoint and can be defined by, see [31],

$$(12.11) \qquad L' := \left(B'|_{\operatorname{ran} B'^+} \right)^{-1} A' P^\perp_{\ker B'}.$$

Hence we can proceed in the calculation (12.6) multiplying (12.6) from the left-hand side by C^{-1}

$$(12.12) \quad 0 = \left(\left(P_{\ker B'} + P^\perp_{\ker B'} L' P^\perp_{\ker B'} - \frac{1}{2} P^\perp_{\ker B'} I_\pm \right) X(k; \boldsymbol{a}, \boldsymbol{b}) + ik P^\perp_{\ker B'} Y'(k; \boldsymbol{a}, \boldsymbol{b}) \right) \begin{pmatrix} \boldsymbol{\alpha} \\ \boldsymbol{\beta} \end{pmatrix}.$$

Since the projectors $P_{\ker B'}$ and $P^\perp_{\ker B'}$ are mutually orthogonal, we infer from (12.10), the definition of $\mathcal{L}$ in (11.6) and with (12.6), especially the second line therein, that

$$(12.13) \qquad P_{\ker B'} X(k; \boldsymbol{a}, \boldsymbol{b}) \begin{pmatrix} \boldsymbol{\alpha} \\ \boldsymbol{\beta} \end{pmatrix} = 0.$$

In (12.12) we insert between the matrices $I_\pm$ and $X(k; \boldsymbol{a}, \boldsymbol{b})$ the unit matrix $\mathbb{1} = P_{\ker B'} + P^\perp_{\ker B'}$ and apply (12.13)

$$(12.14) \qquad 0 = \left(\left(P_{\ker B'} + P^\perp_{\ker B'} \left(L' - \frac{1}{2} I_\pm \right) P^\perp_{\ker B'} \right) X(k; \boldsymbol{a}, \boldsymbol{b}) + ik P^\perp_{\ker B'} Y'(k; \boldsymbol{a}, \boldsymbol{b}) \right) \begin{pmatrix} \boldsymbol{\alpha} \\ \boldsymbol{\beta} \end{pmatrix}.$$

We realize that $L' - \frac{1}{2} I_\pm$ is also self-adjoint. Thus we denote

$$(12.15) \qquad L'' := L' - \frac{1}{2} I_\pm$$

and make a re-definition:

$$(12.16) \qquad A'' := P_{\ker B'} + P^\perp_{\ker B'} L'' P^\perp_{\ker B'} \quad \text{and} \quad B'' := P^\perp_{\ker B'}.$$

It is obvious that the matrices A'' and B'' fulfil the conditions (11.5). Hence as in section 9 respectively [26], we infer that $A'' \pm ik B''$ is invertible and conclude with quite the same calculation as in [34]

$$(12.17) \qquad 0 = (A'' + ik B'') \left[\mathbb{1} - S''(A, B; k) T(\boldsymbol{a}, \boldsymbol{b}; k) \right] \begin{pmatrix} e^{ik \ln \boldsymbol{a}} & 0 \\ 0 & e^{-ik \ln \boldsymbol{b}} \end{pmatrix} \begin{pmatrix} \boldsymbol{\alpha} \\ \boldsymbol{\beta} \end{pmatrix}.$$

Here we have used the definitions

$$(12.18) \qquad S''(A, B; k) := S(A'', B''; k) := -\frac{A'' - ik B''}{A'' + ik B''} \quad \text{and} \quad T(\boldsymbol{a}, \boldsymbol{b}; k) := \begin{pmatrix} 0 & e^{ik \ln \frac{\boldsymbol{b}}{\boldsymbol{a}}} \\ e^{ik \ln \frac{\boldsymbol{b}}{\boldsymbol{a}}} & 0 \end{pmatrix}.$$

The first and the third matrix in the product of (12.17) are invertible for all $k \in \mathbb{C} \setminus (\pm i\sigma(L''))$ in which $\sigma(L'')$ denotes the spectrum of L''. For a detailed discussion of this, see [27] and [35]. Thus equation (12.17) is equivalent with

$$(12.19) \qquad 0 = \det \left(\mathbb{1} - S''(A, B; k) T(\boldsymbol{a}, \boldsymbol{b}; k) \right) =: F(k) \quad \text{for } k \in \mathbb{C} \setminus (\pm i\sigma(L'')).$$

We remark that the restriction on k concerns only negative eigenvalues $\lambda = k^2$ of H^2_{BK}. Furthermore in (12.2) we have required $k \neq 0$. Hence (12.19) is only a necessary and sufficient condition for $k \in \mathbb{C} \setminus (\pm i\sigma(L'') \cup \{0\})$ being a "wave number" and $\lambda = k^2$ being an eigenvalue of H^2_{BK}. Furthermore, as in section (9), the multiplicity of the eigenvalue λ coincides with the multiplicity of the eigenvalue one of $S''(A, B; k) T(\boldsymbol{a}, \boldsymbol{b}; k)$ for every $k \in \mathbb{C} \setminus (\pm i\sigma(L'') \cup \{0\})$.

13. The eigenvalue zero

For the eigenvalue $\lambda = 0$, which is equivalent to the case $k = 0$, the eigenfunctions are of the form

$$(13.1) \qquad \psi_0(x) = \left(\alpha_1 \frac{1}{\sqrt{x}} + \beta_1 \frac{1}{\sqrt{x}} \ln x, \dots, \alpha_E \frac{1}{\sqrt{x}} + \beta_E \frac{1}{\sqrt{x}} \ln x \right).$$

With a similar calculation as for the case $k \neq 0$ one obtains the equation

$$(13.2) \qquad \left(A'' \begin{pmatrix} \mathbb{1} & \ln \boldsymbol{a} \\ \mathbb{1} & \ln \boldsymbol{b} \end{pmatrix} + B'' \begin{pmatrix} 0 & \mathbb{1} \\ 0 & -\mathbb{1} \end{pmatrix} \right) \begin{pmatrix} \boldsymbol{\alpha} \\ \boldsymbol{\beta} \end{pmatrix} = 0$$

which is necessary and sufficient for $\lambda = 0$ to be an eigenvalue of H_{BK}^2. The matrices A'' and B'' are the same as in (12.16). Then we can proceed as in [27] and get the following result: $\lambda = k^2 = 0$ is an eigenvalue of H_{BK}^2 iff for one value $k' \neq 0$ and then for every $k' \neq 0$

$$(13.3) \qquad F_0(k') := \det(\mathbb{1} - S''(A, B; k')C(\boldsymbol{a}, \boldsymbol{b}; k')) = 0$$

is fulfilled with $S''(A, B; k')$ as in (12.18) and

$$(13.4) \qquad C(\boldsymbol{a}, \boldsymbol{b}; k') := \begin{pmatrix} \frac{\ln\left(\frac{b_1}{a_1}\right)}{2\frac{\mathrm{i}}{k'}+\ln\left(\frac{b_1}{a_1}\right)} & & & \frac{2\frac{\mathrm{i}}{k'}}{2\frac{\mathrm{i}}{k'}+\ln\left(\frac{b_1}{a_1}\right)} & & \\ & \ddots & & & \ddots & \\ & & \frac{\ln\left(\frac{b_E}{a_E}\right)}{2\frac{\mathrm{i}}{k'}+\ln\left(\frac{b_E}{a_E}\right)} & & & \frac{2\frac{\mathrm{i}}{k'}}{2\frac{\mathrm{i}}{k'}+\ln\left(\frac{b_E}{a_E}\right)} \\ \frac{2\frac{\mathrm{i}}{k'}}{2\frac{\mathrm{i}}{k'}+\ln\left(\frac{b_1}{a_1}\right)} & & & \frac{\ln\left(\frac{b_1}{a_1}\right)}{2\frac{\mathrm{i}}{k'}+\ln\left(\frac{b_1}{a_1}\right)} & & \\ & \ddots & & & \ddots & \\ & & \frac{2\frac{\mathrm{i}}{k'}}{2\frac{\mathrm{i}}{k'}+\ln\left(\frac{b_E}{a_E}\right)} & & & \frac{\ln\left(\frac{b_E}{a_E}\right)}{2\frac{\mathrm{i}}{k'}+\ln\left(\frac{b_E}{a_E}\right)} \end{pmatrix}.$$

Furthermore, the multiplicity of the eigenvalue $\lambda = 0$ coincides with the multiplicity of the eigenvalue one of $S''(A, B; k')C(\boldsymbol{a}, \boldsymbol{b}; k')$ for every real $k' \neq 0$. Thus in general there is a difference between the spectral multiplicity of the eigenvalue one of $S''(A, B; 0)T(\boldsymbol{a}, \boldsymbol{b}, 0)$, which we denote by N, and the eigenvalue one of $S''(A, B; k')C(\boldsymbol{a}, \boldsymbol{b}; k')$ with $k' \neq 0$, see [27], [37] and [40].

We now want to summarize the above results and give some immediate consequences of this and the previous sections.

14. Summary and consequences of the results

We have considered all self-adjoint extensions of $(H_{\mathrm{BK}}, D_0^1(\Gamma))$ and $(H_{\mathrm{BK}}^2, D_0^2(\Gamma))$ on compact graphs. In the first case, $k \in \mathbb{C}$ is an eigenvalue of H_{BK} iff (9.10) is fulfilled and the multiplicities of the corresponding eigenvalues k of H_{BK} and one of $\mathcal{S}(A, B)\mathcal{T}(\boldsymbol{a}, \boldsymbol{b})$ are identical. In the second case $k^2 = \lambda$ with $k \in \mathbb{C} \setminus (\pm\mathrm{i}\sigma(L'') \cup \{0\})$ is an eigenvalue of H_{BK}^2 iff (12.19) is fulfilled. Again, the corresponding multiplicities of the eigenvalues coincide. In both cases one can identify each self-adjoint extension of H_{BK} and H_{BK}^2 with a self-adjoint extension of the classical momentum operator p or the kinetic energy operator $-\Delta$ and vice versa.

In the first case, every choice of A and B with (8.10) corresponds to a self-adjoint extension of $(H_{\mathrm{BK}}, D_0^1(\Gamma))$ or $(p, D_0^1(\Gamma))$. Furthermore, in order to achieve the same spectrum, one only has to adjust the lengths of the edges of the graph. Each edge e_i has to be endowed with a length

$$(14.1) \qquad \mathfrak{l}_i := \ln\left(\frac{b_i}{a_i}\right),$$

but the starting point and the endpoints are free. The momentum operator has the same spectrum as H_{BK} if we choose (14.1) as the lengths for the momentum operator, especially in both cases the secular equations will be equal and identical with (9.10). Especially equation (9.10) holds also for the eigenvalue $k = 0$. This is an essential difference to the eigenvalue zero of the negative Laplace operator or the "squared" Berry-Keating operator.

In the second case, one also has to adjust the lengths as before in order to relate the self-adjoint extensions of $(H_{\mathrm{BK}}^2, D_0^2(\Gamma))$ and $(-\Delta, D_0^2(\Gamma))$. However, in oder to attain the same spectrum, except for the case $k \notin \mathbb{C} \setminus (\pm\mathrm{i}\sigma(L'') \setminus \{0\})$, one has to transform the matrices A and B into A'' and B'' as in (12.9) and (12.16). Then the spectrum of the negative Laplacian characterized by A'' and B'' with the previous choice of the lengths will coincide with the spectrum of H_{BK}^2 characterized by A and B in (11.6). Especially the functions $F(k)$ and $F_0(k)$ in (12.19) and (13.3), respectively, will coincide with the corresponding functions for $-\Delta$, see e.g. [27] and [34].

We remark that the transformation of the matrices $A \to A''$ and $B \to B''$ and vice versa cannot be achieved by perturbing the negative Laplacian by a magnetic flux which corresponds to an operator acting on the edges as

$$(14.2) \qquad \left(\frac{\mathrm{d}}{\mathrm{d}x_j} - \mathrm{i}A_j(x_j)\right)^2 \psi(x_j) \quad \text{for} \quad 1 \le j \le E.$$

Kostrykin and Schrader have shown in [41] that this operator is related to the negative Laplacian $-\Delta$ by a unitary transformation of the corresponding S-matrices. This means that the Laplacian perturbed by a magnetic flux can also be characterized by two matrices A and B obeying (11.7). But with a local gauge transformation this system can be transformed to a quantum graph system with the pure Laplacian which is now characterized by two new matrices $\widetilde{A}$ and $\widetilde{B}$. These new matrices are obtained by the old ones by

$$(14.3) \qquad \widetilde{A} = AU \quad \text{and} \quad \widetilde{B} = BU$$

where U is a diagonal unitary matrix. If we calculate the S-matrices for these systems we obtain

$$(14.4) \qquad S(\widetilde{A}, \widetilde{B}; k) = US(A, B; k)U^+.$$

In particular this means that the S-matrix is k-independent iff the original S-matrix is k-independent. By a result of [42] we conclude that in the sense of (12.10) (see [31]) the corresponding matrix $P^\perp_{\ker B} L P^\perp_{\ker B}$ is zero iff $P^\perp_{\ker \widetilde{B}} \widetilde{L} P^\perp_{\ker \widetilde{B}}$ is zero. This feature is obviously not given by the transformation A, B to A'', B'' especially in (12.15) taking into account that the transformation A, B to A', B' in (12.9) and the corresponding transformation L to L' possess this feature.

Kostrikin and Schrader have shown in [35] that the negative Laplacian $-\Delta$ possesses time-reversal symmetry iff $S^T = S$. Obviously the transformation (14.4) doesn't maintain this symmetry in general.

In both cases we get the same length $\mathfrak{l}_i$ as in (14.1) for the edge e_i of the quantum graph for the corresponding momentum operator or kinetic energy operator. Thus we choose $\mathfrak{l}_i$ for the lengths of the graph and endow it with a metric structure as in section 6.

15. TRACE FORMULAE AND WEYL'S LAW

We are now in the position to give an explicit expressions for the behaviour of the eigenvalue counting functions for large eigenvalues and give trace formulae for the Berry-Keating operator and the "squared" Berry-Keating operator on compact graphs. These results are immediate consequences of sections 7, 10 and 14 and the results in [27]. The proofs of the claims for the Berry-Keating operator are quite analogous to [27] and therefore we only give a short outline of some steps of the proof. Since the trace formulae differ in some details we formulate these formulae in one theorem and one corollary. First of all we introduce an appropriate space of test functions as in [27].

Definition 15.1. For each $r \ge 0$ the space H_r consists of all functions $h : \mathbb{C} \to \mathbb{C}$ satisfying the following conditions:

- h is even, i.e., $h(k) = h(-k)$.
- For each $h \in H_r$ there exists $\delta > 0$ such that h is analytic in the strip $M_{r+\delta} := \{k \in \mathbb{C}; |\operatorname{Im} k| < r + \delta\}$.
- For each $h \in H_r$ there exists $\eta > 0$ such that $h(k) = O\left(\frac{1}{(1+|k|)^{1+\eta}}\right)$ on $M_{r+\delta}$.

We denote by k_n the "energies" respectively "wave numbers" of H_{BK} respectively H^2_{BK} and by g_n the corresponding multiplicities which are identical with the order of the corresponding zeros k_n of $\mathcal{F}$ in (9.10) for $n \in \mathbb{N}_0$ respectively zeros k_n of F in (12.19) for $n \in \mathbb{N}$. $n = 0$ corresponds to the "energy" respectively "wave number" zero and the energies respectively the nonnegative wave numbers are ordered with respect to their absolute value $|k_n|$ in increasing order but the (finitely many) imaginary wave numbers are omitted. Furthermore, we denote the self-adjoint realizations characterized by (8.15) respectively (11.6) by $H_{\mathrm{BK}}(\widetilde{A}, \widetilde{B})$ respectively $H^2_{\mathrm{BK}}(A, B)$. Notice that in the

first case $\widetilde{A}, \widetilde{B} \in \mathrm{Mat}(E \times E, \mathbb{C})$ whereas in the second case $A, B \in \mathrm{Mat}(2E \times 2E, \mathbb{C})$. In addition we denote by $\mathfrak{l}_{\min}$ the minimal length of the graph with respect to the definition of section 6 and defined in (14.1). The minimal positive eigenvalue of L'' in (12.15) is denoted by $\lambda''^{+}_{\min}$ and the unique minimum of the function

$$(15.1) \qquad\qquad \mathfrak{l}(\kappa) := \frac{1}{\kappa} \ln(2E) + \frac{2}{\kappa} \operatorname{artanh}\left(\frac{\kappa}{\lambda''^{+}_{\min}}\right)$$

by σ. For convenience, we denote the total length of the graph by

$$(15.2) \qquad\qquad \mathfrak{L} := \sum_{i=1}^{E} \mathfrak{l}_i.$$

Furthermore, by a hat $\hat{\ }$ we denote the Fourier transform (see (2.16)) and $\cdot * \cdot$ denotes the convolution of two functions in the distributional sense, see e.g. [16]. For convenience, we assume that the graph Γ is local with respect to the S-matrix $S''(A, B; k)$ which means that the scattering between two endpoints is only allowed for adjacent edge ends, see [35] for a precise definition. This has the effect that in the trace formula the periodic orbits are with respect to the classical topology as explained in section 6. Otherwise we must interpret the periodic orbits with respect to the topology induced by the S-matrices which will differ from the one in section 6 and must then interpreted as a quantum mechanical topology. However, in [35] it was shown that there exists always at least one graph, for which the S-matrix is local. In order to interpret the right side of (15.3) for H_{BK} as a sum of periodic orbits, we replace the edges by directed edges and assume that the S-matrix $\mathcal{S}(\widetilde{A}, \widetilde{B})$ is local with respect to the directed edges. This means that $\mathcal{S}(\widetilde{A}, \widetilde{B})_{ij} = 0$ if e_i and e_j share no vertex v_{ij} for which e_j has the direction towards v_{ij} and e_i has the direction away from v_{ij}. Again, it is always possible to find such a graph. We get the following theorem for H_{BK}.

Theorem 15.2. *Let Γ be a compact metric graph and $H_{\mathrm{BK}}(\widetilde{A}, \widetilde{B})$ with the above assumptions be given. Let $h \in H_r$ with any $r \geq 0$. Then the following trace formula holds (where $\hat{h}$ denotes the Fourier transform of h defined as in eq. (2.16))*

$$(15.3) \qquad \sum_{n=0}^{\infty} g_n\, h(k_n) = \quad \mathfrak{L}\, \hat{h}(0) + \sum_{\gamma \in \mathfrak{P}} \left[\mathcal{A}_\gamma \hat{h}(\mathfrak{l}_\gamma) + \overline{\mathcal{A}}_\gamma \hat{h}(\mathfrak{l}_\gamma) \right].$$

The amplitude functions $\mathcal{A}_\gamma$ are constructed from the S-matrix elements with respect to the periodic orbits γ, see [27, 28] for a precise definition of this construction. The proof of this theorem is quite analogous to [27]. Since we have no k-dependence of $\mathcal{S}(A, B)$ in (9.9), we can omit the requirement of the minimal length in contrast to the following corollary 15.3. This also leads to the simple product of the amplitude functions $\mathcal{A}_\gamma$ and the Fourier transform of h in the identity (15.3). Furthermore, since the secular equation (9.8) respectively (9.10) holds also for the eigenvalue zero of H_{BK}, the term $g_0 - \frac{1}{2}N$ does not appear in (15.3) in contrast to (15.4) for H_{BK}^2. For H_{BK}^2 we get the following trace formula.

Corollary 15.3. *Let Γ be a compact metric graph and $H_{\mathrm{BK}}^2(A, B)$ with the above assumptions be given. Let the condition $\mathfrak{l}_{\min} > \mathfrak{l}(\sigma)$ be fulfilled and let $h \in H_r$ with $r \geq \sigma$. Then the following trace formula holds*

$$(15.4) \qquad \begin{aligned} \sum_{n=0}^{\infty} g_n\, h(k_n) = \quad & \mathfrak{L}\, \hat{h}(0) + \left(g_0 - \frac{1}{2}N\right)h(0) - \frac{1}{4\pi} \int_{-\infty}^{+\infty} h(k)\, \frac{\operatorname{Im} \operatorname{tr} S''(A, B; k)}{k}\, \mathrm{d}k \\ & + \sum_{\gamma \in \mathfrak{P}} \left[(\hat{h} * \hat{A}_\gamma)(\mathfrak{l}_\gamma) + (\hat{h} * \hat{\overline{A}}_\gamma)(\mathfrak{l}_\gamma) \right]. \end{aligned}$$

Again, the amplitude functions A_γ are constructed from the S-matrix elements with respect to the periodic orbits γ and N denotes the multiplicity of the eigenvalue one of $S''(A, B; k')C(\boldsymbol{a}, \boldsymbol{b}; k')$ for any $k' \in \mathbb{R} \setminus \{0\}$ (see section 13).

Since we have previously seen that the spectrum of $H^2_{\text{BK}}(A, B)$ coincides with some self-adjoint realization of $-\Delta$ on the graph by adapting the lengths and with the results in [27], we get Weyl's law:

Theorem 15.4. *Given the eigenvalues of some $H^2_{\text{BK}}(A, B)$ in increasing order denoted by $\lambda_n = k^2_n$. Then the asymptotic law holds for the counting function $N(\lambda) := \# \left\{ n; \; k^2_n \leq \lambda \right\}$*

$$(15.5) \qquad\qquad N(\lambda) \sim \frac{\mathfrak{L}}{\pi} \sqrt{\lambda} \quad for \quad \lambda \to \infty.$$

The same asymptotic law holds for $H_{\text{BK}}(A, B)$ replacing λ by k on the left-hand side and replacing $\sqrt{\lambda}$ by k at the right-hand side on the equation. Therefore we can conclude:

Corollary 15.5. *Neither H_{BK} nor H^2_{BK} yields as eigenvalues the nontrivial Riemann zeros if these are self-adjoint realizations on any compact graph.*

16. Simple examples

We shall give a simple example for a wave packet and its time-evolution with respect to the Berry-Keating operator in $\mathcal{H} = L^2(\mathbb{R}_>, \mathrm{d}x)$ discussed in section 2. Furthermore, we give an example for a realization of H_{BK} and H^2_{BK} on the simplest construction of a graph which consists of a single edge. Finally, we present some trace formulae for the presented examples.

Example 16.1. For $\psi(x, 0) = \phi(x)$ in (2.25) we define ($x \in \mathbb{R}_>$)

$$(16.1) \qquad\qquad \phi(x) := \frac{\alpha}{\mathrm{e}^x + 1} \quad \text{with} \quad \alpha = \frac{1}{\sqrt{\ln 2 - \frac{1}{2}}}.$$

(With this choice for α it holds $\|\phi\| = 1$.) From (2.21) we obtain

$$(16.2) \qquad\qquad \psi(x, t) = (U(t)\phi)(x) = \frac{\alpha \mathrm{e}^{-\frac{t}{2}}}{\mathrm{e}^{x\mathrm{e}^{-t}} + 1} \quad \text{with} \quad t \in \mathbb{R}.$$

Thus, we get the large t-asymptotics

$$(16.3) \qquad\qquad \psi \sim \frac{\alpha}{2} \mathrm{e}^{-\frac{t}{2}} \quad \text{for} \quad t \to \infty.$$

On the other hand, with

$$(16.4) \qquad\qquad K_{BK}(x, x_0; t) = \int\limits_{-\infty}^{\infty} \psi_k(x) \overline{\psi}_k(x_0) \mathrm{e}^{-\mathrm{i}kt} \mathrm{d}k,$$

(2.13) and (2.25), we get

$$(16.5) \qquad\qquad \psi(x, t) = \int\limits_{-\infty}^{\infty} A(k) \psi_k(x) \mathrm{e}^{-\mathrm{i}kt} \mathrm{d}k.$$

A direct calculation using (2.18) and the integral representation of $\zeta(s)$ as a Mellin transform (see [43, p.20]) yields

$$(16.6) \qquad\qquad A(k) = \frac{\alpha}{\sqrt{2\pi}} \left(1 - \sqrt{2}\, 2^{\mathrm{i}k}\right) \Gamma\left(\frac{1}{2} - \mathrm{i}k\right) \zeta\left(\frac{1}{2} - \mathrm{i}k\right) \quad,$$

With (see [43, p.13])

$$(16.7) \qquad\qquad \left|\Gamma\left(\frac{1}{2} - \mathrm{i}k\right)\right| \sim \sqrt{2\pi} \mathrm{e}^{-\frac{\pi}{2}|k|} \quad \text{for} \quad |k| \to \infty \quad,$$

we get for the large k-asymptotics of $|A(k)|^2$

$$(16.8) \qquad |A(k)|^2 \sim \alpha^2 \left(3 - 2\sqrt{2} \cos(k \ln 2)\right) \mathrm{e}^{-\pi|k|} \left|\zeta\left(\frac{1}{2} - \mathrm{i}k\right)\right|^2 \quad \text{for} \quad |k| \to \infty \quad,$$

which gives a sufficient condition for $A \in L^2(\mathbb{R}, \mathrm{d}k)$. If we consider the continuous representation (16.5) of $\psi(x,t)$, we see that $\psi(x,t)$ gets no contribution from the wave packet $A(k)$ exactly at the wave numbers k corresponding to the conjectured nontrivial Riemann zeros. This is reminiscent to the absorption spectrum interpretation of the nontrivial Riemann zeros by Connes [11, 12], but of course reveals no insight to the position of the nontrivial Riemann zeros.

Example 16.2. For a single edge $I = [a, b]$ (one-dimensional quantum billiard) the matrices A and B are arbitrary numbers fulfilling (8.10). The equations (8.15) and (9.9) lead there with

$$(16.9) \qquad \qquad \mathcal{S}(A, B) =: \mathrm{e}^{-2\pi \mathrm{i}c}$$

to

$$(16.10) \qquad \begin{aligned} \psi(a) &= \mathcal{S}(A, B)\sqrt{\frac{b}{a}}\psi(b) \\ &= \sqrt{\frac{b}{a}}\mathrm{e}^{-2\pi \mathrm{i}c}\psi(b) \quad \text{with} \quad c \in [0, 1). \end{aligned}$$

The eigenvalue spectrum is given by

$$(16.11) \qquad \qquad k_n = \frac{2\pi}{\ln \frac{b}{a}}(n + c) \quad \text{with} \quad c \in [0, 1) \quad \text{and} \quad n \in \mathbb{Z}.$$

We now want to calculate H_{BK}^2 as defined in (10.2) with (16.10), in particular the S-matrix. In order to distinguish the characterizing matrices, we denote these with the subscript $\cdot_{H_{\mathrm{BK}}}$ and $\cdot_{H_{\mathrm{BK}}^2}$. First, we derive the transformation of $A_{H_{\mathrm{BK}}}, B_{H_{\mathrm{BK}}}$ into $A_{H_{\mathrm{BK}}^2}, B_{H_{\mathrm{BK}}^2}$ for the corresponding operators related by (10.2). We get the additional condition

$$(16.12) \qquad \qquad \psi'(a) = \left(\frac{b}{a}\right)^{\frac{3}{2}}\mathrm{e}^{-2\pi \mathrm{i}c}\psi'(b) \quad \text{with} \quad c \in [0, 1).$$

The two conditions are equivalent to

$$(16.13) \quad \begin{aligned} 0 &= \begin{pmatrix} -1 & \left(\frac{b}{a}\right)^{\frac{1}{2}}\mathrm{e}^{-2\pi \mathrm{i}c} \\ 0 & 0 \end{pmatrix}\Psi_{\mathrm{bv}} + \begin{pmatrix} 0 & 0 \\ 1 & \left(\frac{b}{a}\right)^{\frac{3}{2}}\mathrm{e}^{-2\pi \mathrm{i}c} \end{pmatrix}\Psi_{\mathrm{bv}}' \\ \Leftrightarrow 0 &= \begin{pmatrix} -1 & \left(\frac{b}{a}\right)^{\frac{1}{2}}\mathrm{e}^{-2\pi \mathrm{i}c} \\ 0 & 0 \end{pmatrix}\begin{pmatrix} \frac{1}{a} & 0 \\ 0 & \frac{1}{b} \end{pmatrix}D_{(ab)}\Psi_{\mathrm{bv}} + \begin{pmatrix} 0 & 0 \\ 1 & \left(\frac{b}{a}\right)^{\frac{3}{2}}\mathrm{e}^{-2\pi \mathrm{i}c} \end{pmatrix}\begin{pmatrix} \frac{1}{a} & 0 \\ 0 & \frac{1}{b} \end{pmatrix}D_{(ab)}\Psi_{\mathrm{bv}}' \\ \Leftrightarrow 0 &= \begin{pmatrix} -1 & \left(\frac{a}{b}\right)^{\frac{1}{2}}\mathrm{e}^{-2\pi \mathrm{i}c} \\ 0 & 0 \end{pmatrix}D_{(ab)}\Psi_{\mathrm{bv}} + \begin{pmatrix} 0 & 0 \\ 1 & \left(\frac{b}{a}\right)^{\frac{1}{2}}\mathrm{e}^{-2\pi \mathrm{i}c} \end{pmatrix}D_{(ab)}\Psi_{\mathrm{bv}}'. \end{aligned}$$

Therefore, we define

$$(16.14) \qquad A_{H_{\mathrm{BK}}^2} := \begin{pmatrix} -1 & \left(\frac{a}{b}\right)^{\frac{1}{2}}\mathrm{e}^{-2\pi \mathrm{i}c} \\ 0 & 0 \end{pmatrix} \quad \text{and} \quad B_{H_{\mathrm{BK}}^2} := \begin{pmatrix} 0 & 0 \\ 1 & \left(\frac{b}{a}\right)^{\frac{1}{2}}\mathrm{e}^{-2\pi \mathrm{i}c} \end{pmatrix}$$

and recognize that indeed

$$(16.15) \qquad A_{H_{\mathrm{BK}}^2}B_{H_{\mathrm{BK}}^2}^+ = B_{H_{\mathrm{BK}}^2}A_{H_{\mathrm{BK}}^2}^+ = 0 \quad \text{and} \quad \mathrm{rank}\left(A_{H_{\mathrm{BK}}^2}, B_{H_{\mathrm{BK}}^2}\right) = 2$$

is fulfilled. By a comparison of (16.13) with (11.6), we infer that $A_{H_{\mathrm{BK}}^2}$ and $B_{H_{\mathrm{BK}}^2}$ are two possible matrices to characterize H_{BK}^2 in the sense of (11.6). For $S''\left(A_{H_{\mathrm{BK}}^2}, B_{H_{\mathrm{BK}}^2}; k\right)$, we get

$$(16.16) \qquad S''\left(A_{H_{\mathrm{BK}}^2}, B_{H_{\mathrm{BK}}^2}; k\right) = \begin{pmatrix} 0 & \mathrm{e}^{-2\pi \mathrm{i}c} \\ \mathrm{e}^{2\pi \mathrm{i}c} & 0 \end{pmatrix} = \begin{pmatrix} 0 & \mathcal{S}(A, B) \\ \mathcal{S}(A, B)^+ & 0 \end{pmatrix}$$

and for the secular equation (12.19)

$$(16.17) \qquad \qquad 0 = \left(\mathrm{e}^{\mathrm{i}\left(k \ln\left(\frac{b}{a}\right) + 2\pi c\right)} - 1\right)\left(\mathrm{e}^{\mathrm{i}\left(k \ln\left(\frac{b}{a}\right) - 2\pi c\right)} - 1\right).$$

This leads to the "wave numbers"

$$(16.18) \qquad k_n = \frac{2\pi}{\ln \frac{b}{a}} (n \pm c), \quad n \in \mathbb{Z}$$

with c as in (16.11). Obviously, with (16.18) and (16.11) Weyl's law is fulfilled even for small n. Alternatively, since these are from the classical point of view integrable systems we can perform an EBK-quantization for H_{BK} and H_{BK}^2 [44, 45]. In this semiclassical quantization rule the spectrum consists of energies E_n (for convenience we use now the same letter E_n for k_n respectively λ_n as in the sections 2 respectively 4) for which ($\hbar = 1$)

$$(16.19) \qquad I_n(E_n) = \left(n + \frac{\mu_n}{4} \right) \quad \text{with} \quad n \geq 0$$

is fulfilled. Therein denotes μ_n the so-called Maslov index and

$$(16.20) \qquad I_n(E_n) = \frac{1}{2\pi} \int\limits_{\gamma_n} p \mathrm{d}x$$

the classical action of a periodic orbit γ_n which is a subset of the hypersurface $H_{\mathrm{cl}} = E_n$ respectively $\widetilde{H}_{\mathrm{cl}} = E_n$. For H_{cl} in (1.1) with the ring system structure mentioned in section 3, we get from (16.19)

$$(16.21) \qquad E_n = \frac{2\pi}{\ln \left(\frac{b}{a} \right)} \left(n + \frac{\mu_n}{4} \right)$$

and for $\widetilde{H}_{\mathrm{cl}}$ in (4.1) (also with the ring system structure)

$$(16.22) \qquad \sqrt{E_n} = k_n = \frac{2\pi}{\ln \left(\frac{b}{a} \right)} \left(n + \frac{\mu_n}{4} \right).$$

A comparison of (16.21) with (16.11) yields for the Maslov indices $\mu_n = 4c$ for H_{cl}. For $\widetilde{H}_{\mathrm{BK}}$ we get two Maslov indices, $\mu_n = 4c$ for $n = 0, 2, 4, \ldots$ and $\mu_n = -4c$ for $n = 1, 3, 5, \ldots$. Since a Maslov index is at most defined modulo 4 and because of $c \in [0, 1)$, the above second Maslov indices $\mu_n = -4c$ correspond to the Maslov indices $\tilde{\mu}_n = 4(1 - c)$ for $n = 1, 3, \ldots$. We stress that the EBK-quantization for $\widetilde{H}_{\mathrm{cl}}$ with a classical "hard wall" boundary condition yields

$$(16.23) \qquad \sqrt{E_n} = k_n = \frac{\pi}{\ln \left(\frac{b}{a} \right)} \left(n + \frac{\mu_n}{4} \right),$$

which differs from (16.22) by a factor 2. We mention that the S-matrix elements of $S'' \left(A_{H_{\mathrm{BK}}^2}, B_{H_{\mathrm{BK}}^2}; k \right)$ for Dirichlet (D), Neumann (N) or Robin (R) boundary conditions are given by

$$(16.24) \qquad S'' \left(A_{H_{\mathrm{BK}}^2}, B_{H_{\mathrm{BK}}^2}; k \right)_{ij} = \begin{cases} \delta_{ij} & \text{for } (D), \\ -\delta_{ij} & \text{for } (N), \quad \text{with } \rho_j \in \mathbb{R} \text{ and } i, j \in \{1, 2\} \\ -\delta_{ij} \frac{\rho_j - ik}{\rho_j + ik} & \text{for } (R), \end{cases}$$

which obviously differs from (16.16) and therefore, it cannot originate from a "squared" Berry-Keating operator. If we impose Dirichlet boundary conditions at both interval ends, we get for $F(k)$ in (12.19)

$$(16.25) \qquad F(k) = 1 - \mathrm{e}^{2ik \ln \left(\frac{b}{a} \right)}$$

and thus we obtain for the wave numbers k_n

$$(16.26) \qquad k_n = \frac{\pi}{\ln \left(\frac{b}{a} \right)} n, \quad n \in \mathbb{Z} \setminus \{0\},$$

wherein we have taken into account that $\lambda = k_0^2 = 0$ is not an eigenvalue for the Dirichlet case. In contrast to the Dirichlet case, $\lambda = k_0 = 0$ is an eigenvalue for Neumann boundary conditions at both interval ends and the nonzero wave numbers coincide with the Dirichlet case (16.26). For Robin boundary conditions at both interval ends, we get

$$(16.27) \qquad F(k) = 1 - \frac{(\rho_1 - ik)(\rho_2 - ik)}{(\rho_1 + ik)(\rho_2 + ik)} \mathrm{e}^{2ik \ln \left(\frac{b}{a} \right)}.$$

Again by a comparison of (16.26) with (16.23), we conclude for the Maslov indices for pure Dirichlet and Neumann boundary conditions

$$(16.28) \qquad\qquad \mu_n = 0 \quad \text{for} \quad n \in \mathbb{N}$$

and additionally $\mu_0 = 0$ for the Neumann case. For the Robin boundary conditions on both interval ends the Maslov indices have to be individually calculated for each $n \in \mathbb{N}_0$ by (16.27).

The above considerations underline the fact that the form of the S-matrix (16.16) corresponds to a pure ring system as in the case of the negative Laplacian $-\Delta$, see [35]. The occurrence of possible noninteger "Maslov indices" originates simply from the fact that we have a discontinuous crossover by turning once around in the ring system (one-dimensional torus) in contrast to the "usual" continuity requirement of the wave function, see e.g. [46].

Example 16.3. We shall present a trace formula for the time-evolution operator $U(t)$ in (2.20) and (2.21) for H_{BK} acting on a single edge with the assigned interval $I = [1, b]$:

$$(16.29) \qquad (U(t)\phi)(x) := \sum_{n=-\infty}^{\infty} \psi_n(x) \langle \psi_n, \phi \rangle \, \mathrm{e}^{-\mathrm{i}k_n t}, \quad \phi \in L^2(I, \mathrm{d}x),$$

with the eigenvalues $k_n = \dfrac{2\pi}{\ln b}(n - c)$, $n \in \mathbb{Z}$, $c \in [0, 1)$, and the normalized eigenfunctions

$$(16.30) \qquad \psi_n(x) = \frac{1}{\sqrt{x \ln b}} \mathrm{e}^{\mathrm{i}k_n \ln x} \quad \text{with} \quad n \in \mathbb{Z}.$$

For the corresponding (not retarded) integral kernel of $U(t)$ we get by [15, p.20] (in a distributional sense acting on $\mathcal{D}(I) \subset L^2(I, \mathrm{d}x)$ identified by the continuous representatives; $g(x, x_0; t) := \dfrac{2\pi}{\ln b}[\ln x - \ln x_0 - t])$

$$
\begin{aligned}
(16.31) \qquad K(x, x_0; t) &:= \sum_{n=-\infty}^{\infty} \psi_n(x)\overline{\psi}_n(x_0)\mathrm{e}^{-\mathrm{i}k_n t} = \frac{\mathrm{e}^{-\mathrm{i}cg(x,x_0;t)}}{\sqrt{xx_0}\,\ln b} \sum_{-\infty}^{\infty} \mathrm{e}^{\mathrm{i}g(x,x_0;t)n} \\
&= \frac{2\pi}{\ln b}\frac{\mathrm{e}^{-\mathrm{i}cg(x,x_0;t)}}{\sqrt{xx_0}} \sum_{n=-\infty}^{\infty} \delta(g(x, x_0; t) + 2\pi n) \\
&= \mathrm{e}^{-\mathrm{i}cg(x,x_0;t)} \sum_{n=-\infty}^{\infty} b^{\frac{n}{2}}\mathrm{e}^{\frac{t}{2}}\delta\left(xb^n - x_0\mathrm{e}^t\right).
\end{aligned}
$$

If we take the trace of $U(t)$, we obtain with (16.31) (by defining the "period" $T = \ln b$ [see (2.2)] and the Maslov index $\mu := 4c$)

$$
\begin{aligned}
(16.32) \qquad \mathrm{Tr}\, U(t) &:= \int_1^b K(x, x; t)\mathrm{d}x = \sum_{n=-\infty}^{\infty} \mathrm{e}^{-\mathrm{i}k_n t} \\
&= T \sum_{n=-\infty}^{\infty} \mathrm{e}^{\mathrm{i}\frac{\pi}{2}\mu n}\delta\left(t - nT\right).
\end{aligned}
$$

If we now choose a test function h of H_r (definition 15.1) with an arbitrary $r > 0$, we get by the identity (16.32) and the symmetry of h the trace formula

$$\int\limits_{-\infty}^{\infty} \hat{h}(t)\,\mathrm{Tr}\,U(t)\mathrm{d}t = \sum_{n=-\infty}^{\infty} h(k_n)$$

$$(16.33) \qquad\qquad = T\hat{h}(0) + T\sum_{n=1}^{\infty}\left(\mathrm{e}^{\mathrm{i}\frac{\pi}{2}\mu n}\hat{h}(nT) + \mathrm{e}^{-\mathrm{i}\frac{\pi}{2}\mu n}\hat{h}(-nT)\right)$$

$$= T\hat{h}(0) + 2T\sum_{n=1}^{\infty}\cos\left(\frac{\pi}{2}\mu n\right)\hat{h}(nT).$$

We recall that the S-matrix for this quantum graph is $\mathcal{S}(A,B) = \mathrm{e}^{2\pi\mathrm{i}c} = \mathrm{e}^{\mathrm{i}\frac{\pi}{2}\mu}$ (see (16.9)) and the length of the (single) edge is $\mathfrak{l} = \mathcal{L} = \ln\frac{b}{1} = \ln b$. Since we have a directed edge, there is only one possibility for the orientation of the periodic orbits and therefore, the periodic orbits can be labelled by the natural numbers, and the corresponding lengths of the periodic orbits are $\mathfrak{l}_n = n\ln b$ and all are multiples of one primitive periodic orbit with length $\mathfrak{l}_1 = \ln b = T$. For the amplitude functions we get (see [27]) $\mathcal{A}_n = \mathfrak{l}_1 \mathrm{e}^{2\pi\mathrm{i}cn} = T\mathrm{e}^{\mathrm{i}\frac{\pi}{2}\mu n}$. Applying (15.3) we get (16.33), which confirms the trace formula in Theorem 15.2.

Example 16.4. We shall present a trace formula for the kernel $\widetilde{K}(x,x_0;t)$ of the unitary evolution operator $\mathrm{e}^{-\mathrm{i}tH_{\mathrm{BK}}^2}$ of H_{BK}^2 with Dirichlet boundary conditions (D) on a single edge e with assigned interval $I = [1,b]$. The eigenvalues are given by (16.26), thus the (Feynman-)kernel reads

$$(16.34) \qquad\qquad \widetilde{K}(x,x_0;t) := \sum_{n=1}^{\infty}\psi_n(x)\overline{\psi}_n(x_0)\mathrm{e}^{-\mathrm{i}k_n^2 t}$$

with the normalized eigenfunctions

$$(16.35) \qquad\qquad \psi_n(x) := \sqrt{\frac{2}{\mathfrak{l}}}\,\frac{\sin\left(n\pi\dfrac{\ln x}{\mathfrak{l}}\right)}{\sqrt{x}}, \quad n \in \mathbb{N},$$

where $\mathfrak{l} := \ln b$ denotes the length of the edge e. Using a suitable addition theorem for trigonometric functions, we get two alternative expressions for $\widetilde{K}(x,x_0;t)$ (see [43, p.371])
(16.36)
$\widetilde{K}(x,x_0;t)$

$$= \frac{1}{\sqrt{xx_0}\mathfrak{l}_{\gamma_p}}\left[\Theta_3\left(\frac{1}{\mathfrak{l}_{\gamma_p}}\ln\left(\frac{x}{x_0}\right), -\frac{4\pi}{\mathfrak{l}_{\gamma_p}^2}t\right) - \Theta_3\left(\frac{1}{\mathfrak{l}_{\gamma_p}}\ln\left(xx_0\right), -\frac{4\pi}{\mathfrak{l}_{\gamma_p}^2}t\right)\right]$$

$$= \frac{1}{2\sqrt{xx_0}\sqrt{\mathrm{i}\pi t}}\sum_{n=0}^{\infty}\epsilon_n\left[\mathrm{e}^{\mathrm{i}2n\pi}\exp\left(\mathrm{i}\frac{(\ln x - \ln y + n\mathfrak{l}_{\gamma_p})^2}{4t}\right) + \mathrm{e}^{\mathrm{i}(2n+1)\pi}\exp\left(\mathrm{i}\frac{(\ln x + \ln y + n\mathfrak{l}_{\gamma_p})^2}{4t}\right)\right.$$

$$\left. + \mathrm{e}^{\mathrm{i}2n\pi}\exp\left(\mathrm{i}\frac{(\ln x - \ln y - n\mathfrak{l}_{\gamma_p})^2}{4t}\right) + \mathrm{e}^{\mathrm{i}(2n+1)\pi}\exp\left(\mathrm{i}\frac{(\ln x + \ln y - n\mathfrak{l}_{\gamma_p})^2}{4t}\right)\right],$$

where $\Theta_3(z,\tau)$ denotes the Jacobi theta function and we have defined

$$(16.37) \qquad\qquad \epsilon_n := \begin{cases} \frac{1}{2} & \text{for} \quad n = 0 \\ 1 & \text{for} \quad n > 0 \end{cases}$$

and $\mathfrak{l}_{\gamma_p} := 2\mathfrak{l} = 2\ln b$ is the length of the primitive periodic orbit γ_p of the corresponding classical system. Notice that the summands in the second identity in (16.36) can be interpreted as contributions of free particle kernels at a fixed time t corresponding to the four types of paths $p(x_0,x)$ (see

section 6) joining x_0 and x (see e.g. [42, 47]). For this reason, we define (cp. (4.10) and [20, p.30])

$$\widetilde{K}_p(x, x_0; t) := \frac{1}{2\sqrt{\mathrm{i}\pi t}} \exp\left(\mathrm{i}\frac{\mathfrak{l}_p(x_0, x)^2}{4t}\right) \tag{16.38}$$

where $\mathfrak{l}_p(x_0, x)$ is the length of the path $p(x_0, x)$ (see (6.1)), and we then get by (16.36)

$$\begin{aligned}
\widetilde{K}(x, x_0; t) &= \frac{1}{\sqrt{xx_0}} \sum_{p(x_0, x)} \exp\left(\mathrm{i}\pi n_{p(x_0, x)}\right) \widetilde{K}_p(x, x_0; t) \\
&= \frac{1}{\sqrt{xx_0}} \sum_{p(x_0, x)} \exp\left(-\mathrm{i}\frac{\pi \mu_{p(x_0, x)}}{2}\right) \widetilde{K}_p(x, x_0; t),
\end{aligned} \tag{16.39}$$

where the sum comprises all possible paths $p(x_0, x)$ joining x_0 and x and $n_{p(x_0, x)}$ is defined as the number of reflections of the path $p(x_0, x)$ at the "hard wall" interval endpoints 1 and $\ln b$. $\mu_{p(x_0, x)}$ denotes the Maslov index of the path $p(x_0, x)$ which is given by $\mu_{p(x_0, x)} = 2n_{p(x_0, x)} \mod 4$ in agreement with the "usual" Maslov index for the one-dimensional billiard system corresponding to the negative Laplacian (see [46]), and with (16.28) (in (16.28) the Maslov index corresponds to periodic orbits).

Example 16.5. Finally, we shall present an explicit trace formula (heat kernel) for a single edge with assigned interval $I = [1, b]$ for H_{BK}^2 with Dirichlet boundary conditions (D). We calculate the trace of the heat kernel of $\mathrm{e}^{-tH_{\mathrm{BK}}^2}$ (replacing t by $-\mathrm{i}t$ in (16.34))

$$\widetilde{K}_h(x, x_0; t) := \widetilde{K}(x, x_0; -\mathrm{i}t) = \sum_{k_n} \psi(x)\overline{\psi}_n(x_0)\mathrm{e}^{-k_n^2 t} \tag{16.40}$$

directly and then compare the result with the trace formula (15.4). Therefore, we recall that the wave numbers of H_{BK}^2 with (D) are explicitly given by (16.26). Thus, we obtain for the trace of the heat kernel (setting $\mathfrak{L} := \frac{1}{2}\mathfrak{l}_{\gamma_p} := \ln b$ and [43, p.371])

$$\begin{aligned}
\mathrm{Tr}\, \mathrm{e}^{-tH_{BK}^2} &= \int_1^b \sum_{k_n} \psi(x)\overline{\psi}_n(x)\mathrm{e}^{-k_n^2 t}\mathrm{d}x \\
&= \sum_{k_n} \mathrm{e}^{-k_n^2 t} = \frac{1}{2}\left(\Theta_3\left(0, \mathrm{i}\frac{4\pi}{\mathfrak{l}_{\gamma_p}^2}t\right) - 1\right) = \frac{\mathfrak{l}_{\gamma_p}}{4\sqrt{t\pi}}\left(\sum_{n=-\infty}^{\infty} \exp\left(-\frac{n^2\mathfrak{l}_{\gamma_p}^2}{4t}\right)\right) - \frac{1}{2} \\
&= \frac{\mathfrak{L}}{2\sqrt{\pi t}} - \frac{1}{2} + \sum_{n=1}^{\infty} \frac{\mathfrak{l}_{\gamma_p}}{2\sqrt{\pi t}}\mathrm{e}^{-\frac{(n\mathfrak{l}_{\gamma_p})^2}{4t}}.
\end{aligned} \tag{16.41}$$

Notice that the sums in (16.41) are absolutely convergent whereas in (16.32) the sums are convergent in the topology of $\mathcal{D}'(\mathbb{R})$ (in a distributional sense). In order to compare this result with (15.4), we recall that $C(1, \ln b; k')$ and the S-matrix $S_{(D)}$ for the Dirichlet case is given by (see (13.3) and (16.24))

$$S''_{(D)} = \mathbb{1}_{2\times 2} \quad \text{and} \quad C(1, \ln b; k') = \begin{pmatrix} \frac{\ln b}{2\frac{\mathrm{i}}{k'} + \ln b} & \frac{2\frac{\mathrm{i}}{k'}}{2\frac{\mathrm{i}}{k'} + \ln b} \\ \frac{2\frac{\mathrm{i}}{k'}}{2\frac{\mathrm{i}}{k'} + \ln b} & \frac{\ln b}{2\frac{\mathrm{i}}{k'} + \ln b} \end{pmatrix}. \tag{16.42}$$

It is a simple calculation that the multiplicity g_0 of the eigenvalue one of $S''_{(D)}C(1, \ln b; k')$ is $g_0 = 0$ for any $k' \in \mathbb{R} \setminus \{0\}$. Furthermore, it is obvious that the order N of the zero with wavenumber $k_0 = 0$ of $F(k)$ in (12.19) is $N = 1$, thus $g_0 - \frac{1}{2}N = -\frac{1}{2}$. The multiplicities of the wave numbers k_n are $g_n = 1$ for $n \in \mathbb{N}$. Since Dirichlet boundary condition corresponds to the classical "hard wall" boundary condition, we conclude that the periodic orbits γ are given by all multiples of one primitive periodic orbit γ_p with primitive periodic orbit length $\mathfrak{l}_{\gamma_p} = 2\ln b$. For the amplitude functions A_γ in (15.4) we obtain $A_\gamma = \frac{1}{2}\mathfrak{l}_{\gamma_p}$ (see [27]). Furthermore, it is obvious that $\mathrm{Im}\, S_D = 0$. Using the test function $h(k) := \mathrm{e}^{-k^2 t}$ we obtain the Fourier transform $\hat{h}(x) = \frac{1}{2\sqrt{\pi t}}\mathrm{e}^{-\frac{x^2}{4t}}$. Inserting these quantities in the

trace formula (15.4) we get the trace formula (16.41), which again confirms the trace formula (15.4). We remark that from the small-t asymptotics (16.41) one obtains directly the Weyl asymptotics (15.5) using a proper Karamata-Tauberian theorem.

References

[1] In the comment (included in his collected papers [2]) to his paper on the explicit formulae of number theory [3], A. Weil writes that Hellinger once told him the following: At the occasion of his first course on his theory of integral equations, Hilbert said after having demonstrated that the characteristic values (eigenvalues) of a symmetric kernel are real:"Et avec ce théorème, Messieurs, nous démontrerons l'hypothèse de Riemann". Since Hellinger was a student of Hilbert in Göttingen (since 1904) and later until 1909 Hilbert's assistant, we can assume that the cited statement by Hilbert dates back to these years.

[2] A. Weil. Commentaire 'Sur les "formules explicites" de la théorie des nombres premiers'. In *Scientific works. Collected papers.*, volume II (1951–1964), page 527. Springer, New York, 1979.

[3] A. Weil. Sur les "formules explicites" de la théorie des nombres premiers. *Comm. Sém. Math. Univ. Lund [Medd. Lunds Univ. Mat. Sem.]*, 1952:252–265, 1952.

[4] See Odlyzko's correspondence with Polya: http://www.dtc.umn.edu/∼odlyzko/polya/index.html.

[5] A. Selberg. Harmonic analysis and discontinuous groups in weakly symmetric Riemannian spaces with applications to Dirichlet series. *J. Indian Math. Soc. (N.S.)*, 20:47–87, 1956.

[6] J. Hadamard. Les surfaces à courbures opposeés et leurs lignes geódésiques. *Journal de Mathématique pure et appliqueés*, 4:27–73, 1898.

[7] J. Hadamard. Sur le billard non-Euclidien. *Soc. Sci. Bordeaux*, 147, 1898.

[8] M. C. Gutzwiller. Classical quantization of a Hamiltonian with ergodic behaviour. *Phys. Rev. Lett.*, 45:150–153, 1980.

[9] M. C. Gutzwiller. Periodic orbits and classical quantization conditions. *J. Math. Phys.*, 12:343–358, 1971.

[10] M. V. Berry. Riemann's zeta function: a model for quantum chaos? In T. H. Seligman and Nishioka H., editors, *Quantum Chaos and Statistical Nuclear Physics*, volume 263 of *Lecture Notes in Physics*, pages 1–17. Springer, New York, 1986.

[11] A. Connes. Formule de trace en géométrie non-commutative et hypothèse de Riemann. *C. R. Acad. Sci. Paris Sér. I Math.*, 323:1231–1236, 1996.

[12] A. Connes. Trace formula in noncommutative geometry and the zeros of the Riemann zeta function. *Selecta Math. (N.S.)*, 5(1):29–106, 1999.

[13] M. V. Berry and J. P. Keating. $H = xp$ and the Riemann zeros. In I. V. Lerner, J. P. Keating, and D. E. Khmelnitskii, editors, *Supersymmetry and Trace Formulae: Chaos and Disorder*, volume 263, pages 355–367. Plenum Press, New York, 1999.

[14] M. V. Berry and J. P. Keating. The Riemann zeros and eigenvalue asymptotics. *SIAM Rev.*, 41(2):236–266, 1999.

[15] I. M. Gelfand and G. E. Schilow. *Verallgemeinerte Funktionen (Distributionen). I: Verallgemeinerte Funktionen und das Rechnen mit ihnen*. Hochschulbücher für Mathematik, Bd. 47. VEB Deutscher Verlag der Wissenschaften, Berlin, 1960.

[16] M. Reed and B. Simon. *Methods of Modern Mathematical Physics. II. Fourier Analysis, Self-Adjointness*. Academic Press, New York, 1975.

[17] W. Arendt. Gaussian estimates and interpolation of the spectrum in L^p. *Differential Integral Equations*, 7(5-6):1153–1168, 1994.

[18] W. Arendt. Spectrum and growth of positive semigroups. In *Evolution equations (Baton Rouge, LA, 1992)*, volume 168 of *Lecture Notes in Pure and Appl. Math.*, pages 21–28. Dekker, New York, 1995.

[19] W. Arendt and B. de Pagter. Spectrum and asymptotics of the Black-Scholes partial differential equation in (L^1, L^∞)-interpolation spaces. *Pacific J. Math.*, 202(1):1–36, 2002.

[20] C. Grosche and F. Steiner. *Handbook of Feynman path integrals*, volume 145 of *Springer Tracts in Modern Physics*. Springer-Verlag, Berlin, 1998.

[21] S. Endres and F. Steiner. A simple infinite quantum graph. *Ulmer Seminare 2009*.

[22] M. C. Gutzwiller. *Chaos in classical and quantum mechanics*, volume 1 of *Interdisciplinary Applied Mathematics*. Springer-Verlag, New York, 1990.

[23] F. Black and M. S. Scholes. The pricing of options and corporate liabilities. *Journal of Political Economy*, 81(3):637–54, 1973.

[24] R. C: Merton. Theory of rational option pricing. *Bell Journal of Economics*, 4(1):141–183, 1973.

[25] A. Terras. *Harmonic analysis on symmetric spaces and applications. I*. Springer-Verlag, New York, 1985.

[26] V. Kostrykin and R. Schrader. Kirchhoff's rule for quantum wires. *J. Phys. A*, 32:595–630, 1999.

[27] J. Bolte and S. Endres. The trace formula for quantum graphs with general self adjoint boundary conditions. *Annales Poincaré, manuscript accepted*, 2009.

[28] T. Kottos and U. Smilansky. Periodic orbit theory and spectral statistics for quantum graphs. *Ann. Phys. (NY)*, 274:76–124, 1999.

[29] J. Weidmann. *Lineare Operatoren in Hilberträumen. Teil 1*. Mathematische Leitfäden. B. G. Teubner, Stuttgart, 2000.

[30] M. Reed and B. Simon. *Methods of modern mathematical physics. I*. Academic Press Inc., New York, second edition, 1980. Functional analysis.

[31] P. Kuchment. Quantum graphs. I. Some basic structures. *Waves Random Media*, 14:S107–S128, 2004.

[32] M. Reed and B. Simon. *Methods of Modern Mathematical Physics. IV. Analysis of Operators*. Academic Press, New York, 1978.

[33] W. N. Everitt and L. Markus. Complex symplectic spaces and boundary value problems. *Bull. Amer. Math. Soc. (N.S.)*, 42(4):461–500, 2005.

[34] V. Kostrykin and R. Schrader. Laplacians on metric graphs: eigenvalues, resolvents and semigroups. In G. Berkolaiko, R. Carlson, S. A. Fulling, and P. Kuchment, editors, *Quantum graphs and their applications*, volume 415 of *Contemp. Math.*, pages 201–225. Amer. Math. Soc., Providence, RI, 2006.

[35] V. Kostrykin and R. Schrader. The inverse scattering problem for metric graphs and the traveling salesman problem. *preprint, arxiv:math-ph/0603010*, 2006.

[36] B. Thaller. *The Dirac equation*. Texts and Monographs in Physics. Springer-Verlag, Berlin, 1992.

[37] S. A. Fulling, P. Kuchment, and J. H. Wilson. Index theorems for quantum graphs. *J. Phys. A*, 40:14165–14180, 2007.

[38] E. Schrödinger. A method of determining quantum-mechanical eigenvalues and eigenfunctions. *Proc. Roy. Irish Acad. Sect. A.*, 46:9–16, 1940.

[39] L. Infeld and T. E. Hull. The factorization method. *Rev. Modern Physics*, 23:21–68, 1951.

[40] P. Kurasov and M. Nowaczyk. Inverse spectral problem for quantum graphs. *J. Phys. A*, 38:4901–4915, 2005.

[41] V. Kostrykin and R. Schrader. Quantum wires with magnetic fluxes. *Comm. Math. Phys.*, 237:161–179, 2003.

[42] V. Kostrykin, J. Potthoff, and R. Schrader. Heat kernels on metric graphs and a trace formula. In F. Germinet and P.D. Hislop, editors, *Adventure in Mathematical Physics*, volume 447 of *Contemp. Math.*, pages 175–198. Amer. Math. Soc., Providence, RI, 2007.

[43] W. Magnus, F. Oberhettinger, and R. P. Soni. *Formulas and theorems for the special functions of mathematical physics*. Third enlarged edition. Die Grundlehren der mathematischen Wissenschaften, Band 52. Springer.

[44] A. Einstein. Zum Qantensatz von Sommerfeld und Epstein (in German). *Verh. Deutsche Phys. Ges.*, 19:82–92, 1917.

[45] J. B. Keller. Corrected Bohr-Sommerfeld quantum conditions for nonseparable systems. *Ann. Physics*, 4:180–188, 1958.

[46] H.-J. Stöckmann. *Quantum chaos*. Cambridge University Press, Cambridge, 1999. An introduction.

[47] F. Barra and P. Gaspard. Transport and dynamics on open quantum graphs. *Phys. Rev. E (3)*, 65(1, part 2):016205, 21, 2002.

Sebastian Endres, Frank Steiner: Institut für Theoretische Physik, Universität Ulm, Albert-Einstein-Allee 11, 89081 Ulm, Germany

E-mail address: `sebastian.endres@uni-ulm.de`

E-mail address: `frank.steiner@uni-ulm.de`