

The Berry–Keating operator on $L^2(\mathbb{R}_+, dx)$ and on compact quantum graphs with general self-adjoint realizations

This article has been downloaded from IOPscience. Please scroll down to see the full text article.

2010 J. Phys. A: Math. Theor. 43 095204

(<http://iopscience.iop.org/1751-8121/43/9/095204>)

View [the table of contents for this issue](#), or go to the [journal homepage](#) for more

Download details:

IP Address: 171.66.16.158

The article was downloaded on 03/06/2010 at 08:58

Please note that [terms and conditions apply](#).

The Berry–Keating operator on $L^2(\mathbb{R}_>, dx)$ and on compact quantum graphs with general self-adjoint realizations

Sebastian Endres and Frank Steiner

Institut für Theoretische Physik, Universität Ulm Albert-Einstein-Allee 11, 89081 Ulm, Germany

E-mail: sebastian.endres@uni-ulm.de and frank.steiner@uni-ulm.de

Received 27 July 2009, in final form 22 December 2009

Published 15 February 2010

Online at stacks.iop.org/JPhysA/43/095204

Abstract

The Berry–Keating operator $H_{\text{BK}} := -i\hbar(x \frac{d}{dx} + \frac{1}{2})$ (Berry and Keating 1999 *SIAM Rev.* **41** 236) governing the Schrödinger dynamics is discussed in the Hilbert space $L^2(\mathbb{R}_>, dx)$ and on compact quantum graphs. It has been proved that the spectrum of H_{BK} defined on $L^2(\mathbb{R}_>, dx)$ is purely continuous and thus this quantization of H_{BK} cannot yield the hypothetical Hilbert–Polya operator possessing as eigenvalues the nontrivial zeros of the Riemann zeta function. 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 $H_{\text{BK}}^2 := -x^2 \frac{d^2}{dx^2} - 2x \frac{d}{dx} - \frac{1}{4}$ which is a special case of the Black–Scholes operator used in financial theory of option pricing. 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. While the spectra of both H_{BK} and H_{BK}^2 on any compact quantum graph are discrete, their Weyl asymptotics demonstrate that neither H_{BK} nor H_{BK}^2 can yield as eigenvalues the nontrivial Riemann zeros. Some simple examples are worked out in detail.

PACS numbers: 03.65.Ca, 03.65.Db

1. Introduction: the hypothetical Hilbert–Polya operator

There is an old idea usually attributed to Hilbert¹ and Polya² that the nontrivial (i.e. complex) zeros s_n of the Riemann zeta function $\zeta(s)$ have a spectral interpretation. Writing $s_n := \frac{1}{2} - i\tau_n$, the Riemann hypothesis states that the nonimaginary solutions τ_n of $\zeta(\frac{1}{2} - i\tau_n) = 0$ 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 $\tau_n = i(s_n - \frac{1}{2})$.

Around 1950, Selberg [3] 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 noted 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 [2]. 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 [4, 5] 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 [6] 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 [7], 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 [8] 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 [9] (see also [10]) 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 [11, 12] speculated that the conjectured Hilbert–Polya operator might be some quantization of the extraordinarily simple classical Hamiltonian function $H_{\text{cl}}(x, p)$ of a single coordinate x and its conjugate momentum p :

$$H_{\text{cl}}(x, p) := xp. \quad (1)$$

¹ In the comment (included in his collected papers [1]) to his paper on the explicit formulae of number theory [2], A Weil writes that E 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 See Odlyzko’s correspondence with Polya: <http://www.dtc.umn.edu/odlyzko/polya/index.html>

Inspired by [13, 14], Berry and Keating [11] suggested to investigate quantum graph models of (1), in particular the spectrum of these operators. One of the first researchers who dealt with differential operators on graphs was Roth [15] who derived a trace formula for the heat kernel of the Laplacian with Kirchhoff boundary conditions. von Below [16] considered the heat equation on graphs and derived a characteristic equation for the eigenvalues of the weighted Laplacian on graphs. Some physical quantum graph models were considered by Exner and Šeba [17] who discussed e.g. the scattering problem for a free quantum particle on a star graph. A method to approximate mesoscopic systems like thin branching systems by quantum graphs was discussed by Exner and Post [18] and Post [19]. Carlson [20] used semigroups on graphs to simulate the blood flow in the human arterial system. Kottos and Smilansky [13, 14] introduced quantum graphs as a model for quantum chaos.

In this paper, we study the quantization of the classical Berry–Keating Hamiltonian (1) in the Hilbert space $L^2(\mathbb{R}_>, dx)$ and on compact quantum graphs and give a complete classification of the self-adjoint realizations of the corresponding Berry–Keating operator. In addition, we also study the quantization of the corresponding ‘squared’ operator. It turns out that no self-adjoint realization of (1) exists which yields as eigenvalues the Riemann zeros.

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) 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

$$\dot{x}(t) = \frac{\partial H_{\text{cl}}}{\partial p} = x(t) \quad \text{and} \quad \dot{p}(t) = -\frac{\partial H_{\text{cl}}}{\partial x} = -p(t). \quad (2)$$

Starting at time $t = 0$ at an arbitrary point $(x_0, p_0) \in \mathcal{P}$ in phase space, the unique solutions are [11]

$$x(t) = x_0 e^t \quad \text{and} \quad p(t) = p_0 e^{-t}. \quad (3)$$

Obviously, the point $(0, 0) \in \mathcal{P}$ is an unstable point. We note that the Hamiltonian (1) is time independent corresponding to the conserved ‘energy’ $E := H_{\text{cl}}(x(t), p(t)) = x_0 p_0 \in \mathbb{R}$, 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 [11, 12] 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) by a self-adjoint operator H in \mathcal{H} . With the standard choice $\mathcal{H} := L^2(\mathbb{R}, dx)$, the simplest operator corresponding to (1) is obtained by Weyl ordering of the coordinate operator x (acting by multiplication) and the momentum operator $p = -i\hbar \frac{d}{dx}$ (acting by differentiation) leading to the Berry–Keating operator [11, 12]

$$H_{\text{BK}} := \frac{1}{2}(xp + px) = -i\hbar \left(x \frac{d}{dx} + \frac{1}{2} \right), \quad (4)$$

and the Schrödinger equation

$$i\hbar \frac{\partial \Psi(x, t)}{\partial t} = H_{\text{BK}} \Psi(x, t). \quad (5)$$

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

$$H_{\text{BK}}\psi(x) = \lambda\psi(x). \tag{6}$$

Writing $\lambda = \hbar k$, $k \in \mathbb{R}$, Planck's constant drops out from (6), and the eigenvalue problem reads ($s := -\frac{1}{2} + ik$)

$$x \frac{d\phi_s(x)}{dx} = s\phi_s(x). \tag{7}$$

For $x \in \mathbb{R}$, (7) possesses the general solution

$$\phi_s(x) = c_1 x_+^s + c_2 x_-^s, \tag{8}$$

where x_\pm^s denote the generalized functions (see e.g. [21, p 87])

$$x_+^s := \begin{cases} 0 & \text{for } x \leq 0 \\ x^s & \text{for } x > 0 \end{cases} \quad \text{and} \quad x_-^s := \begin{cases} |x|^s & \text{for } x < 0 \\ 0 & \text{for } x \geq 0, \end{cases} \tag{9}$$

which is well defined for $\text{Re } s > -1$. In [11], 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 ($c_1 = c_2 = c$) $\phi_s^{\text{even}}(x) = c|x|^s$.

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. [22] (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 (6) is then given by

$$\psi_k(x) := \frac{1}{\sqrt{2\pi}} x_+^{-\frac{1}{2}+ik} \quad \text{with } k \in \mathbb{R}, \tag{10}$$

which is obviously not in $L^2(\mathbb{R}_>, dx)$ and satisfies the orthonormality relation (in a distributional sense)

$$\langle \psi_k | \psi_{k'} \rangle := \int_0^\infty \overline{\psi_k(x)} \psi_{k'}(x) dx = \delta(k - k') \tag{11}$$

and the completeness relation

$$\int_{-\infty}^\infty \psi_k(x) \overline{\psi_k(x')} dk = \delta(x - x'). \tag{12}$$

Thus, we have for any $\phi \in L^2(\mathbb{R}_>, dx)$ the spectral decomposition

$$\phi(x) = \int_{-\infty}^\infty A(k) \psi_k(x) dk \tag{13}$$

with

$$A(k) := \langle \psi_k | \phi \rangle = \int_0^\infty \overline{\psi_k(x)} \phi(x) dx \tag{14}$$

and (assuming $\langle \phi | \phi \rangle = 1$)

$$\int_{-\infty}^\infty |A(k)|^2 dk = 1. \tag{15}$$

Forming a general wave packet with a given amplitude $A(k)$ satisfying (13) and (15), one obtains ($x \in \mathbb{R}_>$)

$$\phi(x) = \sqrt{\frac{2\pi}{x}} \hat{A}(\ln x), \tag{16}$$

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

$$\hat{A}(y) := \frac{1}{2\pi} \int_{-\infty}^{\infty} A(k) e^{iky} dk. \tag{17}$$

Let us also mention an alternative to the spectral decomposition (13) for the Berry–Keating operator. Defining the Mellin transform $\check{\phi}$ of ϕ by

$$\check{\phi}(s) := \int_0^{\infty} x^{s-1} \phi(x) dx, \tag{18}$$

we obtain for the wave number amplitude $A(k)$ (see (14))

$$A(k) = \frac{1}{\sqrt{2\pi}} \check{\phi}\left(\frac{1}{2} - ik\right), \tag{19}$$

from which $\phi(x)$ can be recovered by the inverse Mellin transform (convergent at least in mean square, see e.g. [23, p 94])

$$\begin{aligned} \phi(x) &= \frac{1}{2\pi i} \int_{\frac{1}{2}-i\infty}^{\frac{1}{2}+i\infty} \check{\phi}(s) x^{-s} ds = \frac{1}{2\pi} \int_{-\infty}^{\infty} \check{\phi}\left(\frac{1}{2} - ik\right) x^{-\frac{1}{2}+ik} dk \\ &= \int_{-\infty}^{\infty} A(k) \psi_k(x) dk \end{aligned} \tag{20}$$

in agreement with (13).

The unitary group

$$U(t) := \exp\left(-\frac{it}{\hbar} H_{\text{BK}}\right) = e^{-\frac{t}{2}} e^{-tD} \tag{21}$$

generated by the Berry–Keating operator (4) acts on functions $\phi \in \mathcal{H}$ as (see e.g. [24, p 365])

$$(U(t)\phi)(x) = e^{-\frac{t}{2}} \phi(e^{-t}x). \tag{22}$$

Here we have used the relation $H_{\text{BK}} = -i\hbar(D + \frac{1}{2})$, where $D := x\frac{d}{dx}$ is the generator of scaling transformations (dilations). Let us mention that the operator D has been discussed by Arendt [25–27], where $A_p := -D$ is considered as the generator of a semigroup on e.g. $L^p(\mathbb{R}_>, dx)$ ($1 \leq p < \infty$) 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 (6)

$$(U(t)\psi)(x) = e^{-i\frac{\lambda}{\hbar}t} \psi(x), \tag{23}$$

which in turn leads with (22), $\lambda = \hbar k$, $s = -\frac{1}{2} + ik$ and $\kappa := e^{-t} > 0$ ($t < \infty$) to

$$\psi(\kappa x) = \kappa^s \psi(x). \tag{24}$$

This shows that an eigenfunction ψ of H_{BK} must be a homogeneous function with (complex) degree $s = -\frac{1}{2} + ik$. Differentiation of (24) with respect to κ and then setting $\kappa = 1$ leads back to the eigenvalue problem (7) which possesses for $x \in \mathbb{R}_>$ the unique solution (10)

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

$$K_{\text{BK}}(x, x_0; t) = e^{-\frac{t}{2}} \delta(x_0 - x e^{-t}) \Theta(t). \tag{25}$$

We observe that the quantum mechanical time evolution follows in the configuration space exactly the classical trajectory (3). Starting at time $t = 0$ with the initial wavefunction $\phi \in L^2(\mathbb{R}_>, dx)$, one obtains with (25) the wavefunction $\psi(x, t)$ at a later time $t > 0$:

$$\begin{aligned} \psi(x, t) &= \int_0^{\infty} K_{\text{BK}}(x, x_0; t) \phi(x_0) dx_0 \\ &= e^{-\frac{t}{2}} \phi(e^{-t}x) \end{aligned} \tag{26}$$

in complete agreement with (22). 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. [28, p 26],

$$\begin{aligned} G_{\text{BK}}(x, x_0; \lambda) &:= \frac{i}{\hbar} \int_0^\infty e^{\frac{i}{\hbar}(\lambda+i\epsilon)t} K_{\text{BK}}(x, x_0; t) dt \\ &= \int_{-\infty}^\infty \frac{\psi_{k'}(x) \overline{\psi_{k'}(x_0)}}{\hbar k' - \lambda - i\epsilon} dk' \\ &= \frac{2\pi i}{\hbar} \psi_k(x) \overline{\psi_k(x_0)} \Theta(x - x_0), \end{aligned} \tag{27}$$

which satisfies the inhomogeneous time-independent Schrödinger equation (see (6))

$$(H_{\text{BK},x} - \hbar k)G_{\text{BK}}(x, x_0; \hbar k) = \delta(x - x_0). \tag{28}$$

Since the operator (4) acting in the Hilbert space $L^2(\mathbb{R}, dx)$ respectively $L^2(\mathbb{R}_+, dx)$ 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) 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 [11]. It is the purpose of our paper to discuss the self-adjoint realizations on compact quantum graphs and in a forthcoming paper [29] we study a noncompact quantum graph.

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 [11] (see also Connes [9, 10]) 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 $H_{\text{cl}}(x, p)$ in one dimension given by (see e.g. [30])

$$N(E) = \frac{1}{2\pi\hbar} \text{area}(E)(1 + O(\hbar)), \tag{29}$$

where

$$\text{area}(E) := \int_{\mathcal{P}} dx dp \Theta(E - H_{\text{cl}}(x, p)) \tag{30}$$

is the phase-space area under the contour $H_{\text{cl}}(x, p) = E$. Obviously, there is a problem if this formula is applied to the Hamiltonian (1), since the classical motion is not bounded, so that $\text{area}(E)$ is infinite. Therefore, Berry and Keating [11] proposed to regularize the system by a suitable truncation of phase space in such a way that $\text{area}(E)$ becomes finite.

The regularization proposed by Berry and Keating [11] is to truncate x and p by considering the ‘regularized phase space’ $\mathcal{P}_{\text{reg}} := (l_x, \infty) \times (l_p, \infty)$ together with the semiclassical condition $l_x l_p = 2\pi\hbar$. This truncation cuts off not only the ‘small’ coordinate $x \leq l_x$ respectively momentum values $p \leq l_p$, but it leads to a given ‘energy’ $E > 0$ also to a cutoff at the ‘large’ values $x = \frac{E}{l_p}$ respectively $p = \frac{E}{l_x}$ since $E = H_{\text{cl}}(x, p)$ holds. Without specifying the behaviour of the classical motion at the end points of the trajectories, we follow Berry and Keating and obtain from (29) and (30):

$$\begin{aligned} N(E) &= \frac{1}{2\pi\hbar} \left(\int_{l_x}^{\frac{E}{l_p}} \frac{E}{x} dx - l_p \left(\frac{E}{l_p} - l_x \right) \right) (1 + O(\hbar)) \\ &= \frac{1}{2\pi\hbar} E \left(\ln \left(\frac{E}{2\pi\hbar} \right) - 1 \right) + 1 + \dots \end{aligned} \tag{31}$$

Setting $\hbar = 1$ together with a modification of $N(E)$ by adding $-\frac{1}{8}$ to the right-hand side of (31) which was suggested by Berry and Keating [11, 12] 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 (Riemann–von Mangoldt formula):

$$N(E) = \frac{E}{2\pi} \ln\left(\frac{E}{2\pi}\right) - \frac{E}{2\pi} + \frac{7}{8} + O(\ln E). \tag{32}$$

Following the argumentation of Berry and Keating [11, 12] for the modification of $N(E)$, we get for the corresponding Maslov index $\mu = -\frac{1}{2}$. This seems at first somewhat strange since there is no magnetic flux or spinning particle given and, therefore, the Maslov index should be an integer number as in the case of ‘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 $(\frac{E}{l_p}, l_p)$ to the point $(l_x, \frac{E}{l_x})$ 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

$$\tilde{H}_{cl}(x, p) := x^2 p^2, \tag{33}$$

which is the square of the Berry–Keating Hamiltonian (1). Note that (33) can be derived from the Lagrangian

$$L(x, \dot{x}) = \frac{1}{4} \left(\frac{\dot{x}}{x}\right)^2 \tag{34}$$

and that Hamilton’s equations do not decouple in this case as in (2). In fact, one obtains

$$\dot{x}(t) = \frac{\partial \tilde{H}_{cl}}{\partial p} = 2x^2 p(t) \quad \text{and} \quad \dot{p}(t) = -\frac{\partial \tilde{H}_{cl}}{\partial x} = -2xp^2(t), \tag{35}$$

and the solutions are

$$x(t) = x_0 e^{2x_0 p_0 t} \quad \text{and} \quad p(t) = p_0 e^{-2x_0 p_0 t}. \tag{36}$$

If one broadens the phase space to

$$\mathcal{P}_{reg,b} := (l_x, \infty) \times ((l_p, \infty) \cup (-l_p, -\infty)), \tag{37}$$

one now has the possibility of scattering from the end point $(\frac{E}{l_p}, l_p)$ of a trajectory of the form (36) to the end point $(\frac{E}{l_p}, -l_p)$. This corresponds to a reflection on a wall similar to that 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 \tilde{H}_{cl} and H_{BK}^2 respectively as an energy (operator). Further hints to this choice will follow in what follows.

Before investigating the ‘squared’ Berry–Keating operator 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 $\tilde{H} := H_{\text{BK}}^2$ gives (setting from now on $\hbar = 1$)

$$H_{\text{BK}}^2 := \left(-i \left(x \frac{d}{dx} + \frac{1}{2} \right) \right)^2 = -x^2 \frac{d^2}{dx^2} - 2x \frac{d}{dx} - \frac{1}{4}. \quad (38)$$

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 (38) is a special case of the famous Black–Scholes operator [31, 32] introduced to determine the pricing of options in financial theory whose interesting mathematical properties have been discussed e.g. in [25–27].

It is easy to see that the functions $\psi_k(x)$ ($k \in \mathbb{R} \setminus \{0\}$) defined in (10) 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 generalized eigenfunctions:

$$\psi_{0,1}(x) = \frac{1}{\sqrt{2\pi}} x_+^{-\frac{1}{2}} \quad \text{and} \quad \psi_{0,2}(x) = \frac{1}{\sqrt{2\pi}} x_+^{-\frac{1}{2}} \ln x. \quad (39)$$

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

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

$$\tilde{U}(t) := e^{-itH_{\text{BK}}^2} \quad (40)$$

by

$$\psi(x, t) := (\tilde{U}(t)\phi)(x) =: \int_{\mathbb{R}_>} \tilde{K}(x, x_0; t) \phi(x_0) dx_0, \quad (41)$$

where $\phi(x) \in L^2(\mathbb{R}_>, dx)$ is the initial wavefunction at $t = 0$, we obtain (cf [28, p 27])

$$\begin{aligned} \tilde{K}(x, x_0; t) &= \int_{-\infty}^{\infty} \psi_k(x) \bar{\psi}_k(x_0) e^{-ik^2 t} \Theta(t) dk \\ &= (4\pi it x x_0)^{-\frac{1}{2}} e^{i \frac{(\ln x - \ln x_0)^2}{4t}} \Theta(t). \end{aligned} \quad (42)$$

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

$$\left(i \frac{\partial}{\partial t} - H_{\text{BK},x}^2 \right) \tilde{K}(x, x_0; t) = i\delta(x - x_0)\delta(t), \quad (43)$$

i.e. it is the retarded Green’s function. With (41), the action of $\tilde{U}(t)$ on $\phi \in L^2(\mathbb{R}_>, dx)$ is given by ($t > 0$)

$$(\tilde{U}(t)\phi)(x) = (4\pi it)^{-\frac{1}{2}} \int_{-\infty}^{\infty} e^{i \frac{\tau^2}{4t}} e^{-\frac{\tau}{2}} \phi(e^{-\tau} x) d\tau, \quad (44)$$

which expresses the fact that $\tilde{U}(t)$ is a combination of the scaling transformation generated by the operator $D = x \frac{d}{dx}$ (see equation (22)) and the transformation generated by the operator $T := x^2 \frac{d^2}{dx^2}$, since $\tilde{U}(t) = e^{i \frac{t}{4}} e^{iT} e^{2itD}$. Note that the transformation generated by T reads

$$(e^{iT}\phi)(x) = \frac{e^{-i \frac{t}{4}}}{(4\pi it)^{\frac{1}{2}}} \int_{-\infty}^{\infty} e^{i \frac{\tau^2}{4t} + \frac{\tau}{2}} \phi(e^{-\tau} x) d\tau, \quad (45)$$

and that the operators D and T commute. The resolvent kernel (outgoing Green’s function) of H_{BK}^2 is given by (see [28, p 26])

$$\begin{aligned} \tilde{G}(x, x_0; \lambda) &:= i \int_0^{\infty} e^{i(\lambda+i\epsilon)t} \tilde{K}(x, x_0; t) dt \\ &= (4x x_0 (-\lambda - i\epsilon))^{-\frac{1}{2}} e^{-(\lambda-i\epsilon)^{\frac{1}{2}} |\ln x - \ln x_0|}, \end{aligned} \quad (46)$$

which shows that \tilde{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 ($x, x_0 \in \mathbb{R}_{>}$)

$$\begin{aligned} \tilde{G}(x, x_0; k^2) &= \frac{i}{2k\sqrt{xx_0}} e^{ik|\ln x - \ln x_0|} \\ &= \frac{i\pi}{k} \begin{cases} \psi_k(x)\bar{\psi}_k(x_0) & \text{for } x \geq x_0 \\ \bar{\psi}_k(x)\psi_k(x_0) & \text{for } x < x_0 \end{cases} \end{aligned} \quad (47)$$

in agreement with the general form of Green's function of a Sturm–Liouville operator (see e.g. [33, p 112]).

5. Semiclassical estimate for the eigenvalue counting function of the ‘squared’ Berry–Keating operator

Using again the semiclassical formula (29) and the truncation of phase space as discussed in section 3, we obtain for the counting function in the quadratic case

$$\begin{aligned} N(E) &= \frac{1}{2\pi\hbar} 2 \left(\int_{l_x}^{\frac{\sqrt{E}}{l_p}} \frac{\sqrt{E}}{x} dx - l_p \left(\frac{\sqrt{E}}{l_p} - l_x \right) \right) (1 + O(\hbar)) \\ &= 2 \left[\frac{k}{2\pi} \ln \left(\frac{k}{2\pi} \right) - \frac{k}{2\pi} + \frac{7}{8} \right] + \dots, \end{aligned} \quad (48)$$

where we have included the same Maslov index correction as in section 3. 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 $\pm k$. Note that in this case the Riemann zeros are not interpreted as ‘energies’ but rather as ‘momenta’ $\hbar k$ respectively ‘wave numbers’ k . Formula (48) agrees with the well-known universal law that $N(E)$, for a bounded system in d dimensions, grows asymptotically as $N(E) = O(E^{\frac{d}{2}})$, and thus for a one-dimensional system one expects $N(E) = O(\sqrt{E}) = O(k)$, eventually modified by a factor $\ln(\sqrt{E})$.

6. Compact graphs

We shall present a short overview on compact graphs using the notations of [34, 35].

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 $v = \tilde{v}$ 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 final 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 end point. We need the notion of a path and of a periodic orbit of the graph. We slightly differ from the definition in [35] for further convenience. A path $p(w, z) := ((e_i)_{i=1}^n, w, z)$ is a set of a finite sequence of edges $(e_i)_{i=1}^n$ where the points $w, z \in \mathbf{I}$ denote the starting and final points of the path. Furthermore, it is required that

- the edges e_i and e_{i+1} are adjacent,

- the point w must be an element of I_1 and z must be an element of I_n .

The case $w = z$ is admissible and corresponds to a closed path. In [35] or [14] 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 [35]; 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 [35]. 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 $l_p(w, z)$ of the path $p(w, z) := ((e_i)_{i=1}^n, w, z)$ as follows. If $n \geq 2$, we denote by y_1 and y_n the end points 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 $l_p(w, z)$ is defined as

$$l_p(w, z) := \left| \ln \left(\frac{y_1}{w} \right) \right| + \sum_{i=2}^{n-1} \ln \left(\frac{b_i}{a_i} \right) + \left| \ln \left(\frac{y_n}{z} \right) \right|. \tag{49}$$

Similarly, if $n = 2$ ($y_1 = y_n := y$) respectively $n = 1$, we define

$$l_p(w, z) := \left| \ln \left(\frac{y}{w} \right) \right| + \left| \ln \left(\frac{y}{z} \right) \right| \quad \text{respectively} \quad l_p(w, z) := \left| \ln \left(\frac{w}{z} \right) \right|. \tag{50}$$

Furthermore, we define in a natural way the length l_γ of a periodic orbit γ :

$$l_\gamma := \ln \left(\prod_{i=1}^n \frac{b_i}{a_i} \right). \tag{51}$$

In order to define a metric structure of the graph, we need the notion of connectedness. We define w and z as connected iff there exists a path $p(w, z) := ((e_i)_{i=1}^n, w, z)$. 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

$$d_{w,z} := \min\{l_p; p \text{ connects } w \text{ and } z\}. \tag{52}$$

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 $(\det g)(x) = \frac{1}{x^2}$. The reason for our choice of the metric will be explained in sections 7 and 13.

We also need for the interpretation of the trace formula for the Berry–Keating operator H_{BK} in theorem 15.2 the notion of a directed graph in order to interpret the right-hand side of (136) as a sum of periodic orbits. Therefore, we replace the edges by directed edges. This does not affect the lengths of the edges but has of course an influence on the topological properties of the graph such as connectedness and on the set \mathfrak{P} of periodic orbits. Since in this case there are only such paths $p(w, z) := ((e_i)_{i=1}^n, w, z)$ allowed for which for all consecutive edges e_i, e_{i+1} , there exist vertices v_{ij} such that the direction of e_i is towards v_{ij} and e_{i+1} has the direction away from v_{ij} . Then, the definitions for the periodic orbits and for connectedness for directed graphs are the same as for undirected graphs. Again, not necessarily but for convenience we always assume that the directed graph (in the case for the Berry–Keating operator H_{BK}) is connected.

7. The Berry–Keating operator on compact quantum graphs

We define, in accordance with [35],

$$C_0^\infty(\Gamma) := \bigoplus_{i=1}^E C_0^\infty[a_i, b_i] \quad \text{and} \tag{53}$$

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

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:

$$\psi \in L^2(\Gamma) \quad \text{iff} \quad \psi = \bigoplus_{i=1}^E \psi_i \quad \text{with } \psi_i \in L^2(I_i, dx). \tag{54}$$

The first function space in (53) will be a possible operator core for the closed Berry–Keating operator with (57) 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

$$\langle \psi, \phi \rangle := \sum_{j=1}^E \int_{a_j}^{b_j} \overline{\psi_j(x_j)} \phi_j(x_j) dx_j. \tag{55}$$

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

$$H_{\text{BK}}\psi := \left(-i \left(x \frac{d}{dx} + \frac{1}{2} \right) \psi_1, \dots, -i \left(x \frac{d}{dx} + \frac{1}{2} \right) \psi_E \right), \tag{56}$$

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. [36, p 183], we conclude that H_{BK} is closable since the standard momentum operator $p = -i \frac{d}{dx}$ is closable. Furthermore, we note that multiplication by the argument is also a (bounded) bijection from

$$D_0^1(\Gamma) := \bigoplus_{i=1}^E H_0^1[a_i, b_i] \tag{57}$$

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 end points of the intervals and with square integrable weak derivatives. 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 (57). Furthermore, by similar arguments the adjoint operator of $(H_{\text{BK}}, D_0^1(\Gamma))$ is given by $(H_{\text{BK}}, H^1(\Gamma))$ in which

$$H^1(\Gamma) := \bigoplus_{i=1}^E H^1[a_i, b_i] \tag{58}$$

is the set of absolutely continuous functions on the intervals of the graph Γ , cf [36, p 100] possessing square integrable weak derivatives.

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. [37]. The operator $(H_{\text{BK}}, D_0^1(\Gamma))$ is symmetric and it is possible to show that the deficiency indices are (E, E) , compare e.g. [22, 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 a compact resolvent, see also [38]. Thus, by the compact resolvent theorem, cf [39, p 245], and the relatively compact perturbation theorem (cf [39, p 113]) the operator (56) 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 [22, p 138] and [34], see also [40] for a comprehensive discussion. Therefore, we define the complex symplectic form on $H^1(\Gamma) \times H^1(\Gamma)$ (cf [22, p 138]):

$$[\phi, \psi]_1 := \langle \phi, H_{\text{BK}}^+ \psi \rangle_{L^2(\Gamma)} - \langle H_{\text{BK}}^+ \phi, \psi \rangle_{L^2(\Gamma)} \quad \text{for } \phi, \psi \in H^1(\Gamma). \tag{59}$$

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. [22]) the self-adjoint extensions are exactly the maximal $[\cdot, \cdot]_1$ -symmetric subspaces of $H^1(\Gamma)$. We follow the approach by Kostyrykin and Schrader [34] to classify these extensions. By a proper Sobolev embedding theorem we can define the boundary value bv (an element of \mathbb{C}^{2E}) of $\psi \in H^1(\Gamma)$:

$$\Psi_{\text{bv}} := (\psi_1(a_1), \dots, \psi_E(a_E), \psi_1(b_1), \dots, \psi_E(b_E))^T \quad \text{for } \psi \in H^1(\Gamma). \tag{60}$$

For convenience, we also define

$$I_{\pm} := \begin{pmatrix} \mathbb{1}_{E \times E} & 0 \\ 0 & -\mathbb{1}_{E \times E} \end{pmatrix}, \quad D_{(ab)} := \begin{pmatrix} \mathbf{a} & 0 \\ 0 & \mathbf{b} \end{pmatrix}, \tag{61}$$

with (no summation over i)

$$\mathbf{a}_{ij} := \delta_{ij} a_i \quad \text{and} \quad \mathbf{b}_{ij} := \delta_{ij} b_i \quad \text{for } 0 \leq i, j \leq E \tag{62}$$

and

$$J := \begin{pmatrix} 0 & \mathbb{1}_{E \times E} \\ -\mathbb{1}_{E \times E} & 0 \end{pmatrix}, \quad U := \frac{1}{\sqrt{2}} \begin{pmatrix} i\mathbb{1}_{E \times E} & \mathbb{1}_{E \times E} \\ -\mathbb{1}_{E \times E} & -i\mathbb{1}_{E \times E} \end{pmatrix}. \tag{63}$$

By a simple calculation we obtain the identity

$$U(iI_{\pm})U^+ = J. \tag{64}$$

Thus, we obtain for (59) by an integration by parts using the unitarity of U :

$$\begin{aligned} [\psi, \phi]_1 &= \langle \Phi_{\text{bv}}, iI_{\pm} D_{(ab)} \Psi_{\text{bv}} \rangle_{\mathbb{C}^{2E}} \\ &= \langle D_{(ab)}^{\frac{1}{2}} \Phi_{\text{bv}}, iI_{\pm} D_{(ab)}^{\frac{1}{2}} \Psi_{\text{bv}} \rangle_{\mathbb{C}^{2E}} \\ &= \langle U D_{(ab)}^{\frac{1}{2}} \Phi_{\text{bv}}, J U D_{(ab)}^{\frac{1}{2}} \Psi_{\text{bv}} \rangle_{\mathbb{C}^{2E}} \quad \text{for all } \psi, \phi \in H^1(\Gamma). \end{aligned} \tag{65}$$

To define the square root of $D_{(ab)}$ we have used the usual definition of a positive operator ([37, p 196]), which in this case simply means to take the square root of the (diagonal) entries in $D_{(ab)}$. Note that

$$\omega(\cdot, \cdot) := \langle \cdot, J \cdot \rangle_{\mathbb{C}^{2E}} \tag{66}$$

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

- $a, b \in \mathcal{L}$ then $\omega(a, b) = 0$.
 - Whenever for a subspace $\tilde{\mathcal{L}} \supset \mathcal{L}$ the first property holds, it follows $\tilde{\mathcal{L}} = \mathcal{L}$.
- (67)

For the Lagrangian subspaces of \mathbb{C}^{2E} we apply the result of [34]. A subspace \mathcal{L} is Lagrangian iff there exist two matrices $A, B \in \text{Mat}(E \times E, \mathbb{C})$ with

$$\begin{aligned} AB^+ &= BA^+ \quad \text{and} \\ \text{rank}(A, B) &= E. \end{aligned} \tag{68}$$

We then have

$$\mathcal{L} = \left\{ \phi \in \mathbb{C}^{2E}; \phi := \begin{pmatrix} \phi_1 \\ \phi_2 \end{pmatrix} \text{ and } A\phi_1 + B\phi_2 = 0 \right\}. \tag{69}$$

In (68) the matrix (A, B) is formed by the columns of A and B , and we have introduced two maps

$$(\cdot)_i : \mathbb{C}^{2E} \rightarrow \mathbb{C}^E \quad \text{for } 1 \leq i \leq 2 \tag{70}$$

by

$$\phi_i := \begin{cases} (\mathbb{1}, 0)\phi & \text{if } i = 1, \\ (0, \mathbb{1})\phi & \text{if } i = 2. \end{cases} \tag{71}$$

Furthermore, as mentioned in [41], these matrices are not uniquely defined. Two sets of matrices A, B and \tilde{A}, \tilde{B} define the same Lagrangian subspace iff there exists an invertible matrix C with

$$A = C\tilde{A} \quad \text{and} \quad B = C\tilde{B}. \tag{72}$$

Since $UD_{(ab)}^{\frac{1}{2}}$ is a bijection from \mathbb{C}^{2E} onto itself and by (59) and (65) we infer, with the same arguments as in [34], that there is a one-to-one correspondence between the self-adjoint extensions of $(H_{BK}, D_0^1(\Gamma))$ and the Lagrangian subspaces of \mathbb{C}^{2E} . We thus have proved the following proposition.

Proposition 8.1. *Each domain of definition of such a self-adjoint extension is exactly the preimage with respect to (60) of a subspace*

$$\mathcal{L} = \{ \Psi_{bv} \in \mathbb{C}^{2E}; A(UD_{(ab)}^{\frac{1}{2}}\Psi_{bv})_1 + B(UD_{(ab)}^{\frac{1}{2}}\Psi_{bv})_2 = 0 \}, \tag{73}$$

where A and B fulfil (68). The converse is also true.

Because of proposition 8.1, we denote in the following the self-adjoint extensions of $(H_{BK}, D_0^1(\Gamma))$ by $(H_{BK}; A, B)$.

9. Determination of the eigenvalues of H_{BK}

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

$$\psi_k(x) = \left(\alpha_1 \frac{1}{\sqrt{x}} e^{ik \ln x}, \dots, \alpha_E \frac{1}{\sqrt{x}} e^{ik \ln x} \right). \tag{74}$$

We denote the column vector (60) corresponding to ψ_k by $\Psi_{bv,k}$. In order to apply (73) for determining the eigenvalues k and the corresponding eigenvectors ψ_k , we calculate $UD_{(ab)}^{\frac{1}{2}}\Psi_{bv,k}$ using (63):

$$\begin{aligned} UD_{(ab)}^{\frac{1}{2}}\Psi_{bv,k} &= U \begin{pmatrix} e^{ik \ln a} & 0 \\ 0 & e^{ik \ln b} \end{pmatrix} \alpha \\ &= \frac{1}{\sqrt{2}} \begin{pmatrix} i e^{ik \ln a} & e^{ik \ln b} \\ -e^{ik \ln a} & -i e^{ik \ln b} \end{pmatrix} \alpha \\ &= \frac{1}{\sqrt{2}} \begin{pmatrix} i e^{ik \ln a} + e^{ik \ln b} & 0 \\ 0 & -e^{ik \ln a} - i e^{ik \ln b} \end{pmatrix} \alpha. \end{aligned} \tag{75}$$

For convenience, we have used the notations

$$\begin{aligned} (e^{ik \ln a})_{mn} &:= \delta_{mn} e^{ik \ln a_m}, \\ (e^{ik \ln b})_{mn} &:= \delta_{mn} e^{ik \ln b_m} \quad \text{for } 1 \leq m, n \leq E \end{aligned} \tag{76}$$

and

$$\alpha := (\alpha_1, \dots, \alpha_E, \alpha_1, \dots, \alpha_E)^T. \tag{77}$$

Therefore, we get

$$\begin{aligned} \sqrt{2}(UD_{(ab)}^{\frac{1}{2}}\Psi_{bv,k})_1 &= (ie^{ik \ln a} + e^{ik \ln b})\alpha_1 \\ \sqrt{2}(UD_{(ab)}^{\frac{1}{2}}\Psi_{bv,k})_2 &= -(e^{ik \ln a} + ie^{ik \ln b})\alpha_2, \end{aligned} \tag{78}$$

where we have used $(\cdot)_i$ defined in (71).

Taking into account that $\alpha_1 = \alpha_2 =: \tilde{\alpha}$, we obtain for the expression in (73)

$$\begin{aligned} \sqrt{2}[A(UD_{(ab)}^{\frac{1}{2}}\Psi_{bv,k})_1 + B(UD_{(ab)}^{\frac{1}{2}}\Psi_{bv,k})_2] \\ = (A(ie^{ik \ln a} + e^{ik \ln b}) - B(e^{ik \ln a} + ie^{ik \ln b}))\tilde{\alpha} \\ = (i(A + iB)e^{ik \ln a} + (A - iB)e^{ik \ln b})\tilde{\alpha}. \end{aligned} \tag{79}$$

Kostykin and Schrader have shown, see [34], that $A \pm iB$ are invertible under the assumption (68). With the notation

$$C(k) := e^{ik \ln a} \tilde{\alpha} \tag{80}$$

and, because $(A - iB)$ and $(A + iB)^{-1}$ commute (see [42]), we get

$$\begin{aligned} A(UD_{(ab)}^{\frac{1}{2}}\Psi_{bv,k})_1 + B(UD_{(ab)}^{\frac{1}{2}}\Psi_{bv,k})_2 &= 0 \\ \Leftrightarrow (\mathbb{1} - i\frac{A - iB}{A + iB}e^{ik \ln \frac{b}{a}})C(k) &= 0, \end{aligned} \tag{81}$$

with $e^{ik \ln \frac{b}{a}}$ similarly defined as in (76). Due to the similarity of (81) with the secular equation for the common Laplace operator on compact graphs (see [41]), we denote

$$S(A, B) := i\frac{A - iB}{A + iB} \quad \text{and} \quad T(a, b; k) := e^{ik \ln \frac{b}{a}}. \tag{82}$$

It follows with exactly the same arguments as in [34] that $S(A, B)$ is unitary, and we shall call it also the S -matrix of the quantum graph. The unitarity of $T(a, b; k)$ is obvious iff $k \in \mathbb{R}$. Since, for all $k \in \mathbb{C}$, $C(k) = 0$ iff $\tilde{\alpha} = 0$, we have proved the following proposition establishing the secular equation $\mathcal{F}(k) = 0$.

Proposition 9.1. $k_n \in \mathbb{R}$ is an eigenvalue of $(H_{BK}; A, B)$ iff

$$\mathcal{F}(k_n) := \det(\mathbb{1}_{E \times E} - S(A, B)T(a, b; k_n)) = 0. \tag{83}$$

Furthermore, the multiplicity of the eigenvalue one of $S(A, B)T(a, b; k_n)$ coincides with the multiplicity of the eigenvalue k_n of $(H_{BK}; A, B)$.

We remark that the geometric multiplicities and the algebraic multiplicities of $S(A, B)T(a, b; k)$ coincide since this matrix is diagonalizable.

In contrast to the S -matrix of the generic negative Laplacian $-\Delta$ on graphs, the S -matrix $S(A, B)$ is always independent of k (the S -matrix of $-\Delta$ is independent of the wave number k iff $S^+ = S$ (see [41])). 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 $x \in \mathbb{R}$):

$$p := -i\frac{d}{dx}. \tag{84}$$

The calculations are quite analogous (see e.g. [43] for a detailed discussion of this). In fact every self-adjoint extension of p can be characterized by the same matrices A and B as in (68)

and we would get the same S -matrix $S(A, B)$. The only difference in the secular equation between the operators H_{BK} and p then is the form of the second matrix in (82) which in the case of p is given by

$$T(\mathbf{a}, \mathbf{b}; k) := e^{ik(b-a)}. \tag{85}$$

This is one reason why we rather relate H_{BK} to a momentum operator than an energy operator as indicated in section 2. Because of the occurrence of the logarithm in \mathcal{T} , we endow the quantum graph with a metric structure as proposed in section 6. We also mention that proposition 9.1 is valid for all $k \in \mathbb{C}$, in particular for $k = 0$ in contrast to the corresponding proposition 12.1 for H_{BK}^2 . However, the analogy between $p^2 = -\Delta$ 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 (54) and (55). Again, we seek self-adjoint extensions of (38) with respect to $C_0^\infty(\Gamma)$. In order to obtain a self-adjoint operator, the task is to specify an appropriate domain $D(H_{BK}^2)$ for this operator with

$$C_0^\infty(\Gamma) \subset D(H_{BK}^2). \tag{86}$$

One simple possibility is to define H_{BK}^2 as the ‘squared’ Berry–Keating operator, which means

$$\begin{aligned} H_{BK}^2 \psi &:= H_{BK}(H_{BK}\psi), \\ \psi \in D(H_{BK}^2) &:= \{\phi \in D(H_{BK}); H_{BK}\phi \in D(H_{BK})\}. \end{aligned} \tag{87}$$

It follows immediately that H_{BK}^2 is self-adjoint if H_{BK} is self-adjoint using Friedrichs’ extension theorem [22, 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

$$H_{BK}^+ H_{BK} \quad \text{or} \quad H_{BK} H_{BK}^+. \tag{88}$$

This is an idea quite analogous to the concept of supersymmetry, see [44, 45] (the technique of factorization was already introduced by Schrödinger [46] and reviewed in [47]). In [45] this technique has been used but not explicitly mentioned. However, only a certain kind of self-adjoint extension can be attained in such a way. In [45] 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 [41].

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. First, the operator H_{BK}^2 acting on $C_0^\infty(\Gamma)$ or

$$D_0^2(\Gamma) := \bigoplus_{i=1}^E H_0^2[a_i, b_i] \quad \text{with} \quad 0 < a_i < b_i < \infty \tag{89}$$

is symmetric. $H_0^2[a_i, b_i]$ is the set of absolutely continuous functions which possess absolutely continuous derivatives on $[a_i, b_i]$, square integrable weak second derivatives and which together with their first derivatives vanish at the end points of the intervals. Furthermore, H_{BK}^2 acting on $D_0^2(\Gamma)$ is closed and the adjoint operator of $(H_{BK}^2, D_0^2(\Gamma))$ is $(H_{BK}^2, H^2(\Gamma))$. Here

$$H^2(\Gamma) := \bigoplus_{i=1}^E H^2[a_i, b_i] \quad \text{with} \quad 0 < a_i < b_i < \infty \tag{90}$$

is the space of functions being absolutely continuous on the intervals of the graph Γ possessing absolutely continuous derivatives and weak square integrable second derivatives. The deficiency indices are $(2E, 2E)$; thus $(H_{\text{BK}}^2, D_0^2(\Gamma))$ possesses infinitely many self-adjoint extensions. Again, as for H_{BK} the spectrum of every self-adjoint extension is purely discrete and 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. [37]). We shall follow a general approach to find all these self-adjoint extensions, quite analogous as in section 8 and based on [34].

11. Classification of the self-adjoint extensions of the ‘squared’ Berry–Keating operator

First, we define Ψ_{bv} as in (60) for $\psi \in H^2(\Gamma)$ and additionally

$$\Psi'_{\text{bv}} := (\psi'_1(a_1), \dots, \psi'_E(a_E), -\psi'_1(b_1), \dots, -\psi'_E(b_E))^T \quad \text{for } \psi \in H^2(\Gamma), \tag{91}$$

in which ψ'_i is the derivative of ψ_i on the interval I_i . Similarly as in (59), we define a symplectic form on $H^2(\Gamma) \times H^2(\Gamma)$:

$$[\phi, \psi]_2 := \langle \phi, H_{\text{BK}}^{2+} \psi \rangle_{L^2(\Gamma)} - \langle H_{\text{BK}}^{2+} \phi, \psi \rangle_{L^2(\Gamma)} \quad \text{for } \phi, \psi \in H^2(\Gamma). \tag{92}$$

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 $(H_{\text{BK}}^2, D_0^2(\Gamma))$. We shall adapt the definition of J in (63) by

$$J := \begin{pmatrix} 0 & \mathbb{1}_{2E \times 2E} \\ -\mathbb{1}_{2E \times 2E} & 0 \end{pmatrix} \tag{93}$$

and (see (61))

$$\tilde{D}_{(ab)} := \begin{pmatrix} D_{(ab)} & 0 \\ 0 & D_{(ab)} \end{pmatrix}, \quad [\psi]_{\text{bv}} := \begin{pmatrix} \Psi_{\text{bv}} \\ \Psi'_{\text{bv}} \end{pmatrix} \quad \text{for } \psi \in D_0^2(\Gamma). \tag{94}$$

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

$$\begin{aligned} [\psi, \phi]_2 &= \sum_{i=1}^E (b_i^2 \overline{\psi'_i(b_i)} \phi(b_i) - \overline{\psi_i(b_i)} \phi'(b_i)) - a_i^2 \overline{\psi'_i(a_i)} \phi(a_i) - \overline{\psi_i(a_i)} \phi'(a_i)) \\ &= \langle [\psi]_{\text{bv}}, J \tilde{D}_{(ab)}^2 [\phi]_{\text{bv}} \rangle_{\mathbb{C}^{4E}} \\ &= \langle \tilde{D}_{(ab)} [\psi]_{\text{bv}}, J \tilde{D}_{(ab)} [\phi]_{\text{bv}} \rangle_{\mathbb{C}^{4E}}. \end{aligned} \tag{95}$$

Taking the scalar product in the definition of $\omega(\cdot, \cdot)$ in (66) with respect to \mathbb{C}^{4E} , we infer as in section 8 the following proposition.

Proposition 11.1. *The self-adjoint extensions of $(H_{\text{BK}}^2, D_0^2(\Gamma))$ are exactly the preimages of*

$$\begin{aligned} \mathcal{L} &= \{[\phi]_{\text{bv}} \in \mathbb{C}^{4E}; A(\tilde{D}_{(ab)}[\phi]_{\text{bv}})_1 + B(\tilde{D}_{(ab)}[\phi]_{\text{bv}})_2 = 0\} \\ &= \{[\phi]_{\text{bv}} \in \mathbb{C}^{4E}; AD_{(ab)}\Phi_{\text{bv}} + BD_{(ab)}\Phi'_{\text{bv}} = 0\} \end{aligned} \tag{96}$$

with respect to $[\cdot]_{\text{bv}}$ in (94).

In (96) we have used $(\cdot)_i$ defined in (71). The matrices A and B are now elements of $\text{Mat}(2E \times 2E, \mathbb{C})$ with the adopted conditions

$$AB^+ = BA^+ \quad \text{and} \quad \text{rank}(A, B) = 2E. \tag{97}$$

Again, as in section 8 and because of proposition 11.1 we denote the self-adjoint extensions of $(H_{\text{BK}}^2, D_0^2(\Gamma))$ by $(H_{\text{BK}}^2; A, B)$.

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

We want to solve the eigenvalue problem

$$H_{BK}^2 \psi = \lambda \psi. \tag{98}$$

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.

In addition to (98) 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

$$\psi_k(x) = \left(\frac{1}{\sqrt{x}}(\alpha_1 e^{ik \ln x} + \beta_1 e^{-ik \ln x}), \dots, \frac{1}{\sqrt{x}}(\alpha_E e^{ik \ln x} + \beta_E e^{-ik \ln x}) \right). \tag{99}$$

We can proceed as in [34]. Therefore, we compute $\Psi_{bv,k}$ and $\Psi'_{bv,k}$ using the definitions in (61) and (76):

$$\begin{aligned} \Psi_{bv,k} &= D_{(ab)}^{-\frac{1}{2}} \begin{pmatrix} e^{ik \ln a} & e^{-ik \ln a} \\ e^{ik \ln b} & e^{-ik \ln b} \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} \\ \Psi'_{bv,k} &= \left(-\frac{1}{2} D_{(ab)}^{-\frac{3}{2}} \begin{pmatrix} e^{ik \ln a} & e^{-ik \ln a} \\ -e^{ik \ln b} & -e^{-ik \ln b} \end{pmatrix} \right. \\ &\quad \left. + ik D_{(ab)}^{-\frac{3}{2}} \begin{pmatrix} e^{ik \ln a} & e^{-ik \ln a} \\ -e^{ik \ln b} & -e^{-ik \ln b} \end{pmatrix} I_{\pm} \right) \begin{pmatrix} \alpha \\ \beta \end{pmatrix}. \end{aligned} \tag{100}$$

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 (96) defined by the two matrices A and B . We make the identification (cf [41]):

$$X(k; \mathbf{a}, \mathbf{b}) := \begin{pmatrix} e^{ik \ln a} & e^{-ik \ln a} \\ e^{ik \ln b} & e^{-ik \ln b} \end{pmatrix}, \tag{101}$$

$$Y(k; \mathbf{a}, \mathbf{b}) := \begin{pmatrix} e^{ik \ln a} & e^{-ik \ln a} \\ -e^{ik \ln b} & -e^{-ik \ln b} \end{pmatrix} \tag{102}$$

and

$$Y'(k; \mathbf{a}, \mathbf{b}) := \begin{pmatrix} e^{ik \ln a} & -e^{-ik \ln a} \\ -e^{ik \ln b} & e^{-ik \ln b} \end{pmatrix}. \tag{103}$$

Thus, we conclude, with the definition for the bold symbols in accordance with (62),

$$0 \stackrel{\dagger}{=} AD_{(ab)} \Phi_{bv} + BD_{(ab)} \Phi'_{bv} \tag{104}$$

$$\begin{aligned} &= \left(AD_{(ab)}^{\frac{1}{2}} X(k; \mathbf{a}, \mathbf{b}) + BD_{(ab)}^{-\frac{1}{2}} Y(k; \mathbf{a}, \mathbf{b}) \begin{pmatrix} -\frac{1}{2} + ik & 0 \\ 0 & -\frac{1}{2} - ik \end{pmatrix} \right) \begin{pmatrix} \alpha \\ \beta \end{pmatrix} \\ &= \left(\left(AD_{(ab)}^{\frac{1}{2}} - \frac{1}{2} BD_{(ab)}^{-\frac{1}{2}} I_{\pm} \right) X(k; \mathbf{a}, \mathbf{b}) + ik BD_{(ab)}^{-\frac{1}{2}} Y(k; \mathbf{a}, \mathbf{b}) \right) \begin{pmatrix} \alpha \\ \beta \end{pmatrix}. \end{aligned} \tag{105}$$

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

$$AD_{(ab)}^{\frac{1}{2}} (BD_{(ab)}^{-\frac{1}{2}})^{\dagger} = AB^{\dagger}. \tag{106}$$

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

$$\text{rank}(AD_{(ab)}^{\frac{1}{2}}, BD_{(ab)}^{-\frac{1}{2}}) = \text{rank}(A, B) = 2E. \tag{107}$$

Therefore, we define

$$AD_{(ab)}^{\frac{1}{2}} =: A' \quad \text{and} \quad BD_{(ab)}^{-\frac{1}{2}} =: B' \quad (108)$$

and observe that A' and B' also fulfil conditions (97). Therefore, we can apply a theorem of Kuchment [38]. It states that two matrices A' and B' fulfil (97) iff there exists an invertible matrix C with

$$A' = CP_{\ker B'} + CP_{\ker B'}^{\perp} L' P_{\ker B'}^{\perp} \quad \text{and} \quad B' = CP_{\ker B'}^{\perp}. \quad (109)$$

In (109) we have defined $P_{\ker B'}$ as the projector onto the kernel of B' and $P_{\ker B'}^{\perp}$ as the corresponding orthogonal projector. The matrix L' is self-adjoint and can be defined by (see [38])

$$L' := (B'|_{\text{ran} B'^{\perp}})^{-1} A' P_{\ker B'}^{\perp}. \quad (110)$$

Hence, we can proceed in the calculation (104) by multiplying (105) from the left-hand side by C^{-1} :

$$0 = \left(\left(P_{\ker B'} + P_{\ker B'}^{\perp} L' P_{\ker B'}^{\perp} - \frac{1}{2} P_{\ker B'}^{\perp} I_{\pm} \right) X(k; \mathbf{a}, \mathbf{b}) + ik P_{\ker B'}^{\perp} Y'(k; \mathbf{a}, \mathbf{b}) \right) \begin{pmatrix} \alpha \\ \beta \end{pmatrix}. \quad (111)$$

Since the projectors $P_{\ker B'}$ and $P_{\ker B'}^{\perp}$ are mutually orthogonal, we infer from (109), the definition of \mathcal{L} in (96) and with the first line of (105), that

$$P_{\ker B'} X(k; \mathbf{a}, \mathbf{b}) \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = 0. \quad (112)$$

In (111) we insert between the matrices I_{\pm} and $X(k; \mathbf{a}, \mathbf{b})$ the unit matrix $\mathbb{1} = P_{\ker B'} + P_{\ker B'}^{\perp}$ and apply (112)

$$0 = \left(\left(P_{\ker B'} + P_{\ker B'}^{\perp} \left(L' - \frac{1}{2} I_{\pm} \right) P_{\ker B'}^{\perp} \right) X(k; \mathbf{a}, \mathbf{b}) + ik P_{\ker B'}^{\perp} Y'(k; \mathbf{a}, \mathbf{b}) \right) \begin{pmatrix} \alpha \\ \beta \end{pmatrix}. \quad (113)$$

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

$$L'' := P_{\ker B'}^{\perp} \left(L' - \frac{1}{2} I_{\pm} \right) P_{\ker B'}^{\perp} \quad (114)$$

and make a redefinition:

$$A'' := P_{\ker B'} + L'' \quad \text{and} \quad B'' := P_{\ker B'}^{\perp}. \quad (115)$$

It is obvious that the matrices A'' and B'' fulfil conditions (95). Hence as in section 9 respectively [34], we infer that $A'' \pm ikB''$ is invertible and conclude with quite the same calculation as in [41]:

$$0 = (A'' + ikB'')[\mathbb{1} - S''(A, B; k)T(\mathbf{a}, \mathbf{b}; k)] \begin{pmatrix} e^{ik \ln a} & 0 \\ 0 & e^{-ik \ln b} \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix}. \quad (116)$$

Here we have used the definitions

$$S''(A, B; k) := S(A'', B''; k) := -\frac{A'' - ikB''}{A'' + ikB''} \quad \text{and} \quad (117)$$

$$T(\mathbf{a}, \mathbf{b}; k) := \begin{pmatrix} 0 & e^{ik \ln \frac{b}{a}} \\ e^{ik \ln \frac{b}{a}} & 0 \end{pmatrix}.$$

The first and the third matrix in the product of (116) 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 [35] and [42]. Thus, we have proved the following proposition.

Proposition 12.1. k^2 with $k \in \mathbb{C} \setminus (\pm i\sigma(L'') \cup \{0\})$ is an eigenvalue of $(H_{BK}^2; A, B)$ iff

$$F(k) := \det(\mathbb{1}_{2E \times 2E} - S''(A, B; k)T(\mathbf{a}, \mathbf{b}; k)) = 0. \tag{118}$$

Furthermore, as in section 9, the multiplicity of the eigenvalue $\lambda = k^2$ coincides with the multiplicity of the eigenvalue one of $S''(A, B; k)T(\mathbf{a}, \mathbf{b}; k)$ for every $k \in \mathbb{C} \setminus (\pm i\sigma(L'') \cup \{0\})$.

We remark that the restriction on k concerns only non-positive eigenvalues $\lambda = k^2$ of H_{BK}^2 .

13. The eigenvalue zero

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

$$\psi_0(x) = \left(\alpha_1 \frac{1}{\sqrt{x}} + \beta_1 \frac{1}{\sqrt{x}} \ln x, \dots, \alpha_E \frac{1}{\sqrt{x}} + \beta_E \frac{1}{\sqrt{x}} \ln x \right). \tag{119}$$

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

$$\left(A'' \begin{pmatrix} \mathbb{1}_{E \times E} & \ln \mathbf{a} \\ \mathbb{1}_{E \times E} & \ln \mathbf{b} \end{pmatrix} + B'' \begin{pmatrix} 0 & \mathbb{1}_{E \times E} \\ 0 & -\mathbb{1}_{E \times E} \end{pmatrix} \right) \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = 0 \tag{120}$$

which is necessary and sufficient for $\lambda = 0$ to be an eigenvalue of $(H_{BK}^2; A, B)$. The matrices A'' and B'' are the same as in (115). Then we can proceed as in [35] and get the following proposition.

Proposition 13.1. $\lambda = k^2 = 0$ is an eigenvalue of $(H_{BK}^2; A, B)$ iff for one value $k' \neq 0$ and then for every $k' \neq 0$

$$F_0(k') := \det(\mathbb{1} - S''(A, B; k')C(\mathbf{a}, \mathbf{b}; k')) = 0 \tag{121}$$

is fulfilled with $S''(A, B; k')$ as in (117) and

$$C(\mathbf{a}, \mathbf{b}; k') := \begin{pmatrix} \frac{\ln \left(\frac{b_1}{a_1} \right)}{2 \frac{i}{k'} + \ln \left(\frac{b_1}{a_1} \right)} & 0 & \frac{2 \frac{i}{k'}}{2 \frac{i}{k'} + \ln \left(\frac{b_1}{a_1} \right)} & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & \frac{\ln \left(\frac{b_E}{a_E} \right)}{2 \frac{i}{k'} + \ln \left(\frac{b_E}{a_E} \right)} & 0 & \frac{2 \frac{i}{k'}}{2 \frac{i}{k'} + \ln \left(\frac{b_E}{a_E} \right)} \\ \frac{2 \frac{i}{k'}}{2 \frac{i}{k'} + \ln \left(\frac{b_1}{a_1} \right)} & 0 & \frac{\ln \left(\frac{b_1}{a_1} \right)}{2 \frac{i}{k'} + \ln \left(\frac{b_1}{a_1} \right)} & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & \frac{2 \frac{i}{k'}}{2 \frac{i}{k'} + \ln \left(\frac{b_E}{a_E} \right)} & 0 & \frac{\ln \left(\frac{b_E}{a_E} \right)}{2 \frac{i}{k'} + \ln \left(\frac{b_E}{a_E} \right)} \end{pmatrix}. \tag{122}$$

Furthermore, the multiplicity of the eigenvalue $\lambda = 0$ coincides with the multiplicity of the eigenvalue one of $S''(A, B; k')C(\mathbf{a}, \mathbf{b}; k')$ for every real $k' \neq 0$.

Thus, in general there is a difference between the spectral multiplicity of the eigenvalue one of $S''(A, B; 0)T(\mathbf{a}, \mathbf{b}, 0)$, which we denote by N , and that of the eigenvalue one of $S''(A, B; k')C(\mathbf{a}, \mathbf{b}; k')$ with $k' \neq 0$, see [35, 45, 48].

In order to relate the self-adjoint extensions of $(H_{BK}^2, D_0^2(\Gamma))$ to the self-adjoint extensions of the Laplacian $-\Delta$ one has to adjust the lengths as before. However, in order to attain the same spectrum, except for the case $k \notin \mathbb{C} \setminus (\pm i\sigma(L'') \setminus \{0\})$, one has to transform the matrices

A and B into A'' and B'' as in (108) and (115). 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 (96). Especially, the functions $F(k)$ and $F_0(k)$ in (118) and (121), respectively, will coincide with the corresponding functions for $-\Delta$, see e.g. [35] and [41].

We remark that the transformation of the matrices $A \rightarrow A''$ and $B \rightarrow B''$ and vice versa (actually we consider below the converse direction) cannot be achieved by perturbing the negative Laplacian by a magnetic flux which corresponds to an operator acting on the edges as

$$\left(\frac{d}{dx_j} - iA_j(x_j)\right)^2 \psi(x_j) \quad \text{for } 1 \leq j \leq E. \quad (123)$$

Kostrykin and Schrader have shown in [49] 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 (97). But with a local gauge transformation this system can be transformed into a quantum graph system with the pure Laplacian which is now characterized by two new matrices \tilde{A} and \tilde{B} . These new matrices are obtained by the old ones by

$$\tilde{A} = AU \quad \text{and} \quad \tilde{B} = BU \quad (124)$$

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

$$S(\tilde{A}, \tilde{B}; k) = US(A, B; k)U^+. \quad (125)$$

In particular this means that the S -matrix is k -independent iff the original S -matrix is k -independent. By a result of [50] we conclude that in the sense of (109) (see [38]) the corresponding matrix $P_{\ker B}^\perp L P_{\ker B}^\perp$ is zero iff $P_{\ker \tilde{B}}^\perp \tilde{L} P_{\ker \tilde{B}}^\perp$ is zero. This feature is obviously not given by the transformation A, B into A'', B'' especially in (114) taking into account that the transformation A, B into A', B' in (108) and the corresponding transformation L into L' possess this feature.

Kostrykin and Schrader have shown in [42] that the negative Laplacian $-\Delta$ possesses time-reversal symmetry iff $S^T = S$. Obviously, the transformation (125) does not maintain this symmetry in general.

In both cases (H_{BK} and H_{BK}^2) we get the same length l_i for the edge e_i of the quantum graph for the corresponding momentum operator or kinetic energy operator. Thus, we choose l_i for the lengths of the graph and endow it with a metric structure as in section 6.

14. Connection between H_{BK} and H_{BK}^2

We also want to reveal the link between H_{BK} and H_{BK}^2 , the last one considered as the ‘squared’ Berry–Keating operator as in (87). Therefore, we are starting from $(H_{\text{BK}}; A, B)$ with the corresponding S -matrix $S(A, B)$ and then calculate $(H_{\text{BK}}^2; \tilde{A}, \tilde{B})$ with the corresponding S -matrix $S(\tilde{A}, \tilde{B})$. Using definitions (73) we obtain from (87) the two (necessary and sufficient) equations, setting $\phi := H_{\text{BK}}\psi$,

$$\begin{aligned} A(UD_{(ab)}^{\frac{1}{2}}\Psi_{\text{bv}})_1 + B(UD_{(ab)}^{\frac{1}{2}}\Psi_{\text{bv}})_2 &= 0 \\ A(UD_{(ab)}^{\frac{1}{2}}\Phi_{\text{bv}})_1 + B(UD_{(ab)}^{\frac{1}{2}}\Phi_{\text{bv}})_2 &= 0. \end{aligned} \quad (126)$$

Making the definitions

$$\psi(\mathbf{a}) = (\psi_1(a_1), \dots, \psi_E(a_E))^T \quad \text{and} \quad \psi(\mathbf{b}) = (\psi_1(b_1), \dots, \psi_E(b_E))^T \quad (127)$$

equations (126) can be transformed into (see definition (62))

$$\begin{aligned} \psi(a) &= \left(\frac{b}{a}\right)^{\frac{1}{2}} \mathcal{S}(A, B)\psi(b) \\ \psi'(a) &= \left(\frac{b}{a}\right)^{\frac{3}{2}} \mathcal{S}(A, B)\psi'(b). \end{aligned} \tag{128}$$

This is equivalent to the equation

$$\begin{pmatrix} -\mathbb{1} & (\frac{a}{b})^{\frac{1}{2}} \mathcal{S}(A, B) \\ 0 & 0 \end{pmatrix} D_{(ab)}\Psi_{bv} + B \begin{pmatrix} 0 & 0 \\ \mathbb{1} & (\frac{b}{a})^{\frac{1}{2}} \mathcal{S}(A, B) \end{pmatrix} D_{(ab)}\Psi'_{bv} = 0. \tag{129}$$

Comparing (129) with (96), we infer for the matrices (one possible choice) \tilde{A} and \tilde{B} :

$$\tilde{A} = \begin{pmatrix} -\mathbb{1} & (\frac{a}{b})^{\frac{1}{2}} \mathcal{S}(A, B) \\ 0 & 0 \end{pmatrix}, \quad \tilde{B} = \begin{pmatrix} 0 & 0 \\ \mathbb{1} & (\frac{b}{a})^{\frac{1}{2}} \mathcal{S}(A, B) \end{pmatrix}. \tag{130}$$

It is a simple calculation that indeed the matrices \tilde{A} and \tilde{B} fulfil (97). In order to calculate $S(\tilde{A}, \tilde{B})$ we make two observations. First, we infer from (106) and (130) that $L' = 0$ in the decomposition (109). Furthermore, we note that

$$\begin{aligned} \ker \tilde{B}'^{\perp} &= \text{span} \left\{ \begin{pmatrix} \mathcal{S}(A, B)e_i \\ e_i \end{pmatrix}; i = 1, \dots, E \right\}, \\ \ker \tilde{B}' &= \text{span} \left\{ \begin{pmatrix} \mathcal{S}(A, B)e_i \\ -e_i \end{pmatrix}; i = 1, \dots, E \right\}, \end{aligned} \tag{131}$$

where span denotes the linear span of the corresponding vectors, and the vectors e_i span the space \mathbb{C}^E . Therefore, by (114) we conclude

$$L'' = L' = 0. \tag{132}$$

Thus, by (117) and after an easy (but lengthy) calculation we obtain for the S -matrix of $(H_{BK}^2; \tilde{A}, \tilde{B})$

$$S(\tilde{A}, \tilde{B}) = \begin{pmatrix} 0 & \mathcal{S}(A, B) \\ \mathcal{S}(A, B)^+ & 0 \end{pmatrix}. \tag{133}$$

Therefore, we have proved the following proposition.

Proposition 14.1. $(H_{BK}^2; \tilde{A}, \tilde{B})$ is the ‘squared’ operator of some $(H_{BK}; A, B)$ in the sense of (87) iff the corresponding S -matrices fulfil (133).

We remark that a similar relation holds for the usual Laplace operator $-\Delta$ and the momentum operator p on compact graphs.

15. Trace formulae and Weyl’s law

We are now in the position to give 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 the results in [35]. The proofs of the claims for the Berry–Keating operator are quite analogous to [35] 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 [35].

Definition 15.1. For each $r \geq 0$ the space H_r consists of all functions $h : \mathbb{C} \rightarrow \mathbb{C}$ 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 $M_{r+\delta}$, $k \rightarrow \infty$.

We denote by k_n the ‘energies’ respectively ‘wave numbers’ of H_{BK} respectively H_{BK}^2 and by g_n the corresponding multiplicities which are identical with the order of the corresponding zeros k_n of \mathcal{F} in (83) for $n \in \mathbb{N}_0$ respectively zeros $k_n \neq 0$ of F in (118) 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. However, the (finitely many) imaginary wave numbers are omitted. Furthermore, we denote the self-adjoint realizations characterized by (73) respectively (96) by $(H_{\text{BK}}; A, B)$ respectively $(H_{\text{BK}}^2; \tilde{A}, \tilde{B})$. Note that in the first case $A, B \in \operatorname{Mat}(E \times E, \mathbb{C})$ whereas in the second case $\tilde{A}, \tilde{B} \in \operatorname{Mat}(2E \times 2E, \mathbb{C})$. In addition, we denote by l_{\min} the minimal length of the graph with respect to the definition of section 6. The minimal positive eigenvalue of L'' in (114) is denoted by λ''_{\min} and the unique minimum of the function

$$l(\kappa) := \frac{1}{\kappa} \ln(2E) + \frac{2}{\kappa} \operatorname{artanh} \left(\frac{\kappa}{\lambda''_{\min}} \right) \tag{134}$$

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

$$\mathcal{L} := \sum_{i=1}^E l_i. \tag{135}$$

Furthermore, by a hat $\hat{\cdot}$ we denote the Fourier transform (see (17)) and $\cdot * \cdot$ denotes the convolution of two functions in the distributional sense, see e.g. [22]. 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 end points is only allowed for adjacent edge ends, see [42] 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 be interpreted as a quantum mechanical topology. However, in [42] it was shown that there exists always at least one graph, for which the S -matrix is local. In order to interpret the right-hand side of (136) for H_{BK} as a sum of periodic orbits, we replace the edges by directed edges as mentioned in section 6. Furthermore, we assume that the S -matrix $\mathcal{S}(A, B)$ is local with respect to the directed edges. This means that $\mathcal{S}(A, B)_{ij} = 0$ 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 obtain the following theorem for H_{BK} .

Theorem 15.2 (Trace formula for H_{BK}). Let Γ be a compact metric graph and $(H_{\text{BK}}; A, B)$ 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 equation (17) and g_n the multiplicity of the eigenvalue k_n):

$$\sum_{n=0}^{\infty} g_n h(k_n) = \mathcal{L} \hat{h}(0) + 2 \sum_{\gamma \in \mathfrak{P}} \operatorname{Re}(\mathcal{A}_\gamma) \hat{h}(l_\gamma). \tag{136}$$

The amplitude functions \mathcal{A}_γ are constructed from the S -matrix elements with respect to the periodic orbits γ , see [14, 35] for a precise definition of this construction. The proof of this theorem is quite analogous to [35]. Since we have no k -dependence of $\mathcal{S}(A, B)$ in (82), we can omit the requirement of the minimal length in contrast to corollary 15.3. This also leads to the simple product of the real part of the amplitude functions \mathcal{A}_γ and the Fourier transform of h in the identity (136). Furthermore, since the secular equation (81) respectively (83) holds also for the eigenvalue zero of H_{BK} , the term $g_0 - \frac{1}{2}N$ does not appear in (136) in contrast to (137) for H_{BK}^2 , where N denotes the multiplicity of the (possible) zero $k_0 = 0$ of $F(k)$. For H_{BK}^2 we get the following trace formula.

Theorem 15.3 (Trace formula for H_{BK}^2). *Let Γ be a compact metric graph and $(H_{\text{BK}}^2; \tilde{A}, \tilde{B})$ with the above assumptions be given. Let the condition $l_{\min} > l(\sigma)$ be fulfilled and let $h \in H_r$ with $r \geq \sigma$. Then the following trace formula holds:*

$$\sum_{n=0}^{\infty} g_n h(k_n) = \mathfrak{L} \hat{h}(0) + \left(g_0 - \frac{1}{2}N \right) h(0) - \frac{1}{4\pi} \int_{-\infty}^{+\infty} h(k) \frac{\text{Im tr } S''(A, B; k)}{k} dk + \sum_{\gamma \in \mathfrak{P}} [(\hat{h} * \hat{A}_\gamma)(l_\gamma) + (\hat{h} * \hat{\tilde{A}}_\gamma)(l_\gamma)]. \tag{137}$$

Again, the amplitude functions A_γ are constructed from the S -matrix elements with respect to the periodic orbits γ and g_0 denotes the multiplicity of the eigenvalue one of $S''(A, B; k')C(\mathbf{a}, \mathbf{b}; k')$ for any $k' \in \mathbb{R} \setminus \{0\}$ (see section 13).

Since we have previously seen that the spectrum of $(H_{\text{BK}}^2; \tilde{A}, \tilde{B})$ coincides with some self-adjoint realization of $-\Delta$ on the graph by adapting the lengths and with the results in [35], we get Weyl’s law.

Theorem 15.4 (Weyl’s law for H_{BK}^2). *Given the eigenvalues of some $(H_{\text{BK}}^2; \tilde{A}, \tilde{B})$ in increasing order denoted by $\lambda_n = k_n^2$. Then for the counting function $N(\lambda) := \#\{n; k_n^2 \leq \lambda\}$ the following asymptotic law holds:*

$$N(\lambda) \sim \frac{\mathfrak{L}}{\pi} \sqrt{\lambda} \quad \text{for } \lambda \rightarrow \infty. \tag{138}$$

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 on the right-hand side of the equation, i.e. we have the following.

Theorem 15.5 (Weyl’s law for H_{BK}). *Given the positive eigenvalues of some $(H_{\text{BK}}; A, B)$ in increasing order denoted by $\lambda_n = k_n$. Then for the counting function $N(k) := \#\{n; k_n \leq k\}$ the following asymptotic law holds:*

$$N(k) \sim \frac{\mathfrak{L}}{\pi} k \quad \text{for } k \rightarrow \infty. \tag{139}$$

Theorem 15.5 can be proved by a suitable Karamata–Tauberian theorem (see e.g. [51] and [35]) or alternatively by applying theorem 15.4 to the ‘squared’ operator H_{BK}^2 of H_{BK} in the sense of (87) (the spectrum of the eigenvalues of H_{BK} and the wave numbers of H_{BK}^2 coincides then and therefore the corresponding eigenvalue respectively wave number counting functions are the same). Comparing theorems 15.4 and 15.5 with the asymptotics of the counting function for the nontrivial Riemann zeros (32), we therefore can conclude the following.

Theorem 15.6 (No-go theorem). *Neither H_{BK} nor H_{BK}^2 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 $\mathcal{H} = L^2(\mathbb{R}_>, dx)$ discussed in section 2. Furthermore, we give an example for a realization of H_{BK} and H_{BK}^2 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 (26) we define ($x \in \mathbb{R}_>$)

$$\phi(x) := \frac{\alpha}{e^x + 1} \quad \text{with} \quad \alpha = \frac{1}{\sqrt{\ln 2 - \frac{1}{2}}}. \tag{140}$$

(With this choice for α it holds $\|\phi\| = 1$.) From (22) we obtain

$$\psi(x, t) = (U(t)\phi)(x) = \frac{\alpha e^{-\frac{t}{2}}}{e^{xe^{-t}} + 1} \quad \text{with} \quad t \in \mathbb{R}. \tag{141}$$

Thus, we get the large- t asymptotics

$$\psi \sim \frac{\alpha}{2} e^{-\frac{t}{2}} \quad \text{for} \quad t \rightarrow \infty. \tag{142}$$

On the other hand, with

$$K_{BK}(x, x_0; t) = \int_{-\infty}^{\infty} \psi_k(x) \bar{\psi}_k(x_0) e^{-ikt} dk, \tag{143}$$

(14) and (26), we get

$$\psi(x, t) = \int_{-\infty}^{\infty} A(k) \psi_k(x) e^{-ikt} dk. \tag{144}$$

A direct calculation using (19) and the integral representation of $\zeta(s)$ as a Mellin transform (see [52, p 20]) yields

$$A(k) = \frac{\alpha}{\sqrt{2\pi}} (1 - \sqrt{2} 2^{ik}) \Gamma\left(\frac{1}{2} - ik\right) \zeta\left(\frac{1}{2} - ik\right). \tag{145}$$

With (see [52, p 13])

$$\left| \Gamma\left(\frac{1}{2} - ik\right) \right| \sim \sqrt{2\pi} e^{-\frac{\pi}{2}|k|} \quad \text{for} \quad k \in \mathbb{R}, \quad |k| \rightarrow \infty, \tag{146}$$

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

$$|A(k)|^2 \sim \alpha^2 (3 - 2\sqrt{2} \cos(k \ln 2)) e^{-\pi|k|} \left| \zeta\left(\frac{1}{2} - ik\right) \right|^2 \quad \text{for} \quad k \in \mathbb{R}, \quad |k| \rightarrow \infty, \tag{147}$$

which gives a sufficient condition for $A \in L^2(\mathbb{R}, dk)$. If we consider the continuous representation (144) 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 [9, 10], 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 (68). Equations (73) and (82) lead then with

$$S(A, B) =: e^{-2\pi ic} \tag{148}$$

to

$$\psi(a) = S(A, B) \sqrt{\frac{b}{a}} \psi(b) = \sqrt{\frac{b}{a}} e^{-2\pi ic} \psi(b) \quad \text{with} \quad c \in [0, 1). \tag{149}$$

The eigenvalue spectrum is given by

$$k_n = \frac{2\pi}{\ln \frac{b}{a}}(n + c) \quad \text{with } c \in [0, 1) \quad \text{and } n \in \mathbb{Z}. \quad (150)$$

We now want to calculate H_{BK}^2 as defined in (87) with (149), in particular the S -matrix and then compare it with the results in section 14. In order to distinguish the characterizing matrices, we denote these with the subscripts $\cdot_{H_{\text{BK}}}$ and $\cdot_{H_{\text{BK}}^2}$. First, we derive the transformation of $A_{H_{\text{BK}}}, B_{H_{\text{BK}}}$ into $A_{H_{\text{BK}}^2}, B_{H_{\text{BK}}^2}$ for the corresponding operators related by (87). We get the additional condition

$$\psi'(a) = \left(\frac{b}{a}\right)^{\frac{3}{2}} e^{-2\pi ic} \psi'(b) \quad \text{with } c \in [0, 1). \quad (151)$$

The two conditions are equivalent to

$$\begin{aligned} 0 &= \begin{pmatrix} -1 & (\frac{b}{a})^{\frac{1}{2}} e^{-2\pi ic} \\ 0 & 0 \end{pmatrix} \Psi_{\text{bv}} + \begin{pmatrix} 0 & 0 \\ 1 & (\frac{b}{a})^{\frac{3}{2}} e^{-2\pi ic} \end{pmatrix} \Psi'_{\text{bv}} \\ \Leftrightarrow 0 &= \begin{pmatrix} -1 & (\frac{b}{a})^{\frac{1}{2}} e^{-2\pi ic} \\ 0 & 0 \end{pmatrix} \begin{pmatrix} \frac{1}{a} & 0 \\ 0 & \frac{1}{b} \end{pmatrix} D_{(ab)} \Psi_{\text{bv}} \\ &\quad + \begin{pmatrix} 0 & 0 \\ 1 & (\frac{b}{a})^{\frac{3}{2}} e^{-2\pi ic} \end{pmatrix} \begin{pmatrix} \frac{1}{a} & 0 \\ 0 & \frac{1}{b} \end{pmatrix} D_{(ab)} \Psi'_{\text{bv}} \\ \Leftrightarrow 0 &= \begin{pmatrix} -1 & (\frac{a}{b})^{\frac{1}{2}} e^{-2\pi ic} \\ 0 & 0 \end{pmatrix} D_{(ab)} \Psi_{\text{bv}} + \begin{pmatrix} 0 & 0 \\ 1 & (\frac{b}{a})^{\frac{1}{2}} e^{-2\pi ic} \end{pmatrix} D_{(ab)} \Psi'_{\text{bv}}. \end{aligned} \quad (152)$$

Therefore, we define

$$A_{H_{\text{BK}}^2} := \begin{pmatrix} -1 & (\frac{a}{b})^{\frac{1}{2}} e^{-2\pi ic} \\ 0 & 0 \end{pmatrix} \quad \text{and} \quad B_{H_{\text{BK}}^2} := \begin{pmatrix} 0 & 0 \\ 1 & (\frac{b}{a})^{\frac{1}{2}} e^{-2\pi ic} \end{pmatrix} \quad (153)$$

and recognize that indeed

$$A_{H_{\text{BK}}^2} B_{H_{\text{BK}}^2}^+ = B_{H_{\text{BK}}^2} A_{H_{\text{BK}}^2}^+ = 0 \quad \text{and} \quad \text{rank}(A_{H_{\text{BK}}^2}, B_{H_{\text{BK}}^2}) = 2 \quad (154)$$

is fulfilled. By a comparison of (152) with (96), we infer that $A_{H_{\text{BK}}^2}$ and $B_{H_{\text{BK}}^2}$ are two possible matrices to characterize H_{BK}^2 in the sense of (96). For $S''(A_{H_{\text{BK}}^2}, B_{H_{\text{BK}}^2}; k)$, we get

$$S''(A_{H_{\text{BK}}^2}, B_{H_{\text{BK}}^2}; k) = \begin{pmatrix} 0 & e^{-2\pi ic} \\ e^{2\pi ic} & 0 \end{pmatrix} = \begin{pmatrix} 0 & S(A, B) \\ S(A, B)^+ & 0 \end{pmatrix} \quad (155)$$

in complete agreement with (133) and for the secular equation (118)

$$0 = (e^{i(k \ln(\frac{b}{a}) + 2\pi c)} - 1)(e^{i(k \ln(\frac{b}{a}) - 2\pi c)} - 1). \quad (156)$$

This leads to the ‘wave numbers’

$$k_n = \frac{2\pi}{\ln \frac{b}{a}}(n \pm c), \quad n \in \mathbb{Z}, \quad (157)$$

with c as in (150). Obviously, with (157) and (150) 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 [53, 54]. 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 sections 2 respectively 4) for which ($\hbar = 1$)

$$I_n(E_n) = \left(n + \frac{\mu_n}{4}\right) \quad \text{with } n \geq 0 \quad (158)$$

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

$$I_n(E_n) = \frac{1}{2\pi} \int_{\gamma_n} p \, dx \tag{159}$$

is the classical action of a periodic orbit γ_n which is a subset of the hypersurface $H_{\text{cl}} = E_n$ respectively $\tilde{H}_{\text{cl}} = E_n$. For H_{cl} in (1) with the ring system structure mentioned in section 3, we get from (158)

$$E_n = \frac{2\pi}{\ln(\frac{b}{a})} \left(n + \frac{\mu_n}{4} \right), \tag{160}$$

and for \tilde{H}_{cl} in (33) (also with the ring system structure)

$$\sqrt{E_n} = k_n = \frac{2\pi}{\ln(\frac{b}{a})} \left(n + \frac{\mu_n}{4} \right). \tag{161}$$

A comparison of (160) with (150) yields for the Maslov indices $\mu_n = 4c$ for H_{cl} . For \tilde{H}_{BK} we get two Maslov indices: $\mu_n = 4c$ for $n = 0, 2, 4, \dots$ and $\mu_n = -4c$ for $n = 1, 3, 5, \dots$. 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 $n = 1, 3, \dots$. We stress that the EBK-quantization for \tilde{H}_{cl} with a classical ‘hard wall’ boundary condition yields

$$\sqrt{E_n} = k_n = \frac{\pi}{\ln(\frac{b}{a})} \left(n + \frac{\mu_n}{4} \right), \tag{162}$$

which differs from (161) by a factor 2. We mention that the S -matrix elements of $S''(A_{H_{\text{BK}}^2}, B_{H_{\text{BK}}^2}; k)$ for Dirichlet (D), Neumann (N) or Robin (R) boundary conditions are given by

$$S''(A_{H_{\text{BK}}^2}, B_{H_{\text{BK}}^2}; k)_{ij} = \begin{cases} -\delta_{ij} & \text{for } D, \\ \delta_{ij} & \text{for } N, \\ -\delta_{ij} \frac{\rho_j - ik}{\rho_j + ik} & \text{for } R, \end{cases} \quad \text{with } \rho_j \in \mathbb{R} \text{ and } i, j \in \{1, 2\}, \tag{163}$$

which obviously differ from (155) and, therefore, cannot originate from a ‘squared’ Berry-Keating operator. If we impose Dirichlet boundary conditions at both interval ends, we get for $F(k)$ in (118)

$$F(k) = 1 - e^{2ik \ln(\frac{b}{a})} \tag{164}$$

and thus we obtain for the wave numbers k_n :

$$k_n = \frac{\pi}{\ln(\frac{b}{a})} n, \quad n \in \mathbb{Z} \setminus \{0\}, \tag{165}$$

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 (165). For Robin boundary conditions at both interval ends, we get

$$F(k) = 1 - \frac{(\rho_1 - ik)(\rho_2 - ik)}{(\rho_1 + ik)(\rho_2 + ik)} e^{2ik \ln(\frac{b}{a})}. \tag{166}$$

Again, by a comparison of (165) with (162), we conclude for the Maslov indices for pure Dirichlet and Neumann boundary conditions

$$\mu_n = 0 \quad \text{for } n \in \mathbb{N} \tag{167}$$

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 (166).

The above considerations underline the fact that the form of the S -matrix (155) corresponds to a pure ring system as in the case of the negative Laplacian $-\Delta$, see [42]. 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 wavefunction, see e.g. [55].

Example 16.3. We shall present a trace formula for the time-evolution operator $U(t)$ in (21) and (22) for H_{BK} acting on a single edge with the assigned interval $I = [1, b]$:

$$(U(t)\phi)(x) := \sum_{n=-\infty}^{\infty} \psi_n(x) \langle \psi_n, \phi \rangle e^{-ik_n t}, \quad \phi \in L^2(I, dx), \quad (168)$$

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

$$\psi_n(x) = \frac{1}{\sqrt{x \ln b}} e^{ik_n \ln x} \quad \text{with } n \in \mathbb{Z}. \quad (169)$$

For the corresponding (not retarded) integral kernel of $U(t)$ we get by [21, p 20] (in a distributional sense acting on $\mathcal{D}(I) \subset L^2(I, dx)$ identified by the continuous representatives; $g(x, x_0; t) := \frac{2\pi}{\ln b} [\ln x - \ln x_0 - t]$)

$$\begin{aligned} K(x, x_0; t) &:= \sum_{n=-\infty}^{\infty} \psi_n(x) \bar{\psi}_n(x_0) e^{-ik_n t} = \frac{e^{icg(x, x_0; t)}}{\sqrt{xx_0 \ln b}} \sum_{n=-\infty}^{\infty} e^{ig(x, x_0; t)n} \\ &= \frac{2\pi}{\ln b} \frac{e^{icg(x, x_0; t)}}{\sqrt{xx_0}} \sum_{n=-\infty}^{\infty} \delta(g(x, x_0; t) + 2\pi n) \\ &= e^{icg(x, x_0; t)} \sum_{n=-\infty}^{\infty} b^{\frac{n}{2}} e^{\frac{i}{2}n} \delta(xb^n - x_0 e^t). \end{aligned} \quad (170)$$

If we take the trace of $U(t)$, we obtain with (170) (by defining the ‘period’ $T = \ln b$ (see (3)) and the Maslov index $\mu := 4c$)

$$\begin{aligned} \text{Tr } U(t) &:= \int_1^b K(x, x; t) dx = \sum_{n=-\infty}^{\infty} e^{-ik_n t} \\ &= T \sum_{n=-\infty}^{\infty} e^{-i\frac{\pi}{2}\mu n} \delta(t - nT). \end{aligned} \quad (171)$$

If we now choose a test function h of H_r (definition 15.1) with an arbitrary $r > 0$, we get by identity (171) and the symmetry of h the trace formula

$$\begin{aligned} \int_{-\infty}^{\infty} \hat{h}(t) \text{Tr } U(t) dt &= \sum_{n=-\infty}^{\infty} h(k_n) \\ &= T \hat{h}(0) + T \sum_{n=1}^{\infty} (e^{-i\frac{\pi}{2}\mu n} \hat{h}(nT) + e^{i\frac{\pi}{2}\mu n} \hat{h}(-nT)) \\ &= T \hat{h}(0) + 2T \sum_{n=1}^{\infty} \cos\left(\frac{\pi}{2}\mu n\right) \hat{h}(nT). \end{aligned} \quad (172)$$

We recall that the S -matrix for this quantum graph is $\mathcal{S}(A, B) = e^{-2\pi ic} = e^{-i\frac{\pi}{2}\mu}$ (see (148)), and the length of the (single) edge is $l = \mathfrak{L} = \ln \frac{b}{1} = \ln b$. 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 $l_n = n \ln b$ and all are multiples of one primitive periodic orbit with length $l_1 = \ln b = T$. For the amplitude functions we get (see [35]) $\mathcal{A}_n = l_1 e^{-2\pi icn} = T e^{-i\frac{\pi}{2}\mu n}$. Applying (136) we get (172), which confirms the trace formula in theorem 15.2.

Example 16.4. We shall present a trace formula for the kernel $\tilde{K}(x, x_0; t)$ of the unitary evolution operator $e^{-itH_{\text{BK}}^2}$ 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 (165); thus the (Feynman-)kernel reads

$$\tilde{K}(x, x_0; t) := \sum_{n=1}^{\infty} \psi_n(x) \bar{\psi}_n(x_0) e^{-ik_n^2 t} \tag{173}$$

with the normalized eigenfunctions

$$\psi_n(x) := \sqrt{\frac{2}{l}} \frac{\sin\left(n\pi \frac{\ln x}{l}\right)}{\sqrt{x}}, \quad n \in \mathbb{N}, \tag{174}$$

where $l := \ln b$ denotes the length of the edge e . Using a suitable addition theorem for trigonometric functions, we get two alternative expressions for $\tilde{K}(x, x_0; t)$ (see [52, p 371]):

$$\begin{aligned} \tilde{K}(x, x_0; t) &= \frac{1}{\sqrt{x x_0} l_{\gamma_p}} \left[\Theta_3\left(\frac{1}{l_{\gamma_p}} \ln\left(\frac{x}{x_0}\right), -\frac{4\pi}{l_{\gamma_p}^2} t\right) - \Theta_3\left(\frac{1}{l_{\gamma_p}} \ln(x x_0), -\frac{4\pi}{l_{\gamma_p}^2} t\right) \right] \\ &= \frac{1}{2\sqrt{x x_0} \sqrt{i\pi t}} \sum_{n=0}^{\infty} \epsilon_n \left[e^{i2n\pi} \exp\left(i \frac{(\ln x - \ln x_0 + n l_{\gamma_p})^2}{4t}\right) \right. \\ &\quad + e^{i(2n+1)\pi} \exp\left(i \frac{(\ln x + \ln x_0 + n l_{\gamma_p})^2}{4t}\right) \\ &\quad + e^{i2n\pi} \exp\left(i \frac{(\ln x - \ln x_0 - n l_{\gamma_p})^2}{4t}\right) \\ &\quad \left. + e^{i(2n+1)\pi} \exp\left(i \frac{(\ln x + \ln x_0 - n l_{\gamma_p})^2}{4t}\right) \right], \tag{175} \end{aligned}$$

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

$$\epsilon_n := \begin{cases} \frac{1}{2} & \text{for } n = 0 \\ 1 & \text{for } n > 0. \end{cases} \tag{176}$$

$l_{\gamma_p} := 2l = 2 \ln b$ is the length of the primitive periodic orbit γ_p of the corresponding classical system. Note that the summands in the second identity in (175) 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. [50, 56]). For this reason, we define (cf (42)

and [28, p 30])

$$\tilde{K}_p(x, x_0; t) := \frac{1}{2\sqrt{i\pi t}} \exp\left(i \frac{l_p(x_0, x)^2}{4t}\right) \tag{177}$$

where $l_p(x_0, x)$ is the length of the path $p(x_0, x)$ (see (49)), and we then get by (175)

$$\begin{aligned} \tilde{K}(x, x_0; t) &= \frac{1}{\sqrt{xx_0}} \sum_{p(x_0, x)} \exp(i\pi n_{p(x_0, x)}) \tilde{K}_p(x, x_0; t) \\ &= \frac{1}{\sqrt{xx_0}} \sum_{p(x_0, x)} \exp\left(-i \frac{\pi \mu_{p(x_0, x)}}{2}\right) \tilde{K}_p(x, x_0; t), \end{aligned} \tag{178}$$

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 end points 1 and $\ln b$. $\mu_{p(x_0, x)}$ denotes the Maslov index of the path $p(x_0, x)$ which is given by $\mu_{p(x_0, x)} = 2n_{p(x_0, x)} \bmod 4$ in agreement with the ‘usual’ Maslov index for the one-dimensional billiard system corresponding to the negative Laplacian (see [55]), and with (167) (in (167) 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 $e^{-tH_{\text{BK}}^2}$ (replacing t by $-it$ in (173))

$$\tilde{K}_h(x, x_0; t) := \tilde{K}(x, x_0; -it) = \sum_{k_n} \psi(x) \bar{\psi}_n(x_0) e^{-k_n^2 t} \tag{179}$$

directly and then compare the result with the trace formula (137). Therefore, we recall that the wave numbers of H_{BK}^2 with (D) are explicitly given by (165). Thus, we obtain for the trace of the heat kernel (setting $\mathcal{L} := \frac{1}{2}l_{\gamma_p} := \ln b$ and [52, p 371])

$$\begin{aligned} \text{Tr } e^{-tH_{\text{BK}}^2} &= \int_1^b \sum_{k_n} \psi(x) \bar{\psi}_n(x) e^{-k_n^2 t} dx = \sum_{k_n} e^{-k_n^2 t} \\ &= \frac{1}{2} \left(\Theta_3\left(0, i \frac{4\pi}{l_{\gamma_p}^2} t\right) - 1 \right) \\ &= \frac{l_{\gamma_p}}{4\sqrt{t\pi}} \left(\sum_{n=-\infty}^{\infty} \exp\left(-\frac{n^2 l_{\gamma_p}^2}{4t}\right) \right) - \frac{1}{2} \\ &= \frac{\mathcal{L}}{2\sqrt{\pi t}} - \frac{1}{2} + \sum_{n=1}^{\infty} \frac{l_{\gamma_p}}{2\sqrt{\pi t}} e^{-\frac{(nl_{\gamma_p})^2}{4t}}. \end{aligned} \tag{180}$$

Note that the sums in (180) are absolutely convergent whereas in (171) the sums are convergent in the topology of $\mathcal{D}'(\mathbb{R})$ (in a distributional sense). In order to compare this result with (137), we recall that $C(1, \ln b; k')$ and the S -matrix $S_{(D)}$ for the Dirichlet case are given by (see (121) and (163))

$$S''_{(D)} = -\mathbb{1}_{2 \times 2} \quad \text{and} \quad C(1, \ln b; k') = \begin{pmatrix} \frac{\ln b}{2\frac{i}{k'} + \ln b} & \frac{2\frac{i}{k'}}{2\frac{i}{k'} + \ln b} \\ \frac{2\frac{i}{k'}}{2\frac{i}{k'} + \ln b} & \frac{\ln b}{2\frac{i}{k'} + \ln b} \end{pmatrix}. \tag{181}$$

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 wave

number $k_0 = 0$ of $F(k)$ in (118) 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 a 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 $l_{\gamma_p} = 2 \ln b$. For the amplitude functions A_γ in (137) we obtain $A_\gamma = \frac{1}{2}l_{\gamma_p}$ (see [35]). Furthermore, it is obvious that $\text{Im } S_D = 0$. Using the test function $h(k) := e^{-k^2 t}$ we obtain the Fourier transform $\hat{h}(x) = \frac{1}{2\sqrt{\pi t}} e^{-\frac{x^2}{4t}}$. Inserting these quantities in the trace formula (137) we get the trace formula (180), which again confirms the trace formula (137). We remark that from the small- t asymptotics (180) one obtains directly the Weyl asymptotics (138) using a proper Karamata–Tauberian theorem.

17. Summary and conclusions

We have studied the quantization of the extraordinarily simple classical Hamiltonian $H_{cl}(x, p) = xp$ about which Berry and Keating [11, 12] speculated that some quantization of it might yield the hypothetical Hilbert–Polya operator (see footnotes 1 and 2) [1, 2, 8–10] possessing as eigenvalues the nontrivial Riemann zeros. Two quantum Hamiltonians respectively Schrödinger operators have been considered: the original Berry–Keating operator $H_{BK} := -i\hbar(x \frac{d}{dx} + \frac{1}{2})$ obtained from H_{cl} by Weyl ordering, and the so-called squared Berry–Keating operator $H_{BK}^2 := -x^2 \frac{d^2}{dx^2} - 2x \frac{d}{dx} - \frac{1}{4}$ which is a special case of the famous Black–Scholes operator [31, 32] used in the financial theory of option pricing.

In section 2, we have given a complete description of the quantum dynamics generated by H_{BK} acting in the Hilbert space $L^2(\mathbb{R}_>, dx)$. While the one-dimensional quantum system governed by H_{BK} possesses many interesting properties, one of our main results of section 2 is that the spectrum of H_{BK} is purely continuous corresponding to scattering states. Since there are no bound states corresponding to a discrete spectrum, it is obvious that this specific quantization of the Berry–Keating operator cannot possess the Riemann zeros as part of its spectrum. Let us point out, however, that in the simple example 16.1 we have studied the quantum dynamics of H_{BK} for the particular square-integrable wavefunction (141) for which it turns out that the spectral decomposition consists of a continuous wave number spectrum, $k \in \mathbb{R}$, into which infinitely many absorption lines located exactly at the wave numbers $k_n = \tau_n \in \mathbb{R}$ corresponding to the nontrivial Riemann zeros satisfying the Riemann hypothesis are embedded. To our knowledge, there is, however, no relation of this occurrence of the Riemann zeros to the absorption spectrum interpretation of Connes [9, 10].

Analogous results have been obtained in section 4 for the ‘squared’ Berry–Keating operator H_{BK}^2 acting in the Hilbert space $L^2(\mathbb{R}_>, dx)$. We have proved that in this case the spectrum is purely continuous too and thus there holds again a ‘no-go theorem’ with respect to the identification of H_{BK}^2 with the hypothetical Hilbert–Polya operator.

In the main part of our paper, we have dealt with the quantum dynamics of H_{BK} respectively H_{BK}^2 on compact quantum graphs introduced in section 6. After having defined the Berry–Keating operator H_{BK} on compact graphs in section 7, we have given in proposition 8.1 a complete classification of all self-adjoint extensions of H_{BK} on compact quantum graphs in terms of two matrices A and B satisfying conditions (68). In proposition 9.1 we have established a secular equation valid for any self-adjoint realization in form of a determinant whose zeros determine the discrete spectrum of H_{BK} .

In sections 10–13, we have studied the quantization of the ‘squared’ Berry–Keating operator H_{BK}^2 on compact quantum graphs. Proposition 11.1 provides the complete classification of all self-adjoint realizations of H_{BK}^2 again in terms of matrices A and B

satisfying in this case conditions (97). For the discrete spectrum of H_{BK}^2 , we have given in proposition 12.1 the corresponding secular equation for $\lambda = k^2 \neq 0$. The zero eigenvalue $\lambda = k^2 = 0$ of H_{BK}^2 plays a special role which we have discussed in section 13 leading to the additional secular equation (121). Furthermore, in section 14 we have discussed the conditions under which H_{BK}^2 is the square of H_{BK} in the sense of (87), see proposition 14.1.

Based on the results derived in the previous sections, we have been able to state several theorems in section 15. In theorems 15.2 and 15.3 we have given an exact trace formula for H_{BK} respectively H_{BK}^2 for a large class of test functions $h(k)$ belonging to the space H_r defined in definition 15.1. The trace formulae establish a deep connection between the eigenvalue spectra of H_{BK} respectively H_{BK}^2 and the length spectra of the periodic orbits of the corresponding classical dynamics.

As an important consequence of the trace formulae, we have derived the Weyl asymptotics for H_{BK} (for H_{BK}^2 we have used results in [35]). The Weyl asymptotics of these operators have been given in theorems 15.5 and 15.4, respectively. A comparison with the expected Weyl asymptotics (48) respectively (32) for the nontrivial Riemann zeros demonstrates clearly that neither H_{BK} nor H_{BK}^2 can yield as eigenvalues the nontrivial zeros of the Riemann zeta function if these operators are self-adjoint realizations on any compact quantum graph, see theorem 15.6.

Finally, we have presented in section 16 four simple examples illustrating some aspects of the quantum dynamics of H_{BK} respectively H_{BK}^2 .

Acknowledgments

We would like to thank Wolfgang Arendt, Jens Bolte and Jan Eric Sträng for very helpful discussions and fruitful hints and Wolfgang Arendt for drawing our attention to [25–27]. SE would like to thank the graduate school ‘Analysis of evolution, information and complexity’ of the Land Baden–Württemberg for the stipend which has enabled this paper.

References

- [1] Weil A 1979 Commentaire ‘Sur les ‘formules explicites’ de la théorie des nombres premiers’ *Scientific Works. Collected Papers* (1951–1964) vol 2 (New York: Springer) p 527
- [2] Weil A 1952 Sur les ‘formules explicites’ de la théorie des nombres premiers *Commun. Sém. Math. Univ. Lund [Medd. Lunds Univ. Mat. Sem.]* **1952** 252–65
- [3] Selberg A 1956 Harmonic analysis and discontinuous groups in weakly symmetric Riemannian spaces with applications to Dirichlet series *J. Indian Math. Soc. (NS)* **20** 47–87
- [4] Hadamard J 1898 Les surfaces à courbures opposées et leurs lignes géodésiques *J. Math. Pure Appl.* **4** 27–73
- [5] Hadamard J 1898 Sur le billard non-Euclidien *Soc. Sci. Bordeaux, Proc. Verbaux* **147**
- [6] Gutzwiller M C 1980 Classical quantization of a Hamiltonian with ergodic behaviour *Phys. Rev. Lett.* **45** 150–3
- [7] Gutzwiller M C 1971 Periodic orbits and classical quantization conditions *J. Math. Phys.* **12** 343–58
- [8] Berry M V 1986 Riemann’s zeta function: a model for quantum chaos? *Quantum Chaos and Statistical Nuclear Physics (Lecture Notes in Physics vol 263)* ed T H Seligman and H Nishioka (New York: Springer) pp 1–17
- [9] Connes A 1996 Formule de trace en géométrie non-commutative et hypothèse de Riemann *C. R. Acad. Sci., Paris* **323** 1231–6
- [10] Connes A 1999 Trace formula in noncommutative geometry and the zeros of the Riemann zeta function *Sel. Math. (NS)* **5** 29–106
- [11] Berry M V and Keating J P 1999 $H = xp$ and the Riemann Zeros *Supersymmetry and Trace Formulae: Chaos and Disorder* ed I V Lerner, J P Keating and D E Khmelnitskii vol 263 (New York: Plenum) pp 355–67
- [12] Berry M V and Keating J P 1999 The Riemann zeros and eigenvalue asymptotics *SIAM Rev.* **41** 236–66
- [13] Kottos T and Smilansky U 1997 Quantum chaos on graphs *Phys. Rev. Lett.* **79** 4794–7
- [14] Kottos T and Smilansky U 1999 Periodic orbit theory and spectral statistics for quantum graphs *Ann. Phys., NY* **274** 76–124

- [15] Roth J-P 1983 Spectre du laplacien sur un graphe *C. R. Acad. Sci., Paris* **296** 793–5
- [16] von Below J 1985 A characteristic equation associated to an eigenvalue problem on c^2 -networks *Linear Algebr. Appl.* **71** 309–25
- [17] Exner P and Šeba P 1989 Free quantum motion on a branching graph *Rep. Math. Phys.* **28** 7–26
- [18] Exner P and Post O 2005 Convergence of spectra of graph-like thin manifolds *J. Geom. Phys.* **54** 77–115
- [19] Post O 2006 Spectral convergence of quasi-one-dimensional spaces *Ann. Henri Poincaré* **7** 933–73
- [20] Carlson R 2006 Linear network models related to blood flow *Quantum Graphs and Their Applications (Contemp. Math.* vol 415) (Providence, RI: American Mathematical Society) pp 65–80
- [21] Gelfand I M and Schilow G E 1960 *Verallgemeinerte Funktionen (Distributionen): I. Verallgemeinerte Funktionen und das Rechnen mit ihnen Hochschulbücher für Mathematik, Bd. 47.* VEB Deutscher (Berlin: Verlag der Wissenschaften)
- [22] Reed M and Simon B 1975 *Methods of Modern Mathematical Physics: II. Fourier Analysis, Self-Adjointness* (New York: Academic)
- [23] Titchmarsh E C 1948 *Introduction to the Theory of Fourier Integrals* (Oxford: Clarendon)
- [24] Weidmann J 2003 *Lineare Operatoren in Hilberträumen. Teil II Mathematische Leitfäden. [Mathematical Textbooks]* (Stuttgart: B G Teubner)
- [25] Arendt W 1994 Gaussian estimates and interpolation of the spectrum in L^p *Differ. Integral Equ.* **7** 1153–68
- [26] Arendt W 1995 Spectrum and growth of positive semigroups *Evolution Equations (Baton Rouge, LA, 1992) (Lecture Notes in Pure and Application Mathematics vol 168)* (New York: Dekker) pp 21–8
- [27] Arendt W and de Pagter B 2002 Spectrum and asymptotics of the Black–Scholes partial differential equation in (L^1, L^∞) -interpolation spaces *Pacific J. Math.* **202** 1–36
- [28] Grosche C and Steiner F 1998 *Handbook of Feynman Path Integrals (Springer Tracts in Modern Physics vol 145)* (Berlin: Springer)
- [29] Endres S and Steiner F 2009 A simple infinite quantum graph *Ulmer Seminare 2009* **14** 187–201
- [30] Gutzwiller M C 1990 *Chaos in Classical and Quantum Mechanics (Interdisciplinary Applied Mathematics vol 1)* (New York: Springer)
- [31] Black F and Scholes M S 1973 The pricing of options and corporate liabilities *J. Pol. Econ.* **81** 637–54
- [32] Merton R C 1973 Theory of rational option pricing *Bell J. Econ.* **4** 141–83
- [33] Terras A 1985 *Harmonic Analysis on Symmetric Spaces and Applications: I* (New York: Springer)
- [34] Kostyrykin V and Schrader R 1999 Kirchhoff’s rule for quantum wires *J. Phys. A: Math. Gen.* **32** 595–630
- [35] Bolte J and Endres S 2009 The trace formula for quantum graphs with general self adjoint boundary conditions *Ann. Poincaré* **10** 189–223
- [36] Weidmann J 2000 *Lineare Operatoren in Hilberträumen. Teil I Mathematische Leitfäden* (Stuttgart: B G Teubner)
- [37] Reed M and Simon B 1980 *Methods of modern mathematical physics: I Functional Analysis* 2nd edn (New York: Academic)
- [38] Kuchment P 2004 Quantum graphs: I. Some basic structures *Waves Random Media* **14** S107–28
- [39] Reed M and Simon B 1978 *Methods of Modern Mathematical Physics: IV. Analysis of Operators* (New York: Academic)
- [40] Everitt W N and Markus L 2005 Complex symplectic spaces and boundary value problems *Bull. Am. Math. Soc. (NS)* **42** 461–500
- [41] Kostyrykin V and Schrader R 2006 Laplacians on metric graphs: eigenvalues, resolvents and semigroups *Quantum Graphs and their Applications (Contemporary Mathematics vol 415)* ed G Berkolaiko, R Carlson, S A Fulling and P Kuchment (Providence, RI: American Mathematical Society) pp 201–25
- [42] Kostyrykin V and Schrader R 2006 The inverse scattering problem for metric graphs and the traveling salesman problem arXiv:math-ph/0603010
- [43] Carlson R 1999 Inverse eigenvalue problems on directed graphs *Trans. Am. Math. Soc.* **351** 4069–88
- [44] Thaller B 1992 *The Dirac equation Texts and Monographs in Physics* (Berlin: Springer)
- [45] Fulling S A, Kuchment P and Wilson J H 2007 Index theorems for quantum graphs *J. Phys. A: Math. Theor.* **40** 14165–80
- [46] Schrödinger E 1940 A method of determining quantum-mechanical eigenvalues and eigenfunctions *Proc. R. Irish Acad. A* **46** 9–16
- [47] Infeld L and Hull T E 1951 The factorization method *Rev. Modern Phys.* **23** 21–68
- [48] Kurasov P and Nowaczyk M 2005 Inverse spectral problem for quantum graphs *J. Phys. A: Math. Gen.* **38** 4901–15
- [49] Kostyrykin V and Schrader R 2003 Quantum wires with magnetic fluxes *Commun. Math. Phys.* **237** 161–79
- [50] Kostyrykin V, Potthoff J and Schrader R 2007 Heat kernels on metric graphs and a trace formula *Adventure in Mathematical Physics (Contemporary Mathematics vol 447)* ed F Germinet and P D Hislop (Providence, RI: American Mathematical Society) pp 175–98

- [51] Karamata J 1931 Neuer Beweis und Verallgemeinerung einiger Tauberian-Sätze *Math. Z.* **33** 294–9
- [52] Magnus W, Oberhettinger F and Soni R P 1966 *Formulas and Theorems for the Special Functions of Mathematical Physics (Die Grundlehren der mathematischen Wissenschaften, Band 52)* 3rd enlarged edn (New York: Springer)
- [53] Einstein A 1917 Zum Qantensatz von Sommerfeld und Epstein (in German) *Verh. Deutsche Phys. Ges.* **19** 82–92
- [54] Keller J B 1958 Corrected Bohr–Sommerfeld quantum conditions for nonseparable systems *Ann. Phys.* **4** 180–8
- [55] Stöckmann H-J 1999 *Quantum Chaos: An Introduction* (Cambridge: Cambridge University Press)
- [56] Barra F and Gaspard P 2002 Transport and dynamics on open quantum graphs *Phys. Rev. E* **65** 016205, 21