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JENS BOLTE, SEBASTIAN EGGER AND STEFAN KEPPELER

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Mathematisches Forschungsinstitut Oberwolfach gGmbH (MFO)
Schwarzwaldstrasse 9-11
77709 Oberwolfach-Walke
Germany

Tel +49 7834 979 50
Fax +49 7834 979 55
Email admin@mfo.de
URL www.mfo.de

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The Berry-Keating operator on a lattice

Jens Bolte¹, Sebastian Egger², and Stefan Keppeler³

Abstract

We construct and study a version of the Berry-Keating operator with a built-in truncation of the phase space, which we choose to be a two-dimensional torus. The operator is a Weyl quantisation of the classical Hamiltonian for an inverted harmonic oscillator, producing a difference operator on a finite, periodic lattice. We investigate the continuum and the infinite-volume limit of our model in conjunction with the semiclassical limit. Using semiclassical methods, we show that a specific combination of the limits leads to a logarithmic mean spectral density as it was anticipated by Berry and Keating.

¹Department of Mathematics, Royal Holloway, University of London, Egham, TW20 0EX, United Kingdom, jens.bolte@rhul.ac.uk

²Department of Mathematics, Technion–Israel Institute of Technology, 629 Amado Building, Haifa 32000, Israel, egger@tx.technion.ac.il

³Fachbereich Mathematik, Universität Tübingen, Auf der Morgenstelle 10, 72076 Tübingen, Germany, stefan.keppeler@uni-tuebingen.de

1 Introduction

Phase-space methods in quantum mechanics are often used in a semiclassical context because they link (pseudo-)differential operators and functions on a classical phase space, see, e.g., [Zwo12]. In such a context the phase space is a cotangent bundle of a manifold (the configuration space) and, hence, is not compact. In contrast, quantisations on compact phase spaces lead to operators in finite dimensional Hilbert spaces. The latter approach is frequently used to quantise symplectic maps on tori [BD96, DEG03], the most prominent example being the cat map [HB80]. However, one can also quantise Hamiltonian flows on tori and therefore obtain a phase-space representation of a Schrödinger equation in a finite dimensional Hilbert space. In this context the Hamiltonian operator can be interpreted as a difference operator on a finite lattice with periodic boundary conditions. If the classical phase space is a two-dimensional torus one has two length parameters available in addition to the semiclassical parameter. In models with difference operators on periodic lattices these length scales can be used to perform a continuum limit as well as an infinite volume limit.

In this paper we explore the various limits in a discrete variant of the Berry-Keating operator that was introduced in [BK99a]. The latter is a differential operator with a self-adjoint realisation in $L^2(\mathbb{R})$ and, therefore, can be represented in the phase space $T^*\mathbb{R}$. Inspired by the work of Connes [Con96, Con99], Berry and Keating intended to define a self-adjoint operator whose spectrum is related to the non-trivial zeros of the Riemann zeta function. In particular, the mean spectral density of this operator should follow the same asymptotic, logarithmic law as that of the Riemann zeros. To this end they considered a quantisation of the classical Hamiltonian $H(q, p) = qp$. The first obstacle that needed to be addressed was that the naive version of the operator has a purely continuous spectrum, which is related to the fact that the energy surfaces in phase space are not compact. For that reason Berry and Keating suggested a truncation of these energy surfaces [BK99a, BK99b], however, without defining an operator that would correspond to that truncation. Using standard semiclassical techniques, they then showed that the truncated energy surfaces would lead to the desired form of the mean spectral density. Later, a modification was suggested [SRL11] to overcome the problems with the phase-space truncation, and this was subsequently improved in [BK11]. These modifications keep the non-compact phase space $T^*\mathbb{R}$, but add terms to the classical Hamiltonian in such a way that its energy surfaces are compact, yet the resulting semiclassical spectral density has the same leading asymptotic behaviour as before. After quantisation, however, the additional terms lead to non-local contributions to the quantum Hamiltonian.

In other approaches two-dimensional, semi-inverted oscillators were related to the Riemann zeta function and its zero-count [BKRT97], and versions of the Berry-Keating operator on a half-line as well as on quantum graphs were investigated [ES10]. The connection of the Berry-Keating operator with local versions of the Riemann hypothesis was studied in [Sre11]. More recently, a PT-symmetric, non-hermitian variant of the Berry-Keating operator [BBM16] as well as a version in polymeric quantum mechanics [BMM16] were studied.

Our proposal differs from previous approaches in that we use a two-dimensional torus as phase space, but keep the classical Hamiltonian (up to a linear canonical transformation). Weyl quantisation on this compact phase space will immediately produce a self-adjoint operator in an N -dimensional Hilbert space that, therefore, will have a discrete, even finite, spectrum. The number N of eigenvalues tends to infinity in the semiclassical limit, which in this context is well known to be the limit $N \rightarrow \infty$. The model allows us to study various limits of the operator and its spectrum, including semiclassical, continuum and infinite-volume limits, or combinations thereof. We also use semiclassical methods that are mainly based on a Gutzwiller trace formula which we proved previously [BEK15]. In that context we identify a way to choose the length scales of the torus in such a way that they produce the same cut-off as it was imposed in [BK99a]. As a consequence, the semiclassical approximation of the spectral density is the same as in [BK99a].

The paper is organised as follows. In Section 2 we review the model of Berry and Keating and then introduce our model. In the next section we analyse the continuum and the infinite-volume limit. This is first done very explicitly in the example of the quantisation of the symbol ξ^2 , and then qualitatively for our model. Section 4 is devoted to a semiclassical calculation of the spectral density in our model. The result is compared to numerical data in the following section. We present our conclusions in Section 6. Two appendices contain a proof of a lemma in Section 2 and the calculation of the matrix elements of our model operator, respectively.

2 The model

Berry and Keating [BK99a, BK99b] consider the operator

$$H_{\text{BK}} = \frac{\hbar}{i} x \frac{d}{dx} + \frac{\hbar}{2i}, \quad (2.1)$$

which is a (Weyl) quantisation of the symbol $h_{\text{BK}}(q, p) = qp$ on the phase space $\mathbb{T}^*\mathbb{R}$. Their intention is to count the number of eigenvalues in spectral intervals, however, the operator H_{BK} defined on a suitable domain in $L^2(\mathbb{R})$ has a continuous spectrum and no eigenvalues. They, therefore, suggest a cut-off in phase space to enforce the energy surfaces $h_{\text{BK}}^{-1}(E) \subset \mathbb{T}^*\mathbb{R}$ to be compact. One would expect a modification of the operator (2.1) that reflects the truncation of the energy surfaces to possess a purely discrete spectrum. However, no definition of an operator is given.

The cut-off procedure they suggest is to only consider the subset

$$\{(q, p) \in \mathbb{T}^*\mathbb{R}; q \geq L_q, p \geq L_p\}, \quad (2.2)$$

of phase space, where $L_q > 0$ and $L_p > 0$ are parameters satisfying $L_q L_p = 2\pi\hbar$. Before the truncation the energy surface consists of the points $(q, p) \in \mathbb{T}^*\mathbb{R}$ on the two branches of the hyperbola $qp = E$. After the truncation only the part in the first quadrant satisfying

$$L_q \leq q \leq \frac{E}{L_p} \quad \text{and} \quad L_p \leq p \leq \frac{E}{L_q} \quad (2.3)$$

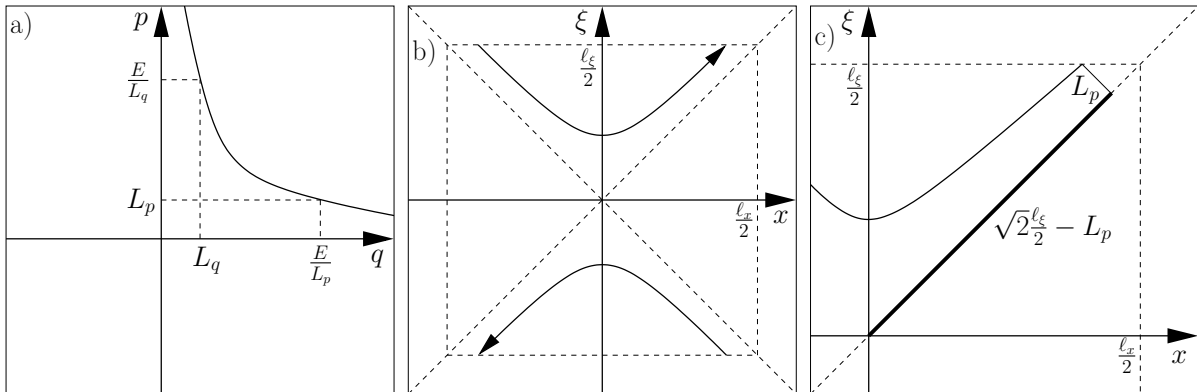


Figure 1: Energy surfaces (a) for the classical Hamiltonian corresponding to the Berry-Keating operator, with cut-off parameters L_q and L_p , and (b) for the rotated Hamiltonian (2.5), with fundamental domain characterised by ℓ_x and ℓ_ξ ; (c) relation between $L_{q,p}$ and $\ell_{x,\xi}$, see Sec. 4.

remains, see Figure 1(a). This has finite volume, suggesting that a related operator would possess a purely discrete spectrum. Berry and Keating also propose that one should identify p with $-p$ and/or q with $-q$ in a yet to be specified way.

With the last suggestion in mind we propose to ‘compactify’ phase space independent of E in that $\mathbb{T}^*\mathbb{R}$ is replaced by a torus, \mathbb{R}^2/Γ , where $\Gamma \cong \mathbb{Z}^2$ is a lattice. Any observable then has to be a function on \mathbb{R}^2 that is periodic with respect to Γ . If the lattice were chosen such that it acts on points in \mathbb{R}^2 as $(q, p) \mapsto (q + na, p + mb)$, with some fixed parameters $a, b > 0$ and integers n, m , observables would have to be functions f that are periodic in q and p . The symbol $h_{\text{BK}}(q, p) = qp$ clearly does not have this property, so one would need to restrict it to a fundamental domain of Γ , say, $0 \leq q \leq a$, $0 \leq p \leq b$, and extend it periodically to \mathbb{R}^2 . The result would be a function on \mathbb{R}^2 that is not continuous.

One can achieve an improvement by introducing new coordinates,

$$x = \frac{p - q}{\sqrt{2}} \quad \text{and} \quad \xi = \frac{p + q}{\sqrt{2}}. \quad (2.4)$$

The map $(q, p) \mapsto (x, \xi)$ is symplectic (a canonical transformation), and the symbol h_{BK} is transformed to

$$h(x, \xi) = \frac{\xi^2 - x^2}{2}. \quad (2.5)$$

One then defines the lattice $\ell_x\mathbb{Z} \oplus \ell_\xi\mathbb{Z}$ acting on \mathbb{R}^2 as $(x, \xi) \mapsto (x + n\ell_x, \xi + m\ell_\xi)$, $n, m \in \mathbb{Z}$. Restricting $h(x, \xi)$ to a fundamental domain $(-\ell_x/2, \ell_x/2) \times (-\ell_\xi/2, \ell_\xi/2)$ of the lattice and extending it periodically to \mathbb{R}^2 then gives a continuous, albeit not differentiable, function. Hence, the Fourier series for h will have improved convergence properties over the Fourier series for h_{BK} . As opposed to some alternative suggestions this procedure maintains the symmetry in x and ξ , at least when choosing $\ell_x = \ell_\xi$. A fundamental domain of the lattice as well as an energy surface of h are shown in Figure 1(b).

Returning to operators defined in $L^2(\mathbb{R})$, a (Weyl) quantisation of the symbol (2.5) produces the Hamiltonian operator for an inverted oscillator,

$$H = -\frac{\hbar^2}{2} \frac{d^2}{dx^2} - \frac{1}{2}x^2, \quad (2.6)$$

that one can define on the domain $C_0^\infty(\mathbb{R})$.

Proposition 1. *The operator H has the following properties:*

- (i) *Defined on the domain $C_0^\infty(\mathbb{R})$, it is essentially self-adjoint. (For simplicity we denote its self-adjoint extension also as H .)*
- (ii) *It is unitarily equivalent to the operator H_{BK} defined in (2.1).*
- (iii) *H has a purely absolutely continuous spectrum, $\sigma(H) = \sigma_{\text{ac}}(H) = \mathbb{R}$.*

Proof. The proof uses standard arguments:

- (i) This property follows from [Wei03, Satz 17.15].
- (ii) The symbol h of the operator H was obtained from the symbol h_{BK} of the operator H_{BK} through the linear symplectic map (2.4). A combination of [Fol89, Eq. (2.1)] with [Fol89, Eq. (4.23)] therefore yields that H and H_{BK} are unitarily equivalent. More specifically, by referring to the Heisenberg equations of motion for a harmonic oscillator one can confirm that, indeed,

$$e^{i\frac{\pi}{4\hbar}H_{\text{osc}}} H_{\text{BK}} e^{-i\frac{\pi}{4\hbar}H_{\text{osc}}} = H, \quad \text{where} \quad H_{\text{osc}} = -\frac{\hbar^2}{2} \frac{d^2}{dx^2} + \frac{1}{2}x^2. \quad (2.7)$$

- (iii) In [Per83, Proposition 6.2] as well as in [Wei03, Satz 24.6] it is shown that the spectrum of H_{BK} is \mathbb{R} and is purely absolutely continuous. By (ii) the same then holds for the operator H .

□

We now turn to constructing a model operator by Weyl quantising the equivalent of the symbol (2.5) on the torus $\mathbb{R}^2/\ell_x\mathbb{Z} \oplus \ell_\xi\mathbb{Z}$. Hence, for all $n, m \in \mathbb{Z}$ we set

$$h(x, \xi) = \frac{(\xi - m\ell_\xi)^2 - (x - n\ell_x)^2}{2}, \quad \text{if} \quad \begin{cases} (m - \frac{1}{2})\ell_\xi \leq \xi < (m + \frac{1}{2})\ell_\xi \\ (n - \frac{1}{2})\ell_x \leq x < (n + \frac{1}{2})\ell_x \end{cases}. \quad (2.8)$$

This function has a representation as a Fourier series,

$$h(x, \xi) = \sum_{n, m \in \mathbb{Z}} h_{mn} e^{2\pi i \left(\frac{m\xi}{\ell_\xi} - \frac{nx}{\ell_x} \right)}, \quad (2.9)$$

with coefficients

$$h_{mn} = \begin{cases} \frac{\ell_\xi^2 - \ell_x^2}{24}, & \text{if } (m, n) = (0, 0) \\ \frac{1}{4\pi^2} \left(\ell_\xi^2 \frac{(-1)^m}{m^2} (1 - \delta_{m0}) \delta_{n0} - \ell_x^2 \frac{(-1)^n}{n^2} (1 - \delta_{n0}) \delta_{m0} \right), & \text{if } (m, n) \neq (0, 0) \end{cases}. \quad (2.10)$$

The Weyl quantisation on the torus was introduced in [HB80], for details see, e.g., [BD96, DEG03]. It assigns to the function (2.8) with Fourier coefficients (2.10) an operator

$$\text{op}_N(h) := \sum_{m, n \in \mathbb{Z}} h_{mn} T^{m, n} \quad (2.11)$$

acting in \mathbb{C}^N . When h is real valued and \mathbb{C}^N is equipped with the standard inner product, $\text{op}_N(h)$ is self-adjoint. Here the unitary operators

$$T^{m, n} = e^{i\pi \frac{nm}{N}} T^{m, 0} T^{0, n} \quad (2.12)$$

in \mathbb{C}^N are defined through the actions

$$(T^{m, 0} \psi)_l := \psi_{l+m} \quad \text{and} \quad (T^{0, n} \psi)_l := e^{-\frac{2\pi i l n}{N}} \psi_l \quad (2.13)$$

on $\psi = (\psi_l) \in \mathbb{C}^N$, where we use the convention that $\psi_{l+N} = \psi_l$. The operators $T^{m, 0}$ and $T^{0, n}$ represent translations in the x - and ξ -directions, respectively. The integer $N \in \mathbb{N}$ is a semiclassical parameter, such that $N \rightarrow \infty$ is the semiclassical limit. It satisfies the relation

$$2\pi \hbar N = \ell_\xi \ell_x. \quad (2.14)$$

Therefore, the Weyl quantisation of the symbol (2.8) is

$$\begin{aligned} \text{op}_N(h) &= \frac{\ell_\xi^2 - \ell_x^2}{24} T^{0, 0} + \frac{\ell_\xi^2}{4\pi^2} \sum_{m=1}^{\infty} \frac{(-1)^m}{m^2} (T^{m, 0} + T^{-m, 0}) \\ &\quad - \frac{\ell_x^2}{4\pi^2} \sum_{n=1}^{\infty} \frac{(-1)^n}{n^2} (T^{0, n} + T^{0, -n}), \end{aligned} \quad (2.15)$$

and acts on a vector $\psi = (\psi_l) \in \mathbb{C}^N$ as

$$\begin{aligned} (\text{op}_N(h)\psi)_l &= \frac{\ell_\xi^2 - \ell_x^2}{24} \psi_l + \frac{\ell_\xi^2}{4\pi^2} \sum_{m=1}^{\infty} \frac{(-1)^m}{m^2} (\psi_{l+m} + \psi_{l-m}) \\ &\quad - \frac{\ell_x^2}{4\pi^2} \sum_{n=1}^{\infty} \frac{(-1)^n}{n^2} (e^{-\frac{2\pi i l n}{N}} + e^{\frac{2\pi i l n}{N}}) \psi_l \\ &= \frac{\ell_\xi^2}{24} \psi_l + \frac{\ell_\xi^2}{4\pi^2} \sum_{m=1}^{\infty} \frac{(-1)^m}{m^2} (\psi_{l+m} + \psi_{l-m}) - \frac{1}{2} \left(\frac{\ell_x}{N} \right)^2 \psi_l. \end{aligned} \quad (2.16)$$

It can hence be seen as a difference operator on a lattice with N points and periodic boundary conditions.

The spectrum $\sigma(\text{op}_N(h))$ of $\text{op}_N(h)$ consists of N real eigenvalues E_n .

Lemma 1. *When $l_x = l_\xi$ the spectrum of $\text{op}_N(h)$ is symmetric about zero, i.e., $E_n \in \sigma(\text{op}_N(h))$ implies that $-E_n \in \sigma(\text{op}_N(h))$.*

We prove this lemma in Appendix A.

Below we wish to study the distribution of the eigenvalues of $\text{op}_N(h)$ in the semiclassical limit $N \rightarrow \infty$. We intend our approach to provide an approximation to the operator (2.6) and, therefore, keep the value of \hbar fixed. Due to the relation (2.14), the semiclassical limit $N \rightarrow \infty$ can then be achieved by sending l_ξ and/or l_x to infinity.

3 Continuum and infinite volume limit

Before studying spectral properties of the operator $\text{op}_N(h)$ in various combinations of the limits $l_\xi \rightarrow \infty$ and $l_x \rightarrow \infty$, we want to explore their interpretation in some more detail. It is obvious from the set-up that l_x measures the extension of the model in ‘configuration space’, whereas l_ξ is the corresponding measure in ‘momentum space’. One may then view vectors $\psi = (\psi_n) \in \mathbb{C}^N$ as functions evaluated at the N equidistant points

$$x_n = \frac{n l_x}{N} \in \left[-\frac{l_x}{2}, \frac{l_x}{2} \right), \quad (3.1)$$

where $-\frac{N}{2} \leq n < \frac{N}{2}$. The distance between neighbouring points can be expressed as

$$\frac{l_x}{N} = \frac{2\pi\hbar}{l_\xi} \quad (3.2)$$

by making use of the relation (2.14). As we keep \hbar fixed, taking $l_\xi \rightarrow \infty$ corresponds to a continuum limit, in which difference operators approximate differential operators. In contrast, taking $l_x \rightarrow \infty$ corresponds to an infinite-volume limit. Both limits are semiclassical in the sense of Weyl quantisation on a torus as they imply $N \rightarrow \infty$.

When a symbol only depends on either x or ξ , the spectrum of its quantisation can be determined explicitly. As a simplification of (2.8) we therefore choose

$$a(\xi) = (\xi - m l_\xi)^2, \quad \text{if } \left(m - \frac{1}{2}\right) l_\xi \leq \xi < \left(m + \frac{1}{2}\right) l_\xi, \quad m \in \mathbb{Z}, \quad (3.3)$$

with Fourier expansion

$$a(\xi) = \frac{l_\xi^2}{12} + \frac{l_\xi^2}{\pi^2} \sum_{n=1}^{\infty} \frac{(-1)^n}{n^2} \cos\left(\frac{2\pi}{l_\xi} n \xi\right). \quad (3.4)$$

Its quantisation is

$$\text{op}_N(a) = \frac{l_\xi^2}{12} + \frac{l_\xi^2}{2\pi^2} \sum_{n=1}^{\infty} \frac{(-1)^n}{n^2} (T^{n,0} + T^{-n,0}). \quad (3.5)$$

We define plane waves $\psi^{(\nu)} = (\psi_m^{(\nu)}) \in \mathbb{C}^N$ as

$$\psi_m^{(\nu)} = e^{\frac{i}{\hbar} \frac{\nu \ell_\xi}{N} \frac{m \ell_x}{N}} = e^{2\pi i \frac{\nu m}{N}}. \quad (3.6)$$

Choosing $\nu \in \mathbb{Z}$ with $-\frac{N}{2} \leq \nu < \frac{N}{2}$ ensures that the N momenta satisfy

$$\frac{\nu \ell_\xi}{N} \in \left[-\frac{\ell_\xi}{2}, \frac{\ell_\xi}{2} \right). \quad (3.7)$$

Plane waves can easily be seen to be eigenfunctions of the operators $T^{n,0}$,

$$(T^{n,0} \psi^{(\nu)})_m = e^{2\pi i \frac{\nu n}{N}} \psi_m^{(\nu)}, \quad (3.8)$$

and consequently

$$(\text{op}_N(a) \psi^{(\nu)})_m = \left(\frac{\ell_\xi^2}{12} + \frac{\ell_\xi^2}{\pi^2} \sum_{n=1}^{\infty} \frac{(-1)^n}{n^2} \cos\left(2\pi \frac{\nu n}{N}\right) \right) \psi_m^{(\nu)} = \left(\frac{\nu \ell_\xi}{N} \right)^2 \psi_m^{(\nu)}. \quad (3.9)$$

It is convenient to express the eigenvalues $E_\nu^N = \left(\frac{\nu \ell_\xi}{N} \right)^2$ in several ways,

$$E_\nu^N = \ell_\xi^2 \frac{\nu^2}{N^2} \quad (3.10a)$$

$$= \left(\frac{2\pi \hbar}{\ell_x} \right)^2 \nu^2 \quad (3.10b)$$

$$= 2\pi \hbar \frac{\ell_\xi}{\ell_x} \frac{\nu^2}{N}. \quad (3.10c)$$

We note in passing that

$$\inf \sigma(\text{op}_N(a)) = 0 \quad \text{and} \quad \sup \sigma(\text{op}_N(a)) = \begin{cases} \frac{\ell_\xi^2}{4} & \text{for } N \text{ even} \\ \frac{\ell_\xi^2}{4} \left(\frac{N-1}{N} \right)^2 & \text{for } N \text{ odd} \end{cases}, \quad (3.11)$$

and that the nearest-neighbour separation of eigenvalues (for non-negative ν) is

$$s_\nu^N = E_{\nu+1}^N - E_\nu^N = \ell_\xi^2 \frac{2\nu + 1}{N^2} \quad (3.12a)$$

$$= \left(\frac{2\pi \hbar}{\ell_x} \right)^2 (2\nu + 1) \quad (3.12b)$$

$$= 2\pi \hbar \frac{\ell_\xi}{\ell_x} \frac{2\nu + 1}{N}. \quad (3.12c)$$

We now discuss the behaviour of the spectrum in the continuum- and/or infinite-volume limit:

1. *Continuum limit in finite volume*, i.e., l_x fixed, $l_\xi \rightarrow \infty$: From (3.10b) one sees that the eigenvalues, even before taking the limit, are the same as eigenvalues of the operator $-\hbar^2 \frac{d^2}{dx^2}$ on an interval $[-l_x/2, l_x/2]$ with periodic boundary conditions. The only effect of the limit $N \rightarrow \infty$ hence is a growing number of eigenvalues, eventually covering the entire spectrum of the differential operator. The separation of neighbouring eigenvalues (3.12b) is unaffected.
2. *Infinite volume limit on the lattice* $\frac{2\pi\hbar}{l_\xi}\mathbb{Z}$, i.e., l_ξ fixed, $l_x \rightarrow \infty$: In this limit the expression on the right-hand side of (3.5) for the operator $\text{op}_N(a)$ is unaffected by the limit; $\text{op}_N(a)$ remains a difference operator, albeit on a growing lattice that tends to an infinite lattice in the limit. From (3.11) we see that the spectrum remains in the finite interval $[0, \ell_\xi^2/4]$, whereas (3.12a) shows that the eigenvalues become dense everywhere in this interval.
3. *Continuum limit in infinite volume*, i.e., $l_x \rightarrow \infty$ and $l_\xi \rightarrow \infty$: Combining the two previous cases one might expect a convergence (in a suitable sense) of the difference operator $\text{op}_N(a)$ to the differential operator $-\hbar^2 \frac{d^2}{dx^2}$ acting in $L^2(\mathbb{R})$. The spectrum is expected to approach a ‘continuous’ spectrum $[0, \infty)$. Indeed, (3.11) implies that $\sup \sigma(\text{op}_N(a)) \rightarrow \infty$ in this case, but whether the eigenvalues become dense depends on how fast l_x and l_ξ go to ∞ , and the answer can be different in different ranges. To illustrate this we set

$$l_\xi = AN^\alpha, \quad l_x = BN^{1-\alpha} \quad (3.13)$$

with $\alpha \in (0, 1)$ and constants A, B satisfying $AB = 2\pi\hbar$ in order to comply with (2.14). Then according to (3.10c) and (3.12c),

$$E_\nu^N = A^2 N^{2\alpha-2} \nu^2 \quad \text{and} \quad s_\nu^N = A^2 N^{2\alpha-2} (2\nu + 1). \quad (3.14)$$

Thus, at a fixed range in the spectrum, i.e. when ν grows like $N^{1-\alpha}$, the eigenvalues become dense for every $\alpha > 0$. Near the supremum of the spectrum, i.e., when ν grows proportional to N , the eigenvalues only become dense if $\alpha < \frac{1}{2}$, i.e., if l_x grows faster than l_ξ .

When $l_x = l_\xi$, the operators $\text{op}_N(a)$ and $\text{op}_N(b)$, where $b(x) = x^2$, are unitarily equivalent via the discrete Fourier transform, see (A.6). Therefore, the operators have the same spectrum and the above discussion applies to $\text{op}_N(b)$ too. However, even when $l_x \neq l_\xi$ can one carry over the above analysis to $\sigma(\text{op}_N(b))$; one only needs to swap l_ξ and l_x .

For the operator $\text{op}_N(h)$ we expect a qualitatively similar behaviour. We first note that since

$$\text{op}_N(h) = \frac{1}{2}(\text{op}_N(a) - \text{op}_N(b)), \quad (3.15)$$

and both $\text{op}_N(a)$ and $\text{op}_N(b)$ are positive operators, the min-max principle allows us to bound the spectrum of $\text{op}_N(h)$ from above and below in terms of the upper bounds $E_{a,\max} = \ell_\xi^2/4$ and $E_{b,\max} = \ell_x^2/4$ for $\text{op}_N(a)$ and $\text{op}_N(b)$, respectively,

$$-\frac{\ell_x^2}{8} \leq \text{op}_N(h) \leq \frac{\ell_\xi^2}{8}. \quad (3.16)$$

In the various cases of sending ℓ_ξ and/or ℓ_x to infinity we make the following observations:

1. *Continuum limit in finite volume*, i.e., ℓ_x fixed, $\ell_\xi \rightarrow \infty$: The explicit form (B.11) of the matrix elements of $\text{op}_N(h)$ show that in this limit $\text{op}_N(a)$ dominates, so that $\text{op}_N(b)$ can be seen as a perturbation. Hence, as $\ell_\xi \rightarrow \infty$ the eigenvalues of $\text{op}_N(h)$ will asymptotically be given by (one half of) the right-hand side of (3.10) (ν fixed). This will describe large eigenvalues; at the bottom of the spectrum the contribution of $\text{op}_N(b)$ will have an effect. As can be seen from (3.16), in the limit the spectrum will be contained in $[-\ell_x^2/8, \infty)$. We expect the limiting operator to be

$$-\frac{\hbar^2}{2} \frac{d^2}{dx^2} - \frac{1}{2} x^2 \quad (3.17)$$

on the interval $[-\ell_x/2, \ell_x/2]$ with periodic boundary conditions.

2. *Infinite volume limit on the lattice* $\frac{2\pi\hbar}{\ell_\xi}\mathbb{Z}$, i.e., ℓ_ξ fixed, $\ell_x \rightarrow \infty$: This limit describes the opposite case to the previous one, in that $\text{op}_N(a)$ will be a perturbation of $-\text{op}_N(b)$. Asymptotically, the eigenvalues will be given by $-\frac{1}{2}$ times the right-hand side of (3.10) with ℓ_x instead of ℓ_ξ . The limiting spectrum will be contained in $(-\infty, \ell_\xi^2/8]$.
3. *Continuum limit in infinite volume*, specifically, $\ell := \ell_x = \ell_\xi \rightarrow \infty$: From (B.11) one obtains that all matrix elements of $\text{op}_N(h)$ contain a factor ℓ^2 , hence the eigenvalues will have the same factor and otherwise be independent of ℓ . The only conclusion one can draw from the bounds (3.16) is that the limiting spectrum will be contained in \mathbb{R} . We expect the limiting operator to be H (2.6), whose spectrum is described in Proposition 1.

The semiclassical discussion in the following section will confirm this picture.

4 Semiclassics

For a semiclassical analysis of the spectrum of $\text{op}_N(h)$ we need to determine some classical quantities, including the energy surface and periodic orbits of the Hamiltonian flow, as well as their actions and periods. We first note that

$$-\frac{\ell_x^2}{8} \leq E \leq \frac{\ell_\xi^2}{8}, \quad (4.1)$$

which is the classical equivalent to (3.16). For these values of E the energy surface is

$$\Sigma_E = \left\{ (x, \xi) \in \left(-\frac{\ell_x}{2}, \frac{\ell_x}{2} \right) \times \left(-\frac{\ell_\xi}{2}, \frac{\ell_\xi}{2} \right); \frac{\xi^2 - x^2}{2} = E \right\}. \quad (4.2)$$

When $\ell_\xi = \ell_x$, the energy surface is always connected. Otherwise, depending on the values for ℓ_ξ, ℓ_x, E it is either connected or consists of two connected components. The latter case occurs when either $\ell_\xi > \ell_x$ and

$$0 < E < \frac{\ell_\xi^2 - \ell_x^2}{8}, \quad (4.3)$$

or when $\ell_x > \ell_\xi$ and

$$\frac{\ell_\xi^2 - \ell_x^2}{8} < E < 0. \quad (4.4)$$

In all other cases Σ_E is connected. Likewise, when Σ_E is connected, there is only one primitive periodic orbit p of the Hamiltonian flow. Its period t_p then is the volume (in Liouville measure) of Σ_E . When Σ_E has two components, however, there are two primitive periodic orbits p and p^{-1} , where the latter is the time reversal of the former. In this case the volume of Σ_E is the sum of t_p and $t_{p^{-1}}$, i.e., $2t_p$.

When one keeps ℓ_x fixed and increases ℓ_ξ , only in the small range $\ell_\xi^2 - \ell_x^2 < 8E < \ell_\xi^2$ will Σ_E be connected. In the large energy range (4.3) Σ_E has two components. As E grows, these components approach the two components of the energy surface

$$\Sigma_E^0 := \left\{ (x, \xi); \xi = \pm\sqrt{2E} \right\} \quad (4.5)$$

of $\xi^2/2$. A Bohr-Sommerfeld quantisation of the energy surfaces Σ_E hence demonstrates that semiclassical approximations of large eigenvalues of $\text{op}_N(h)$ in the range (4.3) approach semiclassical approximations of the eigenvalues of the operator $-\frac{\hbar^2}{2} \frac{d^2}{dx^2}$ on the interval $[-\ell_x/2, \ell_x/2]$ with periodic boundary conditions. (The latter are identical with the exact eigenvalues (3.10b).) Near the bottom of the spectrum one would approximate eigenvalues with Bohr-Sommerfeld quantisations of surfaces Σ_E at small, positive values of E , which deviate essentially from the corresponding energy surfaces Σ_E^0 . There will also be a limited range of negative energies with connected Σ_E whose quantisations may approximate negative eigenvalues. Thus, the semiclassical picture conforms with our discussion in Section 3.

When ℓ_x grows while ℓ_ξ is kept fixed, the above discussion applies after having swapped x and ξ as well as positive E and negative E . In the case $\ell_x = \ell_\xi$ all energy surfaces are connected and there is a complete symmetry in x and ξ . After Bohr-Sommerfeld quantisation this leads to a semiclassical equivalent of Lemma 1.

We now calculate the action S_p and period t_p of the single primitive periodic orbit p in the case of a connected energy surface at positive energy E ,

$$S_p = \oint_p \xi dx \quad \text{and} \quad t_p = \frac{dS_p}{dE}. \quad (4.6)$$

At negative energy one has to swap x and ξ , but otherwise gets the same expressions. In the fundamental domain the primitive orbit p consists of the two sections of the hyperbola $\xi^2 - x^2 = 2E$ between the points $(x_-, \ell_\xi/2)$ and $(x_+, \ell_\xi/2)$, and $(x_+, -\ell_\xi/2)$ and $(x_-, -\ell_\xi/2)$,

respectively, as shown in Figure 1(b). Here we have defined $x_{\pm} = \pm\sqrt{\ell_{\xi}^2/4 + 2E}$. Thus, for the action we find

$$\begin{aligned} S_p &= 2 \int_{x_-}^{x_+} \sqrt{x^2 + 2E} \, dx + \ell_{\xi}(x_+ - x_-) \\ &= 4E \operatorname{arsinh} \sqrt{\frac{\ell_{\xi}^2}{8E} - 1} - \frac{\ell_{\xi}}{2} \sqrt{\ell_{\xi}^2 - 8E}. \end{aligned} \quad (4.7)$$

The derivative of this result yields the period,

$$t_p = 4 \operatorname{arsinh} \sqrt{\frac{\ell_{\xi}^2}{8E} - 1}. \quad (4.8)$$

With these classical quantities available, we can use them in the trace formula that was proven in [BEK15]. Choosing a test function $\rho \in C^{\infty}(\mathbb{R})$ with Fourier transform $\hat{\rho} \in C_0^{\infty}(\mathbb{R})$, denoting the eigenvalues of $\operatorname{op}_N(\hbar)$ as E_n , the Maslov index of the primitive periodic orbit p as σ_p [BEK15], and with the notation as above, this trace formula reads

$$\sum_n \rho\left(\frac{E_n - E}{\hbar}\right) = \sum_{k \in \mathbb{Z}} \frac{t_p \hat{\rho}(kt_p)}{2\pi} e^{\frac{i}{\hbar} k S_p - i \frac{\pi}{2} k \sigma_p} + O(\hbar). \quad (4.9)$$

Using a suitable Tauberian theorem [BPU95, Theorem 6.3], this expression allows us to determine the leading semiclassical behaviour of the local eigenvalue counting function to be

$$N(E; r) := \#\{n; |E_n - E| \leq r\hbar\} \sim \frac{r}{\pi} t_p \quad \text{as } \hbar \rightarrow 0. \quad (4.10)$$

This means that the leading asymptotic behaviour of the spectral density is given by

$$d(E) \sim \frac{t_p}{2\pi\hbar} = \frac{2}{\pi\hbar} \operatorname{arsinh} \sqrt{\frac{\ell_{\xi}^2}{8E} - 1}. \quad (4.11)$$

We now propose to link our length-parameters ℓ_{ξ}, ℓ_x to the truncation (2.2) of the phase space introduced by Berry and Keating. Their parameters L_q, L_p measure the closest distance of the truncated hyperbola $qp = E$ to the coordinate axes. In our coordinates this would be the closest distance of the hyperbola $\xi^2 - x^2 = 2E$ to the asymptotes $\xi = \pm x$. The truncation at E/L_p on the q -axis in [BK99a] then corresponds to the distance

$$\sqrt{2} \frac{\ell_{\xi}}{2} - L_p \quad (4.12)$$

on the asymptote $\xi = x$, see Figure 1(c) for an illustration. Equating these quantities and using the value $L_p = \sqrt{2\pi}$ (in units where $\hbar = 1$) as in [BK99a] gives

$$\ell_{\xi} = \frac{E + 2\pi}{\sqrt{\pi}}, \quad (4.13)$$

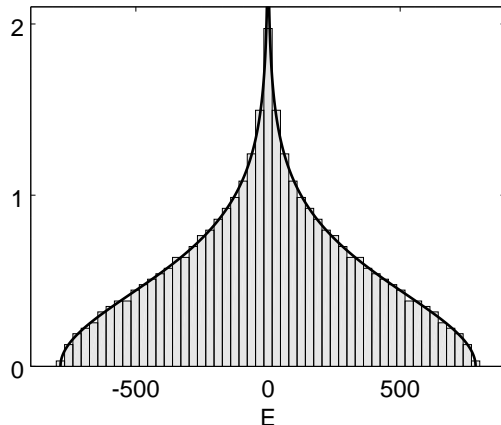


Figure 2: Histogram (grey) of the eigenvalues of $\text{op}_N(h)$ for $N = 1000$, $\hbar = 1$ and $\ell_x = \ell_\xi = \sqrt{2\pi N}$ compared to the semiclassical estimate (thick black line) for the density (4.11).

hence linking the torus-length scale to the energy. With this identification the action (4.7) and the period (4.8) become

$$\begin{aligned} S(E) &= 4E \operatorname{arsinh} \left(\frac{E - 2\pi}{\sqrt{8\pi E}} \right) - \frac{E^2}{2\pi} + 2 \\ &= 2E \log \frac{E}{2\pi} - \frac{E^2}{2\pi} + 2 \end{aligned} \quad (4.14)$$

and

$$t_p = 4E \operatorname{arsinh} \left(\frac{E - 2\pi}{\sqrt{8\pi E}} \right) = 2 \log \left(\frac{E}{2\pi} \right). \quad (4.15)$$

Using this in the expression on the right-hand side of (4.11) then leads us to expect a logarithmic mean spectral density

$$\bar{d}(E) = \frac{1}{\pi} \log \left(\frac{E}{2\pi} \right). \quad (4.16)$$

We note that this is twice the value which Berry and Keating [BK99a] found in their model. The factor of two arises from the fact that in [BK99a] only one branch of the hyperbola was considered, whereas we have taken both branches into account.

5 Numerical results

In order to illustrate the findings of Section 4 we have numerically diagonalised the Hamiltonian $\text{op}_N(h)$, whose matrix elements are given in Eq. (B.11). We set $\hbar = 1$ and are

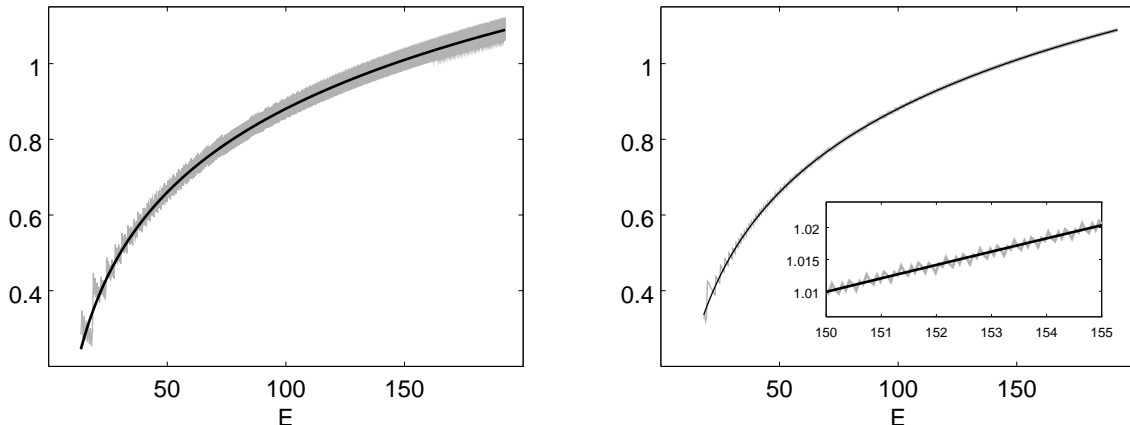


Figure 3: Numerical estimate d^K (grey) of the mean spectral density compared to the semiclassical asymptotics \bar{d} (black), see Eq. (4.16). The left panel is for $K = 2$; one observes fluctuations of d^K around \bar{d} . For $K = 3$ (right panel) the lines are hardly distinguishable at higher energies; small rapid fluctuations are visible upon magnification (inset).

interested in the simultaneous continuum and infinite-volume limits. For simplicity, we therefore choose $\ell_x = \ell_\xi = \sqrt{2\pi N}$, thus satisfying the condition (2.14).

We first test the accuracy of the semiclassical arguments leading to the estimate (4.11) for the spectral density. To this end we show a histogram of the eigenvalues of $\text{op}_N(h)$ for $N = 1000$ in Figure 2. The overall behaviour is well described by Eq. (4.11), which is plotted for comparison.

Now we want to compare the logarithmic mean density (4.16) to the numerical data, where we have to satisfy the condition (4.13). However, since we have already fixed ℓ_ξ in terms of N , this relation now reads

$$\sqrt{2\pi N} = \frac{E + 2\pi}{\sqrt{\pi}}. \quad (5.1)$$

It can thus be implemented in the following way. For each value of N – recall that N labels matrices of different size, and thus different spectra – we have to determine the spectral density at the energy

$$E = \pi\sqrt{2N} - 2\pi. \quad (5.2)$$

The latter we do as follows. We first determine the K eigenvalues which are closest to the given energy E . Of these we determine the minimal and the maximal value E_{\min}^K and E_{\max}^K , respectively. We then estimate the local spectral density as

$$d^K(E) = \frac{K - 1}{E_{\max}^K - E_{\min}^K}. \quad (5.3)$$

In Figure 3 we compare the spectral densities d^K obtained from spectra with $10K \leq N \leq 2000$ to the logarithmic semiclassical estimate (4.16) and observe a good agreement.

6 Conclusions

Our goal was to introduce a self-adjoint quantum Hamiltonian as a modification of the Berry-Keating operator [BK99a, BK99b] that has, to leading order, an eigenvalue count resembling the logarithmic law of the Riemann zeros. In order to achieve this we followed the suggestion of a phase-space truncation made in [BK99a, BK99b]. In contrast to previous approaches [SRL11, BK11] we did not modify the classical Hamiltonian to achieve compact energy surfaces, but we replaced the non-compact phase space $T^*\mathbb{R}$ by a torus. We then demonstrated that Weyl quantisation on a torus provides a powerful tool to construct operators and to analyse their properties. This setting enabled us to use the three available parameters, the two length scales and the semiclassical parameter, to perform various limits, including a continuum and an infinite-volume limit.

Representing the quantum Hamiltonian in Weyl quantisation offers the opportunity to use semiclassical methods in order to study spectral properties. Based on the Gutzwiller trace formula for our setting [BEK15], we derived a semiclassical expression for the spectral density which, however, is not of the desired logarithmic form. It rather expresses the spectral density in the vicinity of a fixed energy E , with fixed length parameters and in a semiclassical approximation. However, it does fit a numerically computed spectral density very well. As in the (semi-)classical calculation provided in [BK99a, BK99b], we had to link the torus length scales to the energy; this can be done in a similar way as in [BK99a, BK99b], producing the same leading term.

Our model provides a clean and direct implementation of the original proposal made by Berry and Keating, avoiding ad hoc modifications as well as non-local terms in the quantum Hamiltonian as they were suggested in [SRL11, BK11]. The original model was based on the work of Connes [Con96, Con99], and central to it was the idea to provide a quantisation of the classical Hamiltonian $H(q, p) = qp$, with the expectation that the hyperbolic nature of the classical dynamics would provide the necessary instability to produce a spectrum that would be able to mimic the ‘spectrum’ of Riemann zeros, whose correlations on the scale of the mean level spacing can be modelled by random-matrix theory (see, e.g., [BK99b] and references therein). In one degree of freedom, however, classical dynamics are integrable and, therefore, one cannot truly expect such a mimicking to happen. This is reflected by the fact that we had to use a family of operators, parametrised by the semiclassical parameter N , and to link the size of the torus to the energy E . We then counted eigenvalues around E in an N -dependent way, eventually leading to the desired logarithmic spectral density. In that way our analysis clearly demonstrates the limitations of modelling the Riemann zeros with the eigenvalues of an operator that is a quantisation (of an established nature) of $H(q, p) = qp$.

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A Proof of Lemma 1

Along the symbol $a(\xi)$ defined in (3.3), whose Fourier series is (3.4), we define

$$b(x) = (x - n\ell_x)^2, \quad \text{if } \left(n - \frac{1}{2}\right)\ell_x \leq x < \left(n + \frac{1}{2}\right)\ell_x, \quad n \in \mathbb{Z}, \quad (\text{A.1})$$

with Fourier expansion

$$b(x) = \frac{\ell_x^2}{12} + \frac{\ell_x^2}{\pi^2} \sum_{n=1}^{\infty} \frac{(-1)^n}{n^2} \cos\left(\frac{2\pi}{\ell_x} nx\right), \quad (\text{A.2})$$

and quantisation

$$\text{op}_N(b) = \frac{\ell_x^2}{12} + \frac{\ell_x^2}{2\pi^2} \sum_{n=1}^{\infty} \frac{(-1)^n}{n^2} (T^{0,n} + T^{0,-n}). \quad (\text{A.3})$$

Hence, $h(x, \xi) = \frac{1}{2}(a(\xi) - b(x))$.

We also introduce the discrete Fourier transform F , which is a unitary operator on \mathbb{C}^N defined as

$$(F\psi)_k := \frac{1}{\sqrt{N}} \sum_{l=0}^{N-1} e^{-2\pi i \frac{kl}{N}} \psi_l, \quad (\text{A.4})$$

where we recall the periodicity $\psi_{l+N} = \psi_l$. A short calculation then shows that

$$F^{-1}T^{m,0}F = T^{0,m}, \quad \text{hence} \quad FT^{0,m}F^{-1} = T^{m,0}. \quad (\text{A.5})$$

When $\ell_x = \ell_\xi$, a comparison of (3.5) and (A.3) hence yields that

$$F^{-1} \text{op}_N(a)F = \text{op}_N(b). \quad (\text{A.6})$$

Moreover, since F^2 is a parity operator, $(F^2\psi)_l = \psi_{-l}$, it follows that

$$F^2 \text{op}_N(b)F^{-2} = \text{op}_N(b), \quad \text{hence} \quad \text{op}_N(a) = F \text{op}_N(b)F^{-1} = F^{-1} \text{op}_N(b)F. \quad (\text{A.7})$$

Thus,

$$\begin{aligned} F^{-1}2 \text{op}_N(h)F &= F^{-1} \text{op}_N(a)F - F^{-1} \text{op}_N(b)F \\ &= \text{op}_N(b) - \text{op}_N(a) = -2 \text{op}_N(h). \end{aligned} \quad (\text{A.8})$$

As $F^{-1} \text{op}_N(h)F$ and $\text{op}_N(h)$ have the same spectra, the lemma is proven. \square

B Matrix elements

In this appendix we calculate the matrix elements $\text{op}_N(h)_{k,l}$ of the operator with Weyl symbol (2.8).

The matrix elements $A_{k,l}$ of an operator A are defined by

$$(A\psi)_k = \sum_{-\frac{N}{2} \leq k < \frac{N}{2}} A_{k,l} \psi_l. \quad (\text{B.1})$$

In order to calculate the matrix elements of a Weyl operator (2.11) we need the matrix elements of the unitary phase-space translation operators $T^{m,n}$. From Eqs. (2.12) and (2.13) one concludes that

$$(T^{m,n}\psi)_k = \sum_{-\frac{N}{2} \leq k < \frac{N}{2}} e^{-i\pi \frac{nm}{N}} e^{-2\pi i \frac{kn}{N}} \delta_{k+m,l} \psi_l, \quad (\text{B.2})$$

from which the matrix elements are read off as

$$(T^{m,n})_{k,l} = e^{-i\pi \frac{nm}{N}} e^{-2\pi i \frac{kn}{N}} \delta_{k+m,l}. \quad (\text{B.3})$$

Here it is understood that our convention $\psi_{l+N} = \psi_l$ implies that all indices are to be taken modulo N .

Since phase space is a torus, the resulting periodicity of translations imply that for fixed N we can always view a Weyl operator as the quantisation of a symbol that is a finite trigonometric polynomial instead of the in general infinite series (2.11).

Lemma 2. *Let $f \in C(\mathbb{R}^2/(\ell_x\mathbb{Z} \oplus \ell_y\mathbb{Z}))$ be a Weyl symbol with quantisation $\text{op}_N(f)$. Then there exists a (generally N -dependent) symbol g that is a finite trigonometric polynomial, such that*

$$\text{op}_N(f) = \text{op}_N(g). \quad (\text{B.4})$$

We remark that a similar statement can be found in [Lig16, Theorem 1].

Proof. We explicitly construct g . First observe the following periodicity property of the phase space translations,

$$T^{m+\mu N, n+\nu N} = (-1)^{m\nu+n\mu+\mu\nu N} T^{m,n}, \quad (\text{B.5})$$

which follows from (B.3) by a direct computation. Hence,

$$\begin{aligned} \text{op}_N(f) &= \sum_{m,n \in \mathbb{Z}} f_{m,n} T^{m,n} = \sum_{m,n=0}^{N-1} \sum_{\mu,\nu \in \mathbb{Z}} f_{m+\mu N, n+\nu N} T^{m+\mu N, n+\nu N} \\ &= \sum_{m,n=0}^{N-1} \sum_{\mu,\nu \in \mathbb{Z}} f_{m+\mu N, n+\nu N} (-1)^{m\nu+n\mu+\mu\nu N} T^{m,n}. \end{aligned} \quad (\text{B.6})$$

Defining

$$g_{m,n} = \sum_{\mu,\nu \in \mathbb{Z}} f_{m+\mu N, n+\nu N} (-1)^{m\nu+n\mu+\mu\nu N}, \quad 0 \leq m, n < N-1, \quad (\text{B.7})$$

concludes the proof. \square

We now use this result to determine the matrix elements of $\text{op}_N(h)$, see (2.11). To this end we first choose $f(x, \xi) = a(\xi)/2$, with a defined in Eq. (3.3), for the symbol in Lemma 2. Then $f_{m,n} = a_m \delta_{n0}$ and, likewise, $g_{m,n} = 0$ for all $n \neq 0$. For $m \neq 0$ we have, cf. (3.4),

$$\begin{aligned} g_{m,0} &= \frac{\ell_\xi^2}{4\pi^2} \sum_{\mu \in \mathbb{Z}} \frac{(-1)^{m+\mu N}}{(m+\mu N)^2} = \frac{\ell_\xi^2 (-1)^m}{4\pi^2 N^2} \sum_{\mu \in \mathbb{Z}} \frac{(-1)^{\mu N}}{(\mu + \frac{m}{N})^2} \\ &= \frac{\ell_\xi^2 (-1)^m}{4N^2 \sin^2(\pi \frac{m}{N})} \begin{cases} 1 & \text{if } N \text{ even} \\ \cos(\pi \frac{m}{N}) & \text{if } N \text{ odd} \end{cases}, \end{aligned} \quad (\text{B.8})$$

where we have used [DLMF, Eq. 5.15.6] to evaluate the sums. The remaining coefficient is

$$g_{0,0} = \frac{\ell_\xi^2}{24} + \frac{\ell_\xi^2}{2\pi^2} \sum_{\mu=1}^{\infty} \frac{(-1)^{\mu N}}{\mu^2 N^2} = \frac{\ell_\xi^2}{24N^2} \begin{cases} (N^2 + 2) & \text{if } N \text{ even} \\ (N^2 - 1) & \text{if } N \text{ odd} \end{cases}. \quad (\text{B.9})$$

The second term of the symbol (2.8), $h - a/2 = b/2$, cf. (A.1), is a function of x only, and thus its quantisation is diagonal in the chosen representation,

$$(\text{op}_N(b/2)\psi)_l = -\frac{1}{2} \left(\frac{l}{N} \ell_x \right)^2 \psi_l. \quad (\text{B.10})$$

Finally, the matrix elements of $\text{op}_N(h)$ read

$$\text{op}_N(h)_{k,l} = \left(g_{0,0} - \frac{1}{2} \left(\frac{k}{N} \ell_x \right)^2 \right) \delta_{k,l} + \sum_{m=1}^{N-1} g_{m,0} \delta_{k+m,l}, \quad (\text{B.11})$$

with the coefficients $g_{m,0}$ given in Eqs. (B.8) and (B.9).

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