



Inferring topology of quantum phase space

With an appendix by Laurent Charles

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Abstract

Does a semiclassical particle remember the phase space topology? We discuss this question in the context of the Berezin–Toeplitz quantization and quantum measurement theory by using tools of topological data analysis. One of its facets involves a calculus of Toeplitz operators with piecewise-constant symbols developed in an appendix by Laurent Charles.

Keywords Persistent homology · Barcode · Berezin–Toeplitz quantization · Quantum measurement

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1 Introduction

We discuss an application of persistent homology to the quantum-classical correspondence, a fundamental principle stating that quantum mechanics contains the classical one as the limiting case when the Planck constant \hbar tends to 0. Paraphrasing (Stöckmann 1999, Chapter 7) this means that in this limit, mathematical structures of Hamiltonian dynamics on closed symplectic manifolds are hidden somewhere in the algebraic and probabilistic formalism of matrix quantum mechanics. While a vast literature explores quantum footprints of dynamical phenomena, such as transition to chaos (Stöckmann 1999), not much is known about the ones of phase space topology. In fact, on the quantum side, topological phenomena can be elusive. For instance, according to the tunneling effect (Merzbacher 2002), a quantum particle may commute between different connected components of an energy level set in the phase space, thus “getting wrong” about the topology of this set.

In the present paper we make a step towards the understanding of quantum footprints of phase space topology in the framework of quantum measurement theory. Specifically, we deal with the following problem. Suppose that the phase space of a semiclassical system is equipped with a finite collection of sensors. An experimentalist, having an access to an ensemble of particles, registers each of them at a “nearby” sensor and gathers the statistics. Is it possible to guess the homology of the phase space on the basis of the data thus obtained? We shall show, within a specific probabilistic model of registration, that such a topological inference is feasible provided the sensors form a sufficiently dense net in the phase space and the experimentalist can tune the range of the sensors. Roughly speaking, a sensor z has range a if it cannot detect particles located at distance $\geq a$ from z . Here is a sketch of the proposed recipe.

1. Take two special values of the range, $a < b$, which depend on the local geometry of the sensor network, and which are assumed to be known in advance. Then, for each value of the range $s \in \{a, b\}$ perform two consecutive registrations and calculate, for all distinct sensors z and w , the probability $p_{zw,s}$ of registration at z and w .
2. Fix a real $m > 0$. Form a pair of simplicial complexes Q_s , $s \in \{a, b\}$, whose vertices are the sensors, and whose simplices are formed by subsets σ of vertices satisfying $p_{zw,s} > \hbar^m$ for all distinct $z, w \in \sigma$. Here we assume that the Planck constant \hbar is small enough.
3. With a right choice of a and b , Q_a will be a subset of Q_b . The image of the inclusion morphism in homology $H(Q_a) \rightarrow H(Q_b)$ turns out to be isomorphic to the homology of the phase space.

For a rigorous statement, see Theorem 3.3, formulated in Sect. 3 and proved in Sect. 4. These sections contain brief preliminaries on persistent homology and relevant methods of topological data analysis. The mathematical model of registration is discussed

in Sects. 2 and 5. In Sect. 6 we discuss some special situations where one can infer the homotopy type of the phase space without using persistent homology. One of them involves a calculus of Toeplitz operators with piecewise-constant symbols developed in an appendix by Laurent Charles. The paper ends with an outline of further research directions.

2 Registration: setting the stage

In this section we present a mathematical model of the registration procedure used in order to infer topology of the phase space. We first introduce a classical registration procedure, and then discuss its quantum counterpart.

We assume that the phase space is a closed symplectic manifold (M, ω) . Our concept of registration procedure (Polterovich 2012) involves a finite open cover $\mathcal{U} = \{U_1, \dots, U_N\}$ of M , interpreted as a small-scale coarse-graining of M , and a subordinated partition of unity f_1, \dots, f_N , where $f_i : M \rightarrow [0, 1]$ is a smooth function supported in U_i and $\sum_i f_i = 1$.

The classical registration procedure assigns to every point $z \in M$ a unique $i \in \Omega_N := \{1, \dots, N\}$ with probability $f_i(z)$. Thus it provides an answer to the question “to which of the sets U_i does z belong?” While the question is ambiguous due to overlaps between the sets U_i , the ambiguity is resolved with the help of the partition of unity. Since f_i is supported in U_i , the output is “the truth, but not the whole truth”.

Recall that a classical state is a Borel probability measure on M . If ν is a state, one readily calculates (see Sect. 5 below) the probability p_i^C that the classical system prepared in the state ν is registered in U_i :

$$p_i^C = \int f_i d\nu, \tag{1}$$

where C stands for classical.

This registration procedure has a natural quantum version in the context of Berezin–Toeplitz quantization. To realize it we assume that the symplectic structure ω is quantizable, i.e., its cohomology class divided by 2π is integral. The reader is invited to think of the 2-dimensional sphere of area 2π , which appears as the phase space of the quantum spin system in the classical limit. The Berezin–Toeplitz quantization is given by a family of finite-dimensional complex Hilbert spaces \mathcal{H}_{\hbar} , where \hbar is the Planck constant (considered as a small parameter), together with linear maps T_{\hbar} from $C^\infty(M)$ to the space of Hermitian operators $\mathcal{L}(\mathcal{H}_{\hbar})$. The maps T_{\hbar} , which are defined by the integration against an $\mathcal{L}(\mathcal{H}_{\hbar})$ -valued positive operator valued measure (POVM), satisfy the quantum-classical correspondence principle, which will be recalled in Sect. 5. The quantum counterpart of the partition of unity f_1, \dots, f_N is a POVM on a finite set $\{1, \dots, N\}$ consisting of Hermitian operators $F_{1,\hbar}, \dots, F_{N,\hbar}$ such that

$$F_{j,\hbar} = T_{\hbar}(f_j) \in \mathcal{L}(\mathcal{H}_{\hbar}).$$

Let \mathcal{S}_{\hbar} be the set of quantum states, i.e., the positive trace 1 operators from $\mathcal{L}(\mathcal{H}_{\hbar})$. Recall that every quantum state $\rho \in \mathcal{S}_{\hbar}$ determines a Borel probability measure $\mu_{\rho, \hbar}$ on M by the formula

$$\int f d\mu_{\rho, \hbar} = \text{trace}(T_{\hbar}(f)\rho) \quad \forall f \in C^{\infty}(M) .$$

Intuitively speaking, the measure $\mu_{\rho, \hbar}$, called the Husimi measure, governs the distribution of a quantum particle in the phase space. By definition, the probability $p_{i, \hbar}^{\text{Q}}$ of the quantum registration at i when the system is in the state ρ equals

$$p_{i, \hbar}^{\text{Q}} = \text{trace}(F_{i, \hbar}\rho) = \int f_i d\mu_{\rho, \hbar} , \quad (2)$$

in an analogy with the classical Eq. (1). Here Q stands for quantum.

A key role in our strategy of phase space learning is played by *repeated registration*: prepare the system in the “maximally mixed state” ρ_0 and perform two consecutive independent registrations. In the classical case the state ρ_0 is the normalized symplectic volume μ , and in the quantum case $\rho_0 = \frac{1}{\dim \mathcal{H}_{\hbar}} \mathbb{1}$.

In the classical case, the probability of the outcome ij of the repeated registration equals

$$p_{ij}^{\text{C}} = \int_M f_i f_j d\mu , \quad (3)$$

see Sect. 5.

In the quantum case, in order to calculate the probability $p_{ij, \hbar}^{\text{Q}}$ of the outcome ij of the repeated registration, one has to take into account the quantum state reduction. We assume that the latter is described by the Lüders rule recalled below in Sect. 5. We denote by $\mathcal{O}(\hbar^{\infty})$ a sequence which decays faster than any power of \hbar .

Proposition 2.1 *Assume that the system is prepared in the maximally mixed state. Then for the repeated registration*

$$p_{ij, \hbar}^{\text{Q}} = \frac{\text{trace}(F_{i, \hbar} F_{j, \hbar})}{\dim \mathcal{H}_{\hbar}} = p_{ij}^{\text{C}} + \mathcal{O}(\hbar) . \quad (4)$$

Furthermore, if the supports of f_i and f_j are disjoint, then $p_{ij, \hbar}^{\text{Q}} = \mathcal{O}(\hbar^{\infty})$.

The proof is given in Sect. 5.

3 Topological analysis of registration data

In this section we show that under certain geometric assumptions on open covers and partitions of unity, one can infer the homology of the quantum phase space by performing two pairs of consecutive registrations. Our main result is stated in Theorem 3.3 below.

Fix a Riemannian metric on the phase space M . Denote by d the corresponding distance function and by $B(z, r)$ the open metric ball of radius r centered in $z \in M$. Take $r' > 0$ such that every ball of radius $4r'$ in M is a convex normal neighbourhood of its center (that is, any two of its points can be connected by a unique globally minimal geodesic lying in the ball).

The role of a sensor network mentioned in the introduction will be played by a finite subset $Z \subset M$. We assume that Z is an $r/2$ -net in M , $r > 0$, that is, the balls $B(z, r/2)$, $z \in Z$, cover M . Furthermore, we fix a constant $\lambda > 1$ and assume that

$$r'/r > 4\lambda^4 . \tag{5}$$

Consider the cover \mathcal{U}_ϵ of M by the balls of radius $\lambda\epsilon/2$ centered in the points of Z , where

$$\epsilon \in \mathcal{I} := [2r\lambda, 2r'/\lambda] .$$

Take any partition of unity $\{f_z^{(\epsilon)}\}$, $z \in Z$, subordinated to \mathcal{U}_ϵ with the following property:

Assumption ♠: For every $z \in Z$ and $\epsilon \in \mathcal{I}$

$$B(z, \epsilon/(2\lambda)) \subset \text{Interior}(\text{supp } f_z^{(\epsilon)}) \subset \text{supp } f_z^{(\epsilon)} \subset B(z, \lambda\epsilon/2) .$$

We shall also need the following condition which relates partitions of unity $\{f_z^{(\epsilon)}\}$ for different values of ϵ :

Assumption ♣: For every $z \in Z$,

$$\text{supp } f_z^{(\epsilon_1)} \subset \text{supp } f_z^{(\epsilon_2)} \text{ for } \epsilon_1, \epsilon_2 \in \mathcal{I}, \epsilon_1 < \epsilon_2 . \tag{6}$$

Finally, pick $a, b \in \mathcal{I}^0$ (where \mathcal{I}^0 stands for the interior of \mathcal{I}) with

$$b/a > 4\lambda^2 . \tag{7}$$

Such a choice is possible due to (5). Under certain circumstances, that will be clarified below, we shall additionally postulate the following.

Assumption ◇: For every $s \in \{a, b\}$ and $z, w \in Z$, if the interiors of the supports of $f_z^{(s)}$ and $f_w^{(s)}$ are disjoint, then the supports are disjoint.

For instance, if the boundaries of the support of $f_z^{(s)}$ are generic smooth s -dependent families of embedded hypersurfaces, assumption (◇) holds true for all but a finite number of values of the parameter s . Thus this assumption can be ensured to hold by a small perturbation of any pair a, b satisfying (7).

Example 3.1 Assume, for instance, that for every $z \in Z$ and $s \in \mathcal{I}$, the support of $f_z^{(s)}$ is the closure of $B(z, s)$. Then (◇) fails only for s taking value in the finite set

$$s \in \{d(z, w)/2 : z, w \in Z, z \neq w\} \cap \mathcal{I} .$$

Convention \heartsuit : We fix $m > 0$, and a and b from \mathcal{I}^0 satisfying (7). If $m \geq 1$, we assume in addition that a, b satisfy \diamondsuit .¹

As in the previous section, for every $\epsilon \in \mathcal{I}$ we consider the quantum repeated registration procedure with respect to the sensor network Z and the partition of unity $\{f_z^{(\epsilon)}\}$, and write $p_{zw, \hbar, \epsilon}^Q$ for the probabilities of the outcome z, w . Here we bookkeep the dependence on ϵ in our notation. Form the complex $Q_{m, \hbar, \epsilon}$ as follows: the vertices are the points of Z , and the subset $\sigma \subset Z$ forms a simplex of $Q_{m, \hbar, \epsilon}$ whenever $p_{zw, \hbar, \epsilon}^Q \geq \hbar^m$ for all $z, w \in \sigma$ with $z \neq w$.

Proposition 3.2 $Q_{m, \hbar, a} \subset Q_{m, \hbar, b}$ for all sufficiently small \hbar .

For a sufficiently small \hbar define the vector space $X_{m, \hbar, a, b}$ as the image of the natural morphism

$$H(Q_{m, \hbar, a}) \rightarrow H(Q_{m, \hbar, b})$$

in homology. Here and below we use homology with coefficients in a field. Now we are ready to formulate our main result under assumptions \spadesuit , \clubsuit and convention \heartsuit .

Theorem 3.3 *The space $X_{m, \hbar, a, b}$ is isomorphic to the homology of the phase space $H(M)$ for every sufficiently small $\hbar > 0$.*

The proofs of Proposition 3.2 and Theorem 3.3 occupy the next section.

4 Persistent homology: proofs

In this section we prove Theorem 3.3. First, we compare the complex $Q_{m, \hbar, \epsilon}$ with its classical analogue (Proposition 4.1), next we observe that the latter is in some sense close to the Vietoris–Rips complex of the sensor network Z (Proposition 4.2), and finally we deduce the theorem by using methods of topological data analysis involving persistence modules and their barcodes. For reader's convenience, some preliminaries on the latter subject are given in Sect. 4.2.

4.1 The classical complex

For every $\epsilon \in \mathcal{I}$ consider the classical repeated registration procedure with respect to the sensor network Z and the partition of unity $\{f_z^{(\epsilon)}\}$, and write $p_{zw, \epsilon}^C$ for the probabilities of the outcome z, w . Form the complex C_ϵ as follows. Its vertices are the points of Z , and the subset $\sigma \subset Z$ forms a simplex of C_ϵ whenever $p_{zw, \epsilon}^C > 0$ for all $z, w \in \sigma$ with $z \neq w$.

Proposition 4.1 *For fixed m, ϵ and a sufficiently small \hbar ,*

$$C_\epsilon = Q_{m, \hbar, \epsilon} \tag{8}$$

¹ We thank Laurent Charles for noticing that assumption \diamondsuit is not needed when $m < 1$.

provided ϵ satisfies (\diamond) .

Proof For $\epsilon \in \mathcal{I}$ put

$$\gamma_\epsilon = \min \left\{ p_{zw,\epsilon}^C : z, w \in Z, z \neq w, p_{zw,\epsilon}^C > 0 \right\}. \tag{9}$$

Note that $\gamma_\epsilon > 0$. Applying formula (4) in Proposition 2.1, we see that

$$p_{zw,\epsilon}^C > 0 \Rightarrow p_{zw,\epsilon}^C \geq \gamma_\epsilon \Rightarrow p_{zw,\hbar,\epsilon}^Q \geq \gamma_\epsilon + \mathcal{O}(\hbar) \geq \hbar^m,$$

provided \hbar is less than a constant depending on m and ϵ . Therefore, $C_\epsilon \subset Q_{m,\hbar,\epsilon}$.

The proof of the opposite inclusion splits into two cases. If $m \geq 1$, by assumption (\diamond) and the second statement of Proposition 2.1,

$$\begin{aligned} p_{zw,\hbar,\epsilon}^Q \geq \hbar^m &\Rightarrow \text{supp } f_z^{(\epsilon)} \cap \text{supp } f_w^{(\epsilon)} \neq \emptyset \\ &\Rightarrow \text{Interior}(\text{supp } f_z^{(\epsilon)}) \cap \text{Interior}(\text{supp } f_w^{(\epsilon)}) \neq \emptyset \Rightarrow p_{zw,\epsilon}^C = \int_M f_z^{(\epsilon)} f_w^{(\epsilon)} d\mu > 0. \end{aligned}$$

If $m < 1$, formula (4) in Proposition 2.1 implies that

$$p_{zw,\epsilon}^C = 0 \Rightarrow p_{zw,\hbar,\epsilon}^Q = \mathcal{O}(\hbar) \leq \hbar^m.$$

In both cases we get that $C_\epsilon \supset Q_{m,\hbar,\epsilon}$, which completes the proof. □

In particular, for all sufficiently small \hbar ,

$$Q_{m,\hbar,a} = C_a \text{ and } Q_{m,\hbar,b} = C_b, \tag{10}$$

where a and b satisfy (\heartsuit) .

4.2 Persistence modules and their barcodes

Next, we focus on the family of complexes C_t , $t \in \mathcal{I}$. Note that assumption (\clubsuit) guarantees that $C_t \subset C_s$ for $s > t$ and hence C_s is a *filtered complex*. Combining this with (10), we deduce Proposition 3.2.

We shall study the filtered complex $\{C_s\}$ by using techniques of persistence modules, see Edelsbrunner (2014), Chazal et al. (2016), Oudot (2015) for an introduction.² Let us recall some preliminaries. A *pointwise finite-dimensional persistence module* is a family of finite-dimensional vector spaces V_a , $a \in \mathbb{R}_+$, over a field \mathcal{F} together with *persistence morphisms* $\pi_{ab}^V : V_a \rightarrow V_b$, $a < b$, such that $\pi_{bc}^V \circ \pi_{ab}^V = \pi_{ac}^V$ when $a < b < c$. An important example is given by an *interval module* $\mathcal{F}(I)$, where I is an interval (that is, a connected subset) of \mathbb{R}_+ ; this module is defined as $\mathcal{F}(I)_a = \mathcal{F}$ for

² **Warning:** Here and below we work with persistence modules parameterized by positive real numbers \mathbb{R}_+ . The group \mathbb{R}_+ acts by multiplication on the set of parameters. The notion of interleaving and the stability theorem are adjusted accordingly.

$a \in I$, and 0 otherwise, and $\pi_{ab}^{\mathcal{F}(I)} = \mathbb{1}$ for $a, b \in I$, and 0 otherwise. According to the *normal form theorem*, for every persistence module V there exists a unique collection of intervals with multiplicities, which is called a *barcode* and denoted by $\mathcal{B}(V)$, so that $V = \bigoplus_{I \in \mathcal{B}(V)} \mathcal{F}(I)$.

The following notion (see Chazal et al. 2016) is crucial for our purposes. Two persistence modules V and W are said to be K -interleaved ($K > 1$) if there exist linear maps $\phi_a : V_a \rightarrow W_{Ka}$ and $\psi_a : W_a \rightarrow V_{Ka}$ that commute with the respective persistence morphisms and satisfy

$$\phi_a \circ \psi_{a/K} = \pi_{a/K, Ka}^W, \quad \psi_a \circ \phi_{a/K} = \pi_{a/K, Ka}^V, \quad \forall a \in \mathbb{R}_+.$$

According to a deep *stability theorem*, one can erase certain (not necessarily all) bars in the barcodes $\mathcal{B}(V)$ and $\mathcal{B}(W)$ with the ratio of the endpoints $\leq K^2$ so that the rest of the bars are matched in one-to-one manner as follows: if a bar $I \in \mathcal{B}(V)$ with endpoints $a < b$ corresponds to a bar $J \in \mathcal{B}(W)$ with endpoints $a' < b'$ then

$$K^{-1} \leq a/a' \leq K, \quad K^{-1} \leq b/b' \leq K.$$

For a persistence module V , define the subspaces

$$P_{st}(V) := \text{Image}(\pi_{st}^V), \quad s < t.$$

Suppose that we are given a family of finite simplicial complexes D_s , with s running over an interval $\mathcal{J} \subset \mathbb{R}_+$ and $D_s \subset D_t$ for $s < t$. Consider a persistence module V which equals $H(D_s)$ for $s \in \mathcal{J}$ and vanishes outside \mathcal{J} (for the idea of such a truncation, see e.g. Chazal et al. (2016)). By definition, the persistence morphisms π_{st}^V are the inclusion morphisms in homology for $s, t \in \mathcal{J}$ and they vanish otherwise. For $s, t \in \mathcal{J}$, $s < t$ the space $P_{st}(V)$ is called the *persistent homology* of D . We shall denote $V = \overline{H}(D)_{\mathcal{J}}$.

Apply the above construction to the family of classical complexes C_s , $s \in \mathcal{I}$. In light of Proposition 4.1,

$$P_{ab}(V) = X_{m, \hbar, a, b}, \quad (11)$$

where the latter space is taken from Theorem 3.3 and $V := \overline{H}(C)_{\mathcal{I}}$.

4.3 Interleaving with the Vietoris–Rips complex

Recall Edelsbrunner (2014), Oudot (2015) that the *Vietoris–Rips complex* R_t , $t > 0$ of the subset $Z \subset (M, d)$ playing the role of our sensor network is defined as the complex whose vertices are the points of Z , and a subset $\sigma \subset Z$ forms a simplex of R_t whenever the diameter of σ is $< t$. Apply the truncation construction to R_t , $t \in \mathcal{J} := [2r, 2r']$ and get the persistence module $W := \overline{H}(R)_{\mathcal{J}}$. We keep notation V for $\overline{H}(C)_{\mathcal{I}}$.

Proposition 4.2 *The persistence modules V and W are λ -interleaved.*

Proof We employ assumption (\spadesuit) . For $s \in [2r, 2r'/\lambda^2]$ and $z, w \in Z$,

$$d(z, w) < s \Rightarrow B(z, s/2) \cap B(w, s/2) \neq \emptyset \Rightarrow p_{zw, \lambda s}^C > 0,$$

so $R_s \subset C_{\lambda s}$. Furthermore, for $t \in [2r\lambda, 2r'/\lambda]$,

$$p_{zw, t}^C > 0 \Rightarrow B(z, t\lambda/2) \cap B(w, t\lambda/2) \neq \emptyset \Rightarrow d(z, w) < t\lambda,$$

so $C_t \subset R_{\lambda t}$.

Define the morphisms $\phi_s : W_s \rightarrow V_{\lambda s}$ and $\psi_t : V_t \rightarrow W_{\lambda t}$ as the inclusion morphisms in homology when $s \in [2r, 2r'/\lambda^2]$ and, respectively, $t \in [2r\lambda, 2r'/\lambda]$, and as 0 otherwise. A direct inspection shows that they provide the desired λ -interleaving. \square

Proof of Theorem 3.3 We continue using the notations V, W as above. A standard comparison between the Vietoris–Rips and the Čech complexes, see Oudot (2015), shows that the persistence module W is 2-interleaved with a module Y such that $Y_t = H(M)$ for $t \in (r, 4r')$, and $Y_t = 0$ otherwise. It follows from Proposition 4.2 that V and Y are 2λ -interleaved. Now let us apply the stability theorem. To any bar of $\mathcal{B}(V)$ containing $[a, b]$, where $a, b \in (2r\lambda, 2r'/\lambda)$ and $b/a > 4\lambda^2$, corresponds a unique bar of $\mathcal{B}(Y)$. On the other hand, $\mathcal{B}(Y)$ has exactly $\dim H(M)$ bars of the form $(r, 4r')$, and therefore to each such bar corresponds a bar of $\mathcal{B}(V)$ containing $(2r\lambda, 2r'/\lambda)$, and hence containing $[a, b]$. It follows that $\mathcal{B}(V)$ possesses exactly $\dim H(M)$ bars containing $[a, b]$, which yields $P_{ab}(V) = H(M)$. Applying (11), we complete the proof of the theorem. \square

5 Registration: proofs

In this section we prove some auxiliary facts on the classical and quantum registration procedure used above. In the course of the proof, we recall a number of basic facts about Berezin–Toeplitz quantization.

Derivation of formula (1): Preparation of a system in the classical state ν means choosing an M -valued random variable Z which is uniformly distributed with respect to ν , i.e., the probability of finding Z in a subset $U \subset M$ equals $\nu(U)$. Let R be another random variable (registration) taking values in $\{1, \dots, N\}$ and defined on the same space of elementary events as Z . By definition, $f_i(z)$ is the conditional probability $\mathbb{P}(R = i | Z = z)$, which in turn means (again, by definition; recall that in general Z is a continuous random variable) that for every $U \subset M$ the joint probability $\mathbb{P}(R = i, Z \in U)$ is given by

$$\mathbb{P}(R = i, Z \in U) = \int_U \mathbb{P}(R = i | Z = z) d\nu(z).$$

Taking here $U = M$ and recalling that in our interpretation $p_i^C := \mathbb{P}(R = i)$, we get (1). \square

Derivation of formula (3): We assume that the first and the second registrations, denoted by R_1 and R_2 , respectively, are random variables defined on the same space of elementary events as Z , which are conditionally independent given Z : $\mathbb{P}(R_1 = i, R_2 = j | Z = z) = f_i(z)f_j(z)$. It follows that

$$p_{ij}^C = \mathbb{P}(R_1 = i, R_2 = j) = \int_M f_i f_j d\mu ,$$

which proves (3). □

Proof of Proposition 2.1 We shall use the following properties of the Berezin–Toeplitz quantization, see Bordemann et al. (1994), Charles (2016):

- **(normalization)** $T_{\hbar}(1) = \mathbb{1}$;
- **(quasi-multiplicativity)** $\|T_{\hbar}(fg) - T_{\hbar}(f)T_{\hbar}(g)\|_{op} = \mathcal{O}(\hbar)$;
- **(trace correspondence)**

$$\left| \text{trace}(T_{\hbar}(f)) - \frac{\text{Volume}(M)}{(2\pi\hbar)^n} \int_M f d\mu \right| \leq \text{const} \cdot \|f\|_{L^1} \hbar^{-(n-1)} ,$$

for all $f, g \in C^\infty(M)$.

Here $\|\cdot\|_{op}$ denotes the operator norm. In the quasi-multiplicativity, $\mathcal{O}(\hbar)$ stands for a remainder which depends on \hbar, f and g and whose operator norm is $\leq \text{const} \cdot \hbar$ as $\hbar \rightarrow 0$.

Taking $f = 1$ in the trace correspondence, we get

$$\dim \mathcal{H}_{\hbar} = \frac{\text{Volume}(M)}{(2\pi\hbar)^n} (1 + \mathcal{O}(\hbar)) ,$$

and hence

$$\frac{\text{trace}(T_{\hbar}(f))}{\dim \mathcal{H}_{\hbar}} = \int_M f d\mu \cdot (1 + \mathcal{O}(\hbar)) . \tag{12}$$

In conjunction with (2), this proves that

$$p_{i,\hbar}^Q = \frac{\text{trace}(F_{i,\hbar})}{\dim \mathcal{H}_{\hbar}} = p_i^C (1 + \mathcal{O}(\hbar)) .$$

Let us focus now on the repeated registration. According to the Lüders rules of state reduction Busch et al. (2016), a.k.a. wave function collapse, after the first registration the system will be in the state

$$\eta := \frac{F_{i,\hbar}^{1/2} \rho_0 F_{i,\hbar}^{1/2}}{\text{trace}(F_{i,\hbar} \rho_0)} = \frac{F_{i,\hbar}}{\text{trace}(F_{i,\hbar})} ,$$

if the result of the registration equals i . Thus the probability of the outcome ij equals

$$p_{ij,\hbar}^Q = \text{trace}(F_{i,\hbar} \rho_0) \cdot \text{trace}(F_{j,\hbar} \eta) = \frac{\text{trace}(F_{i,\hbar} F_{j,\hbar})}{\dim \mathcal{H}_{\hbar}} . \tag{13}$$

By the quasi-multiplicativity,

$$\text{trace}(F_{i,\hbar}F_{j,\hbar}) = \text{trace}(T_{\hbar}(f_i f_j) + \mathcal{O}(\hbar)) .$$

Thus, by (12),

$$p_{ij,\hbar}^Q = \int_M f_i f_j d\mu + \mathcal{O}(\hbar) = p_{ij}^C + \mathcal{O}(\hbar) ,$$

which proves (4).

The last statement of the proposition follows from the fact that $T_{\hbar}(fg) = \mathcal{O}(\hbar^\infty)$ whenever f and g have disjoint supports. This is an immediate consequence of the exponential decay of the scalar product between distinct coherent states as $\hbar \rightarrow 0$, see Bordemann et al. (1994), Charles and Polterovich (2018). □

6 Discussion: do we really need barcodes?

Here we discuss the role of topological data analysis in our approach to inferring topology of the quantum phase space. Recall that important ingredients of our model are a family of covers of the phase space by metric balls (the “location areas” of the sensors placed in their centers) and a family of partitions of unity representing probabilities in the registration procedure. We observe (see Sect. 6.1) that the shape of the supports of the functions from these partitions matters. Roughly speaking, when these supports are close to the balls forming the cover, persistence barcodes become redundant and one can reconstruct homology, and sometimes even the homotopy type of the phase space, by less sophisticated tools.

Furthermore, in Sect. 6.2, we explore a special situation of piecewise constant (and thus, discontinuous!) partitions of unity whose supports simply coincide with the balls of the cover. In this case, on the classical side it is elementary to infer the nerve of the cover and therefore to recover the homotopy type of the phase space. However, quantization of discontinuous functions is a non-trivial task, since the remainders in the quantum-classical correspondence are sensitive to the smoothness of observables. Nevertheless, in this setting we can also infer the topology of the quantum phase space by using the theory of Toeplitz operators with piecewise-constant symbols, as developed in the appendix by Laurent Charles.

6.1 The shape of supports matters

Here we use the notation of Sect. 4 above. Denote by $\Gamma \subset \mathbb{R}_+$ the finite set of all distances $d(z, w)$, where $z, w \in Z, z \neq w$. Take any connected component of $\mathbb{R}_+ \setminus \Gamma$ which is bounded away from 0 and ∞ , and consider its intersection, say Δ , with $\mathcal{J} = [2r, 2r']$. Observe that the Vietoris–Rips complex R_t does not change when t runs through Δ . Take such a t , and assume that the parameter $\lambda > 1$ is close to 1 so that

$$(t/\lambda, \lambda t) \subset \Delta . \tag{14}$$

Recall that λ appears in assumption (\spadesuit) on functions $f_z^{(t)}, z \in Z$, from the partitions of unity playing the role of probabilities in our registration model: the support of $f_z^{(t)}$ is sandwiched between the balls of radii $t/(2\lambda)$ and $\lambda t/2$. Roughly speaking, λ measures the deviation of the support from the metric ball $B(z, t)$.

The proof of Proposition 4.2 together with inclusion (14) yield

$$R_{t/\lambda} \subset C_t \subset R_{t\lambda}, \tag{15}$$

and hence, since $R_{t/\lambda} = R_t = R_{t\lambda}$, we conclude that $C_t = R_t$.

Sometimes, for an individual value of the parameter, the Rips complex associated to a finite subset carries important topological information about the ambient manifold. For instance, by a theorem of Latschev (2001), for every sufficiently small $t > 0$ there exists $r > 0$ such that R_t is homotopically equivalent to M for every r -net Z in M . Take such t , and choose $r > 0$ small enough so that $t \in \mathcal{J}$ and Latschev’s theorem holds. Choosing Z to be a generic $r/2$ -net, we can ensure that $t \notin \Gamma$. Next, pick $\lambda > 1$ so close to 1 that $C_t = R_t$. Finally, assume that (\diamond) holds for t , which, for instance, is the case when the boundaries of the supports of the functions $f_z^{(t)}$ are smooth and intersect transversally. Then (8) guarantees that for a given m and a sufficiently small \hbar we have $Q_{m,\hbar,t} = C_t$. This shows that, for specially chosen sensor nets Z and for λ sufficiently close to 1, the quantum complex $Q_{m,\hbar,t}$ has the homotopy type of M . Let us mention that in this case we reached a stronger conclusion without applying the stability theorem for persistence modules which plays a crucial role in our proof of Theorem 3.3.

However, for values of λ that are large compared to the ratios of the consecutive points in Γ , the above argument fails, since “sandwiching” (15) does not allow one to detect topology of the classical complex C in terms of the Vietoris–Rips complex R . At this point the stability theorem enters the play, and we do not see a shortcut.

6.2 Inferring the nerve of a cover

Let (M, μ) be a probability space endowed with a finite cover $\mathcal{U} = \{U_1, \dots, U_N\}$ by measurable subsets. The measure μ represents the initial distribution of a particle in M . In this section we deal with a version of the registration procedure involving a special partition of unity of the following form. Denote by χ_i the indicator function of U_i , and put $\chi := \sum_k \chi_k, f_i := \chi_i/\chi$. The functions f_i vanish outside U_i and form a partition of unity. For a vector $I := (i_1, \dots, i_k)$ with $i_j \in \Omega_N := \{1, \dots, N\}$ put $U_I := U_{i_1} \cap \dots \cap U_{i_k}$. The probability of k -times repeated registration in the sets U_{i_1}, \dots, U_{i_k} equals by definition

$$p_I^C := \int_M f_{i_1} \cdots f_{i_k} d\mu = \int_{U_I} \chi^{-k}(z) d\mu(z). \tag{16}$$

Example 6.1 Consider a toy case when M is a finite set. A cover \mathcal{U} can be regarded as a hypergraph with the set of vertices M and with edges $U_i, i = 1, \dots, N$. Introduce a probability measure μ on M by

$$\mu(z) = \chi(z)/S, \text{ where } S := \sum_{z \in M} \chi(z).$$

In other words, the probability of a vertex is proportional to the number of edges containing it. Consider two-times repeated registration and look at the conditional probability $\mathbb{P}(j|i)$, $i, j \in \Omega_N$, of getting j as the second outcome provided the first one is i . Note that $\mathbb{P}(j|i) = p_{ij}^C/p_i^C$, where, by (16),

$$p_i^C = \sharp(U_i)/S, \quad p_{ij}^C = S^{-1} \cdot \sum_{z \in U_i \cap U_j} \chi^{-1}(z),$$

and \sharp denotes the cardinality. It follows that

$$\mathbb{P}(j|i) = \frac{\sum_{z \in U_i \cap U_j} \chi^{-1}(z)}{\sharp(U_i)},$$

which, interestingly enough, coincides with the transition probability of the random walk on the edges of a hypergraph as defined in Avin et al. (2010). **Warning:** our model of k -times repeated registration differs from this random walk at time k when $k \geq 3$ because our experimentalist registers all the way *the same* particle $z \in M$. Rather, the random walk models an “absent-minded experimentalist”, who at each step bookkeeps the outcome of the previous registration, but loses track of the specific particle, and therefore chooses it at random within the subset corresponding to this outcome.

Suppose now that M is a closed manifold equipped with a quantizable symplectic form ω . Write μ for the (normalized) symplectic volume. Let \mathcal{U} be any finite cover of M by open subsets with smooth boundaries.

Denote by $\Theta_k, k = 1, \dots, N$, the set of vectors $I = (i_1, \dots, i_k) \subset \Omega_N^k$ with strictly increasing coordinates: $i_1 < \dots < i_k$. Such vectors are identified with subsets of Ω_N . Recall that the nerve of the cover \mathcal{U} is a simplicial complex $L(\mathcal{U})$ with vertices Ω_N whose k -simplices are formed by vectors $I \in \Theta_k$ with $U_I \neq \emptyset$. The latter condition holds if and only if $p_I^C > 0$. It follows that the repeated classical registration procedure detects the nerve of the cover. In particular, if the cover is *good*, i.e., all the sets U_I for all values of k are either empty or contractible, the nerve lemma guarantees that $L(\mathcal{U})$ has the homotopy type of M .

Consider now k -times repeated quantum registration. Put $F_{i, \hbar} = T_{\hbar}(f_i)$, where T_{\hbar} stands for the Berezin–Toeplitz quantization. A straightforward calculation involving the Lüders rule and state reduction (cf. Sect. 5) shows that the probability p_I^Q of k -times repeated registration in $I := (i_1, \dots, i_k)$ equals

$$p_{I, \hbar}^Q := \frac{\text{trace} \left(F_{i_k, \hbar}^{1/2} \cdots F_{i_2, \hbar}^{1/2} F_{i_1, \hbar} F_{i_2, \hbar}^{1/2} \cdots F_{i_k, \hbar}^{1/2} \right)}{\dim \mathcal{H}_{\hbar}}. \tag{17}$$

Theorem 6.2 (*L. Charles*) $p_{I,\hbar}^Q = p_I^C + \mathcal{O}(\hbar^{1/8})$.

The proof is given in the Appendix written by Laurent Charles (see Corollary A.3). A delicate point in this theorem is that the functions f_i are non-smooth, which makes the standard results on the quantum-classical correspondence unapplicable in this case.

Fix now any $m < 1/8$, and consider the simplicial complex with vertices $\{1, \dots, N\}$ such that the vector $I \in \Theta_k$ forms a simplex whenever $p_I^Q > \hbar^m$. By Theorem 6.2, this complex coincides with the nerve $L(\mathcal{U})$ for all sufficiently small \hbar . Hence, for good covers, we inferred the homotopy type of the phase space.

7 Further directions

We conclude the paper with an outline of further research directions and open problems.

The subject of the present note is related to manifold learning, a technique of inferring topology of low-dimensional submanifolds of \mathbb{R}^n from sufficiently dense samples (see e.g. Niyogi et al. 2008). The motivation comes from dimensionality reduction in data analysis. While closed symplectic manifolds (i.e., phase spaces) do not naturally arise as submanifolds of linear spaces, many interesting examples appear as the *Marsden-Weinstein reduction* of symplectic manifolds equipped with a Hamiltonian Lie group action (Marsden and Weinstein 1974). It would be interesting to explore whether the topology of a reduced phase space can be reconstructed from quantum data.

It is tempting to apply the technique of the present note to the tunneling effect discussed in the introduction. Assume that we are given a classical Hamiltonian g on M . Let ξ_{\hbar} be a generic linear combination of pure eigenstates of the quantum Hamiltonian $T_{\hbar}(g)$ with the eigenvalues from a sufficiently small neighborhood of λ , where λ is a regular value of g . Suppose that the initial state of the system equals ξ_{\hbar} . Can we infer the homology of the level set $\{g = \lambda\}$ from the statistics of consecutive registrations by means of a sufficiently dense system of sensors?

Another natural question is whether one can infer the *symplectic topology* of quantum phase space. While reconstructing the symplectic structure seems to be out of reach, it is possible to detect certain quantum footprints of symplectic rigidity, see e.g. Polterovich (2016).

Can we recover the homotopy type of the quantum phase space? In this note we did this for rather special partitions of unity, see Sects. 6 and 6.2, while for more general partitions considered in Sect. 3 we restricted ourselves to a modest topological information, such as homology with coefficients in a field. Detecting the homotopy type in this generality might be plausible, cf. Latschev (2001), Niyogi et al. (2008), but seemingly requires new ideas.

Let us mention, for the record, that for the standard Berezin–Toeplitz quantization of closed Kähler manifolds the dimension of the quantum Hilbert space \mathcal{H}_{\hbar} is given by the Hirzebruch–Riemann–Roch formula (Ma and Marinescu 2011), which carries certain topological information. For instance, if M is a closed real surface of genus g equipped with a quantizable symplectic form, then

$$\dim \mathcal{H}_{\hbar} = \frac{\text{Area}(M)}{2\pi \hbar} + 1 - g .$$

However, I am unable to come up with any *gedankenexperiment* which would enable us to detect $\dim \mathcal{H}_{\hbar}$.

Finally, an intriguing link between topological data analysis and quantum mechanics, which goes another way around, appears in Lloyd et al. (2016). In this paper, the authors propose a quantum algorithm for calculating persistent homology. It would be interesting to implement this algorithm for inferring topology of a quantum phase space along the lines of Sect. 3 above. This might shed some light on how topological structures arise in an intrinsic way in matrix quantum mechanics.

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Appendix: Toeplitz operators with piecewise constant symbol (by Laurent Charles³)

In Berezin–Toeplitz quantization, we consider a symplectic compact manifold M , a set $\Lambda \subset \mathbb{R}_{>0}$ having 0 as a limit point, and for any $\hbar \in \Lambda$, a Hermitian complex line bundle L_{\hbar} and a finite-dimensional subspace \mathcal{H}_{\hbar} of $C^{\infty}(M, L_{\hbar})$. The space \mathcal{H}_{\hbar} has a natural scalar product $\langle \Psi, \Psi' \rangle_{\mathcal{H}_{\hbar}} = \int_M (\Psi, \Psi') d\nu$, where (Ψ, Ψ') is the pointwise scalar product and ν the Liouville measure⁴ of M . To any function $f \in C^{\infty}(M)$, we associate an endomorphism $T_{\hbar}(f) : \mathcal{H}_{\hbar} \rightarrow \mathcal{H}_{\hbar}$ such that

$$\langle T_{\hbar}(f)\Psi, \Psi' \rangle_{\mathcal{H}_{\hbar}} = \int_M (\Psi, \Psi')(x) f(x) d\nu(x), \quad \Psi, \Psi' \in \mathcal{H}_{\hbar}, \quad (18)$$

When the spaces \mathcal{H}_{\hbar} are conveniently defined, the family $(T_{\hbar}, \hbar \in \Lambda)$ enjoys usual semi-classical properties. Typically, for a Kähler manifold M equipped with a positive line bundle L , we choose $\Lambda := \{\hbar = 1/k, k \in \mathbb{N}^*\}$, $L_{\hbar} := L^{\otimes k}$ and define \mathcal{H}_{\hbar} as the space of holomorphic sections of L^k . These definitions can be extended to any quantizable M , cf. Ma and Marinescu (2011) or Charles (2016) for instance. For the purpose of this appendix, we only need that the reproducing kernel of \mathcal{H}_{\hbar} satisfies the two estimates (22) and (23).

In the definition (18) of $T_{\hbar}(f)$, instead of a smooth function f , we can more generally consider any distribution $f \in C^{-\infty}(M)$. Indeed, in equation (18), the pointwise

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⁴ The Liouville measure of the previous sections is $\mu(A) = \nu(A)/\nu(M)$.

scalar product (Ψ, Ψ') is a smooth function, so the integral of f against $(\Psi, \Psi')d\nu$ still makes sense and defines an endomorphism $T_{\hbar}(f)$. The map $T_{\hbar} : C^{-\infty}(M) \rightarrow \text{End}(\mathcal{H}_{\hbar})$ is linear and positive in the sense that $T_{\hbar}(f) \geq 0$ when $f \geq 0$. The question is whether the asymptotic properties of $T_{\hbar}(f)$ still hold, in particular the estimates of the trace and the product.

Proposition A.1 *For any $f \in C^{-\infty}(M)$, we have*

$$\text{tr}(T_{\hbar}(f)) = (2\pi\hbar)^{-n} \left(\int_M f d\nu \right) (1 + \mathcal{O}(\hbar))$$

The proof is an immediate generalization of the smooth case and will be given later. For the multiplicative properties of T_{\hbar} , the regularity is crucial. For instance, let us recall two estimates proved in Barron et al. (2014). Let $R_{\hbar}(f, g) = T_{\hbar}(f)T_{\hbar}(g) - T_{\hbar}(fg)$. When f and g are both of class C^{ℓ} with $\ell = 1$ or 2 , $\|R_{\hbar}(f, g)\| = \mathcal{O}(\hbar^{\ell/2})$. When f and g are only assumed to be continuous, $\|R_{\hbar}(f, g)\|$ tends to 0 in the semiclassical limit $\hbar \rightarrow 0$. It is not proved that these estimates are sharp, but we believe they are.

Our goal is to extend these multiplicative properties to a subalgebra of $L^{\infty}(M)$ containing the characteristic functions of smooth domains. By a smooth domain, we mean a 0-codimensional smooth submanifold with boundary. For any endomorphism T of \mathcal{H}_{\hbar} , we introduce its Schatten norm normalized by the dimension $d(\hbar) = \dim \mathcal{H}_{\hbar}$,

$$\|T\|_p := \left(\frac{\text{tr}|T|^p}{d(\hbar)} \right)^{1/p}, \quad p \in [1, \infty).$$

If (T_{\hbar}) is a family of endomorphisms depending on \hbar , we write $T_{\hbar} = \mathcal{O}_p(\hbar^m)$ for $\|T_{\hbar}\|_p = \mathcal{O}(\hbar^m)$. For any measurable set A of M , denote by $\chi_A \in L^{\infty}(M)$ its characteristic function. We say that A is a *good set* if

$$T_{\hbar}(\chi_A)^2 = T_{\hbar}(\chi_A) + \mathcal{O}_1(\hbar^{1/2}). \quad (19)$$

We say that a function $f \in L^{\infty}(M)$ is a *simple function* if it has the form

$$f = \sum_{i=1}^m \lambda_i \chi_{A_i} \quad (20)$$

where $m \in \mathbb{N}$, $\lambda_1, \dots, \lambda_m$ are real numbers and A_1, \dots, A_m are good sets.

Theorem A.2 *1. Any smooth domain of M is a good set.*

2. The good sets form an algebra, that is, they are closed under taking complement, finite intersection and finite union.

3. If $f, g \in L^{\infty}(M)$ are simple functions, then fg is simple and

$$T_{\hbar}(f)T_{\hbar}(g) = T_{\hbar}(fg) + \mathcal{O}_2(\hbar^{1/4}).$$

4. If f is simple and takes only non-negative values, then $f^{1/2}$ is simple and

$$T_{\hbar}(f)^{1/2} = T_{\hbar}(f^{1/2}) + \mathcal{O}_4(\hbar^{1/8}).$$

Interestingly, only the first assertion relies on the estimates (22) and (23) of the Bergman kernel. The proof of the other assertions is independent and does not use any difficult result.

Corollary A.3 *Let f_1, \dots, f_m be m simple non-negative functions. Let $P_{\hbar} = T_{\hbar}(f_1)^{1/2} \cdots T_{\hbar}(f_m)^{1/2}$. Then*

$$\frac{1}{d(\hbar)} \operatorname{tr}(P_{\hbar}^* P_{\hbar}) = \frac{1}{\nu(M)} \int_M f_1 \cdots f_m \, d\nu + \mathcal{O}(\hbar^{1/8}).$$

Remark It is essential that we use a Schatten norm in the definition (19) of a good set. Indeed, for any measurable set A , $0 \leq T_{\hbar}(\chi_A) \leq 1$, so $0 \leq T_{\hbar}(\chi_A) - T_{\hbar}(\chi_A)^2 \leq 1/4$. When A is a good domain such that A and its complement are non-empty, we will prove in a forthcoming paper that $T_{\hbar}(\chi_A)$ has an eigenvalue $\lambda(\hbar)$ converging to $1/2$ when $\hbar \rightarrow 0$. Therefore,

$$\|T_{\hbar}(\chi_A)^2 - T_{\hbar}(\chi_A)\| \rightarrow 1/4.$$

The curious reader can think about the case where M is the two-sphere and A a hemisphere. In this case, we can explicitly compute the spectrum of $T_{\hbar}(\chi_A)$, as we learned from Douçot and Estienne (2017), cf. also Barron and Polterovich (2015). □

Proofs

Let (Ψ_i) be an orthonormal basis of \mathcal{H}_{\hbar} and define the Bergman kernel

$$K_{\hbar}(x, y) = \sum_{i=1}^{d(\hbar)} \Psi_i(x) \otimes \overline{\Psi}_i(y) \in L_x^k \otimes \overline{L}_y^k, \quad x, y \in M, \tag{21}$$

where \overline{L} is the conjugate line bundle of L . We will need the diagonal estimate

$$K_{\hbar}(x, x) = (2\pi\hbar)^{-n} (1 + \mathcal{O}(\hbar)), \tag{22}$$

where we identify $L_x^k \otimes \overline{L}_x^k$ with \mathbb{C} by using the metric of L . The second estimate we need is

$$|K_{\hbar}(x, y)| \leq C_m \hbar^{-n} e^{-\hbar^{-1}d(x,y)^2/C} + C_m \hbar^m \tag{23}$$

for any $m \in \mathbb{N}$, with some positive constants C and C_m independent of x, y . Here d is any distance on M obtained by embedding M into an Euclidean space and restricting

the Euclidean distance. In the Kähler case, (22) was first proved in Bouche (1990) and was subsequently extended in Zelditch (1998) to convergence in the C^∞ -topology. Estimate (23) follows from Corollary 1 of Charles (2003).

Proof of Proposition A.1 We have

$$\begin{aligned} \text{tr}(T_{\hbar}(f)) &= \sum_{i=1}^{d(\hbar)} \langle T_{\hbar}(f)\Psi_i, \Psi_i \rangle = \int_M f(x)K_{\hbar}(x, x)d\nu(x) \\ &= (2\pi\hbar)^{-n} \left(\int_M f d\nu \right) (1 + \mathcal{O}(\hbar)) \end{aligned}$$

by (22), which holds in the C^∞ -topology. □

In the sequel, to lighten the notation, we set $T_A := T_{\hbar}(\chi_A)$ for any measurable set A of M . We denote by A^c the complement of A .

Lemma A.4 *A measurable set A of M is good if and only if*

$$\int_{A \times A^c} |K_{\hbar}(x, y)|^2 d\nu(x) d\nu(y) = \mathcal{O}(\hbar^{-n+1/2}). \tag{24}$$

Proof Since $0 \leq T_A \leq 1$, $T_A - T_A^2 \geq 0$. Hence

$$\|T_A^2 - T_A\|_1 = \frac{1}{d(\hbar)} \text{tr}(T_A - T_A^2) = \frac{1}{d(\hbar)} \text{tr}(T_A(1 - T_A)).$$

Using that $d(\hbar) = (2\pi\hbar)^{-n}\nu(M)(1 + \mathcal{O}(\hbar))$, we see that A is good if and only if $\text{tr}(T_A(1 - T_A)) = \mathcal{O}(\hbar^{-n+1/2})$. To conclude the proof, observe that for any measurable subsets A and B

$$\text{tr}(T_A T_B) = \int_{A \times B} |K_{\hbar}(x, y)|^2 d\nu(x) d\nu(y). \tag{25}$$

Indeed, computing the trace in the orthogonal basis (Ψ_i) , we have

$$\begin{aligned} \text{tr}(T_A T_B) &= \sum_{i,j} \langle T_A \Psi_i, \Psi_j \rangle \langle T_B \Psi_j, \Psi_i \rangle \\ &= \sum_{i,j} \int_{A \times B} (\Psi_i, \Psi_j)(x) (\Psi_j, \Psi_i)(y) d\nu(x) \nu(y). \end{aligned}$$

By the definition (21) of the Bergman kernel,

$$\begin{aligned} |K_{\hbar}(x, y)|^2 &= \sum_{i,j} (\Psi_i(x) \otimes \bar{\Psi}_i(y), \Psi_j(x) \otimes \bar{\Psi}_j(y)) \\ &= \sum_{i,j} (\Psi_i, \Psi_j)(x) (\Psi_j, \Psi_i)(y), \end{aligned}$$

which proves (25). □

Proof of assertion 1 of Theorem A.2 We will deduce from estimate (23) that any smooth domain A in M satisfies (24). Consider a finite cover $(U_\alpha, 1 \leq \alpha \leq N)$ of M such that each U_α is the domain of a coordinate system (x_i) in which $A \cap U_\alpha = \{x \in U_\alpha; x_1(x) \geq 0\}$. Denote by Δ the diagonal of M^2 . Let $(f_\alpha, 0 \leq \alpha \leq N)$ be a partition of unity of M^2 subordinated to the cover $(\Delta^c, U_1^2, \dots, U_m^2)$. It suffices to show that for each α

$$\int_{A \times A^c} f_\alpha(x, y) |K_\hbar(x, y)|^2 d\nu(x) d\nu(y) = \mathcal{O}(\hbar^{-n+1/2}). \tag{26}$$

For $\alpha = 0$, this follows from the fact that $\text{supp } f_0 \cap \Delta = \emptyset$, so that $|K_\hbar(x, y)| = \mathcal{O}(\hbar^{-\infty})$ uniformly on $\text{supp } f_0$. Let $\alpha \geq 1$ and choose a coordinate system (x_i) on U_α as above. Introduce on U_α^2 the coordinate system

$$s_i(x, y) = x_i(x), \quad t_i(x, y) = x_i(x) - x_i(y), \quad x, y \in U_\alpha.$$

Then by (23) there exists a constant C such that for any $(x, y) \in \text{supp } f_\alpha$, we have

$$|K_\hbar|^2 \leq C \hbar^{-2n} e^{-\hbar^{-1}|t|^2/C} + C \hbar^{-n+1/2},$$

where $|t|^2 = \sum t_i^2$. Furthermore $(A \times \overline{A^c}) \cap U_\alpha^2 = \{0 \leq s_1 \leq t_1\}$. So the integral in (26) is bounded above by

$$\hbar^{-2n} \int_{0 \leq s_1 \leq t_1, |s'|_\infty \leq M} e^{-\hbar^{-1}|t|^2/C} ds dt + \mathcal{O}(\hbar^{-n+1/2}),$$

where $|s'|_\infty = \max(|s_2|, \dots, |s_{2n-1}|)$ and M is chosen so that the support of f_α is contained in $\{|s'|_\infty \leq M\}$. Integrating with respect to the s_i 's and making the change of variable $t = t \hbar^{-1/2}$, we obtain

$$\begin{aligned} \hbar^{-2n} \int_{0 \leq s_1 \leq t_1, |s'|_\infty \leq M} e^{-\hbar^{-1}|t|^2/C} ds dt &= \hbar^{-2n} (2M)^{2n-1} \int_{0 \leq t_1} t_1 e^{-\hbar^{-1}|t|^2/C} dt \\ &= \hbar^{-n+1/2} (2M)^{2n-1} \int_{\mathbb{R}_+ \times \mathbb{R}^{2n-1}} t_1 e^{-|t|^2/C} dt. \end{aligned}$$

Hence, the estimate (26) holds. □

Proof of assertion 2 of Theorem A.2 Since $T_{A^c} = 1 - T_A, T_A - T_A^2 = T_{A^c} - T_{A^c}^2$, so A is a good set if and only if A^c is a good set. The intersection of two good sets A, B is good because

$$(A \cap B) \times (A \cap B)^c \subset (A \times A^c) \cup (B \times B^c)$$

and thanks to Lemma A.4. □

Proof of assertion 3 of Theorem A.2 It suffices to prove that for any good sets A and B ,

$$T_A T_B = T_{A \cap B} + \mathcal{O}_2(\hbar^{1/2}). \quad (27)$$

We first show that

$$d(\hbar)^{-1} \operatorname{tr}(T_A T_B) = \mu(A \cap B) + \mathcal{O}(\hbar^{1/2}), \quad (28)$$

with $\mu(A \cap B) = \nu(A \cap B)/\nu(M)$. Introduce the good sets $a = A \setminus B$, $b = B \setminus A$ and $C = A \cap B$. Then A is the disjoint union of a and C , so $T_A = T_a + T_C$. In the same way, $T_B = T_b + T_C$. Therefore,

$$T_A T_B = T_a T_b + T_a T_C + T_C T_b + T_C^2. \quad (29)$$

Since a and b are disjoint, we deduce from (25) that

$$0 \leq \operatorname{tr}(T_a T_b) \leq \operatorname{tr}(T_a(1 - T_a)).$$

Further, since a is good, we obtain that $d(\hbar)^{-1} \operatorname{tr}(T_a T_b) = \mathcal{O}(\hbar^{1/2})$. By the same argument, $d(\hbar)^{-1} \operatorname{tr}(T_a T_C) = \mathcal{O}(\hbar^{1/2})$ and $d(\hbar)^{-1} \operatorname{tr}(T_C T_b) = \mathcal{O}(\hbar^{1/2})$. Finally, since C is good,

$$d(\hbar)^{-1} \operatorname{tr} T_C^2 = d(\hbar)^{-1} \operatorname{tr} T_C + \mathcal{O}(\hbar^{1/2}) = \mu(C) + \mathcal{O}(\hbar^{1/2})$$

by Proposition A.1. Summing the various estimates, we get (28).

Second, we compute the Hilbert-Schmidt norm of $T_A T_B$. We will use the following consequence of the Hölder inequality: for any \hbar -dependent endomorphisms S, S', T of \mathcal{H}_\hbar ,

$$\begin{aligned} S &= S' + \mathcal{O}_p(\hbar^m) \quad \text{and} \quad \|T\| = \mathcal{O}(1) \\ \Rightarrow \quad \frac{1}{d(\hbar)} \operatorname{tr}(ST) &= \frac{1}{d(\hbar)} \operatorname{tr}(S'T) + \mathcal{O}(\hbar^m). \end{aligned} \quad (30)$$

We have:

$$\begin{aligned} \|T_A T_B\|_2^2 &= d(\hbar)^{-1} \operatorname{tr}(T_A^2 T_B^2) \\ &= d(\hbar)^{-1} \operatorname{tr}(T_A^2 T_B) + \mathcal{O}(\hbar^{1/2}) \quad \text{because } B \text{ is good and by (30)} \\ &= d(\hbar)^{-1} \operatorname{tr}(T_A T_B) + \mathcal{O}(\hbar^{1/2}) \quad \text{because } A \text{ is good and by (30)} \\ &= \mu(A \cap B) + \mathcal{O}(\hbar^{1/2}) \quad \text{by (28)}. \end{aligned} \quad (31)$$

Now we come to the proof of (27). With $C = A \cap B$, we have

$$\|T_A T_B - T_C\|_2^2 = d(\hbar)^{-1} \operatorname{tr}(T_A^2 T_B^2 + T_C^2 - T_A T_B T_C - T_C T_B T_A).$$

Next, by (31),

$$d(\hbar)^{-1} \operatorname{tr}(T_A^2 T_B^2) = \mu(C) + \mathcal{O}(\hbar^{1/2}), \quad d(\hbar)^{-1} \operatorname{tr} T_C^2 = \mu(C) + \mathcal{O}(\hbar^{1/2}). \quad (32)$$

To estimate the trace of $T_A T_B T_C$, we use as above the sets $a = A \setminus B$ and $b = B \setminus A$. By (29),

$$T_A T_B T_C = T_a T_b T_C + T_a T_C^2 + T_C T_b T_C + T_C^3.$$

Using that C is good and (30), we have

$$d(\hbar)^{-1} \operatorname{tr}(T_C^3) = d(\hbar)^{-1} \operatorname{tr}(T_C^2) + \mathcal{O}(\hbar^{1/2}) = \mu(C) + \mathcal{O}(\hbar^{1/2})$$

by (28). Similarly, using that C is good, (30) and (28), we have

$$d(\hbar)^{-1} \operatorname{tr}(T_a T_C^2) = d(\hbar)^{-1} \operatorname{tr}(T_a T_C) + \mathcal{O}(\hbar^{1/2}) = \mathcal{O}(\hbar^{1/2}),$$

because $a \cap C = \emptyset$. By the same argument, $d(\hbar)^{-1} \operatorname{tr}(T_b T_C^2) = \mathcal{O}(\hbar^{1/2})$. Finally, C being good, $d(\hbar)^{-1} \operatorname{tr}(T_a T_b T_C) = d(\hbar)^{-1} \operatorname{tr}(T_a T_b T_C^2) + \mathcal{O}(\hbar^{1/2})$, and by the Hölder inequality,

$$\left| \frac{1}{d(\hbar)} \operatorname{tr}(T_a T_b T_C^2) \right| \leq \|T_C T_a\|_2 \|T_b T_C\|_2 = \mathcal{O}(\hbar^{1/4}) \mathcal{O}(\hbar^{1/4}) = \mathcal{O}(\hbar^{1/2}),$$

where we have applied (31) to C, a and b, C and used the fact that these sets are pairwise disjoint. Gathering these estimates we conclude that

$$d(\hbar)^{-1} \operatorname{tr}(T_A T_B T_C) = \mu(C) + \mathcal{O}(\hbar^{1/2}). \quad (33)$$

Exchanging A and B , we get the same estimate for $d(\hbar)^{-1} \operatorname{tr}(T_B T_A T_C)$. Now (33) and (32) imply that $\|T_A T_B - T_C\|_2^2 = \mathcal{O}(\hbar^{1/2})$. \square

Proof of assertion 4 of Theorem A.2 Since the good sets are closed under taking the complement and finite intersections, we see that any simple function f can be written as a sum (20) with the A_i being pairwise disjoint good sets. We can furthermore assume that these sets are non-empty. Assume that f is non-negative, then all the coefficients λ_i are non-negative. Then $f^{1/2}$ is simple. Set $S_{\hbar}(f) = T_{\hbar}(f^{1/2})^2$. By the third assertion of Theorem A.2, we have

$$S_{\hbar}(f) = T_{\hbar}(f) + \mathcal{O}_2(\hbar^{1/4}). \quad (34)$$

Using that the square root is an operator monotone function, we have

$$\|\sqrt{S_{\hbar}(f)} - \sqrt{T_{\hbar}(f)}\|_4 \leq \|\sqrt{|S_{\hbar}(f) - T_{\hbar}(f)|}\|_4 = \|S_{\hbar}(f) - T_{\hbar}(f)\|_2^{1/2}$$

and the right-hand side is a $\mathcal{O}(\hbar^{1/8})$ by (34). In other words, $T_{\hbar}(f^{1/2}) = T_{\hbar}(f)^{1/2} + \mathcal{O}_4(\hbar^{1/8})$. \square

Proof of Corollary A.3 By assertion 4 of Theorem A.2 and (30), we have

$$\frac{1}{d(\hbar)} \operatorname{tr}(P_{\hbar}^* P_{\hbar}) = \frac{1}{d(\hbar)} \operatorname{tr}(Q_{\hbar}^* Q_{\hbar}) + \mathcal{O}(\hbar^{1/8}),$$

with $Q_{\hbar} = T_{\hbar}(f_1) \cdots T_{\hbar}(f_m)$. By assertion 3 of Theorem A.2,

$$Q_{\hbar}^* Q_{\hbar} = T_{\hbar}(f_1 \cdots f_m) + \mathcal{O}(\hbar^{1/4}).$$

Hence, by (30) and Proposition A.1,

$$\frac{1}{d(\hbar)} \operatorname{tr}(Q_{\hbar}^* Q_{\hbar}) = \frac{1}{\nu(M)} \int_M f_1 \cdots f_m \, d\nu + \mathcal{O}(\hbar^{1/4}),$$

and the result follows. \square

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