MAT656 --- Topics in Dynamical Systems: Introduction to Quantum Chaos

Announcements

Course Information

Problem Sets

Lecture Notes

Course Instructor

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Tentative Schedule

(More a ``chronological list of topics" than a ``schedule" *per se*; topics will not necessarily cover exactly one week)

Dates	Торіс	Notes
1/31 2/4	Introduction	
2/7 2/11	Brief Review of Fourier Analysis	
2/14 2/18	Basics of Quantum Mechanics, Quantization	
2/21 2/25	Eigenvalue Spacing Statistics	
2/28 3/4	Quantum Ergodicity and the QUE Conjecture	
3/7 3/11	Toy Models	
3/14 3/18	Ergodic Theory and Entropy	
3/21 3/25	Quantum Limits for the Baker's Maps	
3/28 4/1	Quantum Limits for Cat Maps	
4/4 4/8	Graph Eigenfunctions	
4/11 4/15	A Little Measure Rigidity	
4/18 4/22	SPRING RECESS, no classes	
4/27 4/29	A Little More Measure Rigidity	No class on 4/25
5/2 5/6	Hecke Operators and Arithmetic QUE	
5/9 5/13	Hyperbolic Surfaces and the Ehrenfest Time	

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MAT656 — Topics in Dynamical Systems: Introduction to Quantum Chaos Spring 2011 Shimon Brooks MWF 10:40-11:35, Physics P123

1 Introduction

Sir Michael Berry famously wrote that, "There is no quantum chaos, in the sense of exponential sensitivity to initial conditions, but there are several novel quantum phenomena which reflect the presence of classical chaos. The study of these phenomena is quantum chaology." (The name never stuck...)

It has become increasingly clear over the last few decades that there will be no precise "dictionary" between notions of chaos in classical mechanics to equivalent notions in quantum mechanics (one important exception is Shnir'lman's **Quantum Ergodicity Theorem**, which describes what the correct analogue of ergodicity should be in quantum-mechanical systems). On the other hand, there are some conjectures about how chaos "should be" reflected in quantum systems; eg. the 1977 **Berry-Tabor Conjecture** and 1984 **Bohigas-Giannoni-Schmit Conjecture**. More recently, there have been suggestions regarding more specific cases, such as the 1994 **Quantum Unique Ergodicity Conjecture** of Rudnick-Sarnak for the geodesic flow on a Riemannian manifold of negative sectional curvature.

In this course, we will attempt to lay out the current state of conjectured understanding, and also discuss some rigorous results and numerical data known to date. In this way, we hope to open up some of the tantalizing open problems in the field, while also explaining the tools available at present (and their limitations). We will focus mainly on simpler "toy models" of quantum chaos, that capture many of the ideas, without much of the complicated analysis of more general settings.

2 Outline of the Course

- Introduction, some Questions, and some Pictures.
- Brief Review of Basics of Quantum Mechanics.
- Universality in Eigenvalue Statistics?
- Quantum Ergodicity and Shnir'lman's Theorem.
- Quantum Unique Ergodicity? Conjectures and Examples.
- Entropy of Quantum Limits.
- Further Topics: Hyperbolic Surfaces, Arithmetic QUE, ...

3 Course Structure

The class meets **MWF 10:40-11:35AM** (at least for now), in **room P123** in the Physics building. I will have **office hours on Thursday 1-3PM** (subject to change), at my **office in 5D-148**.

There will be Problem Sets throughout the semester containing practice exercises, along with some more elementary proofs that will be skipped during the lectures.

I will (hopefully be able to) maintain lecture notes throughout the semester. The lecture notes, along with problem sets, announcements, and all other course information will be available at

 $http://www.math.sunysb.edu/\sim sbrooks/qcSp11.html$

4 Some References

There is no prescribed textbook for the course; there exist books and articles that treat the subject from a variety of different angles and with varying degrees of generality, but none are sufficiently suited to our approach in this course. As mentioned above, lecture notes will be updated throughout the semester and made available on the website.

Below is a sampling of references, approaching the theory from different angles. It would be good to find one that suits your taste— but do not neglect the other approaches! The beauty of the field lies in the ability to combine ideas from the different intersecting theories.

WARNING — Beware of differing conventions and notations!

- *Quantum Chaos: a Brief First Visit*, by Stephan De Bièvre. Good introductory article from the mathematical physics viewpoint.
- Anatomy of Quantum Chaotic Eigenstates, by Stéphane Nonnenmacher. More comprehensive article, closest to the spirit of this course.
- Arithmetic Quantum Chaos, by Peter Sarnak. The canonical introduction to number-theoretic aspects.
- An Introduction to Semiclassical and Microlocal Analysis, by André Martinez. A very readable introduction to pseudo-differential operators and quantization.
- Recent Developments in Mathematical Quantum Chaos, by Steve Zelditch. More comprehensive, more analytic treatment.

Problem Sets

Problem Set I, due Monday 2/21

Contents

1. Review of Some Fourier Analysis	2
1.1. Fourier Analysis on $\mathbb{Z}/N\mathbb{Z}$	2
1.2. Fourier Transform on \mathbb{T} and \mathbb{R}	7
1.3. Fourier Series and Equidistribution	20
1.4. Some Comments about the Fourier Transform on \mathbb{R}^d	23
1.5. The Semi-classical Fourier Transform	25
2. A Brief Introduction to Basics of Quantum Mechanics	27
2.1. The Hamiltonian Formulation of (Classical) Mechanics	27
2.2. Quantum Mechanics on \mathbb{R}	30
2.3. Quantization of Observables	36
2.4. Quantum Dynamics and Egorov's Theorem	47
2.5. Anti-Wick Quantization	50
2.6. Eigenstates and Definite Values	54
2.7. Quantization on Manifolds	55
3. Eigenvalue Spacing Statistics	56
3.1. Weyl's Law	57
3.2. Completely Integrable Systems: Invariant Tori and the	
Berry-Tabor Conjecture	58
3.3. Chaotic Systems: Random Matrices and the Bohigas-	
Giannoni-Schmit Conjecture	60
3.4. Arithmetic Symmetries	62
3.5. Gross Omission — Random Matrices and L -functions	63
4. Eigenfunctions and Quantum Ergodicity	
5. Toy Model I — the Baker's Maps	68
5.1. The Classical Map	69
5.2. Walsh-quantized baker's map	69

LECTURE NOTES — INTRO TO QUANTUM CHAOS, SPRING 2011

WORK IN PROGRESS — USE WITH APPROPRIATE CAUTION

Please send comments and corrections to sbrooks@math.sunysb.edu

LECTURE NOTES INTENDED AS REFERENCE GUIDE ONLY EXPOSITORY MATERIAL, NO CLAIM TO ORIGINALITY

1. Review of Some Fourier Analysis

For now, we will be content to review some basic facts about abelian Fourier analysis, on the groups \mathbb{R} , $\mathbb{T} = \mathbb{R}/\mathbb{Z}$, and $\mathbb{Z}/N\mathbb{Z}$.

Throughout, we denote $e(x) := e^{2\pi i x}$.

1.1. Fourier Analysis on $\mathbb{Z}/N\mathbb{Z}$. We will begin with the Fourier transform on $\mathbb{Z}/N\mathbb{Z}$. Here, since everything is nice and finite, the analysis is simpler— later, we will take advantage of this to work with finite-dimensional toy models of quantum chaos— so we will quickly run through the essential facts, before we extend them to \mathbb{T} and \mathbb{R} .

Lemma 1.1. For any $N \in \mathbb{N}$, and any integer $m \neq 0 \pmod{N}$, we have

$$\sum_{j=0}^{N-1} e(mj/N) = 0$$

Therefore, we see that

$$\frac{1}{N}\sum_{j=0}^{N-1}e(mj/N) = \begin{cases} 1 & m \equiv 0 \pmod{N} \\ 0 & m \neq 0 \pmod{N} \end{cases} := \delta_0$$

Proof: Notice that the terms $e^{2\pi i m j/N}$ form a geometric series, with common ratio $e^{2\pi i m/N}$. We have an explicit formula for the sum of a geometric series:

$$\sum_{j=0}^{N-1} e^{2\pi i m j/N} = \frac{e^{2\pi i m (0)/N} - e^{2\pi i m (N-1+1)/N}}{1 - e^{2\pi i m/N}}$$
$$= \frac{e^0 - e^{2\pi i m}}{1 - e^{2\pi i m/N}}$$
$$= \frac{1-1}{1 - e^{2\pi i m/N}} = 0$$

since $m \neq 0 \pmod{N}$ implies that the denominator $1 - e^{2\pi i m/N} \neq 0$. \Box

Remark: It is clear that the above Lemmas can also be extended to several dimensions; for $\vec{m} \in (\mathbb{Z}/N\mathbb{Z})^d$, we have

$$\frac{1}{N^d} \sum_{x_1, \dots, x_d=0}^{N-1} e^{2\pi i \vec{m} \cdot \vec{x}/N} d\vec{x} = \begin{cases} 1 & \vec{m} = \vec{0} \\ 0 & \vec{m} \neq \vec{0} \end{cases}$$

 $\mathbf{2}$

$$\frac{1}{N^d} \sum_{x_1,\dots,x_d=0}^{N-1} e^{2\pi i \vec{m} \cdot \vec{x}/N} = \frac{1}{N^d} \sum_{x_1,\dots,x_d=0}^{N-1} e^{2\pi i m_1 x_1/N} e^{2\pi i m_2 x_2/N} \cdots e^{2\pi i m_d x_d/N}$$
$$= \prod_{j=1}^d \frac{1}{N} \sum_{x_j=1}^{N-1} e^{2\pi i m_j x_j/N} dx_j$$
$$= \prod_{j=1}^d \delta_{m_j=0} = \delta_{\vec{0}}$$

Definition 1.1. If $f \in \mathbb{C}^N$ is a function on $\mathbb{Z}/N\mathbb{Z}$, then we define its Fourier transform $\hat{f} \in \mathbb{C}^N$ to be

$$\hat{f}(m) := \frac{1}{\sqrt{N}} \sum_{x \in \mathbb{Z}/N\mathbb{Z}} f(x) e^{-2\pi i m x/N}$$

(the $\frac{1}{\sqrt{N}}$ is a convenient normalization that will make the Fourier transform unitary; see below.)

The Fourier transform would be pretty useless without the following crucial fact:

Lemma 1.2 (Fourier Inversion). For any $f \in \mathbb{C}^N$, we have

$$f(x) = \frac{1}{\sqrt{N}} \sum_{m \in \mathbb{Z}/N\mathbb{Z}} \hat{f}(m) e^{2\pi i m x/N}$$

Proof: Write

$$\frac{1}{\sqrt{N}} \sum_{m \in \mathbb{Z}/N\mathbb{Z}} \hat{f}(m) e^{2\pi i m x/N} = \frac{1}{\sqrt{N}} \sum_{m \in \mathbb{Z}/N\mathbb{Z}} \left(\frac{1}{\sqrt{N}} \sum_{y \in \mathbb{Z}/N\mathbb{Z}} f(y) e^{-2\pi i m y/N} \right) e^{2\pi i m x/N}$$
$$= \sum_{y} f(y) \frac{1}{N} \sum_{m} e^{2\pi i m (x-y)/N}$$
$$= \sum_{y} f(y) \delta_0(x-y) = f(x)$$

Put another way, this calculation shows that the N functions $\{\frac{1}{\sqrt{N}}e^{2\pi i j(\cdot)/N}\}_{j=0}^{N-1}$ form an orthonormal basis of the N-dimensional space \mathbb{C}^N of functions

on $\mathbb{Z}/N\mathbb{Z}$, with respect to the usual inner product

$$\langle f,g\rangle = \sum_{j=0}^{N-1} f(j)\overline{g(j)}$$

on the Hilbert space \mathbb{C}^N . The Fourier transform \hat{f} simply gives the coefficients of f when expressed in this basis, given by the inner product of f with the unit vector

$$\left\langle f, \frac{1}{\sqrt{N}} e^{2\pi i m(\cdot)/N} \right\rangle = \sum_{x=0}^{N-1} f(x) \overline{\frac{1}{\sqrt{N}}} e^{2\pi i m x/N}$$
$$= \frac{1}{\sqrt{N}} \sum_{x=0}^{N-1} f(x) e^{-2\pi i m x/N}$$
$$= \hat{f}(m)$$

This also explains the $\frac{1}{\sqrt{N}}$ normalizing factor; it normalizes the basis to be unit vectors.

Lemma 1.3 (Plancherel Formula). The Fourier transform is unitary with respect to the usual inner product on \mathbb{C}^N ; that is,

$$\langle f, g \rangle = \langle f, \hat{g} \rangle$$

Proof: Write

$$\begin{split} \langle \hat{f}, \hat{g} \rangle &= \sum_{m=0}^{N-1} \frac{1}{\sqrt{N}} \sum_{x=0}^{N-1} f(x) e^{-2\pi i m x/N} \frac{1}{\sqrt{N}} \sum_{y=0}^{N-1} g(y) e^{-2\pi i m y/N} \\ &= \sum_{x,y=0}^{N-1} f(x) \overline{g(y)} \frac{1}{N} \sum_{m=0}^{N-1} e^{2\pi i m (y-x)/N} \\ &= \sum_{x,y=0}^{N-1} f(x) \overline{g(y)} \delta_0(y-x) \\ &= \sum_{x=0}^{N-1} f(x) \overline{g(y)} = \langle f, g \rangle \end{split}$$

In particular, $||\hat{f}||_2^2 = ||f||_2^2$ (this is nothing more than the Pythagorean Theorem applied to our orthonormal basis.)

We also have the following important properties of the Fourier transform:

Lemma 1.4. (1) $\widehat{fg} = \widehat{f} * \widehat{g}$

5

(2) $\widehat{f * g} = \widehat{f}\widehat{g}$ (3) f is real-valued iff $\widehat{f}(-m) = \overline{\widehat{f}(m)}$ for all $m \in \mathbb{Z}/N\mathbb{Z}$. (4) \widehat{f} is real valued iff $f(-x) = \overline{f(x)}$ for all $x \in \mathbb{Z}/N\mathbb{Z}$.

Proof:

(1) Use Fourier inversion to write

$$\begin{aligned} \widehat{fg}(m) &= \frac{1}{\sqrt{N}} \sum_{x=0}^{N-1} f(x) g(x) e^{-2\pi i m x/N} \\ &= \frac{1}{\sqrt{N}} \sum_{x=0}^{N-1} f(x) \frac{1}{\sqrt{N}} \sum_{n=0}^{N-1} \widehat{g}(n) e^{2\pi n x/N} e^{-2\pi i m x} \\ &= \frac{1}{\sqrt{N}} \sum_{n=0}^{N-1} \widehat{g}(n) \frac{1}{\sqrt{N}} \sum_{x=0}^{N-1} f(x) e^{-2\pi i (m-n)/N} \\ &= \frac{1}{\sqrt{N}} \sum_{n=0}^{N-1} \widehat{g}(n) \widehat{f}(m-n) \\ &= \left(\widehat{g} * \widehat{f}\right)(m) \end{aligned}$$

(2) Similar to above; see also Lemma below on \mathbb{Z} .

(3) If f is real-valued, then $f(x) = \overline{f(x)}$ for all x, so

$$\hat{f}(-m) = \frac{1}{\sqrt{N}} \sum_{x=0}^{N-1} f(x) e^{-2\pi i (-m)x/N}$$
$$= \frac{1}{\sqrt{N}} \sum_{x=0}^{N-1} f(x) e^{2\pi i m x/N}$$
$$= \frac{1}{\sqrt{N}} \sum_{x=0}^{N-1} \overline{f(x)} e^{-2\pi i m x/N} = \overline{\hat{f}(m)}$$

Now, if $\hat{f}(-m) = \overline{\hat{f}(m)}$ for all m, then in particular, we see that $\hat{f}(0) \in \mathbb{R}$. We consider two cases: either N is even, or odd.

If N is odd, then from the Fourier inversion formula we see that

$$\begin{split} f(x) &= \frac{1}{\sqrt{N}} \sum_{m \in \mathbb{Z}/N\mathbb{Z}} \hat{f}(m) e^{2\pi i m x/N} \\ &= \frac{1}{\sqrt{N}} \hat{f}(0) + \frac{1}{\sqrt{N}} \sum_{j=1}^{N/2} \left(\hat{f}(j) e^{2\pi i j x/N} + \hat{f}(-j) e^{2\pi i (-j) x/N} \right) \\ &= \frac{1}{\sqrt{N}} \hat{f}(0) + \frac{1}{\sqrt{N}} \sum_{j=0}^{N/2} \left(\hat{f}(j) e^{2\pi i j x/N} + \overline{\hat{f}(j)} e^{2\pi i (j) x/N} \right) \\ &= \frac{1}{\sqrt{N}} \hat{f}(0) + \frac{1}{\sqrt{N}} \sum_{j=0}^{N/2} 2Re\left(\hat{f}(j) e^{2\pi i j x/N} \right) \in \mathbb{R} \end{split}$$

If N is even, then we also have $\hat{f}(\frac{N}{2}) = \hat{f}(-\frac{N}{2}) \in \mathbb{R}$, so we can repeat the same argument to show that

$$\begin{split} f(x) &= \frac{1}{\sqrt{N}}\hat{f}(0) + \frac{1}{\sqrt{N}}\hat{f}(N/2)e^{2\pi i(\frac{N}{2})/N} + \frac{1}{\sqrt{N}}\sum_{j=0}^{\frac{N-1}{2}}2Re\left(\hat{f}(j)e^{2\pi ijx/N}\right) \\ &= \frac{1}{\sqrt{N}}\hat{f}(0) + \frac{1}{\sqrt{N}}\hat{f}(N/2)e^{\pi i} + \frac{1}{\sqrt{N}}\sum_{j=0}^{\frac{N-1}{2}}2Re\left(\hat{f}(j)e^{2\pi ijx/N}\right) \\ &= \frac{1}{\sqrt{N}}\hat{f}(0) - \frac{1}{\sqrt{N}}\hat{f}(N/2) + \frac{1}{\sqrt{N}}\sum_{j=0}^{\frac{N-1}{2}}2Re\left(\hat{f}(j)e^{2\pi ijx/N}\right) \end{split}$$

and again all terms in the sum are real.

(4) Same argument as above, using Fourier inversion in place of the Fourier transform.

Lemma 1.5. Let $e^{2\pi i y X/N}$ be the multiplication operator

$$\left[e^{2\pi i y X/N} f\right](x) = e^{2\pi i y x/N} f(x)$$

and T_h be the translation operator

$$[T_h f](x) = f(x+h)$$

Then

$$e^{\widehat{2\pi i X/N}}f = T_{-y}\hat{f}$$
$$\widehat{T_yf} = e^{2\pi i y X/N}\hat{f}$$

Proof: For the first statement, write

$$\widehat{e^{2\pi i X} f}(m) = \sum_{x \in \mathbb{Z}/N\mathbb{Z}} \left[e^{2\pi i y X} f \right](x) e^{-2\pi i m x/N}$$
$$= \sum_{x \in \mathbb{Z}/N\mathbb{Z}} e^{2\pi i y x} f(x) e^{-2\pi i m x/N}$$
$$= \sum_{x \in \mathbb{Z}/N\mathbb{Z}} f(x) e^{-2\pi i (m-y) x/N}$$
$$= \widehat{f}(m-y)$$

For the second statement, we have

$$\begin{split} \widehat{T_y f}(m) &= \sum_{x \in \mathbb{Z}/N\mathbb{Z}} \left[T_y f \right] e^{-2\pi i m x/N} \\ &= \sum_{x \in \mathbb{Z}/N\mathbb{Z}} f(x+y) e^{-2\pi i m (x+y)/N} e^{2\pi i m y/N} \\ &= e^{2\pi i y m/N} \widehat{f}(m) \end{split}$$

as required. \Box

Remark: This Lemma shows a certain duality between multiplication by exponentials and translations in the Fourier transform. This duality will play a large role in understanding the Uncertainty Principle, and its connection to the Fourier transform.

1.2. Fourier Transform on \mathbb{T} and \mathbb{R} . Though many of the properties of the Fourier transform are captured in the finite setting described above, there is a much more intricate structure when we include smoothness. We will for the most part assume that all functions we consider are of class C^{∞} (though we will be forced to consider distributions as well), and so we will often assume this in place of the sharpest possible hypotheses.

Lemma 1.6. For any $m \in \mathbb{Z} \setminus 0$, we have

$$\int_{\mathbb{T}} e^{2\pi i m x} dx = 0$$

Proof: This can be integrated explicitly by the Fundamental Theorem of Calculus:

$$\int_0^1 e^{2\pi i m x} dx = \frac{1}{2\pi i m} \left(e^{2\pi i m (1)} - e^{2\pi i m (0)} \right)$$
$$= \frac{1}{2\pi i m} (1-1) = 0$$

 $\overline{7}$

since $m \neq 0$. \Box

8

Some care must be taken in the analogous statement for \mathbb{R} , since the integral $\int_{\mathbb{R}} e^{i\xi x} dx$ does not converge absolutely. However, we will see that this works in the sense of **distributions**.

Definition 1.2. • If $f \in C^{\infty}(\mathbb{T})$, then we define its Fourier transform (or Fourier series) $\hat{f} \in \mathbb{C}^{\mathbb{Z}}$ to be

$$\hat{f}(m) := \int_{\mathbb{T}} f(x) e^{-2\pi i m x} dx$$

• If $f \in C_c^{\infty}(\mathbb{R})$ (smooth with compact support), then we define its Fourier transform $\hat{f} \in C^{\infty}(\mathbb{R})$ to be

$$\hat{f}(\xi) := \int_{\mathbb{R}} f(x) e^{-2\pi i \xi x} dx$$

Note that, since f has compact support, the integral converges absolutely; it is also smooth since we can differentiate under the integral sign.

The space $C_c^{\infty}(\mathbb{R})$ will turn out to be the wrong space to work with over \mathbb{R} , but for now it is convenient and will suffice. For later reference, though, we introduce the **Schwartz space**

$$\mathcal{S}(\mathbb{R}) := \{ f \in C^{\infty}(\mathbb{R}) : \forall j, k \in \mathbb{N}, \forall x \in \mathbb{R}, \quad |(1+x^2)^j \partial^k f(x)| < \infty \}$$

of smooth functions that decay rapidly (faster than any polynomial) along with all of their derivatives. It is clear that $C_c^{\infty} \subset \mathcal{S}(\mathbb{R})$, but there are many other important Schwartz functions, such as the Gaussians $G_{\alpha}(x) := e^{-\alpha x^2}$.

Exercise 1.1. Show that the Gaussian $G_{\alpha} \in \mathcal{S}(\mathbb{R})$ for any $\alpha > 0$.

Exercise 1.2. Show that for $f \in \mathcal{S}(\mathbb{R})$, the integral $\hat{f}(\xi) = \int_{\mathbb{R}} f(x)e^{2\pi i\xi x} dx$ converges absolutely.

Lemma 1.7.

$$\int_{\mathbb{R}} e^{-\pi x^2} dx = 1$$

Proof: This is a trick (that should be!) taught in every multivariable calculus class. Consider the *square* of the integral

$$\left(\int_{\mathbb{R}} e^{-\pi x^2} dx\right)^2 = \iint_{\mathbb{R}^2} e^{-\pi (x^2 + y^2)} dx dy$$

Now convert the integral over \mathbb{R}^2 into polar coordinates to get

$$\int_{\theta=0}^{2\pi} \int_{r=0}^{\infty} e^{-\pi r^2} r dr d\theta = 2\pi \int_{r=0}^{\infty} e^{-\pi r^2} r dr$$
$$= \int_{u=0}^{\infty} e^{-u} du = 1$$

by the change of variables $u = \pi r^2$. \Box

Lemma 1.8. The Gaussian $G_{\pi}(x) = e^{-\pi x^2}$ is its own Fourier transform; i.e., $G_{\pi} = \widehat{G}_{\pi}$.

Proof: Write

$$\widehat{G_{\pi}}(\xi) = \int_{\mathbb{R}} G_{\pi}(x) e^{-2\pi i \xi x} dx$$
$$= \int_{\mathbb{R}} e^{-\pi (x^2 + 2i\xi x)} dx$$
$$= \int_{\mathbb{R}} e^{-\pi (x + i\xi)^2} e^{-\pi \xi^2} dx$$
$$= G_{\pi}(\xi) \int_{\mathbb{R}} e^{-\pi (x + i\xi)^2} dx$$

It remains to show that $\int_{\mathbb{R}} e^{-\pi(x+i\xi)^2} dx = 1$. But notice that this is the integral of $e^{-\pi z^2}$ over the contour $Im(z) = \xi$. Since $e^{-\pi z^2}$ is holomorphic, and decays as $Re(z) \to \pm \infty$, we can shift the contour of integration back to \mathbb{R} without changing its value. Thus, using the previous Lemma,

$$\int_{\mathbb{R}} e^{-\pi(x+i\xi)^2} dx = \int_{\mathbb{R}} e^{-\pi x^2} dx = 1$$

as required. \Box .

Lemma 1.9. Let $f \in \mathcal{S}(\mathbb{R})$, and for any $\lambda \in \mathbb{R}$, set $R_{\lambda}f(x) = f(\lambda x)$. Then

$$\widehat{R_{\lambda}f} = \lambda^{-1}R_{\lambda^{-1}}\hat{f}$$

Proof: Write

$$\widehat{R_{\lambda}f} = \int_{\mathbb{R}} R_{\lambda}f(x)e^{-2\pi i\xi x}dx$$
$$= \int_{\mathbb{R}} f(\lambda x)e^{2\pi i\xi x}dx$$
$$= \lambda^{-1}\int_{u\in\mathbb{R}} f(u)e^{2\pi i\frac{\xi}{\lambda}u}du$$
$$= \lambda^{-1}\widehat{f}\left(\frac{\xi}{\lambda}\right)$$

by change of variable $u = \lambda x$. \Box

Corollary 1.1. For $\alpha > 0$,

$$\widehat{G_{\alpha}} = \sqrt{\frac{\pi}{\alpha}} G_{\pi^2/\alpha}$$

To see this, simply note that $G_{\alpha} = R_{\sqrt{\alpha/\pi}}G_{\pi}$, and recall that G_{π} is its own Fourier transform.

This is a very important theme that will recur again and again the more localized a function is in the "space variable" x, the more spread out its Fourier transform will be in the "frequency variable" ξ , and vice versa. This will be manifested in the Heisenberg Uncertianty Principle, Theorem 1.3 below.

Lemma 1.10. For the Fourier transform on either \mathbb{Z} or \mathbb{R} , we have

$$\widehat{f \ast g} = \widehat{f}\widehat{g}$$

Recall that we proved the analogous fact for the discrete Fourier transform in Lemma 1.4(2).

Proof: First, consider the Fourier transform on \mathbb{T} . We have

$$\widehat{f * g}(m) = \int_{0}^{1} (f * g)(x)e^{-2\pi i m x} dx$$

$$= \int_{x=0}^{1} \int_{y=0}^{1} f(y)g(x-y)dye^{-2\pi i m x} dx$$

$$= \int_{y=0}^{1} \int_{x=0}^{1} f(y)g(x-y)e^{-2\pi i m y}e^{-2\pi i m (x-y)} dxdy$$

$$= \int_{y=0}^{1} f(y)e^{-2\pi m y} \int_{x=0}^{1} g(x-y)e^{-2\pi i m (x-y)} dxdy$$

$$= \int_{y=0}^{1} f(y)e^{-2\pi m y} \hat{g}(m)dy = \hat{f}(m)\hat{g}(m)$$

10

by doing the change of variables $x \mapsto x + y$ in the x integral.

For the Fourier transform on \mathbb{R} , repeat the above argument, taking $f, g \in \mathcal{S}(\mathbb{R})$ to avoid issues in the order of integration.

We now wish to prove the Fourier inversion formulae for these Fourier transforms. However, convergence issues come into play, since the Fourier transforms now live on non-compact spaces \mathbb{Z} and \mathbb{R} . The utility of the following fact cannot be understated:

Lemma 1.11. If $f \in C^{\infty}(\mathbb{T})$ (resp. $\mathcal{S}(\mathbb{R})$), then $\hat{f}(m) = O(m^{-2})$ (resp. $\hat{f}(\xi) \leq (1+\xi^2)^{-1}$). Therefore, the Fourier expansion $\sum_{m \in \mathbb{Z}} \hat{f}(m) e^{2\pi i m x}$ (resp. $\int_{\mathbb{R}} \hat{f}(\xi) e^{2\pi i \xi x} d\xi$) converges absolutely.

Proof: Get used to integrating by parts!! It is a trick that will recur again and again in semiclassical analysis.

For the \mathbb{T} statement, consider

$$\hat{f}(m) = \int_0^1 f(x) e^{-2\pi i m x} dx$$

and integrate by parts twice; we wish to differentiate f (this doesn't hurt too much, since $f \in C^2$) while integrating the exponential term. Integrating by parts the first time gives

$$\hat{f}(m) = \int_0^1 f(x)e^{-2\pi i m x} dx = \frac{1}{2\pi i m} \int_0^1 f'(x)e^{-2\pi i m x} dx$$

and integrating by parts again yields

$$\hat{f}(m) = \left(\frac{1}{2\pi i m}\right)^2 \int_0^1 f''(x) e^{-2\pi i m x} dx = O(m^{-2} \cdot ||f''||_\infty) = O_f(m^{-2})$$

since $f \in C^{\infty}(\mathbb{T}) \subset C^{2}(\mathbb{T})$ implies that f'' is uniformly bounded.

For the $\mathbb R$ statement, do the same (double) integration by parts to get

$$\hat{f}(\xi) = \int_{\mathbb{R}} f(x)e^{2\pi i\xi x} dx = \left(\frac{1}{2\pi i\xi}\right)^2 \int_{\mathbb{R}} f''(x)e^{-2\pi i\xi x} dx$$

(here, the boundary terms vanish since $f \in \mathcal{S}(\mathbb{R})$ vanishes at the boundary.) Now, since $f \in \mathcal{S}(\mathbb{R})$, we know that $f'' \in L^1(\mathbb{R})$, and so the integral $\int_{\mathbb{R}} f''(x)e^{-2\pi i\xi x}dx$ converges absolutely, and uniformly in ξ . Thus, we have $\hat{f}(\xi) \leq_f (1+\xi^2)^{-1}$, as required. \Box **Definition 1.3.** The **Dirichlet kernel of order** n on \mathbb{T} is the function

$$D_n(x) := \sum_{j=-n}^n e^{2\pi i j x} = \frac{\sin 2\pi (n+\frac{1}{2})x}{\sin 2\pi \frac{x}{2}}$$

To justify the expression on the right, simply use the formula for summing a geometric series

$$\sum_{j=-n}^{n} e^{2\pi i j x} = \frac{e^{2\pi i (-n)x} - e^{2\pi i (n+1)x}}{1 - e^{2\pi i x}}$$
$$= \frac{e^{2\pi i (-n-\frac{1}{2})x} - e^{2\pi i (n+\frac{1}{2})x}}{e^{-2\pi i \frac{1}{2}x} - e^{2\pi i \frac{1}{2}x}}$$
$$= \frac{\sin 2\pi (n+\frac{1}{2})x}{\sin 2\pi \frac{x}{2}}$$

multiplying top and bottom by $e^{-2\pi i \frac{1}{2}x}$ in the second line, and recalling that $\sin \theta = \frac{1}{2i}(e^{i\theta} - e^{-i\theta})$.

Remark: Note that by Lemma 1.6

$$\widehat{D_n}(m) = \begin{cases} 1 & |m| \le k \\ 0 & |m| > k \end{cases}$$

Therefore, multiplying \widehat{f} by $\widehat{D_n}$ cuts off the Fourier series of f at k terms; by Lemma 1.10, this means that $f * D_n$ is a function whose Fourier transform matches that of f up to the k-th terms, but then vanishes.

We also note that $\int_{\mathbb{T}} D_n(x) dx = 1$ for every *n*. On the other hand, D_n oscillates wildly, and in fact $\int_0^1 |D_n(x)| dx$ gets quite large. A better kernel is the Fejér kernel:

Definition 1.4. The Fejér kernel of order n on \mathbb{T} is the function

$$F_n(x) := \frac{1}{n} \sum_{k=0}^{n-1} D_k(x) = \sum_{j=-n}^n \frac{n-|j|}{n} e^{2\pi i j x}$$

Remark: As with the Dirichlet kernel, we see from Lemma 1.6 that

$$\widehat{F_n}(m) = \begin{cases} \frac{n - |m|}{n} & |m| \le n\\ 0 & |m| > n \end{cases}$$

The utility of the Fejér kernel becomes much more apparent from the following fact:

Lemma 1.12.

$$F_n(x) = \frac{1}{n} \left(\frac{\sin(2\pi \frac{nx}{2})}{\sin(2\pi \frac{x}{2})} \right)^2 \ge 0$$

Moreover, for any $\delta > 0$, we have

$$\lim_{n \to \infty} \int_{|x| > \delta} F_n(x) dx = 0$$

Proof: From the previous expression of D_n , we can write

$$nF_{n}(x) = \sum_{k=0}^{n-1} D_{k}(x) = \frac{1}{\sin 2\pi \frac{x}{2}} \sum_{k=0}^{n-1} \sin 2\pi (n + \frac{1}{2})x$$

$$= \frac{1}{\sin 2\pi \frac{x}{2}} Im \left(\sum_{k=0}^{n-1} e^{2\pi i (n + \frac{1}{2})x} \right)$$

$$= \frac{1}{\sin 2\pi \frac{x}{2}} Im \left(\frac{e^{2\pi i \frac{1}{2}x} - e^{2\pi i (n + \frac{1}{2})x}}{1 - e^{2\pi i x}} \right)$$

$$= \frac{1}{\sin 2\pi (\frac{x}{2})} Im \left(\frac{1 - e^{2\pi i n x}}{-2i \sin 2\pi \frac{x}{2}} \right)$$

$$= \frac{1}{\sin 2\pi (\frac{x}{2})} Re \left(\frac{1 - e^{2\pi i n x}}{2 \sin 2\pi \frac{x}{2}} \right)$$

$$= \frac{1}{\sin^{2} 2\pi (\frac{x}{2})} \left[\frac{1}{2} (1 - \cos 2\pi n x) \right]$$

$$= \frac{1}{\sin^{2} 2\pi (\frac{x}{2})} \left(\sin^{2} \frac{2\pi n x}{2} \right) = \left(\frac{\sin(2\pi \frac{n x}{2})}{\sin(2\pi \frac{x}{2})} \right)^{2}$$

since $\frac{1}{2}(1 - \cos \theta) = \sin^2 \frac{\theta}{2}$.

For the second property, note that $F_n(x) \leq \frac{1}{n\sin 2\pi\delta/2}$ for $|x| > \delta$, which clearly goes to 0 as $n \to \infty$. Since \mathbb{T} has total measure 1, this means that $\int_{|x|>\delta} F_n(x)dx \to 0$. \Box

Remark: Note that we now have the Fejér kernels on \mathbb{T} , and the normalized Gaussian kernels on \mathbb{R} , that are "good kernels" satisfying the following conditions:

•

$$\int_{\mathbb{T}} F_n(x) dx = \int_{\mathbb{T}} |F_n(x)| dx = 1$$
$$\int_{\mathbb{R}} \sqrt{\frac{\pi}{\alpha}} G_\alpha(x) dx = \int_{\mathbb{R}} \left| \sqrt{\frac{\pi}{\alpha}} G_\alpha(x) \right| dx = 1$$

• For any $\delta > 0$, we have

$$\lim_{n \to \infty} \int_{|x| > \delta} |F_n(x)| dx = 0$$
$$\lim_{\alpha \to \infty} \int_{|x| > \delta} \left| \sqrt{\frac{\pi}{\alpha}} G_\alpha(x) \right| dx = 0$$

This means that for any $f \in C(\mathbb{T})$, we have $f * F_n \to f$ uniformly as $n \to \infty$. If f is smooth, then more is true; eg. for $f \in \mathcal{S}(\mathbb{R})$, we have $f * \sqrt{\frac{\pi}{\alpha}} G_{\alpha} \to f$ in the C^k -norm, for any k.

Lemma 1.13 (Uniqueness of Fourier Series). Let $f \in C(\mathbb{T})$ such that $\hat{f}(m) = 0$ for all m. Then $f \equiv 0$.

Proof: Suppose not, and let $x_0 \in \mathbb{T}$ such that $f(x_0) \neq 0$. Then by continuity, $f(x) \neq 0$ on a neighborhood of x_0 .

Consider $\int_{\mathbb{T}} f(x) F_n(x-x_0) dx$. Since

$$F_n(x-x_0) = \sum_{j=-n}^n \frac{n-|j|}{n} e^{2\pi i j(x-x_0)} = \sum_{j=-n}^n \left(\frac{n-|j|}{n} e^{-2\pi i j x_0}\right) e^{2\pi i j x}$$

and f is orthogonal to each term in the expansion, we must have $\int f(x)F_n(x-x_0)dx = 0$. On the other hand, for n sufficiently large, the convolution $\int f(x)F_n(x-x_0)dx \to f(x_0) \neq 0$, which gives the contradiction. \Box

Theorem 1.1 (Fourier Inversion on \mathbb{T}). For $f \in C^{\infty}(\mathbb{T})$, we have

$$f(x) = \sum_{m \in \mathbb{Z}} \hat{f}(m) e^{2\pi i m x}$$

Proof: Notice that by Lemma 1.10

$$\widehat{f * F_n}(m) = \begin{cases} \frac{n - |m|}{n} \widehat{f}(m) & n \ge m\\ 0 & n \le m \end{cases}$$

By Lemma 1.13, we see that

$$f * F_n = \sum_{m=-n}^n \frac{n - |m|}{n} \hat{f}(m) e^{2\pi i m x}$$

Recall also by Theorem 1.11 that $\hat{f}(m) \leq m^{-2}$.

Since $f * F_n \to f$, we have for all ϵ , and $n > n(\epsilon)$ sufficiently large, that

$$|f(x) - (f * F_n)(x)| < \epsilon$$

14

and, therefore,

$$\left| f(x) - \sum_{m=-n}^{n} \frac{n - |m|}{n} \widehat{f}(m) e^{2\pi i m x} \right| < \epsilon$$

for n sufficiently large. On the other hand,

$$\left| \sum_{m \in \mathbb{Z}} \hat{f}(m) e^{2\pi i m x} - \sum_{m=-n}^{n} \frac{n - |m|}{n} \hat{f}(m) e^{2\pi i m x} \right|$$
$$= \left| \sum_{m=-n}^{n} \frac{|m|}{n} \hat{f}(m) e^{2\pi i m x} + \sum_{|m| > n} \hat{f}(m) e^{2\pi i m x} \right|$$

Now, since $\hat{f}(m) \lesssim m^{-2}$ decays sufficiently fast, we can select $M(\epsilon)$ such that $\sum_{|m|>M(\epsilon)} |\hat{f}(m)| < \epsilon$. Now divide

$$\begin{aligned} \left| \sum_{m \in \mathbb{Z}} \hat{f}(m) e^{2\pi i m x} - \sum_{m=-n}^{n} \frac{n - |m|}{n} \hat{f}(m) e^{2\pi i m x} \right| \\ &= \left| \sum_{m=-n}^{n} \frac{|m|}{n} \hat{f}(m) e^{2\pi i m x} + \sum_{|m| > n} \hat{f}(m) e^{2\pi i m x} \right| \\ &\leq \sum_{|m| \le M(\epsilon)} \frac{|m|}{n} \left| \hat{f}(m) \right| + \sum_{|m| > M(\epsilon)} \left| \hat{f}(m) \right| \\ &< 2\epsilon \end{aligned}$$

if n is chosen large enough so that the first sum is less than ϵ (i.e., $n > \epsilon^{-1} \sum_{|m| \le M(\epsilon)} |m| |\hat{f}(m)).$ Putting everything together, we have

$$\begin{aligned} \left| f(x) - \sum_{m \in \mathbb{Z}} \hat{f}(m) e^{2\pi i m x} \right| \\ &\leq \left| f(x) - \sum_{m=-n}^{n} \frac{n - |m|}{n} \hat{f}(m) e^{2\pi i m x} \right| + \left| \sum_{m \in \mathbb{Z}} \hat{f}(m) e^{2\pi i m x} - \sum_{m=-n}^{n} \frac{n - |m|}{n} \hat{f}(m) e^{2\pi i m x} \right| \\ &< \epsilon + 2\epsilon = 3\epsilon \end{aligned}$$

Since this holds for any $\epsilon > 0$, we are done. \Box

Lemma 1.14. If $f, g \in \mathcal{S}(\mathbb{R})$, then

$$\int_{\mathbb{R}} f(x)\hat{g}(x)dx = \int_{\mathbb{R}} \hat{f}(y)g(y)dy$$

Proof: Write

$$\begin{split} \int_{\mathbb{R}} f(x)\hat{g}(x)dx &= \int_{x\in\mathbb{R}} f(x)\int_{y\in\mathbb{R}} g(y)e^{-2\pi ixy}dy\\ &= \int_{y\in\mathbb{R}} \int_{x\in\mathbb{R}} f(x)e^{-2\pi ixy}g(y)dy\\ &= \int_{y\in\mathbb{R}} \hat{f}(y)g(y)dy \end{split}$$

using the decay of $f, g \in \mathcal{S}(\mathbb{R})$ to interchange the order of integration.

Theorem 1.2 (Fourier Inversion on \mathbb{R}). For $f \in \mathcal{S}(\mathbb{R})$, we have

$$f(x_0) = \int_{\mathbb{R}} \hat{f}(\xi) e^{2\pi i \xi x_0} d\xi$$

Proof: Take $g_{\alpha}(y) = e^{2\pi i x_0 y} G_{\alpha^{-1}}(y) \in \mathcal{S}(\mathbb{R})$ in Lemma 1.14. This gives

$$\int_{x \in \mathbb{R}} f(x)\hat{g}_{\alpha}(x)dx = \int_{y \in \mathbb{R}} \hat{f}(y)g(y)$$

Note that $\hat{g}_{\alpha}(x) = \sqrt{\pi \alpha} G_{\pi^2 \alpha}(x - x_0)$, so that

$$\int_{x \in \mathbb{R}} f(x) \hat{g}_{\alpha}(x) dx \to f(x_0)$$

as $\alpha \to \infty$, so the left hand side converges to $f(x_0)$. On the other hand, $g_{\alpha}(y) \to e^{2\pi i x_0 y}$ pointwise as $\alpha \to \infty$, and since $f \in \mathcal{S}(\mathbb{R})$ decays rapidly, we have

$$\hat{f}g_{\alpha} \to \hat{f}e^{2\pi i x_0 y}$$

in $L^1(\mathbb{R})$ as well. Thus the right-hand side converges to $\int_{y \in \mathbb{R}} \hat{f}(y) e^{2\pi i y x_0}$ and, replacing y with ξ , we are done. \Box

Remark: It is convenient to describe Fourier inversion as saying that

$$\sum_{m \in \mathbb{Z}} e^{2\pi i m x} = \delta_0$$
$$\int_{\mathbb{R}} e^{2\pi i \xi x} dx = \delta_0$$

as distributions on $\mathbb T$ and $\mathbb R,$ respectively. This is ubiquitous in calculations!

Lemma 1.15 (Plancherel Theorem). We have the following unitarity properties of the Fourier transform:

16

• For $f, g \in C^{\infty}(\mathbb{T})$, we have

$$\int_0^1 f(x)\overline{g(x)}dx = \sum_{m \in \mathbb{Z}} \hat{f}(m)\overline{\hat{g}(m)}$$

• For $f, g \in \mathcal{S}(\mathbb{R})$, we have

$$\int_{\mathbb{R}} f(x)\overline{g(x)}dx = \int_{\mathbb{R}} \hat{f}(\xi)\overline{\hat{g}(\xi)}d\xi$$

In particular, $||f||_{L^2} = ||\hat{f}||_{L^2}$.

Proof: For the \mathbb{T} statement, write

$$\sum_{m \in \mathbb{Z}} \hat{f}(m)\hat{g}(m) = \sum_{m \in \mathbb{Z}} \int_{x=0}^{1} f(x)e^{-2\pi i m x} dx \overline{\hat{g}(m)}$$
$$= \int_{x=0}^{1} f(x) \sum_{m \in \mathbb{Z}} \overline{\hat{g}(m)}e^{2\pi i m x} dx$$
$$= \int_{x=0}^{1} f(x)\overline{g(x)} dx$$

using Fourier inversion.

The \mathbb{R} statement follows similarly. \Box .

Remark: Note that for this, we only required g to be smooth; of course, we could also have reversed the roles and required only f to be smooth. In other words, this works just as well when one of f or g is replaced with a distribution.

Lemma 1.16. Consider the operators

$$[Xf](x) = xf(x) [e^{2\pi i y X} f](x) = e^{2\pi i y x} f(x) [Df](x) = (2\pi i)^{-1} f'(x)$$

Then for $f \in C^{\infty}(\mathbb{T})$ we have

$$\widehat{Df}(m) = (m)\widehat{f}(m)$$

$$e^{2\pi i y X} \widehat{f}(m) = \widehat{f}(m-y)$$

For $f \in \mathcal{S}(\mathbb{R})$, we have

$$\widehat{Df}(\xi) = (\xi)\widehat{f}(\xi)$$
$$\widehat{Xf}(\xi) = -\frac{1}{2\pi i}\widehat{f'}(\xi)$$
$$e^{2\pi i y X}\widehat{f}(\xi) = \widehat{f}(\xi - y)$$

Proof: Exercise.

Corollary 1.2. The Fourier transform maps $\mathcal{S}(\mathcal{R})$ into (and therefore, by inversion, onto) itself.

This is a big reason why $\mathcal{S}(\mathbb{R})$ is the right space to consider for the Fourier transform on \mathbb{R} .

Lemma 1.17. With the operators X and D on $\mathcal{S}(\mathbb{R})$ as in Lemma 1.16, we have the following commutation relation

$$[D, X]f = (2\pi i)^{-1}f$$

Proof: First,

$$[D(Xf)](x) = [Xf]'(x) = (2\pi i)^{-1} \frac{d}{dx} (xf(x)) = (2\pi i)^{-1} (f(x) + xf'(x))$$

On the other hand,

$$[X(Df)](x) = x[Df](x) = x(2\pi i)^{-1}f'(x) = (2\pi i)^{-1}xf'(x)$$

Therefore,

$$\begin{bmatrix} [D, X]f \end{bmatrix}(x) = [D(Xf)](x) - [X(Df)](x) = (2\pi i)^{-1}(f(x) + xf'(x)) - (2\pi i)^{-1}xf'(x)) = (2\pi i)^{-1}f(x)$$

A (striking) consequence of this property is the following fact:

Theorem 1.3 (Heisenberg Uncertainty Principle). With notations as in Lemma 1.16, we have for any $f \in S(\mathbb{R})$

$$||Xf||_{L^2} \cdot ||Df||_{L^2} \ge \frac{1}{4\pi} ||f||_{L^2}^2$$

Proof: Consider, for real numbers $a, b \in \mathbb{R}$ to be chosen later, that

$$0 \leq ||(aX + ibD)f||_{L^{2}}^{2} = a^{2}||Xf||_{L^{2}}^{2} + b^{2}||Df||_{L^{2}}^{2} + \langle aXf, ibDf \rangle + \langle ibDf, aXf \rangle = a^{2}||Xf||_{L^{2}}^{2} + b^{2}||Df||_{L^{2}}^{2} - iab\Big(\langle Xf, Df \rangle - \langle Df, Xf \rangle\Big)$$

Noting that X and D are both self-adjoint, we can write

$$\begin{split} \langle Xf, Df \rangle - \langle Df, Xf \rangle &= \langle DXf, f \rangle - \langle XDf, f \rangle \\ &= \langle [D, X]f, f \rangle \\ &= (2\pi i)^{-1} ||f||_{L^2}^2 \end{split}$$

Thus,

$$0 \le a^2 ||Xf||_{L^2}^2 + b^2 ||Df||_{L^2}^2 - \frac{ab}{2\pi} ||f||_{L^2}^2$$

Now set $a = ||Df||_{L^2}$ and $b = ||Xf||_{L^2}$, and divide through by $ab = ||Xf||_{L^2}||Df||_{L^2}$ to get

 $0 \le ||Df||_{L^2} ||Xf||_{L^2} + ||Xf||_{L^2} ||Df||_{L^2} - (2\pi)^{-1} ||f||_{L^2}^2$

and the result follows. \Box

Remark: Let's interpret what this means. For simplicity, suppose that f is a function such that both $|f|^2$ and $|\hat{f}|^2$ have mean 0; i.e., both

$$\int_{\mathbb{R}} x |f(x)|^2 dx = 0$$
$$\int_{\mathbb{R}} \xi |f(\xi)|^2 d\xi = 0$$

Then the variances of f and \hat{f} are given by the second moments

$$\int_{\mathbb{R}} x^2 |f(x)|^2 dx = ||Xf||_{L^2}^2$$
$$\int_{\mathbb{R}} \xi^2 |\hat{f}(\xi)|^2 d\xi = ||\widehat{Df}||_{L^2}^2 = ||Df||_{L^2}^2$$

applying Lemmas 1.15 and 1.16 in the second equation. Thus Theorem 1.3 says that the variance of f and \hat{f} cannot both be arbitrarily small; the more one localizes f, the more widely distributed \hat{f} becomes, and vice versa.

Corollary 1.3. For any $\hbar > 0$, we have

$$||Xf||_{L^2} \cdot ||2\pi\hbar Df||_{L^2} \ge \frac{\hbar}{2} ||f||_{L^2}^2$$

Exercise 1.3. The point of this exercise is to show that, for the Gaussians G_{α} , equality is achieved in the Heisenberg Uncertainty Principle; *i.e.*, we have

$$\left(\int_{\mathbb{R}} x^2 |G_{\alpha}(x)|^2 dx\right)^{\frac{1}{2}} \left(\int_{\mathbb{R}} \xi^2 |\widehat{G_{\alpha}}(\xi)|^2 d\xi\right)^{\frac{1}{2}} = \frac{1}{4\pi} ||G_{\alpha}||_{L^2}^2$$

(1) Using some changes of variable and Corollary 1.1, show that it is sufficient to prove the case of $\alpha = \pi$; i.e., that

$$||XG_{\pi}||_{2}^{2} = \frac{1}{4\pi}||G_{\pi}||_{2}^{2}$$

(2) Use an integration by parts argument to show that

$$||XG_{\pi}||_{2}^{2} = \int_{\mathbb{R}} x^{2} e^{-2\pi x^{2}} dx = \frac{1}{4\pi} ||G_{\pi}||_{2}^{2}$$

Exercise 1.4. The point of this exercise is to show that f and \hat{f} cannot both be compactly supported.

(1) Show that, if f has compact support, then its Fourier transform

$$\hat{f}(z) = \int_{\mathbb{R}} f(x) e^{-2\pi i x z} dx$$

can be extended to a holomorphic function of $z \in \mathbb{C}$.

- (2) Use this to show that the set $\{z : \hat{f}(z) = 0\}$ must be discrete.
- (3) Deduce a contradiction from the assumption that \hat{f} is compactly supported on \mathbb{R} .

1.3. Fourier Series and Equidistribution. An important observation about Fourier coefficients is that, for $f \in C^{\infty}(\mathbb{T})$, the 0-th coefficient $\hat{f}(0) = \int_0^1 f(x) dx$ is the average of f over \mathbb{T} . Thus, the remaining Fourier coefficients determine, in a sense that can be made more precise, how f deviates from its average. A classical example is Weyl's Equidistribution Theorem:

Theorem 1.4 (Weyl). Let $\alpha \in \mathbb{R} \setminus \mathbb{Q}$ be irrational. Then the multiples $\{n\alpha \mod 1\}_{n=1}^{\infty}$ are equidistributed in \mathbb{T} (with respect to Lebesgue measure) as $n \to \infty$.

Proof: We write $\{n\alpha\} = n\alpha \mod 1$ to be the fractional part of $n\alpha$. To say that the sequence $\{n\alpha\}$ is equidistributed means that, for any interval $[a, b] \subset [0, 1)$, we have

$$\lim_{N \to \infty} \frac{1}{N} \# \{ n \le N : \{ n\alpha \} \in [a, b] \} = l([a, b]) = b - a$$

or, setting $\chi_{[a,b]}$ to be the characteristic function of the interval [a,b] (extended to be a 1-periodic function on \mathbb{R})

$$\frac{1}{N}\sum_{n=1}^{N}\chi_{[a,b]}(n\alpha) = \int_{0}^{1}\chi_{[a,b]}(x)dx$$

It is more convenient to smooth out the characteristic function, and consider instead smooth 1-periodic functions $f \in C^{\infty}(\mathbb{T})$ that approximates $\chi_{[a,b]}$ in L^1 ; it is sufficient to show that

$$\lim_{N \to \infty} \frac{1}{N} \sum_{n=1}^{N} f(n\alpha) = \int_{0}^{1} f(x) dx = \hat{f}(0)$$

for all smooth $f \in C^{\infty}(\mathbb{T})$, since we can take smooth functions f_+ and f_- such that $f_+(x) \geq \chi_{[a,b]}(x) \geq f_-(x)$ everywhere, while f_+ and f_-

are L^1 -close to $\chi_{[a,b]}$, giving

$$\begin{split} \int_0^1 \chi_{[a,b]}(x) dx &- \epsilon \quad < \quad \int_0^1 f_-(x) dx = \lim_{N \to \infty} \frac{1}{N} \sum_{n=1}^N f_-(n\alpha) \\ &\leq \quad \lim_{N \to \infty} \frac{1}{N} \sum_{n=1}^N \chi_{[a,b]}(n\alpha) \\ &\leq \quad \lim_{N \to \infty} \frac{1}{N} \sum_{n=1}^N f_+(n\alpha) = \int_0^1 f_+(x) dx \\ &< \quad \int_0^1 \chi_{[a,b]}(x) dx + \epsilon \end{split}$$

So, consider $f \in C^{\infty}(\mathbb{T})$. By Fourier inversion, we can write

$$\frac{1}{N}\sum_{n=1}^{N}f(n\alpha) = \frac{1}{N}\sum_{n=1}^{N}\sum_{m=-\infty}^{\infty}\hat{f}(m)e^{2\pi i n\alpha}$$
$$= \sum_{m=-\infty}^{\infty}\hat{f}(m)\frac{1}{N}\sum_{n=1}^{N}e^{2\pi i m n\alpha}$$

The term m = 0 in the sum gives us $\hat{f}(0)$, which is exactly what we want; the problem is to eliminate the other terms. By the Lemma 1.11, the Fourier coefficients \hat{f} decay rapidly (and thus the sum over m is absolutely convergent, uniformly in N); therefore it is sufficient to show that

$$\frac{1}{N}\sum_{n=1}^{N}e^{2\pi i m n \alpha} \to 0$$

as $N \to \infty$; this is known as Weyl's criterion.

To finish, note that the above sum is a geometric series, and so

$$\left|\frac{1}{N}\sum_{n=1}^{N}e(mn\alpha)\right| = \frac{1}{N}\frac{|e(m\alpha) - e((N+1)m\alpha)|}{|1 - e(m\alpha)|} = O\left(\frac{1}{N}\right)$$

for any $m \in \mathbb{Z}$, since $e(m\alpha) \neq 1$ (α is irrational!) is independent of N, and the numerator is bounded by 2. \Box

Here is another important fact, that we will use later on— informally, it is a generalization of Weyl's argument, to the case where there are a few more non-zero Fourier coefficients. For a measure (or, more generally, a distribution) μ , we define the Fourier transform of μ via

$$\hat{\mu}(m) := \int e^{-2\pi i m x} d\mu(x)$$

Lemma 1.18. Suppose μ is a probability measure on \mathbb{T} , such that

$$\sum_{|m| \le M} |\hat{\mu}(m)| \le k$$

(think of M as being much larger than k, so that there are few sizable Fourier coefficients).

Then for any interval I of length $\geq M^{-1}$, we have

$$\mu(I) \lesssim k \cdot l(I)$$

where l(I) is the (Lebesgue) length of I. In other words, up to a factor of k, the mass of μ is evenly distributed up to scale M^{-1} .

Proof: It is sufficient to consider intervals of length M^{-1} , since we can cover a larger interval by smaller intervals to get the statement.

Let x_0 be the midpoint of such an interval, and consider the convolution of $F_{M/2}$ with μ at x_0 ,

$$\int_{\mathbb{T}} F_{M/2}(x-x_0) d\mu(x)$$

Since

22

$$F_{M/2}(x - x_0) = \sum_{m = -M/2}^{M/2} c_m e^{2\pi i m x}$$

with each $|c_m| \leq 1$, we have

$$\left|\int_{\mathbb{T}} F_{M/2}(x-x_0)d\mu(x)\right| \le k$$

On the other hand, since $F_{M/2} \ge 0$ and μ is a positive measure, we have

$$k \ge \int_{\mathbb{T}} F_{M/2}(x - x_0) d\mu(x) \ge \int_{I} F_{M/2}(x - x_0) d\mu(x)$$

and, noting that $\sin(x) \le x$ and that $\frac{\sin(x)}{x}$ is decreasing for $|x| \le \pi/4$, we have for $|x - x_0| < 1/2M$ that

$$F_{M/2}(x - x_0) = \frac{2}{M} \left(\frac{\sin(\frac{\pi}{2}M(x - x_0))}{\sin(\pi(x - x_0))} \right)^2$$

$$\geq \frac{2}{M} \left(\frac{\sin(\frac{\pi}{2}M(x - x_0))}{\pi(x - x_0)} \right)^2$$

$$\geq \frac{M}{2} \left(\frac{\sin(\frac{\pi}{2}M(x - x_0))}{\frac{\pi}{2}M(x - x_0)} \right)^2$$

$$\geq \frac{M}{2} \left(\frac{\sin(\pi/4)}{\pi/4} \right)^2 \gtrsim M$$

Therefore, we have

$$k \geq \int_{I} F_{M/2}(x - x_{0})d\mu(x)$$

$$\gtrsim \int_{I} Md\mu$$

$$= M\mu(I)$$

and the result follows. \Box

1.4. Some Comments about the Fourier Transform on \mathbb{R}^d . As noted before, there is not too much mystery in generalizing the Fourier transform to several dimensions. For example, for $f \in \mathcal{S}(\mathbb{R}^d)$ (defined in the obvious way, replacing powers of x with polynomial functions in the d variables, and replacing derivatives with respect to x with all derivatives), we define

$$\hat{f}(\xi) = \int_{\mathbb{R}^d} f(x) e^{-2\pi i \xi \cdot x} dx$$

where x and ξ are now in \mathbb{R}^d , and we use the usual dot product

$$\xi \cdot x := \xi_1 x_1 + \xi_2 x_2 + \dots + \xi_d x_d$$

Since the exponential satisfies

$$e^{-2\pi i\xi \cdot x} = \prod_{j=1}^d e^{-2\pi i\xi_j x_j}$$

the Fourier transform on \mathbb{R}^d inherits the properties of the Fourier transform on \mathbb{R} simply by repeating the arguments, integrating one variable at a time.

In particular, we have:

• Fourier Inversion:

$$f(x) = \int_{\mathbb{R}^d} \hat{f}(\xi) e^{2\pi i \xi \cdot x} d\xi$$

• Scaling Property: If $[R_{\lambda}(f)](x) = f(\lambda x)$ for $\lambda \in \mathbb{R}$, then

$$R_{\lambda}(f) = \lambda^{-d} \hat{f}(\xi/\lambda)$$

(Note the scale factor of λ^{-d} , since we are changing variables $x \to \lambda x$ in d dimensions!)

• Plancherel Theorem:

$$\langle f,g\rangle = \langle \hat{f},\hat{g}\rangle$$

• Multiplication and Convolution:

$$\widehat{f * g} = \widehat{f} \widehat{g} \widehat{fg} = \widehat{f} * \widehat{g}$$

• Multiplication Operators and Differentiation: If X_j is the operator of multiplication by x_j , and D_j is the differential operator $(2\pi i)^{-1} \frac{\partial}{\partial x_j}$, then

$$\widehat{X_j f} = -D_j \widehat{f}
\widehat{D_j f} = X_j \widehat{f}
\widehat{e^{2\pi i y X_j}} f(\xi) = \widehat{f}(\xi_1, \xi_2, \dots, \xi_j - y, \dots, \xi_d)$$

• Our favorite Schwartz function on \mathbb{R}^d , the Gaussian $G_{\pi} = e^{-\pi |x|^2}$, is its own Fourier transform. Hence

$$\widehat{G_{\alpha}} = \left(\frac{\pi}{\alpha}\right)^{d/2} G_{\pi^2/\alpha}$$

and yields equality in the Heisenberg Uncertainty Principle (see below).

There are several points regarding the Fourier transform on \mathbb{R}^d , however, that deserve attention. The first is the Uncertainty Principle: note that while

$$[D_i, X_i] = (2\pi i)^{-1} Id$$

for each j, the operators D_j and X_k commute whenever $j \neq k$, since

$$\frac{\partial}{\partial x_j}(x_k f) = x_k \frac{\partial}{\partial x_j} f$$

So the Uncertainty Principle holds in each coordinate individually.

Another point to consider is that we have many different coordinate systems in \mathbb{R}^d (and nobody likes depending on a particular coordinate system, especially when we move from \mathbb{R}^d to manifolds). It will be of particular interest to us to consider polar coordinates, and we begin with the following Lemma:

Lemma 1.19. Let $R \in SO(d)$ be a rotation of \mathbb{R}^d , and denote T_R the operator $T_R f(x) = f(Rx)$. Then

$$\widehat{T_R f} = T_R \widehat{f}$$

i.e., the Fourier transform commutes with rotations.

24

Proof: Since det R = 1, we can change variables $x \mapsto R^{-1}x$ to get

$$\widehat{T_R f}(\xi) = \int_{\mathbb{R}^d} f(Rx) e^{-2\pi i x \cdot \xi} dx$$
$$= \int_{\mathbb{R}^d} f(x) e^{-2\pi i R^{-1} x \cdot \xi} dx$$
$$= \int_{\mathbb{R}^d} f(x) e^{-2\pi i x \cdot R\xi} dx$$
$$= \widehat{f}(R\xi)$$

since R preserves the dot product, whereby $R^{-1}x \cdot \xi = x \cdot R\xi$. One particularly nice consequence is that

Corollary 1.4. Let $f \in \mathcal{S}(\mathbb{R})$ be a radial function; i.e., f(x) = f(|x|)(or, equivalently, f(Rx) = f(x) for all rotations $R \in SO(d)$ for all x. Then \hat{f} is also a radial function.

A nice example is (again) our friends the Gaussians. *Proof:* This follows from the last Lemma, since

$$\hat{f}(R\xi) = T_R \hat{f}(\xi) = \widehat{T_R f}(\xi) = \hat{f}(\xi)$$

because $T_R f = f$. \Box

Another related property is the following important fact:

Exercise 1.5. Let

$$\Delta = \frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} + \dots + \frac{\partial^2}{\partial x_d^2}$$

be the Laplacian operator on \mathbb{R}^d . Show that

$$\widehat{\Delta f}(\xi) = -4\pi^2 |\xi|^2 \widehat{f}(\xi)$$

So the Laplacian, which is invariant under rotations, is sent by the Fourier transform to the operator of multiplication by a radial function $-4\pi^2 |\xi|^2$.

1.5. The Semi-classical Fourier Transform. As hinted above in Corollary 1.3, we would like to be able to control the degree of uncertainty in our Fourier transforms $(\frac{1}{4\pi}$ is a very interesting number, but does not conform to the quantum mechanics of our universe; at least not in our usual units). In everyday life the uncertainty is very small (about 1.05×10^{-34} in SI units). For the semiclassical theory, \hbar will always be a small (positive) parameter tending to 0.

In order to get the right uncertainty, then, we need to reparametrize our Fourier transform. Thus we define: **Definition 1.5.** For $f \in \mathcal{S}(\mathbb{R})$, we define the \hbar -semiclassical Fourier transform

$$\mathcal{F}_{\hbar}(f)(\xi) = (2\pi\hbar)^{-1/2} \int_{\mathbb{R}} f(x) e^{-\frac{i}{\hbar}\xi x} dx$$

Note that this is nothing but the usual Fourier transform, rescaled by a factor of $2\pi\hbar$; i.e.

$$\mathcal{F}_{\hbar}(f)(2\pi\hbar\xi) = (2\pi\hbar)^{-1/2}\hat{f}(\xi)$$

Note that the normalizing factor of $(2\pi\hbar)^{-1/2}$ insures that \mathcal{F}_{\hbar} remains unitary.

It is clear that the semiclassical Fourier transform is inverted via

$$f(x) = (2\pi\hbar)^{-1/2} \int_{\mathbb{R}} \mathcal{F}_{\hbar}(\xi) e^{\frac{i}{\hbar}x\xi} d\xi$$

Remark: The importance of the parameter \hbar will become apparent later on; for now, let us be content to examine its effect on the Heisenberg Uncertainty Principle— since the Fourier transform is rescaled by a factor of $2\pi\hbar$, the function \mathcal{F}_{\hbar} is much more localized than \hat{f} , by a factor of $2\pi\hbar$. This leads to the semiclassical version of Heisenberg's Uncertainty Principle, stated in Corollary 1.3. This is actually a physical law, when the appropriate (very small) constant \hbar is used; though in the semiclassical sense, it is measuring the degree to which one can simultaneously localize f and $\mathcal{F}_{\hbar}f$ as $\hbar \to 0$. Notice, of course, that as $\hbar \to 0$, the right-hand side of Corollary 1.3 tends to 0 as well.

We also wish to record the following important fact:

Lemma 1.20. Consider the operator $H = -\hbar^2 \Delta$ on $\mathcal{S}(\mathbb{R})$. Then

$$\mathcal{F}_{\hbar}(Hf)(\xi) = |\xi|^2 \mathcal{F}_{\hbar}(f)(\xi)$$

Proof: Recall from Exercise 1.5 that $\widehat{\Delta f}(\xi) = -|2\pi\xi|^2 \widehat{f}(\xi)$. Therefore

$$\mathcal{F}_{\hbar}(Hf)(\xi) = \frac{1}{\sqrt{2\pi\hbar}} \widehat{Hf}(\xi/2\pi\hbar)$$

$$= -\frac{1}{\sqrt{2\pi\hbar}} \hbar^2 \widehat{\Delta f}(\xi/2\pi\hbar)$$

$$= \frac{1}{\sqrt{2\pi\hbar}} \hbar^2 |\xi/\hbar|^2 \widehat{f}(\xi/2\pi\hbar)$$

$$= |\xi|^2 \frac{1}{\sqrt{2\pi\hbar}} \widehat{f}(\xi/2\pi\hbar)$$

$$= |\xi|^2 \mathcal{F}_{\hbar}(\xi)$$

as required. \Box

Remark: One can also define a semiclassical Fourier transform on the torus, by setting for $f \in C^{\infty}(\mathbb{T})$

$$\mathcal{F}_{\hbar}f(2\pi\hbar m) = (2\pi\hbar)^{-1/2}\hat{f}(m)$$

which is now defined on $2\pi\hbar\mathbb{Z}$. (The discrete Fourier transform is in a sense already "semi-classical", and we will see it arise out of \mathcal{F}_{\hbar} on \mathbb{T} when we discuss the so-called "cat map" models).

2. A Brief Introduction to Basics of Quantum Mechanics

In this section, we give a "crash course" in the basic foundations of quantum mechanics. We will not try to motivate the discussion physically, nor try to discuss philosophical consequences of the physical theory. From our point of view, it is simply an abstract (and bizarre) mathematical model of mechanics, whose only redeeming feature is that some very smart people have found that it works (i.e., its predictions agree disturbingly well with experimental data).

2.1. The Hamiltonian Formulation of (Classical) Mechanics. Let's first recall Newton's Law of classical mechanics, given by the second order ODE

$$F = \frac{dp}{dt} = m\frac{d^2q}{dt^2}$$

where $p = m \frac{dq}{dt} \in \mathbb{R}^d$ is the momentum of a particle moving in \mathbb{R}^d , m its mass, and $q \in \mathbb{R}^d$ its position. F is the (net) force acting on the particle, which we will always assume to be conservative; i.e., given by $F = -\nabla V(q)$ for some potential function V of the position. This immediately implies that the motion of the particle is determined initial conditions $(q_0, p_0) \in \mathbb{R}^{2d}$, and in fact the motion is a flow on \mathbb{R}^{2d} determined by solving the ODE (we will always assume that the solution exists for all time).

Hamilton recognized that Newton's Law can be reformulated by introducing the **Hamiltonian function** $H = \frac{|p|^2}{2m} + V(q)$, and observing that

$$\frac{\partial H}{\partial p_j} = \frac{1}{m} p_j = \frac{1}{m} \cdot m \frac{dq_j}{dt}$$
$$= \frac{dq_j}{d_t}$$

for $j = 1, \ldots d$, while Newton's Law implies that

$$-\frac{\partial H}{\partial q_j} = -\frac{dV}{dq_j} = F_j$$
$$= \frac{dp_j}{dt}$$

At first, this just looks like a silly way to write one 2nd order equation as a system of 2 1st order equations. But it becomes a bit less silly, and a bit more useful, with the following important observation:

Lemma 2.1. Let $f \in C^{\infty}(\mathbb{R}^{2d})$, and suppose z(t) = (q(t), p(t)) is a solution of Hamilton's equations for some Hamiltonian H. Then,

$$\frac{df}{dt} = \{f, H\}$$

Here we introduce the **Poisson bracket**

(1)
$$\{f,g\} = \frac{\partial f}{\partial q}(z)\frac{\partial g}{\partial p}(z) - \frac{\partial f}{\partial q}(z)\frac{\partial g}{\partial p}(z)$$
$$= \sum_{j=1}^{d} \frac{\partial f}{\partial q_j}(z)\frac{\partial g}{\partial p_j}(z) - \frac{\partial f}{\partial q_j}(z)\frac{\partial g}{\partial p_j}(z)$$

In particular, a function $f \in C^{\infty}(\mathbb{R}^{2d})$ is invariant under the motion governed by H iff $\{f, H\} = 0$.

Proof of Lemma 2.1:

$$\frac{d}{dt}f(z(t)) = \frac{\partial f}{\partial q}(z(t))q'(t) + \frac{\partial f}{\partial p}(z(t))p'(t)$$
$$= \frac{\partial f}{\partial q}\frac{\partial H}{\partial p}(z(t)) - \frac{\partial f}{\partial p}\frac{\partial H}{\partial q}(z(t))$$
$$= \{f, H\}(z(t))$$

We pause for some terminology, into which we can translate the above Lemma. We consider $z(t) = (q(t), p(t)) \in \mathbb{R}^{2d}$ to be the **state** of the particle at time t, in the sense that knowing z(t) tells you everything you need to know about the particle at time t to determine its path. We call \mathbb{R}^{2d} the **phase space** for the motion; this is the space on which the motion takes place, as the particle moves from state to state. Any (smooth) function f on \mathbb{R}^{2d} is called an **observable**, in the sense that it's something about the particle you can measure at any point in its motion. Examples of observables are

- A position coordinate $f(q, p) = q_j$
- A momentum coordinate $f(q, p) = p_j$
- The potential f(q, p) = V(q)

- The Hamiltonian itself $f(q, p) = H(q, p) = \frac{1}{2m}|p|^2 + V(q)$
- The angular momentum $f(q, p) = L_3(q, p) = q_1p_2 p_1q_2$
 - (the terminology and notation come from the case d = 3)
- Anything else you might care to measure about your particle.

So, the Hamiltonian function (or "observable") gives rise to a flow Φ_t^H on the phase space \mathbb{R}^{2d} , and an observable f is invariant under this flow iff $\{f, H\} = 0$. We call such an f a **constant of the motion**. Observe that $\{H, H\} = 0$ trivially, so that the Hamiltonian is a constant of the motion. In fact, observe that the Hamiltonian is nothing but the total energy of the particle (kinetic energy + potential energy), so this observation states that energy is conserved.

Example 2.1. Let d = 2, and suppose that V = V(r) is a radial function. Then the angular momentum L_3 is a constant of the motion.

Proof: Compute

$$\{L_3, H\} = \sum_{j=1}^{2} \frac{\partial L_3}{\partial q_j} \frac{\partial H}{\partial p_j} - \frac{\partial L_3}{\partial p_j} \frac{\partial H}{\partial q_j}$$
$$= \left(p_2 \frac{p_1}{m} - (-q_2) \frac{dV}{dq_1} \right) + \left((-p_1) \frac{p_2}{m} - q_1 \frac{dV}{dq_2} \right)$$
$$= (q_2, -q_1) \cdot \nabla V$$

But since V is radial, its gradient ∇V points radially (inward or outward, depending on the sign), and is therefore orthogonal to the vector field $(q_2, -q_1)$. \Box

Definition 2.1. A Hamiltonian $H \in C^{\infty}(\mathbb{R}^{2d})$ is called **completely integrable** iff there exist d independent constants of the motion $\{f_i\}$ (that is, the Jacobian of the map $x \mapsto \{f_1(x) = H(x), f_2(x), \dots, f_d(x)\}$ has full rank d) such that

$$\{f_i, f_j\} = 0$$

for all i, j = 1, ... d.

Example 2.2. Note that, for a particle moving in \mathbb{R}^2 (with phase space \mathbb{R}^4), a Hamiltonian is completely integrable if there exists any constant of the motion (besides H).

- Circular billiards preserve angular momentum about the center. (More generally, elliptic billiards preserve angular momentum about either focus.)
- Rectangular billiards preserve linear momentum in each direction (up to sign, which changes during reflection).

It can be shown (Liouville-Arnold Theorem) that in the completely integrable case, the common level surfaces of the constants of the motion are tori, on which the Hamiltonian flow acts by translation. Thus, for completely integrable Hamiltonians, the flow is *not* exponentially unstable (toral translations can only have linear instability).

The following observation is also important:

Theorem 2.1 (Liouville). *The Hamiltonian flow preserves phase space volume.*

Proof: Essentially follows from the fact that the Hamiltonian vector field

$$X_H = \left(\frac{\partial H}{\partial p_1}, \frac{\partial H}{\partial p_2}, \dots, \frac{\partial H}{\partial p_d}, -\frac{\partial H}{\partial q_1}, \dots, -\frac{\partial H}{\partial q_d}\right)$$

generating the flow defined by Hamilton's equations is divergence-free, as is clear from straightforward calculation (the derivatives of positive terms with respect to q_j cancel with the derivatives of the negative terms with respect to p_j). \Box

2.2. Quantum Mechanics on \mathbb{R} .

2.2.1. Quantum States. In quantum mechanics, the first change is that the state of a particle is no longer described by a point in phase space; rather, it is given by a vector in a Hilbert space. For a particle moving along \mathbb{R} , the space of states is $L^2(\mathbb{R})$; such a state $\psi \in \mathbb{R}$ is often called the "wave function" of the particle. We will always take our states to be unit vectors, i.e. we require that $||\psi||_{L^2} = 1$.

The position and momentum of the particle no longer have definite values. Rather, the probability measure $|\psi(q)|^2 dq$ gives the probability density of the particle being found near q; more precisely, given an interval A, the probability of finding the particle in A is given by

$$Prob(q \in A) = \int_{A} |\psi(q)|^2 dq$$

Remark: We will often say, eg., that "1/2 of the mass of the particle is in A", rather than "the probability of finding the particle in A is 1/2". Mathematically there is no real difference here; either way, we mean that $\int_A |\psi|^2 dq = 1/2$. Physically speaking, the latter is probably more correct, since upon measurement, the particle will either be in A or not. But in our idealized universe, no definitive experiments will actually be performed, and it will be more intuitive (to me) to simply imagine a particle whose mass is smeared out over \mathbb{R} according to the distribution $|\psi|^2$. The momentum density of the particle is given by the measure $|\mathcal{F}_{\hbar}(\psi)(p)|^2 dp$. Note that, by the unitarity of \mathcal{F}_{\hbar} , this is also a probability measure. In this way, the Heisenberg Uncertainty Principle of Corollary 1.3 is given its usual physical meaning— one cannot give both the position and momentum of a particle to arbitrary accuracy; if the position is known to high accuracy (meaning that $|\psi|^2$ is highly localized), then its momentum will be accordingly uncertain ($\mathcal{F}_{\hbar}(\psi)$ will be more widely spread out).

2.2.2. Observables. Since the state of a particle is no longer a point in phase space, it's no longer relevant to measure some observable quantity by evaluating a function on phase space. Rather, we need a new way to understand observables and their "evaluation" on states $\psi \in L^2(\mathbb{R})$.

The easiest way to understand this is by considering the "position observable" formerly known as f(q, p) = q. We have already stated that we can't measure the position of the particle exactly; rather, we can understand the "average position" or the expected value of the position as

$$\mathbb{E}(q) = \int_{\mathbb{R}} q |\psi(q)|^2 dq$$

Paraphrasing, we can say that the expected value of the position observable (for the state ψ) is given by

$$\mathbb{E}_{\psi}(f(q,p)=q) = \langle Q\psi,\psi\rangle$$

where we have introduced the operator $Q\psi(q) = q\psi(q)$

Similarly, we can see that a diagonal matrix coefficient of the operator $P: \psi \mapsto -i\hbar \frac{d\psi}{dq}$ gives the expected value of the momentum for the state ψ

$$\begin{split} \mathbb{E}_{\psi}(f(q,p) = p) &= \langle P\psi, \psi \rangle \\ &= \langle \mathcal{F}_{\hbar}(P\psi), \mathcal{F}_{\hbar}(\psi) \rangle \\ &= \int_{\mathbb{R}} p |\mathcal{F}_{\hbar}(\psi)|^2 dp \end{split}$$

In general, we would like to associate to each classical $f \in C^{\infty}(\mathbb{R}^2)$ an *operator* on $L^2(\mathbb{R})$, denoted Op(f), such that the matrix coefficient

$$\mathbb{E}_{\psi}(f) = \langle Op(f)\psi, \psi \rangle$$

gives the average value of the observable f for the state ψ .

Example 2.3. • If f(q, p) = f(q) is a function only of position, then by analogy with the position operator Q (and by the same reasoning), the operator Op(f) should be multiplication by f. Thus,

$$\langle Op(f)\psi,\psi\rangle = \int_{\mathbb{R}} f(q)|\psi(q)|^2 dq$$

By the same token, if f(q, p) = f(p) is a function only of momentum, then we should take the ħ-Fourier transform inside the inner product, and apply the same logic. Thus, in particular, if f(p) is a polynomial in p, then Op(f) will be a differential operator on L²(ℝ).

Example 2.4. Extending the analogy with Q and P above, we should write

$$H = \frac{1}{2m}P^2 + V(Q)$$

as the Hamiltonian operator on $L^2(\mathbb{R})$. Since $P^2 = -\hbar^2 \frac{d^2}{dq^2}$, we get

$$\mathbb{E}_{\psi}(H) = \langle H\psi, \psi \rangle = \int_{\mathbb{R}} \left(-\frac{d^2\psi}{dq^2}(q)\overline{\psi(q)} + V(q)|\psi(q)|^2 \right) dq$$

Note that we have abused notation and used H to stand for both the Hamiltonian function on \mathbb{R}^2 and its quantization Op(H) as an operator on $L^2(\mathbb{R})$. Some use $\hat{H} = Op(H)$, but then one runs into other notation problems because of the Fourier transform... in any case, the convention H = Op(H) is widespread, so even if you don't like it, you'll have to get used to it anyway!

Remark: One might be (and probably should be) concerned that these operators are not bounded on $L^2(\mathbb{R})$, so it's not clear why the expectation \mathbb{E}_{ψ} should exist for these observables. We won't tread into this issue, since for most of this course we will be working with compact domains; for now, let's adopt the "physicists' convention" that vectors in $L^2(\mathbb{R})$ are actually Schwartz functions.

2.2.3. The Schrödinger Equation. An important remaining question is, what becomes of the equations of motion? The state of a particle over time is no longer a flow of points in phase space; we need instead a law governing the time evolution of a wave function.

The quantum evolution is given by Schrödinger's Equation

$$\begin{aligned} \frac{\partial}{\partial t}\psi_t(q) &= -\frac{i}{\hbar}H\psi_t(q) \\ &= \frac{i\hbar}{2m}\frac{\partial^2}{\partial q^2}\psi_t(q) - \frac{i}{\hbar}V(q)\psi_t(q) \end{aligned}$$

32

We often write $U_t = e^{-\frac{i}{\hbar}Ht}$ for the evolution operator sending $\psi_0 \mapsto \psi_t$. The "U" here stands for unitary, since the evolution is unitary, as can be seen by

$$\begin{aligned} \frac{d}{dt} \int_{\mathbb{R}} |\psi_t(x)|^2 dx &= \frac{\partial}{\partial t} \langle \psi_t, \psi_t \rangle = \left\langle \frac{\partial}{\partial t} \psi_t, \psi_t \right\rangle + \left\langle \psi_t, \frac{\partial}{\partial t} \psi_t \right\rangle \\ &= \left\langle -\frac{i}{\hbar} H \psi_t, \psi_t \right\rangle + \left\langle \psi_t, -\frac{i}{\hbar} H \psi_t \right\rangle \\ &= -\frac{i}{\hbar} \left(\langle H \psi_t, \psi_t \rangle - \langle \psi_t, H \psi_t \rangle \right) \end{aligned}$$

and the unitarity follows from the fact that H is symmetric (assuming as we always will— that V is real-valued, and doing an integration by parts with the differential operator P).

This calculation brings out the importance of H being symmetric; without this assumption, the Schrödinger flow need not be unitary, which violates the interpretations of $|\psi|^2$ and $|\mathcal{F}_{\hbar}\psi|^2$ as probability densities. This property is the quantum analogue of Theorem 2.1.

2.2.4. The Ehrenfest Equations. There is a nice way to (try to) justify the analogy with classical mechanics, by showing that there are equations analogous to Hamilton's equations that are satisfied by the Schrödinger flow. These equations are called the Ehrenfest equations, and are given by

$$\frac{d}{dt} \mathbb{E}_{\psi_t}(q) = \frac{1}{m} \mathbb{E}_{\psi_t}(p)$$
$$\frac{d}{dt} \mathbb{E}_{\psi_t}(p) = -\mathbb{E}_{\psi_t}\left(\frac{dV}{dq}\right)$$

satisfied by any solution ψ_t of Schrödinger's equation, as we show below. Notice that these are extremely similar to Hamilton's equations, and it even seems at first glance like the average postion and momentum $\mathbb{E}_{\psi_t}(q)$ and $\mathbb{E}_{\psi_t}(p)$ satisfy an ODE! Unfortunately, this is not quite the case, since in general

$$-\mathbb{E}_{\psi_t}\left(\frac{dV}{dq}\right) \neq \frac{dV}{dq}(\mathbb{E}_{\psi_t}(q))$$

i.e., the average value of the force F = -V'(q) is not equal to the force evaluated at the average position $\mathbb{E}_{\psi_t}(q)$.

Now we "prove" the Ehrenfest equations, by assuming that $\psi_t \in \mathcal{S}(\mathbb{R})$. Of course, there isn't much mystery here— simply write out what the time derivatives are, and replace $\partial_t \psi_t$ via the Schrödinger

equation:

$$\frac{d}{dt}\mathbb{E}_{\psi_t}(q) = \left\langle Q\frac{\partial}{\partial t}\psi_t, \psi_t \right\rangle + \left\langle Q\psi_t, \frac{\partial}{\partial t}\psi_t \right\rangle$$
$$= 2Re\left(\int_{\mathbb{R}} q\left(\frac{i\hbar}{2m}\psi_t''(q) - \frac{i}{\hbar}V(q)\psi_t(q)\right)\overline{\psi_t(q)}dq\right)$$

Now, the potential term (with the "V" term) clearly vanishes, since it is proportional to the imaginary part of

$$\int_{\mathbb{R}} qV(q) |\psi_t(q)|^2 dq$$

which is real-valued. It remains to check the term with ψ''_t , for which we apply integration by parts to get

$$\frac{d}{dt}\mathbb{E}_{\psi_t}(q) = -\frac{\hbar}{m}Im\left(\int_{\mathbb{R}}q\left(\psi_t''(q)\right)\overline{\psi_t(q)}dq\right) \\
= \frac{\hbar}{m}Im\left(\int_{\mathbb{R}}q|\psi_t'(q)|^2dq + \int_{\mathbb{R}}\psi_t'(q)\overline{\psi_t(q)}dq\right) \\
= -\frac{i\hbar}{2m}\left(\langle\psi_t',\psi_t\rangle - \langle\psi_t,\psi_t'\rangle\right)$$

since the term $\int_{\mathbb{R}} q |\psi_t'(q)|^2 dq$ is real. But this last line can be rewritten

$$\frac{d}{dt}\mathbb{E}_{\psi_t}(q) = \frac{1}{2m}\left(\langle (-i\hbar)\psi'_t, \psi_t \rangle + \langle \psi_t, (-i\hbar)\psi'_t \rangle\right) \\
= \frac{1}{2m}\left(\langle P\psi_t, \psi_t \rangle + \langle \psi_t, P\psi_t \rangle\right) \\
= \frac{1}{2m}2\langle P\psi_t, \psi_t \rangle \\
= \frac{1}{2m}\mathbb{E}_{\psi_t}(p)$$

since P is symmetric.

Exercise 2.1. In this exercise, (continue to) assume that $\psi_t \in \mathcal{S}(\mathbb{R})$.

• Show the second Ehrenfest equation

$$\frac{d}{dt}\mathbb{E}_{\psi_t}(p) = -\mathbb{E}_{\psi_t}\left(\frac{dV}{dq}\right)$$

is satisfied by any solution of the Schrödinger equation.

• Show that the expected value of H is preserved under the Schrödinger flow (conservation of energy); i.e., we have

$$\frac{d}{dt}\mathbb{E}_{\psi_t}(H) := \frac{d}{dt} \langle H\psi, \psi \rangle = 0$$

34

2.2.5. Commutators. Recall that the Hamiltonian formulation gave us a convenient way to understand the time dependence of an observable f, evaluated for the state $(q(t), p(t)) \in \mathbb{R}^{2d}$ of a (moving) particle. In particular, we saw that the value of the observable is conserved iff the observable Poisson-commutes with the Hamiltonian, H.

There is a similarly lovely description of the time dependence of the average value of a quantum observable operator F acting on $L^2(\mathbb{R})$:

Lemma 2.2. Let ψ_t be a solution of Schrödinger's equation, and H the Hamiltonian operator. Then for any quantum observable F, we have

$$\frac{d}{dt}\langle F\psi_t,\psi_t\rangle = \frac{1}{i\hbar}\langle [F,H]\psi_t,\psi_t\rangle$$

Here, the bracket denotes the usual commutator operator $[F, H] := F \circ H - H \circ F$. Notice again the conservation of energy, since [H, H] = 0 trivially.

Proof: Here we go again,

$$\begin{aligned} \frac{d}{dt} \langle F\psi_t, \psi_t \rangle &= \langle F\partial_t\psi_t, \psi_t \rangle + \langle F\psi_t, \partial_t\psi_t \rangle \\ &= \left\langle -\frac{i}{\hbar}FH\psi_t, \psi_t \right\rangle + \left\langle F\psi_t, -\frac{i}{\hbar}H\psi_t \right\rangle \\ &= \frac{1}{i\hbar} \langle [F, H]\psi_t, \psi_t \rangle \end{aligned}$$

since H is self-adjoint. Thus, we see that F is a **constant of the motion** iff F commutes with H.

This gives us another correspondence in the classical \leftrightarrow quantum dictionary

$$\{f,g\} \longleftrightarrow \frac{1}{i\hbar}[Op(f), Op(g)]$$

which you can check by hand for the observables we listed above (see also Lemma 2.3 below).

Example 2.5 (Canonical Commutation Relations). Observe that

$$[Q_j, P_k] = \begin{cases} i\hbar Id & j = k\\ 0 & j \neq k \end{cases}$$
$$= i\hbar \delta_j(k) Id$$

where Id is the identity operator. It's straightforward to check that $\{q_j, p_k\} = \delta_j(k)$. Recall that this fact implies the Heisenberg Uncertainty Principle, which explains its conspicuous title.

2.3. Quantization of Observables. It is now very natural to ask: given a smooth (classical) observable $f \in C^{\infty}(\mathbb{R})$, is there always a naturally defined operator Op(f) on $L^2(\mathbb{R})$ on the quantum side? What are its properties— eg., is Op(f) a bounded operator if f is a bounded function?

Unfortunately, the answer is "no"— or at least, "not quite". One can understand the issue from the simple example of f(q, p) = qp. At first glance, one is tempted to define Op(f) = QP, with the position and momentum operators Q = Op(f(q, p) = q) and P = Op(f(q, p) = p)defined above. The problem with this is that f(q, p) = qp = pq, so it seems equally valid to write Op(f) = PQ, and the operators P and Qdo not commute. Thus $QP \neq PQ$, and our naively defined quantization of f(q, p) = qp is not well-defined.

However, one can hope to find solace (and a satisfactory solution) by recalling that, as $\hbar \to 0$, the operators P and Q almost commute; more precisely, they commute up to a factor of \hbar . Thus, asymptotically there is no difference between PQ and QP, and we can hope to capture this asymptotic equivalence to work out a theory of **quantization** sending smooth observables to linear operators in a relatively reasonable— even if not canonical— way.

Let's look at the example above of f(q, p) = qp. If we decide to take $Op^{L}(f) = QP$ (the "L" stands for left-quantization¹), then we can write via Fourier inversion

$$[Op^{L}(f)\psi](q) = q \cdot \frac{1}{\sqrt{2\pi\hbar}} \int_{p\in\mathbb{R}} p\mathcal{F}_{\hbar}(f)e^{\frac{i}{\hbar}qp}dp$$

$$= \frac{1}{2\pi\hbar} \int_{p\in\mathbb{R}} qp \cdot e^{\frac{i}{\hbar}qp} \int_{q'\in\mathbb{R}} \psi(q')e^{-\frac{i}{\hbar}q'p}dq'dp$$

$$= \frac{1}{2\pi\hbar} \iint f(q,p)\psi(q')e^{\frac{i}{\hbar}(q-q')p}dq'dp$$

On the other hand, using $Op^{R}(f) = PQ$ ("right-quantization") gives

$$[Op^R(f)\psi](q) = \frac{1}{2\pi\hbar} \iint f(q',p)\psi(q')e^{\frac{i}{\hbar}(q-q')p}dq'dp$$

Another possibility, called **Weyl quantization**, is to "split the difference" between left and right quantization, and define

$$[Op^W(f)\psi](q) = \frac{1}{2\pi\hbar} \iint f\left(\frac{q+q'}{2}, p\right)\psi(q')e^{\frac{i}{\hbar}(q-q')p}dpdq'$$

¹This is sometimes called "standard quantization" in the literature; which is rather unfortunate, because for us, the Weyl quantization is much more natural.

One can see that Op^W has the pleasant property of sending real-valued functions to symmetric operators:

$$\begin{aligned} \langle Op^{W}(f)\psi_{1},\psi_{2}\rangle &= \int [Op^{W}(f)\psi_{1}](q)\overline{\psi_{2}(q)}dq \\ &= \iiint f\left(\frac{q+q'}{2},p\right)\psi_{1}(q')e^{\frac{i}{\hbar}(q-q')p}\overline{\psi_{2}(q)}dqdq'dp \\ &= \iiint \psi_{1}(q')\overline{f\left(\frac{q+q'}{2},p\right)\psi_{2}(q)}e^{\frac{i}{\hbar}(q'-q)p}dqdq'dp \\ &= \int \psi_{1}(q')\overline{[Op^{W}(f)\psi_{2}](q')}dq' \\ &= \langle\psi_{1},Op^{W}(f)\psi_{2}\rangle\end{aligned}$$

using the fact that f is real valued in the third line. This only works because the definition of f is symmetric in q and q', which is not the case for left and right quantizations!

Exercise 2.2. Let f(q, p) = qp as in the above discussion. Show that

$$Op^{W}(f) = \frac{1}{2}(QP + PQ)$$

where $Q\psi(q) = q\psi(q)$ and $P\psi(q) = -i\hbar \frac{d\psi}{dq}$ are the position and momentum operators as above.

Each of these quantizations of f is an example of a **pseudodiffer**ential operator, which is the general name given to an operator A of the form

$$A\psi(x) = \frac{1}{2\pi\hbar} \iint a(x, y, \xi)\psi(y)e^{\frac{i}{\hbar}(x-y)\xi}dyd\xi$$

for some smooth function a, called the **symbol** of A. The terminology comes from the fact that, when a is polynomial in ξ , you get differential operators; thus pseudodifferential operators generalize the usual differential operators.

Pseudodifferential operators have many wonderful applications to various branches of analysis, but we won't concern ourselves here with the general theory. For now, we will be content to discuss a specific class of pseudodifferential operators adapted to our problem, and examine some of its properties. For us, the symbol a will always be of the form

$$a(p,q) = \sum_{j=0}^{\infty} \hbar^j a_j(p,q)$$

for some sequence of smooth functions a_j , and unless otherwise specified, $Op(a) = Op^W(a)$. The function a_0 will be called the **principle** **symbol** of the "**complete symbol**" *a*. The idea is that we imagine $\hbar \to 0$, and under some growth assumptions on the a_j , the principal symbol dominates. For now, we take the a_j to be \hbar -independent (this will have to be loosened later on, but is just fine for introducing the theory), and we further assume that:

(2)
$$\exists M > 0 \text{ such that } ||a_j||_{C^k} \leq M^{j+k} \quad \forall k \in \mathbb{N}$$

This will ensure not only that the series $\sum \hbar^j a_j$ converges for \hbar sufficiently small, but also that we can apply certain differential operators that will be important in the arguments. So statements presented here should be understood in the sense of "there exists a reasonable class of symbols, such that for any symbol a in this class, the statement holds".

We can now state the main results of this section:

Theorem 2.2. Let a be a complete symbol satisfying (2). Then $Op^W(a) = Op^L(a_1) = Op^R(a_2)$ for some symbols a_1 and a_2 satisfying (2), whose principle symbols are equal to the principal symbol of a.

Remark: Since Weyl quantization is the only one among our three "obvious" quantizations with the property that $Op^W(f)$ is self-adjoint whenever f is real-valued, it will be the "default" quantization that we will use the most. However, we will meet other important quantizations as well, that have other important properties!

Theorem 2.3. Suppose a and b are complete symbols (satisfying (2)). Then $Op(a) \circ Op(b) = Op(c)$ for some complete symbol c (also satisfying (2)), such that the principal symbol of c is $c_0 = a_0b_0$.

Thus our operators form an algebra, which is commutative to first order. This is consistent with the idea that the $\hbar \to 0$ limit should recover classical mechanics, where the algebra $C^{\infty}(\mathbb{R})$ of observables is commutative.

2.3.1. Quantization(s) of Characters. Before proving these statements, let's look at some key examples, and see what Theorems 2.2 and 2.3 say:

Example 2.6. Suppose a(q, p) = uq + vp is a linear function, for some $u, v \in \mathbb{R}$. Then

$$Op^W(a) = Op^L(a) = Op^R(a) = uQ + vP$$

given by

$$[Op(a)\psi](q) = uq\psi(q) - iv\hbar\psi'(q)$$

More generally, if a(q, p) = f(q) + g(p), then all three of these quantizations will agree—because we don't have to worry about noncommutativity! Thus, these symbols trivially satisfy Theorem 2.2. Now, given two linear symbols $a(q, p) = u_1q + v_1p$ and $b(q, p) = u_2q + v_2p$, we have

$$Op(a) \circ Op(b) = (u_1Q + v_1P)(u_2Q + v_2P)$$

= $u_1u_2Q^2 + u_1v_2QP + u_2v_1PQ + v_1v_2P^2$
= $u_1u_2Op(q^2) + u_1v_2Op^L(qp) + u_2v_1Op^R(qp) + v_1v_2Op(p^2)$

But we already saw that $[Q, P] = i\hbar Id$, so that

$$Op(a) \circ Op(b)$$

$$= u_1 u_2 Op(q^2) + u_1 v_2 QP + u_2 v_1 (QP - [Q, P]) + v_1 v_2 Op(p^2)$$

$$= u_1 u_2 Op(q^2) + u_1 v_2 Op^L(qp) + u_2 v_1 Op^L(qp) - i\hbar u_2 v_1 Op(1) + v_1 v_2 Op(p^2)$$

$$= Op^L (u_1 u_2 q^2 + (u_1 v_2 + u_2 v_1) qp + v_1 v_2 p^2 - i\hbar u_2 v_1)$$

So $Op(a) \circ Op(b) = Op^{L}(c)$, for a symbol $c(q, p) = c_0(q, p) + i\hbar u_2 v_1$ with principal symbol

$$c_0 = ab = u_1u_2q^2 + (u_1v_2 + u_2v_1)qp + v_1v_2p^2$$

and Theorem 2.3 is satisfied for Op^L . A similar calculation shows that the statement holds true for Op^R and Op^W as well; only the \hbar proportional term of c changes, leaving the principal symbol equal to $c_0 = ab$.

Example 2.7. Suppose $a(q,p) = e^{\frac{i}{\hbar}(uq+vp)}$ for some $u, v \in \mathbb{R}$. Then

$$\begin{bmatrix} Op^{L}(a)\psi \end{bmatrix}(q) = e^{\frac{i}{\hbar}uq}\psi(q+v) \begin{bmatrix} Op^{R}(a)\psi \end{bmatrix}(q) = e^{\frac{i}{\hbar}u(q+v)}\psi(q+v) \begin{bmatrix} Op^{W}(a)\psi \end{bmatrix}(q) = e^{\frac{i}{\hbar}uq}e^{\frac{i}{2\hbar}uv}\psi(q+v)$$

Note that this example essentially shows us what to do for any smooth symbol a, since we can decompose it into a linear combination of these exponentials via (inverse) Fourier transform.

Remark: These are sometimes called the **translation operators**, since (up to the constant phase factor $e^{\frac{i}{\hbar}tuv}$) they translate by the vector (v, u) in phase space; i.e. they translate the position by $q \mapsto q + v$, and the momentum by $p \mapsto p + u$.

Remark: You will notice that each of these three operators is *unitary*, and, in particular, bounded on L^2 , even though their symbols are not Schwartz-class. This is a first indication that the quantized operators are more sensitive to local properties (boundedness, smoothness) than

decay. In fact, this example shows us that the norm of Op(a) is really controlled by the decay of the *Fourier transform* of a.

Proof: First, let's do the case u = 0, in which case all three quantizations (remember, they have to agree when a is independent of q!) give translation by v. Recall that

$$[Op(a)\psi](q) = \frac{1}{2\pi\hbar} \iint \psi(q')a(q,p)e^{\frac{i}{\hbar}(q-q')p}dpdq'$$

$$= \frac{1}{\sqrt{2\pi\hbar}} \iint \mathcal{F}_{\hbar}(\psi)(p)e^{\frac{i}{\hbar}(vp)}e^{\frac{i}{\hbar}qp}dp$$

$$= \frac{1}{\sqrt{2\pi\hbar}} \iint \mathcal{F}_{\hbar}(\psi)(p)e^{\frac{i}{\hbar}(q+v)p}dpd$$

$$= \psi(q+v)$$

from Fourier inversion.

Remark: This operator is sometimes written as $e^{\frac{i}{\hbar}vP}$. Recalling that $P = -i\hbar \frac{d}{dx}$, we get the statement that $e^{v\frac{d}{dx}}\psi(q) = \psi(q+v)$. One can think of this as a Fourier-analytic way of saying that the exponential map takes the tangent vector $t\frac{d}{dx}$ to translation by t.

Continuation of Proof of Example 2.7: For Op^L , remember that we "do the p part first", which means that we first translate by v, and afterwards multiply by $e^{\frac{i}{\hbar}uq}$. More precisely,

$$\begin{split} \left[Op^{L}(a)\psi\right](q) &= \frac{1}{2\pi\hbar} \iint \psi(q')a(q,p)e^{\frac{i}{\hbar}(q-q')p}dpdq' \\ &= \frac{1}{2\pi\hbar} \iint \psi(q')e^{\frac{i}{\hbar}(uq+vp)}e^{\frac{i}{\hbar}(q-q')p}dpdq' \\ &= e^{\frac{i}{\hbar}uq}\frac{1}{2\pi\hbar} \iint \psi(q')e^{\frac{i}{\hbar}vp}e^{\frac{i}{\hbar}(q-q')p}dpdq' \\ &= e^{\frac{i}{\hbar}uq}\psi(q+v) \end{split}$$

as above.

For Op^R , we first do the *q*-part, multiplying by the function $e^{\frac{i}{\hbar}uq}$ to get $\tilde{\psi}(q) = e^{\frac{i}{\hbar}uq}$, and then apply the *p* part, translating $\tilde{\psi}$ by $q \mapsto q + v$ to get

$$[Op^R(a)\psi](q) = \tilde{\psi}(q+v) = e^{\frac{i}{\hbar}u(q+v)}\psi(q+v)$$

To be precise, we have

$$\begin{split} \left[Op^{R}(a)\psi\right](q) &= \frac{1}{2\pi\hbar} \iint \psi(q')a(q',p)e^{\frac{i}{\hbar}(q-q')p}dpdq'\\ &= \frac{1}{2\pi\hbar} \iint \psi(q')e^{\frac{i}{\hbar}(uq'+vp)}e^{\frac{i}{\hbar}(q-q')p}dpdq'\\ &= \frac{1}{2\pi\hbar} \int_{p\in\mathbb{R}} e^{\frac{i}{\hbar}vp}e^{\frac{i}{\hbar}qp} \left(\int_{q'\in\mathbb{R}} \psi(q')e^{\frac{i}{\hbar}uq'}e^{-\frac{i}{\hbar}q'p}dq'\right)dp\\ &= \frac{1}{\sqrt{2\pi\hbar}} \int e^{\frac{i}{\hbar}(q+v)p}\mathcal{F}_{\hbar}(\psi)(p-u)dp \end{split}$$

Notice now, that in order to perform the Fourier inversion, we have to change variables to p' = p - u, which gives us

$$\begin{bmatrix} Op^{R}(a)\psi \end{bmatrix}(q) = \frac{1}{\sqrt{2\pi\hbar}} \int e^{\frac{i}{\hbar}(q+v)(p'+u)} \mathcal{F}_{\hbar}(\psi)(p')dp' \\ = e^{\frac{i}{\hbar}(q+v)u} \frac{1}{\sqrt{2\pi\hbar}} \int e^{\frac{i}{\hbar}(q+v)p'} \mathcal{F}_{\hbar}(\psi)(p')dp' \\ = e^{\frac{i}{\hbar}(q+v)u}\psi(q+v)$$

We leave it as an exercise to do the final calculation, for $Op^W(a)$. \Box Exercise 2.3. Let $a(q, p) = e^{\frac{i}{\hbar}(uq+vp)}$. Show that

$$[Op^{W}(a)\psi](q) = e^{\frac{i}{2\hbar}uv}e^{\frac{i}{\hbar}uq}\psi(q+v)$$

Notice that the quantizations differ only by the factor of $e^{\frac{i}{\hbar}tuv}$ appearing in front; for Op^L we take t = 0, for Op^R we take t = 1, and for Op^W we take t = 1/2. Imagine now that we take an \hbar -independent symbol $a(q, p) = e^{i(xq+yp)}$; this is the same as taking $x = \hbar u$ and $y = \hbar v$ in Example 2.7. Thus, we find that

$$\begin{bmatrix} Op^{L}(a)\psi \end{bmatrix}(q) = e^{iuq}\psi(q+\hbar v) \begin{bmatrix} Op^{R}(a)\psi \end{bmatrix}(q) = e^{iu(q+\hbar v)}\psi(q+\hbar v) \begin{bmatrix} Op^{W}(a)\psi \end{bmatrix}(q) = e^{iuq}e^{i\hbar uv}\psi(q+v)$$

and the three quantizations differ only by a factor of

$$e^{it\hbar uv} = 1 + \sum_{j=1}^{\infty} \hbar^j \frac{(ituv)^j}{j!}$$

Thus we see how Theorem 2.2 is satisfied; we have $Op^W(a) = Op^L(a_1) = Op^R(a_2)$ with

$$a_1 = a + \sum_{j=1}^{\infty} \hbar^j \frac{\left(-\frac{1}{2}iuv\right)^j}{j!} a$$
$$a_2 = a + \sum_{j=1}^{\infty} \hbar^j \frac{\left(\frac{1}{2}iuv\right)^j}{j!} a$$

whose principle symbols are equal to a.

42

For the composition statement of Theorem 2.3, notice that for two such exponential symbols $a(q, p) = \exp(i(u_1q + v_1p))$ and $b(q, p) = \exp(i(u_2q + v_2p))$, their product $c_0 = \exp(i((u_1 + u_2)q + (v_1 + v_2)p))$ is again of the same form, and is supposed to be the principal symbol of $Op(a) \circ Op(b)$. By Theorem 2.2 (which we just checked for these symbols) it's sufficient to show this for Op^L , which turns out to be the most convenient for this purpose, since

$$\begin{aligned} \left[Op^{L}(a) \circ Op^{L}(b)\psi \right](q) &= e^{iu_{1}q} [Op^{L}(b)\psi](q + \hbar v_{1}) \\ &= e^{iu_{1}q} e^{iu_{2}(q + \hbar v_{1})}\psi(q + \hbar v_{1} + \hbar v_{2}) \\ &= e^{i\hbar u_{2}v_{1}} \cdot \left[Op^{L}(c_{0})\psi \right](q) \\ &= \left[Op^{L}(e^{i\hbar u_{2}v_{1}}c_{0})\psi \right](q) \end{aligned}$$

and by again expanding the factor $e^{i\hbar u_2 v_1}$ in a Taylor series, we get the complete symbol $c = e^{i\hbar u_2 v_1} c_0$ with principal symbol c_0 .

It's also worth noting the asymmetry in the factor $e^{i\hbar u_2 v_1}$; in fact, if we computed $Op^L(b) \circ Op^L(a)$ instead, we would get a different factor $e^{i\hbar u_1 v_2}$. This shows that Op(a) and Op(b) do not commute, but that their commutator is proportional to \hbar . In general, Theorem 2.3 shows that the commutator [Op(a), Op(b)] is a pseudodifferential operator whose principal symbol vanishes; it can be shown that in this case the next term in the expansion of the symbol (which is the dominant term as $\hbar \to 0$) is proportional to $\hbar\{a, b\}$; another indication of the correspondence between commutators on the quantum side and Poisson brackets on the classical side (see Lemma 2.3). You can check this directly for the exponential symbols we just did!

2.3.2. Smooth Observables. Suppose now that $a \in \mathcal{S}(\mathbb{R}^2)$, which in particular means that $\mathcal{F}_{\hbar}(a)$ (understood now as a 2-dimensional (semiclassical) Fourier transform) decays nicely; in particular, we have $\mathcal{F}_{\hbar}(a) \in L^1(\mathbb{R}^2)$, and we use Fourier inversion to write

$$a(q,p) = \frac{1}{2\pi\hbar} \iint \mathcal{F}_{\hbar}(a)(\xi,\eta) e^{\frac{i}{\hbar}(\xi,\eta) \cdot (q,p)} d\xi d\eta$$

Therefore, we can extend Example 2.7 by linearity to quantize a: let $e_{\xi,\eta}(q,p) := \exp\left(\frac{i}{\hbar}(\xi,\eta) \cdot (q,p)\right) = \exp\left(\frac{i}{\hbar}(\xi q + \eta p)\right)$, and define

$$Op(a) = \frac{1}{2\pi\hbar} \iint \mathcal{F}_{\hbar}(a)(\xi,\eta) \cdot Op(e_{\xi,\eta}) d\xi d\eta$$

since each $Op(e_{\xi,\eta})$ is unitary on $L^2(\mathbb{R})$, and $\mathcal{F}_{\hbar}(a)$ is in L^1 , the operator Op(a) is bounded on L^2 .

Remark: Recall from Lemma 1.11 that the L^1 -norm of \hat{a} — and thus, by a change of variable, the L^1 -norm of $(2\pi\hbar)^{-1}\mathcal{F}_{\hbar}(a)$ — can be controlled by the first few derivatives of a (the requisite number of derivatives depends only on the dimension d of the phase space \mathbb{R}^d); thus, the norm of Op(a) can be bounded in terms of the first first k(d) derivatives of a. This is a general fact— the Calderón-Vaillancourt Theorem states that, if a and its derivatives are each bounded on \mathbb{R}^{2d} (but even if a is not a Schwartz function), then the operator Op(a) is bounded on $L^2(\mathbb{R}^d)$ by $||a||_{C^k(\mathbb{R}^{2d})}$ for some k = k(d) depending only on the dimension d. We won't need this level of generality, so we won't give the proof.

We now wish to prove Theorems 2.2 and 2.3 under the assumption that $\mathcal{F}_{\hbar}(a) \in L^1(\mathbb{R}^2)$. The general idea is to use Example 2.7 for each Fourier component $\mathcal{F}_{\hbar}(a)(\xi,\eta)$, but we need to correctly interpret the step where we take the Taylor expansion $e^{i\hbar\xi\eta} = \sum \hbar^j (i\xi\eta)^j / j!$, since we are integrating over all $(\xi,\eta) \in \mathbb{R}^2$.

Proof of Theorem 2.2: We will actually give an explicit formula for the symbols, namely

$$a_{1} = a + \sum_{j=1}^{\infty} \hbar^{j} \frac{\left(-\frac{1}{2}i\right)^{j}}{j!} \frac{\partial^{2j}a}{\partial q^{j}\partial p^{j}}$$
$$a_{2} = a + \sum_{j=1}^{\infty} \hbar^{j} \frac{\left(\frac{1}{2}i\right)^{j}}{j!} \frac{\partial^{2j}a}{\partial q^{j}\partial p^{j}}$$

We begin by writing

$$Op(a) = Op^{W}(a) = \frac{1}{2\pi\hbar} \iint \mathcal{F}_{\hbar}(a)(\xi,\eta) \cdot Op^{W}(e_{\xi,\eta}) d\xi d\eta$$

quantizing each Fourier component individually according to Example 2.7; the integral converges absolutely as long as $\mathcal{F}_{\hbar}(a) \in L^1(\mathbb{R}^2)$, since each $Op(e_{\xi,\eta})$ is unitary.

Recall also from Example 2.7 that

$$Op^{W}(e_{\xi,\eta}) = e^{\frac{i}{2\hbar}\xi\eta}Op^{L}(e_{\xi,\eta})$$
$$= e^{-\frac{i}{2\hbar}\xi\eta}Op^{R}(e_{\xi,\eta})$$

Therefore, we have

$$Op^{W}(a) = \frac{1}{2\pi\hbar} \iint e^{\frac{i}{2\hbar}\xi\eta} \mathcal{F}_{\hbar}(a)(\xi,\eta) \cdot Op^{L}(e_{\xi,\eta}) d\xi d\eta$$
$$= \frac{1}{2\pi\hbar} \iint \sum_{j=0}^{\infty} \frac{\left(\frac{i}{2}\right)^{j}}{j!} \frac{\xi^{j}\eta^{j}}{\hbar^{j}} \mathcal{F}_{\hbar}(a)(\xi,\eta) \cdot Op^{L}(e_{\xi,\eta}) d\xi d\eta$$

Now, recall that \mathcal{F}_{\hbar} has the property that

$$\frac{-i\xi}{\hbar} \mathcal{F}_{\hbar}(a) = \mathcal{F}_{\hbar}\left(\frac{\partial a}{\partial q}\right)$$
$$\frac{-i\eta}{\hbar} \mathcal{F}_{\hbar}(a) = \mathcal{F}_{\hbar}\left(\frac{\partial a}{\partial p}\right)$$

which means that

$$\frac{\xi\eta}{\hbar}\mathcal{F}_{\hbar}(a) = -\hbar\mathcal{F}_{\hbar}\left(\frac{\partial^2 a}{\partial q \partial p}\right)$$

so that we get

$$Op^{W}(a) = \frac{1}{2\pi\hbar} \iint \sum_{j=0}^{\infty} \frac{\left(\frac{i}{2}\right)^{j}}{j!} \frac{\xi^{j} \eta^{j}}{\hbar^{j}} \mathcal{F}_{\hbar}(a)(\xi,\eta) \cdot Op^{L}(e_{\xi,\eta}) d\xi d\eta$$

$$= \frac{1}{2\pi\hbar} \iint \sum_{j=0}^{\infty} \frac{\left(\frac{i}{2}\right)^{j}}{j!} (-\hbar)^{j} \mathcal{F}_{\hbar} \left[\left(\frac{\partial^{2}}{\partial q \partial p}\right)^{j} a \right] (\xi,\eta) \cdot Op^{L}(e_{\xi,\eta}) d\xi d\eta$$

$$= \frac{1}{2\pi\hbar} \iint \mathcal{F}_{\hbar} \left[\sum_{j=0}^{\infty} \frac{\left(-\frac{i}{2}\right)^{j}}{j!} \hbar^{j} \left(\frac{\partial^{2}}{\partial q \partial p}\right)^{j} a \right] (\xi,\eta) \cdot Op^{L}(e_{\xi,\eta}) d\xi d\eta$$

$$= Op^{L}(a_{1})$$

with

$$a_1 = \sum_{j=0}^{\infty} \hbar^j \frac{\left(-\frac{1}{2}i\right)^j}{j!} \frac{\partial^{2j}a}{\partial q^j \partial p^j} = a + \sum_{j=1}^{\infty} \hbar^j \frac{\left(-\frac{1}{2}i\right)^j}{j!} \frac{\partial^{2j}a}{\partial q^j \partial p^j}$$

as required. The argument for Op^R is identical, substituting $-\frac{1}{2\hbar}$ for $\frac{1}{2\hbar}$. \Box

We now turn to the composition theorem. The ideas are the same, though the implementation gets a bit messier, since we now have two operators Op(a) and Op(b), which each need to be decomposed into Fourier components, and then make sense of the resulting Fourier transforms. There will now be four Fourier parameters $\xi_1, \eta_1, \xi_2, \eta_2$, and the formulas will get a bit longer. To simplify the exposition, we will

44

restrict ourselves to left-quantization Op^L , though it's clear the calculations may be carried out identically for Op^R or Op^W . In any case, Theorem 2.2 shows that it doesn't matter!

Proof of Theorem 2.3: Once again, write

$$Op^{L}(a) = \frac{1}{2\pi\hbar} \iint \mathcal{F}_{\hbar}(a)(\xi_{1},\eta_{1}) \cdot Op(e_{\xi_{1},\eta_{1}})d\xi d\eta$$
$$Op^{L}(b) = \frac{1}{2\pi\hbar} \iint \mathcal{F}_{\hbar}(b)(\xi_{2},\eta_{2}) \cdot Op(e_{\xi_{2},\eta_{2}})d\xi d\eta$$

and recall from Example 2.7 that

$$Op^{L}(e_{\xi_{1},\eta_{1}}) \circ Op^{L}(e_{\xi_{2},\eta_{2}}) = e^{\frac{i}{\hbar}\xi_{2}\eta_{1}}Op(e_{\xi_{1},\eta_{1}} \cdot e_{\xi_{2},\eta_{2}})$$

Therefore, we have

$$\begin{aligned} Op^{L}(a) \circ Op^{L}(b) \\ &= \frac{1}{(2\pi\hbar)^{2}} \iiint \mathcal{F}_{\hbar}(a)(\xi_{1},\eta_{1})\mathcal{F}_{\hbar}(b)(\xi_{2},\eta_{2})Op^{L}(e_{\xi_{1},\eta_{1}}) \circ Op^{L}(e_{\xi_{2},\eta_{2}})d\xi_{1}d\eta_{1}d\xi_{2}d\eta_{2} \\ &= \frac{1}{(2\pi\hbar)^{2}} \iiint \mathcal{F}_{\hbar}(a)(\xi_{1},\eta_{1})\mathcal{F}_{\hbar}(b)(\xi_{2},\eta_{2})e^{\frac{i}{\hbar}\xi_{2}\eta_{1}}Op^{L}(e_{\xi_{1},\eta_{1}} \cdot e_{\xi_{2},\eta_{2}})d\xi_{1}d\eta_{1}d\xi_{2}d\eta_{2} \\ &= \frac{1}{(2\pi\hbar)^{2}} \iiint \mathcal{F}_{\hbar}(a)(\xi_{1},\eta_{1})\mathcal{F}_{\hbar}(b)(\xi_{3}-\xi_{1},\eta_{3}-\eta_{1})e^{\frac{i}{\hbar}(\xi_{3}-\xi_{1})\eta_{1}}Op^{L}(e_{\xi_{3},\eta_{3}})d\xi_{1}d\eta_{1}d\xi_{3}d\eta_{3} \end{aligned}$$

where $\xi_3 = \xi_1 + \xi_2$ and $\eta_3 = \eta_1 + \eta_2$, since

$$e_{\xi_1,\eta_1} \cdot e_{\xi_2,\eta_2} = e_{\xi_3,\eta_3}$$

(This is basically the same calculation one does to show that $\hat{ab} = \hat{a} * \hat{b}$).

Ideally, we would like to integrate over ξ_1 and η_1 to get

$$\iint \mathcal{F}_{\hbar}(a)(\xi_1,\eta_1)\mathcal{F}_{\hbar}(b)(\xi_3-\xi_1,\eta_3-\eta_1)d\xi_1d\eta_1=\mathcal{F}_{\hbar}(a)*\mathcal{F}_{\hbar}(b)$$

but there is a factor $\exp(-\frac{i}{\hbar}(\xi_3 - \xi_1)\eta_1)$ that is interfering.

As before, though, in the proof of Theorem 2.2, we can expand this exponential in a Taylor series, and transform multiplication of $\mathcal{F}_{\hbar}(a)(\xi_1,\eta_1)$ by η_1 and $\mathcal{F}_{\hbar}(b)(\xi_3-\xi_1)$ by $(\xi_3-\xi_1)$ as differential operators inside \mathcal{F}_{\hbar} :

$$\frac{1}{2\pi\hbar} \iint \mathcal{F}_{\hbar}(a)(\xi_{1},\eta_{1})\mathcal{F}_{\hbar}(b)(\xi_{3}-\xi_{1},\eta_{3}-\eta_{1})e^{\frac{i}{\hbar}(\xi_{3}-\xi_{1})\eta_{1}}d\xi_{1}d\eta_{1}$$

$$= \frac{1}{2\pi\hbar} \iint \sum_{k=0}^{\infty} \frac{(-i\hbar)^{k}}{k!} \left(\frac{-i\eta_{1}}{\hbar}\right)^{k} \mathcal{F}_{\hbar}(a)(\xi_{1},\eta_{1}) \cdot \left(\frac{-i(\xi_{3}-\xi_{1})}{\hbar}\right)^{k} \mathcal{F}_{\hbar}(b)(\xi_{3}-\xi_{1},\eta_{3}-\eta_{1})d\xi_{1}d\eta_{1}$$

$$= \frac{1}{2\pi\hbar} \iint \sum_{k=0}^{\infty} \frac{(-i\hbar)^{k}}{k!} \mathcal{F}_{\hbar}\left(\frac{\partial^{k}a}{\partial p^{k}}\right) (\xi_{1},\eta_{1}) \mathcal{F}_{\hbar}\left(\frac{\partial^{k}b}{\partial q^{k}}\right) (\xi_{3}-\xi_{1},\eta_{3}-\eta_{1})d\xi_{1}d\eta_{1}$$

$$= \frac{1}{2\pi\hbar} \sum_{k=0}^{\infty} \frac{(-i\hbar)^{k}}{k!} \mathcal{F}_{\hbar}\left(\frac{\partial^{k}a}{\partial p^{k}}\right) * \mathcal{F}_{\hbar}\left(\frac{\partial^{k}b}{\partial q^{k}}\right) (\xi_{3},\eta_{3})$$

$$= \mathcal{F}_{\hbar}(ab)(\xi_{3},\eta_{3}) + \sum_{k=1}^{\infty} \hbar^{k} \frac{(-i)^{k}}{k!} \mathcal{F}_{\hbar}\left(\frac{\partial^{k}a}{\partial p^{k}}\frac{\partial^{k}b}{\partial q^{k}}\right) (\xi_{3},\eta_{3})$$

since $\frac{1}{2\pi\hbar} \mathcal{F}_{\hbar}(f) * \mathcal{F}_{\hbar}(g) = \mathcal{F}_{\hbar}(fg)$. Therefore we get

$$Op^{L}(a) \circ Op^{L}(b) = \iint \mathcal{F}_{\hbar}(c)(\xi_{3},\eta_{3})Op^{L}(e_{\xi_{3},\eta_{3}})d\xi_{3}d\eta_{3} = Op^{L}(c)$$

where

$$c = ab - i\hbar \frac{\partial a}{\partial p} \frac{\partial b}{\partial q} + \sum_{k=2}^{\infty} \hbar^k \left(\frac{i^k}{k!}\right) \frac{\partial^k a}{\partial p^k} \frac{\partial^k b}{\partial q^k}$$

and we are done. \Box

2.3.3. Gross Omission: The Method of Stationary Phase. If you sense that there is a more general principle at work here in the calculations of the preceding section, then you are right— these are special examples of a more general principal called the **method of stationary phase**. Generally speaking, the idea is that given a **phase function** $\phi(x,\xi)$ with exactly one critical point (x_0,ξ_0) that is not degenerate, one can get an asymptotic expansion about (x_0,ξ_0) in powers of \hbar for the integral

$$\int_{\mathbb{R}^2} f(x,\xi) e^{\frac{i}{\hbar}\phi(x,\xi)} dx d\xi = \sum_{k=0}^{\infty} \hbar^k D_{2k} f(x_0,\xi_0)$$

where the D_{2k} are differential operators of order at most 2k. For a complete proof, see eg. Martinez[?] or Evans-Zworksi[?]; we will only sketch the ideas involved, since the full force will not be needed in the course.

The first idea is that the extremely rapid oscillations of $e^{\frac{i}{\hbar}\phi(x,\xi)}$ away from the critical point of ϕ imply that the integral is really over a small neighborhood of the critical point; more precisely, if $B = B_{\epsilon}(x_0, y_0)$ is the ball of radius ϵ around the critical point, then

$$\int_{\mathbb{R}^2 \setminus B} f(x,\xi) e^{\frac{i}{\hbar}\phi(x,\xi)} dx d\xi = O_{\phi,\epsilon,f}(\hbar^{\infty})$$

which means that for any $N \in \mathbb{N}$, there exists a constant $C(\phi, \epsilon, f, N)$ such that the integral is $\leq C(\phi, \epsilon, f, N)\hbar^N$. This is established by integrating by parts N times in the integral.

Without loss of generality, we may assume that $x_0 = 0 = \xi_0$ by doing a change of variable. Next, one approximates $\phi(x,\xi)$ near the critical point (0,0) by a non-degenerate quadratic form $Q(x,\xi)$, and use the Plancherel Theorem 1.15 for the (ordinary) Fourier transform to obtain

$$\int_{\mathbb{R}^2 \setminus B} f(x,\xi) e^{\frac{i}{\hbar}Q(x,\xi)} dx d\xi = \int_{\mathbb{R}^2 \setminus B} \hat{f}(y,\eta) \widehat{e^{\frac{i}{\hbar}Q(\cdot)}}(y,\eta) dy d\eta$$

Now, the Fourier transform of $e^{\frac{i}{\hbar}Q(\cdot)}$, like the Fourier transform of a Gaussian (corresponding to the quadratic form $Q(x,\xi) = x^2 + \xi^2$), is proportional to $e^{i\hbar Q^{-1}(y,\eta)}$, which can be expanded in a Taylor series as we did in the last section. Each term in the Taylor expansion is of the form $\hbar^k P_{2k}$, where each P_{2k} is a polynomial in y, η of degree 2k; moving this inside the Fourier transform, it becomes a differential operator of order 2k. So we are left with

$$\int \left[\sum_{k=0}^{\infty} \hbar^k D_{2k} f\right](y,\eta) dy d\eta = \sum_{k=0}^{\infty} \hbar^k D_{2k} f(0,0)$$

by Fourier inversion.

2.4. Quantum Dynamics and Egorov's Theorem. At the end of the proof of Theorem 2.3, we explicitly calculated the next term of the semiclassical expansion: namely, we saw that $Op^{L}(a) \circ Op^{L}(b) = Op^{L}(c)$ with

$$c = ab - i\hbar \frac{\partial a}{\partial p} \frac{\partial b}{\partial q} + \sum_{k=2}^{\infty} \hbar^k \left(\frac{(-i)^k}{k!} \right) \frac{\partial^k a}{\partial p^k} \frac{\partial^k b}{\partial q^k}$$

We had a good reason for computing this term explicitly, since it gives

Lemma 2.3. Let a, b be complete symbols. Then for any of our quantizations Op^W, Op^L, Op^R , we have the commutator formula

$$\left[Op(a), Op(b)\right] = i\hbar Op(c)$$

where c has principal symbol given by the Poisson bracket $\{a, b\}$.

Proof: We first show this for Op^L . From the expression above for $Op^L(a) \circ Op^L(b)$, we have

$$[Op^L(a), Op^L(b)] = Op^L(a) \circ Op^L(b) - Op^L(b) \circ Op^L(a)$$

= $Op^L(c_1) - Op^L(c_2)$

with

$$c_{1} = ab - i\hbar \frac{\partial a}{\partial p} \frac{\partial b}{\partial q} + \sum_{k=2}^{\infty} \hbar^{k} \left(\frac{(-i)^{k}}{k!} \right) \frac{\partial^{k} a}{\partial p^{k}} \frac{\partial^{k} b}{\partial q^{k}}$$
$$c_{2} = ab - i\hbar \frac{\partial b}{\partial p} \frac{\partial a}{\partial q} + \sum_{k=2}^{\infty} \hbar^{k} \left(\frac{(-i)^{k}}{k!} \right) \frac{\partial^{k} b}{\partial p^{k}} \frac{\partial^{k} a}{\partial q^{k}}$$

Subtracting $c_1 - c_2$, we see that the leading terms cancel, and the difference of the second terms gives exactly $i\hbar\{a,b\}$.

Now, replacing Op^L by either Op^W or Op^R doesn't change the principle symbol of c on the right-hand side, by Theorem 2.2, and the same is true for the leading term on the left-hand side. It remains to see what happens with the \hbar -linear term on the left-hand side. We have

$$Op^{W}(f) = Op^{L}(f + \hbar \tilde{f}_{1} + O(\hbar^{2}))$$

$$Op^{R}(f) = Op^{L}(f + \hbar \tilde{f}_{2} + O(\hbar^{2}))$$

(here $g = O(\hbar^2)$ means that $g = \hbar^2 \tilde{g}$ for some symbol \tilde{g}). On the other hand, looking at the \hbar -linear term of the commutator gives

$$\frac{1}{\hbar} \Big(\Big[Op^W(a), Op^W(b) \Big] - \Big[Op^L(a), Op^L(b) \Big] \Big) \\
= Op^L(\tilde{a}_1) \circ Op^L(b) + Op^L(a) \circ Op^L(\tilde{b}_1) - Op^L(\tilde{b}_1) \circ Op^L(a) - Op^L(b) \circ Op^L(\tilde{a}_1) + O(\hbar) \\
= O(\hbar)$$

since compositions of Op^{L} 's commute to first order, and so the terms cancel modulo $O(\hbar)$. The same is true for Op^{R} . \Box

We now apply this to Lemma 2.2, to get

Lemma 2.4. Let $f \in C^{\infty}(\mathbb{R}^2)$ be a smooth observable such that $||f||_{C^k} \leq M^k$ for some constant M (i.e., f is an \hbar -independent symbol satisfying (2)), and Op(f) one of our three quantizations. Then for any L^2 -normalized solutions u_t, v_t of Schrödinger's equation, we have

$$\frac{a}{dt}\langle Op(f)u_t, v_t\rangle = \langle Op(\{f, H\})u_t, v_t\rangle + O(\hbar)$$

48

Proof: Lemma 2.2 shows² that

$$\frac{d}{dt}\langle Op(f)u_t, v_t \rangle = \frac{1}{i\hbar} \langle [Op(f), H]u_t, v_t \rangle$$

But now Lemma 2.3 says that

$$\frac{1}{i\hbar}[Op(f),H] = Op(\{f,H\}) + \hbar Op(\tilde{f})$$

for some symbol \tilde{f} , such that $Op(\tilde{f})$ is bounded on $L^2(\mathbb{R})$. Therefore, since u_t and v_t are unit vectors, we have

$$\hbar \langle Op(f)u_t, v_t \rangle = O(\hbar)$$

and the statement follows. \Box

Recalling from Lemma 2.1 that the Hamiltonian flow Φ_t^H satisfies

$$\frac{d}{dt}f(\Phi_t^H(z)) = \{f, H\}(z)$$

we define

$$f_t = f \circ \Phi_t^H$$

$$F_t = e^{\frac{i}{\hbar}Ht} Op(f) e^{-\frac{i}{\hbar}Ht}$$

to be the classical and quantum evolutions of the obervable f and Op(f), respectively (to understand why F_t corresponds to the Schrödinger evolution of Op(f), consider a solution $\psi_t = e^{-\frac{i}{\hbar}Ht}\psi$ of Schrödinger's equation, and write

$$\langle Op(f)\psi_t,\psi_t\rangle = \langle Op(f)e^{-\frac{i}{\hbar}Ht}\psi,e^{-\frac{i}{\hbar}Ht}\psi\rangle = \langle F_t\psi,\psi\rangle$$

since the Schrödinger operator $e^{-\frac{i}{\hbar}Ht}$ is unitary by section 2.2.3).

We want to understand the relationship between $Op(f_t)$ and F_t ; in other words, the relationship between the classical evolution governed by Hamilton's equations and the quantum evolution given by Schrödinger's equation. We can now give the main result giving this correspondence:

Theorem 2.4 (Egorov). For any smooth observable $f \in C^{\infty}(\mathbb{R})$ (satisfying 2), and any fixed time t, we have

$$||e^{\frac{i}{\hbar}Ht}Op(f)e^{-\frac{i}{\hbar}Ht} - Op(f \circ \Phi_t^H)|| = O_t(\hbar)$$

in the operator norm on $L^2(\mathbb{R}^2)$.

²More precisely, the proof of the Lemma, since the Lemma is only stated for the case u = v.

Remark: Egorov's Theorem is actually a more general statement about the propagation of singularities by PDEs, but Theorem 2.4 is the consequence of Egorov's Theorem that will concern us.

Proof of Theerem 2.4: First, by unitarity of the Schrödinger evolution we have

$$||e^{\frac{i}{\hbar}Ht}Op(f)e^{-\frac{i}{\hbar}Ht} - Op(f_t)|| = ||Op(f) - e^{-\frac{i}{\hbar}Ht}Op(f_t)e^{\frac{i}{\hbar}Ht}||$$

and so we may estimate the latter. For this, we'll take two unit vectors $u, v \in \mathcal{S}(\mathbb{R})$ and estimate the matrix coefficient

$$\left\langle \left(Op(f) - e^{-\frac{i}{\hbar}Ht} Op(f_t) e^{\frac{i}{\hbar}Ht} \right) u, v \right\rangle$$

Note that for t = 0, where both operators are equal to Op(f), this matrix coefficient is exactly 0; so it is sufficient to show that the derivative

$$\frac{d}{dt}\left\langle \left(Op(f) - e^{-\frac{i}{\hbar}Ht}Op(f_t)e^{\frac{i}{\hbar}Ht}\right)u, v\right\rangle = \frac{d}{dt}\left\langle e^{-\frac{i}{\hbar}Ht}Op(f_t)e^{\frac{i}{\hbar}Ht}u, v\right\rangle = O(\hbar)$$

and then integrate up to time t.

Now take u_t and v_t to be the solutions of Schrödinger's equation with initial conditions $u_0 = u$ and $v_0 = v$, and observe that

$$\frac{d}{dt}\left\langle e^{-\frac{i}{\hbar}Ht}Op(f_t)e^{\frac{i}{\hbar}Ht}u,v\right\rangle = \frac{d}{dt}\left\langle Op(f_t)u_{-t},v_{-t}\right\rangle$$

Applying Lemma 2.4 (with a minus sign, since u_{-t} and v_{-t} are being propagated backwards) and recalling that $\frac{d}{dt}(f_t) = \{f, H\}$, we have

$$\frac{d}{dt} \langle Op(f_t)u_{-t}, v_{-t} \rangle = \left\langle \frac{d}{dt} Op(f_t)u_{-t}, v_{-t} \right\rangle - \left\langle Op(\{f_t, H\})u_{-t}, v_{-t} \right\rangle + O(\hbar)$$

$$= \left\langle Op(\{f_t, H\})u_{-t}, v_{-t} \right\rangle - \left\langle Op(\{f_t, H\})u_{-t}, v_{-t} \right\rangle + O(\hbar)$$

$$= O(\hbar)$$

as required. \Box

Remark: One sees from the argument that the error term in Theorem 2.4 can, in general, depend exponentially on t. This implies that there is a constant c, such that the classical and quantum evolutions differ by a "small" error (that vanishes as $\hbar \to 0$) up to time $c |\log \hbar|$. This will be a recurring theme when we discuss the Ehrenfest time.

2.5. Anti-Wick Quantization. Another question one might want to ask about quantization is positivity— is it true that, if $f \ge 0$ is a positive function, then Op(f) is positive-definite? Of course, by now we know that, in general, it only makes sense to ask for this to hold up to \hbar ; in fact, for the quantizations we've discussed so far, it's not true that Op(f) is positive-definite whenever $f \ge 0$, when \hbar is fixed. However, there is another quantization for which this property *does* hold for arbitrary $\hbar > 0$, called the **Anti-Wick quantization**. That this quantization is positive is obvious from the construction, but we will also show that it agrees with our previous quantizations, at least to first order (i.e., they have the same principal symbol).

To discuss the Anti-Wick quantization, we need to introduce the concept of a **coherent state**. Let the function $g_{0,0}$ be given by the L^2 -normalized Gaussian

$$g_{0,0}(q) = (\pi\hbar)^{-1/4} e^{-\frac{1}{2\hbar}q^2}$$

Note that this Gaussian is symmetric about q = 0, and is equal to its \hbar -Fourier transform, which is therefore symmetric about p = 0. Moreover, $g_{0,0}$ (and therefore also $\mathcal{F}_{\hbar}(g_{0,0})$) is localized up to $\sqrt{\hbar}$ near 0 (in the sense that once $x > C\sqrt{\hbar}$, the value of $g_{0,0}(x) < e^{-Cx^2}$ decays very rapidly). We will often say that $g_{0,0}$ has width³ $\sqrt{\hbar/2}$.

We call $g_{0,0}$ the **coherent state centered at** (0,0). The terminology comes from the fact that $g_{0,0}$ is optimally jointly localized in position and momentum near 0. We then use the translation operators from Example 2.7 to define the **coherent state centered** at (x,ξ) by

$$g_{x,\xi}(q) := Op^{W}(e_{-\xi,x})g_{0,0}(q) = e^{-\frac{i}{2\hbar}x\xi}e^{\frac{i}{\hbar}\xi q}g_{0,0}(q-x)$$

Observe that $g_{x,\xi}$ is optimally jointly localized in position near x, and momentum near ξ .

An important property is that any wave function can be decomposed into a superposition of coherent states:

Lemma 2.5 (Coherent State Decomposition). Let $u \in L^2(\mathbb{R})$. Then we have

$$u = \frac{1}{2\pi\hbar} \iint_{\mathbb{R}^2} \langle u, g_{x,\xi} \rangle g_{x,\xi} dx d\xi$$

in $L^2(\mathbb{R})$. In other words, for any Schwartz function $v \in \mathcal{S}(\mathbb{R})$, we have

$$\langle u, v \rangle = \frac{1}{2\pi\hbar} \iint_{\mathbb{R}^2} \langle u, g_{x,\xi} \rangle \langle g_{x,\xi}, v \rangle dxd\xi$$

$$\int_{-\infty}^{\infty}q^2g_{0,0}^2(q)dq=\frac{\hbar}{2}$$

 $^{^3\}mathrm{For}$ more precise (but perhaps less intuitive) terminology, notice that the variance of $|g_{0,0}|^2$

so that the "width" is given by the *standard deviation* of the probability measure $|g_{0,0}(q)|^2 dq$.

Proof: Write

$$\iint_{\mathbb{R}^2} \langle u, g_{x,\xi} \rangle \langle g_{x,\xi}, v \rangle dx d\xi$$

=
$$\iint_{(x,\xi)\in\mathbb{R}^2} \int_{q_1\in\mathbb{R}} \int_{q_2\in\mathbb{R}} u(q_1) \overline{g_{x,\xi}(q_1)} g_{x,\xi}(q_2) \overline{v(q_2)} dq_1 dq_2 dx d\xi$$

=
$$\iint_{q_1,q_2\in\mathbb{R}} u(q_1) \overline{v(q_2)} \iint_{x,\xi\in\mathbb{R}} g_{x,\xi}(q_2) \overline{g_{x,\xi}(q_1)} dx d\xi dq_1 dq_2$$

We claim that

$$\iint g_{x,\xi}(q_2)\overline{g_{x,\xi}(q_1)}dxd\xi = 2\pi\hbar\delta_0(q_1 - q_2)$$

from which the Lemma follows. To prove the claim, recall by Fourier inversion that $\int e^{\frac{i}{\hbar}\xi(q_2-q_1)}d\xi = 2\pi\hbar\delta(q_2-q_1)$, and write

$$\begin{aligned} \iint g_{x,\xi}(q_2) \overline{g_{x,\xi}(q_1)} dx d\xi \\ &= \int_{x=-\infty}^{\infty} \int_{\xi=-\infty}^{\infty} e^{-\frac{i}{2\hbar}x\xi} e^{\frac{i}{\hbar}\xi q_2} g_{0,0}(q_2 - x) \overline{e^{-\frac{i}{2\hbar}x\xi} e^{\frac{i}{\hbar}\xi q_1} g_{0,0}(q_1 - x)} d\xi dx \\ &= \int_{x=-\infty}^{\infty} \int_{\xi=-\infty}^{\infty} e^{\frac{i}{\hbar}\xi(q_2 - q_1)} g_{0,0}(q_2 - x) \overline{g_{0,0}(q_1 - x)} d\xi dx \\ &= \int_{x=-\infty}^{\infty} g_{0,0}(q_2 - x) \overline{g_{0,0}(q_1 - x)} \int_{\xi\in\mathbb{R}} e^{\frac{i}{\hbar}\xi(q_2 - q_1)} d\xi dx \\ &= \int_{x=-\infty}^{\infty} g_{0,0}(q_2 - x) \overline{g_{0,0}(q_1 - x)} 2\pi \hbar \delta(q_2 - q_1) dx \\ &= ||g_{0,0}||_{L^2}^2 2\pi \hbar \delta(q_2 - q_1) = 2\pi \hbar \delta(q_2 - q_1) \end{aligned}$$

as claimed. \Box

Thus, we see that any wave function u can be decomposed into optimally-localized pieces. The map

$$u \mapsto \frac{1}{\sqrt{2\pi\hbar}} \langle u, g_{x,\xi} \rangle$$

from $L^2(\mathbb{R}) \to L^2(\mathbb{R}^2_{x,\xi})$, which is unitary by Lemma 2.5, is called the **microlocal transform** or **FBI transform** of u (named after Fourier-Bros-Iagolnitzer). The term "microlocal" is supposed to evoke intuition of being localized to scale $\sqrt{\hbar}$ in both position and momentum.

Equipped with such a decomposition, it makes sense to define the Anti-Wick quantization of f as

$$[Op^{AW}(f)\psi](q) := \frac{1}{2\pi\hbar} \iint_{(x,\xi)\in\mathbb{R}^2} f(x,\xi)\langle\psi,g_{x,\xi}\rangle g_{x,\xi}dxd\xi$$

52

Intuitively, you multiply each coherent state component of ψ — the piece localized near (x, ξ) — by the function $f(x, \xi)$.

Remark: The choice of Weyl quantization in the definition of coherent states here is not significant; either left or right quantization could be substituted without affecting Lemma 2.5, since the terms distinguishing the quantizations of $e_{-\xi,x}$ are of the form $e^{-\frac{i}{\hbar}tx\xi}$ and cancel with their complex conjugates in the integral.

Remark: It is clear that this quantization makes sense not only for smooth f, but even just $f \in L^{\infty}(\mathbb{R}^2)$. How can this be? The convolution with $g_{x,\xi}$ in the definition of the quantization smooths out the function f, so that it behaves like the quantization of a Schwartz function (see below Lemma 2.6).

Remark: Putting in the constant function f(q, p) = 1, we get the so-called **resolution of the identity**

$$Id = Op^{AW}(1) = \frac{1}{2\pi\hbar} \int_{(x,\xi)\in\mathbb{R}^2} |g_{x,\xi}\rangle \langle g_{x,\xi}| dxd\xi$$

that appears in the literature.

Important(!) Remark: This quantization assigns positive-define operators to positive functions— if $f(x,\xi) \ge 0$ for all $(x,\xi) \in \mathbb{R}^2$, then

$$\langle Op^{AW}(f)\psi,\psi\rangle = \frac{1}{2\pi\hbar} \iint f(x,\xi) \left|\langle\psi,g_{x,\xi}\rangle\right|^2 dxd\xi \ge 0$$

Lemma 2.6. Let $f \in \mathcal{S}(\mathbb{R}^2)$. Then we have

$$||Op^{AW}(f) - Op^{W}(f)|| = O_f(\hbar)$$

Thus, the Anti-Wick quantization is asymptotically equivalent to the three quantizations we already know.

Proof: We leave as an exercise (see below) to show that

$$Op^{AW}(f) = Op^{W}(f * G)$$

for the Gaussian $G(x,\xi) = e^{-\frac{1}{\hbar}(x^2+\xi^2)}$. Then, since $f * G \to f$ in C^k for any k, as $\hbar \to 0$, the Lemma follows from the remark of section 2.3.2, that for $f \in \mathcal{S}(\mathbb{R}^2)$, the operator Op(f) is bounded⁴ by $||Op(f)|| \leq ||f||_{C^2}$.

Exercise 2.4. Assume that $f \in \mathcal{S}(\mathbb{R})$, and set $G(x,\xi) = e^{\frac{1}{\hbar}(x^2+\xi^2)}$.

⁴As remarked there, the Calderón-Vaillancourt Theorem removes the decay assumption on f, and so this Lemma actually holds for more general $f \in C^{\infty}(\mathbb{R})$ under mild growth conditions.

(1) Show that

$$Op^{W}(f * G)\psi(q) = \iiint_{q',x,\xi \in \mathbb{R}} \psi(q')f(x,\xi) \left(\int_{p \in \mathbb{R}} G\left(\frac{q+q'-2x}{2}, p-\xi\right) e^{\frac{i}{\hbar}(q-q')p}dp\right) dxd\xi dpdq'$$

- (2) Do the integral over p first, evaluating the expression in parentheses using the formula for the ħ-Fourier transform of a Gaussian.
- (3) Use the fact that

$$\frac{a^2 + b^2}{2} = \left(\frac{a+b}{2}\right)^2 + \left(\frac{a-b}{2}\right)^2$$

to show that this expression from part (2) is equal to $g_{x,\xi}(q)g_{x,\xi}(q')$. (4) Conclude that $Op^W(f * G) = Op^{AW}(f)$.

2.6. Eigenstates and Definite Values. We've seen how we can calculate the expected value of a quantum observable, given a specified quantization Op, and we've seen some examples of various quantizations and their properties.

In general, this is the best one can hope to do in terms of "evaluating" observables in the quantum world. However, there are some observables that admit definite evaluation, at least for some states. As a silly example, take the constant classical observable f(q, p) = C. It doesn't matter where you are or where you're going; the observable takes the value C. Of course, $\mathbb{E}_{\psi}(f(q, p) = C) = C$ trivially for any L^2 -normalized state ψ , but it would be very strange indeed if quantum mechanics did not allow some mechanism for giving this observable a *definite* value, instead of just an average value, of C.

So let's agree to assign the identity operator a definite value of 1 for all states. But this is not without consequence— what if a state ψ cannot distinguish between an operator Op(f) and a scalar operator $C \cdot Id$? In other words, if ψ is an eigenvector of Op(f), then Op(f) acts on ψ as a scalar multiple of Id, and therefore we should agree that ψ has a definite value for the observable Op(f), given by its eigenvalue.

Remark: Note that the operators Q and P have no L^2 -eigenvectors an eigenvector of Q would have to be a δ function (why?), which is not in L^2 ; an eigenvector of P is an exponential $\psi(q) = e^{ikq}$ for some $k \in \mathbb{R}$, which is also not in L^2 . So there is still no state with definite position or momentum! On the other hand, waves like e^{ikq} do have a definite momentum— and a definite energy— which is one of the motivating facts behind the development of quantum mechanics. Eigenvectors of an observable are often called **eigenstates** or **pure states** for the observable. An important example is H, the Hamiltonian operator. Since the observable H corresponds to the total energy of the particle, eigenfunctions of H are states of definite energy. Note that Schrödinger's equation implies that if $\psi = \psi_0$ is such a state, then the Schrödinger evolution acts on the eigenspace of ψ by a scalar λ_{ψ} , and in fact

$$e^{-\frac{i}{\hbar}Ht}\psi = e^{-\frac{i}{\hbar}\lambda_{\psi}t}\psi$$

so that the evolution is by a phase factor of absolute value 1 (this is also immediate from the fact that the Schrödinger evolution is unitary). Multiplication by a factor $e^{-\frac{i}{\hbar}\lambda_{\psi}t}$ does not change $|\psi|$ or $|\mathcal{F}_{\hbar}(\psi)|$, so the position and momentum distributions for ψ remain unchanged by the Schrödinger evolution. Thus, these distributions are invariant under the quantum evolution! We often call such a ψ a steady-state for the Schrödinger evolution— in this case, ψ_t is not exactly fixed, since it changes by a phase factor, but this factor has no physical significance; the physically meaningful distributions $|\psi_t|$ and $\mathcal{F}_{\hbar}(\psi)|$ remain constant.

2.7. Quantization on Manifolds. We will soon wish to work with dynamical systems on compact— or perhaps finite volume— manifolds, rather than \mathbb{R}^d . For the systems we have in mind (toy models and hyperbolic surfaces), we will establish quantization procedures that are more amenable to each setting. However, it is worth remarking that for any smooth manifold M, one can use the standard pseudodifferential calculus on \mathbb{R}^d in a local chart to define a quantization on M.

Namely, given an atlas of charts $U_j \subset M$ and smooth diffeomorphisms $\phi_j : U_j \to \tilde{U}_j \subset \mathbb{R}^d$, we can define local (Darboux) coordinates on the cotangent bundle T^*M via the map

$$\Phi_j: (p,q) \mapsto (\phi_j(q), d\phi_j(q)^{-1}p) \in \mathbb{R}^{2d}$$

One can then take a partition of unity $\chi_k \in C_0^{\infty}(U_{j(k)})$ satisfying $\sum_k \chi_k^2 = 1$, and define for $f \in C^{\infty}(T^*M)$

$$Op(f)\psi = \sum_{k} \chi_k \Big[Op(f \circ \Phi_j(k))(\chi_k \psi \circ \phi_{j(k)}^{-1}) \Big] \circ \phi_{j(k)}$$

Of course, this definition depends on the choice of quantization on \mathbb{R}^{2d} , the choice of local coordinates, and the partition of unity— but it is not hard to be convinced that these choices only change the symbol by lower order terms, and that the operator Op(f) is asymptotically well-defined.

Since we will not use this quantization in the course, we won't enter into any of these details; however, it is good to know that there is at the very least *some* way to extend the results from \mathbb{R}^d to manifolds, so that we may ask questions about the latter.

3. EIGENVALUE SPACING STATISTICS

We now turn to the main objects of study for this course: the Hamiltonian operator

$$H = \frac{1}{2m}P^2 + V(Q)$$

We wish to understand the relationship between this operator, which generates the Schrödinger evolution of a quantum particle, and the classical dynamics generated by the Hamiltonian flow to which H corresponds.

We will now assume that the dynamics take place on a compact manifold, on which the potential vanishes. Two main examples are

- Billiard flow on a compact domain $D \subset \mathbb{R}^2$ (with boundary).
- Geodesic flow on a compact Riemann surface M without boundary.

We will introduce more examples (so-called "toy models) in section ??, but for now, let's keep these two examples in mind. Notice that since there is no potential, the classical Hamiltonian is simply $\frac{1}{2m}|p|^2$, and so the Hamiltonian operator is the scaled Laplacian $H = -\frac{1}{2m}\hbar^2\Delta$ (for billiards with boundary, we have the Dirichlet boundary condition $\psi|_{\partial D} = 0$ which prevents the particle from leaving the domain).

Since our operator H is self-adjoint, we have an orthonormal basis of $L^2(D)$ or $L^2(M)$ consisting of eigenfunctions of H. Of course, to understand the operator H means to understand how it acts on L^2 , which in turn means understanding its eigenvalues and eigenfunctions. So the question becomes, what properties of the eigenvalues and eigenfunctions of H reflect properties of the classical dynamics?

In this section, we discuss some conjectures about properties of the eigenvalues that are supposed to reflect dynamical information about the classical system. Very little is known about these conjectures, and later sections will be devoted to the eigenfunctions— about which much more can be said.

Notational Remark: From here on, we will assume that the particle has mass 1 and (definite) energy H = 1/2. Thus, the spectrum of the operator H determines which values of \hbar are admissible (of course, in physics, it goes the other way around— \hbar is fixed, and determines which energy levels are admissible...). Thus when we take $\hbar \to 0$, we are taking \hbar along a discrete sequence of values accumulating at 0. On the flip side, if $H\psi = \frac{1}{2}\psi$ for small \hbar , this means that ψ is an eigenfunction of Δ of large eigenvalue $2\hbar^{-2}$, since

$$-\hbar^2 \Delta \psi = H\psi = \frac{1}{2}\psi$$

So the semiclassical limit $\hbar \to 0$ is the same as the large eigenvalue limit of the Laplacian.

3.1. Weyl's Law. A fundamental result (which we will not prove here) is Weyl's law, which gives the asymptotic number of eigenvalues (counted with multiplicity) of H. Note that this result is *uniform*, and does not depend on the dynamics of the classical system! We set |D| to be the area of D, and set $N(\lambda)$ to be the number of eigenvalues λ_j (with multiplicity) such that $\lambda_j \leq \lambda$.

Theorem 3.1 (Weyl's Law in Dimension 2). We have

$$N(\lambda) \sim \frac{|D|}{4\pi} \lambda$$

This can also be extended to the Laplace-Beltrami operator on a manifold without too much trouble.

Exercise 3.1. Verify Weyl's Law for a rectangular billiard with sides of length a and b.

- (1) For any eigenfunction ψ , use the Dirichlet boundary condition to expand ϕ in a Fourier sine series in each coordinate (separation of variables).
- (2) Conclude that eigenvalues are of the form $\frac{m^2}{a^2} + \frac{n^2}{b^2}$ for integers m and n, and give an explicit basis of eigenfunctions.
- (3) Use Gauss' result that the number of integer lattice points inside an ellipse $\frac{x^2}{a^2} + \frac{y^2}{b^2} \leq C$ is asymptotic to the area $C\pi ab$ of the ellipse. Check how many lattice points actually correspond to the same eigenfunction!
- (4) Compare the number of basis eigenfunctions in the previous part with the number you get from Weyl's Law.

For most domains, the eigenvalues and eigenfunctions are extremely difficult to compute explicitly. Thus, it is something of a miracle that their total number is, at least asymptotically, easy to calculate (though the remainder term is much harder, even for the square billiard— this is Gauss' circle problem!). In any case, the generality of Weyl's Law shows that the total number of eigenvalues is not sensitive to the dynamics; if there is dynamical information encoded in the spectrum, we will have to look at the finer structure of the spectrum to see it. As we will see, it is conjectured that one should look at the spacings between consecutive eigenvalues to distinguish completely integrable systems from chaotic dynamics.

3.2. Completely Integrable Systems: Invariant Tori and the Berry-Tabor Conjecture. The first conjecture in this direction came in 1977:

Conjecture 3.1 (Berry-Tabor, 1977). For a "generic" completely integrable Hamiltonian system, the spacing between consecutive eigenvalues of the corresponding Hamiltonian operator should obey Poisson statistical laws.

The word "generic" is used very loosely (and dangerously) here; perhaps the most illuminating definition for generic here is "unless there's a good reason for the conjecture to fail". Indeed, there are examples eg., square billiards; see below— where this is false, but for arithmetic reasons which are "not generic" in a usual, measure-theoretic sense.

Let's also discuss what "Poisson statistical laws" are. Informally speaking (we won't give the rigorous characterization here), we're talking about the spacings between consecutive occurences of *independent* random events. A good prototypical example to have in mind is coinflips: suppose we are flipping a fair coin once every second, and looking at the time between consecutive results of heads. Each flip is independent of the preceding ones, so given that a heads has just occurred, the probability of getting a heads on the next flip (so that the spacing between the consecutive flips is 1 second) is 1/2. The probability that the spacing is exactly 2 seconds is the joint probability of a tails followed by a heads, which is 1/4. It's clear that the probability of waiting exactly t seconds for the next head is $\left(\frac{1}{2}\right)^t$. In particular, the probability density decays exponentially with time.

This is a general picture of what happens for the spacings between independent random events. If the probability of an event occurring in any time interval is independent of the last occurrence, then the joint probability of the event not occurring over the course of many intervals should decay exponentially. Thus, the spacing statistics should look like an exponential decay, as in Figure 1.

Thus, Berry-Tabor are conjecturing that the spacings between consecutive eigenvalues for a completely integrable Hamiltonian should look like those of numbers that were randomly and independently selected, asymptotically as the eigenvalues go to ∞ .

Why? Here's a vague heuristic argument. We know that, in the completely integrable case, the phase space is foliated into invariant

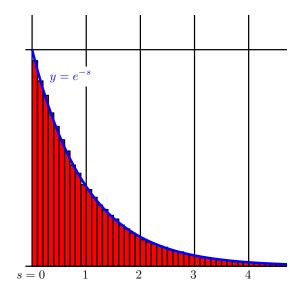


FIGURE 1. Normalized gaps between the first 250,000 eigenvalues of a rectangle with side/bottom ratio $5^{1/4}$ and area 4π , compared to the expected probability density e^{-s} of a Poisson process. Picture from Rudnick[?].

tori. We also know that these tori are level sets for an integral of the motion f, that by definition Poisson commutes with the Hamiltonian H, so that the corresponding quantizations commute up to small error: $[Op(f), H] = O(\hbar^2)$. It is natural to imagine (and a rigorous version of this was proved by Schnir'lman[?]) that the Hamiltonian operator H approximately commutes with projection to the invariant tori, and for small \hbar — or large eigenvalue— we can imagine the phase space as being broken up into disjoint blocks of invariant tori, each with its own H-spectrum, that are independent of each other. As $\hbar \to 0$, we can take a finer and finer subdivision into more and more such invariant blocks of tori.

Now, essentially by "Weyl's law", each block of phase space will contribute a chunk of the spectrum proportional to its volume. Thus, the spectrum of H can be thought of as coming from a collection of independently chosen values, from the many disjoint blocks of invariant tori. In this way, their statistics should resemble those of independent random variables.

Conjecture 3.1 is not known (yet) to hold for a single case. On the other hand, there are some known counterexamples. Notice that, for the square billiard, the eigenvalues must be (proportional to) integers, and occur with high multiplicity. The probability density for level spacings collapses to a δ measure at 0. The same thing happens for any rectangle whose sides are rational multiples of each other. In some sense, one can view the δ measure at 0 as a degenerate limit of the Poisson distribution, and one believes that under diophantine conditions, rectangular billiards should obey the Berry-Tabor Law. But so far, very little is known.

3.3. Chaotic Systems: Random Matrices and the Bohigas-Giannoni-Schmit Conjecture. At the other extreme, we have the "chaotic" systems, and a conjecture about the spacings between consecutive eigenvalues for their Hamiltonian operators.

Conjecture 3.2 (Bohigas-Giannoni-Schmit, 1984). The spacings between eigenvalues of a chaotic Hamiltonian operator "generically" follow the spacing laws for eigenvalues of large random matrices.

The idea of using statistical properties of large random matrices to model complicated systems has a long history in physics, beginning with Wigner, who suggested using eigenvalues of large random matrices to model the energy levels of heavy atoms (the complex interactions between large numbers of subatomic particles make the heavy atoms difficult— if not impossible— to analyze directly). One might call this a quantum version of statistical mechanics.

In any case, it is not at all obvious what the correct notion of "random matrices" is. First of all, we should restrict ourselves to matrices that have some semblance to the Hamiltonian operators they're trying to model; in particular, since our Hamiltonians are self-adjoint, one should consider matrices with similar symmetry. Consider, then, the space of $N \times N$ real symmetric matrices, where N is large. This space is N(N + 1)/2-dimensional, since the matrix is determined by its values along the diagonal and in the upper triangular region (the lower triangular region is determined by symmetry). One natural notion of a random symmetric matrix is the so-called "GOE", which stands for Gaussian Orthogonal Ensemble. It comes from the following two assumptions:

- Each of the N(N+1)/2 matrix elements are chosen independently.
- The probability distribution is invariant under conjugation by orthogonal matrices (i.e., orthogonal change of basis).

It turns out that these very natural conditions force the (independent) matrix elements to be Gaussian-distributed in \mathbb{R} . In fact, the orthogonal-invariance condition requires all off-diagonal elements to

be chosen from the same Gaussian distribution, and all diagonal elements to be chosen from the same Gaussian distribution (the variance of the diagonal elements turns out to be twice the variance of the offdiagonal ones, essentially because each off-diagonal term appears twice in the matrix, and each diagonal term appears once). It can also be shown that the probability density of a matrix A is proportional to $e^{-C(N) \cdot Tr(A)^2}$ for some constant C(N) depending on the size of the matrices.

A conjecture that has its roots back in the work of Wigner states that the statistics of eigenvalues of GOE matrices should hold for any "reasonable" probability distribution on the space of real-symmetric matrices, in which matrix elements are chosen independently. We will not enter into a discussion of this fascinating theory here, but we note that this type of universality is very encouraging for the hope of extrapolating to arbitrary "generic" chaotic Hamiltonian operators.

The level spacings between consecutive eigenvalues of GOE matrices are distributed according to the probability measure

$$\mu_{GOE}(s) = \frac{\pi}{2}se^{-\frac{\pi s^2}{4}}$$

which looks like the picture in Figure 2. We won't prove this here, but there is one glaring feature that distinguishes it from the Poisson distribution, and which is not too difficult to understand— namely, the density vanishes at 0. This is often referred to as **level repulsion**, since the eigenvalues (or energy levels) tend to repel each other, in the sense that the probability of finding another eigenvalue very close to a given one is very small.

Why is this? Consider a double eigenvalue; this means that there is a two-dimensional space on which the matrix acts as a scalar multiple of the identity. By an orthogonal change of basis— which we may do, since our distribution is invariant under orthogonal transformations— we can

assume that our matrix has the form
$$\begin{pmatrix} \lambda & 0 \\ 0 & \lambda \\ & M \end{pmatrix}$$
 for an $(N-2) \times (N-2)$

2) symmetric matrix M. Note that the condition of having a double eigenvalue forces *two* conditions on this upper left block of the matrix the diagonal terms must be equal, and the off-diagonal terms must vanish. More precisely, if these two eigenvalues are very close together, it forces two conditions on the entries in the 2×2 block— the diagonal terms must be close, and the off-diagonal term(s) must be small (this is one condition, since one off-diagonal term determines the other by symmetry). Since all (3) matrix elements are chosen independently,

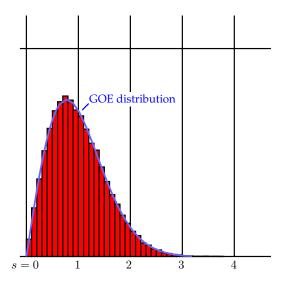


FIGURE 2. Normalized gaps between 50,000 eigenvalues of a chaotic billiard, compared to the expected probability density $\frac{\pi}{2}se^{-\frac{\pi s^2}{4}}$ of GOE matrices. Picture from Rudnick[?].

satisfying these two independent conditions simultaneously forces the probability density to vanish.

3.4. Arithmetic Symmetries. Like the Berry-Tabor Conjecture 3.1, almost nothing is known towards the Bohigas-Giannoni-Schmit Conjecture 3.2. However, there are some counterexamples "known", in the sense that numerical evidence overwhelmingly suggests that the eigenvalue spacings are not GOE-distributed, for some special examples. Once again, this is (assumed to be) due to special arithmetic nuances.

For example, if we take $M = SL(2, \mathbb{Z}) \setminus \mathbb{H}$ to be the modular surface, then numerics have shown quite convincingly that the eigenvalue spacings obey *Poissonian* statistics, rather than GOE. It's as though the geodesic flow on T^*M were completely integrable! Of course, this is not the case, and M is not foliated into invariant tori by any integral of the motion. There is, however, an interesting foliation lurking in the background— called the Hecke correspondence— which we will now introduce briefly.

Recall that $SL(2, \mathbb{R})$ acts on \mathbb{H} by Möbius transformations. In general, once we quotient by a subgroup, there is no reason to believe that matrices in $SL(2, \mathbb{R})$ should act on $\Gamma \setminus \mathbb{H}$ in any meaningful way; the only way for this to happen is if the action preserves the Γ -invariance.

If $\Gamma = SL(2,\mathbb{Z})$, however, there *are* some matrices are permuted by $SL(2,\mathbb{Z})$. Namely, let M_p be the set of 2×2 integer matrices of determinant p. Then $SL(2,\mathbb{Z})$ acts on M_p by multiplication. We can embed $M_p \hookrightarrow SL(2,\mathbb{R})$ by dividing by \sqrt{p} , and $SL(2,\mathbb{Z})$ leaves this set invariant; thus the quotient $SL(2,\mathbb{Z}) \setminus M_p \hookrightarrow SL(2,\mathbb{Z}) \setminus \mathbb{H}$.

We can now define the *p*-Hecke operator $T_p: L^2(M) \circlearrowleft$ by

$$T_p(f)(x) = \frac{1}{\sqrt{p}} \sum_{\alpha \in SL(2,\mathbb{Z}) \setminus M_p} f(\alpha.x)$$

Since each α acts by isometries, this operator T_p commutes with Δ on $L^2(M)$. One can also show that T_p commutes with T_q whenever (p,q) = 1; that is, whenever p and q are relatively prime. Thus, in particular, the set $\{T_p\}$ for p prime forms a large family of self-adjoint operators that commute with each other and with Δ . Notice how heavily this construction relies on the arithmetic!

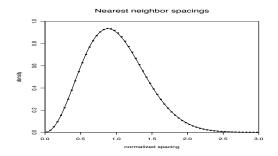
It is the existence of such a family that is (thought to be) responsible for the Poissonian spacings between eigenvalues. Indeed, it's as though each T_p eigenspace is contributing its own "spectrum" independently, just as each block of invariant tori contributed its own piece of the spectrum in the completely integrable case.

Sadly, virtually nothing can be proved about any of this!

3.5. Gross Omission — Random Matrices and *L*-functions. I would be remiss if I did not at least mention one other fascinating aspect of the eigenvalue spacings of random matrices. Have a look at Figure 3— does this look like it might be a graph representing the consecutive spacings of eigenvalues of a chaotic Hamiltonian⁵ operator?

In fact, this plot comes from consecutive spacings of zeroes of the Riemann zeta function on the critical line. It is very tempting to guess that the zeroes $s = \frac{1}{2} + it$ of the zeta function are given by eigenvalues of $\frac{1}{2} + iH$ for some chaotic Hamiltonian operator H. If true, then this would immediately imply the Riemann hypothesis, since self-adjoint Hamiltonian operators have real eigenvalues— in fact, the idea that zeroes of the zeta function could be given by eigenvalues of a self-adjoint operator goes back to Hilbert and Polya, well before the

⁵Actually, the solid curve in the figure corresponds to the GUE ensemble of complex Hermitian matrices, rather than real symmetric ones; we won't be too concerned with the difference between these ensembles here, but properties of the classical Hamiltonian (conjecturally) govern whether GOE or GUE is the correct random matrix model.



64

FIGURE 3. Normalized gaps between 10 billion consecutive zeroes of $\zeta(s)$, starting from around zero number 1.3×10^{16} , from Odlyzko[?].

numerics⁶ of Odlyzko. What these numerics suggest is that the mysterious "Riemann zeta function Hamiltonian"— if it exists— should come from the quantization of a chaotic Hamiltonian.

The same spacing statistics are expected to hold for all L-functions (and for other spacing statistics); see eg. [?] for a more detailed account.

4. Eigenfunctions and Quantum Ergodicity

We now turn to studying the eigenfunctions of H. For simplicity, we will restrict the discussion in this section to $H = -\hbar^2 \Delta$ on $L^2(M)$, where $M = \Gamma \setminus \mathbb{H}$ is a hyperbolic Riemann surface and Δ its Laplacian. This operator corresponds to $H = Op(|p|^2)$, where $|p|^2$ is the energy of a particle of mass 1/2 moving freely on M at unit speed. In other words, H is a Hamiltonian for the geodesic flow on M.

There are many questions that one can ask regarding the eigenstates of H for small \hbar (which correspond to eigenfunctions of Δ of large eigenvalue \hbar^{-2}). A very general— and rather vague— idea, that can be traced back to M. Berry, is that these eigenstates should resemble "random waves" in the semiclassical limit. Whether or not this is true (and it isn't, in general; as with the eigenvalue spacing conjectures, there are arithmetic counterexamples), intuition leads us to believe that, as steady-states of the Schrödinger evolution, these eigenstates should be "spread out" rather than localizing in small sets. There are many different notions of "spread out": for example,

⁶Actually, Montgomery was the first to compute spacings between zeroes of $\zeta(s)$, and Dyson was the one who suggested that they be compared with random matrix statistics. This is itself is a wonderful folklore story, of which many versions can be found.

Conjecture 4.1 (Iwaniec-Sarnak). Let ϕ_j be a sequence of eigenfunctions of Δ on M, with eigenvalues $\lambda_j \to \infty$. Assume that $||\phi_j||_{L^2} = 1$. Then $||\phi_j||_{L^p} = O_{p,\epsilon}(\lambda^{\epsilon})$ for all $2 , and any <math>\epsilon > 0$.

Conjecture 4.1 is very deep⁷, and far out of reach at the present. A more modest goal is "weak" equidistribution:

Conjecture 4.2 (Quantum Unique Ergodicity, Rudnick-Sarnak '94). Let M be a compact Riemannian manifold of negative sectional curvature, and $\{\phi_j\}$ an orthonormal basis of $L^2(M)$ consisting of eigenfunctions of Δ on M. Then for any $f \in C(M)$, we have

$$\int_M f(x) |\phi_j(x)|^2 dVol(x) \to \int_M f(x) dVol(x)$$

i.e., the measures $|\phi_j|^2 dVol$ converge in the weak-* topology to the uniform measure dVol.

Moreover, the microlocal lifts

$$\mu_j: f \mapsto \langle Op(f)\phi_j, \phi_j \rangle$$

converge weak-* to the uniform (Liouville) measure in S^*M .

Some comments are in order regarding Conjecture 4.2. First, note that the second statement implies the first, since taking $f \in C^{\infty}(M) \subset C^{\infty}(S^*M)$ gives

$$\langle Op(f)\phi_j,\phi_j\rangle_{L^2(S^*M)} = \int_M f(x)|\phi_j(x)|^2 dVol(x)$$

since in this case Op(f) is simply multiplication by f. The significance of the stronger statement is that it deals with distributions on S^*M — where the dynamics take place— which, as we will see (Egorov's Theorem) are asymptotically invariant under the geodesic flow. One can also show that these distributions are asymptotically positive (à la Anti-Wick quantization), and thus weak-* limit points of the μ_j are geodesic-flow-invariant probability measures (due to the L^2 -normalization of the eigenfunctions). Thus, the second statement is the one most suited to ergodic theory. Such a weak-* limit point of the μ_j is called a **quantum limit**. So Conjecture 4.2 is stating that there is a *unique* quantum limit; namely Liouville measure on S^*M (that Liouville measure is a quantum limit at all will be established by Quantum Ergodicity, Theorem 4.1 below). This (partially) explains the terminology.

⁷For example, when applied to congruence surfaces, Conjecture 4.1 would imply the Lindelöf Hypothesis for ζ and some other classical *L*-functions.

Lemma 4.1. Any quantum limit is a positive measure, invariant under the geodesic flow on S^*M .

Proof: Let $f \in C^{\infty}(S^*M)$. Since $H\psi_j = \frac{1}{2}\psi_j$ $e^{-\frac{i}{\hbar}Ht}\phi_i = e^{-\frac{i}{\hbar}\frac{1}{2}t}\phi_i$

and $e^{-\frac{i}{\hbar}\frac{1}{2}t}\overline{e^{-\frac{i}{\hbar}\frac{1}{2}t}} = 1$, we have

66

$$\begin{aligned} \langle Op(f)\phi_j,\phi_j\rangle &= \langle Op(f)e^{-\frac{i}{\hbar}Ht}\phi_j, e^{-\frac{i}{\hbar}Ht}\phi_j\rangle \\ &= \langle e^{\frac{i}{\hbar}Ht}Op(f)e^{-\frac{i}{\hbar}Ht}\phi_j,\phi_j\rangle \\ &= \langle Op(f\circ g_t)\phi_j,\phi_j\rangle + O_f(\hbar) \end{aligned}$$

by Egorov's Theorem. Thus as $\hbar \to 0$ we have

$$|\mu_j(f) - \mu_j(f \circ g_t)| \to 0$$

for any smooth $f \in C^{\infty}(S^*M)$, and so any weak-* limit point of the μ_i must be g_t -invariant.

Since we may replace our choice of Op(f) by a positive quantization $Op^+(f)$ (eg. by a local Anti-Wick construction) up to an error of $O(\hbar)$ in the operator norm, and since $||\phi_j|| = 1$, we have for f non-negative

$$\langle Op(f)\phi_j,\phi_j\rangle = \langle Op^+(f)\phi_j,\phi_j\rangle + O(\hbar) \ge O(\hbar)$$

and μ_i is asymptotically a positive measure. \Box

Remark: You might wonder whether this condition is already restrictive. If the flow were *uniquely ergodic*, then there would be only one invariant measure; but the geodesic flow on a compact manifold is not uniquely ergodic. For example, given a closed geodesic, one can take the normalized length measure on the geodesic. In general, there are many, many measures invariant under the geodesic flow.

The first step towards classifying quantum limits is the following Quantum Ergodicity Theorem, which shows that the uniform measure is the "generic" quantum limit, when the classical flow is ergodic.

Theorem 4.1 (Quantum Ergodicity, Shnir'lman-Zelditch-Colin de Verdière). Let M be a Riemannian manifold, such that the geodesic flow on Mis ergodic. Then almost all eigenfunctions become equidistributed; precisely, given any orthonormal basis $\{\phi_j\}$ of $L^2(M)$ consisting of eigenfunctions of Δ , there exists a subsequence $\{\phi_{j_k}\}$ of asymptotic density 1 such that μ_{j_k} converge weak-* to Liouville measure on S^*M .

Remarks:

• By asymptotic density 1, we mean that

$$\lim_{k \to \infty} \frac{k}{\#\{j \le j_k\}} = 1$$

• Theorem 4.1 implies that, if there are exceptional sequences of eigenfunctions that converge to a singular measure, they are sparse. In fact, in the toy models that we will meet later on, there *are* such sparse exceptional sequences, and their construction relies in an obvious way on selecting very special eigenfunctions.

Sketch of Proof: The analytic input is an average over the spectrum, of the form:

(3)
$$\lim_{\lambda \to \infty} \frac{1}{N(\lambda)} \sum_{\lambda_j \le \lambda} \langle Op(f)\phi_j, \phi_j \rangle = \int_{S^*M} f d\mu_L$$

where μ_L is Liouville measure on S^*M . If Op(f) is supported on the finite-dimensional span of $\{\phi_j : \lambda_j \leq \Lambda\}$, then this is established⁸ by writing the trace of Op(f) in two ways— the left-hand side as a sum over the eigenvalues, and the right-hand side as an integral of the kernel over the diagonal. One then takes a suitable limit of cutoffs approximating Op(f) to get the general statement.

The set of probability measures on M is weak-* compact, and so if the complete sequence μ_j does not converge to μ_L , then there exist other weak-* limit points (quantum limits) of the μ_j . So suppose that there is a sequence $E = \{\phi_{j_i}\}$ of eigenfunctions, such that

$$\lim_{\lambda_{j_l} \to \infty} \langle Op(f)\phi_{j_l}, \phi_{j_l} \rangle = \int_{S^*M} f d\mu_{\text{bad}}$$

for some singular measure μ_{bad} . Then we can rewrite the average (3) as

$$\begin{split} \int_{S^*M} f d\mu_L &\sim \quad \frac{1}{N(\lambda)} \sum_{\lambda_j \leq \lambda} \langle Op(f)\phi_j, \phi_j \rangle \\ &= \quad \frac{1}{N(\lambda)} \sum_{\lambda_{j_l} \leq \lambda, \phi_{j_l} \in E} \langle Op(f)\phi_{j_l}, \phi_{j_l} \rangle + \frac{1}{N(\lambda)} \sum_{\lambda_{j_k} \leq \lambda, \phi_{j_k} \notin E} \langle Op(f)\phi_{j_k}, \phi_{j_k} \rangle \end{split}$$

Clearly, the first sum on the right tends to $\lim_{\lambda\to\infty} \frac{\#\lambda_{j_l}\leq\lambda}{N(\lambda)}\mu_{\text{bad}}(f)$. But then this gives a decomposition of μ_L into distinct invariant measures! Since μ_L is ergodic for the geodesic flow on M, such a decomposition must be trivial, and so the weight $\lim_{\lambda\to\infty} \frac{\#\lambda_{j_l}\leq\lambda}{N(\lambda)}$ of μ_{bad} in the decomposition must be 0, and the exceptional set E has density 0.

⁸In practice, it's better to first average over a chunk of the spectrum, that's moving to higher and higher eigenvalues, and then deduce the estimate for the full average.

68

Since this holds for an arbitrary symbol $f \in C^{\infty}(S^*M)$, one can take a countable base for which the statement is satisfied, and then take a countable intersection of full density subsequences to get the statement for *all* symbols in $C^{\infty}(S^*M)$. \Box

Remark: Note that we used the ergodicity of the geodesic flow, but nothing more. In the toy models that we will meet in the next section, where the classical dynamics are ergodic— in fact, uniformly hyperbolic— Quantum Ergodicity can be proven along the lines of this argument, but QUE fails; we will exhibit explicit (sparse) sequences of eigenfunctions whose microlocal lifts have a singular component. Thus, QUE requires more than just ergodicity.

Remark: The terminology has two meanings: firstly, since quantum ergodicity is implied by ergodicity of the classical flow, it is the correct analogue of ergodicity for quantum systems (Zelditch has shown that under some conditions, the converse is also true; but this is not automatic). Secondly, it has an interpretation as a quantum version of Birkhoff's Pointwise Ergodic Theorem ??: just as almost every orbit is equidistributed classically, we have a statement that almost every quantum limit is equidistributed.

Remark: If the classical flow is *uniquely ergodic*, meaning that there are no invariant measures other than Liouville measure, then QUE is automatically satisfied by Lemma 4.1.

5. Toy Model I — the Baker's Maps

The QUE problem is hard. So, it makes sense to look for easier problems to study, that are sufficiently analogous, and can provide good intuition as to what to look for in the harder problems. As it turns out, some of these toy models lead to juicy questions of their own, whose resolution could help gain a better understanding of the theory.

So what is a "toy model"? What we require is a "chaotic" dynamical system $T: X \to X$ that's well understood, and admits some reasonable quantum model: i.e., a sequence of small numbers $\hbar \to 0$, and

- A Hilbert space of states \mathcal{H} (analogous to $L^2(M)$)
- A quantization of observables $f \in C^{\infty}(X) \mapsto Op(f) \in Hom(\mathcal{H})$ such that Op(f) is asymptotically positive-definite whenever f is positive
- A quantization of the dynamics $\tilde{T} : \mathcal{H} \to \mathcal{H}$ satisfying an Egorov property

$$\tilde{T}^{-1}Op(f)\tilde{T} \sim Op(f \circ T)$$

Given such a framework, we can take a sequence of normalized eigenfunctions ϕ_i of \tilde{T} , and study the microlocal lift

$$\mu_j(f) = \langle Op(f)\phi_j, \phi_j \rangle_{\mathcal{H}}$$

By the Egorov property and asymptotic positivity, weak-* limit points of the μ_i will be positive *T*-invariant measures on *X*.

5.1. The Classical Map. Our first toy model is a quantization of the D-baker's maps, or 2-sided shift on D symbols, where $D \ge 2$ is an integer. In this case (and for our other toy model, the cat maps in section ??), the space $X = \mathbb{T}^2$, though for baker's maps it is best to identify points $(q, p) \in \mathbb{T}^2$ with a 2-sided infinite sequence

$$(q, p) \leftrightarrow \ldots \epsilon'_2 \epsilon'_1 \cdot \epsilon_1 \epsilon_2 \ldots \qquad \epsilon_i, \epsilon'_i \in [0, D-1] \cap \mathbb{Z}$$

coming from the D-adic expansions

$$q = 0.\epsilon_1\epsilon_2..$$

$$p = 0.\epsilon'_1\epsilon'_2$$

(This identification is not quite 1-to-1, since eg. $\ldots 00 \cdot 100 \ldots$ and $\ldots 11 \cdot 011 \ldots$ both correspond to the point $(1/D, 0) \in \mathbb{T}^2$, but this only happens on a countable set of measure 0, and may be disregarded.)

The dynamics are given by the map

$$B(q,p) = \left(Dq \mod 1, \frac{p + \lfloor Dq \rfloor}{D} \right) \in \mathbb{T}^2$$

which is identified with the shift on Σ , the space of double-sided sequences with the product topology. See Figure ?? for a picture; the name comes from the intuition of cutting and stretching out the dough in strips. It is well known that the shift supports piles and piles of invariant measures— including, but not limited to, Bernoulli measures of arbitrary entropy (see section ??).

5.2. Walsh-quantized baker's map. We will now describe a quantum model for the baker's maps. Our semiclassical parameter will be given by $2\pi\hbar = D^{-k}$, where $k \in \mathbb{N}$ is a parameter tending to ∞ in the semi-classical limit. Our Hilbert space \mathcal{H}_{D^k} of quantum states is finitedimensional, isomorphic to \mathbb{C}^{D^k} . If we consider an orthonormal basis $\{e_0, \ldots, e_{D-1}\}$ of \mathbb{C}^D , then we take $\{e_{\epsilon_0} \otimes \cdots \otimes e_{\epsilon_{k-1}} : \epsilon_i \in [0, D-1] \cap \mathbb{Z}\}$ to be our orthonormal basis of \mathcal{H}_{D^k} . These vectors correspond to "position eigenstates", and are "lifted" to the phase-space as characteristic functions of (right-sided) cylinder sets of length k, i.e., sets of the form $\{\{a_n\} : a_i = \epsilon_i \text{ for } i = 0, \ldots, k-1\}$. Such cylinder sets correspond to vertical strips of width D^{-k} on \mathbb{T}^2 . For "momentum eigenstates", we employ the discrete D-Fourier Transform

$$(\mathcal{F}_D)_{jk} = \frac{1}{\sqrt{D}} e^{2\pi i k j/D}$$

as follows. The orthonormal set $\{\mathcal{F}_D^* e_{\epsilon_{-k}} \otimes \cdots \otimes \mathcal{F}_D^* e_{\epsilon_{-1}}\}$ is the basis for the momentum representation of states in \mathcal{H}_{D^k} . They lift to characteristic functions of left-sided cylinder sets, i.e. sets of the form $\{\{a_n\}: a_i = \epsilon_i \text{ for } i = -1, \ldots, -k\}$, corresponding to horizontal strips on \mathbb{T}^2 . Analogously, we take "coherent states" to be vectors of the form

(4)
$$\boldsymbol{\epsilon' \cdot \epsilon} := e_{\epsilon_0} \otimes \cdots \otimes e_{\epsilon_{\lfloor k/2 \rfloor}} \otimes \mathcal{F}_D^* e_{\epsilon_{-\lceil k/2 \rceil+1}} \otimes \cdots \otimes \mathcal{F}_D^* e_{\epsilon_{-1}}$$

that lift to characteristic functions of disjoint rectangles $R(\epsilon' \cdot \epsilon) \subset \mathbb{T}^2$, each of area D^{-k} , that are approximately square. This achieves a joint localization in both position and momentum.

A family of quantizations is described in [?] for each k, corresponding to different choices of "coherent states", and they show the asymptotic equivalence in the semiclassical limit $k \to \infty$ for all $f \in Lip(\Sigma)$, the space of Lipschitz functions with respect to the shift metric. Therefore we consider $Lip(\Sigma)$ to be our space of observables, and define "the" Anti-Wick quantization to be

$$Op_k^{AW}(f)\psi := Op_{k,\lfloor k/2\rfloor}(f)\psi = D^k \sum_{\boldsymbol{\epsilon'}\cdot\boldsymbol{\epsilon}} \left(\int_{R(\boldsymbol{\epsilon'}\cdot\boldsymbol{\epsilon})} f(x)dx\right) \langle \boldsymbol{\epsilon'}\cdot\boldsymbol{\epsilon}|\psi\rangle\langle \boldsymbol{\epsilon}'\cdot\boldsymbol{\epsilon}|\psi\rangle\langle \boldsymbol{\epsilon'}\cdot\boldsymbol{\epsilon}|\psi\rangle\langle \boldsymbol{\epsilon}'\cdot\boldsymbol{\epsilon}|\psi\rangle\langle \boldsymbol{\epsilon'}\cdot\boldsymbol{\epsilon}|\psi\rangle\langle \boldsymbol{\epsilon'}\cdot\boldsymbol{\epsilon}|\psi\rangle\langle \boldsymbol{\epsilon}'\cdot\boldsymbol{\epsilon}|\psi\rangle\langle \boldsymbol{\epsilon}'\cdot\boldsymbol$$

for all $f \in Lip(\Sigma)$, where the sum runs over the D^k basis vectors of the form (4). The "Husimi measures", which will serve as our microlocal lifts for this model, are then given by

$$\mu_{\psi}(f) = \langle Op_k^{AW}(f)\psi|\psi\rangle = \sum_{R(\boldsymbol{\epsilon'\cdot\epsilon})} D^k |\langle\psi|\boldsymbol{\epsilon'\cdot\epsilon}\rangle|^2 \int_{R(\boldsymbol{\epsilon'\cdot\epsilon})} f(x)dx$$

Note that these are positive measures for all k.

The quantization of the baker's map is defined to be the operator B_{D^k} , whose action on \mathcal{H}_{D^k} is given by

$$B_{D^k}(v_1 \otimes v_2 \otimes \cdots \otimes v_k) = v_2 \otimes \cdots \otimes v_k \otimes \mathcal{F}_D^* v_1$$

We can now show that B_{D^k} satisfies the Egorov property for observables $f \in Lip(\Sigma)$ (see [?, Proposition 3.2])

Lemma 5.1. For $f \in Lip(\Sigma)$, we have

$$||B_{D^k}^{-1}Op_k^{AW}(f)B_{D^k} - Op_k^{AW}(f \circ B)|| \lesssim ||f||_{\infty} D^{-k/2}$$

as $k \to \infty$.

Now we take a sequence $\{\psi_j \in \mathcal{H}_{D^{k_j}}\}$ of eigenvectors of $B_{D^{k_j}}$, normalized so that $||\psi_j|| = 1$, and examine the Husimi (probability) measures μ_{ψ_j} as $k_j \to \infty$. By the Egorov property (5.1), any quantum limit of $\{\mu_{\psi_j}\}$ is a *B*-invariant probability measure on \mathbb{T}^2 , and the problem is to understand which of the myriad *B*-invariant measures arise as such a limit.

Lemma 5.2 (Quantum Ergodicity for Walsh-quantized baker's maps). For each k, and any choice of orthonormal basis of \mathcal{H}_k of B_k -eigenvectors, there is a subset E_k of basis vectors such that

$$\lim_{k \to \infty} \frac{|E_k|}{\dim \mathcal{H}_k} = 0$$

• For any sequence $\{\phi_k \in \mathcal{H}_k\}$ of basis eigenvectors such that each $\phi_k \notin E_k$, the microlocal lifts

$$\mu_k : f \in Lip(\Sigma) \mapsto \langle Op^{AW}(f)\phi_k, \phi_k \rangle_{\mathcal{H}_k}$$

as measures on \mathbb{T}^2 converge weak-* to Lebesgue measure.

Proof: For each $Op_k^{AW}(f) : \mathcal{H}_k \circlearrowleft$, write the trace of $Op_k^{AW}(f)$ in two different (orthonormal) bases:

$$TrOp_k^{AW}(f) = \sum_{i=1}^{D^k} \langle Op_k^{AW}(f)\phi_k^{(i)}, \phi_k^{(i)} \rangle$$
$$TrOp_k^{AW}(f) = \sum_{j=1}^{D^k} D^k \int_{R_k} f = D^k \int_{\mathbb{T}^2} f(x) dx$$

We have used an orthonormal basis of eigenfunctions in the first expansion, and an orthonormal basis of coherent states in the second (there is a small miracle in this model that the coherent states are actually orthogonal!). Equating both expressions, we get

$$\frac{1}{D^k} \sum_{i=1}^{D^k} \langle Op_k(f)\phi_k^{(i)}, \phi_k^{(i)} \rangle = \int_{\mathbb{T}^2} f(x) dx$$

i.e., the average of $\mu_k^{(i)}(f)$ over the full spectrum of B_k in \mathcal{H}_k is equal to Lebesgue measure. As above in Theorem 4.1, if we can divide this average into two non-trivial measures, this would contradict the ergodicity of Lebesgue measure; thus if there are some eigenvectors $\phi_k^{(i)}$ such that $\mu_k^{(i)}$ do *not* converge to Lebesgue measure, then their weight in the average must tend to 0 as $k \to \infty$. \Box

Problem Set I MAT656, Spring 2011

Exercise 1. Show that the Gaussian G_{α} defined by $G_{\alpha}(x) = e^{-\alpha x^2}$ belongs to the Schwartz class

$$\mathcal{S}(\mathbb{R}) := \left\{ f \in C^{\infty}(\mathbb{R}) : \forall j, k \in \mathbb{N}, \forall x \in \mathbb{R}, \quad \left| (1+x^2)^j \frac{d^k}{dx^k} f(x) \right| < \infty \right\}$$

for any $\alpha > 0$.

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Exercise 2. Show that for $f \in \mathcal{S}(\mathbb{R})$, the integral $\hat{f}(\xi) = \int_{\mathbb{R}} f(x)e^{2\pi i\xi x} dx$ converges absolutely.

Exercise 3. Consider the operators

$$[Xf](x) = xf(x) [e^{2\pi i y X} f](x) = e^{2\pi i y x} f(x) [Df](x) = (2\pi i)^{-1} f'(x)$$

Show that for $f \in C^{\infty}(\mathbb{T})$ we have

$$\widehat{Df}(m) = (m)\widehat{f}(m)$$
$$e^{2\pi i y X} \widehat{f}(x) = \widehat{f}(m-y)$$

and that for $f \in \mathcal{S}(\mathbb{R})$, we have

$$\begin{array}{rcl} \widehat{Df}(\xi) &=& (\xi)\widehat{f}(\xi) \\ \widehat{Xf} &=& -\frac{1}{2\pi i}\widehat{f'}(\xi) \\ e^{2\widehat{\pi iyX}}\widehat{f}(x) &=& \widehat{f}(\xi-y) \end{array}$$

Exercise 4. The point of this exercise is to show that, for the Gaussians G_{α} , equality is achieved in the Heisenberg Uncertainty Principle; *i.e.*, we have

$$\left(\int_{\mathbb{R}} x^2 |G_{\alpha}(x)|^2 dx\right)^{\frac{1}{2}} \left(\int_{\mathbb{R}} \xi^2 |\widehat{G_{\alpha}}(\xi)|^2 d\xi\right)^{\frac{1}{2}} = \frac{1}{4\pi} ||G_{\alpha}||_{L^2}^2$$

(1) Using some changes of variable and Corollary ??, show that it is sufficient to prove the case of $\alpha = \pi$; i.e., that

$$||XG_{\pi}||_{2}^{2} = \frac{1}{4\pi} ||G_{\pi}||_{2}^{2}$$

(2) Use an integration by parts argument to show that

$$||XG_{\pi}||_{2}^{2} = \int_{\mathbb{R}} x^{2} e^{-2\pi x^{2}} dx = \frac{1}{4\pi} ||G_{\pi}||_{2}^{2}$$

Exercise 5. The point of this exercise is to show that f and \hat{f} cannot both be compactly supported.

(1) Show that, if f has compact support, then its Fourier transform

$$\hat{f}(z) = \int_{\mathbb{R}} f(x) e^{-2\pi i x z} dx$$

can be extended to a holomorphic function of $z \in \mathbb{C}$.

- (2) Use this to show that the set $\{z : \hat{f}(z) = 0\}$ must be discrete.
- (3) Deduce a contradiction from the assumption that \hat{f} is compactly supported on \mathbb{R} .

Exercise 6. Let

$$\Delta = \frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} + \dots + \frac{\partial^2}{\partial x_d^2}$$

be the Laplacian operator on \mathbb{R}^d . Show that

$$\widehat{\Delta f}(\xi) = -4\pi^2 |\xi|^2 \widehat{f}(\xi)$$