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Hermite/Laguerre-Gaussian Modes & Lower Bounds for Quasimodes of Semiclassical Operators

A dissertation submitted in partial satisfaction
of the requirements for the degree
Doctor of Philosophy in Mathematics

by

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The dissertation of Michael James VanValkenburgh is approved.

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Publications

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Abstract of the Dissertation

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Professor Michael Hitrik, Chair

In the first part of the dissertation, we are concerned with local lower bounds for (i) quasimodes of semiclassical Schrödinger operators on domains with boundary and for (ii) Bargmann transforms of certain functions. On domains with boundary, the main tool is a boundary Carleman estimate, essentially due to Lebeau and Robbiano. It is more elementary to prove lower bounds for Bargmann transforms, since Bargmann transforms map to weighted spaces of holomorphic functions.

In the second part of the dissertation, we study the manipulation of Hermite-Gaussian modes and Laguerre-Gaussian modes for use in laser physics, building on the work of Calvo and Picón. Specifically, we classify the self-adjoint extensions of Calvo and Picón's operators, and we study the associated unitary propagators using methods from semiclassical analysis.

CHAPTER 1

Introduction

Each of the following chapters has its own introduction, and each may be read independently of the others. However, for convenience, we further condense the dissertation's main results into this global introduction.

The work presented here addresses two unrelated problems, although there are some overlapping techniques. In the first part, Chapters 2 and 3, we are concerned with local lower bounds for quasimodes of semiclassical Schrödinger operators on domains with boundary (Chapter 2) and for Bargmann transforms of certain functions (Chapter 3). On domains with boundary the main tool is a boundary Carleman estimate used in varying forms by Lebeau and Robbiano [LR95] and Burq [Bur98], [Bur02]. Since a proof of the relevant estimate is not explicitly given in the literature, we provide a full proof (modeled after that of Lebeau and Robbiano) in Appendix A. On the other hand, it is more elementary to prove lower bounds for Bargmann transforms, since Bargmann transforms map to weighted spaces of holomorphic functions; hence we may use complex-analytic techniques. In the second part of the dissertation, Chapters 4, 5, and 6, we study the manipulation of Hermite-Gaussian modes and Laguerre-Gaussian modes for use in laser physics, building on the work of Calvo and Picón [CP08]. Specifically, we classify the self-adjoint extensions of Calvo and Picón's operators, and we study the associated unitary propagators using methods from semiclassical analysis. The Weierstrass $\wp$-function plays a role in this work, and we include

Appendix B for the necessary background.

In Chapter 2, we prove quantitative unique continuation results for the semiclassical Schrödinger operator on smooth, bounded domains. These take the form of exponentially decreasing (in h) local lower bounds for exponentially precise quasimodes. We also show that these lower bounds are sharp in h, and that, moreover, the hypothesized quasimode accuracy is also sharp. To be more precise, while still referring to the introduction of Chapter 2 for further details, we consider a smooth bounded domain $\Omega \subset \mathbb{R}^n$, a semiclassical Schrödinger operator $P(h)$ on Ω, and a uniformly bounded spectral parameter $E(h)$. For $\beta > 0$ and $h_0 > 0$, we say that $u = u(\cdot\,; h)$, with $||u||_{L^2(\Omega)} = 1$, is a (β, h_0)-exponentially precise quasimode of $P(h)$ if

$$||(P(h) - E(h))u||_{L^2(\Omega)} = \mathcal{O}(e^{-\beta/h})$$

for all $h \in (0, h_0)$. The main results of Chapter 2 are then the following theorems:

Theorem 1.1. *Let ω be an open subset of Ω. Then there exist constants $C > 0$, $\alpha > 0$, $h_0 > 0$, and $\beta_0 > 0$ such that*

$$Ce^{-\alpha/h} \leq ||u(\cdot\,; h)||_{L^2(\omega)}$$

for all (β, h_0)-exponentially precise quasimodes u with $\beta > \beta_0$.

Theorem 1.2. *Let $\Gamma \subset \partial\Omega$ be a connected component of the boundary of Ω. Then there exist constants $C > 0$, $\alpha > 0$, $h_0 > 0$, and $\beta_0 > 0$ such that*

$$Ce^{-\alpha/h} \leq ||hNu(\cdot\,; h)||_{L^2(\Gamma)}$$

for all (β, h_0)-exponentially precise quasimodes u with $\beta > \beta_0$. (Here Nu denotes the normal derivative of u.)

In Chapter 3, we study local lower bounds for the Bargmann transform and give applications to quasimodes of elliptic semiclassical pseudodifferential operators and to functions with limited smoothness. We use the conventions such that the Bargmann transform is defined for $u \in \mathcal{S}'(\mathbb{R}^n)$, $z \in \mathbb{C}^n$, by

$$Tu(z;h) = (\pi h)^{-3n/4} \int e^{i\phi(z,y)/h} u(y)\, dy$$

with

$$\phi(z,y) = i\left(\frac{z^2}{2} + \frac{y^2}{2} - \sqrt{2}\, zy\right).$$

Our main result is then the following (essentially complex-analytic) theorem, which, for greater flexibility, we state for a general semiclassical indexing set.

Theorem 1.3. *Let $H \subset (0,1]$, $0 \in \overline{H}$, and let $u(\cdot\,;h) \in L^2(\mathbb{R}^n)$ for $h \in H$. Assume that there exist constants $h_{00} > 0$, $c_{00} > 0$, $\beta \geq 0$ and some compact set $K \subset\subset \mathbb{C}^n$ such that*

$$c_{00} e^{-\beta/h} ||u(\cdot\,;h)||_{L^2(\mathbb{R}^n)} \leq ||Tu(\cdot\,;h)||_{L^\infty(K)} \quad \forall h \in (0, h_{00}) \cap H.$$

Then for any open set $\omega \subset \mathbb{C}^n$ there exist constants $\alpha > 0$, $c_0 > 0$, and $h_0 > 0$ such that

$$c_0 e^{-\alpha/h} ||u(\cdot\,;h)||_{L^2(\mathbb{R}^n)} \leq ||Tu(\cdot\,;h)||_{H_\Phi(\omega)} \quad \forall h \in (0, h_0) \cap H.$$

We then turn to problems in laser physics, initially inspired by J. B. Rosenzweig's talk entitled "Accelerator Physics: New Light Sources and Medical Imaging Techniques." Recent developments in laser physics have called renewed attention to Laguerre-Gaussian beams of paraxial light [ABP03], and in Chapter 4 we give an original treatment of the corresponding Laguerre-Gaussian modes for the two-dimensional harmonic oscillator, which appear in the transversal plane at the laser beam's waist. We see how they arise as Wigner transforms of Hermite-Gaussian modes, and we proceed to find a closed form for their own Wigner transforms, providing an alternative to the methods of Simon and Agarwal [SA00]. Our main observation is that the Wigner transform intertwines the creation and annihilation operators for the two classes of modes.

In Chapter 5, we build on recent work of the physicists Gabriel F. Calvo and Antonio Picón [CP08]. Calvo and Picón defined a class of operators, for use in quantum communication, that allows arbitrary manipulations of the three lowest two-dimensional Hermite-Gaussian modes $\mathcal{H}_{\mathcal{T}} = \{|0,0\rangle, |1,0\rangle, |0,1\rangle\}$. Our work continues the study of those operators, and our results fall into two categories. For one, we show that the generators of the operators have infinite deficiency indices, and we explicitly describe all self-adjoint realizations. And secondly we investigate semiclassical approximations of the propagators. The basic method is to start from a semiclassical Fourier integral operator ansatz and then construct approximate solutions of the corresponding evolution equations. In doing so, we give a complete description of the Hamilton flow, which in most cases is given by elliptic functions; the necessary background is given in Appendix B. We find that the semiclassical approximation behaves well when acting on sufficiently localized initial conditions, for example, finite sums of semiclassical Hermite-Gaussian modes, since near the origin the Hamilton trajectories trace out the bounded components of elliptic curves.

In Chapter 6, we continue the study, from a semiclassical viewpoint, of Calvo and Picón's operators, as manipulating photon states in quantum communication. In the preceding chapter, we defined a one-dimensional model operator and studied it analytically before moving on to Calvo and Picón's full two-dimensional operators. In Chapter 6, we show how the one-dimensional operator may also be useful as an experimental model, since it allows manipulations of two-dimensional

Laguerre-Gaussian modes; the intensity distributions (in physical space) of the Laguerre-Gaussian modes then approximately flow along the elliptic curves studied earlier. Since the Wigner transform is fundamental in the study of Laguerre-Gaussian modes, we give a slightly expanded treatment of the Wigner transform in the context of Calvo and Picón's work.

CHAPTER 2

Exponential Lower Bounds for Quasimodes of Semiclassical Schrödinger Operators

2.1 Introduction

In this chapter we establish quantitative unique continuation results for the semiclassical Schrödinger operator on smooth, compact domains. We consider a smooth, open, bounded, and connected domain $\Omega \subset \mathbb{R}^n$, and we let $G = (g^{ij}) \in C^\infty(\overline{\Omega})^{n^2}$ be a positive definite symmetric matrix with real entries. Then, with Δ denoting the "Laplacian" associated to this matrix,

$$\Delta = \sum_{i,j} \partial_{x^i}\, g^{ij}(x)\ \partial_{x^j},$$

and with $V \in C^\infty(\overline{\Omega}, \mathbb{R})$ as our potential, we take as our Schrödinger operator

$$P(h) := -h^2 \Delta + V.$$

For simplicity, we will only consider the Dirichlet realization of P; that is, we will only allow P to act on the domain

$$\mathcal{D}(P) := H^2(\Omega) \cap H^1_0(\Omega)$$

corresponding to "zero boundary conditions". Our unique continuation results will take the form of local L^2 lower bounds for certain quasimodes of this operator.

For a uniformly bounded spectral parameter

$$E(h) \in [a,b], \quad \text{for some } -\infty < \min V \leq a \leq b < \infty,$$

and for some $\beta > 0$ and $h_0 > 0$, we consider (β, h_0)-exponentially precise quasimodes of $P(h)$:

$$u(\cdot\,; h) \in \mathcal{D}(P) \quad \text{such that} \quad \begin{cases} ||u||_{L^2(\Omega)} = 1, & \text{and} \\ ||(P(h) - E(h))u||_{L^2(\Omega)} = \mathcal{O}(e^{-\beta/h}) \end{cases}$$

for all $h \in (0, h_0)$. Throughout this chapter we allow $\beta = \infty$, which corresponds to exact eigenfunctions.

The following theorems are our main results:

Theorem 2.1. *Let ω be an open subset of Ω. Then there exist constants $C > 0$, $\alpha > 0$, $h_0 > 0$, and $\beta_0 > 0$ such that*

$$Ce^{-\alpha/h} \leq ||u(\cdot\,; h)||_{L^2(\omega)}$$

for all (β, h_0)-exponentially precise quasimodes u with $\beta > \beta_0$.

Theorem 2.2. *Let $\Gamma \subset \partial\Omega$ be a connected component of the boundary of Ω. Then there exist constants $C > 0$, $\alpha > 0$, $h_0 > 0$, and $\beta_0 > 0$ such that*

$$Ce^{-\alpha/h} \leq ||hNu(\cdot\,; h)||_{L^2(\Gamma)}$$

for all (β, h_0)-exponentially precise quasimodes u with $\beta > \beta_0$.

Here, as in the rest of the chapter, n denotes the outward unit normal,

$$\nabla^i = \sum_j (G^{1/2})^{ij} \partial_{x^j}, \qquad \text{and } N = \sum_{i,j} n_i g^{ij} \partial_{x^j}.$$

We will give simple examples showing that these lower bounds are sharp in h. Moreover, in both theorems the quasimode accuracy is also sharp; that is, we will show that there are $\mathcal{O}(e^{-\beta/h})$ quasimodes for which the theorems do not hold, when $\beta > 0$ is relatively small.

Despite the fact that the statements of our results are rather simple and natural, they do not seem to be treated in the literature, at least not in this context. We therefore believe that a short, explicit proof could be useful. Results of this type, stated as "doubling properties" of eigenfunctions of the Laplacian on Riemannian manifolds, with or without boundary, have been proven by Donnelly and Fefferman [DF88], [DF90]. Their Carleman estimate (or "quantitative Aronszajn inequality") is different from the one used here (Theorem 2.3), and it is valid for Lipschitz metrics on smooth, closed manifolds, which allows them to use the estimate after reflecting across the boundary. Jerison and Lebeau further studied "doubling properties", but for *sums* of eigenfunctions of the Laplacian [JL99]. Moreover, we were particularly inspired by Theorem 7.6 in the course notes of Evans and Zworski, which gives exponential estimates from below for certain semiclassical Schrödinger operators on $\mathbb{R}^n$ that are elliptic at infinity [EZ07].

The basic tool in this chapter is a boundary Carleman estimate, which we now describe.

Let Ω_0 and $G_0 = (g_0^{ij})$ be temporary placeholders for Ω and $G = (g^{ij})$. Then our semiclassical Schrödinger operator has principal symbol (in the sense of h-differential operators)

$$p(x,\xi) = \sum_{i,j} \xi_i \, g_0^{ij}(x) \, \xi_j + V, \quad (x,\xi) \in \overline{\Omega_0} \times \mathbb{R}^n,$$

and for $\varphi \in C^\infty(\overline{\Omega_0}, \mathbb{R})$ we let

$$p_\varphi(x,\xi) := p(x, \xi + i\varphi'_x), \tag{2.1}$$

which is the leading semiclassical symbol of the conjugated operator

$$P_\varphi := e^{\varphi/h} \circ P \circ e^{-\varphi/h}.$$

This operator is given explicitly by

$$P_\varphi = \sum_{i,j} (hD_{x^i} + i\varphi'_{x^i}) \circ g_0^{ij}(x) \circ (hD_{x^j} + i\varphi'_{x^j}) + V, \qquad D_x = \frac{1}{i}\partial_x.$$

Now suppose that φ is a Carleman weight, meaning that $\varphi \in C^\infty(\overline{\Omega_0}, \mathbb{R})$ and that

$$p_\varphi(x,\xi) = E(h) \Rightarrow \frac{1}{i}\{\overline{p_\varphi}, p_\varphi\}(x,\xi) \geq c > 0 \tag{2.2}$$

uniformly with respect to h, for some constant $c > 0$. Here we are using the Poisson bracket, given, for $f, g \in C^\infty$, by

$$\{f,g\} := \sum_{j=1}^{n} \left(\frac{\partial f}{\partial \xi_j} \frac{\partial g}{\partial x^j} - \frac{\partial f}{\partial x^j} \frac{\partial g}{\partial \xi_j} \right).$$

With this set-up, we have the following boundary Carleman estimate, which may be found as Proposition 3.2 of Burq's paper [Bur02]. (We give a complete proof in Appendix A.)

Theorem 2.3. *Let Γ be a union of connected components of $\partial\Omega_0$, and let φ be a Carleman weight on $\overline{\Omega_0}$ such that $\nabla\varphi \neq 0$ on Ω_0 and such that $N\varphi\Big|_{\partial\Omega_0} \neq 0$. If $N\varphi\Big|_{\Gamma} < 0$, then there exist constants $c > 0$ and $h_1 > 0$ such that*

$$\int_{\Omega_0} |(P_\varphi(h) - E(h))f|^2 + h \int_{\partial\Omega_0 \setminus \Gamma} \left\{ |f|^2 + |h\nabla f|^2 \right\} \\ \geq ch \int_{\Omega_0} \left\{ |f|^2 + |h\nabla f|^2 \right\}$$

for every $h \in (0, h_1)$ and every $f \in C^\infty(\overline{\Omega_0})$ with $f|_\Gamma \equiv 0$.

Remark 2.4. Estimates of this type, and their application to unique continuation problems, have a long, distinguished history. Hörmander's classic text [Hor63] contains a systematic treatment of such estimates in the boundary-less case. The estimates up to the boundary were originally proven by Lebeau and Robbiano in the case when $V \equiv 0$ and $E(h) \equiv 0$ [LR95], and Burq later observed that their proof extends to more general operators, including semiclassical Schrödinger operators of the type considered here [Bur02]. In all cases, the proof uses a partition of unity to reduce to local results; in the presence of the boundary, a change of variables is then applied to locally straighten the boundary segment. This is possible because the induced error terms do not affect the estimate (but possibly taking a smaller $h_1 > 0$).

Moreover, Theorem 2.3 may be generalized to a more useful form–the form used in this chapter–due to the fact that it is at heart a local result. If the function f vanishes in a neighborhood of some boundary component Γ_0, then the result still holds, even if the condition $N\varphi\Big|_{\Gamma_0} \neq 0$ fails to hold. For completeness, we give the full proof in Appendix A.

A central problem in the use of Carleman estimates is the construction of suitable Carleman weights, and a classical technique is to convexify a function which has no critical points (see, for example, [Hor63], p.205, and [Bur98]). In the proof of Theorem 2.1 we put the critical points inside the set ω, then apply the Carleman estimate to the complement of ω. In the proof of Theorem 2.2, we use two Carleman weights with a certain compatibility condition that allows us to piece together two Carleman estimates; this follows a method of Burq [Bur98].

As pointed out by the referee of our paper [Van09a], our method for constructing Carleman weights is similar to that used by Chae, Imanuvilov, and Kim in the context of control theory [CIK96]. For a connected bounded domain $\Omega \subset \mathbb{R}^n$

with boundary $\partial\Omega \in C^2$, they construct and then convexify a function $\psi \in C^2(\overline{\Omega})$ which vanishes on $\partial\Omega$ and has its critical points in a given fixed subdomain of Ω. In our case, however, it is important that the normal derivatives of ψ on connected components of $\partial\Omega$ have predetermined signs, and we do not need ψ to vanish on $\partial\Omega$.

We prove Theorems 2.1 and 2.2 in Sections 2.2 and 2.3, respectively, where we also give remarks on the sharpness of the estimates.

From now on we will omit "(h)" where the h-dependence is obvious. And in stating estimates we sometimes find it convenient to write $X \lesssim Y$ or $Y \gtrsim X$ whenever $X \leq CY$ for some constant $C > 0$, which could possibly depend on n, the dimension of Ω.

2.2 A Local Lower Bound

In proving Theorem 2.1 we begin with a useful elliptic estimate:

Proposition 2.5. *Let χ, $u \in C^\infty(\overline{\Omega}, \mathbb{C})$. Then*

$$h^2 \int |\chi|^2 |\nabla u|^2 \lesssim \int_{supp\chi} (|(P - E(h))u|^2 + |u|^2) + h^2 \int_{\partial\Omega} |\chi|^2 |uNu|$$

for all h small enough.

Proof. The first part of the proof is an integration by parts:

$$\begin{aligned}\int \Big((P - E(h))u\Big)\, \overline{u}|\chi|^2 &= h^2 \int \nabla u \cdot \nabla(\overline{u}|\chi|^2) - h^2 \int_{\partial\Omega} \overline{u}|\chi|^2 N u \\ &\qquad + \int (V - E(h))|\chi u|^2 \\ &= h^2 \int |\chi|^2 |\nabla u|^2 + 2h^2 \int \overline{u} \nabla u \cdot \mathrm{Re}\,(\overline{\chi} \nabla \chi) \\ &\qquad - h^2 \int_{\partial\Omega} \overline{u}|\chi|^2 N u + \int (V - E(h))|\chi u|^2.\end{aligned}$$

Then, by elementary estimates,

$$\begin{aligned}
h^2 \int |\chi|^2 |\nabla u|^2 &\lesssim \int |\chi(P-E(h))u|^2 + \int |\chi u|^2 \\
&\qquad + h^2 \int_{\partial\Omega} |\chi|^2 |uNu| + h^2 \int |u\nabla\chi||\chi\nabla u| \\
&\lesssim \int |\chi(P-E(h))u|^2 + \int (|\chi|^2 + |\nabla\chi|^2)|u|^2 \\
&\qquad + h^2 \int_{\partial\Omega} |\chi|^2 |uNu| + h^4 \int |\chi|^2 |\nabla u|^2.
\end{aligned}$$

We absorb the last term on the right side into the left side to conclude the proof. □

We can apply Proposition 2.5 to quasimodes with "zero boundary conditions". These necessarily belong to the domain of (the Dirichlet realization of) P, which is

$$\mathcal{D}(P) := H^2(\Omega) \cap H^1_0(\Omega).$$

Hence the computations in the preceding proof are still justified. We can equip this set of functions with semiclassical norms; for instance, in the following lemma we control the semiclassical Sobolev norm H^1_h, given by

$$||u||_{H^1_h} := \left(\int (|u|^2 + |h\nabla u|^2) \right)^{1/2}.$$

Lemma 2.6. *Let $u \in H^2(\Omega) \cap H^1_0(\Omega)$ be such that*

$$||(P-E(h))u||_{L^2(\Omega)} = \mathcal{O}(f(h))||u||_{L^2(\Omega)}$$

for some function $f \geq 0$. Also let ω, $\tilde{\omega}$ be open subsets of Ω such that $\tilde{\omega} \subset\subset \omega \subset\subset \Omega$. Then

$$||u||_{H^1_h(\tilde{\omega})} \lesssim ||u||_{L^2(\omega)} + \mathcal{O}(f(h))||u||_{L^2(\Omega)}.$$

Proof. Let $\chi \in C^\infty(\overline{\Omega})$ be such that $0 \le \chi \le 1$, $\chi \equiv 1$ on $\tilde{\omega}$, and such that $\operatorname{supp}\chi \subset \omega$. Then, by Proposition 2.5, we have

$$\begin{aligned} ||u||^2_{H^1_h(\tilde{\omega})} &= \int_{\tilde{\omega}} \left[|u|^2 + |h\nabla u|^2\right] \\ &\lesssim \int_{\tilde{\omega}} |u|^2 + \int_{\operatorname{supp}\chi} (|(P - E(h))u|^2 + |u|^2) \\ &\lesssim ||u||^2_{L^2(\omega)} + \mathcal{O}(f(h)^2)||u||^2_{L^2(\Omega)}. \end{aligned}$$

□

We now construct a Carleman weight in the standard way: by "convexifying" a function which has no critical points, an idea that goes back at least to Hörmander's classic book ([Hor63], p.205). Moreover, we will find a Carleman weight whose outward normal derivative is negative everywhere on $\partial\Omega$, so that in using the Carleman estimate, Theorem 2.3, we may discard the boundary term.

It is convenient to start with a Morse function–that is, a smooth real-valued function on Ω having no degenerate critical points. For this we may first take *any* $\psi_{00} \in C^\infty(\overline{\Omega})$ with $N\psi_{00}|_{\partial\Omega} < 0$. We then smoothly extend it to a neighborhood of $\overline{\Omega}$, and approximate the extension by a Morse function ψ_0 in the C^1 topology, so that $N\psi_0|_{\partial\Omega} < 0$. We can do this because, for any smooth manifold X, Morse functions are dense in $C^\infty(X, \mathbb{R})$ (see, for instance, [GG73]). Moreover, we choose ψ_0 to be non-negative on $\overline{\Omega}$, simply by adding a sufficiently large constant.

Now let $x_1, \ldots, x_N$ be the (necessarily finitely many) critical points of ψ_0 on $\overline{\Omega}$; we then know that they are away from $\partial\Omega$. Also let ω_0 be an open subset of Ω such that $\omega_0 \subset\subset \Omega$.

Lemma 2.7. *There exists a diffeomorphism $\varkappa : \overline{\Omega} \to \overline{\Omega}$ such that $\varkappa(x) = x$ near $\partial\Omega$ and such that $\varkappa(x_j) \in \omega_0\ \forall j$.*

Proof. For each x_j we take a simple smooth curve $\gamma_j : [0,1] \mapsto \Omega$ such that $\gamma_j(0) = x_j$ and $\gamma_j(1) \in \omega_0$. We may choose the curves such that the $\gamma_j([0,1])$ are pairwise disjoint. Let N_j be a neighborhood of $\gamma_j([0,1])$ such that the N_j are pairwise disjoint.

We take a C^∞ vector field X_j such that $X_j(\gamma_j(t)) = \gamma_j'(t)\ \forall t \in [0,1]$ and such that X_j is zero outside of N_j.

Since X_j is a compactly supported C^∞ vector field, it induces a flow which fixes $\overline{\Omega} \cap \complement N_j$ and which induces a diffeomorphism $\varkappa_j$ of $\overline{\Omega}$, the time 1 flow of X_j, taking x_j into ω_0. Then $\varkappa := \varkappa_1 \circ \cdots \circ \varkappa_N$ is the desired diffeomorphism. $\square$

Let $\psi := \psi_0 \circ \varkappa^{-1}$. Then ψ has finitely many critical points, all of which are contained in ω_0, and $N\psi\Big|_{\partial\Omega} < 0$.

Finally, let

$$\varphi := e^{\gamma\psi},$$

where $\gamma > 0$ is to be determined.

Proposition 2.8. *For γ large enough, φ is a Carleman weight on $\overline{\Omega}\backslash\omega_0$.*

Proof. We have $\varphi' = \gamma e^{\gamma\psi}\psi'$, $\varphi'' = e^{\gamma\psi}(\gamma^2\psi'{}^t\psi' + \gamma\psi'')$, and $p_\varphi = E(h)$ implies that ${}^t\xi G\varphi' = 0$ and ${}^t\xi G\xi + V = {}^t\varphi' G\varphi' + E(h)$. Hence

$$p_\varphi = E(h) \quad \text{implies} \quad |\xi| \leq C\gamma e^{\gamma\psi} \tag{2.3}$$

where the bound is independent of h, as $E(h) \in [a, b]$. We now compute

$$\begin{aligned}
\{\mathrm{Re} p_\varphi, \mathrm{Im} p_\varphi\} &= 4^t\xi G\varphi'' G\xi + 4^t\varphi' G\varphi'' G\varphi' + 2G'(\varphi', \varphi', G\varphi') \\
&\quad + 4G'(\varphi', \xi, G\xi) - 2G'(\xi, \xi, G\varphi') + 2\{V, {}^t\varphi' G\xi\} \\
&= 4e^{\gamma\psi}\gamma^t\xi G\psi'' G\xi + 4e^{3\gamma\psi}(\gamma^4({}^t\psi' G\psi')^2 + \gamma^{3t}\psi' G\psi'' G\psi') \\
&\quad + 2e^{3\gamma\psi}\gamma^3 G'(\psi', \psi', G\psi') + 4\gamma e^{\gamma\psi} G'(\xi, \psi', G\xi) \\
&\quad - 2\gamma e^{\gamma\psi} G'(\xi, \xi, G\psi') + 2\gamma e^{\gamma\psi}\{V, {}^t\psi' G\xi\} \\
&= 4e^{3\gamma\psi}(\gamma^4({}^t\psi' G\psi')^2 + O(\gamma^3)) - 2\gamma e^{\gamma\psi t} V' G\psi'.
\end{aligned}$$

where in the last line we have used (2.3). Since $|\psi'| > 0$ in $\overline{\Omega}\backslash\omega_0$, and since G is of course positive definite, the γ^4 term dominates the γ^3 term when γ is sufficiently large. The term with the potential is also dominated, since we have chosen $\psi \geq 0$ for this very purpose. Hence φ is a Carleman weight on $\overline{\Omega}\backslash\omega_0$ for $\gamma > 0$ large enough. $\square$

Proof. (of Theorem 2.1.) Let ω_0, ω_1, and ω_2 be open subsets of Ω such that $\omega_0 \subset\subset \omega_1 \subset\subset \omega_2 \subset\subset \omega$, where the critical points of our chosen Carleman weight are in ω_0 as above.

Let $\chi \in C^\infty(\overline{\Omega})$ be such that $0 \leq \chi \leq 1$ and

$$\chi \equiv \begin{cases} 0 & \text{near } \overline{\omega_1} \\ 1 & \text{near } \complement\omega_2. \end{cases}$$

Let

$$M_1 := \max_{\overline{\Omega}\backslash\omega_1} \varphi, \qquad M_2 := \max_{\overline{\omega_2}\backslash\omega_1} \varphi, \qquad \text{and} \qquad m := \min_{\overline{\Omega}\backslash\omega_1} \varphi$$

and note that $M_2 > m$ when φ is our chosen Carleman weight.

Using our chosen weight φ we apply the boundary Carleman estimate (Theorem 2.3) to $f = e^{\varphi/h}\chi u$ on $\overline{\Omega}\backslash\omega_0$, with $\Gamma = \partial\Omega$ and where we use the fact that

χ vanishes near $\partial\omega_0$ (see Remark 2.4):

$$
\begin{aligned}
ch^{1/2}||e^{\varphi/h}\chi u||_{L^2(\Omega)} &\leq ||e^{\varphi/h}(P-E(h))\chi u||_{L^2(\Omega)} \\
&= ||e^{\varphi/h}[P,\chi]u + e^{\varphi/h}\chi(P-E(h))u||_{L^2(\Omega)} \\
&\lesssim he^{M_2/h}||u||_{H_h^1(\omega_2)} + e^{(M_1-\beta)/h} \\
&\lesssim he^{M_2/h}(||u||_{L^2(\omega)} + e^{-\beta/h}) + e^{(M_1-\beta)/h}.
\end{aligned}
$$

We have used Lemma 2.6 in the last step.

Hence

$$
\begin{aligned}
e^{m/h}||\chi u||_{L^2(\Omega)} &\lesssim h^{1/2}e^{(M_2-\beta)/h} + h^{1/2}e^{M_2/h}||u||_{L^2(\omega)} + h^{-1/2}e^{(M_1-\beta)/h} \\
&\lesssim e^{(M_2-\beta)/h} + e^{M_2/h}||u||_{L^2(\omega)} + h^{-1/2}e^{(M_1-\beta)/h}
\end{aligned}
$$

which gives, with $\alpha := M_2 - m > 0$,

$$
\begin{aligned}
1 &\lesssim ||\chi u||_{L^2(\Omega)} + ||u||_{L^2(\omega)} \\
&\lesssim e^{(\alpha-\beta)/h} + e^{\alpha/h}||u||_{L^2(\omega)} + ||u||_{L^2(\omega)} + h^{-1/2}e^{(M_1+\alpha-M_2-\beta)/h} \\
&\lesssim e^{(\alpha-\beta)/h} + e^{\alpha/h}||u||_{L^2(\omega)} + h^{-1/2}e^{(M_1+\alpha-M_2-\beta)/h}.
\end{aligned}
$$

That is,

$$
e^{-\alpha/h} - e^{-\beta/h} - h^{-1/2}e^{(M_1-M_2-\beta)/h} \lesssim ||u||_{L^2(\omega)}.
$$

proving the result for quasimodes of accuracy $\mathcal{O}(e^{-\beta/h})$, with, say,

$$
\beta > \alpha + \max_{\overline{\Omega}\setminus\omega_1}\varphi - \max_{\overline{\omega_2}\setminus\omega_1}\varphi =: \beta_0 \ (\geq \alpha). \tag{2.4}
$$

$\square$

Remark 2.9. Theorem 2.1 is sharp in h, both in terms of the quasimode accuracy and in terms of the lower bound. For the former, we consider quasimodes in the case where Agmon estimates are relevant; we construct these quasimodes by simply multiplying an eigenfunction by a suitable cutoff function. To be precise, we let $E \in \mathbb{R}$ and let V be a potential such that the compact set (the classically allowed region)

$$K := \{x \in \overline{\Omega};\ V(x) \leq E\}$$

is non-empty and is contained in Ω; hence the classically forbidden region

$$\{x \in \overline{\Omega};\ V(x) > E\} \neq \emptyset$$

contains a neighborhood of $\partial\Omega$. We then let $\chi \in C_0^\infty(\Omega)$ be such that $\chi = 1$ near K. Then $\mathrm{supp}\nabla\chi \subset \{x \in \Omega;\ V(x) > E\}$. We then consider a family of Dirichlet eigenfunctions $u(\cdot\,; h)$ such that

$$\begin{cases} Pu = (E + \lambda(h))u, & \\ ||u||_{L^2(\Omega)} = 1, & \text{and} \\ \lambda(h) \to 0 & \text{as } h \to 0. \end{cases}$$

Then

$$[-h^2\Delta, \chi]u = -h^2(\Delta\chi)u - 2h^2\nabla\chi \cdot \nabla u$$

and hence

$$\begin{aligned} ||(P - E - \lambda(h))(\chi u)||_{L^2(\Omega)} &\leq h^2||(\Delta\chi)u||_{L^2(\Omega)} + 2h^2||\nabla\chi \cdot \nabla u||_{L^2(\Omega)} \\ &\leq Ch^2(||u||_{L^2(\mathrm{supp}\nabla\chi)} + ||\nabla u||_{L^2(\mathrm{supp}\nabla\chi)}) \\ &\leq Ch^2(e^{-\epsilon/h} + ||\nabla u||_{L^2(\mathrm{supp}\nabla\chi)}) \end{aligned}$$

for some $\epsilon > 0$, as given by Agmon estimates (see, for example, the book of Dimassi and Sjöstrand [DS99] or that of Helffer [Hel88]). We now let U be an open set containing $\mathrm{supp}\nabla\chi$ and such that $\overline{U}$ is contained in the interior of the classically forbidden region. Then Lemma 2.6, combined with another Agmon estimate, gives (possibly with a different $\epsilon > 0$)

$$\begin{aligned} ||(P - E - \lambda(h))(\chi u)||_{L^2(\Omega)} &\lesssim h^2 e^{-\epsilon/h} + h||u||_{L^2(U)} \\ &\lesssim h^2 e^{-\epsilon/h} + he^{-\epsilon/h} \end{aligned} \tag{2.5}$$

for all $h > 0$ sufficiently small. Moreover, these same Agmon estimates show that

$$||\chi u||_{L^2(\Omega)} = 1 - \mathcal{O}(e^{-\delta/h})$$

for some $\delta > 0$ and for all $h > 0$ sufficiently small. Hence χu can be renormalized without affecting the estimate (2.5), thus resulting in a normalized quasimode which vanishes in an open set.

In summary, for $e^{-\beta/h}$ quasimodes, with β sufficiently large, we have our lower bound. But there are *other* $e^{-\epsilon/h}$ quasimodes (with $\epsilon > 0$ related to the Agmon metric) which vanish identically in an h-independent open subset whose closure is contained in the interior of the classically forbidden region.

Moreover, from this discussion of Agmon estimates, it is clear that the lower bound in Theorem 2.1 is sharp in h.

Remark 2.10. It may be possible to extend the proof to smooth, compact, connected, and oriented Riemannian manifolds, with or without boundary. For example, if M is such a manifold without boundary, we let $\omega_0 \subset M$ be open. As before, let $\psi \in C^\infty(M)$ be a nonnegative Morse function such that $\nabla\psi \neq 0$ on $M \backslash \omega_0$. Then $\varphi := e^{\gamma\psi}$, with $\gamma >> 1$, is a Carleman weight on $M \backslash \omega_0$, so we can apply the interior Carleman estimate on $M \backslash \omega_0$ (see Remark 2.4).

We again have that the result is sharp in terms of h, as the following concrete example shows. On the sphere S^2, with usual spherical coordinates

$$(x_1, x_2, x_3) = (\sin\theta\cos\varphi, \sin\theta\sin\varphi, \cos\theta),$$

we consider the functions

$$f_n(\theta, \varphi) = (\sin\theta)^n(\cos\varphi + i\sin\varphi)^n.$$

These are called "zonal harmonics".

Then, letting Δ denote the spherical Laplacian,

$$\Delta = \frac{\partial^2}{\partial\theta^2} + \frac{\cos\theta}{\sin\theta}\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2},$$

we get

$$-\Delta f_n = n(n+1)f_n.$$

We must now study the norm of f_n:

$$\begin{aligned}\int_{S^2}|f_n|^2 &= 4\pi\int_0^1(1-x^2)^n dx = 2\pi\int_0^1(1-t)^n t^{-1/2}dt \\ &= 2\pi B(\frac{1}{2}, n+1) \\ &= 4^{n+1}\pi\frac{(n!)^2}{(2n+1)!} \\ &\approx \frac{4\pi^{3/2}n^{1/2}}{2n+1},\end{aligned}$$

where

$$B(\frac{1}{2}, n+1) = 2\Big(\frac{2\times 4\times 6...(2n)}{1\times 3\times 5...(2n+1)}\Big)$$

is a so-called beta function. The important point is that we get some power of n, which is inconsequential against an exponential factor.

Now for local estimates, we have

$$\int_\omega |f_n|^2 dS = \iint_\omega |\sin\theta|^{2n+1}d\theta d\varphi.$$

If we are looking at a set ω where, say, $(0 \le)\sin\theta \le e^{-1}$, we get

$$\int_\omega |f_n|^2 dS \lesssim e^{-2n}.$$

With $h^{-2} := n(n+1)$ and letting F_h denote the corresponding *normalized* eigenfunction, we get that

$$||F_n||_{L^2(\omega)} \lesssim e^{-\alpha/h}$$

for some $\alpha > 0$ for all $h > 0$ small enough.

2.3 A Lower Bound for Normal Derivatives

We now turn to the proof of Theorem 2.2, where the main ideas came from a careful reading of a paper of Burq [Bur98]. Thus, following Burq, we will use "compatible Morse functions", as constructed in the following proposition, whose proof can be found in [Bur98], Appendix A. We are allowing $\Gamma = \partial\Omega$, in which case some of the conditions are void. In any case, we take Γ to be a connected component of $\partial\Omega$.

Proposition 2.11. *There exist Morse functions ψ_1, ψ_2 on a neighborhood of $\overline{\Omega}$ such that*

$$N\psi_i\Big|_{\partial\Omega\setminus\Gamma} < 0 \qquad \textit{and} \qquad N\psi_i\Big|_{\Gamma} > 0, \qquad i = 1, 2,$$

and such that, for $x \in \Omega$, we have

$$\{\nabla\psi_i(x) = 0\} \Longrightarrow \{\nabla\psi_{i+1}(x) \neq 0 \quad \textit{and} \quad \psi_{i+1}(x) > \psi_i(x)\} \qquad (\psi_3 \equiv \psi_1). \tag{2.6}$$

We call (2.6) the "compatibility condition".

Proof. (of Theorem 2.2.) Let ψ_1 and ψ_2 be compatible Morse functions, which we may assume are nonnegative. Let $\{x_{ij}\}$ be the (finitely many) critical points of ψ_i in $\overline{\Omega}$, and let $\epsilon > 0$ be small enough so that

(i) the balls $B(x_{ij}, 2\epsilon)$ are all disjoint (i and j varying) and have closures contained in Ω, and

(ii) $\psi_{i+1} > \psi_i$ on $B(x_{ij}, 2\epsilon)$ $\qquad (\psi_3 \equiv \psi_1)$.

Let $\chi_i \in C^\infty(\overline{\Omega})$, for $i = 1, 2$, be such that $0 \le \chi_i \le 1$ and such that

$$\chi_i = \begin{cases} 0 & \text{near} \quad \overline{\bigcup_j B(x_{ij}, \epsilon)} \\ 1 & \text{near} \quad \bigcap_j \complement B(x_{ij}, 2\epsilon) \cap \overline{\Omega}. \end{cases}$$

Also, let

$$\Omega_i := \overline{\Omega} \cap \bigcap_j \complement B(x_{ij}, \epsilon),$$

so that $\nabla \psi_i \neq 0$ on Ω_i.

We now let $\varphi_i := e^{\gamma \psi_i}$, with $\gamma > 0$ taken large enough so that φ_i is a Carleman weight on Ω_i, which follows from Proposition 2.8. Our boundary Carleman estimate, Theorem 2.3, applied to $f = \exp(\varphi_i/h)\, \chi_i u$ on Ω_i then gives the upper bound

$$\begin{aligned} ch \int_{\Omega_i} \Big\{ e^{2\varphi_i/h} |\chi_i u|^2 + e^{2\varphi_i/h} |\varphi_i' \chi_i u + h \nabla(\chi_i u)|^2 \Big\} \\ \le \int_{\Omega_i} e^{2\varphi_i/h} |(P - E(h))(\chi_i u)|^2 \\ + h \int_{\cup_j \partial B(x_{ij}, \epsilon) \cup \Gamma} \Big\{ |e^{\varphi_i/h} \chi_i u|^2 + |hN(e^{\varphi_i/h} \chi_i u)|^2 \Big\} \\ = \int_{\Omega_i} e^{2\varphi_i/h} |(P - E(h))(\chi_i u)|^2 \\ + h \int_\Gamma e^{2\varphi_i/h} |hN(\chi_i u)|^2. \end{aligned}$$

Together with an elementary lower bound, this gives the estimate

$$\begin{aligned} h \int_{\Omega_i} \Big\{ |\chi_i u|^2 + |h \nabla(\chi_i u)|^2 \Big\} e^{2\varphi_i/h} \\ \lesssim \int_{\mathfrak{A}_i} |[P, \chi_i] u|^2 e^{2\varphi_i/h} + h \int_\Gamma |hNu|^2 e^{2\varphi_i/h} + e^{2(M_i - \beta)/h} \end{aligned}$$

where $M_i := \max_{\Omega_i} \varphi_i$ and $\mathfrak{A}_i := \cup_j (B(x_{ij}, 2\epsilon) \backslash B(x_{ij}, \epsilon))$.

This implies that

$$\int_{\complement(\cup_j B(x_{ij},2\epsilon))\cap\Omega} \Big\{|u|^2 + |h\nabla u|^2\Big\} e^{2\varphi_i/h}$$
$$\lesssim h\int_{\mathfrak{A}_i}\Big\{|u|^2+|h\nabla u|^2\Big\}e^{2\varphi_i/h} + \int_\Gamma |hNu|^2 e^{2\varphi_i/h} + h^{-1}e^{2(M_i-\beta)/h}.$$

Adding the two estimates, for $i=1,2$, we get

$$\begin{aligned}\sum_{i=1}^2 \int_{\complement(\cup_j B(x_{ij},2\epsilon))\cap\Omega} &\Big\{|u|^2 + |h\nabla u|^2\Big\} e^{2\varphi_i/h}\\
&\lesssim \sum_{i=1}^2\Big[h\int_{\mathfrak{A}_i}\Big\{|u|^2+|h\nabla u|^2\Big\}e^{2\varphi_i/h} + \int_\Gamma |hNu|^2 e^{2\varphi_i/h} + h^{-1}e^{2(M_i-\beta)/h}\Big]\\
&\lesssim \sum_{i=1}^2\Big[h\int_{\mathfrak{A}_i}\Big\{|u|^2+|h\nabla u|^2\Big\}e^{2\varphi_{i+1}/h} + \int_\Gamma |hNu|^2 e^{2\varphi_i/h} + h^{-1}e^{2(M_i-\beta)/h}\Big]\end{aligned}$$

with $\varphi_3 \equiv \varphi_1$, where we have used that $\psi_{i+1} > \psi_i$ on $B(x_{ij}, 2\epsilon)$, with $\psi_3 \equiv \psi_1$ (see (ii) above).

But $\mathcal{A}_1 \subset \complement(\cup_j B(x_{2j}, 2\epsilon))\cap\Omega$ and $\mathcal{A}_2 \subset \complement(\cup_j B(x_{1j}, 2\epsilon))\cap\Omega$, so we can absorb the "$\mathcal{A}$" terms. This gives

$$\begin{aligned}\int_{\complement(\cup_j B(x_{1j},2\epsilon))\cap\Omega}\Big\{|u|^2+|h\nabla u|^2\Big\}e^{2\varphi_1/h} + \int_{\complement(\cup_j B(x_{2j},2\epsilon))\cap\Omega}\Big\{|u|^2+|h\nabla u|^2\Big\}e^{2\varphi_2/h}\\
\lesssim \int_\Gamma |hNu|^2 e^{2\varphi_1/h} + \int_\Gamma |hNu|^2 e^{2\varphi_2/h}\\
+ h^{-1}e^{2(M_1-\beta)/h} + h^{-1}e^{2(M_2-\beta)/h}.\end{aligned}$$

We let

$$\begin{aligned}M &:= \max(\max_\Gamma \varphi_1, \max_\Gamma \varphi_2),\\
m &:= \min(\min_{\overline{\Omega}} \varphi_1, \min_{\overline{\Omega}} \varphi_2), \qquad \text{and}\\
\tilde{M} &:= \max(M_1, M_2),\end{aligned}$$

and we note that $M > m$, by the positivity of the (outward) normal derivatives of the Carleman weights on Γ:

$$N\varphi_i\Big|_\Gamma > 0.$$

We then have

$$e^{2m/h}\int_{\Omega}\left\{|u|^2+|h\nabla u|^2\right\}\lesssim e^{2M/h}\int_{\Gamma}|hNu|^2+h^{-1}e^{2(\tilde{M}-\beta)/h}.$$

We may now simply omit the gradient term on the left side and take β such that $\beta > \tilde{M} - m =: \beta_0$. Hence there exist $c_0 > 0$ and $h_0 > 0$ such that

$$c_0 e^{-(M-m)/h} \leq ||hNu||_{L^2(\Gamma)} \qquad \forall h \in (0, h_0)$$

hence proving the theorem. $\square$

Remark 2.12. Just as in the previous section, we may use Agmon estimates to show that the h-dependence in Theorem 2.2 is sharp, both for the stated quasimode accuracy and for the lower bound. As in Remark 2.9, we consider the case when the classically allowed region

$$\{x \in \overline{\Omega};\, V(x) \leq E\}$$

is a non-empty subset of the open set Ω. Then a neighborhood of the boundary of Ω is contained in the classically forbidden region

$$\{x \in \overline{\Omega};\, V(x) > E\}.$$

Then, precisely as in Remark 2.9, we can use a cutoff function to create exponentially precise quasimodes which vanish in an h-independent neighborhood of Γ.

To show that the lower bound in Theorem 2.2 is sharp in terms of h, we recall a well-known argument for estimating normal derivatives of eigenfunctions; we learned this from papers of Burq [Bur05] and Hassell and Tao [HT02], where the relevant estimates are called “Rellich-type estimates”. For simplicity, we take G to be the identity matrix.

Lemma 2.13. *Let $u(\cdot\,;h)$ be a Dirichlet eigenfunction of P. Then, for any differential operator A,*

$$\int_\Omega u[P,A]u = h^2 \int_{\partial\Omega} \frac{\partial u}{\partial n} Au. \tag{2.7}$$

Proof. Let $E(h)$ be the eigenvalue corresponding to $u(\cdot\,;h)$. Then

$$\begin{aligned}\int_\Omega u[P,A]u &= \int_\Omega \Big[u(P-E(h))Au - Au(P-E(h))u\Big] \\ &= h^2 \int_\Omega \Big[Au\Delta u - u\Delta Au\Big],\end{aligned}$$

and so, by Green's formula and the fact that u vanishes on the boundary, we get the desired identity. ☐

We now choose an operator A so that $||\partial_n u||^2_{L^2(\partial\Omega)}$ is recoverable from (2.7). For this, we use geodesic normal coordinates near $\partial\Omega$, that is, coordinates (r,y) near $\partial\Omega$ such that r is the distance to $\partial\Omega$. Then we choose

$$A = \chi(r)\frac{\partial}{\partial r},$$

where $\chi \in C_0^\infty(\mathbb{R})$ and is such that, for some $\delta > 0$,

$$\chi = \begin{cases} 1 & \text{for } 0 \le r \le \delta/2 \\ 0 & \text{for } r \ge \delta. \end{cases}$$

We take $\delta > 0$ so that the coordinates (r,y) are smooth for $r \in [0,\delta]$. Then the right side of (2.7) is just

$$\int_{\partial\Omega} \left| h\frac{\partial u}{\partial n}\right|^2.$$

As for the left side of (2.7), we simply consider

$$\int_\Omega u[P,A]u = h^2 \int_\Omega u[-\Delta, A]u + \int_\Omega u[V,A]u.$$

Letting

$$N_\delta(\partial\Omega) := \{x \in \Omega;\ \mathrm{dist}(x, \partial\Omega) \le \delta\}$$

it is clear that $[V, A]$ is a smooth function, supported in $N_\delta(\partial\Omega)$, and that $[-\Delta, A]$ is a second-order differential operator with smooth coefficients supported in $N_\delta(\partial\Omega)$. Hence

$$\begin{aligned} \int_{\partial\Omega} \left| h \frac{\partial u}{\partial n} \right|^2 &= \left| \int_\Omega u[P, A]u \right| \\ &\lesssim \int_{N_\delta(\partial\Omega)} \left(|u|^2 + |h\nabla u|^2 \right). \end{aligned}$$

If $\delta > 0$ is moreover small enough so that $N_\delta(\partial\Omega)$ is in the interior of the classically forbidden region, Agmon estimates, as in Remark 2.9, show that

$$\int_{N_\delta(\partial\Omega)} \left(|u|^2 + |h\nabla u|^2 \right) \lesssim e^{-c/h}$$

for some $c > 0$ and for all $h > 0$ sufficiently small. So we finally arrive at the estimate

$$\int_{\partial\Omega} \left| h \frac{\partial u}{\partial n} \right|^2 \lesssim e^{-c/h}.$$

CHAPTER 3

Exponential Lower Bounds for the Bargmann Transform

3.1 Introduction

The Bargmann transform's primary feature is that it unitarily maps $L^2(\mathbb{R}^n)$ onto the Fock space

$$H_\Phi = \mathrm{Hol}(\mathbb{C}^n) \cap L^2(\mathbb{C}^n;\, e^{-2\Phi/h} L(dz)),$$

where h is the semiclassical parameter, $\Phi(z) = |z|^2/2$, and $L(dz)$ is Lebesgue measure on $\mathbb{C}^n$, in such a way that it intertwines the creation operator with multiplication by z and the annihilation operator with holomorphic differentiation with respect to z [Bar61], [Fol89]. We use the conventions such that the Bargmann transform is defined for $u \in \mathcal{S}'(\mathbb{R}^n)$, $z \in \mathbb{C}^n$, by

$$Tu(z;h) = (\pi h)^{-3n/4} \int e^{i\phi(z,y)/h} u(y)\, dy$$

with

$$\phi(z,y) = i\left(\frac{z^2}{2} + \frac{y^2}{2} - \sqrt{2}\, zy\right). \tag{3.1}$$

Using this definition, T intertwines the creation operator

$$a_k^\dagger = (2h)^{-1/2}\left(x_k - h\frac{\partial}{\partial x_k}\right)$$

with multiplication by $h^{-1/2} z_k$:

$$T(a_k^\dagger u)(z;h) = h^{-1/2} z_k Tu(z;h),$$

and it intertwines the annihilation operator

$$a_k = (2h)^{-1/2}\left(x_k + h\frac{\partial}{\partial x_k}\right)$$

with the holomorphic derivative operator:

$$T(a_k u)(z;h) = \sqrt{h}\frac{\partial}{\partial z_k}Tu(z;h).$$

About ten years after the publication of Bargmann's paper [Bar61], Bros and Iagolnitzer defined what is now called the FBI (Fourier, Bros, Iagolnitzer) transform, a close relative of the Bargmann transform, and found that it characterizes local analyticity and is thus useful in axiomatic quantum field theory [BI73], [Iag93]. Córdoba and Fefferman [CF78] and then Sjöstrand [Sjo82], [Sjo96] later put the Bargmann transform and the FBI transform in a larger framework, considering them as special cases of so-called generalized Bargmann-FBI transforms, and viewed as Fourier integral operators with complex phases, associated to complex canonical transformations. Indeed, one may check that (3.1) is an admissible phase in the sense of Sjöstrand:

$$\det(\phi''_{zy}) \neq 0 \qquad \text{and} \qquad \operatorname{Im}\phi''_{yy} > 0.$$

Hence associated to the Bargmann transform T is the (complex linear, in this case) canonical transformation given by

$$\kappa_T : \mathbb{C}^{2n} \ni (y, -\phi'_y(z,y)) \mapsto (z, \phi'_z(z,y)) \in \mathbb{C}^{2n}, \tag{3.2}$$

and

$$\kappa_T(\mathbb{R}^{2n}) = \Lambda_\Phi := \left\{\left(z, \frac{2}{i}\frac{\partial\Phi}{\partial z}(z)\right); \, z \in \mathbb{C}^n\right\},$$

where, as before,

$$\Phi(z) = \sup_{y\in\mathbb{R}^n} -\operatorname{Im}\phi(z,y) = |z|^2/2.$$

To make precise the connection with local analyticity, for $u \in \mathcal{S}'(\mathbb{R}^n)$ let $SS_a(u)$ be the smallest closed subset of $\mathbb{R}^n$ outside of which u is analytic. Then the Bargmann transform of u characterizes $SS_a(u)$; in fact, it characterizes the analytic wavefront set $WF_a(u)$ of u, and $\Pi\, WF_a(u) = SS_a(u)$, where $\Pi : T^*\mathbb{R}^n\backslash 0 \to \mathbb{R}^n$ is the natural projection [Sjo82]. The analytic wavefront set WF_a is defined as follows. The point $(y_0, \eta_0) \in T^*\mathbb{R}^n$ is not in $WF_a(u)$ if and only if there exists a neighborhood ω of $\Pi_z(\kappa_T(y_0, \eta_0)) =: z_0 \in \mathbb{C}^n$ and some $\delta > 0$ such that $||Tu(\cdot\,; h)||_{H_\Phi(\omega)} = \mathcal{O}(e^{-\delta/h})$.

Hence the Bargmann transform, when applied to h-independent tempered distributions, gives a characterization of local analyticity in terms of certain exponentially decreasing upper bounds. When dealing with a family of h-dependent tempered distributions—for example, quasimodes of semiclassical operators—these upper bounds still have meaning and are in fact a main object of study [Mar02]. The purpose of this chapter is to study the corresponding exponentially decreasing *lower* bounds for the Bargmann transform.

Our main result is the following theorem, which, for greater flexibility, we state for a general semiclassical indexing set.

Theorem 3.1. *Let $H \subset (0, 1]$, $0 \in \overline{H}$, and let $u(\cdot\,; h) \in L^2(\mathbb{R}^n)$ for $h \in H$. Assume that there exist constants $h_{00} > 0$, $c_{00} > 0$, $\beta \geq 0$ and some compact set $K \subset\subset \mathbb{C}^n$ such that*

$$c_{00} e^{-\beta/h} ||u(\cdot\,; h)||_{L^2(\mathbb{R}^n)} \leq ||Tu(\cdot\,; h)||_{L^\infty(K)} \quad \forall h \in (0, h_{00}) \cap H.$$

Then for any open set $\omega \subset \mathbb{C}^n$ there exist constants $\alpha > 0$, $c_0 > 0$, and $h_0 > 0$ such that

$$c_0 e^{-\alpha/h} ||u(\cdot\,; h)||_{L^2(\mathbb{R}^n)} \leq ||Tu(\cdot\,; h)||_{H_\Phi(\omega)} \quad \forall h \in (0, h_0) \cap H.$$

Clearly the hypothesis is a necessary condition. We may additionally assume that ω is a neighborhood of the origin, since translation acts in the following way: for any $w \in \mathbb{C}^n$ we have

$$Tu(z+w;h) = e^{z\overline{w}/h} e^{|w|^2/(2h)+i(\operatorname{Re} w)(\operatorname{Im} w)/h} T\left(\tau_{\sqrt{2}\operatorname{Re} w}^{\sqrt{2}\operatorname{Im} w} u\right)(z;h),$$

where for $\alpha, \beta \in \mathbb{R}^n$ we denote by τ_α^β the translation in phase space

$$\left(\tau_\alpha^\beta u\right)(x) = e^{i\beta x/h} u(x+\alpha).$$

In particular,

$$|Tu(z+w;h)| = e^{(\operatorname{Re} z \operatorname{Re} w + \operatorname{Im} z \operatorname{Im} w)/h} e^{|w|^2/(2h)} \left| T\left(\tau_{\sqrt{2}\operatorname{Re} w}^{\sqrt{2}\operatorname{Im} w} u\right)(z;h)\right|.$$

Now there are u such that the hypothesis is not satisfied. For example, in one dimension we consider the h-dependent normalized L^2 functions given by

$$u(x;h) := (\pi h)^{-1/4} e^{ixf(h)/h} e^{-x^2/(2h)}, \quad x \in \mathbb{R},$$

where f is an arbitrary function. This is called the *coherent state* centered at $(0, f(h))$; it is localized to a neighborhood of $x_0 = 0$ of size $\sqrt{h}$, and its h-Fourier transform is localized to a neighborhood of $\xi_0 = f(h)$ of size $\sqrt{h}$. And we may explicitly compute the Bargmann transform:

$$Tu(z;h) = (\pi h)^{-1/2} \exp\left(-\frac{1}{2h} z^2 + \frac{1}{4h}(\sqrt{2}\, z + i f(h))^2\right).$$

If $f(h)$ is bounded for all $h > 0$ sufficiently small, we will have the desired local lower bound. However, if $f(h) = h^{-\nu}$ for $\nu > 0$, for example, we have

$$|Tu(z;h)| = (\pi h)^{-1/2} \exp\left(-\frac{1}{\sqrt{2}} h^{-\nu-1} \operatorname{Im} z - \frac{1}{4} h^{-2\nu-1}\right).$$

In Section 3.2 we give a proof Theorem 3.1, starting with the one-dimensional case, which is the heart of the matter. The extension to n dimensions then follows easily. In Section 3.3 we give a class of functions to which the theorem applies: quasimodes of semiclassical pseudodifferential operators that are elliptic at infinity, hence preventing the quasimodes from concentrating at infinity. And, finally, Section 3.4 gives an application to functions in $C_0^k(\mathbb{R}^n)$.

We emphasize that our theorem is a result of the hypothesized lower bound and just two properties of the Bargmann transform: the elementary estimate

$$|Tu(z;h)| \leq (\pi h)^{-n/2} e^{|z|^2/(2h)} ||u||_{L^2(\mathbb{R}^n)} \tag{3.3}$$

and the fact that Tu is holomorphic in z. The basic approach is more or less standard and may be found, for example, embedded in Sjöstrand's paper [Sjo01]; however, we believe that a self-contained presentation could be useful.

3.2 The Proof of Theorem 3.1

We begin with a proof of the one-dimensional case. For this, we recall Jensen's formula and its application in estimating zeros of holomorphic functions.

Let $f(z)$ be holomorphic in a neighborhood of the disc $\overline{D(0,R)} = \{z \in \mathbb{C};\, |z| \leq R\}$ and such that $f(0) \neq 0$. Let $z_1, \ldots, z_N$ be the zeros of f on $\overline{D(0,R)}$, repeated according to multiplicity. Then Jensen's formula (see, for example, [Ahl78]) says

$$\log|f(0)| + \sum_{j=1}^{N} \log\left|\frac{R}{z_j}\right| = \frac{1}{2\pi} \int_0^{2\pi} \log|f(Re^{i\theta})|\, d\theta.$$

A standard application of this formula is the estimation of zeros of holomorphic functions. Let $N(R/2)$ denote the number of zeros z_j of f with $|z_j| \leq R/2$.

Then

$$\frac{1}{2\pi}\int_0^{2\pi} \log|f(Re^{i\theta})|\,d\theta - \log|f(0)| = \sum_{j=1}^{N} \log\left|\frac{R}{z_j}\right|$$
$$\geq N(R/2)\log 2.$$

In particular, we then have

$$N(R/2) \leq (\log 2)^{-1}\left[\max_{|z|\leq R} \log|f(z)| - \log|f(0)|\right].$$

The preceding results easily extend to the case of a disc $D(a,R)$ of radius R centered at a point $a \in \mathbb{C}$. We will particularly need the following: If f is holomorphic near $\overline{D(a,R)}$ and is such that $f(a) \neq 0$, then

$$N_a(R/2) \leq (\log 2)^{-1}\left[\max_{|z-a|\leq R} \log|f(z)| - \log|f(a)|\right]$$

where $N_a(R/2)$ denotes the number of zeros of f in $\overline{D(a,R/2)}$.

We continue with the proof of the theorem. Without loss of generality, we take $||u(\cdot\,;h)||_{L^2(\mathbb{R}^n)} = 1$. Let $R_K > 1$ be such that $K \subset \overline{D(0,R_K)}$, and let $z(h)$ be a point in $\overline{D(0,R_K)}$ where $\max_{z\in\overline{D(0,R_K)}} |Tu(z;h)|$ is attained. By the maximum principle, $|z(h)| = R_K$ for all h.

We let $N_{z(h)}(100R_K)$ denote the number of zeros of $Tu(\cdot\,;h)$ in the disc of radius $100R_K$ centered at $z(h)$. Then

$$N_{z(h)}(100R_K) \leq (\log 2)^{-1}\left[\max_{|z-z(h)|\leq 200R_K} \log|Tu(z;h)| - \log|Tu(z(h);h)|\right].$$

Hence, using (3.3)[1],

$$
\begin{aligned}
&N_{z(h)}(100R_K) \\
&\qquad \leq (\log 2)^{-1}\left[\max_{|z-z(h)|\leq 200R_K}\log\left((\pi h)^{-n/2}e^{|z|^2/(2h)}\right)-\log|Tu(z(h);h)|\right] \\
&\qquad \leq (\log 2)^{-1}\left[\frac{n}{2}\log\left(\frac{1}{\pi h}\right)+\frac{(200R_K+R_K)^2}{2h}-\log|Tu(z(h);h)|\right].
\end{aligned}
\tag{3.4}
$$

Now our hypothesis says that

$$
-\log|Tu(z(h);h)| \leq \frac{\beta}{h}-\log c_{00},
$$

which then gives

$$
N_{z(h)}(100R_K) \leq (\log 2)^{-1}\left[\frac{n}{2}\log\left(\frac{1}{\pi h}\right)+\frac{(201R_K)^2}{2h}+\frac{\beta}{h}-\log c_{00}\right].
$$

In particular, we have the following bound on the number of zeros in a disc of radius $50R_K$ centered at the origin:

$$
N(50R_K)=\mathcal{O}(1/h) \quad \text{as } h\to 0.
$$

This gives us control on the degree of the polynomial in the factorization of Tu, which we turn to now.

Let $\rho \in (0,1)$ and consider the disc of radius $R_\rho := 2(R_K+\rho)$ centered at $z(h)$. We note that $\overline{D(0,\rho)} \subset \overline{D(z(h),\frac{1}{2}R_\rho)}$ for all $h \in (0,h_{00})\cap H$. For any fixed $\epsilon \in (0,1)$ (independent of h), let $R_\rho(\epsilon) := R_\rho+\epsilon$. For convenience, in what follows we omit the h's from our notation in places where the h-dependence is obvious.

[1]Of course, we are in the case $n=1$, but we write as if forced to use the slightly worse estimate (3.8), since that is the relevant change for the general n-dimensional case.

Let $\{z_j\}_{j=1}^N$ be the zeros of Tu in $|z - z(h)| \leq R_\rho(\epsilon)$. We then have the factorization

$$Tu(z;h) = e^{G(z)} \prod_{j=1}^N (z - z_j)\,, \text{ for } |z - z(h)| \leq R_\rho(\epsilon), \tag{3.5}$$

where G and $1/G$ are holomorphic.

Our first step is to get a pointwise bound from below for the polynomial in (3.5). There is more than one way to do it, but perhaps the most elegant is to use the following elementary lemma from [Sjo01]:

Lemma 3.2. *Let $x_1, \ldots, x_N \in \mathbb{R}$, and let $I \subset \mathbb{R}$ be an interval of length $|I| \in (0, \infty)$. Then there exists $x \in I$ such that*

$$\prod_{j=1}^N |x - x_j| \geq e^{-N(1+\log(2/|I|))}.$$

By this lemma, there exists some $R \in [R_\rho, R_\rho(\epsilon)]$ such that we have

$$\prod_{j=1}^N |z - z_j| \geq e^{-CN} \qquad \text{when} \quad |z - z(h)| = R.$$

Here C depends only on ϵ, K, and ρ. Writing

$$e^{G(z)} = \frac{u(z)}{\prod_{j=1}^N (z - z_j)}$$

and applying the maximum principle on the disc $D(z(h), R)$, we have

$$\begin{aligned} e^{\operatorname{Re} G(z)} &\leq e^{CN} \max_{|z-z(h)|=R} |Tu(z;h)| \\ &\leq (\pi h)^{-n/2} e^{CN} \max_{|z-z(h)|=R} e^{|z|^2/(2h)} \end{aligned}$$

We then use the estimate $N = \mathcal{O}(1/h)$, to obtain, for $|z - z(h)| \leq R$, and in particular for $|z - z(h)| \leq R_\rho$,

$$\operatorname{Re} G(z) \leq C/h$$

for h small enough, perhaps with a new constant C (depending only on ϵ, K, and ρ).

We then consider the function

$$g(z) := C/h - \operatorname{Re} G(z),$$

which is a positive harmonic function in $|z - z(h)| \leq R_\rho$. Then Harnack's Inequality applies:

$$\frac{R_\rho - r}{R_\rho + r} g(z(h)) \leq g(z) \leq \frac{R_\rho + r}{R_\rho - r} g(z(h)) \quad \text{for } |z - z(h)| = r < R_\rho.$$

Rewriting in terms of G, the upper bound says

$$\left(\frac{R_\rho + r}{R_\rho - r}\right) \operatorname{Re} G(z(h)) \leq \operatorname{Re} G(z) + \left(\frac{2r}{R_\rho - r}\right)\left(\frac{C}{h}\right)$$

for $|z - z(h)| = r < R_\rho$, and hence

$$\begin{aligned} |Tu(z;h)| &= e^{\operatorname{Re} G(z)} \prod_{j=1}^{N} |z - z_j| \\ &\geq \exp\left(\frac{R_\rho + r}{R_\rho - r} \operatorname{Re} G(z(h)) - \left(\frac{2r}{R_\rho - r}\right)\left(\frac{C}{h}\right)\right) \prod_{j=1}^{N} |z - z_j|. \end{aligned}$$

So, for $|z - z(h)| = r \leq \frac{1}{2} R_\rho$, we have

$$|Tu(z;h)| \geq \exp\left(c_{13} \operatorname{Re} G(z(h)) - \frac{2C}{h}\right) \prod_{j=1}^{N} |z - z_j|, \tag{3.6}$$

where

$$c_{13} := \begin{cases} 1 & \text{if } \operatorname{Re} G(z(h)) \geq 0 \\ 3 & \text{if } \operatorname{Re} G(z(h)) \leq 0 \end{cases}.$$

But clearly

$$\begin{aligned} e^{c_{13} \operatorname{Re} G(z(h))} &\geq |Tu(z(h);h)|^{c_{13}} \prod_{j=1}^{N} |z(h) - z_j|^{-c_{13}} \\ &\geq |Tu(z(h);h)|^{c_{13}} (5R_K)^{-c_{13} N} \\ &\geq |Tu(z(h);h)|^{c_{13}} e^{-C/h} \end{aligned}$$

where the last line follows from the bound on the number of zeros. Now, by the choice of the $z(h)$ (the points where the maxima are attained),

$$e^{c_{13}\operatorname{Re} G(z(h))} \geq c_{00}^{c_{13}} e^{-(c_{13}\beta+C)/h}. \tag{3.7}$$

So, in summary, combining (3.6) and (3.7),

$$|Tu(z;h)| \geq c_0 e^{-C/h} \prod_{j=1}^{N} |z - z_j|$$

for $|z - z(h)| \leq \frac{1}{2}R_\rho = R_K + \rho$.

The next step is to bound $\prod_{j=1}^{N} |z - z_j|$ from below for $|z - z(h)| \leq R_K + \rho$. We note that the degrees of these ($z(h)$-dependent) polynomials are bounded by C_0/h as $h \to 0$, where $C_0 > 0$ is independent of $z(h)$.

We consider the general case of a holomorphic polynomial $p_N(z)$ of degree N with leading coefficient a_N. Now, with respect to the inner product

$$\langle f|g\rangle := \int_{|z|\leq\rho} f\overline{g}\, L(dz),$$

the monomials $k_j(z) := z^j$, $j = 0, 1, 2, \ldots$, are mutually orthogonal. We can expand p_N with respect to this basis:

$$p_N(z) = \sum_{j=0}^{N} a_j z^j,$$

and then, by orthogonality, we have Parseval's identity:

$$\begin{aligned}||p_N||^2_{L^2(|z|\leq\rho)} &= \sum_{j=0}^{N} |a_j|^2 \int_{|z|\leq\rho} |z|^{2j}\, L(dz) \\ &\geq |a_N|^2 \int_{|z|\leq\rho} |z|^{2N}\, L(dz).\end{aligned}$$

But we compute

$$\int_{|z|\leq\rho} |z|^{2N}\, L(dz) = \frac{\pi}{N+1} e^{2(N+1)\log\rho}.$$

In summary,

$$||p_N||_{L^2(|z|\le\rho)} \ge |a_N| \left(\frac{\pi}{N+1}\right)^{1/2} e^{(N+1)\log\rho}.$$

Hence, letting $N(h)$ denote the number of zeros of $Tu(z;h)$ in $|z - z(h)| \le R_\rho(\epsilon)$, we have

$$\begin{aligned}
||Tu||_{H_\Phi(|z|\le\rho)} &\ge c_0 e^{-C/h} \left|\left| e^{-\Phi/h} \prod_{j=1}^{N(h)} |z - z_j| \right|\right|_{L^2(|z|\le\rho)} \\
&\ge c_0 e^{-C/h - \rho^2/(2h)} \left|\left| \prod_{j=1}^{N(h)} |z - z_j| \right|\right|_{L^2(|z|\le\rho)} \\
&\ge c_0 e^{-C/h} (N(h)+1)^{-1/2} e^{(N(h)+1)\log\rho}.
\end{aligned}$$

The constants C and c_0 of course changed from line to line; also, the estimate on Φ is very crude but sufficient for our purposes. (Alternatively, one may use that the monomials z^j are mutually orthogonal in the weighted space $H_\Phi(\mathbb{C}^n)$, but then the loss appears when considering $||p_N||_{H_\Phi(|z|\le\rho)}$.) We once again use that $N(h) \le C_0 h^{-1}$ for all $h \in (0, h_0) \cap H$, where $C_0 > 0$ is independent of $z(h)$, so

$$||Tu||_{H_\Phi(|z|\le\rho)} \ge c_0 e^{-C/h} \left(\frac{C_0}{h} + 1\right)^{-1/2} e^{-(C_0/h)\log(1/\rho)}.$$

So finally we see that there exist $c_0 > 0$, $\alpha > 0$, and $h_0 > 0$ such that

$$||Tu||_{H_\Phi(|z|\le\rho)} \ge c_0 e^{-\alpha/h} \quad \forall h \in (0, h_0) \cap H.$$

This concludes the proof of the theorem in the one-dimensional case.

For the general case, we again let $K \subset \overline{B(0; R_K)} = \{z \in \mathbb{C}^n;\ |z| \le R_K\}$ and let $z(h) \in \mathbb{C}^n$ be the points where the maxima are attained, so that $|z(h)| = R_K$. We then consider the function $Tu(w\frac{z(h)}{|z(h)|}; h)$, which is holomorphic in $w \in \mathbb{C}$ and which satisfies the pointwise upper bound

$$\left| Tu\left(w\frac{z(h)}{|z(h)|}; h\right)\right| \le (\pi h)^{-n/2} e^{|w|^2/(2h)}. \tag{3.8}$$

For our purposes, this upper bound is no worse than (3.3). We may then apply the arguments of the previous section, since all the constants were explicit, and, in particular, were independent of the orientation of the $z(h)$. Hence for any $\rho \in (0,1)$ there exist $c_0 > 0$, $h_0 > 0$, and $\alpha > 0$ such that

$$\begin{aligned}
c_0 e^{-\alpha/h} &\leq \left|\left| Tu\left(w\frac{z(h)}{|z(h)|};h\right) e^{-|w|^2/(2h)}\right|\right|_{L^2(|w|\leq\rho)} \\
&\lesssim \left|\left| Tu\left(w\frac{z(h)}{|z(h)|};h\right)\right|\right|_{L^\infty(|w|\leq\rho)} \\
&\leq ||Tu(\cdot\,;h)||_{L^\infty(|z|\leq\rho)} \\
&\lesssim ||Tu(\cdot\,;h)||_{L^2(|z|\leq\rho')} \qquad \text{for any } \rho' > \rho \text{ (by Cauchy's Integral Formula)} \\
&\leq e^{(\rho')^2/(2h)}||Tu||_{H_\Phi(|z|\leq\rho')},
\end{aligned}$$

for all $h \in (0,h_0) \cap H$. This proves the theorem in its full generality.

3.3 Application to Quasimodes of Elliptic Operators

The application to elliptic operators takes place in a rather general setting. We first recall the basic definitions but refer to, e.g., [DS99], [EZ07], or [Mar02] for details.

Definition 3.3. *A C^∞ function $m : T^*\mathbb{R}^n \to (0,\infty)$ is called an* order function *if for any multi-indices α and β there exists a constant $C_{\alpha\beta}$ such that*

$$|\partial_x^\alpha \partial_\xi^\beta m(x,\xi)| \leq C_{\alpha\beta} m(x,\xi) \quad \forall (x,\xi) \in T^*\mathbb{R}^n.$$

And we use the following classes of symbols:

Definition 3.4. *Given an order function m, a function $a(\cdot\,;h) \in C^\infty(T^*\mathbb{R}^n)$, with $h \in (0,h_0)$ for some $h_0 > 0$, is in $S_{2n}(m)$ if for any multi-indices α and β*

there exists a constant $C_{\alpha\beta}$ *such that*

$$|\partial_x^\alpha \partial_\xi^\beta a(x,\xi;h)| \leq C_{\alpha\beta} m(x,\xi) \quad \forall (x,\xi) \in T^*\mathbb{R}^n \text{ and } \forall h \in (0,h_0).$$

Now let m be an order function such that $m \geq 1$, and let $p = p(\cdot\,;h) \in S_{2n}(m)$. For a uniformly bounded spectral parameter $E(h) \in [a,b]$, for some $-\infty < a \leq b < \infty$, it is clear that $p - E(h) \in S_{2n}(m)$. Moreover, we assume that $p - E(h)$ is elliptic at infinity in this class; that is, we assume that there exist $C > 0$, $h_0 > 0$, and a compact set $\tilde{K} \subset\subset T^*\mathbb{R}^n$ such that

$$|p - E(h)| \geq \frac{1}{C} m \quad \text{outside of } \tilde{K} \qquad \forall h \in (0,h_0).$$

We take the Weyl quantization of this symbol, $P := \mathrm{Op}_h^W(p)$, defined by

$$\left(\mathrm{Op}_h^W(p)u\right)(x) := (2\pi h)^{-n} \iint_{T^*\mathbb{R}^n} e^{i(x-y)\xi/h} p\left(\frac{x+y}{2}, \xi; h\right) u(y)\, dy\, d\xi,$$

although for the arguments that follow we can just as easily take, for example, the Kohn-Nirenberg quantization.

We now consider L^2 quasimodes of P of accuracy $o(1)$:

$$||(P - E(h))u||_{L^2(\mathbb{R}^n)} = o(1)||u||_{L^2(\mathbb{R}^n)}, \quad u(\cdot\,;h) \in L^2(\mathbb{R}^n).$$

Then our theorem applies to u. To show this, we begin by reducing to the case where $m = 1$. Noting that $1/m \in S_{2n}(1/m) \subset S_{2n}(1)$ (as $m \geq 1$), we simply consider the operator

$$P_2 := \mathrm{Op}_h^W(1/m)(P - E(h)),$$

whose symbol is

$$p_2(x,\xi;h) := m(x,\xi)^{-1}[p(x,\xi;h) - E(h)] + hr \in S_{2n}(1), \quad \text{where } r \in S_{2n}(1);$$

hence this operator is elliptic at infinity in the class $S_{2n}(1)$. Also, since $S_{2n}(1)$ gives rise to L^2-bounded pseudodifferential operators, and $\mathrm{Op}_h^W(1/m)$ is such an operator, we have that

$$||P_2 u|| = ||\mathrm{Op}_h^W(1/m)(P - E(h))u||_{L^2} = o(1)||u||_{L^2}.$$

We now show that the ellipticity of P_2 at infinity implies the lower bound in the hypothesis of Theorem 3.1. We recall that κ_T is the complex canonical transformation (3.2) associated to T when interpreted as a Fourier integral operator with complex phase. Explicitly, in this case we have

$$\kappa_T : \mathbb{C}^{2n} \ni (y, w) \mapsto \left(\frac{1}{\sqrt{2}}(y - iw), \frac{-i}{\sqrt{2}}(y + iw) \right) \in \mathbb{C}^{2n}.$$

We then let $K := \kappa_T(\tilde{K})$, with $\tilde{K}$ as in the ellipticity condition for p_2.

Lemma 3.5. *Under the above hypotheses, there is a constant $C > 0$ such that*

$$(1/C)||Tu||_{H_\Phi} \leq ||Tu||_{H_\Phi(K)} \leq C||Tu||_{H_\Phi} \quad \textit{for all } h \textit{ sufficiently small.}$$

Proof. By unitarity and the fundamental result on approximation by multiplication operators (see, e.g., [Mar02] p.93 or Section 12 of [Sj]), we have

$$\begin{aligned} o(1)||Tu||^2_{H_\Phi} &= ||TP_2 u||^2_{H_\Phi} \\ &= ||p_2 \circ \kappa_T^{-1}|_{\Lambda_\Phi} Tu||^2_{H_\Phi} + \mathcal{O}(h)||Tu||^2_{H_\Phi}. \end{aligned}$$

Hence

$$||p_2 \circ \kappa_T^{-1}|_{\Lambda_\Phi} Tu||^2_{H_\Phi} = o(1)||Tu||^2_{H_\Phi}.$$

We then use the ellipticity at infinity:

$$\begin{aligned} o(1)||Tu||^2_{H_\Phi} &= ||p_2 \circ \kappa_T^{-1}|_{\Lambda_\Phi} Tu||^2_{H_\Phi(K)} + ||p_2 \circ \kappa_T^{-1}|_{\Lambda_\Phi} Tu||^2_{H_\Phi(\complement K)} \\ &\geq ||p_2 \circ \kappa_T^{-1}|_{\Lambda_\Phi} Tu||^2_{H_\Phi(K)} + \frac{1}{C^2}||Tu||^2_{H_\Phi(\complement K)}. \end{aligned}$$

For h small enough, we can absorb part of the left side into the right side, giving

$$\begin{aligned}
o(1)||Tu||^2_{H_\Phi(K)} &\geq ||p_2 \circ \kappa_T^{-1}|_{\Lambda_\Phi} Tu||^2_{H_\Phi(K)} + \frac{1}{2C^2}||Tu||^2_{H_\Phi(\complement K)} \\
&\geq \frac{1}{2C^2}||Tu||^2_{H_\Phi(\complement K)}.
\end{aligned}$$

Hence

$$\begin{aligned}
||Tu||^2_{H_\Phi} &= ||Tu||^2_{H_\Phi(K)} + ||Tu||^2_{H_\Phi(\complement K)} \\
&\leq ||Tu||^2_{H_\Phi(K)} + o(1)||Tu||^2_{H_\Phi(K)} \\
&\leq \mathcal{O}(1)||Tu||^2_{H_\Phi(K)} \\
&\leq \mathcal{O}(1)||Tu||^2_{H_\Phi}
\end{aligned}$$

which proves the lemma. □

Without loss of generality, for the remainder of this section we assume that the $u = u(h)$ are normalized: $||u||_{L^2(\mathbb{R}^n)} = 1$.

We now take $R_K > 1$ to be large enough so that $K \subset B(0, R_K)$. Then the lemma says that $||Tu(\cdot\,; h)||_{H_\Phi(B(0,R_K))} \sim 1$ for all h sufficiently small. In particular, there exist $C > 0$ and $h_0 > 0$ such that

$$\begin{aligned}
\frac{1}{C} &\leq ||e^{-|z|^2/(2h)} Tu||_{L^2(|z| \leq R_K)} \\
&\leq ||Tu||_{L^2(|z|\leq R_K)} \quad \forall h \in (0, h_0).
\end{aligned}$$

We thus have the following simple corollary:

Corollary 3.6. *There exist $h_{00} > 0$ and $c_{00} > 0$ such that*

$$c_{00} \leq \max_{|z| \leq R_K} |Tu(z; h)| \quad \forall h \in (0, h_{00}).$$

Hence the hypothesis of Theorem 3.1 is satisfied, with $\beta = 0$.

3.4 Application to Function in $C_0^k(\mathbb{R}^n)$

We now use Theorem 3.1 to obtain lower bounds for Bargmann transforms of functions in $C_0^{nk}(\mathbb{R}^n)$, for $k \in \{1, 2, \ldots\}$.

The method presented in the previous sections is not unique to our choice of the phase $\phi(z, y) = i\left(\frac{z^2}{2} + \frac{y^2}{2} - \sqrt{2}zy\right)$. For example, one may check that the argument also holds for the phase

$$\phi(z, y) = (i/2)(z - y)^2, \tag{3.9}$$

which is also common in the literature [Sjo96]. This choice is convenient in that we may write the Bargmann transform as a convolution. Moreover, the associated complex canonical transformation is

$$\kappa_T : \mathbb{C}^{2n} \ni (y, w) \mapsto (y - iw, w) \in \mathbb{C}^{2n},$$

and our weighted space H_Φ has $\Phi(z) = |\operatorname{Im} z|^2/2$. In this section we choose to work with the phase (3.9), and we use the real variables $(x, \xi) \in \mathbb{R}^{2n}$ in place of the complex variable $z = x - i\xi \in \mathbb{C}^n$.

Here we will restrict our attention to $u \in C_0^{nk}(\mathbb{R}^n)$ that are h-independent, in which case we have the following improved preliminary lower bound, the main result of this section:

Proposition 3.7. *Let $u \in C_0^{nk}(\mathbb{R}^n)$, with $k \in \{1, 2, \ldots\}$. Let $U \subset \mathbb{R}^n$ be a bounded open set such that $\operatorname{supp} u \subset U$, and let $R > 0$. Then there exists a constant $h_0 > 0$ such that*

$$(1 - \mathcal{O}(h^{k/2}))||u||^2_{L^2(\mathbb{R}^n)} \leq ||Tu(\cdot\,; h)||^2_{H_\Phi(U \times \{|\xi| \leq R\})} \qquad \forall h \in (0, h_0).$$

Then, given this proposition, we can apply Theorem 3.1 to get local H_Φ lower bounds on Tu.

Proof. (of Proposition 3.7) We begin with the one-dimensional case, where we first get exponential *upper* bounds on the set

$$\{(x,\xi) \in \mathbb{R}^2;\, x \notin U\}.$$

Integrating in ξ over all of $\mathbb{R}$, with the weight $\exp(-2\Phi/h) = e^{-\xi^2/h}$, we get

$$\begin{aligned}
\int |Tu(x,\xi;h)|^2 e^{-\xi^2/h} d\xi \\
&= 2^{-1}(\pi h)^{-3/2} \iiint e^{i(x-y)\xi/h} e^{-(x-y)^2/(2h)} e^{-i(x-w)\xi/h} \\
&\qquad e^{-(x-w)^2/(2h)} u(y)\overline{u(w)}\, dy\, dw\, d\xi \\
&= (\pi h)^{-1/2} \iint \left[(2\pi h)^{-1} \int e^{i(w-y)\xi/h}\, d\xi\right] e^{-(x-y)^2/(2h)} \\
&\qquad e^{-(x-w)^2/(2h)} u(y)\overline{u(w)}\, dy\, dw \\
&= (\pi h)^{-1/2} \iint \delta(w-y) e^{-(x-y)^2/(2h)} \\
&\qquad e^{-(x-w)^2/(2h)} u(y)\overline{u(w)}\, dy\, dw \\
&= (\pi h)^{-1/2} \int e^{-(x-y)^2/h} |u(y)|^2\, dy.
\end{aligned}$$

Then, for $\delta := \operatorname{dist}(\complement U, \operatorname{supp} u)$,

$$\begin{aligned}
||Tu||^2_{H_\Phi(x\in\complement U)} &\leq (\pi h)^{-1/2} e^{-\delta^2/(2h)} \iint_{x\in\,\complement U} e^{-(x-y)^2/(2h)} |u(y)|^2\, dy\, dx \\
&\leq \sqrt{2} e^{-\delta^2/(2h)} ||u||^2_{L^2(\mathbb{R})}.
\end{aligned}$$

It thus remains to find a lower bound for

$$||Tu||^2_{H_\Phi(|\xi|\leq R)} = \iint_{|\xi|\leq R} |Tu(x,\xi;h)|^2 e^{-\xi^2/h} dx\, d\xi.$$

We start by integrating in x, over all of $\mathbb{R}$:

$$\begin{aligned}
\int |Tu(x,\xi;h)|^2 e^{-\xi^2/h} dx = 2^{-1}(\pi h)^{-3/2} \iiint e^{i(w-y)\xi/h} e^{-(x-y)^2/(2h)} e^{-(x-w)^2/(2h)} \\
u(y)\overline{u(w)}\, dy\, dw\, dx.
\end{aligned}$$

By taking the x-integration first, we get

$$\int |Tu(x,\xi;h)|^2 e^{-\xi^2/h} dx = (2\pi h)^{-1} \iint e^{i(w-y)\xi/h} e^{-(w-y)^2/(4h)} u(y)\overline{u(w)}\, dy\, dw.$$

We then integrate over $|\xi| \le R$, which gives

$$\iint_{|\xi|\le R} |Tu(x,\xi;h)|^2 e^{-\xi^2/h} dx\, d\xi$$
$$= \frac{1}{\pi} \iint \frac{\sin(R(w-y)/h)}{w-y} e^{-(w-y)^2/(4h)} u(y)\overline{u(w)} dy\, dw.$$

For convenience we replace R by $R\pi$. Then we finally arrive at the expression

$$||Tu||^2_{H_\Phi(|\xi|\le R\pi)} = \iint u(y) K_h(y-w)\overline{u(w)} dy\, dw, \tag{3.10}$$

where

$$K_h(x) := \frac{\sin(R\pi x/h)}{\pi x} e^{-x^2/(4h)}.$$

Now we show that K_h behaves like an approximate identity. By a change of variables we have

$$\int K_h(x) dx = \frac{1}{\pi} \int \frac{\sin x}{x} \exp\left(-\frac{hx^2}{4R^2\pi^2}\right) dx.$$

We then use Parseval's formula to get

$$\int K_h(x) dx = 2R\sqrt{\frac{\pi}{h}} \int_0^1 e^{-\pi^2 R^2 x^2/h} dx$$
$$= \frac{2}{\sqrt{\pi}} \int_0^{\pi R/\sqrt{h}} e^{-t^2} dt.$$

That is,

$$\int K_h(x) dx = 1 - \frac{2}{\sqrt{\pi}} \operatorname{Erfc}\left(\frac{\pi R}{\sqrt{h}}\right),$$

where Erfc is the complementary error function

$$\operatorname{Erfc}(x) = \int_x^\infty e^{-t^2} dt.$$

But Erfc has the well-known asymptotic expansion

$$\mathrm{Erfc}(x) = \frac{1}{2}e^{-x^2}\left[\sum_{m=0}^{M-1}\frac{(-1)^m\Gamma(m+\frac{1}{2})}{x^{2m+1}\Gamma(\frac{1}{2})} + \mathcal{O}(|x|^{-2M-1})\right]$$

as $x \to \infty$, for $M = 1, 2, 3, \ldots$ So, in particular,

$$\int K_h(x)dx = 1 - \frac{1}{\sqrt{\pi}}e^{-\pi^2R^2/h}\left[\frac{\sqrt{h}}{\pi R} + \mathcal{O}(h^{3/2})\right]. \tag{3.11}$$

Lemma 3.8. *$K_h = \delta_0 + \mathcal{O}(h^{k/2})$ in $\mathcal{D}'^k(\mathbb{R})$ as $h \to 0$.*

Proof. For $\phi \in C_0^k(\mathbb{R})$, we have the Taylor expansion

$$\phi(x) = \sum_{j=0}^{k-1}\frac{\phi^{(j)}(0)}{j!}x^j + k\int_0^1(1-t)^{k-1}\phi^{(k)}(tx)\frac{x^k}{k!}dt.$$

Hence

$$\begin{aligned}\int K_h(x)\phi(x)dx = \phi(0)\int K_h(x)dx + \sum_{j=1}^{k-1}\frac{\phi^{(j)}(0)}{j!}\int K_h(x)x^j dx \\ + k\int_0^1(1-t)^{k-1}\frac{1}{k!}\left[\int K_h(x)\phi^{(k)}(tx)x^k dx\right]dt.\end{aligned}$$

But an induction argument involving integration by parts shows that, when $j \in \{1, 2, \ldots\}$,

$$\int K_h(x)x^j dx = \mathcal{O}(e^{-\pi^2R^2/h}).$$

Also, we have that the Taylor remainder term is bounded by a constant times

$$\begin{aligned}\left(\int |K_h(x)||x|^k dx\right)||\phi||_{C^k} &\leq \left(\frac{1}{\pi}\int e^{-x^2/(4h)}|x|^{k-1}dx\right)||\phi||_{C^k} \\ &= \mathcal{O}(h^{k/2})||\phi||_{C^k}.\end{aligned}$$

So

$$\int K_h(x)\phi(x)dx = \phi(0) + \mathcal{O}(h^{k/2})||\phi||_{C^k}.$$

□

Finally, we put it all together to get

$$\begin{aligned}||Tu||^2_{H_\Phi(|\xi|\le R\pi)} &= \iint u(y)K_h(y-w)\overline{u(w)}dy\,dw \\ &= ||u||^2_{L^2(\mathbb{R})} + \mathcal{O}(h^{k/2})||u||_{L^1(\mathbb{R})}||u||_{C^k(\mathbb{R})} \\ &= (1+\mathcal{O}(h^{k/2}))||u||^2_{L^2(\mathbb{R})},\end{aligned}$$

which completes the proof of the proposition in the one-dimensional case.

For the general case, we obtain exponential upper bounds on the set

$$\{(x,\xi)\in\mathbb{R}^{2n}\,;x\notin U\}$$

in exactly the same way as in the one-dimensional case.

We next consider the cube

$$Q_R := \{\xi\in\mathbb{R}^n; |\xi_j|\le R,\ j=1,2,\dots,n\},$$

and wish to find a lower bound for

$$\iint_{\mathbb{R}^n\times Q_R} |Tu(x,\xi;h)|^2 e^{-\xi^2/h}dxd\xi.$$

We start by integrating in x, over all of $\mathbb{R}^n$:

$$\int |Tu(x,\xi;h)|^2e^{-\xi^2/h}dx = 2^{-n}(\pi h)^{-3n/2}\iiint e^{i(w-y)\xi/h}e^{-(x-y)^2/(2h)}e^{-(x-w)^2/(2h)} \\ u(y)\overline{u(w)}\,dy\,dw\,dx.$$

By performing the x-integration first, we get

$$\int |Tu(x,\xi;h)|^2e^{-\xi^2/h}dx = (2\pi h)^{-n}\iint e^{i(w-y)\xi/h}e^{-(w-y)^2/(4h)}u(y)\overline{u(w)}\,dy\,dw.$$

Then integrating over Q_R gives

$$\iint_{\mathbb{R}^n\times Q_R}|Tu(x,\xi;h)|^2e^{-\xi^2/h}dx\,d\xi = \pi^{-n}\iint\prod_{j=1}^n\left[\left(\frac{1}{w_j-y_j}\right)\sin\left(\frac{R}{h}(w_j-y_j)\right)\right] \\ e^{-(w-y)^2/(4h)}u(y)\overline{u(w)}\,dy\,dw.$$

As before, we replace R by $R\pi$ for convenience. Then

$$||Tu||^2_{H_\Phi(\mathbb{R}^n \times Q_{R\pi})} = \iint u(y) K_h(y-w) \overline{u(w)} dy\, dw,$$

where

$$K_h(x) := \prod_{j=1}^{n} \left[\frac{\sin(R\pi x_j/h)}{\pi x_j} e^{-x_j^2/(4h)} \right].$$

That is,

$$K_h = K_h^1 \otimes \cdots \otimes K_h^n,$$

where

$$K_h^j(x_j) := \frac{\sin(R\pi x_j/h)}{\pi x_j} e^{-x_j^2/(4h)}.$$

Then, from (3.11), we have that

$$\int K_h(x) dx = 1 + \mathcal{O}(e^{-\pi^2 R^2/h}).$$

Now, to show that K_h inherits convergence properties from the K_h^j, we need a distribution-theoretical lemma:

Lemma 3.9. *Let X_1 and X_2 be open subsets of $\mathbb{R}^{n_1}$ and $\mathbb{R}^{n_2}$, respectively. Let $u_j, u \in \mathcal{D}'^k(X_1)$ and $v_j, v \in \mathcal{D}'^\ell(X_2)$, for $j = 1, 2, \ldots$, be such that*

$$u = u_j + \mathcal{O}(f(j)) \quad \text{in } \mathcal{D}'^k(X_1)$$

and

$$v = v_j + \mathcal{O}(g(j)) \quad \text{in } \mathcal{D}'^\ell(X_2),$$

for some positive, bounded functions f and g. Then

$$u \otimes v = u_j \otimes v_j + \mathcal{O}(\max\{f(j), g(j)\}) \qquad \text{in } \mathcal{D}'^{k+\ell}(X_1 \times X_2).$$

Proof. Let K be a compact subset of $X_1 \times X_2$, and let K_i, $i = 1, 2$, be the projection of K onto X_i. Then, by hypothesis, there exists a constant $C > 0$ such that

$$|v(\phi_2) - v_j(\phi_2)| \leq Cg(j) \sum_{|\alpha| \leq \ell} \sup|\partial^\alpha \phi_2| \qquad \forall \phi_2 \in C_0^\ell(K_2).$$

In particular,

$$\begin{aligned} |v(\phi(x_1, \cdot)) - v_j(\phi(x_1, \cdot))| &\leq Cg(j) \sum_{|\alpha| \leq \ell} \sup_{x_2} |\partial_{x_2}^\alpha \phi(x_1, x_2)| \\ &\leq Cg(j) \sum_{|\alpha| \leq \ell} \sup|\partial^\alpha \phi| \qquad\qquad \forall \phi \in C_0^\ell(K). \end{aligned}$$

Moreover, for $\phi \in C_0^{k+\ell}(K)$ we define

$$\psi_j(x_1) := v_j(\phi(x_1, \cdot))$$

and

$$\psi(x_1) := v(\phi(x_1, \cdot)),$$

which are all in $C_0^k(K_1)$ by Theorem 2.1.3 in [Hor03]. Then, as we have just shown,

$$|\psi(x_1) - \psi_j(x_1)| \leq Cg(j)||\phi||_{C^\ell(X_1 \times X_2)}.$$

Additionally, by Theorem 2.1.3 in [Hor03],

$$\begin{aligned} \partial_{x_1}^\alpha \psi_j(x_1) &\equiv \partial_{x_1}^\alpha v_j(\phi(x_1, \cdot)) \\ &= v_j(\partial_{x_1}^\alpha \phi(x_1, \cdot)) \end{aligned}$$

for $|\alpha| \leq k$; then a repetition of the above argument shows that

$$|\partial_{x_1}^\alpha \psi(x_1) - \partial_{x_1}^\alpha \psi_j(x_1)| \leq Cg(j)||\phi||_{C^{\ell+|\alpha|}(X_1 \times X_2)}.$$

Hence

$$\psi = \psi_j + \mathcal{O}(g(j))||\phi||_{C^{k+\ell}(X_1 \times X_2)} \qquad \text{in } C_0^k(X_1)$$

in the sense that

$$\sup |\partial^\alpha(\psi_j - \psi)| = \mathcal{O}(g(j))||\phi||_{C^{k+\ell}(X_1\times X_2)}$$

for every $|\alpha| \leq k$ and where $\operatorname{supp}(\psi_j - \psi) \subset K_1(\subset\subset X_1)$ for all j.

Now, due to the hypothesized convergence property of the u_j,

$$|u_j(\tilde{\psi})| \leq C \sum_{|\alpha|\leq k} \sup |\partial^\alpha \tilde{\psi}| \qquad \forall \tilde{\psi} \in C_0^k(K_1)$$

for some constant $C > 0$ independent of j. Hence

$$\begin{aligned}
|u(\psi) - u_j(\psi_j)| &\leq |u(\psi) - u_j(\psi)| + |u_j(\psi - \psi_j)| \\
&\leq \mathcal{O}(f(j))||\psi||_{C^k} + \mathcal{O}(1)||\psi - \psi_j||_{C^k} \\
&\leq \mathcal{O}(\max\{f(j), g(j)\})||\phi||_{C^{k+\ell}(X_1\times X_2)}.
\end{aligned}$$

And so, by Theorem 5.1.1 in [Hor03],

$$\begin{aligned}
(u \otimes v - u_j \otimes v_j)(\phi) &= u(\psi) - u_j(\psi_j) \\
&= \mathcal{O}(\max\{f(j), g(j)\})||\phi||_{C^{k+\ell}(X_1\times X_2)}.
\end{aligned}$$

That is,

$$u \otimes v = u_j \otimes v_j + \mathcal{O}(\max\{f(j), g(j)\}) \qquad \text{in } \mathcal{D}'^{k+\ell}(X_1 \times X_2).$$

$\square$

Now, by the one-dimensional case, we have that

$$K_h^j = \delta_0 + \mathcal{O}(h^{k/2}) \qquad \text{in } \mathcal{D}'^k(\mathbb{R}) \text{ as } h \to 0,$$

for all $j = 1, 2, \ldots, n$. Hence Lemma 3.9 shows that

$$K_h = K_h^1 \otimes \cdots \otimes K_h^n = \delta_0 \otimes \cdots \otimes \delta_0 + \mathcal{O}(h^{k/2}) \qquad \text{in } \mathcal{D}'^{nk}(\mathbb{R}^n).$$

Therefore

$$||Tu||^2_{H_\Phi(\mathbb{R}^n\times Q_{R\pi})} = \int |u(y)|^2dy + \mathcal{O}(h^{k/2})||u||_{L^1}||u||_{C^{nk}} \text{ as } h \to 0,$$

which, together with the upper bound on

$$||Tu||^2_{H_\Phi(\complement U\times\mathbb{R}^n)},$$

completes the proof of Proposition 3.7 in the general case. $\square$

CHAPTER 4

Laguerre-Gaussian Modes and the Wigner Transform

4.1 Introduction

In the early 1990s it was observed that a Laguerre-Gaussian (LG) beam of paraxial light has a well-defined orbital angular momentum and that such a beam may be created from a Hermite-Gaussian (HG) beam by way of an astigmatic optical system [ABS92]. This discovery was soon to find applications, for example, in biology (for "optical tweezers") and in the study of quantum entanglement [ABP03]. Additionally, recent experiments suggest that beams with orbital angular momentum might be generated *in situ*, in free electron lasers [HAR07].

In this chapter we consider the corresponding LG modes for the two-dimensional harmonic oscillator, which appear in the transversal plane at the laser beam's waist. Indeed, one may use the operator algebra of the harmonic oscillator to study the analytical forms of the HG and LG beams [NA93], [VN04]. Here we demonstrate that the LG modes arise as Wigner transforms of HG modes, and we proceed to find their own Wigner transforms. Our methods provide an alternative to those of Gase [Gas95] and those of Simon and Agarwal [SA00]; in particular, Simon and Agarwal were first to discover the closed form expression that we rederive here, using our new point of view.

We define the d-dimensional Wigner transform as

$$W_d(f,g)(\vec{x},\vec{\xi}) = (2\pi)^{-d/2} \int e^{i\vec{p}\cdot\vec{\xi}} \overline{f\left(\frac{\vec{x}+\vec{p}}{\sqrt{2}}\right)} g\left(\frac{\vec{x}-\vec{p}}{\sqrt{2}}\right) d\vec{p}$$

for functions f, g of d variables. If $d = 1$, we omit the subscript. The Wigner transform is often restricted to the case when $f \equiv g$, and then one writes $W_d(f) := W_d(f,f)$. More generally, we define the extended Wigner transform, of a function F of $2d$ variables, as

$$\tilde{W}_d(F)(\vec{x},\vec{\xi}) = (2\pi)^{-d/2} \int e^{i\vec{p}\cdot\vec{\xi}} F\left(\frac{\vec{x}+\vec{p}}{\sqrt{2}}, \frac{\vec{x}-\vec{p}}{\sqrt{2}}\right) d\vec{p}.$$

This more general transform is fundamental for the study of LG modes; this is our main insight and provides the central theme for the chapter.

Our main results are summarized in the following theorem.

Theorem 4.1. *Let h_j denote the j^{th} Hermite function, so that $h_{jk}(x,y) = h_j(x)h_k(y)$ are the HG modes.*

- ***(a)*** *The extended Wigner transform intertwines the creation and annihilation operators of the HG and LG modes.*
- ***(b)*** *The LG modes are precisely $\tilde{W}(h_{jk})$: the extended Wigner transforms of the HG modes.*
- ***(c)*** *The Wigner transforms of the LG modes are given by*

$$W_2(\tilde{W}(h_{jk}), \tilde{W}(h_{mn}))(\vec{x},\vec{\xi}) = \tilde{W}(h_{jm})\left(\frac{x_1+\xi_2}{\sqrt{2}}, \frac{\xi_1-x_2}{\sqrt{2}}\right) \tilde{W}(h_{kn})\left(\frac{x_1-\xi_2}{\sqrt{2}}, \frac{\xi_1+x_2}{\sqrt{2}}\right). \tag{4.1}$$

We remark that part (b) of the theorem follows from part (a) and the fact that $\tilde{W}(h_{00}) = h_{00}$.

In the case $(j,k) = (m,n)$, the formula (4.1) was proven by Simon and Agarwal, using the metaplectic representation, and in fact their proof extends to the general case without modification [SA00]. The generalization should be useful in light of the relationship between the Wigner transform and the Weyl quantization of observables. Indeed, for any tempered distribution $\sigma \in \mathcal{S}'(\mathbb{R}^{2d})$ we may define the Weyl quantization of σ as the [pseudodifferential] operator given by

$$\left(\mathrm{Op}^W(\sigma)u\right)(x) = 2^{-3d/2}\pi^{-d} \iint \exp\left(\frac{i(x-y)\xi}{\sqrt{2}}\right) \sigma\left(\frac{x+y}{\sqrt{2}}, \xi\right) u(y)\, dy\, d\xi.$$

The normalization factor is chosen so that $\mathrm{Op}^W(1)$ is the identity operator. Then it is easy to check that for any Schwartz functions $f, g \in \mathcal{S}(\mathbb{R}^d)$ we have

$$\langle f|\mathrm{Op}^W(\sigma)g\rangle = 2^{-d}\pi^{-d/2} \iint \sigma(x,\xi) W_d(f,g)(x,\xi)\, dx\, d\xi.$$

For an exposition of the Weyl calculus of pseudodifferential operators, the reader may consult the book of Gerald Folland [Fol89].

In Section 4.2 we review the theory of the one-dimensional harmonic oscillator. Since this subject is very well known, we will be brief, so the section is mostly a means of setting up notation for the following sections. In Section 4.3, we review the theory of the two-dimensional harmonic oscillator. Our primary reference for Sections 4.2 and 4.3 is the classic book of Messiah [Mes58].

In Section 4.4 we write the $\{Q\}$-representation in terms of complex variables, which provides a clean expression for the LG modes in terms of Laguerre polynomials. The connection with LG modes of paraxial light is briefly exhibited in Section 4.5.

The LG modes are expressed as Wigner transforms in Section 4.6, and in Section 4.7 we calculate their own Wigner transforms.

4.2 The One-dimensional Harmonic Oscillator

We begin by setting up the notation for the one-dimensional harmonic oscillator, given by

$$H = \frac{1}{2}(P^2 + Q^2), \quad \text{where } [Q, P] = i.$$

We set

$$a = \frac{1}{\sqrt{2}}(Q + iP) \quad \text{and} \quad a^\dagger = \frac{1}{\sqrt{2}}(Q - iP)$$

so that

$$[a, a^\dagger] = 1 \quad \text{and} \quad H = \frac{1}{2}(aa^\dagger + a^\dagger a).$$

Moreover, we define

$$N = a^\dagger a$$

so that

$$H = N + \frac{1}{2}.$$

It is well known that $\mathrm{Spec}(N) = \{0, 1, 2, \ldots\}$ consists of nondegenerate eigenvalues and that $a^\dagger$ and a are the "ladder operators": the creation and annihilation operators, respectively. The associated eigenvectors form a complete set, so we can normalize to get an orthonormal basis of eigenvectors for the observable N:

$$|0\rangle, \quad |1\rangle, \quad |2\rangle, \ldots$$

corresponding to the eigenvalues

$$0, \quad 1, \quad 2, \ldots$$

In the $\{Q\}$-Representation (that is, the Schrödinger representation where states are considered as functions of position) the ladder operators are written as

$$a = \frac{1}{\sqrt{2}}\left(x + \frac{d}{dx}\right)$$

and

$$a^\dagger = \frac{1}{\sqrt{2}}\left(x - \frac{d}{dx}\right).$$

The ground state h_0 satisfies

$$\left[\frac{d}{dx} + x\right] h_0(x) = 0,$$

so that

$$h_0(x) = \pi^{-1/4} e^{-x^2/2}.$$

Using the ladder operators, we get the rest of the eigenvectors, which are precisely the Hermite functions:

$$\begin{aligned} h_n(x) &= \pi^{-1/4}(n!)^{-1/2} 2^{-n/2}\left(x - \frac{d}{dx}\right)^n e^{-x^2/2} \\ &= \pi^{-1/4}(n!)^{-1/2} 2^{-n/2}(-1)^n e^{x^2/2}\frac{d^n}{dx^n}e^{-x^2} \\ &= \pi^{-1/4}(n!)^{-1/2} 2^{-n/2} e^{-x^2/2} H_n(x) \end{aligned}$$

where the H_n are the Hermite polynomials

$$H_n(x) = (-1)^n e^{x^2}\frac{d^n}{dx^n}e^{-x^2}.$$

4.3 The Two-Dimensional Isotropic Harmonic Oscillator

In two dimensions, we have

$$H = \frac{1}{2}(P_1^2 + P_2^2 + Q_1^2 + Q_2^2)$$

with creation and annihilation operators inherited from the one-dimensional case:

$$\begin{aligned} a_j^\dagger &= \frac{1}{\sqrt{2}}(Q_j - iP_j), \\ a_j &= \frac{1}{\sqrt{2}}(Q_j + iP_j), \qquad j = 1, 2. \end{aligned}$$

These are interpreted as creation and annihilation operators, respectively, of quanta of type $j \in \{1, 2\}$. They satisfy

$$[a_i, a_j] = [a_i^\dagger, a_j^\dagger] = 0,$$

$$[a_i, a_j^\dagger] = \delta_{ij}.$$

And we have the corresponding "number operators"

$$N_j = a_j^\dagger a_j, \qquad j = 1, 2,$$

with

$$N = N_1 + N_2$$

representing the total number.

Now the eigenvalues for

$$H = N + 1$$

are

$$\{1, 2, 3, \ldots\}$$

and the eigenvalue j has degeneracy j. Hence there are many possible choices of eigenbasis. One often simply takes the basis consisting of tensor products of the one-dimensional eigenvectors, corresponding to the complete set of commuting observables $\{N_1, N_2\}$. The elements of this basis are given by

$$|n_1 n_2\rangle = (n_1! n_2!)^{-1/2} a_1^{\dagger n_1} a_2^{\dagger n_2} |00\rangle.$$

These are precisely the HG modes; in the Schrödinger representation, they are tensor products of Hermite functions.

However, here we will construct another basis.

The angular momentum operator L is defined by

$$L = Q_1 P_2 - Q_2 P_1 = i(a_1 a_2^\dagger - a_1^\dagger a_2),$$

and one may check that it is a constant of motion. We will show that $\{N, L\}$ is another complete set of commuting observables.

Let

$$A_\pm = \frac{1}{\sqrt{2}}(a_1 \mp i a_2)$$

and

$$A_\pm^\dagger = \frac{1}{\sqrt{2}}(a_1^\dagger \pm i a_2^\dagger).$$

Then

$$[A_r, A_s] = [A_r^\dagger, A_s^\dagger] = 0 \qquad \text{and}$$

$$[A_r, A_s^\dagger] = \delta_{rs} \qquad \text{for } r, s \in \{+, -\}.$$

We think of $A_r^\dagger$, A_r as creation and annihilation operators, respectively, of quanta of type $r \in \{+, -\}$, so then

$$N_r = A_r^\dagger A_r$$

represents the number of "r quanta".

Hence the problem of finding eigenvectors common to N_+ and N_- is formally equivalent to finding eigenvectors common to N_1 and N_2. So by the usual arguments we see that

$$\mathrm{Spec}(N_+) = \mathrm{Spec}(N_-) = \{0, 1, 2, \ldots\}$$

and that these two observables, N_+ and N_-, form a complete set of commuting observables: to each (n_+, n_-) there is a common eigenvector, denoted by $|n_+ n_-\rangle$, that is unique to within a constant.

In fact,

$$A_+|00\rangle = A_-|00\rangle = 0$$

and the states

$$|n_+ n_-\rangle = (n_+! n_-!)^{-1/2} A_+^{\dagger n_+} A_-^{\dagger n_-} |00\rangle$$

form a complete orthonormal eigenbasis common to N_+ and N_-:

$$N_+|n_+ n_-\rangle = n_+|n_+ n_-\rangle$$

and

$$N_-|n_+ n_-\rangle = n_-|n_+ n_-\rangle.$$

We find that

$$N = N_+ + N_-$$

and that

$$L = N_+ - N_-.$$

Hence N and L form a complete set of commuting observables. Moreover,

$$[L, A_\pm^\dagger] = \pm A_\pm^\dagger$$

and

$$[L, A_\pm] = \mp A_\pm,$$

so when they act upon an eigenvector of L, $A_+^\dagger$ and A_- increase L by one unit, and $A_-^\dagger$ and A_+ decrease L by one unit. So it is natural to consider N_+ as the number of particles with positive charge, N_- as the number of particles with negative charge, and L as the total charge (to within a constant).

4.4 The Two-Dimensional Isotropic Harmonic Oscillator in the $\{Q\}$-Representation

In the $\{Q\}$-representation, we write

$$\begin{aligned} a_1 &= \frac{1}{\sqrt{2}}\left(x + \frac{\partial}{\partial x}\right), \qquad & a_2 &= \frac{1}{\sqrt{2}}\left(y + \frac{\partial}{\partial y}\right), \\ a_1^\dagger &= \frac{1}{\sqrt{2}}\left(x - \frac{\partial}{\partial x}\right), \qquad & a_2^\dagger &= \frac{1}{\sqrt{2}}\left(y - \frac{\partial}{\partial y}\right), \end{aligned} \tag{4.2}$$

so that we have

$$\begin{aligned} A_+ &= \frac{1}{2}\left(x + \frac{\partial}{\partial x} - i\left(y + \frac{\partial}{\partial y}\right)\right), \\ A_- &= \frac{1}{2}\left(x + \frac{\partial}{\partial x} + i\left(y + \frac{\partial}{\partial y}\right)\right), \\ A_+^\dagger &= \frac{1}{2}\left(x - \frac{\partial}{\partial x} + i\left(y - \frac{\partial}{\partial y}\right)\right), \\ A_-^\dagger &= \frac{1}{2}\left(x - \frac{\partial}{\partial x} - i\left(y - \frac{\partial}{\partial y}\right)\right). \end{aligned} \tag{4.3}$$

In complex notation, these take a simple form. We write $z = x + iy$, so that

$$\frac{\partial}{\partial z} = \frac{1}{2}\left(\frac{\partial}{\partial x} + \frac{1}{i}\frac{\partial}{\partial y}\right) \qquad \text{and} \qquad \frac{\partial}{\partial \overline{z}} = \frac{1}{2}\left(\frac{\partial}{\partial x} - \frac{1}{i}\frac{\partial}{\partial y}\right).$$

Then

$$\begin{aligned} A_+ &= \frac{1}{2}\overline{z} + \frac{\partial}{\partial z}, \qquad & A_- &= \frac{1}{2}z + \frac{\partial}{\partial \overline{z}}, \\ A_+^\dagger &= \frac{1}{2}z - \frac{\partial}{\partial \overline{z}}, \qquad & A_-^\dagger &= \frac{1}{2}\overline{z} - \frac{\partial}{\partial z}. \end{aligned}$$

Moreover, we can write

$$A_+^\dagger = -e^{z\overline{z}/2}\frac{\partial}{\partial \overline{z}}e^{-z\overline{z}/2} \qquad \text{and} \qquad A_-^\dagger = -e^{z\overline{z}/2}\frac{\partial}{\partial z}e^{-z\overline{z}/2}.$$

The ground state is given by

$$u_0(z, \overline{z}) = \pi^{-1/2}e^{-z\overline{z}/2} \equiv \langle z, \overline{z}|00\rangle,$$

and of course we get all other eigenvectors by applying the creation operators to this. These are precisely the LG modes. Explicitly,

$$\begin{aligned}\langle z,\overline{z}|n_+n_-\rangle &= \langle z,\overline{z}|(n_+!n_-!)^{-1/2}A_+^{\dagger n_+}A_-^{\dagger n_-}|00\rangle \\ &= \pi^{-1/2}(n_+!n_-!)^{-1/2}(-1)^{n_++n_-}e^{z\overline{z}/2}\left(\frac{\partial}{\partial\overline{z}}\right)^{n_+}\left(\frac{\partial}{\partial z}\right)^{n_-}e^{-z\overline{z}}.\end{aligned}$$

We will now formulate this in terms of Laguerre polynomials.

First suppose that $n_+ \geq n_-$. Then

$$\begin{aligned}\langle z,\overline{z}|n_+n_-\rangle &= \pi^{-1/2}(n_+!n_-!)^{-1/2}(-1)^{n_++n_-}e^{z\overline{z}/2}\left(\frac{\partial}{\partial z}\right)^{n_-}\left[(-z)^{n_+}e^{-z\overline{z}}\right] \\ &= \pi^{-1/2}(n_+!n_-!)^{-1/2}(-1)^{n_-}e^{z\overline{z}/2}\overline{z}^{(n_--n_+)}\left(\frac{\partial}{\partial(z\overline{z})}\right)^{n_-}\left[(z\overline{z})^{n_+}e^{-z\overline{z}}\right].\end{aligned}$$

We define the Laguerre polynomials by

$$L_n^\alpha(x) = \frac{x^{-\alpha}e^x}{n!}\frac{d^n}{dx^n}\left(e^{-x}x^{n+\alpha}\right)$$

for $n \geq 0$ and $\alpha > -1$. Then we see that, when $n_+ \geq n_-$,

$$\langle z,\overline{z}|n_+n_-\rangle = \pi^{-1/2}\left(\frac{n_-!}{n_+!}\right)^{1/2}(-1)^{n_-}z^{(n_+-n_-)}e^{-z\overline{z}/2}L_{n_-}^{n_+-n_-}(z\overline{z}).$$

On the other hand, if $n_+ \leq n_-$, similar arguments show that

$$\langle z,\overline{z}|n_+n_-\rangle = \pi^{-1/2}\left(\frac{n_+!}{n_-!}\right)^{1/2}(-1)^{n_+}\overline{z}^{(n_--n_+)}e^{-z\overline{z}/2}L_{n_+}^{n_--n_+}(z\overline{z}).$$

We summarize this in the following theorem:

Theorem 4.2. *We consider the states $|n_+n_-\rangle$ in the $\{Q\}$-representation with position coordinates $(x,y) \in \mathbb{R}^2$, and we write $z = x + iy$. Then*

$$\langle z,\overline{z}|n_+n_-\rangle = \begin{cases}\pi^{-1/2}\left(\frac{n_-!}{n_+!}\right)^{1/2}(-1)^{n_-}z^{(n_+-n_-)}e^{-z\overline{z}/2}L_{n_-}^{n_+-n_-}(z\overline{z}) & \text{if } n_+ \geq n_-, \\ \pi^{-1/2}\left(\frac{n_+!}{n_-!}\right)^{1/2}(-1)^{n_+}\overline{z}^{(n_--n_+)}e^{-z\overline{z}/2}L_{n_+}^{n_--n_+}(z\overline{z}) & \text{if } n_+ \leq n_-.\end{cases}$$

4.5 Comparison With LG Modes of Paraxial Light

The time-harmonic field amplitudes of LG optical modes are expressed in cylindrical coordinates, with propagation coordinate z along the beam axis, as

$$\tilde{u}_{p,\ell}(\mathbf{r}) \propto e^{-i\Phi(\mathbf{r})} e^{-r^2/w(z)^2} \left(\frac{r\sqrt{2}}{w(z)}\right)^{|\ell|} L_p^{|\ell|}\left(\frac{2r^2}{w(z)^2}\right)$$

where the phase is

$$\Phi(\mathbf{r}) = \ell\phi - kz + \frac{kr^2}{2R(z)} - (2p + \ell + 1)\Psi(z)$$

and where again $L_p^{|\ell|}$ is the Laguerre polynomial with radial and azimuthal indices p and ℓ, respectively. The term $\Psi(z) = \tan^{-1}(z/z_R)$ is part of the Gouy phase, $R(z) = (z_R^2 + z^2)/z$ is the radius of curvature, $w(z) = w_0\sqrt{1 + (z/z_R)^2}$ is the beam waist, and $z_R = kw_0^2/2$ is the Rayleigh range. We see that the total phase evolves helically along the propagation coordinate z. For more on this, see, for example, [ABP03], [HAR07], [Sie86].

In the transversal plane at the beam waist (z=0), we get

$$\tilde{u}_{p,\ell}(\mathbf{r}) \propto e^{-i\ell\phi} e^{-r^2/w_0^2} \left(\frac{r\sqrt{2}}{w_0}\right)^{|\ell|} L_p^{|\ell|}\left(\frac{2r^2}{w_0^2}\right),$$

which is essentially what we have in Theorem 4.2.

4.6 LG Modes Are Wigner Transforms

Physicists in the optics community recently computed the Wigner transforms of LG modes [Gas95], [SA00]. Surprisingly, the states $|n_+ n_-\rangle$ are already themselves Wigner transforms of Hermite functions. The Hermite functions, as in Section 4.2, are given by

$$h_j(x) = \pi^{-1/4}(j!)^{-1/2}2^{-j/2}(-1)^j e^{x^2/2}\frac{d^j}{dx^j}e^{-x^2},$$

which, as we know, satisfy the orthogonality relations

$$\langle h_j | h_k \rangle = \delta_{jk}.$$

And we continue to write the HG modes as

$$h_{jk}(x, y) = h_j(x)h_k(y).$$

Now, for reference, we list the standard properties of the Wigner transform:

$$W(f, g) = \overline{W(g, f)}, \tag{4.4}$$

$$\int W(f, g)(x, \xi)\, d\xi = \sqrt{2\pi}\,\overline{f\left(\frac{x}{\sqrt{2}}\right)}g\left(\frac{x}{\sqrt{2}}\right), \tag{4.5}$$

$$\iint W(f, g)(x, \xi)\, dx\, d\xi = 2\sqrt{\pi}\langle f | g \rangle, \tag{4.6}$$

$$\int W(f, g)(x, \xi)\, dx = \sqrt{2\pi}\,\overline{\hat{f}\left(\frac{\xi}{\sqrt{2}}\right)}\hat{g}\left(\frac{\xi}{\sqrt{2}}\right), \tag{4.7}$$

where $\hat{f}(\xi) = \frac{1}{\sqrt{2\pi}}\int e^{-ix\xi}f(x)\,dx$ is the Fourier transform, and ("Moyal's identity")

$$\langle W(f_1, g_1) | W(f_2, g_2) \rangle = \overline{\langle f_1 | f_2 \rangle}\langle g_1 | g_2 \rangle. \tag{4.8}$$

These properties are well known and are easily checked. But there is another elementary property which seems to be a new observation:

Theorem 4.3. *The extended Wigner transform intertwines the creation operators of the HG and LG modes, and it intertwines the annihilation operators of the HG and LG modes:*

$$A_+^\dagger \tilde{W} = \tilde{W} a_1^\dagger, \qquad A_-^\dagger \tilde{W} = \tilde{W} a_2^\dagger,$$

$$A_+ \tilde{W} = \tilde{W} a_1, \qquad A_- \tilde{W} = \tilde{W} a_2.$$

The proof is a direct calculation, using the expressions (4.2) and (4.3). As a first application, it is now easy to see that the extended Wigner transform commutes with the operators H and N.

Additionally using the fact that $\tilde{W}(h_{00}) = h_{00}$, we have the following corollary:

Corollary 4.4. *We consider the LG modes* $|n_+n_-\rangle$ *in the* $\{Q\}$*-representation with position coordinates* $(x, y) \in \mathbb{R}^2$*. Then we have*

$$\langle x, y|n_+n_-\rangle = W(h_{n_+}, h_{n_-})(x, y).$$

Combining this with Theorem 4.2, we have a formula:

Corollary 4.5. *Suppose* $x, y \in \mathbb{R}$*, and let* $z = x + iy$*. Then*

$$W(h_j, h_k)(x, y) = \begin{cases} \pi^{-1/2}\,(k!/j!)^{1/2}\,(-1)^k z^{j-k} e^{-z\bar{z}/2} L_k^{j-k}(z\bar{z}) & \text{if } j \geq k, \text{ and} \\ \pi^{-1/2}\,(j!/k!)^{1/2}\,(-1)^j \bar{z}^{k-j} e^{-z\bar{z}/2} L_j^{k-j}(z\bar{z}) & \text{if } j \leq k. \end{cases}$$

Corollary 4.5 by itself is not new. For example, two independent proofs may be found in Folland's book [Fol89], although we caution the reader that his statement of the result contains a misprint.

So we have yet another way of understanding the orthogonality relations of the states $|n_+n_-\rangle$: as being inherited from the orthogonality of the Hermite functions. Explicitly,

$$\begin{aligned} \langle m_+m_-|n_+n_-\rangle &= \langle W(h_{m_+}, h_{m_-})|W(h_{n_+}, h_{n_-})\rangle \\ &= \langle h_{m_+}|h_{n_+}\rangle\langle h_{m_-}|h_{n_-}\rangle \\ &= \delta_{m_+n_+}\delta_{m_-n_-}. \end{aligned}$$

As another application of Corollary 4.4, we can think of the LG modes $|n_+n_-\rangle$ as being "interference terms" resulting from the quadratic nature of the Wigner transform. If we apply the Wigner transform to sums of Hermite functions, we get interference terms that are LG modes with nonzero angular momentum. In fact, we have the following polarization identity:

$$\begin{aligned}\langle x, y|n_+n_-\rangle = \frac{1}{4}W(h_{n_+} + h_{n_-})(x,y) - \frac{1}{4}W(h_{n_+} - h_{n_-})(x,y) \\ + \frac{i}{4}W(h_{n_+} - ih_{n_-})(x,y) - \frac{i}{4}W(h_{n_+} + ih_{n_-})(x,y).\end{aligned}$$

One may think of the Wigner transform as being a kind of "product". Just as Hermite functions give rise to two-dimensional HG modes, via the tensor product, Hermite functions also give rise to two-dimensional LG modes, via the Wigner transform. To complete this series of relationships, Simon and Agarwal [SA00] noted that the two-dimensional HG and LG modes are unitarily related by the operator

$$\exp\left(\frac{i\pi}{4}\hat{T}_1\right), \qquad \text{where } \hat{T}_1 = xy - \frac{\partial^2}{\partial x \partial y}.$$

Alternatively, we can use the Wigner transform to again show that the HG and LG modes are unitarily related. For functions F of two variables, we consider the extended Wigner transform of F:

$$\tilde{W}F(x,y) = \frac{1}{\sqrt{2\pi}} \int e^{ipy} F\left(\frac{x+p}{\sqrt{2}}, \frac{x-p}{\sqrt{2}}\right) dp.$$

If we write the $\frac{\pi}{4}$-rotation operator as

$$\begin{aligned}(R^*_{\pi/4}F)(x,p) &= F(R_{\pi/4}(x,p)) \\ &= F\left(\frac{x-p}{\sqrt{2}}, \frac{x+p}{\sqrt{2}}\right),\end{aligned}$$

and if we write the partial Fourier transform as

$$(\mathcal{F}_2F)(x,y) = \frac{1}{\sqrt{2\pi}} \int e^{-ipy} F(x,p)\, dp,$$

then we may write the extended Wigner transform as

$$\tilde{W}F(x,y) = \left(\mathcal{F}_2 R^*_{\pi/4} F\right)(x,y). \tag{4.9}$$

This is clearly a unitary operator, so, in particular, we again see that the HG modes h_{jk} are unitarily related to the LG modes $\tilde{W}(h_{jk})$. Moreover, (4.9) allows a computationally simple, and perhaps more revealing, proof of Theorem 4.3.

The results of this section are surprising, despite their mathematical simplicity. We are accustomed to thinking of the Wigner transform of a function as being a phase space representation of the function, but here the relevant Wigner transform is actually a function of the position vector $(x,y) \in \mathbb{R}^2$, as it is an LG mode. So if we use the Wigner transform to study the phase space properties of LG modes, we are really taking Wigner transforms of Wigner transforms. Gase [Gas95], followed by Simon and Agarwal [SA00], already recently derived expressions for Wigner transforms of LG modes (Gase in terms of a quadruple sum, and Simon and Agarwal in terms of a closed form involving no summation at all). We will do the same in the next section, but now using our new point of view.

4.7 Wigner Transforms of LG Modes

We now proceed to compute the Wigner transforms of the LG modes $\tilde{W}(h_{jk})$. In light of (4.9), the first step is to consider the action of the Wigner transform on partial Fourier transforms.

Lemma 4.6.

$$
\begin{aligned}
&W_2(\mathcal{F}_2 F, \mathcal{F}_2 G)(\vec{x}, \vec{\xi}) \\
&\qquad = \frac{1}{2\pi} \iint e^{i\xi_1 s - i x_2 t} \overline{F\left(\frac{x_1+s}{\sqrt{2}}, \frac{-\xi_2 - t}{\sqrt{2}}\right)} G\left(\frac{x_1 - s}{\sqrt{2}}, \frac{-\xi_2 + t}{\sqrt{2}}\right) ds\, dt.
\end{aligned}
$$

This lemma follows from a direct calculation.

We now apply the lemma to

$$
F = R^*_{\pi/4} h_{jk} \qquad \text{and} \qquad G = R^*_{\pi/4} h_{mn}.
$$

That is,

$$
F(\vec{x}) = h_j\left(\frac{x_1 - x_2}{\sqrt{2}}\right) h_k\left(\frac{x_1 + x_2}{\sqrt{2}}\right)
$$

and similarly for G. Hence the Wigner transforms of the LG modes are given by

$$
\begin{aligned}
&W_2(\tilde{W}(h_{jk}), \tilde{W}(h_{mn}))(\vec{x}, \vec{\xi}) \\
&\qquad = \frac{1}{2\pi} \iint e^{i\xi_1 s - i x_2 t} h_j\left(\frac{(x_1+s)+(\xi_2+t)}{2}\right) h_k\left(\frac{(x_1+s)-(\xi_2+t)}{2}\right) \\
&\qquad\qquad h_m\left(\frac{(x_1-s)+(\xi_2-t)}{2}\right) h_n\left(\frac{(x_1-s)-(\xi_2-t)}{2}\right) ds\, dt.
\end{aligned}
$$

We may simplify this integral by again rotating the variables by $\frac{\pi}{4}$. We state the result as a theorem.

Theorem 4.7. *The Wigner transforms of the LG modes are products of LG modes, given by the formula*

$$
\begin{aligned}
&W_2(\tilde{W}(h_{jk}), \tilde{W}(h_{mn}))(\vec{x}, \vec{\xi}) \\
&\qquad = \tilde{W}(h_{jm})\left(\frac{x_1+\xi_2}{\sqrt{2}}, \frac{\xi_1 - x_2}{\sqrt{2}}\right) \tilde{W}(h_{kn})\left(\frac{x_1 - \xi_2}{\sqrt{2}}, \frac{\xi_1 + x_2}{\sqrt{2}}\right).
\end{aligned}
$$

In the special case $(j,k) = (m,n)$, we have the following formula of Simon and Agarwal [SA00]. It is now proven by combining Corollary 4.5 with Theorem 4.7.

Corollary 4.8. *For $(\vec{x},\vec{\xi}) = (x_1,x_2,\xi_1,\xi_2) \in \mathbb{R}^2 \times \mathbb{R}^2$, we let*

$$Q_0 = \frac{1}{2}(|\vec{x}|^2 + |\vec{\xi}|^2) \qquad \textit{and} \qquad Q_2 = (x_1\xi_2 - x_2\xi_1).$$

Then we have

$$W_2(\tilde{W}(h_{jk}),\tilde{W}(h_{jk}))(\vec{x},\vec{\xi}) = \pi^{-1}(-1)^{j+k}e^{-Q_0}L_j^0(Q_0+Q_2)L_k^0(Q_0-Q_2).$$

For comparison, we also give the Wigner transforms of HG modes:

$$W_2(h_{jk},h_{mn})(\vec{x},\vec{\xi}) = \tilde{W}(h_{jm})(x_1,\xi_1)\tilde{W}(h_{kn})(x_2,\xi_2).$$

In the particular case $(j,k) = (m,n)$, if we let

$$Q_3 = \frac{1}{2}(x_1^2 - x_2^2 + \xi_1^2 - \xi_2^2),$$

then we have the formula

$$W_2(h_{jk},h_{jk})(\vec{x},\vec{\xi}) = \pi^{-1}(-1)^{j+k}e^{-Q_0}L_j^0(Q_0+Q_3)L_k^0(Q_0-Q_3).$$

CHAPTER 5

Manipulation of Semiclassical Photon States

5.1 Introduction

In a series of papers, Gabriel F. Calvo, Antonio Picón, and co-authors studied the manipulation of single-photon states for purposes of quantum communication, from theory to experimental design [CPB06], [CP08], [CPZ08]. They demonstrated the limitations of the metaplectic operators when acting on spatial transverse-field modes, and they showed how one can overcome those limitations with a different family of transformations [CP08]. In particular, they considered the subspace of states spanned by the three lowest Hermite-Gaussian (transverse spatial) modes $\mathcal{H}_{\mathcal{T}} = \{|0,0\rangle, |1,0\rangle, |0,1\rangle\}$ and found a class of operators that would allow arbitrary manipulations of such modes. However, their class of operators includes "non-Gaussian transformations", which are not metaplectic operators. Thus the question arises of what properties of metaplectic operators may be extended, at least partially, to their non-Gaussian transformations. This could lead to the construction of the associated optical system [CP08].

The theory of metaplectic operators is often presented in terms of the Stone-von Neumann theorem (see, for example, the book of G. B. Folland [Fol89]). Rather than attempt to extend the Stone-von Neumann theorem to non-Gaussian transformations, in this chapter we provide an alternative approach, based on the theory of semiclassical Fourier integral operators. We find that a Fourier integral operator ansatz provides approximate solutions to the evolution equations of Calvo and Picón, and in the process we will determine the canonical transformations associated with the non-Gaussian transformations, in the sense of Egorov's theorem. In fact, the canonical transformations are given by the Hamilton flow of the semiclassical Weyl symbols of Calvo and Picón's [now semiclassical] differential operators. The Weyl symbols are dependent on the semiclassical parameter h, so the Hamilton flow is also h-dependent. We take this point of view essentially for three reasons: (1) The operators may be exactly reconstructed from their (h-dependent) Weyl symbols. (2) The flow leaves invariant a disc of radius $\sim \sqrt{h}$, which closes up as $h \to 0$. In the context of laser physics,

$$h = \frac{1}{2}w_0^2,$$

where w_0 denotes the radius of the laser beam's waist. Outside this disc of radius $\sim w_0$, the flow goes to infinity in finite time. This is because the flow propagates along elliptic curves having two components, one bounded and one unbounded. (See Section 5.6 and the Appendix.) And (3) the appropriate version of Egorov's theorem has an error of order $\mathcal{O}(h^2)$, rather than the more typical $\mathcal{O}(h)$. (See Section 5.8.) Moreover, in Section 5.9 we give examples suggesting that we have creation and propagation of singularities along the h-dependent flow.

In this chapter we find that there are fundamental difficulties with the generators of the non-Gaussian transformations. First of all, we show that, although they are clearly symmetric, they have infinite deficiency indices. We are however able to describe all self-adjoint realizations in terms of certain boundary conditions at infinity. And there are difficulties with constructing semiclassical approximations of the unitary groups (the non-Gaussian transformations). We can still find approximate solutions to the evolution equations, but the associated symplectic transformations can blow up in finite time, as they are described in terms of the Weierstrass $\wp$-function, which, as is well-known, has a double pole in every period. However, we show that the semiclassical propagator behaves reasonably well when acting on sufficiently phase-space localized initial conditions, for example, finite sums of semiclassical Hermite-Gaussian modes. This is because, as mentioned above, the Hamilton flow leaves invariant a disc of radius $\sim \sqrt{h}$ centered at the origin.

In Section 5.2 we review the non-Gaussian transformations of Calvo and Picón and show that the generators have infinite deficiency indices. We then describe all self-adjoint realizations in terms of certain boundary conditions at infinity. In Section 5.3 we introduce the semiclassical version of Calvo and Picón's work, so that we can solve their evolution equations approximately, in the semiclassical regime. We illustrate this method in Sections 5.4 and 5.5 by first taking simpler generators and using semiclassical Fourier integral operators to find *exact* solutions to the associated evolution equations, corresponding to "Gaussian transformations". We use the same method for the more difficult non-Gaussian transformations in Sections 5.6 and 5.7, but in that case we only have approximate solutions to the evolution equations. In Section 5.8 we discuss Egorov's theorem and give a property of non-Gaussian transformations that is analogous to a property of metaplectic transformations. We give concluding remarks in Section 5.9, and we include Appendix B for relevant facts regarding elliptic curves.

Notation: We write $D_x = \frac{1}{i}\frac{\partial}{\partial x}$ and similarly for the other variables. Also, we will use the semiclassical Weyl quantization of a symbol σ, defined by

$$\mathrm{Op}_h^W(\sigma)f(x) = (2\pi h)^{-n} \iint e^{i(x-y)\xi/h} \sigma\left(\frac{x+y}{2}, \xi\right) f(y)\, dy\, d\xi.$$

We will mostly be in dimension $n = 1$ or $n = 2$, and we will mostly deal with polynomials σ (hence resulting in semiclassical differential operators with polynomial coefficients).

5.2 The Non-Gaussian Transformations of Calvo and Picón

In this section we recapitulate the recent work of Calvo and Picón [CP08]. They introduced the following eight generators acting on Hermite-Gaussian modes:

$$\hat{\mathcal{T}}_1 = \frac{1}{2}(\hat{a}_x^\dagger \hat{a}_y + \hat{a}_y^\dagger \hat{a}_x),$$

$$\hat{\mathcal{T}}_2 = -\frac{i}{2}(\hat{a}_x^\dagger \hat{a}_y - \hat{a}_y^\dagger \hat{a}_x),$$

$$\hat{\mathcal{T}}_3 = \frac{1}{2}(\hat{a}_x^\dagger \hat{a}_x - \hat{a}_y^\dagger \hat{a}_y),$$

$$\hat{\mathcal{T}}_4 = \frac{1}{2}(\hat{a}_x^\dagger + \hat{a}_x - \hat{a}_x^\dagger \hat{a}_x^\dagger \hat{a}_x - \hat{a}_x^\dagger \hat{a}_x \hat{a}_x - \hat{a}_x^\dagger \hat{a}_y^\dagger \hat{a}_y - \hat{a}_x \hat{a}_y^\dagger \hat{a}_y),$$

$$\hat{\mathcal{T}}_5 = -\frac{i}{2}(\hat{a}_x^\dagger - \hat{a}_x - \hat{a}_x^\dagger \hat{a}_x^\dagger \hat{a}_x + \hat{a}_x^\dagger \hat{a}_x \hat{a}_x - \hat{a}_x^\dagger \hat{a}_y^\dagger \hat{a}_y + \hat{a}_x \hat{a}_y^\dagger \hat{a}_y),$$

$$\hat{\mathcal{T}}_6 = \frac{1}{2}(\hat{a}_y^\dagger + \hat{a}_y - \hat{a}_y^\dagger \hat{a}_y^\dagger \hat{a}_y - \hat{a}_y^\dagger \hat{a}_y \hat{a}_y - \hat{a}_y^\dagger \hat{a}_x^\dagger \hat{a}_x - \hat{a}_y \hat{a}_x^\dagger \hat{a}_x),$$

$$\hat{\mathcal{T}}_7 = -\frac{i}{2}(\hat{a}_y^\dagger - \hat{a}_y - \hat{a}_y^\dagger \hat{a}_y^\dagger \hat{a}_y + \hat{a}_y^\dagger \hat{a}_y \hat{a}_y - \hat{a}_y^\dagger \hat{a}_x^\dagger \hat{a}_x + \hat{a}_y \hat{a}_x^\dagger \hat{a}_x),$$

$$\hat{\mathcal{T}}_8 = \frac{1}{2\sqrt{3}}[-2 + 3(\hat{a}_x^\dagger \hat{a}_x + \hat{a}_y^\dagger \hat{a}_y)],$$

defined in terms of the creation and annihilation operators $\hat{a}_x^\dagger = \frac{1}{\sqrt{2}}\left(x - \frac{\partial}{\partial x}\right)$ and $\hat{a}_x = \frac{1}{\sqrt{2}}\left(x + \frac{\partial}{\partial x}\right)$, respectively, and similarly for the y-variable. We note first of all that $\hat{\mathcal{T}}_4$ and $\hat{\mathcal{T}}_5$ are unitarily related by the Fourier transform $\mathcal{F}$:

$$\hat{\mathcal{T}}_5 = \mathcal{F} \circ \hat{\mathcal{T}}_4 \circ \mathcal{F}^{-1},$$

and that $\hat{\mathcal{T}}_6$ and $\hat{\mathcal{T}}_7$ are obtained from $\hat{\mathcal{T}}_4$ and $\hat{\mathcal{T}}_5$ by simply interchanging the variables x and y.

These generators, within the subspace generated by the lowest three Hermite-Gaussian modes $\mathcal{H}_{\hat{\mathcal{T}}} = \{|0,0\rangle, |1,0\rangle, |0,1\rangle\}$, obey the $SU(3)$ algebra[1]

$$[\hat{\mathcal{T}}_a, \hat{\mathcal{T}}_b] = i f_{abc} \hat{\mathcal{T}}_c$$

$(a, b, c = 1, 2, \ldots 8)$, where the only nonvanishing (up to permutations) structure constants f_{abc} are given by

$$f_{123} = 1, \quad f_{147} = f_{165} = f_{246} = f_{257} = f_{345} = f_{376} = 1/2,$$

and

$$f_{458} = f_{678} = \sqrt{3}/2.$$

We note that the triad of generators

$$\Gamma_1 \equiv \{\hat{\mathcal{T}}_1, \hat{\mathcal{T}}_2, \hat{\mathcal{T}}_3\}$$

gives a $SU(2)$ group that conserves the mode order. The remaining two $SU(2)$ groups are formed by the triads

$$\Gamma_2 \equiv \{\hat{\mathcal{T}}_4, \hat{\mathcal{T}}_5, (\hat{\mathcal{T}}_3 + \sqrt{3}\hat{\mathcal{T}}_8)/2\}$$

and

$$\Gamma_3 \equiv \{\hat{\mathcal{T}}_6, \hat{\mathcal{T}}_7, (-\hat{\mathcal{T}}_3 + \sqrt{3}\hat{\mathcal{T}}_8)/2\}.$$

Unitary operators $\hat{U}_{\Gamma_1}$ generated by the first triad give rise to superpositions between the two modes $|1,0\rangle$ and $|0,1\rangle$, leaving invariant the fundamental mode $|0,0\rangle$. Unitarities $\hat{U}_{\Gamma_2}$ and $\hat{U}_{\Gamma_3}$, generated by the second and third triads, produce superpositions between the two modes $|0,0\rangle$ and $|1,0\rangle$ (leaving invariant $|0,1\rangle$), or the modes $|0,0\rangle$ and $|0,1\rangle$ (leaving invariant $|1,0\rangle$), respectively. For reference,

[1] We sum over c, which is only relevant here for $(a, b) = (4, 5)$ and $(a, b) = (6, 7)$.

we state the operations for $\hat{U}_{\Gamma_2}$:

$$\begin{aligned}
e^{it\hat{\mathcal{T}}_4}|0,0\rangle &= \cos(t/2)|0,0\rangle + i\sin(t/2)|1,0\rangle \\
e^{it\hat{\mathcal{T}}_5}|0,0\rangle &= \cos(t/2)|0,0\rangle + \sin(t/2)|1,0\rangle \\
e^{it((\hat{\mathcal{T}}_3+\sqrt{3}\hat{\mathcal{T}}_8)/2)}|0,0\rangle &= e^{-it/2}|0,0\rangle \\
e^{it\hat{\mathcal{T}}_4}|1,0\rangle &= \cos(t/2)|1,0\rangle + i\sin(t/2)|0,0\rangle \\
e^{it\hat{\mathcal{T}}_5}|1,0\rangle &= \cos(t/2)|1,0\rangle - \sin(t/2)|0,0\rangle \\
e^{it((\hat{\mathcal{T}}_3+\sqrt{3}\hat{\mathcal{T}}_8)/2)}|1,0\rangle &= e^{it/2}|1,0\rangle.
\end{aligned}$$

The corresponding operations for $\hat{U}_{\Gamma_1}$ and $\hat{U}_{\Gamma_3}$ are similar.

However, a difficulty arises when attempting to extend to larger subspaces of $L^2(\mathbb{R}^2)$: starting from the smallest natural domain, the domain of [finite] linear combinations of Hermite-Gaussian modes, the symmetric operators $\hat{\mathcal{T}}_4$, $\hat{\mathcal{T}}_5$, $\hat{\mathcal{T}}_6$, and $\hat{\mathcal{T}}_7$ all have multiple self-adjoint realizations.

We first prove that the deficiency indices of $\hat{\mathcal{T}}_4$ are both infinity. For this we consider how $\hat{\mathcal{T}}_4$ acts on the basis of two-dimensional Hermite-Gaussian modes, which we write either as $|m,n\rangle$ or as ψ_m^n, with m being the mode order in the x-variable and n being the mode order in the y-variable. We have that

$$\hat{\mathcal{T}}_4\psi_m^n = \beta_m^n\psi_{m+1}^n + \beta_{m-1}^n\psi_{m-1}^n, \tag{5.1}$$

where

$$\beta_m^n = \frac{1}{2}\sqrt{m+1}(1-m-n).$$

We take the domain of $\hat{\mathcal{T}}_4$ (as an unbounded linear operator) to be the subspace $D(\hat{\mathcal{T}}_4)$ of [finite] linear combinations of Hermite-Gaussian modes. This domain is dense in $L^2(\mathbb{R}^2)$, and $\hat{\mathcal{T}}_4$ is clearly symmetric with this domain. And it is easy to check that the domain of the adjoint operator is

$$D(\hat{\mathcal{T}}_4^*) = \left\{ g = \sum_{m,n=0}^{\infty} g_m^n \psi_m^n \in L^2(\mathbb{R}^2);\ \sum_{m,n=0}^{\infty} |\beta_m^n g_{m+1}^n + \beta_{m-1}^n g_{m-1}^n|^2 < \infty \right\}, \tag{5.2}$$

and that, for $g = \sum_{m,n=0}^{\infty} g_m^n \psi_m^n \in D(\hat{\mathcal{T}}_4^*)$,

$$\hat{\mathcal{T}}_4^* g = \sum_{m,n=0}^{\infty} (\beta_m^n g_{m+1}^n + \beta_{m-1}^n g_{m-1}^n)\psi_m^n.$$

And we occasionally find it convenient to use the formal operator on sequences given by

$$\hat{t}_4 : \quad (g)_m^n \mapsto (\hat{t}_4 g)_m^n := \beta_m^n g_{m+1}^n + \beta_{m-1}^n g_{m-1}^n.$$

Two somewhat degenerate cases occur when $n = 0$ and $n = 1$, so we treat these separately. For $n = 0$, we get

$$\begin{pmatrix} 0 & \frac{1}{2} & 0 & 0 & 0 & 0 & \cdots \\ \frac{1}{2} & 0 & 0 & 0 & 0 & 0 & \\ 0 & 0 & 0 & -\frac{\sqrt{3}}{2} & 0 & 0 & \cdots \\ 0 & 0 & -\frac{\sqrt{3}}{2} & 0 & -2 & 0 & \\ 0 & 0 & 0 & -2 & 0 & -\frac{3}{2}\sqrt{5} & \\ 0 & 0 & 0 & 0 & -\frac{3}{2}\sqrt{5} & \ddots & \ddots \\ 0 & 0 & 0 & 0 & 0 & \ddots & \ddots \\ \vdots & & \vdots & & \vdots & & \ddots \end{pmatrix},$$

and for $n = 1$, we get

$$\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & \cdots \\ 0 & 0 & -\frac{1}{\sqrt{2}} & 0 & 0 & \\ 0 & -\frac{1}{\sqrt{2}} & 0 & -\sqrt{3} & 0 & \cdots \\ 0 & 0 & -\sqrt{3} & 0 & \ddots & \\ 0 & 0 & 0 & \ddots & \ddots & \ddots \\ \vdots & & \vdots & & \ddots & \ddots \end{pmatrix}.$$

In all other cases we have

$$\begin{pmatrix} 0 & \beta_0^n & 0 & 0 & \cdots \\ \beta_0^n & 0 & \beta_1^n & 0 & \\ 0 & \beta_1^n & 0 & \beta_2^n & \\ 0 & 0 & \beta_2^n & 0 & \ddots \\ \vdots & & & \ddots & \ddots \end{pmatrix}$$

where $\beta_m^n < 0$ for all m and n.

Hence $\hat{\mathcal{T}}_4$ acts like a Jacobi matrix for any fixed n, fixing the mode order in the y-variable, and $\hat{\mathcal{T}}_4$ may be decomposed accordingly. To be precise, we consider the orthogonal projection operator onto the n^{th} mode in y:

$$P_n : \ L^2(\mathbb{R}^2) \ni f \mapsto \sum_{m=0}^{\infty} \langle f | \psi_m^n \rangle \psi_m^n. \tag{5.3}$$

Then (5.1) shows that $\hat{\mathcal{T}}_4$ is decomposed according to

$$L^2(\mathbb{R}^2) = \mathcal{H}_n \oplus \mathcal{H}_n^{\perp},$$

where $\mathcal{H}_n$ and $\mathcal{H}_n^{\perp}$ are by definition the kernels of $1 - P_n$ and P_n, respectively. That is, we have (see, for example, the book of Kato [Kat95])

$$P_n D(\hat{\mathcal{T}}_4) \subset D(\hat{\mathcal{T}}_4), \quad \hat{\mathcal{T}}_4 \mathcal{H}_n \subset \mathcal{H}_n, \quad \text{and} \quad \hat{\mathcal{T}}_4 \mathcal{H}_n^{\perp} \subset \mathcal{H}_n^{\perp}.$$

Now, to prove that $\hat{\mathcal{T}}_4$ is not essentially self-adjoint on $D(\hat{\mathcal{T}}_4)$, for any fixed n we consider the equations

$$
\begin{aligned}
(\hat{t}_4 u)_m &= \beta^n_{m-1} u_{m-1} + \beta^n_m u_{m+1} \\
&= z u_m
\end{aligned}
$$

for $z \in \mathbb{C}$. This is a recursion relation for u_{m+1} in terms of u_m and u_{m-1}. In the special case when $n = 0$ we simply take $u_0 = u_1 = 0$; then the solution is uniquely determined by the initial value u_2. If $n = 1$ we simply take u_0=0, so that the solution is uniquely determined by the initial value u_1. In all other cases the solution is completely determined by $u_{-1} = 0$ and the initial value u_0. Hence u_m is the initial condition multiplied by a polynomial in z, which we write as $P_m(z)$.

Let $z \in \mathbb{C}\backslash\mathbb{R}$ and denote by $N_{\overline{z}}$ the orthogonal complement of $\mathcal{R}(\hat{\mathcal{T}}_4 - \overline{z}I)$, called the deficiency subspace of the operator $\hat{\mathcal{T}}_4$. This subspace is precisely the subspace of solutions of the equation

$$\hat{\mathcal{T}}_4^* \phi = z\phi.$$

Considering $D(\hat{\mathcal{T}}_4^*)$, stated in (5.2), we see that $N_{\overline{z}}$ is the subspace given by solutions of the difference equation

$$(\hat{t}_4 u)_m = z u_m, \qquad u_{-1} = 0$$

(or the appropriate modified version for $n = 0$ and $n = 1$. For the remainder we always write the initial condition as u_0, for convenience). Hence for fixed n the deficiency subspace is at most one-dimensional; moreover, it is nonzero if and only if

$$(u_m) = (u_0 P_m(z)) \in \ell^2(\mathbb{N}_0),$$

that is, if

$$\sum_{m=0}^{\infty} |P_m(z)|^2 < \infty.$$

Non-self-adjointness is then a consequence of the following theorem about the infinite Jacobi matrix

$$L = \begin{pmatrix} b_0 & a_0 & 0 & 0 & \cdots \\ a_0 & b_1 & a_1 & 0 & \\ 0 & a_1 & b_2 & a_2 & \\ 0 & 0 & a_2 & b_3 & \ddots \\ \vdots & & & \ddots & \ddots \end{pmatrix}$$

where $a_j > 0$ and $b_j \in \mathbb{R}$ for all j. We can reduce to this case if we multiply $\hat{\mathcal{T}}_4$ by -1. This theorem is from Berezanskii's book ([Ber68], p.507), where one may find a beautiful and elementary proof.

Theorem 5.1. *Assume that $|b_j| \le C$ (j=0,1,...), $a_{j-1}a_{j+1} \le a_j^2$ beginning with some j, and*

$$\sum_{j=0}^{\infty} \frac{1}{a_j} < \infty. \tag{5.4}$$

Then the operator L is not self-adjoint.

It is elementary to show that the hypotheses are satisfied for $a_m = -\beta_m^n$ and $b_m = 0$, for any fixed n. Hence for any fixed n the deficiency indices of the resulting Jacobi matrix are both 1, and so, summing over n, the deficiency indices for $\hat{\mathcal{T}}_4$ are both infinity.

As for the operator $\hat{\mathcal{T}}_5$, we may either use a slight modification of the above methods, or we may simply use the fact that the Fourier transform intertwines $\hat{\mathcal{T}}_4$ and $\hat{\mathcal{T}}_5$. Then, simply by interchanging the roles of the variables x and y, we see that the operators $\hat{\mathcal{T}}_6$ and $\hat{\mathcal{T}}_7$ also have infinite deficiency indices.

The symmetric cubic operators $\hat{\mathcal{T}}_4$, $\hat{\mathcal{T}}_5$, $\hat{\mathcal{T}}_6$, and $\hat{\mathcal{T}}_7$ of Calvo and Picón do however admit self-adjoint extensions. Moreover, using the results of Allahverdiev [All05] we may explicitly classify all of the self-adjoint extensions in terms of certain boundary conditions at infinity. We begin by studying the restriction of $\hat{\mathcal{T}}_4$ to the subspace $\mathcal{H}_n$ given by the projection P_n as in (5.3). We simplify notation by then omitting "n"; in particular, ψ_m now denotes the $(m,n)^{th}$ Hermite-Gaussian mode, and β_m will also lose the superscript "n".

For

$$g = \sum_{m=0}^{\infty} g_m \psi_m \in D(\hat{\mathcal{T}}_4) \cap \mathcal{H}_n$$

and

$$h = \sum_{m=0}^{\infty} h_m \psi_m \in D(\hat{\mathcal{T}}_4) \cap \mathcal{H}_n,$$

we denote by $[g,h]$ the sequence with components $[g,h]_m$ given by

$$[g,h]_m = \beta_m (g_m \overline{h}_{m+1} - g_{m+1} \overline{h}_m).$$

We then have Green's formula:

$$\sum_{m=0}^{M} \{(\hat{t}_4 g)_m \overline{h}_m - g_m (\hat{t}_4 \overline{h})_m\} = -[g,h]_M$$

Since the sequences $(g)_m$, $(h)_m$, $(\hat{t}_4 g)_m$, and $(\hat{t}_4 h)_m$ are all in $\ell^2(\mathbb{N}_0)$, we then have that the limit

$$[g,h]_\infty = \lim_{M \to \infty} [g,h]_M$$

exists and is finite. Hence

$$\langle \hat{t}_4 g | h \rangle - \langle g | \hat{t}_4 h \rangle = -[g,h]_\infty.$$

Now (still for a fixed n) we let

$$u = (u_m) \quad \text{and} \quad v = (v_m)$$

be the solutions of

$$\beta_{m-1}y_{m-1} + \beta_m y_{m+1} = 0 \quad (m \geq 1)$$

satisfying the boundary conditions

$$u_0 = 1, \quad u_1 = 0, \quad v_0 = 0, \quad \text{and} \quad v_1 = \frac{1}{\beta_0}.$$

(We make the appropriate trivial modifications for $n = 0$ and $n = 1$.) We have that $u, v \in D(\hat{\mathcal{T}}_4^*) \cap \mathcal{H}_n$; in fact,

$$(\hat{t}_4 u)_m = 0 \text{ for all } m, \quad (\hat{t}_4 v)_0 = 1, \quad \text{and} \quad (\hat{t}_4 v)_m = 0,\ m \geq 1.$$

With this set-up we have the following results of Allahverdiev [All05]:

Theorem 5.2. (Allahverdiev [All05].) *The domain of the closure of $\hat{\mathcal{T}}_4$ restricted to $\mathcal{H}_n$ consists precisely of those $f \in D(\hat{\mathcal{T}}_4^*) \cap \mathcal{H}_n$ satisfying the boundary conditions*

$$[f, u]_\infty = [f, v]_\infty = 0.$$

For $f \in D(\hat{\mathcal{T}}_4^*) \cap \mathcal{H}_n$ we now define

$$\Gamma_1 f = [f, v]_\infty$$

and

$$\Gamma_2 f = [f, u]_\infty.$$

Then, in the precise sense of unbounded operators on a Hilbert space, we have the following theorem:

Theorem 5.3. (Allahverdiev [All05].) *The operators Γ_1, Γ_2 are (complex-valued, symmetric, linearly independent) boundary values of $\hat{\mathcal{T}}_4$ restricted to $\mathcal{H}_n$.*

And now that we have appropriate boundary values, we have the following well-known description of all self-adjoint extensions:

Theorem 5.4. (Allahverdiev [All05].) *When restricted to $\mathcal{H}_n$, every self-adjoint extension $\hat{\mathcal{T}}_4^h$ of $\hat{\mathcal{T}}_4$ is determined by the equality*

$$\hat{\mathcal{T}}_4^h f = (\hat{t}_4 f)$$

on the functions $f \in D(\hat{\mathcal{T}}_4^*) \cap \mathcal{H}_n$ satisfying the boundary conditions

$$[f, v]_\infty - h[f, u]_\infty = 0 \tag{5.5}$$

for $h \in \mathbb{R} \cup \{\infty\}$. For $h = \infty$ the condition (5.5) should be replaced by $[f, u]_\infty = 0$. Conversely, for an arbitrary $h \in \mathbb{R} \cup \{\infty\}$, the boundary condition (5.5) determines a self-adjoint extension on $\mathcal{H}_n$.

Remark 5.5. Allahverdiev [All05] additionally considers maximal dissipative and accretive extensions of infinite Jacobi matrices. These correspond to $h \in \mathbb{C}$ such that $\operatorname{Im} h \geq 0$ and $\operatorname{Im} h \leq 0$, respectively. He also gives applications to scattering theory.

It remains to consider $\hat{\mathcal{T}}_4$ as acting on the entire space

$$L^2(\mathbb{R}^2) = \bigoplus_{n=0}^{\infty} \mathcal{H}_n.$$

Let $\hat{\mathcal{T}}_4^n$ denote the restriction of $\hat{\mathcal{T}}_4$ to $\mathcal{H}_n$, that is, the operator in $\mathcal{H}_n$ with $D(\hat{\mathcal{T}}_4^n) = D(\hat{\mathcal{T}}_4) \cap \mathcal{H}_n$ such that $\hat{\mathcal{T}}_4^n f = \hat{\mathcal{T}}_4 f \in \mathcal{H}_n$. As we have just shown, the closure of $\hat{\mathcal{T}}_4^n$ is obtained by extending to the space of $f \in D(\hat{\mathcal{T}}_4^{n*})$ satisfying $\Gamma_1^n f = \Gamma_2^n f = 0$. We now prove the analogous result for the larger space.

Theorem 5.6. *The closure of $\hat{\mathcal{T}}_4$ is obtained by extending to the space*

$$\mathcal{D}_{cl} = \{f \in D(\hat{\mathcal{T}}_4^*);\ \Gamma_1^n(P_n f) = \Gamma_2^n(P_n f) = 0\ \forall n\}.$$

Proof. The closure of $\hat{\mathcal{T}}_4$ is of course the adjoint of $\hat{\mathcal{T}}_4^*$, so we are to show that $\mathcal{D}_{cl}$ is equal to

$$D(\hat{\mathcal{T}}_4^{**}) = \{F \in L^2(\mathbb{R}^2);\ \exists H \in L^2(\mathbb{R}^2) \text{ such that } \langle \hat{\mathcal{T}}_4^* g|F\rangle = \langle g|H\rangle\ \forall g \in D(\hat{\mathcal{T}}_4^*)\}.$$

Moreover, we note that $D(\hat{\mathcal{T}}_4^{**}) \subset D(\hat{\mathcal{T}}_4^*)$ since $\hat{\mathcal{T}}_4^{**}$ and $\hat{\mathcal{T}}_4$ have the same adjoint and since $\hat{\mathcal{T}}_4^{**}$ is automatically symmetric.

Now let $F \in \hat{\mathcal{T}}_4^*$ and write

$$F = \sum F_m^n \psi_m^n, \quad g = \sum g_m^n \psi_m^n, \quad \text{and } H = \sum H_m^n \psi_m^n.$$

Then we wish to find those precise conditions on F such that there is some $H \in L^2(\mathbb{R}^2)$ with the property that

$$\langle \hat{\mathcal{T}}_4^* g|F\rangle = \langle g|H\rangle \qquad \forall g \in D(\hat{\mathcal{T}}_4^*).$$

Simply by restricting to $g \in D(\hat{\mathcal{T}}_4)$, we see that it is necessary to have

$$H_m^n = \beta_{m-1}^n F_{m-1}^n + \beta_m^n F_{m+1}^n.$$

So we must find the conditions on F such that

$$\langle \hat{\mathcal{T}}_4^* g|F\rangle = \langle g|\hat{\mathcal{T}}_4^* F\rangle \qquad \forall g \in D(\hat{\mathcal{T}}_4^*).$$

We recall that

$$[g, F]_M^n = \sum_{m=0}^{M} \left(g_m^n \overline{(\hat{t}_4 F)_m^n} - (\hat{t}_4 g)_m^n \overline{F_m^n} \right),$$

so we see that

$$\sum_{n=0}^{\infty} [g, F]_M^n$$

converges absolutely. Moreover, by the dominated convergence theorem,

$$\lim_{M\to\infty}\sum_{n=0}^{\infty}[g,F]_M^n = \sum_{n=0}^{\infty}\lim_{M\to\infty}[g,F]_M^n \equiv \sum_{n=0}^{\infty}[g,F]_\infty^n.$$

Hence

$$\sum_{n=0}^{\infty}[g,F]_\infty^n = \langle g|\hat{\mathcal{T}}_4^* F\rangle - \langle \hat{\mathcal{T}}_4^* g|F\rangle \qquad \forall g \in D(\hat{\mathcal{T}}_4^*).$$

So $D(\hat{\mathcal{T}}_4^{**})$ is precisely the set of $F \in D(\hat{\mathcal{T}}_4^*)$ such that

$$\sum_{n=0}^{\infty}[g,F]_\infty^n = 0 \qquad \forall g \in D(\hat{\mathcal{T}}_4^*).$$

But then this is equivalent to

$$[g,F]_\infty^n \equiv [g,P_n(F)]_\infty^n = 0 \qquad \forall n,\ \forall g \in D(\hat{\mathcal{T}}_4^*) \cap \mathcal{H}_n,$$

which in turn, as shown by Allahverdiev [All05], is equivalent to

$$\Gamma_1^n(P_nF) = \Gamma_2^n(P_nF) = 0 \qquad \forall n.$$

So indeed we have $\mathcal{D}_{cl} = D(\hat{\mathcal{T}}_4^{**})$. □

We have also seen that self-adjoint extensions of $\hat{\mathcal{T}}_4^n$ are in one-to-one correspondence with boundary conditions of the form

$$\Gamma_1^n(f) - h_n\Gamma_2^n(f) = 0$$

for $h_n \in \mathbb{R} \cup \{\infty\}$. Now we define

$$\mathcal{D}_h = \{f \in D(\hat{\mathcal{T}}_4^*);\ \Gamma_1^n(P_nf) - h_n\Gamma_2^n(P_nf) = 0\ \forall n\},$$

and we denote the extension of $\hat{\mathcal{T}}_4$ to this domain as $\hat{\mathcal{T}}_4^h$. We next show that all self-adjoint extensions of $\hat{\mathcal{T}}_4$ are of this form.

Theorem 5.7. *Every self-adjoint extension $\hat{\mathcal{T}}_4^h$ of $\hat{\mathcal{T}}_4$ is determined by extending the domain to a set of the form*

$$\mathcal{D}_h = \{f \in D(\hat{\mathcal{T}}_4^*);\, \Gamma_1^n(P_n f) - h_n \Gamma_2^n(P_n f) = 0 \;\forall n\},$$

where $h = (h_n)_{n=0}^{\infty}$ is an arbitrary sequence with $h_n \in \mathbb{R} \cup \{\infty\}$, and by the rule

$$\hat{\mathcal{T}}_4^h f = (\hat{t}_4 f) \equiv \hat{\mathcal{T}}_4^* f.$$

For $h_n = \infty$ the condition should be replaced by $\Gamma_2^n(P_n f) = 0$. Conversely, for an arbitrary sequence $h = (h_n)_{n=0}^{\infty}$ with $h_n \in \mathbb{R} \cup \{\infty\}$, the set $\mathcal{D}_h$ determines a self-adjoint extension of $\hat{\mathcal{T}}_4$.

Proof. We begin by proving the converse: we take an arbitrary sequence h with $h_n \in \mathbb{R} \cup \{\infty\}$ and prove that the extension $\hat{\mathcal{T}}_4^h$ to the domain $\mathcal{D}_h$ is self-adjoint.

We first show that $\mathcal{D}_h$ is symmetric, that is, we show that

$$\langle \hat{\mathcal{T}}_4^* g | f \rangle = \langle g | \hat{\mathcal{T}}_4^* f \rangle \qquad \forall f, g \in \mathcal{D}_h.$$

As in the proof of Theorem 5.6, we use the identity

$$\sum_{n=0}^{\infty} [g, f]_{\infty}^n = \langle g | \hat{\mathcal{T}}_4^* f \rangle - \langle \hat{\mathcal{T}}_4^* g | f \rangle.$$

But now we may use the identity

$$[g, f]_M^n = [g, u^n]_M^n [\overline{f}, v^n]_M^n - [g, v^n]_M^n [\overline{f}, u^n]_M^n,$$

where u^n and v^n are the functions occurring in the definitions of Γ_1^n and Γ_2^n. Hence, in the limit,

$$[g, f]_{\infty}^n = (\Gamma_2^n P_n g)(\Gamma_1^n P_n \overline{f}) - (\Gamma_1^n P_n g)(\Gamma_2^n P_n \overline{f}).$$

Since g, f are in $\mathcal{D}_h$, we can use the identities

$$\Gamma_1^n(P_n f) - h_n \Gamma_2^n(P_n f) = 0$$

and

$$\Gamma_1^n(P_n g) - h_n \Gamma_2^n(P_n g) = 0$$

to see that $[g, f]_\infty^n = 0$ for all n. Hence $\hat{\mathcal{T}}_4^h$ is a symmetric operator.

To show that $\hat{\mathcal{T}}_4^h$ is a closed operator, we suppose that

$$\mathcal{D}_h \ni f_k \to f \qquad \text{in } L^2(\mathbb{R}^2)$$

and

$$\hat{\mathcal{T}}_4^h f_k \to F \qquad \text{in } L^2(\mathbb{R}^2).$$

Then clearly, for all n,

$$P_n f_k \to P_n f \qquad \text{in } \mathcal{H}_n$$

and

$$P_n \hat{\mathcal{T}}_4^h f_k = \hat{\mathcal{T}}_4^h P_n f_k \to P_n F \qquad \text{in } \mathcal{H}_n.$$

But since $\hat{\mathcal{T}}_4^{h,n}$, the restriction of $\hat{\mathcal{T}}_4^h$ to $\mathcal{H}_n$, is closed (as is $\hat{\mathcal{T}}_4^*$), we then have that $P_n f \in \mathcal{D}_h \cap \mathcal{H}_n$ (hence $f \in \mathcal{D}_h$) and that $\hat{\mathcal{T}}_4^h P_n f = P_n \hat{\mathcal{T}}_4^h f = P_n F$ (hence $\hat{\mathcal{T}}_4^h f = F$). So $\hat{\mathcal{T}}_4^h$ is a closed operator.

Next we show that the deficiency indices of $\hat{\mathcal{T}}_4^h$ are both zero. Suppose $u_\pm \in D(\hat{\mathcal{T}}_4^{h*})$ are such that $u_\pm \in \mathrm{Ker}(\hat{\mathcal{T}}_4^{h*} \mp i)$. Then $P_n u_\pm \in \mathrm{Ker}(\hat{\mathcal{T}}_4^{h,n*} \mp i)$, and, since $\hat{\mathcal{T}}_4^{h,n}$ is self-adjoint, $P_n u_\pm = 0$ for all n. Hence $u_\pm = 0$. So the deficiency indices of $\hat{\mathcal{T}}_4^h$ are both zero, and $\hat{\mathcal{T}}_4^h$ is a closed operator. Hence $\hat{\mathcal{T}}_4^h$ is self-adjoint.

For the other direction, let $\hat{\mathcal{T}}_4^e$, with domain $\mathcal{D}_e$, be some self-adjoint extension of $\hat{\mathcal{T}}_4$, and let $\hat{\mathcal{T}}_4^{e,n}$ be its restriction to $\mathcal{H}_n$. To show that $\hat{\mathcal{T}}_4^{e,n}$ is closed, we suppose that

$$\mathcal{D}_e \cap \mathcal{H}_n \ni f_k \to f \qquad \text{in } \mathcal{H}_n$$

and that

$$\hat{\mathcal{T}}_4^{e,n} f_k \to F \qquad \text{in } \mathcal{H}_n.$$

Then, in particular,

$$\mathcal{D}_e \ni f_k \to f \qquad \text{in } L^2(\mathbb{R}^2)$$

and

$$\hat{\mathcal{T}}_4^e f_k \to F \qquad \text{in } L^2(\mathbb{R}^2).$$

Since $\hat{\mathcal{T}}_4^e$ is closed, we have $f \in \mathcal{D}_e \cap \mathcal{H}_n$ and $\hat{\mathcal{T}}_4^{e,n} f = F$, which proves that $\hat{\mathcal{T}}_4^{e,n}$ is a closed operator. And since the deficiency indices of $\hat{\mathcal{T}}_4^e$ are both zero, it is clear that the deficiency indices of $\hat{\mathcal{T}}_4^{e,n}$ are both zero. Hence $\hat{\mathcal{T}}_4^{e,n}$ is self-adjoint.

Now $\hat{\mathcal{T}}_4^{e,n}$ is a self-adjoint extension of $\hat{\mathcal{T}}_4^n$, so the results of Allahverdiev cited above show that $\hat{\mathcal{T}}_4^{e,n}$ must be given by a boundary condition of the form

$$\Gamma_1^n(f) - h_n \Gamma_2^n(f) = 0$$

for some $h_n \in \mathbb{R} \cup \{\infty\}$. Hence we have $\mathcal{D}_e \subset \mathcal{D}_h$, that is,

$$\hat{\mathcal{T}}_4^e \subset \hat{\mathcal{T}}_4^h,$$

and since both operators are self-adjoint, we then have $\hat{\mathcal{T}}_4^e = \hat{\mathcal{T}}_4^h$. This completes the proof of the theorem. $\square$

We have now categorized all self-adjoint extensions of the operator $\hat{\mathcal{T}}_4$, so we are presented with the basic question: which is the "right" extension? We expect the physics of the problem to dictate the appropriate extension, for which we may return to the original work of Calvo and Picón [CPB06],[CP08],[CPZ08]. They state that the cubic generators, $\hat{\mathcal{T}}_4$, $\hat{\mathcal{T}}_5$, $\hat{\mathcal{T}}_6$, and $\hat{\mathcal{T}}_7$, can be implemented with passive optical elements having higher-than-first-order aberrations (nonquadratic refractive surfaces) [CP08]. Perhaps the physics of the apparatus will determine the "right" self-adjoint extension.

5.3 The Semiclassical Formalism

In the case of Gaussian transformations, one may use the theory of metaplectic operators (sometimes presented in terms of the Stone-von Neumann theorem) to deduce the underlying canonical transformations. However, non-Gaussian transformations are not metaplectic operators, so the arguments must be modified. Calvo and Picón then ask if the Stone-von Neumann theorem can be extended to the case of the above cubic generators, for then "this would enable one to find the explicit form of the symplectic transform and thus the construction of the associated optical system" [CP08]. In the following sections we take a different approach: we approximate the non-Gaussian transformations by semiclassical Fourier integral operators, by starting with the semiclassical Fourier integral operator ansatz and then by solving the resulting eikonal equation and transport equations. This, along with Egorov's theorem (stated in Section 5.8), justifies the claim that the underlying canonical transformation is the Hamilton flow associated to the evolution equation. As a first step, in this section we put the work of Calvo and Picón in the framework of semiclassical analysis.

We wish to construct approximate solutions to the evolution equations associated to the cubic generators $\hat{\mathcal{T}}_4$, $\hat{\mathcal{T}}_5$, $\hat{\mathcal{T}}_6$, and $\hat{\mathcal{T}}_7$, approximate in the sense that we will work in the semiclassical regime. For this we start with the two-dimensional semiclassical ground state

$$|0,0\rangle = (\pi h)^{-1/2} e^{-(x^2+y^2)/(2h)}.$$

To get the other semiclassical Hermite functions, we apply the creation operators

$$\hat{a}_x^\dagger = (2h)^{-1/2}\left(x - h\frac{\partial}{\partial x}\right) \qquad \text{and} \qquad \hat{a}_y^\dagger = (2h)^{-1/2}\left(y - h\frac{\partial}{\partial y}\right).$$

We also have the corresponding annihilation operators

$$\hat{a}_x = (2h)^{-1/2}\left(x + h\frac{\partial}{\partial x}\right) \qquad \text{and} \qquad \hat{a}_y = (2h)^{-1/2}\left(y + h\frac{\partial}{\partial y}\right),$$

so that

$$[\hat{a}_x, \hat{a}_x^\dagger] = 1 \quad \text{and} \quad [\hat{a}_y, \hat{a}_y^\dagger] = 1.$$

The [normalized] semiclassical Hermite functions are then given by

$$|m, n\rangle = (m!n!)^{-1/2}\hat{a}_x^{\dagger\, m}\hat{a}_y^{\dagger\, n}|0, 0\rangle.$$

We again let

$$\hat{\mathcal{T}}_4 = \frac{1}{2}(\hat{a}_x^\dagger + \hat{a}_x - \hat{a}_x^\dagger\hat{a}_x^\dagger\hat{a}_x - \hat{a}_x^\dagger\hat{a}_x\hat{a}_x - \hat{a}_x^\dagger\hat{a}_y^\dagger\hat{a}_y - \hat{a}_x\hat{a}_y^\dagger\hat{a}_y)$$

but now where the creation and annihilation operators are semiclassical. In this context it is more convenient to introduce the semiclassical differential operator

$$\hat{\mathfrak{T}}_4 := -2^{1/2}h^{3/2}\hat{\mathcal{T}}_4.$$

For reference, we note that

$$\hat{\mathfrak{T}}_4 = \frac{1}{2}x\left((hD_x)^2 + (hD_y)^2 + x^2 + y^2\right) - \frac{5}{2}hx - \frac{1}{2}ih^2 D_x, \tag{5.6}$$

and we note that the semiclassical Weyl symbol of $\hat{\mathfrak{T}}_4$ is

$$p_4(x, y, \xi, \eta; h) = \frac{1}{2}x(x^2 + y^2 + \xi^2 + \eta^2) - \frac{5}{2}hx.$$

We then have the permutation properties similar to those in Section 5.2. Explicitly, for $\hat{U}_{\Gamma_2}$ we have

$$
\begin{aligned}
e^{it\hat{\mathfrak{T}}_4/h}|0,0\rangle &= \cos\left(2^{-1/2}h^{1/2}t\right)|0,0\rangle - i\sin\left(2^{-1/2}h^{1/2}t\right)|1,0\rangle \\
e^{it\hat{\mathfrak{T}}_5/h}|0,0\rangle &= \cos\left(2^{-1/2}h^{1/2}t\right)|0,0\rangle - \sin\left(2^{-1/2}h^{1/2}t\right)|1,0\rangle \\
e^{it((\hat{\mathfrak{T}}_3+\sqrt{3}\hat{\mathfrak{T}}_8)/2)/h}|0,0\rangle &= e^{it2^{-1/2}h^{1/2}}|0,0\rangle \\
e^{it\hat{\mathfrak{T}}_4/h}|1,0\rangle &= \cos\left(2^{-1/2}h^{1/2}t\right)|1,0\rangle - i\sin\left(2^{-1/2}h^{1/2}t\right)|0,0\rangle \\
e^{it\hat{\mathfrak{T}}_5/h}|1,0\rangle &= \cos\left(2^{-1/2}h^{1/2}t\right)|1,0\rangle + \sin\left(2^{-1/2}h^{1/2}t\right)|0,0\rangle \\
e^{it((\hat{\mathfrak{T}}_3+\sqrt{3}\hat{\mathfrak{T}}_8)/2)/h}|1,0\rangle &= e^{-it2^{-1/2}h^{1/2}}|1,0\rangle.
\end{aligned}
$$

The operations for $\hat{U}_{\Gamma_1}$ and $\hat{U}_{\Gamma_3}$ are similar. Hence, in this choice of scale, we have permutations of the three lowest Hermite-Gaussian modes when

$$
t : 0 \mapsto \frac{\pi}{\sqrt{2h}}.
$$

5.4 Warm-Up: The FIO Representation of a Gaussian Transformation

For non-Gaussian transformations, the approximate representation by Fourier integral operators will be somewhat complicated, so we begin with a simpler situation: the case of a Gaussian transformation. For the sake of concreteness, we restrict our attention to the semiclassical differential operator

$$
P(h) = -h(\hat{a}_x^\dagger \hat{a}_y^\dagger + \hat{a}_x \hat{a}_y) = -h^2 \frac{\partial^2}{\partial x \partial y} - xy,
$$

though all ten generators of $\hat{U}(S)$, the metaplectic representation of $Sp(4,\mathbb{R})$ (see [CP08]), may be treated in the same way. Our goal is then to solve the evolution equation

$$\begin{cases} (hD_t + P)u = 0 \\ u|_{t=0} = v. \end{cases} \tag{5.7}$$

Following the method outlined in the book of Grigis and Sjöstrand ([GS94], p.129), we try

$$u = U_t v(x, y) = (2\pi h)^{-2} \iint e^{i\varphi(t,x,y,\xi,\eta)/h} a(t) \hat{v}(\xi, \eta)\, d\xi\, d\eta,$$

where φ is a quadratic form in (x, y, ξ, η). Here $\hat{v}$ denotes the semiclassical Fourier transform:

$$\hat{v}(\xi, \eta) = \int e^{-i(x\xi + y\eta)/h} v(x, y)\, dx\, dy.$$

With this ansatz, we arrive at the expression

$$\begin{aligned} (hD_t + h^2 D_x D_y - xy)u = (2\pi h)^{-2} &\iint \left[\frac{\partial\varphi}{\partial t} + \frac{\partial\varphi}{\partial x}\frac{\partial\varphi}{\partial y} - xy\right] e^{i\varphi/h} a(t)\hat{v}(\xi, \eta)\, d\xi\, d\eta \\ - ih(2\pi h)^{-2} &\iint \left[\frac{\partial a}{\partial t} + \frac{\partial^2\varphi}{\partial x \partial y} a\right] e^{i\varphi/h} \hat{v}(\xi, \eta)\, d\xi\, d\eta. \end{aligned}$$

Thus we wish to solve both the eikonal equation,

$$\frac{\partial\varphi}{\partial t} + \frac{\partial\varphi}{\partial x}\frac{\partial\varphi}{\partial y} - xy = 0, \tag{5.8}$$

and also the transport equation,

$$\frac{\partial a}{\partial t} + \frac{\partial^2\varphi}{\partial x \partial y} a = 0. \tag{5.9}$$

It is due to the special form of the operator P that we are able to solve this in such a way that the amplitude a depends only on t. Moreover, we want φ to satisfy

$$\varphi(0, x, y, \xi, \eta) = x\xi + y\eta,$$

and we want a to solve

$$a(0) = 1,$$

so that the initial condition is satisfied in the evolution equation (5.7).

We begin with a solution of the eikonal equation (5.8). The semiclassical Weyl symbol of P is

$$p(x, y, \xi, \eta) = \xi\eta - xy,$$

and we write the semiclassical Weyl symbol of the evolution equation (5.7) as

$$g(t, x, y, \tau, \xi, \eta) = \tau + p(x, y, \xi, \eta),$$

which is actually independent of t. The eikonal equation may then be written in the simple form

$$g(t, x, y, d_t\varphi, d_x\varphi, d_y\varphi) = 0, \tag{5.10}$$

whose solution, which we now sketch, is provided by Hamilton-Jacobi theory.

Hamilton's equations for g are

$$\begin{cases} \dot{t} = \frac{\partial g}{\partial \tau} = 1 \\ \dot{x} = \frac{\partial g}{\partial \xi} = \eta \\ \dot{y} = \frac{\partial g}{\partial \eta} = \xi \\ \dot{\tau} = -\frac{\partial g}{\partial t} = 0 \\ \dot{\xi} = -\frac{\partial g}{\partial x} = y \\ \dot{\eta} = -\frac{\partial g}{\partial y} = x. \end{cases}$$

Hence it is natural to identify the evolution parameter with time t. These equations may be easily solved to give the Hamilton flow of g:

$$\begin{cases} t = t \\ x(t) = x_0 \cosh t + \eta_0 \sinh t \\ y(t) = y_0 \cosh t + \xi_0 \sinh t \\ \tau(t) = \tau_0 \\ \xi(t) = y_0 \sinh t + \xi_0 \cosh t \\ \eta(t) = x_0 \sinh t + \eta_0 \cosh t. \end{cases}$$

One may think of this as just being the Hamilton flow of p, since the flow in the (t, τ) variables is trivial. In this point of view, we may write the Hamilton flow of p in the matrix formulation:

$$\begin{pmatrix} x(t) \\ y(t) \\ \xi(t) \\ \eta(t) \end{pmatrix} = \begin{pmatrix} \cosh t & 0 & 0 & \sinh t \\ 0 & \cosh t & \sinh t & 0 \\ 0 & \sinh t & \cosh t & 0 \\ \sinh t & 0 & 0 & \cosh t \end{pmatrix} \begin{pmatrix} x_0 \\ y_0 \\ \xi_0 \\ \eta_0 \end{pmatrix}.$$

However, for the time being we take the point of view of the Hamilton flow of g. This Hamiltonian system (in a six-dimensional cotangent space) is completely integrable, since we have the three ($= \frac{6}{2}$) independent conserved quantities

$$\begin{cases} g(t, x, y, \tau, \xi, \eta) \\ y^2 - \xi^2 \\ \tau. \end{cases}$$

The fact that we have three conserved quantities corresponds to the fact that the flow is constrained to a Lagrangian submanifold; that is, a three-dimensional submanifold Λ of the cotangent space such that the restriction of the symplectic form σ to Λ is zero (i.e., is *isotropic*):

$$\sigma|_{\Lambda} = 0.$$

To construct a solution of the eikonal equation, the basic idea is to start with a two-dimensional isotropic submanifold Λ' and then to propagate Λ' with respect to the Hamilton flow of g, filling out the whole Lagrangian submanifold Λ. To this end, we let

$$\begin{aligned}\Lambda' &= \{(0, x_0, y_0, \tau_0, \xi_0, \eta_0);\ g(0, x_0, y_0, \tau_0, \xi_0, \eta_0) = \tau_0 + \xi_0\eta_0 - x_0y_0 = 0\} \\ &= \{(0, x_0, y_0, x_0y_0 - \xi_0\eta_0, \xi_0, \eta_0)\},\end{aligned}$$

which we think of as the "submanifold of initial conditions", and where we consider (ξ_0, η_0) as universally fixed. Propagating along the Hamilton flow of g, we thus get the whole manifold Λ:

$$\Lambda = \{(t, x(t), y(t), x(t)y(t) - \xi(t)\eta(t), \xi(t), \eta(t))\}.$$

On the one hand, we may think of a trajectory along the Hamilton flow as being determined by the parameters (t, x_0, y_0). On the other hand, we may think of it is as determined by the parameters (t, x, y), since

$$\begin{cases} x_0 = x\mathrm{sech}t - \eta_0 \tanh t \\ y_0 = y\mathrm{sech}t - \xi_0 \tanh t. \end{cases}$$

Hence, rewriting the variables (ξ_0, η_0) as (ξ, η), we may rewrite Λ as

$$\begin{aligned}\Lambda = \{(t, x, y, (xy - \xi\eta)\mathrm{sech}^2 t - (x\xi + y\eta)\tanh t\,\mathrm{sech}t,& \\ y\tanh t + \xi\mathrm{sech}t,\ x\tanh t + \eta\mathrm{sech}t)\}.&\end{aligned}$$

To conclude the solution of the eikonal equation, we seek a function φ such that Λ is the graph of the gradient of φ, to agree with (5.10), and such that

$\varphi(0,x,y,\xi,\eta) = x\xi + y\eta$. This is easily accomplished, and we thus have the phase:

$$\varphi(t,x,y,\xi,\eta) = (xy - \xi\eta)\tanh t + (x\xi + y\eta)\mathrm{sech} t.$$

And one may now check directly that this is the solution of the eikonal equation.

It is now easy to solve the transport equation (5.9):

$$a(t) = \mathrm{sech} t.$$

So we have the following expression for the solution operator U_t:

$$U_t v(x,y) = \mathrm{sech} t \iint \exp\left(\frac{i}{h}[(xy - \xi\eta)\tanh t + (x\xi + y\eta)\mathrm{sech} t]\right) \hat{v}(\xi,\eta)\,\frac{d\xi\,d\eta}{(2\pi h)^2}.$$

We may use the method of stationary phase (which, in this case, is *exact*) to simplify this expression and get an integral in terms of v. We withhold the details for now, since this will be accomplished in the next section for a different but similar operator.

Also, it is known from the general theory (see, for example, [GS94]) that φ is a generating function of the canonical transformation, which in this case is the Hamilton flow of the symbol p. That is, the Hamilton flow of p is given by

$$\left(\frac{\partial\varphi}{\partial\xi}, \frac{\partial\varphi}{\partial\eta}, \xi, \eta\right) \mapsto \left(x, y, \frac{\partial\varphi}{\partial x}, \frac{\partial\varphi}{\partial y}\right).$$

This can also be checked directly, now that we have an explicit expression for the phase φ.

5.5 The Gyrator Transform

The exact same method may be applied to the semiclassical differential operator

$$T_1 = h(\hat{a}_x^\dagger \hat{a}_y + \hat{a}_y^\dagger \hat{a}_x) = xy - h^2\frac{\partial^2}{\partial x \partial y}.$$

In the previous section, the solution of the evolution equation was exact, so the semiclassical parameter h ultimately played no role. Hence in this section we simply let $h = 1$. In this case, the solution to the evolution equation

$$\begin{cases} (D_t + T_1)u = 0 \\ u|_{t=0} = v \end{cases}$$

for $t \in (-\pi/2, \pi/2)$ is given by

$$u(t,x,y) = (2\pi)^{-2}|\sec t| \iint \exp\left(i[(x\xi + y\eta)\sec t - (xy + \xi\eta)\tan t]\right) \hat{v}(\xi,\eta)\, d\xi\, d\eta. \tag{5.11}$$

It remains to extend the solution to all $t \in \mathbb{R}$.

We may use the method of stationary phase (which is *exact* in this case) to rewrite this integral as a double integral involving v. This simply amounts to a use of the following fact. Let Q be a real, non-degenerate $n \times n$ symmetric matrix. Then the Fourier transform acts as follows (for details, see [GS94], p.21):

$$\mathcal{F} : e^{i\langle x, Qx\rangle/2} \mapsto (2\pi)^{n/2} e^{i(\pi/4)\operatorname{sgn} Q} |\det Q|^{-1/2} e^{-i\langle \xi, Q^{-1}\xi\rangle/2}.$$

After some calculation, for $t \in (0, \pi/2)$ we arrive at the integral expression

$$u(t,x,y) = (2\pi)^{-1}|\sin t|^{-1} \iint v(a,b) \exp\left(i\frac{(xy + ab)\cos t - (ay + xb)}{\sin t} \right) da\, db. \tag{5.12}$$

The righthand side is known as "the gyrator transform" of v [RAC07]. The benefit of this expression is that we may now extend the solution $u(t,x,y)$ to $t \in (0,\pi)$. For $t \in (\pi/2, \pi)$ we may again use the method of stationary phase to return to the expression (5.11). There is no phase shift, since in this example $\operatorname{sgn} \mathrm{Q} = 0$.

Hence we have completely determined $u(t,x,y)$: for $t \in \mathbb{R}\backslash\{(2k+1)\pi/2;\, k \in \mathbb{Z}\}$ it is given by (5.11), and for $t \in \mathbb{R}\backslash\{k\pi;\, k \in \mathbb{Z}\}$ it is given by (5.12). This is analogous to the standard parametrization of the circle by four charts of graph coordinates. In fact, it is not only analogous, but intimately related; the exceptional points for (5.11) (resp. (5.12)) are precisely those for which the Lagrangian submanifolds, swept out by the Hamilton flow of T_1, have degenerate projections onto the (ξ, η) plane (resp. (x, y) plane). (For more on this phenomenon, one may consult Duistermaat's review article [Dui74].)

This unitary group has an important application when $t = \pm\pi/4$: it takes Hermite-Gaussian modes to Laguerre-Gaussian modes. For this we recall the definitions of the extended Wigner transform

$$\tilde{W}F(x,y) = \frac{1}{\sqrt{2\pi}} \int e^{ipy} F\left(\frac{x+p}{\sqrt{2}}, \frac{x-p}{\sqrt{2}}\right) dp$$

and of the (renormalized) partial Fourier transform

$$\mathcal{F}_2 F(x,y) = \frac{1}{\sqrt{2\pi}} \int e^{-ipy} F(x,p) dp.$$

Then one may check that

$$u(\pi/4, x, y) = \tilde{W}(\mathcal{F}_2 v)(x, -y).$$

In the special case when the initial condition is $v = h_{mn}$, the $(m,n)^{th}$ Hermite-Gaussian mode, we have

$$u(\pi/4, x, y) = (-i)^n \tilde{W}(h_{nm})(x, y).$$

Moreover, by taking complex conjugates, we have

$$u(-\pi/4, x, y) = i^n \tilde{W}(h_{mn})(x, y).$$

And we recall from Chapter 4 that $\tilde{W}(h_{mn})$ is precisely the $(m,n)^{th}$ Laguerre-Gaussian mode.

5.6 The FIO Representation of a Non-Gaussian Transformation

We now turn to the more difficult non-Gaussian transformations. The four non-Gaussian transformations used by Calvo and Picón may all be treated by the same methods, so we focus on the operator

$$\hat{\mathcal{T}}_4 = \frac{1}{2}(\hat{a}_x^\dagger + \hat{a}_x - \hat{a}_x^\dagger \hat{a}_x^\dagger \hat{a}_x - \hat{a}_x^\dagger \hat{a}_x \hat{a}_x - \hat{a}_x^\dagger \hat{a}_y^\dagger \hat{a}_y - \hat{a}_x \hat{a}_y^\dagger \hat{a}_y),$$

where the creation and annihilation operators are semiclassical. Moreover, we will make a slight simplification in order to remove inessential complications. Since the operator $\hat{\mathcal{T}}_4$ acts very simply in the y variable, we may instead study the operator

$$\hat{\mathcal{T}} = \frac{1}{2}(\hat{a}_x^\dagger + \hat{a}_x - \hat{a}_x^\dagger \hat{a}_x^\dagger \hat{a}_x - \hat{a}_x^\dagger \hat{a}_x \hat{a}_x)$$

acting on functions of x only. The following arguments may be repeated for $\hat{\mathcal{T}}_4$, but with some slight changes as outlined in Section 5.7.

We renormalize $\hat{\mathcal{T}}$ in order to have a semiclassical differential operator:

$$\begin{aligned}\hat{\mathfrak{T}} &= -2^{1/2} h^{3/2} \hat{\mathcal{T}} \\ &= \frac{1}{2} x(x^2 + (hD_x)^2) - 2hx - \frac{1}{2} i h^2 D_x.\end{aligned}$$

Moreover, later we will need a re-scaled version of this operator, so we consider the slightly more general operator

$$\hat{\mathfrak{T}}_r = \frac{1}{2} x(x^2 + (hD_x)^2) - \frac{r^2}{2} hx - \frac{1}{2} i h^2 D_x$$

for any $r \geq 0$.

The method we use to treat this operator is the same as in the previous sections, but there are some complications. The difficulties may be treated by the general theory, but the solution is not as explicit and exact. Here we wish to remain in the semiclassical setting, and we only expect an asymptotic solution to the corresponding evolution equation:

$$\begin{cases} \left(hD_t + \hat{\mathfrak{T}}_r\right) u = \mathcal{O}(h^\infty) \\ u|_{t=0} = v. \end{cases} \tag{5.13}$$

We will allow the initial conditions v to depend on h. Moreover, for bounded times Duhamel's Principle shows that the semiclassical propagator differs from the exact unitary propagator by $\mathcal{O}(h^\infty)$ (after choosing a self-adjoint realization of the generator).

The semiclassical Weyl symbol of $\hat{\mathfrak{T}}_0$ is

$$p_r(x,\xi;h) = \frac{1}{2}x(x^2+\xi^2) - \frac{r^2}{2}hx,$$

so then Hamilton's equations are

$$\begin{cases} \dot{x} = x\xi \\ \dot{\xi} = -x^2 - \frac{1}{2}(x^2+\xi^2) + \frac{r^2}{2}h. \end{cases} \tag{5.14}$$

Here we have the conserved quantity

$$C = p_r(x,\xi;h).$$

Suppose first that $C \neq 0$, so that, in particular, $x(t) \neq 0$ for all t. Letting

$$w = \frac{1}{x},$$

we have from (5.14) the following differential equation for w:

$$(\dot{w})^2 = 2Cw^3 + r^2hw^2 - 1. \tag{5.15}$$

If $C \neq 0$, this is essentially the same as the differential equation for the famous Weierstrass $\wp$-function:

$$[\wp'(z)]^2 = 4\,[\wp(z)]^3 - g_2\wp(z) - g_3.$$

The two constants g_2 and g_3 are the so-called "invariants". We may then solve Hamilton's equations, giving the Hamilton flow in terms of the Weierstrass $\wp$-function.

To be explicit, for $C \neq 0$ we have

$$x(t) = \frac{1}{2}C\left(\wp(t+t_0) - \frac{1}{12}r^2h\right)^{-1} \tag{5.16}$$

where t_0 is either an arbitrary real constant or an arbitrary real constant plus $\frac{1}{2}\omega_1$, the purely imaginary half-period of $\wp$ (see Appendix B). Here $\wp$ is the Weierstrass $\wp$-function associated to the invariants

$$g_2 = \frac{1}{12}r^4h^2 \qquad \text{and} \qquad g_3 = \frac{1}{4}C^2 - \frac{1}{216}r^6h^3.$$

We then also have

$$\begin{aligned}\xi(t) &= \frac{\dot{x}(t)}{x(t)}\\ &= \frac{-\dot{\wp}(t+t_0)}{\wp(t+t_0) - \frac{1}{12}r^2h}.\end{aligned} \tag{5.17}$$

When $r = 0$ and $C \neq 0$, $\xi(t)$ is always strictly decreasing, which follows simply from Hamilton's equations (5.14). However, when $r > 0$ we have a more complicated behavior, as shown in Figure 5.1. There is a pocket of radius $r\sqrt{h} = \frac{r}{\sqrt{2}}w_0$, where w_0 is in practice the radius of the laser beam's waist.

For $C = 0$, depending on the initial conditions, we have one of the following four cases:

$$\begin{cases} x(t) = 0 \quad \forall t \\ \xi(t) = \sqrt{r^2h}\coth\left(\frac{\sqrt{r^2h}}{2}(t+t_0)\right), \end{cases}$$

$$\begin{cases} x(t) = 0 \quad \forall t \\ \xi(t) = \sqrt{r^2h}\tanh\left(\frac{\sqrt{r^2h}}{2}(t+t_0)\right), \end{cases}$$

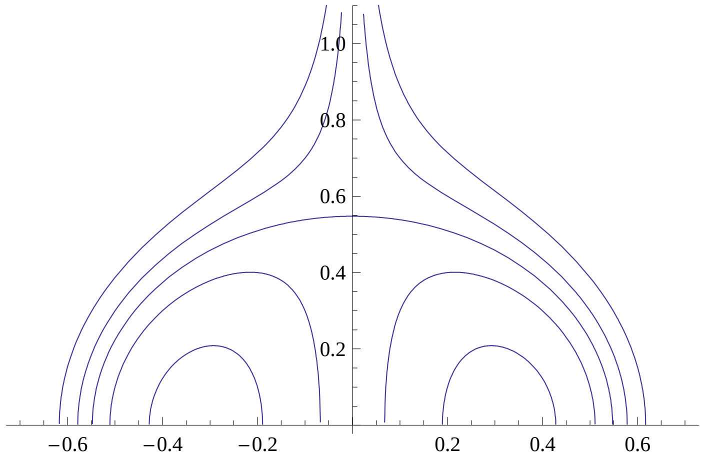

Figure 5.1: Hamilton flow lines in the (x, ξ) upper half plane in the case $h = 1/10$, with variable C_0. The lower half plane is obtained by symmetry.

$$\begin{cases} x(t) = \pm\sqrt{r^2h}\operatorname{sech}(\sqrt{r^2h}(t+t_0)) \\ \xi(t) = -\sqrt{r^2h}\tanh\left(\sqrt{r^2h}(t+t_0)\right), \end{cases}$$

or

$$\begin{cases} (x(t), \xi(t)) = (0, \pm\sqrt{r^2h}) \qquad \forall t \quad \text{(hyperbolic stationary points)}. \end{cases}$$

Of course, we also have the elliptic stationary points $(x, \xi) = (\pm\sqrt{\frac{r^2h}{3}}, 0)$, corresponding to $C = \mp(r^2h/3)^{3/2}$.

Now we look for a solution of the equation (5.13) of the form

$$u = U_t v(x) = (2\pi h)^{-1} \int e^{i\varphi(t,x,\xi)/h} a(t, x, \xi; h)\hat{v}(\xi)\, d\xi. \tag{5.18}$$

Here we are using the semiclassical Fourier transform, given by

$$\hat{v}(\xi) = \int e^{-ix\xi/h} v(x)\, dx.$$

We will even allow the phase φ to depend on h, since we prefer to study the Weyl symbol of $\hat{\mathfrak{T}}_r$, rather than the principal symbol only.

We take φ to be a solution of the now h-dependent eikonal equation

$$\frac{\partial \varphi}{\partial t} + p_r\left(x, \frac{\partial \varphi}{\partial x}; h\right) = 0. \tag{5.19}$$

We may treat this using the same method as before, using Hamilton-Jacobi theory (see, for example, Theorem 5.5 of [GS94]): given any $(x_0, \xi_0) \in \mathbb{R}^2$, there exists a real-valued smooth function $\varphi(t, x; h)$ (with ξ_0 considered as a parameter) defined in a neighborhood of $(0, x_0)$ such that (5.19) is solved and such that

$$\begin{aligned} \varphi(0, x) &= x\xi_0, \\ \frac{\partial \varphi}{\partial t}(0, x_0) &= -\frac{1}{2}x_0(x_0^2 + \xi_0^2) + \frac{r^2}{2}hx_0, \qquad\qquad \text{and} \\ \frac{\partial \varphi}{\partial x}(0, x_0) &= \xi_0. \end{aligned}$$

However we have not yet managed to get a closed-form expression for the Hamilton flow (solely in terms of the initial conditions x_0 and ξ_0) or for the phase φ. Perhaps this is best suited for Laurent expansion methods and numerical methods, but we leave open the possibility that one may find closed-form solutions by brute force.

We next construct the amplitude a. For (5.18) to be a solution of the equation (5.13), the amplitude a must satisfy

$$(hD_t + \hat{\mathfrak{T}}_r)(e^{i\varphi/h}a) = \mathcal{O}(h^\infty),$$

which is equivalent to

$$\left(\frac{\partial \varphi}{\partial t} + hD_t + e^{-i\varphi/h}\hat{\mathfrak{T}}_r e^{i\varphi/h}\right) a = \mathcal{O}(h^\infty).$$

And since φ is a solution of the eikonal equation, we then have

$$\left(hD_t + e^{-i\varphi/h}\hat{\mathfrak{T}}_r e^{i\varphi/h} - p_r\left(x, \frac{\partial\varphi}{\partial x}; h\right)\right) a = \mathcal{O}(h^\infty). \tag{5.20}$$

We simply compute

$$\begin{aligned} &e^{-i\varphi/h}\hat{\mathfrak{T}}_r e^{i\varphi/h} - p_r\left(x, \frac{\partial\varphi}{\partial x}; h\right) \\ &\qquad = -\frac{1}{2}ih\left(x\frac{\partial^2\varphi}{\partial x^2} + \frac{\partial\varphi}{\partial x}\right) + x\frac{\partial\varphi}{\partial x}hD_x + \frac{1}{2}x(hD_x)^2 - \frac{1}{2}ih^2 D_x. \end{aligned}$$

If we let

$$V_t := x\frac{\partial\varphi}{\partial x}\frac{\partial}{\partial x}$$

(which we recall depends on h), then (5.20) becomes

$$\left(\left(\frac{\partial}{\partial t} + \frac{1}{2}\operatorname{div} V_t + V_t\right) + \frac{h}{2i}\left(\frac{\partial}{\partial x}\circ x \circ \frac{\partial}{\partial x}\right)\right) a = \mathcal{O}(h^\infty).$$

It is then natural to define

$$R_1 := \frac{\partial}{\partial t} + \frac{1}{2}\operatorname{div} V_t + V_t$$

and

$$R_2 := \frac{1}{2i}\frac{\partial}{\partial x}\circ x \circ \frac{\partial}{\partial x}.$$

First considering a finite sum, we have

$$(R_1 + hR_2)\sum_{n=0}^{N} h^n a_n = R_1 a_0 + \sum_{n=1}^{N} h^n[R_1 a_n + R_2 a_{n-1}] + h^{N+1}R_2 a_N,$$

so we wish to solve the transport equations

$$\begin{cases} R_1 a_0 = 0 \\ R_1 a_n + R_2 a_{n-1} = 0, \quad n \geq 1 \end{cases}$$

with the initial conditions

$$\begin{cases} a_0(0, x, \xi) = 1 \\ a_n(0, x, \xi) = 0, \quad n \geq 1. \end{cases}$$

There is an elegant solution to the equation

$$\left(\frac{\partial}{\partial t} + \frac{1}{2}\operatorname{div} V_t + V_t\right) a_0 = 0 \tag{5.21}$$

which gives interesting geometric information (see [EZ07] and Appendix A of [HS89]). It is due to the fact that

$$V_t = \frac{\partial p_r}{\partial \xi}\left(x, \frac{\partial \varphi}{\partial x}; h\right)\frac{\partial}{\partial x}.$$

We let

$$\Lambda_{t,\xi} := \left\{\left(x, \frac{\partial \varphi}{\partial x}(t, x, \xi; h)\right)\right\}$$

and we denote the (h-dependent) Hamiltonian flow of p_r by κ (generated by the Hamiltonian vector field H_{p_r}), considered as taking

$$\kappa_{s,t}: \qquad \Lambda_{t-s,\xi} \to \Lambda_{t,\xi}.$$

We then note that

$$\frac{d}{ds}\kappa_{s,t}^* f\Big|_{s=0} = H_{p_r}\Big|_{\Lambda_{t,\xi}} f = V_t f$$

for $f \in C^\infty$.

Considering

$$a_0(t, x, \xi)|dx|^{1/2}$$

as a half-density on $\Lambda_{t,\xi}$, (5.21) then becomes

$$\frac{d}{dt}\kappa_t^*(a_0|dx|^{1/2}) = \left(\frac{\partial}{\partial t} + \mathcal{L}_{V_t}\right)(a_0|dx|^{1/2}) = 0$$

where $\mathcal{L}_{V_t}$ denotes the Lie derivative. That is, the amplitude, interpreted as a half-density, is invariant under the flow. This is the same as

$$\kappa_t^*(a_0(t, x, \xi)|dx|^{1/2}\Big|_{\Lambda_{t,\xi}}) = |dx|^{1/2}\Big|_{\Lambda_{0,\xi}}.$$

Hence

$$\kappa_t^* a_0 = |\partial \kappa_t|^{-1/2},$$

where $\partial\kappa_t$ denotes the differential of the mapping κ_t.

Now we recall that the mapping κ_t may be described in terms of its generating function φ, so that its inverse is given by

$$\kappa_t^{-1}: \quad \left(x, \frac{\partial\varphi}{\partial x}(t,x,\xi;h)\right) \to \left(\frac{\partial\varphi}{\partial\xi}(t,x,\xi;h), \xi\right).$$

Hence

$$\partial(\kappa_t^{-1}\Big|_{\Lambda_{t,\xi}}) = \frac{\partial^2\varphi}{\partial x\partial\xi}.$$

So finally we see that

$$a_0(t,x,\xi) = \left(\frac{\partial^2\varphi}{\partial x\partial\xi}\right)^{1/2}.$$

Remark 5.8. The same argument works for more general operators [EZ07], [HS89]. In particular, the simple operators in Sections 5.4 and 5.5 fit into this framework. In Section 5.4 we had the phase

$$\varphi(t,x,y,\xi,\eta) = (xy - \xi\eta)\tanh t + (x\xi + y\eta)\mathrm{sech}t,$$

so that

$$\det\begin{pmatrix} \frac{\partial^2\varphi}{\partial x\partial\xi} & \frac{\partial^2\varphi}{\partial x\partial\eta} \\ \frac{\partial^2\varphi}{\partial y\partial\xi} & \frac{\partial^2\varphi}{\partial y\partial\eta} \end{pmatrix} = \mathrm{sech}^2 t.$$

And in Section 5.5 we had the phase

$$\varphi(t,x,y,\xi,\eta) = (x\xi + y\eta)\sec t - (xy + \xi\eta)\tan t,$$

so that

$$\det\begin{pmatrix} \frac{\partial^2\varphi}{\partial x\partial\xi} & \frac{\partial^2\varphi}{\partial x\partial\eta} \\ \frac{\partial^2\varphi}{\partial y\partial\xi} & \frac{\partial^2\varphi}{\partial y\partial\eta} \end{pmatrix} = \sec^2 t.$$

We may also solve the higher-order transport equations to construct the full amplitude

$$a \sim \sum_{n=0}^{\infty} h^n a_n$$

in the sense of Borel summation.

To rigorously solve (5.13) one must control the error. For this one uses cutoff functions in phase space and restricts to initial conditions v that are appropriately localized in phase space (for a textbook presentation, see [EZ07]). For example, finite sums of Hermite-Gaussian modes are localized to the origin in phase space, and so are localized to the flow-invariant disc. So fortunately we have good behavior for the physically most relevant initial conditions.

5.7 The Operator $\hat{\mathfrak{T}}_4$

For reference, in this section we give the Hamilton flow for the operator $\hat{\mathfrak{T}}_4$. The methods of the previous section may be applied, with some slight modifications due to the additional parameters.

The semiclassical Weyl symbol of $\hat{\mathfrak{T}}_4$ is

$$p_4(x, y, \xi, \eta; h) = \frac{1}{2}x(x^2 + y^2 + \xi^2 + \eta^2) - \frac{5}{2}hx,$$

so then Hamilton's equations are

$$\begin{cases} \dot{x} = x\xi \\ \dot{y} = x\eta \\ \dot{\xi} = -x^2 - \frac{1}{2}(x^2 + y^2 + \xi^2 + \eta^2) + \frac{5}{2}h \\ \dot{\eta} = -xy. \end{cases} \tag{5.22}$$

Here we have the two conserved quantities

$$\begin{cases} C_0 = p_4(x, y, \xi, \eta; h) \\ C_1^2 = y^2 + \eta^2. \end{cases}$$

For $C_0 \neq 0$ we have the solution

$$x(t) = \frac{1}{2} C_0 \left(\wp(t + t_0) + \frac{1}{12}(C_1^2 - 5h) \right)^{-1} \tag{5.23}$$

where t_0 is either an arbitrary real constant or an arbitrary real constant plus $\frac{1}{2}\omega_1$, the purely imaginary half-period of $\wp$ (see Appendix B). Here $\wp$ is the Weierstrass $\wp$-function associated to the invariants

$$g_2 = \frac{1}{12}(C_1^2 - 5h)^2 \qquad \text{and} \qquad g_3 = \frac{1}{216}(C_1^2 - 5h)^3 + \frac{1}{4} C_0^2.$$

We then also have

$$\xi(t) = \frac{-\dot{\wp}(t + t_0)}{\wp(t + t_0) + \frac{1}{12}(C_1^2 - 5h)}. \tag{5.24}$$

As for y, we have the equation

$$\frac{1}{x} \frac{d}{dt} \left(\frac{1}{x} \dot{y} \right) + y = 0$$

where x is as in (5.23). The solution is given by

$$y(t) = y_0 \cos \int_0^t x(s)\, ds + \eta_0 \sin \int_0^t x(s)\, ds$$

and hence

$$\eta(t) = -y_0 \sin \int_0^t x(s)\, ds + \eta_0 \cos \int_0^t x(s)\, ds$$

where of course

$$y_0^2 + \eta_0^2 = C_1^2.$$

We have very different behavior when $C_0 = 0$, which breaks into multiple cases. If $C_1^2 \geq 5h$, then $x(t) = 0$ for all t. We then have $y(t) \equiv y_0$ and $\eta(t) \equiv \eta_0$. As for ξ, if $C_1^2 > 5h$, then

$$\xi(t) = -\sqrt{C_1^2 - 5h}\ \tan\left(\frac{1}{2}\sqrt{C_1^2 - 5h}\ (t + t_0)\right),$$

where t_0 is an arbitrary constant. And if $C_1^2 = 5h$, then either $\xi \equiv 0$ or $\xi(t) = \frac{2}{t+t_0}$.

On the other hand, if $C_1^2 < 5h$, we have one of the following three cases, depending on the initial conditions. Either

$$\begin{aligned}
x(t) &= \pm\sqrt{5h - C_1^2}\ \operatorname{sech}\left(\sqrt{5h - C_1^2}\ (t + t_0)\right) \\
\xi(t) &= -\sqrt{5h - C_1^2}\ \tanh\left(\sqrt{5h - C_1^2}\ (t + t_0)\right) \\
y(t) &= y_0 \cos \int_0^t x(s)\,ds + \eta_0 \sin \int_0^t x(s)\,ds \\
\eta(t) &= -y_0 \sin \int_0^t x(s)\,ds + \eta_0 \cos \int_0^t x(s)\,ds,
\end{aligned}$$

or, in the case where $x_0 = 0$,

$$\begin{aligned}
&x(t) \equiv 0, \qquad y(t) \equiv y_0, \qquad \eta(t) \equiv \eta_0, \qquad \text{and} \\
&\xi(t) = \sqrt{5h - C_1^2}\ \tanh\left(\frac{1}{2}\sqrt{5h - C_1^2}\ (t + t_0)\right),
\end{aligned}$$

or

$$\begin{aligned}
&x(t) \equiv 0, \qquad y(t) \equiv y_0, \qquad \eta(t) \equiv \eta_0, \qquad \text{and} \\
&\xi(t) = \sqrt{5h - C_1^2}\ \coth\left(\frac{1}{2}\sqrt{5h - C_1^2}\ (t + t_0)\right).
\end{aligned}$$

And we have the stationary points

$$(x, y, \xi, \eta) = (\pm\sqrt{\frac{5}{3}h}, 0, 0, 0)$$

and, for $y_0^2 + \eta_0^2 = C_1^2 \leq 5h$,

$$(x, y, \xi, \eta) = (0, y_0, \pm\sqrt{5h - C_1^2}, \eta_0).$$

5.8 Egorov's Theorem

When dealing with the semiclassical quantization of a quadratic polynomial, one may use the metaplectic representation. This is the method discussed, for example, in the work of Calvo and Picón [CP08]. Here we will simply define the metaplectic representation and note the connection with Egorov's theorem.

Following Folland [Fol89], we write the Schrödinger representation of the Heisenberg group as

$$\rho(p, q, t) = e^{2\pi i(pD+qX+tI)},$$

and we write the metaplectic representation as μ. The metaplectic representation is sometimes described in the language of representation theory as follows. Let $\mathcal{T}$ denote the group of automorphisms of the Heisenberg group $\mathbb{H}_n$ that leave the center pointwise fixed. If $T \in \mathcal{T}$, then the composition $\rho \circ T$ is a new irreducible unitary representation of the Heisenberg group, nontrivial on the center, so the Stone-von Neumann theorem [Fol89] says that there exists a unitary operator $\mu(T)$ on $L^2(\mathbb{R}^n)$ such that

$$\mu(T)\rho(X)\mu(T)^{-1} = \rho \circ T(X), \qquad X \in \mathbb{H}_n.$$

Let us compare this to (one version of) Egorov's Theorem:

$$e^{it\hat{\mathfrak{T}}_4/h}\mathrm{Op}_h^W(q)e^{-it\hat{\mathfrak{T}}_4/h} = \mathrm{Op}_h^W(q_t)$$

with $q_t = q \circ \kappa_t + \mathcal{O}(h^2)$. Since we are dealing with unitary operators and the Weyl quantization, we have an error of order $\mathcal{O}(h^2)$ rather than the more usual $\mathcal{O}(h)$ (see Appendix A of [HS89] or Section 2 of [HS04]). This is in fact one of the main reasons for our using h-dependent canonical transformations. Here $\kappa_t = \exp(tH_{p_4})$ is the (h-dependent) Hamilton flow associated to $\hat{\mathfrak{T}}_4$. Egorov's theorem is a way of justifying the intuition that "the Fourier integral operator $e^{itH/h}$

quantizes the Hamilton flow of H". And there is a wider class of Fourier integral operators that may be considered as quantizations of canonical transformations [GS94].

This has a useful consequence for optics, where the Wigner transform is a widely used tool for studying phase space properties of functions. For this we define the standard n-dimensional semiclassical Wigner transform by

$$W(f,g)(x,\xi) = (2\pi h)^{-n/2} \int e^{-ip\xi/h} f\left(x + \frac{1}{2}p\right) \overline{g\left(x - \frac{1}{2}p\right)}\, dp.$$

Among other useful properties (one may consult Folland's book [Fol89]), we have the norm-preserving property

$$||W(f,g)||_{L^2(\mathbb{R}^{2n})} = ||f||_{L^2(\mathbb{R}^n)}||g||_{L^2(\mathbb{R}^n)},$$

and one may check that for any symbol σ one has

$$\langle \mathrm{Op}_h^W(\sigma) f | g\rangle = (2\pi h)^{-n/2} \iint \sigma(x,\xi) W(f,g)(x,\xi)\, dx\, d\xi.$$

Then, for example, using U_t, the semiclassical approximate propagator for $\hat{\mathfrak{T}}_4$ (with Weyl symbol p_4, having the Hamilton flow κ_t), one has

$$\begin{aligned}\langle \mathrm{Op}_h^W(\sigma) U_t f | U_t g\rangle &= \langle e^{it\hat{\mathfrak{T}}_4/h} \mathrm{Op}_h^W(\sigma) e^{-it\hat{\mathfrak{T}}_4/h} f | g\rangle + \mathcal{O}(h^\infty) \\ &= \langle \mathrm{Op}_h^W(\sigma_t) f | g\rangle + \mathcal{O}(h^\infty),\end{aligned}$$

where $\sigma_t = \sigma \circ \kappa_t + \mathcal{O}(h^2)$. Hence

$$\begin{aligned}\iint \sigma(x,\xi) W(U_t f, U_t g)(x,\xi)\, dx\, d\xi &= \iint \sigma(\kappa_t(x,\xi)) W(f,g)(x,\xi)\, dx\, d\xi + \mathcal{O}(h^2) \\ &= \iint \sigma(x,\xi) W(f,g)(\kappa_{-t}(x,\xi))\, dx\, d\xi + \mathcal{O}(h^2).\end{aligned}$$

Since this is true for all symbols σ, we thus have

$$W(U_t f, U_t g) = W(f,g) \circ \kappa_{-t} + \mathcal{O}(h^2).$$

If we were dealing with a metaplectic operator, the transformation κ would then be a linear symplectic transformation, and the identity would be exact.

5.9 Additional Remarks

Remark 5.9. So far we have concerned ourselves with the manipulation of Hermite-Gaussian modes: those two-dimensional modes generated by applying the x and y creation operators $\hat{a}_x^\dagger$ and $\hat{a}_y^\dagger$ to the fundamental mode $\pi^{-1/2}e^{-(x^2+y^2)/2}$ (one may alternatively use the semiclassical version). But one may also just as easily consider the manipulation of Laguerre-Gaussian modes, generated by applying the creation operators

$$\hat{A}_\pm^\dagger = 2^{-1/2}(\hat{a}_x^\dagger \pm i\hat{a}_y^\dagger)$$

to the fundamental mode. It is no more difficult to use the above methods, since, as seen in Chapter 4, the extended Wigner transform intertwines the two classes of creation operators.

Remark 5.10. We have seen that the Hamilton flows of $\hat{\mathfrak{T}}_4$, $\hat{\mathfrak{T}}_5$, $\hat{\mathfrak{T}}_6$, and $\hat{\mathfrak{T}}_7$ blow up in finite time. One may now ask: what are the consequences for the propagators themselves? As noted by Maciej Zworski [Zwo08], the propagators (the non-Gaussian transformations) may cause certain initial conditions to develop singularities in finite time, since this is precisely what happens for simpler operators.

We consider the following simplification of $\hat{\mathfrak{T}}_5$:

$$Q_1 = \frac{1}{2}(x^2 D_x + D_x \circ x^2).$$

One may explicitly find the deficiency subspaces, the Hamilton flow, and the propagator (which may be viewed as a Fourier integral operator). And there exist smooth $L^2(\mathbb{R})$ initial conditions, namely,

$$u_0(x) = \langle x \rangle^{-\alpha}, \qquad \frac{1}{2} < \alpha < 1,$$

which develop singularities, traveling along the Hamilton flow.

For an example closer yet to $\hat{\mathfrak{T}}_5$, one may consider

$$\begin{aligned} Q_2 &= \frac{1}{2}(x^2 hD_x + hD_x \circ x^2) - 5h^2 D_x \\ &= x^2 hD_x - ihx - 5h^2 D_x. \end{aligned}$$

For reference, we note that the propagator is

$$e^{-itQ_2/h} u_0(t,x) = a(x\sinh(at) + a\cosh(at))^{-1} u_0 \left(a \left(\frac{x\cosh(at) + a\sinh(at)}{x\sinh(at) + a\cosh(at)} \right) \right)$$

where $a = \sqrt{5h}$.

To study creation of singularities in general, one might use the methods of Jared Wunsch [Wun99].

CHAPTER 6

Manipulation of Semiclassical Laguerre-Gaussian Modes: a Model Case

6.1 Introduction

Gabriel F. Calvo and Antonio Picón [CP08] introduced a class of operators which allows arbitrary manipulations of the three lowest-order Hermite-Gaussian (HG) modes for the purposes of quantum communication. In the previous chapter, we (1) classified the self-adjoint extensions of the generators and (2) showed how to construct semiclassical approximations of the associated unitary operators; for the latter, we first considered a simple model operator to illustrate the semiclassical methods in a simplified setting before then moving on to the full operators of Calvo and Picón.

In this chapter, we show that the simplified operator also serves as a model operator from an experimental viewpoint, when considered as manipulating Laguerre-Gaussian (LG) modes of orders $(0,0)$, $(1,0)$, $(0,1)$, and $(1,1)$.

Calvo and Picón introduced the following eight generators acting on Hermite-Gaussian modes:

$$\hat{\mathcal{T}}_1 = \frac{1}{2}(\hat{a}_x^\dagger \hat{a}_y + \hat{a}_y^\dagger \hat{a}_x), \qquad \hat{\mathcal{T}}_2 = -\frac{i}{2}(\hat{a}_x^\dagger \hat{a}_y - \hat{a}_y^\dagger \hat{a}_x), \qquad \hat{\mathcal{T}}_3 = \frac{1}{2}(\hat{a}_x^\dagger \hat{a}_x - \hat{a}_y^\dagger \hat{a}_y),$$

$$\hat{\mathcal{T}}_4 = \frac{1}{2}(\hat{a}_x^\dagger + \hat{a}_x - \hat{a}_x^\dagger \hat{a}_x^\dagger \hat{a}_x - \hat{a}_x^\dagger \hat{a}_x \hat{a}_x - \hat{a}_x^\dagger \hat{a}_y^\dagger \hat{a}_y - \hat{a}_x \hat{a}_y^\dagger \hat{a}_y),$$

$$\hat{\mathcal{T}}_5 = -\frac{i}{2}(\hat{a}_x^\dagger - \hat{a}_x - \hat{a}_x^\dagger\hat{a}_x^\dagger\hat{a}_x + \hat{a}_x^\dagger\hat{a}_x\hat{a}_x - \hat{a}_x^\dagger\hat{a}_y^\dagger\hat{a}_y + \hat{a}_x\hat{a}_y^\dagger\hat{a}_y),$$
$$\hat{\mathcal{T}}_6 = \frac{1}{2}(\hat{a}_y^\dagger + \hat{a}_y - \hat{a}_y^\dagger\hat{a}_y^\dagger\hat{a}_y - \hat{a}_y^\dagger\hat{a}_y\hat{a}_y - \hat{a}_y^\dagger\hat{a}_x^\dagger\hat{a}_x - \hat{a}_y\hat{a}_x^\dagger\hat{a}_x),$$
$$\hat{\mathcal{T}}_7 = -\frac{i}{2}(\hat{a}_y^\dagger - \hat{a}_y - \hat{a}_y^\dagger\hat{a}_y^\dagger\hat{a}_y + \hat{a}_y^\dagger\hat{a}_y\hat{a}_y - \hat{a}_y^\dagger\hat{a}_x^\dagger\hat{a}_x + \hat{a}_y\hat{a}_x^\dagger\hat{a}_x),$$
$$\hat{\mathcal{T}}_8 = \frac{1}{2\sqrt{3}}[-2 + 3(\hat{a}_x^\dagger\hat{a}_x + \hat{a}_y^\dagger\hat{a}_y)],$$

defined in terms of the creation and annihilation operators $\hat{a}_x^\dagger = \frac{1}{\sqrt{2}}\left(x - \frac{\partial}{\partial x}\right)$ and $\hat{a}_x = \frac{1}{\sqrt{2}}\left(x + \frac{\partial}{\partial x}\right)$, respectively, and similarly for the y-variable.

These generators, within the subspace generated by the lowest three Hermite-Gaussian modes $\mathcal{H}_{\hat{\mathcal{T}}} = \{|0,0\rangle, |1,0\rangle, |0,1\rangle\}$, obey the $SU(3)$ algebra

$$[\hat{\mathcal{T}}_a, \hat{\mathcal{T}}_b] = i f_{abc}\hat{\mathcal{T}}_c$$

$(a, b, c = 1, 2, \ldots 8)$, where the only nonvanishing (up to permutations) structure constants f_{abc} are given by

$$f_{123} = 1, \quad f_{147} = f_{165} = f_{246} = f_{257} = f_{345} = f_{376} = 1/2,$$

and

$$f_{458} = f_{678} = \sqrt{3}/2.$$

We note that the triad of generators

$$\Gamma_1 \equiv \{\hat{\mathcal{T}}_1, \hat{\mathcal{T}}_2, \hat{\mathcal{T}}_3\}$$

gives a $SU(2)$ group that conserves the mode order. The remaining two $SU(2)$ groups are formed by the triads

$$\Gamma_2 \equiv \{\hat{\mathcal{T}}_4, \hat{\mathcal{T}}_5, (\hat{\mathcal{T}}_3 + \sqrt{3}\hat{\mathcal{T}}_8)/2\} \qquad \text{and} \qquad \Gamma_3 \equiv \{\hat{\mathcal{T}}_6, \hat{\mathcal{T}}_7, (-\hat{\mathcal{T}}_3 + \sqrt{3}\hat{\mathcal{T}}_8)/2\}.$$

Unitary operators $\hat{U}_{\Gamma_1}$ generated by the first triad give rise to superpositions between the two modes $|1,0\rangle$ and $|0,1\rangle$, leaving invariant the fundamental mode

$|0,0\rangle$. Unitarities $\hat{U}_{\Gamma_2}$ and $\hat{U}_{\Gamma_3}$, generated by the second and third triads, produce superpositions between the two modes $|0,0\rangle$ and $|1,0\rangle$ (leaving invariant $|0,1\rangle$), or the modes $|0,0\rangle$ and $|0,1\rangle$ (leaving invariant $|1,0\rangle$), respectively.

Here we instead consider the one-dimensional operator

$$\hat{\mathcal{T}} = \hat{a}^\dagger + \hat{a} - \hat{a}^\dagger\hat{a}^\dagger\hat{a} - \hat{a}^\dagger\hat{a}\hat{a},$$

acting on the one-dimensional Hermite functions h_n. This is a simplified version of the operator $\hat{\mathcal{T}}_4$ above. We introduced this operator in Chapter 5 since it exhibits the same essential behavior as $\hat{\mathcal{T}}_4$, while leaving out the unessential additional variables. Here we will show that this operator may also be useful in experimental work, as an easier preliminary step before moving to the more complicated operator $\hat{\mathcal{T}}_4$.

One may check that $\hat{\mathcal{T}}h_0 = h_1$ and $\hat{\mathcal{T}}h_1 = h_0$. More generally,

$$\hat{\mathcal{T}}h_n = \beta_n h_{n+1} + \beta_{n-1}h_{n-1}$$

where

$$\beta_n = (1-n)\sqrt{n+1}.$$

So $\hat{\mathcal{T}}$, when acting on the domain of (finite) linear combinations of HG modes, behaves precisely as the infinite Jacobi matrix

$$\begin{pmatrix} 0 & \beta_0 & 0 & 0 & \cdots \\ \beta_0 & 0 & \beta_1 & 0 & \\ 0 & \beta_1 & 0 & \beta_2 & \\ 0 & 0 & \beta_2 & 0 & \ddots \\ \vdots & & & \ddots & \ddots \end{pmatrix} = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 & \cdots & \\ 1 & 0 & 0 & 0 & 0 & 0 & & \\ 0 & 0 & 0 & -\sqrt{3} & 0 & 0 & \cdots & \\ 0 & 0 & -\sqrt{3} & 0 & -4 & 0 & & \\ 0 & 0 & 0 & -4 & 0 & \ddots & & \\ 0 & 0 & 0 & 0 & \ddots & \ddots & \ddots & \\ \vdots & & \vdots & & & \ddots & \ddots & \ddots \end{pmatrix}.$$

Using a theorem from Berezanskii's book ([Ber68], p.507; see also Chapter 5), one can show that the deficiency index of this operator is $(1, 1)$, and hence the space of boundary values is of dimension $2 = 1 + 1$. Moreover, using results of Allahverdiev [All05], one can explicitly classify all self-adjoint extensions in terms of certain boundary values at infinity. This was achieved for the full operators of Calvo and Picón in Chapter 5, using a slight modification of Allahverdiev's methods, but for the simplified operator $\hat{\mathcal{T}}$ the methods of Allahverdiev may be applied without any modification.

We will show that this model operator $\hat{\mathcal{T}}$ allows simple manipulations of LG modes. But first, since the Wigner transform plays a basic role in the theory of LG modes, we recall some relevant facts in the next section.

6.2 The Semiclassical Wigner Transform

The standard n-dimensional semiclassical Wigner transform is defined as

$$W(f, g)(x, \xi) = (2\pi h)^{-n/2} \int e^{-ip\xi/h} f(x + \frac{1}{2}p)\overline{g(x - \frac{1}{2}p)}\, dp, \tag{6.1}$$

where f and g are square-integrable functions of n variables. Then, among other useful properties (one may consult Folland's book [Fol89]), we have the norm-preserving property:

$$||W(f, g)||_{L^2(\mathbb{R}^{2n})} = ||f||_{L^2(\mathbb{R}^n)}||g||_{L^2(\mathbb{R}^n)}.$$

Also, the Wigner transform has an important relationship with Weyl quantization. We recall that the semiclassical Weyl quantization of a symbol σ is the operator $\mathrm{Op}_h^W(\sigma)$ defined by

$$\mathrm{Op}_h^W(\sigma)f(x) = (2\pi h)^{-n} \iint e^{i(x-y)\xi/h}\sigma((x + y)/2, \xi)f(y)dy\, d\xi.$$

Then

$$\langle \mathrm{Op}_h^W(\sigma) f | g \rangle = (2\pi h)^{-n/2} \iint \sigma(x,\xi) W(f,g)(x,\xi) dx\, d\xi.$$

As discussed in Chapter 5, we have an approximate formula for the evolution of the Wigner transform. Let $\hat{\mathfrak{T}}$ be a self-adjoint semiclassical pseudodifferential operator with Hamilton flow κ_t generated by the (possibly h-dependent) Weyl symbol, and let $U_t = e^{-it\hat{\mathfrak{T}}/h}$ be the unitary propagator. (Note: In the previous chapter, U_t sometimes denoted the semiclassical *approximate* unitary propagator.) We then have

$$W(f,g)(\kappa_{-t}(x,\xi)) = W(U_t f, U_t g)(x,\xi) + \mathcal{O}(h^2)||f||_{L^2(\mathbb{R}^n)}||g||_{L^2(\mathbb{R}^n)}.$$

This essentially follows from Egorov's theorem with an $\mathcal{O}(h^2)$ error (see Chapter 5 and references therein).

In the previous chapter, we briefly discussed two-dimensional Wigner transforms. In the present chapter, in the next section, we will consider the case $n = 1$, since LG modes are themselves one-dimensional Wigner transforms of Hermite functions (see Chapter 4).

6.3 The Semiclassical Laguerre-Gaussian Modes

In the context of LG modes, it is more convenient to use an alternative definition of the Wigner transform. We define the (one-dimensional) *extended* Wigner transform, of a function F of two variables, as

$$\tilde{W}(F)(x,\xi) = (2\pi h)^{-1/2} \int e^{ip\xi/h} F\left(\frac{x+p}{\sqrt{2}}, \frac{x-p}{\sqrt{2}}\right) dp.$$

(The sign of the phase is intentionally different from (6.1).) This is clearly a unitary operator; moreover, as shown in Chapter 4, the $(m,n)^{th}$ LG mode is precisely given by $\tilde{W}h_{mn}$, where h_{mn} is the $(m,n)^{th}$ HG mode. For reference, we will now state the main facts in the semiclassical setting.

The zeroth order HG mode is the Gaussian function

$$h_{00}(x,y) = (\pi h)^{-1/2} e^{-(x^2+y^2)/(2h)}.$$

All other HG modes, h_{mn}, may be recovered by applying the creation operators

$$\hat{a}_1^\dagger = (2h)^{-1/2}\left(x - h\frac{\partial}{\partial x}\right) \quad \text{and} \quad \hat{a}_2^\dagger = (2h)^{-1/2}\left(y - h\frac{\partial}{\partial y}\right).$$

That is,

$$h_{mn} = (m!n!)^{-1/2} \hat{a}_1^{\dagger\, m} \hat{a}_2^{\dagger\, n} h_{00}.$$

The corresponding annihilation operators are

$$\hat{a}_1 = (2h)^{-1/2}\left(x + h\frac{\partial}{\partial x}\right) \quad \text{and} \quad \hat{a}_2 = (2h)^{-1/2}\left(y + h\frac{\partial}{\partial y}\right).$$

Alternatively, to recover the LG modes, one applies to h_{00} the creation operators

$$\hat{A}_+^\dagger = \frac{1}{\sqrt{2}}(a_1^\dagger + i a_2^\dagger) \quad \text{and} \quad \hat{A}_-^\dagger = \frac{1}{\sqrt{2}}(a_1^\dagger - i a_2^\dagger).$$

The corresponding LG mode annihilation operators are

$$\hat{A}_+ = \frac{1}{\sqrt{2}}(a_1 - i a_2) \quad \text{and} \quad \hat{A}_- = \frac{1}{\sqrt{2}}(a_1 + i a_2).$$

As discussed in Chapter 4 (but also as one may easily check), the extended Wigner transform intertwines the two classes of creation and annihilation operators:

$$\begin{aligned} \hat{A}_+^\dagger \tilde{W} &= \tilde{W}\hat{a}_1^\dagger, & \qquad \hat{A}_-^\dagger \tilde{W} &= \tilde{W}\hat{a}_2^\dagger, \\ \hat{A}_+ \tilde{W} &= \tilde{W}\hat{a}_1, & \qquad \hat{A}_- \tilde{W} &= \tilde{W}\hat{a}_2. \end{aligned} \tag{6.2}$$

Since $\tilde{W}h_{00} = h_{00}$, this shows that the LG modes are indeed the extended Wigner transforms of the HG modes. Moreover, one may deduce the following familiar analytic expressions for the LG modes. Suppose $x, y \in \mathbb{R}$, and let $z = x + iy$. Then, with h_{jk} denoting the $(j,k)^{th}$ HG mode, the $(j,k)^{th}$ LG mode is

$$\tilde{W}(h_{jk})(x,y) = \begin{cases} (\pi h)^{-1/2}(k!/j!)^{1/2}(-1)^k(z/\sqrt{h})^{j-k}e^{-z\overline{z}/(2h)}L_k^{j-k}(z\overline{z}/h) & \text{if } j \geq k, \text{ and} \\ (\pi h)^{-1/2}(j!/k!)^{1/2}(-1)^j(\overline{z}/\sqrt{h})^{k-j}e^{-z\overline{z}/(2h)}L_j^{k-j}(z\overline{z}/h) & \text{if } j \leq k, \end{cases}$$

where

$$L_n^{\alpha}(x) = \frac{x^{-\alpha}e^x}{n!}\frac{d^n}{dx^n}(e^{-x}x^{n+\alpha})$$

are the Laguerre polynomials. Of particular importance in this chapter are $L_0^0(x) = L_0^1(x) = 1$ and $L_1^0(x) = 1 - x$.

6.4 Manipulation of Semiclassical LG Modes

We first consider the action of the tensor product $\hat{\mathcal{T}} \otimes \hat{\mathcal{T}}$ on tensor products of functions:

$$(\hat{\mathcal{T}} \otimes \hat{\mathcal{T}})(f \otimes \overline{g}) = \hat{\mathcal{T}}(f) \otimes \overline{\hat{\mathcal{T}}(g)}.$$

Then we simply pull back this action to operate on extended Wigner transforms of functions. We write this as follows:

$$(\hat{\mathcal{T}}^{\star}\tilde{W})(f \otimes \overline{g}) := \tilde{W}(\hat{\mathcal{T}}(f) \otimes \overline{\hat{\mathcal{T}}(g)}).$$

Since the extended Wigner transform has the intertwining property (6.2), we see that the pullback operator $\hat{\mathcal{T}}^{\star}$ is precisely the differential operator

$$(\hat{A}_+^{\dagger} + \hat{A}_+ - \hat{A}_+^{\dagger}\hat{A}_+^{\dagger}\hat{A}_+ - \hat{A}_+^{\dagger}\hat{A}_+\hat{A}_+) \circ (\hat{A}_-^{\dagger} + \hat{A}_- - \hat{A}_-^{\dagger}\hat{A}_-^{\dagger}\hat{A}_- - \hat{A}_-^{\dagger}\hat{A}_-\hat{A}_-).$$

However, this point of view only seems to complicate matters.

We are especially interested in the case when $f \otimes \overline{g} = h_{mn}$, the $(m,n)^{th}$ HG mode; then the pullback $\hat{\mathcal{T}}^\star$ acts on LG modes. In particular, $\hat{\mathcal{T}} \otimes \hat{\mathcal{T}}$ acts on the four "binary" HG modes as follows:

$$(\hat{\mathcal{T}} \otimes \hat{\mathcal{T}})h_{00} = h_{11}, \qquad (\hat{\mathcal{T}} \otimes \hat{\mathcal{T}})h_{11} = h_{00},$$
$$(\hat{\mathcal{T}} \otimes \hat{\mathcal{T}})h_{10} = h_{01}, \qquad (\hat{\mathcal{T}} \otimes \hat{\mathcal{T}})h_{01} = h_{10}.$$

Hence

$$(\hat{\mathcal{T}}^\star \tilde{W})h_{00} = \tilde{W}h_{11}, \qquad (\hat{\mathcal{T}}^\star \tilde{W})h_{11} = \tilde{W}h_{00},$$
$$(\hat{\mathcal{T}}^\star \tilde{W})h_{10} = \tilde{W}h_{01}, \qquad (\hat{\mathcal{T}}^\star \tilde{W})h_{01} = \tilde{W}h_{10}.$$

These lowest-order LG modes may be written in polar coordinates as

$$\tilde{W}h_{00} = (\pi h)^{-1/2} e^{-r^2/(2h)}, \qquad \tilde{W}h_{11} = -(\pi h)^{-1/2}(1-(r/\sqrt{h})^2)e^{-r^2/(2h)},$$
$$\tilde{W}h_{10} = (\pi h)^{-1/2}(r/\sqrt{h})e^{i\theta}e^{-r^2/(2h)}, \quad \tilde{W}h_{01} = (\pi h)^{-1/2}(r/\sqrt{h})e^{-i\theta}e^{-r^2/(2h)}.$$

So we see that the pullback $\hat{\mathcal{T}}^\star$ interchanges the LG modes $\tilde{W}h_{00}$ and $\tilde{W}h_{11}$ and simply causes a phase reversal in the LG modes of order one.

For convenience, in order to have a semiclassical differential operator, we define

$$\hat{\mathfrak{T}} = -2^{-1/2}h^{3/2}\hat{\mathcal{T}},$$

and we note that[1]

$$\hat{\mathfrak{T}} = \frac{1}{2}x(x^2 + (hD)^2) - 2hx - \frac{1}{2}ih^2 D,$$

with the notation $D = \frac{1}{i}\frac{\partial}{\partial x}$.

[1]In [Van09b] we mistakenly studied the operator $\frac{1}{2}x(x^2+(hD)^2) - \frac{3}{2}hx - \frac{1}{2}ih^2 D$ with Weyl symbol $\frac{1}{2}x(x^2+\xi^2) - \frac{3}{2}hx$, which is not quite the same as $\hat{\mathfrak{T}}$. However, it was merely given as an example, to illustrate a general method, so in that paper one may simply redefine the operator in the first place.

Just as we defined the pullback of $\hat{\mathcal{T}}$, we may similarly define the pullback of the unitary propagator $U_t = e^{-it\hat{\mathfrak{T}}/h}$:

$$(U_t^\star \tilde{W})(f \otimes \overline{g}) = \tilde{W}(U_t f \otimes \overline{U_t g}).$$

One may check that U_t acts as follows:

$$U_t h_0 = \cos((h/2)^{1/2} t) h_0 + i \sin((h/2)^{1/2} t) h_1.$$

Hence we have

$$\begin{aligned} U_t^\star \tilde{W} h_{00} = \cos^2((h/2)^{1/2} t) \tilde{W} h_{00} + \sin^2((h/2)^{1/2} t) \tilde{W} h_{11} \\ + i \cos((h/2)^{1/2} t) \sin((h/2)^{1/2} t) [\tilde{W} h_{10} - \tilde{W} h_{01}], \end{aligned}$$

where, in polar coordinates,

$$\tilde{W} h_{10} - \tilde{W} h_{01} = (\pi h)^{-1/2} (r/\sqrt{h}) e^{-r^2/(2h)} (2i \sin\theta).$$

This transformation is pictured in Figure 6.1.

As mentioned in Section 6.2, we have an approximate formula for the evolution of the Wigner transform in terms of the Hamilton flow. At the end of this chapter, we will adapt the result to the case of the extended Wigner transform, for the study of LG mode intensities; but first we will explicitly compute the Hamilton flow.

The Weyl symbol of $\hat{\mathfrak{T}}$ is

$$p(x, \xi; h) = \frac{1}{2} x (x^2 + \xi^2) - 2hx.$$

Later we will need a re-scaled version of p, so we consider the slightly more general symbol

$$p_r(x, \xi; h) = \frac{1}{2} x (x^2 + \xi^2) - \frac{1}{2} r^2 h x.$$

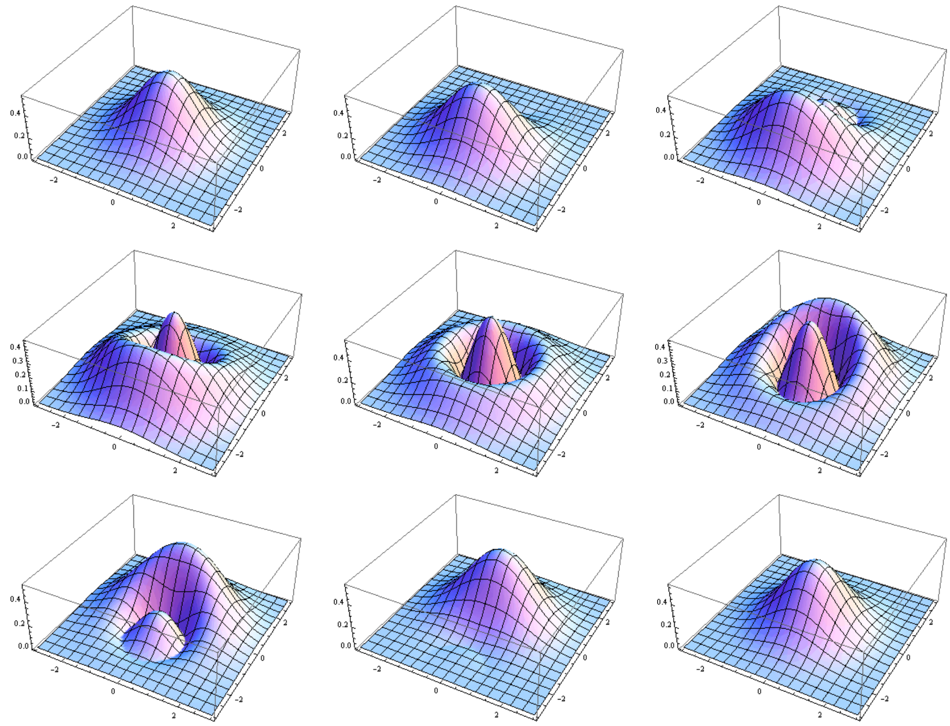

Figure 6.1: For convenience we let $h = 1$ and $T = t/\sqrt{2}$, so that $U^{\star}_{T\sqrt{2}}\tilde{W}h_{00} = \pi^{-1/2}e^{-(x^2+y^2)/2}[\cos(2T) - y\sin(2T) + (x^2+y^2)\sin^2(T)]$. The figure shows the absolute value for $T = k\pi/8$, $k = 0, \ldots, 8$.

Hamilton's equations for this symbol are

$$\begin{cases} \dot{x} = x\xi \\ \dot{\xi} = -\frac{3}{2}x^2 - \frac{1}{2}\xi^2 + \frac{1}{2}r^2h, \end{cases} \tag{6.3}$$

with the conserved quantity $C = p_r(x, \xi; h)$.

First suppose that $C \neq 0$. Then we have

$$x(t) = \frac{1}{2}C\left(\wp(t+t_0) - \frac{1}{12}r^2h\right)^{-1} \qquad \text{and} \qquad \xi(t) = \frac{-\dot{\wp}(t+t_0)}{\wp(t+t_0) - \frac{1}{12}r^2h},$$

where t_0 is either an arbitrary real constant or an arbitrary real constant plus $\frac{1}{2}\omega_1$, the purely imaginary half-period of $\wp$. Here $\wp$ is the Weierstrass $\wp$-function associated to the invariants

$$g_2 = \frac{1}{12}r^4h^2 \qquad \text{and} \qquad g_3 = \frac{1}{4}C^2 - \frac{1}{216}r^6h^3.$$

For further details, one may consult the previous chapter.

When $r = 0$ and $C \neq 0$, $\xi(t)$ is always strictly decreasing, which follows simply from Hamilton's equations (6.3). However, when $r > 0$ we have a more complicated behavior, as shown in Figure 6.2. There is a pocket of radius $r\sqrt{h} = \frac{r}{\sqrt{2}}w_0$, where w_0 is in practice the radius of the laser beam's waist.

For $C = 0$, depending on the initial conditions, we have one of the following four cases:

$$\begin{cases} x(t) = 0 \quad \forall t \\ \xi(t) = \sqrt{r^2h}\coth\left(\frac{\sqrt{r^2h}}{2}(t+t_0)\right), \end{cases}$$

$$\begin{cases} x(t) = 0 \quad \forall t \\ \xi(t) = \sqrt{r^2h}\tanh\left(\frac{\sqrt{r^2h}}{2}(t+t_0)\right), \end{cases}$$

$$\begin{cases} x(t) = \pm\sqrt{r^2h}\,\mathrm{sech}(\sqrt{r^2h}(t+t_0)) \\ \xi(t) = -\sqrt{r^2h}\tanh\left(\sqrt{r^2h}(t+t_0)\right), \end{cases}$$

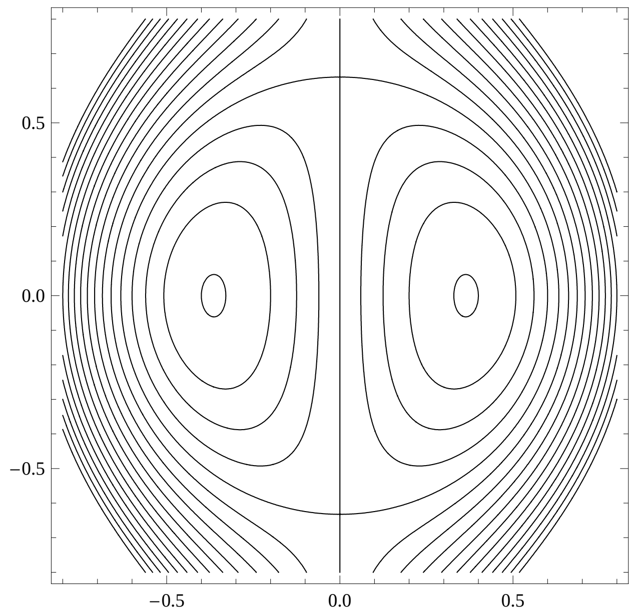

Figure 6.2: Hamilton flow lines in the (x, ξ) plane. Here $h = 1/10$ and $r^2 = 4$.

or

$$\Big\{ (x(t), \xi(t)) = (0, \pm\sqrt{r^2 h}) \qquad \forall t \quad \text{(hyperbolic stationary points)}.$$

Of course, we also have the elliptic stationary points $(x, \xi) = (\pm\sqrt{\frac{r^2 h}{3}}, 0)$, corresponding to $C = \mp(r^2 h/3)^{3/2}$.

Since the LG modes are extended Wigner transforms of HG modes, we now see that the intensity of LG modes evolves according to the Hamilton flow we have just computed. As discussed in Section 6.2, we have that the evolution of the Wigner transform may be approximately described by the Hamilton flow κ_t. However, the extended Wigner transform acts slightly differently with respect to the Weyl quantization:

$$\langle \mathrm{Op}_h^W(\sigma) f | g \rangle = (\pi h)^{-1/2} \iint \tilde{W}(f \otimes \overline{g})(\sqrt{2}\, x, -\sqrt{2}\, \xi) \sigma(x, \xi) \, dx \, d\xi.$$

Even so, the same arguments give the same result, up to some minor re-scaling. Let $\tilde{M}_{\sqrt{2}}$ be the operator given by

$$\tilde{M}_{\sqrt{2}}(x, \xi) = (\sqrt{2}\, x, -\sqrt{2}\, \xi).$$

Then we have

$$\begin{aligned}(U_t^\star \tilde{W})(f \otimes \overline{g}) &= \tilde{W}(U_t f \otimes \overline{U_t g}) \\ &= \tilde{W}(f \otimes \overline{g}) \circ \tilde{M}_{\sqrt{2}} \circ \kappa_{-t} \circ \tilde{M}_{\sqrt{2}}^{-1} + \mathcal{O}(h^2)||f||_{L^2}||g||_{L^2} \\ &= \tilde{W}(f \otimes \overline{g}) \circ \tilde{\kappa}_{-t} + \mathcal{O}(h^2)||f||_{L^2}||g||_{L^2}.\end{aligned}$$

Here

$$\tilde{\kappa}_t := \tilde{M}_{\sqrt{2}} \circ \kappa_t \circ \tilde{M}_{\sqrt{2}}^{-1},$$

which we note is the Hamilton flow of the function

$$\tilde{p} = -2p \circ \tilde{M}_{\sqrt{2}}^{-1}.$$

Up to a re-scaling of t, we then have the Hamilton flow computed earlier, but now in the case $r^2 = 8$.

We are most interested in HG modes and LG modes, so we take $f \otimes \overline{g} = h_{mn}$. We then summarize our work in the following theorem:

Theorem 6.1. *For $\hat{\mathfrak{T}} = -2^{-1/2}h^{3/2}\hat{\mathcal{T}} = -2^{-1/2}h^{3/2}(\hat{a}^\dagger + \hat{a} - \hat{a}^\dagger\hat{a}^\dagger\hat{a} - \hat{a}^\dagger\hat{a}\hat{a})$, having Weyl symbol $p(x, \xi; h) = \frac{1}{2}x(x^2 + \xi^2) - 2hx$, and for $U_t = e^{-it\hat{\mathfrak{T}}/h}$, we have*

$$\begin{aligned}(U_t^\star \tilde{W})(h_{mn}) &\equiv \tilde{W}(U_t h_m \otimes \overline{U_t h_n}) \\ &= \tilde{W}(h_{mn}) \circ \tilde{\kappa}_{-t} + \mathcal{O}(h^2).\end{aligned}$$

Here $\tilde{\kappa}_t$ is the Hamilton flow of the function $\tilde{p}$ given by

$$\begin{aligned}\tilde{p}(x, \xi; h) &= -2p(x/\sqrt{2}, -\xi/\sqrt{2}; h) \\ &= -\frac{1}{\sqrt{2}}\left[\frac{1}{2}x(x^2 + \xi^2) - 4hx\right].\end{aligned}$$

Hence the intensities of the LG modes evolve along elliptic curves, as pictured in Figure 6.2. This was in fact the motivation for the present chapter. Previously, in Chapter 5, we found that the Wigner transforms of HG modes evolve, in four-dimensional phase space $(x, y, \xi, \eta) \in \mathbb{R}^4$, according to a slightly more complicated flow, where the flow in the (x, ξ) plane (with x and ξ dual variables) for certain values of (y, η) appears as in Figure 6.2. Now we have found a situation where the flow along elliptic curves appears in the physical (x, y) plane. If one wishes, one may then consider Wigner transforms of LG modes; formulas for these are given in Chapter 4.

APPENDIX A

A Boundary Carleman Estimate

In Chapter 2, the main tool was a boundary Carleman estimate for the semiclassical Schrödinger operator, as used by Burq [Bur02]. In the case of the Laplacian, the result is due to Lebeau and Robbiano [LR95], whose proof works line-by-line in the more general case; indeed, Burq, in [Bur02], only sketches the argument and refers to Lebeau and Robbiano for details. For completeness, here we will give the full details.

The heart of the matter is the local version, in the positive upper half space $\mathbb{R}^n_+ = \{x_n \geq 0\}$; this is the subject of Sections A.1, A.2, A.3, and A.4. In Section A.5 we prove the global result by reducing to the local result.

A.1 Notation and Definitions

We work in the upper half space $\mathbb{R}^n_+ = \{x_n \geq 0\}$, in the neighborhood $K = \{x \in \mathbb{R}^n_+; |x| \leq r_0\}$ for some $r_0 > 0$, and we let $C_0^\infty(K)$ be the space of functions that are smooth on $\mathbb{R}^n_+$ with support in K. For $f \in C_0^\infty(K)$ we write $f_0 = f|_{x_n=0}$.

We take as our potential $V \in C^\infty(\mathbb{R}^n_+, \mathbb{R})$. Then our Schrödinger operator is

$$P = -h^2\partial_{x_n}^2 + h^2 R(x, \frac{1}{i}\partial_{x'}) + V(x),$$

where R is a second-order differential operator with coefficients smooth in a neighborhood of K, having principal symbol r such that

$$r(x,\xi) \in \mathbb{R} \quad \text{and} \quad \exists c > 0 \quad \text{such that} \quad \forall (x,\xi') \quad \text{we have} \quad r(x,\xi') \geq c|\xi'|^2.$$

As mentioned in Chapter A, the boundary Carleman estimate results from conjugating the operator P by an exponential. For the phase, we let φ be real-valued and smooth in a neighborhood of K, and we let $h \in (0, h_0]$ be a small parameter. The conjugated operator is then

$$P_\varphi := e^{\varphi/h} \circ P \circ e^{-\varphi/h}.$$

With $D_j = \frac{h}{i}\frac{\partial}{\partial x_j}$, by explicit calculation we have [1]

$$\begin{aligned} P_\varphi &= e^{\varphi/h}(D_n^2 + h^2 R(x, \frac{1}{i}\partial_{x'}) + V(x))e^{-\varphi/h} \\ &= (D_n + i\varphi'_{x_n})^2 + h^2 R(x, \frac{1}{i}\partial_{x'} + \frac{i}{h}\varphi'_{x'}) + V(x) \\ &= \sum_{j=0}^{2} h^j P_\varphi^{2-j} \end{aligned}$$

where P_φ^{2-j} is a polynomial in D of order $\leq 2-j$. The principal symbol of P_φ is

$$\begin{aligned} p_\varphi(x,\xi) &= p(x, \xi + i\varphi') \\ &= (\xi_n + i\varphi'_{x_n})^2 + r(x, \xi' + i\varphi'_{x'}) + V(x) \end{aligned}$$

By hypothesis, we will take φ to satisfy

(i) $\forall (x,\xi) \in K \times \mathbb{R}^n, \quad p_\varphi(x,\xi) = 0 \Longrightarrow \{\mathrm{Re} p_\varphi, \mathrm{Im} p_\varphi\}(x,\xi) > 0$, and

(ii) $\forall x \in K, \varphi'_{x_n}(x) \neq 0$

[1] R might have lower-order terms. However, since the statement of our Carleman estimate is invariant under lower-order perturbations (see Section A.5), we may assume that R has no lower-order terms.

The first condition is sometimes called "the Carleman weight condition" or, in Lebeau and Robbiano's work [LR95], "the hypoelliptic hypothesis of Hörmander".

We denote by S^j the space of tangential symbols $a(x, \xi', h)$, which are smooth for x in a neighborhood of K and $\xi \in \mathbb{R}^n$, which are defined for $h \in (0, h_0]$, and which satisfy

$$\forall \alpha, \beta \quad \exists C_{\alpha\beta} \quad \text{such that}, \quad \forall x, \xi', h,$$
$$|\partial_{x'}^{\alpha} \partial_{\xi}^{\beta} a| \leq C_{\alpha\beta}(1 + |\xi'|)^{j-|\beta|}$$

and

$$a(x, \xi', h) \sim \sum_{k=0}^{\infty} a_k(x, \xi') h^k, \qquad a_k \in S^{j-k},$$

in the sense that

$$a - \sum_{k<N} a_k h^k \in h^N S^{j-N}.$$

We let $\mathcal{E}^j$ denote the space of tangential pseudodifferential operators, $A \in \operatorname{Op}(a)$, for $a \in S^j$, defined by

$$A(f)(x) = (2\pi h)^{1-n} \int e^{i(x'-y')\xi'/h} a(x, \xi', h) f(y', x_n) dy' d\xi'.$$

For these operators, $A = \operatorname{Op}(a) \in \mathcal{E}^j$, $a \sim \sum a_k h^k$, we denote by $\sigma(A) = a_0$ the principal symbol of A. Also, we let $\mathcal{D}^j \subset \mathcal{E}^j$ denote the operators A whose symbols $a(x, \xi', h)$ are polynomials in ξ', h.

We let

$$(f|g) = \int_{\mathbb{R}^n_+} f\overline{g}, \qquad ||f||_0^2 = (f|f), \qquad ||f||_1^2 = ||f||_0^2 + \sum_{j=1}^{n} ||h\partial_j f||_0^2.$$

Also, for $f, g \in C_0^{\infty}(K)$ we write

$$(f|g)_0 = \int_{\mathbb{R}^{n-1}} f_0 \overline{g_0}.$$

For $s \in \mathbb{R}$, we write $|f|_s = ||\Lambda^s(f)||_0$, where $\Lambda \in \mathcal{E}^1$ is the operator with symbol

$$\langle \xi' \rangle = (1 + |\xi'|^2)^{1/2}.$$

With

$$\hat{f}_h(x_n, \xi') = \int e^{-ix'\xi'/h} f(x_n, x') dx'$$

we have

$$|f|_s^2 \approx h^{1-n} \int_0^\infty \int \langle \xi' \rangle^{2s} |\hat{f}_h(x_n, \xi')|^2 d\xi' dx_n$$

As final preparation, we state the following basic Gårding inequality:

> If $A \in \mathcal{E}^2$ is such that $\exists c_0 > 0$ such that $\sigma(A)(x, \xi') \geq c_0(1 + |\xi'|^2)$ $\forall (x, \xi') \in K \times \mathbb{R}^{n-1}$, then $\exists c_1 > 0$, $h_1 > 0$ such that $\forall f \in C_0^\infty(K)$ and $\forall h \in (0, h_1]$ we have $\mathrm{Re}(Af|f) \geq c_1 |f|_1^2$

A.2 Integration by Parts

Our conjugated operator P_φ has real and imaginary parts, which we write, respectively, as

$$\tilde{Q}_2 = \frac{1}{2}(P_\varphi + P_\varphi^*), \quad \text{and} \quad \tilde{Q}_1 = \frac{1}{2i}(P_\varphi - P_\varphi^*).$$

Then

$$\begin{cases} P_\varphi = \tilde{Q}_2 + i\tilde{Q}_1 \\ \tilde{Q}_2 = D_n^2 + Q_2 + V; \quad \tilde{Q}_1 = D_n \circ \varphi'_{x_n} + \varphi'_{x_n} \circ D_n + 2Q_1, \end{cases}$$

where $Q_1 \in \mathcal{D}^1$ and $Q_2 \in \mathcal{D}^2$ have as principal symbols

$$\begin{cases} q_2 = \sigma(Q_2) = -(\varphi'_{x_n})^2 + r(x, \xi') - r(x, \varphi'_{x'}) \\ q_1 = \sigma(Q_1) = \tilde{r}(x, \xi', \varphi'_{x'}). \end{cases}$$

Here we denote by $\tilde{r}(x, \xi', \eta')$ the symmetric bilinear form in ξ', η' associated to the real quadratic form $r(x, \xi')$.

We then have

$$\begin{aligned} P_\varphi &= e^{\varphi/h} P e^{-\varphi/h} \\ &= (D_n + i\varphi'_{x_n})^2 + h^2 R(x, \frac{1}{i}\partial_{x'} + \frac{i}{h}\varphi'_{x'}) + V \\ &= D_n^2 + iD_n \circ \varphi'_{x_n} + i\varphi'_{x_n} \circ D_n - (\varphi'_{x_n})^2 + h^2 R(x, \frac{1}{i}\partial_{x'} + \frac{i}{h}\varphi'_{x'}) + V. \end{aligned}$$

Since the only boundary contribution is in the x_n direction, and since we already know that $\tilde{Q}_1$ and $\tilde{Q}_2$ are formally self-adjoint, we only really need to keep track of the D_n terms. In what follows, we will use the symbol "$\equiv$" to reflect this. For $f, g \in C_0^\infty(K)$ we have

$$\begin{aligned} (g|\tilde{Q}_2 f) &\equiv (g|D_n^2 f) \\ &= -(g|\frac{h}{i}D_n f)_0 - \left(g'_{x_n}\middle|\frac{h}{i}D_n f\right) \\ &\equiv -ih(g|D_n f)_0 + \left(g'_{x_n}\middle|\left(\frac{h}{i}\right)^2 f\right)_0 \\ &= -ih(g|D_n f)_0 - ih\left(\frac{h}{i}g'_{x_n}\middle|f\right)_0 \\ &= -ih\Big[(g|D_n f)_0 + (D_n g|f)_0\Big]. \end{aligned}$$

Hence

$$(g|\tilde{Q}_2 f) = (\tilde{Q}_2 g|f) - ih\Big[(g|D_n f)_0 + (D_n g|f)_0\Big].$$

As for $\tilde{Q}_1$, we have

$$\begin{aligned}(g|\tilde{Q}_1 f) &\equiv (g|(D_n \circ \varphi'_{x_n} + \varphi'_{x_n} D_n) f) \\ &\equiv -ih(g|\varphi'_{x_n} f)_0 - ih(\varphi'_{x_n} g|f)_0.\end{aligned}$$

Hence

$$(g|\tilde{Q}_1 f) = (\tilde{Q}_1 g|f) - 2ih(\varphi'_{x_n} g|f)_0.$$

We then have, for $f \in C_0^\infty(K)$,

$$\begin{aligned}||P_\varphi f||_0^2 &= ((\tilde{Q}_2 + i\tilde{Q}_1)f|(\tilde{Q}_2 + i\tilde{Q}_1)f) \\ &= ||\tilde{Q}_2 f||_0^2 + ||\tilde{Q}_1 f||_0^2 + i(\tilde{Q}_1 f|\tilde{Q}_2 f) - i(\tilde{Q}_2 f|\tilde{Q}_1 f).\end{aligned}$$

Moreover, we may write

$$i(\tilde{Q}_1 f|\tilde{Q}_2 f) = i(\tilde{Q}_2 \tilde{Q}_1 f|f) - i\Big[ih[(\tilde{Q}_1 f|D_n f)_0 + (D_n \tilde{Q}_1 f|f)_0]\Big]$$

and

$$-i(\tilde{Q}_2 f|\tilde{Q}_1 f) = -i(\tilde{Q}_1 \tilde{Q}_2 f|f) + i\Big[2ih(\varphi'_{x_n} \tilde{Q}_2 f|f)_0\Big],$$

so we have

$$||P_\varphi f||_0^2 = ||\tilde{Q}_1 f||_0^2 + ||\tilde{Q}_2 f||_0^2 + i([\tilde{Q}_2, \tilde{Q}_1]f|f) + h\mathfrak{B}(f),$$

where

$$\mathfrak{B}(f) = -2(\varphi'_{x_n} \tilde{Q}_2 f|f)_0 + (\tilde{Q}_1 f|D_n f)_0 + (D_n \tilde{Q}_1 f|f)_0.$$

After some computation, we may write the boundary term as

$$\begin{cases} \mathfrak{B}(f) = (2\varphi'_{x_n} D_n f|D_n f)_0 + (A_1 f|D_n f)_0 + (A'_1 D_n f|f)_0 + (A_2 f|f)_0 \\ A_1, A'_1 \in \mathcal{D}^1, \quad \sigma(A_1) = \sigma(A'_1) = 2q_1, \\ \quad A_2 \in \mathcal{D}^2, \quad \sigma(A_2) = -2\varphi'_{x_n}(q_2 + V). \end{cases}$$

A.3 Two Crucial Lemmas

So far, the strategy has been:

1. Integrate by parts so that the commutator shows up, setting up for Gårding's Inequality.

2. Clean up the boundary term. Organize it into its essential parts; separate the D_n from the tangential operators. We will use the usual (interior) estimates for the tangential operators.

3. Next: Rewrite $i[\tilde{Q}_2, \tilde{Q}_1]$ so that we have a factorization that dovetails nicely with the Carleman weight condition.

The following claims are straight-forward computations.

Claim A.1. $i[\tilde{Q}_2, \tilde{Q}_1] \in h[\mathcal{D}^2 + \mathcal{D}^1 D_n + \mathcal{D}^0 D_n^2]$.

Claim A.2. *Since* $\varphi'_{x_n} \neq 0\ \forall x \in K$*, we have*

$$D_n - \frac{1}{2\varphi'_{x_n}}\tilde{Q}_1 \in \mathcal{D}^1 \qquad \text{and} \qquad D_n^2 - \tilde{Q}_2 = -Q_2 - V \in \mathcal{D}^2,$$

which gives

$$i[\tilde{Q}_2, \tilde{Q}_1] = hB_0\tilde{Q}_2 + hB_1\tilde{Q}_1 + hB_2, \qquad B_j \in \mathcal{D}^j.$$

Lemma A.3. *There exists* $C_1 > 0$ *(large) and* $c_0 > 0$ *such that* $\forall (x, \xi') \in K \times \mathbb{R}^{n-1}$ *we have*

$$\frac{C_1}{1 + |\xi'|^2}\Big[q_1^2 + (\varphi'_{x_n})^2(q_2 + V)\Big]^2 + \sigma(B_2) \geq c_0(1 + |\xi'|^2).$$

Proof. We have

$$p_\varphi(x,\xi) = \xi_n^2 + q_2 + V + 2i(\xi_n \varphi'_{x_n} + q_1),$$

so the Carleman weight condition says

$$\begin{cases} \xi_n^2 + q_2 + V = 0 \\ \xi_n \varphi'_{x_n} + q_1 = 0 \end{cases} \quad \text{implies} \quad \{\xi_n^2 + q_2 + V, \xi_n \varphi'_{x_n} + q_1\} > 0.$$

Using the decomposition in Claim A.2, we have

$$\begin{aligned} 2\{\xi_n^2 + q_2 + V, \xi_n \varphi'_{x_n} + q_1\} &= \{\mathrm{Re} p_\varphi, \mathrm{Im} p_\varphi\} \\ &= \frac{1}{h}\sigma(i[\tilde{Q}_2, \tilde{Q}_1]) \\ &= \frac{1}{h}\Big[h\sigma(B_0)(\xi_n^2 + q_2 + V) + h\sigma(B_1)(2\xi_n\varphi'_{x_n} + 2q_1) + h\sigma(B_2)\Big] \\ &= \sigma(B_0)(\xi_n^2 + q_2 + V) + 2\sigma(B_1)(\xi_n \varphi'_{x_n} + q_1) + \sigma(B_2), \end{aligned}$$

so that

$$\begin{cases} \xi_n^2 + q_2 + V = 0 \\ \xi_n \varphi'_{x_n} + q_1 = 0 \end{cases} \quad \text{implies} \quad \sigma(B_2) > 0. \tag{A.1}$$

We would now like to encapsulate both of the conditions of (A.1) into one single condition. Since the statement of the lemma is independent of ξ_n, we might as well take

$$\xi_n = -\frac{q_1}{\varphi'_{x_n}}$$

in order to automatically satisfy the second condition of (A.1). Then the first condition of (A.1) is

$$\frac{q_1^2}{(\varphi'_{x_n})^2} + q_2 + V = 0.$$

That is,

$$q_1^2 + (\varphi'_{x_n})^2(q_2 + V) = 0. \tag{A.2}$$

We note that the left side of (A.2) is a symbol in S^2. Hence we have

$$q_1^2 + (\varphi'_{x_n})^2(q_2 + V) = 0 \quad \Longrightarrow \quad \sigma(B_2) > 0.$$

Since

$$q_2 = -(\varphi'_{x_n})^2 + r(x, \xi') - r(x, \varphi'_{x'})$$

and

$$r(x, \xi') \geq c|\xi'|^2,$$

we have that

$$q_2 + V \geq \tilde{c}|\xi'|^2 \qquad \text{for } |\xi'| \text{ sufficiently large.}$$

Hence

$$q_1^2 + (\varphi'_{x_n})^2(q_2 + V) \geq (\varphi'_{x_n})^2(q_2 + V) \geq c|\xi'|^2 \qquad \text{for } |\xi'| \text{ sufficiently large.}$$

Now, $\sigma(B_2) \in S^2$, so, in particular,

$$|\sigma(B_2)| \leq C_B(1 + |\xi'|)^2.$$

Thus, for $|\xi'|$ sufficiently large and for C_1 chosen sufficiently large,

$$\begin{aligned}
\frac{C_1}{1+|\xi'|^2}\Big[q_1^2{+}(\varphi'_{x_n})^2(q_2 + V)\Big]^2 &+ \sigma(B_2) \\
&\geq \frac{C_1}{1+|\xi'|^2}\Big(c|\xi'|^2\Big)^2 - C_B(1 + |\xi'|)^2 \\
&\geq \frac{C_1 c^2}{8(1+|\xi'|)^2}\Big(1 + |\xi'|\Big)^4 - C_B(1 + |\xi'|)^2 \\
&\geq (\frac{C_1 c^2}{8} - C_B)(1 + |\xi'|^2) \\
&\geq (\frac{C_1 c^2}{8} - C_B)(1 + |\xi'|)^2.
\end{aligned}$$

We now have the result for $|\xi'|$ sufficiently large, so it remains to check it in a compact set.

If $q_1^2 + (\varphi'_{x_n})^2(q_2 + V) = 0$, then $\sigma(B_2) > 0$, and, since we are in a compact set, $\sigma(B_2) \geq c_0(1 + |\xi'|^2)$ here for c_0 small enough. Also, by continuity, we have this in a neighborhood of the set $\{q_1^2 + (\varphi'_{x_n})^2(q_2 + V) = 0\}$. Outside of that neighborhood, but still in our compact set, we have

$$\left(q_1^2 + (\varphi'_{x_n})^2(q_2 + V)\right)^2 > \delta > 0,$$

and $\sigma(B_2)$ is bounded, so again the estimate holds for C_1 big enough. $\square$

The preceding work was preparation, on the level of symbols, for the use of Gårding's Inequality in the next lemma.

Lemma A.4. *There exist $c_1 > 0$, $h_1 > 0$, $G_0 \in \mathcal{E}^0$, $G_1 \in \mathcal{D}^1$ such that for all $h \in (0, h_1]$ and all $f \in C_0^\infty(K)$ we have*

$$||P_\varphi f||_0^2 \geq c_1 h ||f||_1^2 + Re\Big[h\mathfrak{B}(f) + h^2(D_n f + G_1 f|G_0 f)_0\Big].$$

Proof. There are five initial steps.

(1) First we have the identity

$$\begin{aligned} ||P_\varphi f||_0^2 &= ||\tilde{Q}_2 f||_0^2 + ||\tilde{Q}_1 f||_0^2 + i([\tilde{Q}_2, \tilde{Q}_1]f|f) + h\mathfrak{B}(f) \\ &= ||\tilde{Q}_2 f||_0^2 + ||\tilde{Q}_1 f||_0^2 + ((hB_0\tilde{Q}_2 + hB_1\tilde{Q}_1 + hB_2)f|f) + h\mathfrak{B}(f), \end{aligned}$$

so that

$$\begin{aligned} ||P_\varphi f||_0^2 - h\mathrm{Re}[\mathfrak{B}(f)] = ||\tilde{Q}_2 f||_0^2 + ||\tilde{Q}_1 f||_0^2 &+ \mathrm{Re}(h(B_2 f|f)) \\ &+ \mathrm{Re}(h(B_0\tilde{Q}_2 f + B_1\tilde{Q}_1 f|f)). \end{aligned}$$

(2) Secondly, we have the elementary series of estimates

$$\begin{aligned}|h(B_0\tilde{Q}_2 f + B_1\tilde{Q}_1 f|f)| &\leq h||B_0\tilde{Q}_2 f||_0||f||_0 + h|(\tilde{Q}_1 f|\tilde{B}_1 f)| \\ &\lesssim h||\tilde{Q}_2 f||_0||f||_0 + h||\tilde{Q}_1 f||_0|f|_1 \\ &\lesssim h|f|_1(||\tilde{Q}_2 f||_0 + ||\tilde{Q}_1 f||_0) \\ &\lesssim h^{1/2}(||\tilde{Q}_2 f||_0^2 + h|f|_1^2 + ||\tilde{Q}_1 f||_0^2).\end{aligned}$$

(3) Next we use Gårding's Inequality. Let $G \in \mathcal{E}^0$ be such that

$$\sigma(G) = \frac{C_1}{1+|\xi'|^2}(q_1^2 + (\varphi'_{x_n})^2(q_2 + V)).$$

Then

$$\sigma\Big([Q_1^2 + (Q_2+V)(\varphi'_{x_n})^2]G + B_2\Big) = \frac{C_1}{1+|\xi'|^2}(q_1^2 + (\varphi'_{x_n})^2(q_2+V))^2 + \sigma(B_2),$$

so that Lemma A.3 and Gårding's Inequality give

$$\mathrm{Re}\Big([Q_1^2 + (Q_2+V)(\varphi'_{x_n})^2]Gf\Big|f\Big) + \mathrm{Re}(B_2 f|f) \geq C_1|f|_1^2.$$

Hence

$$\begin{aligned}\mathrm{Re}h(B_2 f|f) &\geq C_1 h|f|_1^2 - h\mathrm{Re}\Big([Q_1^2 + (Q_2+V)(\varphi'_{x_n})^2]Gf\Big|f\Big) \\ &= C_1 h|f|_1^2 - h\mathrm{Re}\Big([Q_1^2 + (\varphi'_{x_n})^2(Q_2+V)]f\Big|Gf\Big).\end{aligned}$$

(4) In the fourth initial step, we prove the following:

Claim. We have

$$Q_1 = \frac{1}{2}(\tilde{Q}_1 - [D_n, \varphi'_{x_n}]) - \varphi'_{x_n} D_n$$

and hence

$$||f||_1 \lesssim ||\tilde{Q}_1 f||_0 + |f|_1.$$

Proof of Claim. For the first statement, we simply recall that

$$\tilde{Q}_1 = D_n \circ \varphi'_{x_n} + \varphi'_{x_n} D_n + 2Q_1$$

and

$$\tilde{Q}_1 - [D_n, \varphi'_{x_n}] = 2\varphi'_{x_n} D_n + 2Q_1.$$

As for the estimate, we have

$$\begin{aligned} ||f||_1^2 &= \sum_{j=1}^{n} ||D_j f||_0^2 + ||f||_0^2 \\ &\lesssim |f|_1^2 + ||D_n f||_0^2, \end{aligned}$$

and

$$\begin{aligned} ||D_n f||_0^2 &\lesssim ||\varphi'_{x_n} D_n f||_0^2 \\ &\lesssim ||\tilde{Q}_1 f||_0^2 + ||[D_n, \varphi'_{x_n}] f||_0^2 + ||Q_1 f||_0^2 \\ &\lesssim ||\tilde{Q}_1 f||_0^2 + h^2 ||f||_0^2 + |f|_1^2, \end{aligned}$$

so that

$$||f||_1 \lesssim ||\tilde{Q}_1 f||_0 + |f|_1.$$

(5) We next need the following:[2]

Claim.

$$\begin{aligned} &-\mathrm{Re}\Big((Q_1^2 + (\varphi'_{x_n})^2 (Q_2 + V)) f \Big| G f \Big) \\ &\qquad \geq -\mathrm{Re}\Big(\frac{h}{2i} \varphi'_{x_n} \tilde{Q}_1 f \Big| G f \Big)_0 - c_4 ||f||_1 \Big[||\tilde{Q}_2 f||_0 + ||\tilde{Q}_1 f||_0 + h ||f||_0 \Big). \end{aligned}$$

Proof of Claim. We use the decomposition

$$\begin{aligned} Q_1^2 + (\varphi'_{x_n})^2 (Q_2 + V) = \Big(\varphi'_{x_n} D_n - \frac{1}{2} (\tilde{Q}_1 - [D_n, \varphi'_{x_n}]) \Big) \varphi'_{x_n} D_n \\ + \frac{Q_1}{2} (\tilde{Q}_1 - [D_n, \varphi'_{x_n}]) + (\varphi'_{x_n})^2 (\tilde{Q}_2 - D_n^2) \end{aligned}$$

to establish the following straight-forward result:

$$Q_1^2 + (\varphi'_{x_n})^2 (Q_2 + V) \in (\varphi'_{x_n})^2 \tilde{Q}_2 - \frac{1}{2} D_n \varphi'_{x_n} \tilde{Q}_1 + \mathcal{D}^1 \tilde{Q}_1 + h \mathcal{D}^1 + h \mathcal{D}^0 D_n.$$

[2]Lebeau and Robbiano write "$-$Re" instead of "Re" in the two instances, which is true but not what we need.

The last ingredient in proving the claim is the following integration by parts:

$$\mathrm{Re}(\frac{1}{2}D_n\varphi'_{x_n}\tilde{Q}_1f|Gf) = \mathrm{Re}\ \Big[(-\frac{h}{2i}\varphi'_{x_n}\tilde{Q}_1f|Gf)_0 - \frac{1}{2}(\varphi'_{x_n}\tilde{Q}_1f|D_nGf)\Big].$$

Putting together these five initial estimates, we get

$$\begin{aligned}
||P_\varphi f||_0^2 - \mathrm{Re}[h\mathfrak{B}(f)] &\overset{(i)}{=} ||\tilde{Q}_2f||_0^2 + ||\tilde{Q}_1f||_0^2 + \mathrm{Re}(h(B_2f|f)) \\
&\quad + \mathrm{Re}(h(B_0\tilde{Q}_2f + B_1\tilde{Q}_1f|f)) \\
&\overset{(ii),(iii)}{\geq} ||\tilde{Q}_2f||_0^2 + ||\tilde{Q}_1f||_0^2 + c_1h|f|_1^2 \\
&\quad - h\mathrm{Re}\Big([Q_1^2 + (\varphi'_{x_n})^2(Q_2+V)]f\Big|Gf\Big) \\
&\quad - c_4h^{1/2}(||\tilde{Q}_2f||_0^2 + h|f|_1^2 + ||\tilde{Q}_1f||_0^2) \\
&\geq \frac{1}{2}||\tilde{Q}_2f||_0^2 + \frac{1}{2}||\tilde{Q}_1f||_0^2 + \frac{c_1}{2}h|f|_1^2 \\
&\quad - h\mathrm{Re}\Big([Q_1^2 + (\varphi'_{x_n})^2(Q_2+V)]f\Big|Gf\Big) \\
&\quad \text{(for } h \text{ small enough)} \\
&\overset{(v)}{\geq} \frac{1}{2}||\tilde{Q}_2f||_0^2 + \frac{1}{2}||\tilde{Q}_1f||_0^2 + \frac{c_1}{2}h|f|_1^2 \\
&\quad - h\mathrm{Re}\Big(\frac{h}{2i}\varphi'_{x_n}\tilde{Q}_1f\Big|Gf\Big)_0 \\
&\quad - c_5h||f||_1\Big[||\tilde{Q}_2f||_0 + ||\tilde{Q}_1f||_0 + h||f||_0\Big].
\end{aligned}$$

Moreover, (iv) says $||f||_1^2 \leq c_8(||\tilde{Q}_1f||_0^2 + |f|_1^2)$, so that

$$h|f|_1^2 \geq \frac{h}{c_8}||f||_1^2 - h||\tilde{Q}_1f||_0^2.$$

Hence

$$\begin{aligned}
||P_\varphi f||_0^2 - \mathrm{Re}[h\mathfrak{B}(f)] &\geq \frac{1}{2}||\tilde{Q}_2f||_0^2 + \frac{1}{2}||\tilde{Q}_1f||_0^2 + \frac{c_1h}{2c_8}||f||_1^2 \\
&\quad - \frac{c_1}{2}h||\tilde{Q}_1f||_0^2 - h\mathrm{Re}\Big(\frac{h}{2i}\varphi'_{x_n}\tilde{Q}_1f\Big|Gf\Big)_0 \\
&\quad - c_5h||f||_1\Big[||\tilde{Q}_2f||_0 + ||\tilde{Q}_1f||_0 + h||f||_0\Big].
\end{aligned}$$

Additionally,

$$-h||f||_1||\tilde{Q}_2 f||_0 \geq -\frac{h}{c_{10}}||f||_1^2 - c_{10}h||\tilde{Q}_2 f||_0^2$$

and

$$\begin{aligned}-h||f||_1||\tilde{Q}_1 f||_0 &= -(h^{3/4}||f||_1)(h^{1/4}||\tilde{Q}_1 f||_0)\\ &\geq -\frac{1}{2}(h^{3/2}||f||_1^2 + h^{1/2}||\tilde{Q}_1 f||_0^2),\end{aligned}$$

so, for c_{10} taken sufficiently large, we have

$$\begin{aligned}||P_\varphi f||_0^2 - \mathrm{Re}[h\mathfrak{B}(f)] &\geq \frac{1}{8}||\tilde{Q}_2 f||_0^2 + \frac{1}{16}||\tilde{Q}_1 f||_0^2 + \frac{1}{8}h||f||_1^2\\ &\quad - h\mathrm{Re}\Big(\frac{h}{2i}\varphi'_{x_n}\tilde{Q}_1 f\Big|Gf\Big)_0 - c_9 h^2||f||_1||f||_0\\ &\geq \frac{1}{8}||\tilde{Q}_2 f||_0^2 + \frac{1}{16}||\tilde{Q}_1 f||_0^2 + \frac{1}{16}h||f||_1^2\\ &\quad - h\mathrm{Re}\Big(\frac{h}{2i}\varphi'_{x_n}\tilde{Q}_1 f\Big|Gf\Big)_0.\end{aligned}$$

Moreover,

$$\begin{aligned}(\varphi'_{x_n}\tilde{Q}_1 f|Gf)_0 &= \Big(\varphi'_{x_n}(D_n\circ\varphi'_{x_n} + \varphi'_{x_n}D_n + 2Q_1)f\Big|Gf\Big)_0\\ &= \Big(\varphi'_{x_n}(\frac{h}{i}\varphi''_{x_n x_n} + 2\varphi'_{x_n}D_n + 2Q_1)f\Big|Gf\Big)_0\\ &= (\frac{h}{i}\varphi''_{x_n x_n}f|\varphi'_{x_n}Gf)_0 + (D_n f|2(\varphi'_{x_n})^2 Gf)_0 + (Q_1 f|2\varphi'_{x_n}Gf)_0\\ &= (G_1 f + D_n f|2(\varphi'_{x_n})^2 Gf)_0,\end{aligned}$$

where

$$G_1 f := \frac{h}{2i}\frac{\varphi''_{x_n x_n}}{\varphi'_{x_n}}f + \frac{Q_1}{\varphi'_{x_n}}f \in \mathcal{D}^1.$$

Hence

$$-h^2\mathrm{Re}(\frac{1}{2i}\varphi'_{x_n}\tilde{Q}_1 f|Gf)_0 = h^2\mathrm{Re}(D_n f + G_1 f|G_0 f)_0,$$

with

$$G_0 := \frac{1}{i}(\varphi'_{x_n})^2 G \in \mathcal{E}^0.$$

Finally, we obtain

$$\begin{aligned}||P_\varphi f||_0^2 - \mathrm{Re}[h\mathfrak{B}(f)] &\geq \frac{1}{8}||\tilde{Q}_2 f||_0^2 + \frac{1}{16}||\tilde{Q}_1 f||_0^2 + \frac{1}{16}h||f||_1^2 \\ &\quad + h^2\mathrm{Re}(D_n f + G_1 f|G_0 f)_0 \\ &\geq c_1 h||f||_1^2 + h^2\mathrm{Re}(D_n f + G_1 f|G_0 f)_0,\end{aligned}$$

which proves the lemma. □

A.4 The Main Results

We are now ready to state and prove the local results, beginning with:

Proposition A.5. *Let φ be a Carleman weight such that $\varphi'_{x_n} \neq 0$ on K. Then $\exists\ C > 0$ and $h_1 > 0$ such that for each $h \in (0, h_1]$ and each $g \in C_0^\infty(K)$ we have*

$$\int_{\mathbb{R}_n^+} |Pg|^2 e^{2\varphi/h} + h\int_{\mathbb{R}^{n-1}} \Big\{|g|^2 + |h\nabla g|^2\Big\} e^{2\varphi/h} \geq Ch\int_{\mathbb{R}_n^+} \Big\{|g|^2 + |h\nabla g|^2\Big\} e^{2\varphi/h}.$$

Proof. Let $g = e^{-\varphi/h} f$. Then Lemma A.4 says

$$||e^{\varphi/h}Pg||_0^2 \geq c_1 h||e^{\varphi/h}g||_1^2 + \mathrm{Re}\Big[h\mathfrak{B}(e^{\varphi/h}g) + h^2\Big((D_n + G_1)(e^{\varphi/h}g)\Big|G_0(e^{\varphi/h}g)\Big)_0\Big].$$

An Elementary Inequality:

Let a and b be numbers and $f(x)$ such that $||f||_\infty^2 \leq M < \infty$. Then

$$\begin{aligned}
|a|^2 + |f(x)a + b|^2 &\geq |a|^2 + |fa|^2 + |b|^2 - 2|fa||b| \\
&\geq |a|^2 + |fa|^2 + |b|^2 - \alpha|fa|^2 - \frac{1}{\alpha}|b|^2 \\
&= |a|^2 - (\alpha - 1)|fa|^2 + (1 - \frac{1}{\alpha})|b|^2 \\
&\qquad \text{but we take } \alpha > 1, \text{ so that} \\
&\geq |a|^2 - (\alpha - 1)M|a|^2 + (1 - \frac{1}{\alpha})|b|^2 \\
&= (1 - (\alpha - 1)M)|a|^2 + (1 - \frac{1}{\alpha})|b|^2.
\end{aligned}$$

We also want $1 - (\alpha - 1)M > 0$, ie $\frac{1}{M} + 1 > \alpha$, so we take $1 < \alpha < 1 + \frac{1}{M}$.

This elementary inequality then gives

$$\begin{aligned}
||e^{\varphi/h} g||_1^2 &= ||e^{\varphi/h} g||_0^2 + ||(\nabla\varphi) e^{\varphi/h} g + e^{\varphi/h} h \nabla g||_0^2 \\
&\gtrsim ||e^{\varphi/h} g||_0^2 + ||e^{\varphi/h} h \nabla g||_0^2,
\end{aligned}$$

so

$$\begin{aligned}
||e^{\varphi/h} Pg||_0^2 \geq \tilde{c}_1 h &\Big[||e^{\varphi/h} g||_0^2 + ||e^{\varphi/h} h \nabla g||_0^2 \Big] \\
&+ \mathrm{Re}\Big[h\mathfrak{B}(e^{\varphi/h} g) + h^2 \Big((D_n + G_1)(e^{\varphi/h} g) \Big| G_0(e^{\varphi/h} g) \Big)_0 \Big].
\end{aligned}$$

It thus remains to show

$$\left| \mathrm{Re}\Big[\mathfrak{B}(e^{\varphi/h} g) + h\Big((D_n + G_1)(e^{\varphi/h} g) \Big| G_0(e^{\varphi/h} g) \Big)_0 \Big] \right| \lesssim \int_{\mathbb{R}^{n-1}} \Big\{ |g|^2 + |h \nabla g|^2 \Big\} e^{2\varphi/h}.$$

However, we have

$$\begin{aligned}
\left| \Big((D_n + G_1)(e^{\varphi/h} g) \Big| G_0(e^{\varphi/h} g) \Big)_0 \right| &\lesssim ||D_n(e^{\varphi/h} g)||_0 ||e^{\varphi/h} g||_0 + ||e^{\varphi/h} g||_1 ||e^{\varphi/h} g||_0 \\
&\lesssim ||D_n(e^{\varphi/h} g)||_0^2 + ||e^{\varphi/h} g||_1^2 \\
&\lesssim ||e^{\varphi/h} D_n g||_0^2 + ||e^{\varphi/h} g||_1^2,
\end{aligned}$$

which is even better than we needed, as we did not need to use the small parameter h.

Hence it remains to show

$$|\mathrm{Re}\mathfrak{B}(e^{\varphi/h}g)| \lesssim \int_{\mathbb{R}^{n-1}} \Big\{|g|^2 + |h\nabla g|^2\Big\} e^{2\varphi/h}.$$

We begin by using the decomposition in terms of the A's.

$$\begin{aligned} |\mathfrak{B}(e^{\varphi/h}g)| = \Big| & \Big(2\varphi'_{x_n} D_n(e^{\varphi/h}g)\Big| D_n(e^{\varphi/h}g)\Big)_0 + \Big(A_1(e^{\varphi/h}g)\Big| D_n(e^{\varphi/h}g)\Big)_0 \\ & + \Big(A'_1 D_n(e^{\varphi/h}g)\Big| e^{\varphi/h}g\Big)_0 + \Big(A_2(e^{\varphi/h}g)\Big| e^{\varphi/h}g\Big)_0 \Big| \end{aligned} \tag{A.3}$$

For the first term in (A.3), we estimate

$$||\frac{1}{i}\varphi'_{x_n} e^{\varphi/h}g + e^{\varphi/h}D_n g||_0^2 \lesssim ||e^{\varphi/h}g||_0^2 + ||e^{\varphi/h}D_n g||_0^2.$$

As for the second term,

$$\begin{aligned} \Big|\Big(A_1(e^{\varphi/h}g)\Big| D_n(e^{\varphi/h}g)\Big)_0\Big| &\lesssim ||e^{\varphi/h}g||_1 ||\frac{1}{i}\varphi'_{x_n} e^{\varphi/h}g + e^{\varphi/h}D_n g||_0 \\ &\lesssim ||e^{\varphi/h}g||_1^2 + ||e^{\varphi/h}g||_0^2 + ||e^{\varphi/h}D_n g||_0^2. \end{aligned}$$

The same computation works for the A'_1 term if we integrate by parts first to get

$$\Big(D_n(e^{\varphi/h}g)\Big| \tilde{A}'_1(e^{\varphi/h}g)\Big)_0.$$

For the fourth term, we do another integration by parts, to convert a second-order differential operator into two first-order differential operators:

$$\begin{aligned} \Big|\Big(A_2(e^{\varphi/h}g)\Big| e^{\varphi/h}g\Big)_0\Big| &= \Big|\Big(A''_1(e^{\varphi/h}g)\Big| A'''_1(e^{\varphi/h}g)\Big)_0\Big| \\ &\lesssim ||e^{\varphi/h}g||_1^2. \end{aligned}$$

Finally, to complete the proof of the proposition, we note that

$$\begin{aligned} ||e^{\varphi/h}g||_1^2 &= ||e^{\varphi/h}g||_0^2 + ||h\partial_{x'}(e^{\varphi/h}g)||_0^2 \\ &\lesssim ||e^{\varphi/h}g||_0^2 + ||e^{\varphi/h}h\partial_{x'}g||_0^2. \end{aligned}$$

$\square$

Proposition A.6. *Let φ be a Carleman weight such that*

$$\varphi'_{x_n}(x',0) > 0 \qquad \textit{for each} \qquad (x',0) \in K.$$

Then $\exists\ C > 0$ and $h_1 > 0$ such that for each $h \in (0, h_1]$ and each $g \in C_0^\infty(K)$ satisfying $g_0 = g|_{x_n=0} = 0$ we have

$$\int_{\mathbb{R}_n^+} |Pg|^2 e^{2\varphi/h} \geq Ch \int_{\mathbb{R}_n^+} \Big\{|g|^2 + |h\nabla g|^2\Big\} e^{2\varphi/h}.$$

Proof. Again we let $g = e^{-\varphi/h} f$. Then, since $g_0 = 0$, Lemma A.4 says

$$||e^{\varphi/h} Pg||_0^2 \geq c_1 h ||e^{\varphi/h} g||_1^2 + \mathrm{Re}[h\mathfrak{B}(e^{\varphi/h} g)].$$

But, again since $g_0 = 0$,

$$\begin{aligned}
\mathfrak{B}(e^{\varphi/h} g) &= 2\Big(\varphi'_{x_n} D_n(e^{\varphi/h} g)\Big| D_n(e^{\varphi/h} g)\Big)_0 \\
&= 2\int_{\mathbb{R}^{n-1}} \varphi'_{x_n} |D_n(e^{\varphi/h} g)|^2 \\
&\geq 0.
\end{aligned}$$

Hence

$$\begin{aligned}
||e^{\varphi/h} Pg||_0^2 &\geq c_1 h ||e^{\varphi/h} g||_1^2 \\
&\geq Ch(||e^{\varphi/h} g||_0^2 + ||e^{\varphi/h} h\nabla g||_0^2),
\end{aligned}$$

where the last step follows from our "elementary inequality". $\square$

A.5 From the Local Estimate to a Global Estimate

Let Ω_0 be an oriented Riemannian manifold with boundary $\partial\Omega_0$ and smooth Riemannian metric g_0 such that $\overline{\Omega_0}$ is compact.

We first prove that the following boundary Carleman estimate is a local result.

Proposition A.7. *Let φ be a Carleman weight on Ω_0, and let $\Gamma \subset \partial\Omega_0$ be a union of connected components of $\partial\Omega_0$. If $\frac{\partial\varphi}{\partial n}\Big|_\Gamma < 0$, then there exist constants $c > 0$ and $h_1 > 0$ such that*

$$\int_{\Omega_0} |Pf|^2 e^{2\varphi/h} \geq ch \int_{\Omega_0} \Big[|f|^2 + |h\nabla f|^2\Big] e^{2\varphi/h}$$

for every $h \in (0, h_1)$ and every $f \in C_0^\infty(\Omega_0 \bigcup \Gamma)$ (that is, zero in a neighborhood of $\partial\Omega_0 \backslash \Gamma$) such that $f|_\Gamma \equiv 0$.

Proof. Let $\{U_j\}_{j=1}^N$ be an open cover of $\overline{\Omega_0}$ such that the Carleman estimate is true on each U_j. Let $\sum_{j=1}^N \psi_j \equiv 1$ be a partition of unity adapted to the U_j, and write $f_j = \psi_j f \in C^\infty(U_j)$.

Then, with $P(f_j) = \psi_j Pf + hQ_j f$, where Q_j is a first-order semiclassical differential operator, we have

$$\begin{aligned}
h \int_{\Omega_0} \Big[|f|^2 + |h\nabla f|^2\Big] e^{2\varphi/h} &\lesssim \sum_{j=1}^N h \int_{\Omega_0} \Big[|f_j|^2 + |h\nabla f_j|^2\Big] e^{2\varphi/h} \\
&\lesssim \sum_{j=1}^N \int_{\Omega_0} |Pf_j|^2 e^{2\varphi/h} = \sum_{j=1}^N \int_{\Omega_0} |\psi_j Pf + hQ_j f|^2 e^{2\varphi/h} \\
&\lesssim h^2 \sum_{j=1}^N \int_{\Omega_0} |Q_j f|^2 e^{2\varphi/h} + \int_{\Omega_0} |Pf|^2 e^{2\varphi/h} \\
&\lesssim h^2 \int_{\Omega_0} \Big[|f|^2 + |h\nabla f|^2\Big] e^{2\varphi/h} + \int_{\Omega_0} |Pf|^2 e^{2\varphi/h},
\end{aligned}$$

where the first term on the right side may be absorbed in the left side for h small enough. □

We next show that the Carleman weight condition is invariant under changes of coordinates. This is basically obvious, since it is a condition on a Poisson bracket, but for completeness we give the full details. Let $\varkappa : \mathbb{R}^n_y \to \mathbb{R}^n_x$ be a diffeomorphism, and let p be the real-valued [semiclassical] principal symbol of our [semiclassical] differential operator.

Let φ be a Carleman weight, meaning that $\varphi \in C^\infty(\mathbb{R}^n, \mathbb{R})$ and

$$p_\varphi = 0 \Rightarrow \frac{1}{i}\{\overline{p_\varphi}, p_\varphi\} > 0$$

where $p_\varphi(x,\xi) := p(x, \xi + i\nabla\varphi)$, and let $\tilde{\varkappa}$ be the canonical transformation induced by $\varkappa$, given by

$$(y,\eta) \mapsto (\varkappa(y), ({}^t\varkappa')^{-1}(\eta)) \equiv \tilde{\varkappa}(y,\eta) \equiv (x,\xi).$$

Now let

$$\phi := \varphi \circ \varkappa \qquad \text{and} \qquad \rho := p \circ \tilde{\varkappa}.$$

Then

$$\begin{aligned}
(p_\varphi \circ \tilde{\varkappa})(y,\eta) &= p(\varkappa(y), ({}^t\varkappa')^{-1}\eta + i(\nabla\varphi)(\varkappa(y))) \\
&= p(\varkappa(y), ({}^t\varkappa')^{-1}\eta + i({}^t\varkappa')^{-1}\nabla\phi(y)) \\
&= (p \circ \tilde{\varkappa})(y, \eta + i\nabla\phi(y)) \\
&= \rho(y, \eta + i\nabla\phi(y)) \\
&= \rho_\phi(y,\eta).
\end{aligned}$$

Of course, we also have

$$\begin{aligned}
\{\mathrm{Re}\rho_\phi, \mathrm{Im}\rho_\phi\} &= \{(\mathrm{Re}p_\varphi) \circ \tilde{\varkappa}, (\mathrm{Im}p_\varphi) \circ \tilde{\varkappa}\} \\
&= \{\mathrm{Re}p_\varphi, \mathrm{Im}p_\varphi\} \circ \tilde{\varkappa}.
\end{aligned}$$

These facts together show that, for $(x,\xi) = \tilde{\varkappa}(y,\eta)$,

$$\rho_\phi(y,\eta) = 0 \Longrightarrow p_\varphi(x,\xi) = 0 \Longrightarrow \frac{1}{i}\{\overline{p_\varphi}, p_\varphi\}(x,\xi) > 0 \Longrightarrow \frac{1}{i}\{\overline{\rho_\phi}, \rho_\phi\}(y,\eta) > 0.$$

Thus ϕ is a Carleman weight for ρ. This is what we mean by "the Carleman weight condition is invariant under diffeomorphisms".

To prepare for the application of our local result, which was for a straight boundary, we now review the well known construction of geodesic coordinates with respect to the boundary; our reference for this is Lee and Uhlmann's paper [LU89]. But first we recall the basic objects in Riemannian geometry.

For $f : \Omega \to \mathbb{R}$, the gradient of f is the vector field given by

$$(\nabla f)^i \equiv (\mathrm{grad} f)^i = g^{ij}\frac{\partial f}{\partial x^j}.$$

For X a vector field, the divergence of X is given by

$$\mathrm{div} X = \frac{1}{\sqrt{\det g}}\frac{\partial}{\partial x^i}(\sqrt{\det g}X^i)$$

where $\det g := \det(g_{kl})$.

The Laplacian is given by

$$\Delta f := \mathrm{div}(\mathrm{grad} f) = \frac{1}{\sqrt{\det g}}\frac{\partial}{\partial x^j}(g^{ij}\sqrt{\det g}\frac{\partial f}{\partial x^i}).$$

Gauss's Theorem says that, for X a vector field, Σ the volume element of Ω, σ the volume element on $\partial\Omega$, and n the outward unit normal to the boundary, all with respect to the Riemannian metric, we have $\int_\Omega (\mathrm{div} X)\Sigma = \int_{\partial\Omega}(X \cdot n)\sigma$. We will abbreviate this by omitting the Σ and σ in what follows.

Now let Ω be the interior of a smooth compact n-manifold $\overline{\Omega}$ with boundary, and g a smooth Riemannian metric on $\overline{\Omega}$.

For each $q \in \partial\Omega$, we let $\gamma_q : [0, \epsilon) \to \overline{\Omega}$ denote the unit-speed geodesic starting at q and normal to $\partial\Omega$. We can then smoothly extend any local coordinates for $\partial\Omega$ near $p \in \partial\Omega$, say $\{x^1, ..., x^{n-1}\}$, to coordinates $\{x^1, ..., x^n\}$ for $\overline{\Omega}$ in some neighborhood of p, such that x^n is the parameter along γ_q. These are called the *boundary normal coordinates* determined by $\{x^1, ..., x^{n-1}\}$. Hence $x^n > 0$ in Ω, and $\partial\Omega$ is locally characterized by $x^n = 0$. In these coordinates, the metric g has the form

$$g = \sum_{\alpha,\beta=1}^{n-1} g_{\alpha\beta}(x)dx^\alpha dx^\beta + (dx^n)^2.$$

This change of coordinates introduces a lower-order "error" term, but we now show that the boundary Carleman estimate is invariant under perturbations of this type.

Let Q be a first-order semiclassical differential operator.

Lemma A.8. *Under the assumptions of the global boundary Carleman estimate for P, we then also have the estimate for $P + hQ$, that is,*

$$\int_\Omega |(P+hQ)g|^2 e^{2\varphi/h} + h\int_{\partial\Omega} \Big[|g|^2 + |h\nabla g|^2\Big] e^{2\varphi/h} \geq ch\int_\Omega \Big[|g|^2 + |h\nabla g|^2\Big] e^{2\varphi/h}$$

for every $h \in (0, h_1)$ and every $g \in C^\infty(\overline{\Omega})$.

Proof. We have

$$\begin{aligned} |Pg + hQg|^2 &\geq |Pg|^2 + h^2|Qg|^2 - h^{1/2}|Pg|^2 - h^{3/2}|Qg|^2 \\ &\gtrsim |Pg|^2 - h^{3/2}|Qg|^2, \end{aligned}$$

and also

$$\begin{aligned} ||e^{\varphi/h}Qg||_0^2 &\lesssim ||Q(e^{\varphi/h}g)||_0^2 + ||e^{\varphi/h}g||_0^2 \\ &\lesssim ||e^{\varphi/h}g||_1^2 \\ &= ||e^{\varphi/h}g||_0^2 + ||\frac{1}{i}(\nabla\varphi)g + e^{\varphi/h}\frac{h}{i}\nabla g||_0^2 \\ &\lesssim ||e^{\varphi/h}g||_0^2 + ||e^{\varphi/h}h\nabla g||_0^2 \\ &= \int_\Omega e^{2\varphi/h}\Big[|g|^2 + |h\nabla g|^2\Big]. \end{aligned}$$

Hence, given that we have the estimate for P,

$$\begin{aligned}\int_\Omega |(P+hQ)g|^2 e^{2\varphi/h} + h\int_{\partial\Omega}\Big[|g|^2+|h\nabla g|^2\Big]e^{2\varphi/h} \\ \gtrsim -h^{3/2}\int_\Omega |Qg|^2 e^{2\varphi/h} + h\int_\Omega \Big[|g|^2+|h\nabla g|^2\Big]e^{2\varphi/h} \\ \gtrsim h(1-h^{1/2})\int_\Omega \Big[|g|^2+|h\nabla g|^2\Big]e^{2\varphi/h},\end{aligned}$$

which gives the result for h small enough. □

Clearly, we have a similar result for our local boundary Carleman estimate.

Using the boundary normal coordinates as above, the Laplacian becomes

$$-\Delta_g = D_n^2 + R(x, D_{x'}) + \text{ lower order terms},$$

where the principal symbol of R, $r(x,\xi')$, is such that

$$r(x,\xi)\in\mathbb{R} \quad \text{and} \quad \exists c>0 \quad \text{such that} \quad \forall (x,\xi') \quad \text{we have} \quad r(x,\xi')\geq c|\xi'|^2.$$

Therefore, our operator $P=-h^2\Delta+V$ becomes, in these coordinates,

$$P=(hD_n)^2+R(x,hD_{x'})+hR_1+V$$

where R_1 is a semiclassical differential operator of order one. By the invariance under perturbations mentioned above, the local Carleman estimate thus holds for P.

To prove a global Carleman estimate for a compact oriented Riemannian manifold with boundary, we use a partition of unity. We use the classical *interior* Carleman estimate on interior pieces (vanishing in a neighborhood of the boundary) and the local boundary Carleman estimate on pieces that touch the boundary. We thus obtain a global Carleman estimate for P.

Hence we arrive at the following result:

Let Ω_0 be an oriented Riemannian manifold with smooth boundary $\partial\Omega_0$ and smooth Riemannian metric g_0 such that $\overline{\Omega_0}$ is compact. Let $P := -h^2\Delta + V$, with [semiclassical] principal symbol $p(x,\xi) = {}^t\xi g_0 \xi + V$. Let $p_\varphi(x,\xi) := p(x, \xi + i\nabla\varphi)$. Suppose we have a Carleman weight φ on Ω_0, meaning that $\varphi \in C^\infty(\overline{\Omega_0}, \mathbb{R})$ and

$$p_\varphi(x,\xi) = 0 \Rightarrow \frac{1}{i}\{\overline{p_\varphi}, p_\varphi\}(x,\xi) > 0.$$

Theorem A.9. *Let $\Gamma_1, \Gamma_2 \subset \partial\Omega_0$ each be a union of connected components of $\partial\Omega_0$ such that $\Gamma_1 \cap \Gamma_2 = \emptyset$, and let $N(\Gamma_1)$ be a small neighborhood of Γ_1. Let φ be a Carleman weight on Ω_0 such that $\nabla\varphi \neq 0$ on Ω_0 and such that $\frac{\partial\varphi}{\partial n}\Big|_{\partial\Omega_0\setminus\Gamma_1} \neq 0$. If $\frac{\partial\varphi}{\partial n}\Big|_{\Gamma_2} < 0$, then there exist constants $c > 0$ and $h_1 > 0$ such that*

$$\int_{\Omega_0} |Pf|^2 e^{2\varphi/h} + h\int_{\partial\Omega_0\setminus(\Gamma_1\cup\Gamma_2)} \Big\{|f|^2 + |h\nabla f|^2\Big\} e^{2\varphi/h} \geq ch\int_{\Omega_0} \Big\{|f|^2 + |h\nabla f|^2\Big\} e^{2\varphi/h}$$

for every $h \in (0, h_1)$ and every $f \in C_0^\infty(\overline{\Omega_0}\setminus N(\Gamma_1))$ such that $f|_{\Gamma_2} \equiv 0$.

Remark. Strictly speaking, we should have a local Carleman estimate for a strictly positive density $\lambda(x)dx$, but since we are on a compact manifold, $\lambda \approx 1$, so the estimates are interchangeable.

APPENDIX B

The Weierstrass $\wp$-Function

In Section 5.6 the Weierstrass $\wp$-function played a central role, as elliptic functions were found to parametrize the (h-dependent) Hamilton flow of

$$p_r(x,\xi;h) = \frac{1}{2}x(x^2+\xi^2) - \frac{r^2}{2}hx.$$

Here we briefly describe some useful facts about the $\wp$-function, in the context of our problem. In what follows, we occasionally state (but do not prove) standard results, taken from the textbooks of Ahlfors [Ahl78] and Koblitz [Kob93].

The Weierstrass $\wp$-function is a doubly periodic meromorphic function on the complex plane, say, with periods $\omega_1, \omega_2 \in \mathbb{C}$, with a double pole at each point of the period lattice, including the origin. And it is a solution of the differential equation

$$[\wp'(z)]^2 = 4[\wp(z)]^3 - g_2\wp(z) - g_3, \tag{B.1}$$

where the "invariants" g_2 and g_3 characterize $\wp$ just as well as ω_1 and ω_2. In our case,

$$g_2 = \frac{1}{12}r^4h^2 \quad \text{and} \quad g_3 = \frac{1}{4}C^2 - \frac{1}{216}r^6h^3.$$

Here $C := p_r(x,\xi;h)$ is conserved under the flow. Since the differential equation has constant coefficients, $\wp(z+z_0)$ is also a solution, for any $z_0 \in \mathbb{C}$.

One may factorize the cubic polynomial (B.1):

$$\wp'(z)^2 = 4(\wp(z)-e_1)(\wp(z)-e_2)(\wp(z)-e_3).$$

It is a familiar fact that the roots e_1, e_2, e_3 of $4x^3 - g_2x - g_3$ are distinct if and only if the discriminant is nonzero:

$$\Delta := g_2^3 - 27g_3^2 \neq 0.$$

Moreover, all the roots e_1, e_2, e_3 are real if and only if g_2 and g_3 are real and $\Delta > 0$. In our case,

$$\Delta = \frac{27}{16}C^2\left(\frac{1}{27}r^6h^3 - C^2\right).$$

So if we ignore the trivial case $C = 0$ (see Section 5.6), we have that e_1, e_2, e_3 are distinct if and only if $C^2 \neq \left(\frac{r^2h}{3}\right)^3$, and moreover e_1, e_2, e_3 are real if and only if $C^2 < \left(\frac{1}{3}r^2h\right)^3$.

Suppose that we are in the case $\Delta > 0$. We then order the e_i such that $e_1 < e_3 < e_2$. Then one may choose the periods ω_1 and ω_2 of $\wp$ to be given by

$$\frac{1}{2}\omega_1 = i\int_{-\infty}^{e_1} \frac{dt}{\sqrt{g_3 + g_2t - 4t^3}} \tag{B.2}$$

and

$$\frac{1}{2}\omega_2 = \int_{e_2}^{\infty} \frac{dt}{\sqrt{4t^3 - g_2t - g_3}}, \tag{B.3}$$

where we take the positive branch of the square root and integrate along the real axis. Hence the fundamental domain of $\wp$ in the complex plane is a rectangle with its opposite edges identified.

In our case, in Section 5.6, it is clear that the unbounded flow lines are described by restricting $\wp$ to the real line, since the poles lie on the real line. Also, it is clear that the nondegenerate flow loops are described by restricting $\wp$ to a line of the form

$$L_\alpha = \{t + \alpha;\, t \in \mathbb{R}\}, \quad \text{for some } \alpha \in \mathbb{C}.$$

To determine the value of α, we make use of the addition formula

$$\wp(z+u) = -\wp(z) - \wp(u) + \frac{1}{4}\left(\frac{\wp'(z) - \wp'(u)}{\wp(z) - \wp(u)}\right)^2.$$

For $\wp(t+\alpha)$ to be real for all $t \in \mathbb{R}$, we then only need α to satisfy $\wp(\alpha) \in \mathbb{R}$ and $\wp'(\alpha) \in \mathbb{R}$. But it is well known that

$$e_1 = \wp\left(\frac{\omega_1}{2}\right), \quad e_2 = \wp\left(\frac{\omega_2}{2}\right), \quad e_3 = \wp\left(\frac{\omega_1+\omega_2}{2}\right),$$

and that

$$\wp'\left(\frac{\omega_1}{2}\right) = 0, \quad \wp'\left(\frac{\omega_2}{2}\right) = 0, \quad \text{and} \quad \wp'\left(\frac{\omega_1+\omega_2}{2}\right) = 0.$$

Hence, in light of (B.2) and (B.3), we may simply take $\alpha = \frac{1}{2}\omega_1$.

This shows that the nondegenerate flow loops are parametrized by

$$\mathbb{R} \ni t \mapsto (x(t), \xi(t)),$$

with

$$x(t) = \frac{1}{2}C\left(\wp\left(t+\frac{\omega_1}{2}\right) - \frac{1}{12}r^2h\right)^{-1}$$

and

$$\xi(t) = \frac{-\wp'\left(t+\frac{\omega_1}{2}\right)}{\wp\left(t+\frac{\omega_1}{2}\right) - \frac{1}{12}r^2h}.$$

This can easily be seen in the figures. The fundamental domain of $\wp$ is pictured in Figure B.1. As t traverses the horizonal line (a), $(x(t), \xi(t))$ traces out the curve (a) in Figure B.2. And as $t+\frac{\omega_1}{2}$ traverses the horizontal line (b), $(x(t), \xi(t))$ traces out the curve (b) in Figure B.2. The parameters in Figure B.2 are $r^2 = 3$, $h = 0.1$, and $C = 0.025$. Note in particular that $C^2 < h^3$. When $C^2 = h^3$, the loop reduces to a point, although there is still an unbounded component. And there is only an unbounded component when $C^2 > h^3$.

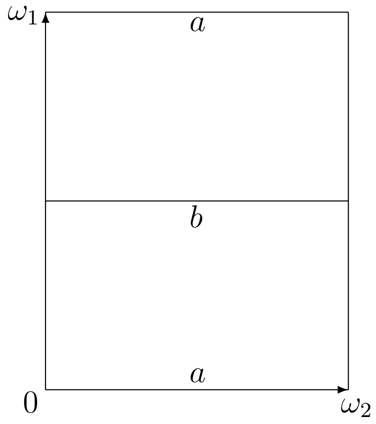

Figure B.1: The fundamental domain of $\wp$. When restricted to either the line (a) or the line (b), $\wp$ is real-valued.

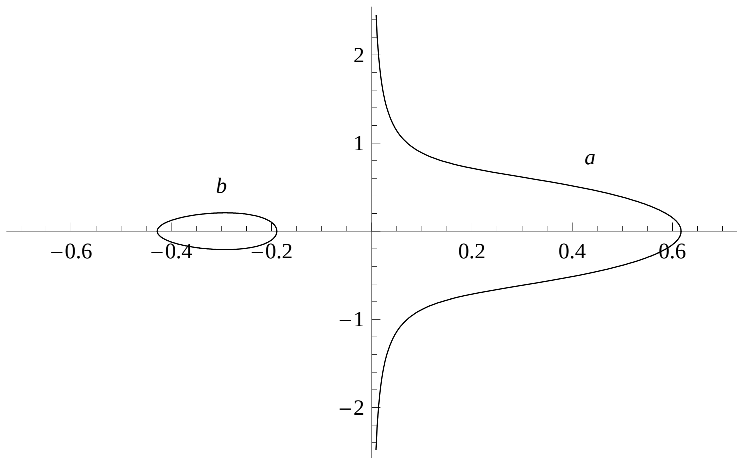

Figure B.2: The elliptic curve parametrized by $(x(t), \xi(t))$. The parameters for the curve are $r^2 = 3$, $h = 0.1$, and $C = 0.025$.

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