

ANNALES
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ON A QUANTUM-CLASSICAL CORRESPONDENCE: FROM GRAPHS TO MANIFOLDS

SUR UNE CORRESPONDANCE
QUANTIQUE-CLASSIQUE : DES GRAPHS
AUX VARIÉTÉS

ABSTRACT. — We establish conditions for which graph Laplacians $\Delta_{\lambda,\epsilon}$ on compact, boundaryless, smooth submanifolds $\mathcal{M}$ of Euclidean space are semiclassical pseudodifferential operators (Ψ DOs). Specifically, the graph Laplacian's kernel bandwidth (*bias term*) $\sqrt{\epsilon}$ must decay faster than the semiclassical parameter h , i.e., $h \gg \sqrt{\epsilon}$, and we compute the symbol. Coupling this with Egorov's theorem and coherent states ψ_h localized at $(x_0, \xi_0) \in T^*\mathcal{M}$, we show that with $U_{\lambda,\epsilon}^t := e^{-it\sqrt{\Delta_{\lambda,\epsilon}}}$ spectrally defined, the (co-)geodesic flow Γ^t on $T^*\mathcal{M}$ is approximated by $\langle U_{\lambda,\epsilon}^{-t} \text{Op}_h(a) U_{\lambda,\epsilon}^t \psi_h, \psi_h \rangle = a \circ \Gamma^t(x_0, \xi_0) + O(h)$.

In the discrete setting, for a normalized graph Laplacian $\Delta_{\lambda,\epsilon,N}$ defined on a set of N points $x_1, \dots, x_N$ sampled i.i.d. from a probability distribution with smooth density, we establish Bernstein-type lower bounds on the probability that $\|U_{\lambda,\epsilon,N}^t u - U_{\lambda,\epsilon}^t u\|_{L^\infty} \leq \delta$ with $U_{\lambda,\epsilon,N}^t := e^{-it\sqrt{\Delta_{\lambda,\epsilon,N}}}$. We apply these bounds to coherent states to show that the geodesic flow on $\mathcal{M}$ can be approximated by matrix dynamics on the discrete sample set. Specifically, *with high probability*, the evolved state concentrates at the projected geodesic x_t of

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$\Gamma^t(x_0, \xi_0)$, satisfying $c_{t,N}^{-1} \sum_{j=1}^N |U_{\lambda,\epsilon,N}^t \psi_h(x_j)|^2 u(x_j) = u(x_t) + O(h)$ for the normalization $c_{t,N} := \sum_{j=1}^N |U_{\lambda,\epsilon,N}^t \psi_h(x_j)|^2$.

RÉSUMÉ. — Nous établissons des conditions sous lesquelles les laplaciens de graphes $\Delta_{\lambda,\epsilon}$ sur des sous-variétés compactes, sans bord et lisses $\mathcal{M}$ de l'espace euclidien sont des opérateurs pseudo-différentiels semi-classiques (Ψ DO). Plus précisément, la largeur de bande du noyau du Laplacien du graphe (*terme de biais*) $\sqrt{\epsilon}$ doit décroître plus rapidement que le paramètre semi-classique h , c'est-à-dire $h \gg \sqrt{\epsilon}$, et nous calculons le symbole. En combinant ceci avec le théorème d'Egorov et les états cohérents ψ_h localisés en $(x_0, \xi_0) \in T^*\mathcal{M}$, nous montrons que, avec $U_{\lambda,\epsilon}^t := e^{-it\sqrt{\Delta_{\lambda,\epsilon}}}$ défini spectralement, le flot (co-)géodésique Γ^t sur $T^*\mathcal{M}$ est approché par $\langle U_{\lambda,\epsilon}^{-t} \text{Op}_h(a) U_{\lambda,\epsilon}^t \psi_h, \psi_h \rangle = a \circ \Gamma^t(x_0, \xi_0) + O(h)$.

Dans le cadre discret, pour un laplacien de graphe normalisé $\Delta_{\lambda,\epsilon,N}$ défini sur un ensemble de N points $x_1, \dots, x_N$ échantillonnés de manière i.i.d. à partir d'une distribution de probabilité à densité régulière, nous établissons des bornes inférieures de type Bernstein sur la probabilité que $\|U_{\lambda,\epsilon,N}^t u - U_{\lambda,\epsilon}^t u\|_{L^\infty} \leq \delta$ avec $U_{\lambda,\epsilon,N}^t := e^{-it\sqrt{\Delta_{\lambda,\epsilon,N}}}$. Nous appliquons ces bornes aux états cohérents pour montrer que le flot géodésique sur $\mathcal{M}$ peut être approximé par une dynamique matricielle sur l'ensemble d'échantillons discrets. Plus précisément, *avec une forte probabilité*, l'état après évolution se concentre sur la géodésique projetée x_t de $\Gamma^t(x_0, \xi_0)$, satisfaisant $c_{t,N}^{-1} \sum_{j=1}^N |U_{\lambda,\epsilon,N}^t \psi_h(x_j)|^2 u(x_j) = u(x_t) + O(h)$ pour la normalisation $c_{t,N} := \sum_{j=1}^N |U_{\lambda,\epsilon,N}^t \psi_h(x_j)|^2$.

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1. Introduction

Given a pointset $\Lambda_N := \{X_1, \dots, X_N\} \subset \mathbb{R}^D$ that is assumed to lie on a submanifold $\Lambda \supset \Lambda_N$, a natural inverse problem asks to approximate the *intrinsic* geometry of Λ , using only this data. Implicitly, there is an isometric embedding $\iota : \mathcal{M} \rightarrow \Lambda \subset \mathbb{R}^D$ of an abstract manifold $\mathcal{M}$, both of which are unknown. Granted sufficient smoothness, such a reconstruction may consist of: an atlas that is prescribed by intrinsic data, e.g., a system of normal coordinates, or operators that are intimately tied to the intrinsic geometry, as in the Laplace–Beltrami⁽¹⁾ operator $\Delta_{\mathcal{M}}$, to name a couple of examples related to the study in this paper. Further, the restriction of functions on Λ to the pointset may be modeled by identifying Λ_N with the canonical basis in $\mathbb{C}^N$, which gives a complex vector space $\mathcal{H}_N \cong \mathbb{C}^N$. Then, for example, a vector in $\mathcal{H}_N$ may be seen as the restriction to Λ_N of a linear combination of N bump functions $u_1, \dots, u_N$ with $u_j(X_j) = 1$ or 0 and pairwise disjoint supports, $\text{supp } u_j \cap \text{supp } u_\ell = \emptyset$ for all $j \neq \ell$. Hence, the question arises as to how the dynamics of functions on $\mathcal{M}$ can be approximated by dynamics in $\mathcal{H}_N$. In many ways the geometry of manifolds is intimately tied with dynamics on them and so these two kinds of problems are interconnected.

Over the last two decades, the theory of graph Laplacians has advanced, giving convergence rates for the recovery of $\Delta_{\mathcal{M}}$ from samples Λ_N drawn from a probability distribution P supported on Λ , as $N \rightarrow \infty$, under various assumptions on $\mathcal{M}$, Λ , P and the kernels used to construct the graph Laplacians [LBB08, CGT22, HAVL05, Sin06]. A common schema is described in [NLCK06] as follows: using a positive, *essentially* locally supported⁽²⁾ smooth function $k : \mathbb{R}_+ \rightarrow \mathbb{R}$, an *averaging* matrix $(\mathcal{A}_{\epsilon, N})_{j, \ell} := k(\|X_j - X_\ell\|_{\mathbb{R}^D}^2 / \epsilon)$ is defined that after row normalisation represents a Markov chain process in discrete time and space. This normalized matrix $\mathcal{A}_{\epsilon, N}$ converges in such settings, with high probability as $N \rightarrow \infty$, to an operator A_ϵ that represents a Markov process in continuous space $\mathcal{M}$ and discrete time with steps of size ϵ ; its transition probability from $x \in \mathcal{M}$ to $y \in \mathcal{M}$ is proportional to $k_\epsilon(x, y) := k(\|\iota(x) - \iota(y)\|_{\mathbb{R}^D}^2 / \epsilon)$. The infinitesimal generator of this Markov process is $\Delta_{\mathcal{M}} + O(\partial^1)$ with $O(\partial^1)$ denoting terms with differential operators of order at most one. Further, in the limit $\epsilon \rightarrow 0$, this Markov process converges to a diffusion process

⁽¹⁾In the following, we define the Laplace–Beltrami operator to be signed so it is *positive semi-definite*: that is, in local coordinates,

$$\Delta_{\mathcal{M}} := -\frac{1}{\sqrt{|g|}} \sum_{j, \ell} \partial_j \sqrt{|g|} g^{j, \ell} \partial_\ell,$$

wherein g is the Riemannian metric on $\mathcal{M}$ and $g^{j, \ell}$ are the (j, ℓ) components of the inverse, g^{-1} .

⁽²⁾This means that if $k \in C^m(\mathbb{R}_+)$, then there are $R_1, \dots, R_m > 0$ such that $\partial^j k$ decays exponentially fast outside of $[0, R_j]$.

with the same infinitesimal generator. The (*random walk*) *discrete* and *continuum* graph Laplacians here are equal, up to a constant factor, to $(I - A_{\epsilon, N})/\epsilon$ and $(I - A_\epsilon)/\epsilon$, respectively, and they give the concrete approximations to the infinitesimal generator.

In this work, we study for smooth, compact, boundaryless manifolds $\mathcal{M}$, with some basic assumptions on Λ and P , the inclusion of graph Laplacians in the framework of semiclassical analysis and switch perspective from diffusion processes to quantum dynamics. The geometric data we are interested in recovering are the geodesics on $\mathcal{M}$, which can be cast as projections of the intrinsic (*co*)-*geodesic* flow $\Gamma^t : T^*\mathcal{M} \rightarrow T^*\mathcal{M}$ governed by the Hamiltonian $|\xi|_{g_x} := \langle g_x^{-1}\xi, \xi \rangle^{\frac{1}{2}}$, wherein g_x is the Riemannian metric at $x \in \mathcal{M}$. This Hamiltonian flow is *quantized* by $e^{-it\sqrt{\Delta_{\mathcal{M}}}}$, in that for times $|t|$ smaller than *Ehrenfest time*, it moves the support of wavepackets localized at (x_0, ξ_0) in *phase space* $T^*\mathcal{M}$ to those localized at $\Gamma^t(x_0, \xi_0)$, which ultimately leads to a linear PDEs approach to accessing geodesics. We use the framework of semiclassical pseudodifferential operators (Ψ DOs) to recover this behaviour with continuum graph Laplacians in place of $\Delta_{\mathcal{M}}$ and a manifold generalization of coherent states for the localized wavepackets. Then, we find probabilistic convergence rates so geodesics can be recovered with matrix dynamics on $\mathcal{H}_N$ using discrete graph Laplacians in place of their continuum counterparts and the restrictions of coherent states to the sample points Λ_N . Along the way, we establish consistency between solutions to discrete wave equations on Λ_N and solutions to wave equations on $\mathcal{M}$.

The dichotomy in the continuum and discrete settings requires completely different considerations. In Section 4, we realise continuum graph Laplacians, denoted $\Delta_{\lambda, \epsilon}$ with $\lambda \geq 0$ a normalization parameter (such that $\lambda = 0$ gives the random walk continuum graph Laplacian) – following [HAVL05], we define these in Section 2.2 – as semiclassical pseudodifferential operators (Ψ DOs). Then, the quantum dynamical perspective is driven by Egorov’s theorem, which tells more generally that if for $h \in [0, h_0)$ with $h_0 > 0$, Q is an order one Ψ DO on $\mathcal{M}$ with real-valued principal symbol $q \in C^\infty(T^*\mathcal{M} \times [0, h_0)_h)$ that generates a Hamiltonian flow $\Theta_q^t : T^*\mathcal{M} \rightarrow T^*\mathcal{M}$ on $T^*\mathcal{M}$ and $\hat{A}$ is a Ψ DO with symbol $a \in C^\infty(T^*\mathcal{M} \times [0, h_0)_h)$, then the operator dynamics $\hat{A}_t := e^{\frac{i}{h}tQ} \hat{A} e^{-\frac{i}{h}tQ}$ remains pseudodifferential and is, up to lower order, the quantization of $a \circ \Theta_q^t$. In this sense, we say that $e^{-\frac{i}{h}tQ}$ *quantizes* the flow Θ_q^t . To retrieve the flow of symbols from their quantized operators, we make use of *coherent states*, which are wavepackets of the form $\tilde{\psi}_h := e^{-\frac{i}{h}\bar{\phi}(\cdot; x_0, \xi_0)}$ localized at $(x_0, \xi_0) \in T^*\mathcal{M}$ with a complex phase ϕ satisfying certain *admissibility conditions* as defined in Section 2.4 that say roughly that $\tilde{\psi}_h$ locally resembles $e^{-\frac{\|\cdot - x_0\|^2}{2h}} e^{\frac{i}{h}\langle (\cdot - x_0), \xi_0 \rangle}$. The coherent states are essentially Schwartz kernels of a Fourier–Bros–Iagolnitzer (FBI) transform defined on manifolds [WZ01] and since the latter are well-known to essentially *diagonalize* Ψ DOs over $T^*\mathcal{M}$, we can recover the flow of symbols through the diagonal matrix elements of Ψ DOs in the basis of coherent states. That is, if $\psi_h := \tilde{\psi}_h / \|\tilde{\psi}_h\|_{L^2}$ is a normalized coherent state, then the flow is approximated by $\langle \hat{A}_t \psi_h, \psi_h \rangle_{L^2}$ in the sense that up to Ehrenfest time

$$T_E(h, \rho; q) := |t| \leq T + \frac{\rho}{C_q} \log(1/h),$$

we have $|\langle \hat{A}_t \psi_h, \psi_h \rangle_{L^2} - a \circ \Theta_q^t(x_0, \xi_0)| \lesssim h^{1-2\rho}$ for a constant $C_q > 0$ determined by the dynamics generated by q and $h \in (0, h_0]$ (see Section 5). This relationship between operator dynamics in the space of Ψ DOs and Hamiltonian mechanics on *phase space* $T^*\mathcal{M}$ is an instance of *quantum-classical correspondence*.

The order one Ψ DO $h\sqrt{\Delta_{\mathcal{M}}}$ quantizes $|\xi|_{g_x}$ and therefore, the geodesic flow is quantized by $U^t := e^{-it\sqrt{\Delta_{\mathcal{M}}}}$, which can be defined by spectral theory. While previous works (e.g., [HAVL05]) have shown that $\Delta_{\lambda,\epsilon} = \Delta_{\mathcal{M}} + O(\partial^1) + O(\epsilon)$ and it is certainly true that Egorov's theorem is agnostic to the $O(\partial^1)$ terms since the semiclassical principal symbol of $h\sqrt{\Delta_{\mathcal{M}} + O(\partial^1)}$ is just $|\xi|_{g_x}$, the method of approximation goes through a Taylor series expansion so that the $O(\epsilon)$ term consists of higher order operators. This indeed raises an issue in both, including $h^2\Delta_{\lambda,\epsilon}$ in the class of Ψ DOs and quantizing the geodesic flow through it, which can briefly be put as: the semiclassical parameter $h > 0$ sets the wavelength at which the pseudodifferential calculus resolves functions, so if the diffusion scale $\sqrt{\epsilon}$ is greater than the semiclassical wavelength h , then the corresponding symbol is concentrated *below* this wavelength and hence, its content goes undetected by the quantization procedure. This perspective is expounded in more detail and drives the analysis in Section 4.

A perhaps more direct way to see the issue in approximating U^t with $U_{\lambda,\epsilon}^t := e^{-it\sqrt{\Delta_{\lambda,\epsilon}}}$ is the following: it is well-known from microlocal analysis, or indeed discernible from Egorov's theorem that U^t propagates wavepackets localized in phase space along geodesics. That is, if the FBI transform (or physically, the *Husimi function*, which is its squared modulus) at wavelength h of $u_h \in C^\infty(\mathcal{M} \times (0, h_0)_h)$ is localized to a $\sqrt{h}$ neighbourhood of $(x_0, \xi_0) \in T^*\mathcal{M}$, then for t smaller than the injectivity radius at x_0 , the Husimi function of $U^t[u_h]$ is localized to roughly a $\sqrt{h}$ neighbourhood of $\Gamma^t(x_0, \xi_0)$. On the other hand, by functional calculus, we find that

$$(1.1) \quad U_{\lambda,\epsilon}^t[u_h] = f(0)u_h + A_{\lambda,\epsilon}[Df(A_{\lambda,\epsilon})[u_h]],$$

wherein $f(z) := e^{-itc\sqrt{(1-z)/\epsilon}}$ for a constant $c > 0$ and $Df := (f(z) - f(0))/z$. Recall that for $\lambda = 0$, $A_{0,\epsilon} = A_\epsilon$ represents a Markov process with transition probabilities being close to one in roughly $\sqrt{\epsilon}$ -balls and decaying exponentially outside of them; in fact, this is true for all $\lambda \geq 0$. Therefore, the second term of the right-hand side of (1.1) will be diffused to at least a $\sqrt{\epsilon}$ -ball and we can calculate that the Husimi function at wavelength h of the Schwartz kernel for $A_{\lambda,\epsilon} : u(\cdot) \mapsto \int_{\mathcal{M}} k_{\lambda,\epsilon}(\cdot, y)u(y) p(y) d\nu_g(y)$ (we assume P has smooth density p with respect to the volume form ν_g on $\mathcal{M}$) at a fixed $y \in \mathcal{M}$ is localized in phase space to balls of radius roughly $h/\sqrt{\epsilon}$ around $0 \in T_{\alpha_x}^*\mathcal{M}$ for all α_x in a neighbourhood of y . Hence, if $\epsilon \gtrsim h^2$, then for h sufficiently small, the Husimi function for $U_{\lambda,\epsilon}^t[u_h]$ will retain the support of its initial condition at all times, which is in stark contrast to the behaviour of $U^t[u_h]$. On the other hand, if $\epsilon \ll h^2$, then the Husimi functions of the two terms on the right-hand side of (1.1) can interact and there is chance for cancellations to occur.

In Section 4, we find that essentially $\epsilon \ll h^2$ is also sufficient for $h^2\Delta_{\lambda,\epsilon}$ to be a Ψ DO. Its symbol approximates $|\xi|_{g_x}^2$ within distance roughly $h/\sqrt{\epsilon}$ of the zero section in $T^*\mathcal{M}$ and outside of this, it is of order zero for any fixed h . Still, as a *semiclassical* Ψ DO, this makes the graph Laplacian an order *two* Ψ DO, but clearly

not elliptic. We find that on application to coherent states ψ_h , due to their localizing of Ψ DOs to $\sqrt{h}$ -balls in phase space, we can approximately quantize Γ^t with $U_{\lambda,\epsilon}^t$. Indeed, in Theorems 4.4 and 5.2 we show under the assumptions:

- (1) $\mathcal{M}$ is a compact, boundaryless C^∞ manifold and,
- (2) P is a probability distribution on Λ so that with respect to the volume form ν_g on $\mathcal{M}$, there is a positive density $p := dP \circ \iota / d\nu_g \in C^\infty$,

that the following quantum-classical correspondence holds.

THEOREM A (*Quantum-classical correspondence for the graph Laplacian*). — Let $\lambda \geq 0$ and $h \in (0, 1]$. Then, for all $\alpha \geq 1$, $h^2 \Delta_{\lambda, h^{2+\alpha}}$ is a semiclassical Ψ DO in $h^0 \Psi^2$ as defined in Section 2.3, whose principal symbol q in any fixed neighbourhood of $0 \in T^* \mathcal{M}$ is $|\xi|_{g_x}^2 + O(h)$. Furthermore, let ψ_h be an L^2 normalized coherent state localized at $(x_0, \xi_0) \in T^* \mathcal{M} \setminus 0$ and denote by $\Gamma^t : T^* \mathcal{M} \rightarrow T^* \mathcal{M}$ the (co-)geodesic flow. Then, there exist $h_0 > 0$ and a constant $C_q > 0$ depending on the Hamiltonian dynamics generated by q such that for all $|t|$ smaller than Ehrenfest time $T_E(h, \rho; q) := T + (\rho/C_q) \log(1/h)$ for $T \geq 0$ and $\rho \in [0, 1/2]$, we have for all $h \in (0, h_0]$ that:

- (1) $U_{\lambda, h^{2+\alpha}}^t \psi_h$ is localized in phase space near $(x_t, \xi_t) := \Gamma^t(x_0, \xi_0)$ at scale $h^{1/2-\tilde{\rho}}$ for all $\tilde{\rho} \in (\rho, 1/2]$, in the sense that for any $\chi_\rho^c \in C^\infty(T^* \mathcal{M})$ belonging to the symbol class $h^0 S_\rho^0$ as per Section 2.3 and supported outside of a ball around (x_t, ξ_t) at this scale, the functions $\text{Op}_h(\xi^\beta \chi_\rho^c) U_{\lambda, h^{2+\alpha}}^t \psi_h$ have L^∞ norm $O(h^M)$ for all $\beta \in \mathbb{N}_0^n$ and $M \in \mathbb{N}$ and,
- (2) given $a \in C^\infty(T^* \mathcal{M})$ belonging to the symbol class $h^0 S^0$ with its quantization $A := \text{Op}_h(a) \in h^0 \Psi^0$,

$$\left\langle U_{\lambda, h^{2+\alpha}}^{-t} A U_{\lambda, h^{2+\alpha}}^t \psi_h(\cdot; x_0, \xi_0), \psi_h(\cdot; x_0, \xi_0) \right\rangle_{L^2(\mathcal{M})} = a \circ \Gamma^t(x_0, \xi_0) + O(h^{1-2\rho}).$$

These properties are put to use in Section 6, wherein we study the convergence of the discrete counterparts to the preceding constructions in the continuum setting. Namely, the propagator we use is $U_{\lambda,\epsilon,N}^t := e^{-it\sqrt{\Delta_{\lambda,\epsilon,N}}}$, which is defined by functional calculus and acts on $\mathcal{H}_N$ equipped with the inner product $\langle u, v \rangle_N := \frac{1}{N} \sum_{j=1}^N u(x_j) \overline{v(x_j)}$ that gives the norm $\|\cdot\|_N := \sqrt{\langle \cdot, \cdot \rangle_N}$. This vector space structure approaches $L^2(\mathcal{M}, p d\nu_g)$ as $N \rightarrow \infty$, so it becomes important to normalize vectors to reduce the effect of the sampling density p . The matrix $U_{\lambda,\epsilon,N}^t$ is not unitary, so the initial state is a *time-dependent* normalization of the coherent state ψ_h , that is, we set $\psi_{h,t,N} := U_{\lambda,\epsilon,N}^t \psi_h / \|U_{\lambda,\epsilon,N}^t \psi_h\|_N$. Importantly, the probabilistic consistency rates of the discrete constructions depend on the L^∞ norm of $U_{\lambda, h^{2+\alpha}}^t \psi_h$, owing to the pointwise consistency results they are based upon (see Section 2). For this, the phase space localization to within a ball of radius $h^{1/2-\tilde{\rho}}$ gives a stark improvement over a priori L^∞ bounds from functional calculus: indeed, applying a frequency cut-off Ψ DO implies that $\|U_{\lambda, h^{2+\alpha}} \psi_h\|_{L^\infty} \lesssim h^{-(1/2+\tilde{\rho})n/2}$ (see Section 6.3). Then, under the additional assumption that Λ_N is a set of i.i.d. random vectors on $\mathbb{R}^D$ with law P and ι has a bounded second fundamental form, in Theorem 6.25 we arrive at the following consistency result.

THEOREM B (Quantum-classical correspondence for the discrete graph Laplacian). *Let $\lambda \geq 0$, $\alpha \geq 1$, $(x_0, \xi_0) \in T^*\mathcal{M}$ and $|t|$ be smaller than Ehrenfest time $T_E(h, \rho; q)$ for $\rho \in [0, 1/2)$. Then, for ψ_h a coherent state localized at (x_0, ξ_0) and given $u \in C^\infty$ and $\tilde{\rho} \in (\rho, 1/2]$ a localizing parameter, there are constants $h_0, C > 0$ such that we have for all $h \in (0, h_0]$ and $\epsilon := h^{2+\alpha}$,*

$$\Pr \left[\left| \left\langle \left| U_{\lambda, \epsilon, N}^t \psi_{h, t, N}(x_j) \right|^2, u \right\rangle_N - u(x_t) \right| > h^{1-2\rho} \right] \leq \exp \left(- \frac{N h^{n(2+3\tilde{\rho})+4} \epsilon^{\frac{5}{2}n+4}}{C|t|^8} \right).$$

As an application of this, we recover in $\mathcal{X}_N := \iota^{-1}[\Lambda_N]$ the geodesic flow on $\mathcal{M}$ to times that increase with $1/h$. We note at this point that the timeframe is dictated by the length of time to which the quantum-classical correspondence holds; one way to characterize this is the duration of time to which coherent states stay localized near a trajectory, rather than spreading apart. As stated, the Ehrenfest time $T_E(h, \rho; q)$ accounts only for the *worst-case scenario*, in that the constant C_q is an upper bound on the maximal Lyapunov exponent for dynamics near $\{|\xi|_{g_x} = |\xi_0|_{g_{x_0}}\}$ and when this is positive, we have the $\log(1/h)$ scaling for the quantum-classical correspondence. This is the case, for example, in chaotic dynamics or geodesic flows in the negative curvature regime. On the other hand, in completely integrable systems such as the flows on flat tori and surfaces of revolution, the scaling is of order $h^{-1/2+\delta}$ for all $\delta > 0$ [BR02].

Altogether, applying the preceding theorem using *coordinate functions* with either local coordinates or the extrinsic coordinates $\iota_1, \dots, \iota_D$, we find in Proposition 6.29 that,

PROPOSITION C (Observing geodesics: the mean case). — *Let ψ_h be a coherent state localized at $(x_0, \xi_0) \in T^*\mathcal{M}$, $|t|$ less than Ehrenfest time $T_E(h, \rho; q)$ for $\rho \in [0, 1/2)$, $\tilde{\rho} \in (\rho, 1/2]$ a localizing parameter, $\lambda \geq 0$ and $\alpha \geq 1$.*

- *Extrinsic case: Define the global extrinsic sample mean $\bar{x}_{N, t}$ to be the closest point in Λ_N to*

$$\bar{\iota}_N^t(x_0, \xi_0) := (\bar{\iota}_{N,1}^t(x_0, \xi_0), \dots, \bar{\iota}_{N,D}^t(x_0, \xi_0)),$$

with

$$\bar{\iota}_{N,j}^t(x_0, \xi_0) := \left\langle \left| U_{\lambda, \epsilon, N}^t \psi_{h, t, N} \right|^2, \iota_j \right\rangle_N.$$

That is, $\bar{x}_{N, t} := \arg \min_{X \in \Lambda_N} \|X - \bar{\iota}_N^t(x_0, \xi_0)\|_{\mathbb{R}^D}$. Then, there are constants $h_{\iota, \max} > 0$ and $C \geq 1$ such that for all $h \in (0, h_{\iota, \max}]$ and $\epsilon := h^{2+\alpha}$,

$$\Pr \left[d_g(\iota^{-1}(\bar{x}_{N, t}), x_t) > h^{1-2\rho} \right] \leq \exp \left(- \frac{N h^{(2+3\tilde{\rho})n+4} \epsilon^{\frac{5}{2}n+4}}{C|t|^8} \right).$$

- *Local case: Let $\mathcal{O}_t \subset \mathcal{M}$ be an open neighbourhood of a maximizer $\hat{x}_{N, t}$ of $|U_{\lambda, \epsilon, N}^t \psi_h|^2$ over $\mathcal{X}_N$ and $u : \mathcal{O}_t \rightarrow V_t \subset \mathbb{R}^n$ its C^∞ diffeomorphic coordinate mapping. Given a smooth cut-off $\chi \in C_c^\infty(\mathbb{R}^n, [0, 1])$ with $\text{supp } \chi \subset V_t$, define the local sample mean $\bar{x}_{N, u, t}$ to be the closest point in $\mathcal{V}_N := u[\mathcal{X}_N \cap \mathcal{O}_t]$ to*

$$\bar{u}_N^t(x_0, \xi_0) := (\bar{u}_{N,1}^t(x_0, \xi_0), \dots, \bar{u}_{N,n}^t(x_0, \xi_0)),$$

with

$$\bar{u}_{N,j}^t(x_0, \xi_0) := \left\langle \left| U_{\lambda, \epsilon, N}^t \psi_{h,t,N} \right|^2, (\chi \circ u) u_j \right\rangle_N.$$

That is, $\bar{x}_{N,u,t} := \arg \min_{X \in \mathcal{V}_N} \|X - \bar{u}_N^t(x_0, \xi_0)\|_{\mathbb{R}^n}$. Then, there are constants $h_{u,\max} > 0$ and $C \geq 1$ such that for all $h \in (0, h_{u,\max}]$, if $\bar{\mathcal{B}}_t := \{\|u(\hat{x}_{N,t}) - v\|_{\mathbb{R}^n} \leq h^{1/2-\tilde{\rho}}\} \subset V_t$, then for any smooth cut-off $\chi \in C_c^\infty(\mathbb{R}^n, [0, 1])$ with $\text{supp } \chi \subset V_t$ that is $\chi \equiv 1$ on $\bar{\mathcal{B}}_t$, we have with $\epsilon := h^{2+\alpha}$,

$$\Pr \left[d_g \left(u^{-1}(\bar{x}_{N,u,t}), x_t \right) > h^{1-2\rho} \right] \leq \exp \left(- \frac{N h^{(2+3\tilde{\rho})n+4} \epsilon^{\frac{5}{2}n+4}}{C |t|^8} \right).$$

On the way to these consistency results, we have studied in Section 6 the consistency between certain matrix dynamics on $\mathcal{H}_N$ and operator dynamics on $C^\infty(\mathcal{M})$. An intermediary result of independent interest is that for $u \in C^\infty$, a natural *extension* of $U_{\lambda, \epsilon, N}^t[u]$ to $\mathcal{M}$ is, with high probability, close to $U_{\lambda, \epsilon}^t[u]$ in L^∞ norm. The extension is realized by a discrete version of (1.1), namely, for any $x \in \mathcal{M}$ we have,

$$(1.2) \quad U_{\lambda, \epsilon, N}^t[u](x) = f(0)u(x) + A_{\lambda, \epsilon, N}[Df(A_{\lambda, \epsilon, N})[u_h]](x).$$

Here, $Df(A_{\lambda, \epsilon, N})$ is an $N \times N$ matrix over $\mathcal{H}_N$ as defined by spectral calculus, while $A_{\lambda, \epsilon, N}$ naturally extends to a finite-rank operator on $L^2(\mathcal{M})$, for example in the $\lambda = 0$ case by the fact that $A_{\epsilon, N}[v](x) = \langle v, k_\epsilon(x, \cdot) \rangle_N / \langle k_\epsilon(x, \cdot), 1 \rangle_N$. Thus, (1.2) is essentially a Nyström extension to the manifold. With this formalism at hand, we find in Theorem 6.14 that,

THEOREM D (Consistency of half-wave propagations). — *Let $\lambda \geq 0$ and $\epsilon \in (0, 1]$. Then, we have for any $t \in \mathbb{R}$ and $u \in L^\infty(\mathcal{M})$ that if there is $K_u > 0$ such that for all $|s| \leq |t|$, $\|U_{\lambda, \epsilon}^s[u]\|_\infty \leq K_u$, then there are constants $C, C_0 \geq 1$ such that for all*

$$\frac{K_u^{\frac{1}{2}} \epsilon^{-\left(\frac{5}{8}n+1\right)}}{C_0 N^{\frac{1}{4}}} \leq \delta < C_0,$$

$$\Pr \left[\left\| U_{\lambda, \epsilon, N}^t[u] - U_{\lambda, \epsilon}^t[u] \right\|_\infty > \delta \right] \leq \exp \left(- \frac{N \delta^4 \epsilon^{\frac{5}{2}n+4}}{C K_u^2 |t|^8} \right).$$

In connection to the semiclassical nature of $\Delta_{\lambda, \epsilon}$ for $\epsilon \ll h^2$, it may be possible to have a generic bound K_u by appealing to semiclassical Strichartz-type estimates to arrive at an $L^1 \rightarrow L^\infty$ bound on $U_{\lambda, \epsilon}^t$, as used for example in the proof of [Zwo12, Theorem 10.8]. Alternatively, a bound is attainable directly from inspection of (1.1) combined with spectral theory and we give that in the corollary to Theorem 6.14. As mentioned above, the phase space localization of coherent state propagation gives a super-quadratic improvement over this bound by a standard application of semiclassical Sobolev estimates and a Littlewood–Paley decomposition in frequency space. We have applied this in Section 6.3 to achieve the consistency rates mentioned above for the quantum-classical correspondence of the discrete graph Laplacian.

The discrete results we present justify the use of spectral manipulations of the discrete graph Laplacian for approximating solutions to wave equations and ultimately, geodesic flows, on $\mathcal{M}$ through linear computations on the dataset Λ_N . In Section 6.5

we indicate an algorithm of this sort for approximating geodesics of $\mathcal{M}$ in Λ_N . More careful constructions, including the construction of coherent states from the dataset, are deployed in [KS22], where several examples are given, both for model cases of a sphere and torus as well as for real-world datasets and convergence rates are shown. The consistency analysis we study is independent of arguments from the spectral convergence of graph Laplacians to $\Delta_{\mathcal{M}}$, which is currently a very active topic, both in the probabilistic [CM20, GTGHS20, GTS18, WR21] and deterministic [BIK14] settings; in this regard, we mention in Section 4.2 connections between the semiclassical framework and analysis of the spectrum. In particular, we discuss how semiclassical calculus yields information about frequency localizations of eigenfunctions of $\Delta_{\lambda,\epsilon}$ with eigenvalues $\gtrsim 1/\epsilon^{3/4}$, a regime well beyond where existing spectral convergence analyses, even in the continuum, break down ($\ll 1/\sqrt{\epsilon}$). An interesting direction would be to apply the consistency of half-wave propagations in Theorem 6.14 to the study of these spectral problems.

Outline

We proceed as follows: in Section 2 we state the assumptions on $\mathcal{M}, \iota, P$ and the *kernel function* k used to construct the graph Laplacians. Then, we state some basic geometric lemmas that will be used later and come to the definitions of the graph Laplacians. We give some of their basic spectral properties and in Section 2.2.1 we reprove a well-known result on the pointwise consistency of the application of discrete averaging operators $A_{\lambda,\epsilon,N}$ to L^∞ functions, following [Hei05], but give more explicit details on the dependence on the L^∞ norm of the function. This allows further convergence results to be stated in terms of these norms, which may depend on ϵ , as is the case for example with the coherent states we use later. Then, we provide some background on Ψ DOs, mainly to state the forms of quantization we consider and set some notation and in Section 2.4 we recall the notion of an FBI transform on a smooth, compact manifold as explicated in [WZ01]. In Section 3 we give an explicit form to the Husimi function of a coherent state; this simply follows from the Schwartz kernel of the operator that projects functions in $L^2(T^*\mathcal{M})$ onto the range of the FBI transform and indeed, we follow the discussion in [WZ01]. The results in this section are likely well-known, but to the best of the author's knowledge, not explicitly written down in literature and perhaps not directly accessible to a wider audience interested in the topics of this study, so we provide them in some detail. We briefly discuss in Section 3.1 some practical considerations in the construction of coherent states from the data, Λ_N ; this program is carried out in more detail in [KS22].

We study the connection between semiclassical analysis and graph Laplacians in Section 4. Then, we study the propagation of coherent states in Section 5. We include a version of Egorov's theorem suited to our purposes: namely, it features a quantum-classical correspondence for observables localized to balls of radius $h^{1/2-\tilde{\rho}}$ in phase space for $\tilde{\rho} \in (\rho, 1/2]$ and up to Ehrenfest time $T_E(h, \rho; q)$ and wherein the classical flow is given by the principal symbol q of the generator of the quantum dynamics. The former feature plays an essential role in establishing the propagation of coherent

states, while the latter captures of the local approximation of the unit-speed geodesic flow by the dynamics of graph Laplacians. This is likely part of folklore, but to the author's knowledge, not explicated in literature. The method of proof in Theorem 5.2 is essentially to reduce to this situation by using the coherent state to *microlocalize* the generator $\sqrt{\Delta_{\lambda,\epsilon}}$ to a $\Theta(1/h)$ neighbourhood of ξ_0/h in frequency space; with this, we quickly conclude the localization properties of the propagated coherent state.

In Section 6 we study the discrete problems over Λ_N and establish probabilistic convergence rates to bridge the gap to the continuum, $N \rightarrow \infty$ setting. After extending pointwise consistency of the averaging matrix $A_{\lambda,\epsilon,N}$ to L^∞ consistency, the methods become deterministic applications of union bounds of events based on this. It is only at the end of our sequence of constructions that we invoke a probabilistic method, in order to associate a sample point in an $O(h^{1-2\rho})$ neighbourhood of the sample mean $\bar{x}_{N,\cdot,t}$ of the propagated coherent state. Along the way, we study the square roots of graph Laplacians and apply properties of the Schwartz kernels of Markov operators and matrix elements of Markov matrices, in order to establish the L^∞ consistency of $\sqrt{\Delta_{\lambda,\epsilon,N}}[u]$ with $\sqrt{\Delta_{\lambda,\epsilon}}[u]$. The singular part of the spectrum of the graph Laplacian introduces variances that we control by a kind of *Tikhonov regularization* through spectral shifts $(\Delta_{\lambda,\epsilon,N} + \varepsilon I)^{1/2}$ and $(\Delta_{\lambda,\epsilon} + \varepsilon I)^{1/2}$ for small values of the regularization parameter $\varepsilon > 0$. This yields consistency of the unperturbed model when tuned to the *optimal* ratio δ^2/ϵ of noise variance to bias. When decoupled from the noise variance, this introduces a *bias-variance tradeoff* in the resolution of dynamics with respect to the continuum graph Laplacian. Upon tuning $\varepsilon \sim h^{-1}$ to the semiclassical frequency regime, these perturbations in themselves enjoy the same quantum-classical correspondence on the continuum side and we find improved convergence rates to semiclassical propagation and the geodesic flow from the discrete side. From the stand-point of standard statistical inference, this seems paradoxical as the *bias floor* in terms of the unperturbed square root graph Laplacians grows as $\sim h^{-1/2}$. However, by evolving coherent states we impose a *microlocal bias* through phase space localization, adjusted for quantum-classical correspondence, so that the *effective* bias floor drops to order $\sim h$. We have presented both models concurrently and in Section 6.7 we have summarized the dominating consistency rates for each model through various parts of our constructions that may be of independent interest. Combined with a data-driven construction of coherent states that we discuss in Section 6.6 and that is detailed in the companion work [KS22] by M. Sarovar and the present author, this yields statistical estimators for the unit speed geodesic flow to long times, with convergence rates that follow a power law in the number of samples, wherein the exponents are independent of the extrinsic dimension D and depend only on the effective manifold dimension n .

Our methods also yield an alternative statistical estimator for the geodesic flow at *all* speeds. Using essentially a subset of the constructions in Section 6, one finds the L^∞ consistency of the discrete Schrödinger propagation $e^{-ith\Delta_{\lambda,\epsilon,N}}[u]$ with $e^{-ith\Delta_{\lambda,\epsilon}}[u]$. Then, the propagation of coherent states and quantum-classical correspondence results all transfer to this setting rather directly, with similar probabilistic convergence rates. However, the half-wave propagator yields significantly better approximations and improved stability with respect to parameters ϵ and h in practice, for the unit

speed flow. We expect this to be attributed to the inherently hyperbolic nature of its dynamics. In Appendix A, we give a numerical example of this for the simple case of uniformly random samples drawn from the unit circle in $\mathbb{R}^2$. While the asymptotics are similar to order $h^{1-2\rho}$ error rates up to Ehrenfest time, it would appear that there are discretization errors at higher orders with large coefficients that make Schrödinger propagation less stable within computationally feasible sample sizes. This is suggested by the fact that the Schrödinger propagator is dispersive, consisting of superpositions of waves traveling at different speeds. These combine in the propagation of an initial condition to fill the frequency space at all magnitudes corresponding to the part of the spectrum where the initial condition has significant overlap. Viewing $e^{-ith\Delta_{\lambda,\epsilon}}\psi_h$ as the semiclassical FBI transform at (x_0, ξ_0) of one component of the Schwartz kernel for $e^{-ith\Delta_{\lambda,\epsilon}}$, the task of the coherent state is to effectively *filter out* all singularities aside from those localized near x_0 with frequencies near ξ_0/h . On the discrete side, the effective sample size required to resolve the FBI transform of a Fourier integral operator by essentially performing Monte Carlo integration is likely to increase rapidly with the amount of frequency space that the wavefront set occupies. It is based on this heuristic and the consistently higher performance of the half-wave propagator in applications and numerical experiments conducted in [KS22] that we have made it the principal character of our study.

2. Preliminaries

We will discuss the necessary results for manifold learning and semiclassical analysis. To set the stage, there is an *unknown manifold* $\mathcal{M}$, on which we wish to implement operators and dynamics and whose geometry we wish to learn; we always operate under the following assumptions:

ASSUMPTIONS 2.1. — *The manifold $\mathcal{M}$ is C^∞ , compact, boundaryless, of dimension $n := \dim \mathcal{M}$ with Riemannian metric g giving the geodesic distance function $d_g : \mathcal{M} \times \mathcal{M} \rightarrow \mathbb{R}_+$ and embedded as $\Lambda \subset \mathbb{R}^D$ through a smooth isometry $\iota : \mathcal{M} \xrightarrow{\sim} \Lambda \subset \mathbb{R}^D$ with $D \geq n + 1$. The second fundamental form of Λ (see [Hei05, Lemma 2.22]) has bounded norm and*

$$\kappa := \inf_{x \in \mathcal{M}} \inf_{y \in \mathcal{M} \setminus B_{\pi\rho}(x,g)} |\iota(x) - \iota(y)| > 0,$$

wherein $\rho := \inf\{\gamma \text{ unit-speed geodesic in } \mathcal{M} \mid |\partial_t^2[\iota \circ \gamma]|\}$, termed the minimum radius of curvature, is positive due to Λ having bounded second fundamental form (see [Hei05, Section 2.2.1]). Samples $X_1, \dots, X_N$ are drawn i.i.d. from a fixed probability distribution P concentrated on Λ such that $P \circ \iota^{-1}$ is absolutely continuous with respect to the volume measure on $\mathcal{M}$ and has smooth, positive density $p \in C^\infty(\mathcal{M})$.

Remark 2.2. — The conditions on Λ give control on its extrinsic geometry through the intrinsic geometry of $\mathcal{M}$: in particular, [Hei05, Lemma 2.22] tells that for all $x, y \in \mathcal{M}$ such that $|\iota(x) - \iota(y)| \leq \kappa/2$, we have $d_g(x, y)/2 \leq |\iota(x) - \iota(y)| \leq d_g(x, y) \leq \kappa$.

A common way to think of the samples $X_1, \dots, X_N$ is through a *graph structure* with vertices $\mathcal{X}_N := \{x_1, \dots, x_N\}$, wherein $x_j := \iota^{-1}(X_j)$ for each $j \in [N]$. In this

setting, the graph connectivity is given by an adjacency matrix that uses the embedding ι and is defined as one of the *discrete averaging operators* $A_{\lambda,\epsilon,N}$ defined in Section 2.2. We can also view $\mathcal{X}_N$ as a set of basis elements giving rise to a vector space structure and endow it with an inner product in which these are orthogonal. Then, the restriction of C^∞ functions to $\mathcal{X}_N$ can be seen as vectors in this space and with appropriate weighting schema, the discrete structures that emerge, begin to parallel certain weighted L^2 spaces. Such representations form the basis from which discrete constructions — particularly functions of averaging operators that encode certain dynamics — are extended to the full, *continuum* space $\mathcal{M}$. The basic principles of this point of view are treated in [Hei05] and briefly in [HAVL05]; we will utilise it primarily in Section 6.

The general notation used throughout the following sections is summarized in Appendix B and more specific notation is listed there for quick reference; when some notation is introduced for the time, it will be defined in context.

2.1. Geometric properties

We will often need to switch to normal coordinates and expand them in Taylor series about a point of interest. Affecting this, we have a classical theorem of Riemann:

LEMMA 2.3 (Expansion of Normal Coordinates). — *Let $x \in \mathcal{M}$ and $V_x \subset \mathbb{R}^n$ be a neighbourhood of the origin in normal coordinates centered at x . Then, for $\exp_x : V_x \rightarrow \mathcal{M}$ defined via the identification $T_x \mathcal{M} \cong \mathbb{R}^n$, we have $D \exp_x(v) = I_n + O(|v|^2)$ and $(g \circ \exp_x)(v) = I_n + O(|v|^2)$.*

In practice, direct access to normal coordinates is seldom achievable. However, projection onto the tangent space at a point on Λ also provides local coordinates and for *shrinking* neighbourhoods, this approximates normal coordinates reasonably well:

LEMMA 2.4 (Normal to Projection Coordinates). — *Let $\mathcal{U} \subset \mathcal{M}$ be a neighbourhood and $V_x \subset \mathbb{R}^n \cong T_{\iota(x)} \Lambda$ for some $x \in \mathcal{U}$. If $\gamma : \mathcal{U} \rightarrow V_x$ are local coordinates provided by the orthogonal projection $\iota(\mathcal{U}) \rightarrow V_x$ and $s_x(y) := \exp_x^{-1}(y)$, then $s_x \circ \gamma^{-1}(v) = v + O(|v|^3)$ and $D[s_x \circ \gamma^{-1}](v) = I + O(|v|^3)$.*

Proof. — This is [Laf04, Lemma 5]. □

Another option is to work directly with extrinsic coordinates provided by the embedding map $\iota : \mathcal{M} \rightarrow \Lambda$. To this end, we have the following expansion, useful for integration formulae:

LEMMA 2.5 (Extrinsic to Normal Coordinates). — *Let $\mathcal{U} \subset \mathcal{M}$ be a neighbourhood of $x \in \mathcal{M}$ contained inside the normal neighbourhood of x and $s_x(y) := \exp_x^{-1}(y)$. Then,*

- (1) $D[\iota \circ s_x^{-1}](0) = D[\iota](x)$ and
- (2) for all $y \in \mathcal{U}$, $|\iota(x) - \iota(y)|^2 = d_g(x, y)^2 + O(d_g(x, y)^4)$.

Proof. — These are both shown in the [ABH21, Proof of Lemma 2.1]. □

We will also need the following information on the growth of covering numbers on compact manifolds using balls of decaying radii:

LEMMA 2.6 (Bishop–Günther inequality). — *Let $\rho > 0$ be fixed and define $\mathcal{N}(\rho)$ to be the minimal number of (geodesic) balls of radius ρ that cover $\mathcal{M}$. Then, there exist positive constants $C_{\mathcal{M}}$ and $C'_{\mathcal{M}}$ depending only on the dimension, volume, sectional curvature and injectivity radius of $\mathcal{M}$ such that if $0 < \rho \leq C'_{\mathcal{M}}$, then $\mathcal{N}(\rho) \leq C_{\mathcal{M}}\rho^{-n}$.*

Proof. — The volume of $B(x, \rho)$ for $x \in \mathcal{M}$ is $V(x) \geq \rho^n/C''_{\mathcal{M}}$ when $\rho \leq C'_{\mathcal{M}}$ for some constants $C'_{\mathcal{M}}, C''_{\mathcal{M}} > 0$ independent of x that are provided by the Bishop–Günther inequality and depend only on the sectional curvature, injectivity radius and dimension of $\mathcal{M}$. Therefore, $\mathcal{N}(\rho) \leq \text{vol}(\mathcal{M})/(\inf V) \leq C_{\mathcal{M}}\rho^{-n}$ with $C_{\mathcal{M}} := \text{vol}(\mathcal{M})C''_{\mathcal{M}}$. $\square$

2.2. Laplacians: from graphs to manifolds

As alluded to in the introduction, there are now well-established schema for approximating Laplace–Beltrami operators, modulo lower-order terms, from the Euclidean distances of samples $X_1, \dots, X_N$ of a smooth isometric embedding of $\mathcal{M}$ satisfying the Assumptions. Namely, the objects of study are adjacency matrices of weighted graphs on these samples and taking on a certain form, which we call *averaging operators*. We now fix the terminology:

DEFINITION 2.7 (Kernel functions). — *A kernel function is a monotonically decreasing function $k : \mathbb{R}_+ \rightarrow \mathbb{R}_+$ that is smooth on $(0, \infty)$ with all derivatives having exponential decay: that is, for each $m \geq 0$, there are constants $R_{k,m}, A_{k,m} > 0$ so that for all $t > R_{k,m}$,*

$$|\partial_t^m k(t)| \leq e^{-A_{k,m}t}$$

and that satisfies $k(t) > \|k\|_{\infty}/2$ on $[0, r_k)$ for some $r_k > 0$. We denote $R_k := R_{k,0}$.

Kernel functions are the basic building blocks for the graph structures leading to the operators of interest. Using them, we can make,

DEFINITION 2.8 (Averaging operators). — *Let there be $N > 0$ random vectors $X_1, \dots, X_N \subset \Lambda$ with law P as per the Assumptions 2.1 and for each $j \in [N]$, denote $x_j := \iota^{-1}(X_j)$. Let $k : \mathbb{R}_+ \rightarrow \mathbb{R}_+$ be a kernel function. Then, fixing $k : \mathbb{R}_+ \rightarrow \mathbb{R}_+$ a kernel function and letting $k_{\epsilon} : \mathcal{M} \times \mathcal{M} \rightarrow \mathbb{R}$ be given by $k_{\epsilon} : (x, y) \mapsto \epsilon^{-\frac{n}{2}} k(|\iota(x) - \iota(y)|^2/\epsilon)$ for $\epsilon > 0$, we define the discrete and continuum averaging operators as*

$$(2.1) \quad (\mathcal{A}_{\epsilon,N})_{j,j'} := \frac{1}{N} k_{\epsilon}(x_j, x_{j'}), \quad \mathcal{A}_{\epsilon} : u \mapsto \int_{\mathcal{M}} k_{\epsilon}(x, y) u(y) p(y) d\nu_g(y),$$

respectively. Further, with⁽³⁾ $p_{\epsilon,N}(x) := \mathcal{A}_{\epsilon,N}[1](x)$ and $p_{\epsilon}(x) := \mathcal{A}_{\epsilon}[1](x)$ we define

$$A_{\epsilon,N} := \text{diag}(p_{\epsilon,N}^{-1}) \mathcal{A}_{\epsilon,N}, \quad A_{\epsilon} := \frac{1}{p_{\epsilon}} \mathcal{A}_{\epsilon},$$

⁽³⁾We abuse notation by writing $A[1]$ to refer interchangeably to the action of an operator on the constant function $f \equiv 1$ or the action of a matrix on the all-ones vector $(1, \dots, 1)^T$.

called the discrete and continuum renormalized averaging operators, respectively. More generally, let $\lambda \geq 0$ and define

$$k_{\lambda,\epsilon,N}(x, y) := k_\epsilon(x, y) / [p_{\epsilon,N}(x)p_{\epsilon,N}(y)]^\lambda \quad \text{and} \quad k_{\lambda,\epsilon}(x, y) := k_\epsilon(x, y) / [p_\epsilon(x)p_\epsilon(y)]^\lambda.$$

With this,

$$(\mathcal{A}_{\lambda,\epsilon,N})_{j,j'} := k_{\lambda,\epsilon,N}(x_j, x_{j'}), \quad \mathcal{A}_{\lambda,\epsilon} : u \mapsto \int_{\Lambda} k_{\lambda,\epsilon}(x, y) u(y) p(y) d\nu_g(y)$$

are the discrete and continuum λ -averaging operators, respectively and

$$A_{\lambda,\epsilon,N} := \text{diag}(\mathcal{A}_{\lambda,\epsilon,N}[1]^{-1}) \mathcal{A}_{\lambda,\epsilon,N}, \quad A_{\lambda,\epsilon} : u \mapsto (\mathcal{A}_{\lambda,\epsilon}[1])^{-1} \mathcal{A}_{\lambda,\epsilon}[u]$$

are the discrete and continuum λ -renormalized averaging operators, respectively.

Notation 2.9. — We will denote for every $\lambda \geq 0$, $p_{\lambda,\epsilon} := \mathcal{A}_{\lambda,\epsilon}[1]$.

The main use of these operators is to approximate the Laplace–Beltrami operator on the manifold. Therefore, we also make the

DEFINITION 2.10 (Graph Laplacians). — Let c_2 and c_0 be the second and zeroth order moments of $k(\|\cdot\|^2)$ on $\mathbb{R}^n$. We define

$$\Delta_{\lambda,\epsilon,N} := \frac{2c_0}{c_2} \frac{I - A_{\lambda,\epsilon,N}}{\epsilon}, \quad \Delta_{\lambda,\epsilon} := \frac{2c_0}{c_2} \frac{I - A_{\lambda,\epsilon}}{\epsilon},$$

which we call the discrete and continuum λ -renormalized graph Laplacians, respectively. Note that when $\lambda = 0$, $A_{\lambda,\epsilon,N} = A_{\epsilon,N}$ and $A_{\lambda,\epsilon} = A_\epsilon$.

Remark 2.11. — In using the above terminologies, we will often omit the *discrete* and *continuum* specifications as well as *λ -renormalized* when the symbols and context make the regime sufficiently clear. The symbolic expressions are adapted from [HAVL05], while the terminology is non-standard.

We will use the spectral properties of $A_{\lambda,\epsilon,N}$ and $A_{\lambda,\epsilon}$ and the simplest way to access those is to see that they are symmetrized by conjugation via $\sqrt{p_{\lambda,\epsilon,N}}$ and $\sqrt{p_{\lambda,\epsilon}}$ respectively. That is, we have,

LEMMA 2.12. — Let for all $\lambda \geq 0$ and $\epsilon > 0$,

$$A_{\lambda,\epsilon,N}^{(s)} := \sqrt{p_{\lambda,\epsilon,N}} A_{\lambda,\epsilon,N} \frac{1}{\sqrt{p_{\lambda,\epsilon,N}}}, \quad A_{\lambda,\epsilon}^{(s)} := \sqrt{p_{\lambda,\epsilon}} A_{\lambda,\epsilon} \frac{1}{\sqrt{p_{\lambda,\epsilon}}}.$$

Then,

- (1) $A_{\lambda,\epsilon,N}^{(s)}$ and $A_{\lambda,\epsilon}^{(s)}$ are symmetric and their spectra coincide with those of $A_{\lambda,\epsilon,N}$ and $A_{\lambda,\epsilon}$, respectively,
- (2) the spectrum of $A_{\lambda,\epsilon}$ is contained in $[-1, 1]$ with $\sigma = 1$ a simple eigenvalue and all other eigenvalues lying strictly in $(-1, 1)$ and there are constants $C_1, C_2 > 0$ such that for all $\epsilon \in (0, C_1]$, the same holds for $A_{\lambda,\epsilon,N}$ with probability at least $1 - C_2 \epsilon^{-\frac{n}{2}} e^{-N \epsilon^{\frac{n}{2}} / C_2}$,
- (3) $A_{\lambda,\epsilon,N}^{(s)}$ and $A_{\lambda,\epsilon}^{(s)}$ fix $\sqrt{p_{\lambda,\epsilon,N}}$ and $\sqrt{p_{\lambda,\epsilon}}$, respectively and,

- (4) for any connected open subset $D \subset \mathbb{C}$ with $[-1, 1] \subset \bar{D}$ and $f : \bar{D} \rightarrow \mathbb{C}$ analytic on D with an absolutely convergent Taylor series on $[-1, 1]$,

$$f(A_{\lambda, \epsilon, N}) = \frac{1}{\sqrt{p_{\lambda, \epsilon, N}}} f(A_{\lambda, \epsilon, N}^{(s)}) \sqrt{p_{\lambda, \epsilon, N}}, \quad f(A_{\lambda, \epsilon}) = \frac{1}{\sqrt{p_{\lambda, \epsilon}}} f(A_{\lambda, \epsilon}^{(s)}) \sqrt{p_{\lambda, \epsilon}}$$

with $\epsilon \in (0, C_1]$ and probability at least $1 - C_2 \epsilon^{-\frac{n}{2}} e^{-N \epsilon^{\frac{n}{2}} / C_2}$ in the former case of application to $A_{\lambda, \epsilon, N}$.

Proof. — The properties (1) and (3) follow immediately from the definitions of $A_{\lambda, \epsilon, N}^{(s)}$ and $A_{\lambda, \epsilon}^{(s)}$. The spectral property (2) for $A_{\lambda, \epsilon}$ follows from the Krein–Rutman theorem along with the fact that it is a compact operator that maps $1 \mapsto 1$ and non-negative, non-zero C^∞ functions to positive C^∞ functions: indeed, then for example [Du06, Theorem 1.2, Chapter 1] applies.

In the case of $A_{\lambda, \epsilon, N}$, the Perron–Frobenius theorem applies to give (2) as soon as the matrix gives a connected graph. This follows from covering $\mathcal{M}$ by sufficiently small balls such that for any ball in the cover, k_ϵ is bounded below on all nearest neighbour balls. Then, any two points can be reached by a path of balls in this cover such that $k_\epsilon \gg 0$ on adjacent balls and with high probability, there is a sample point in every ball, which gives a connected graph. The details are as follows. Let $x_1^*, \dots, x_M^* \in \mathcal{M}$ be points such that⁽⁴⁾ $\bigcup_{j \in [M]} B_j = \mathcal{M}$ with $B_j := B_{\mathcal{M}}(x_j^*, \sqrt{r_k \epsilon} / 8)$. Now for each $j \in [M]$, let $Y_j : \mathcal{M} \rightarrow \{0, 1\}$ map $Y_j[B_j] = 1$ and $Y_j[\mathcal{M} \setminus B_j] = 0$. Each Y_j gives N i.i.d. random variables when applied to the sample points $x_1, \dots, x_N$ and since $\nu_g(B_{\mathcal{M}}(x_j, \sqrt{r_k \epsilon} / 8)) \approx (r_k \epsilon)^{\frac{n}{2}} / 8^n$, this is a Bernoulli process with mean $N \epsilon^{\frac{n}{2}} / C_{\mathcal{M}}$ for some constant $C_{\mathcal{M}} > 0$. Therefore, by a Chernoff bound, $\Pr[\#(\{x_1, \dots, x_N\} \cap B_j) \geq 1] > 1 - e^{-N \epsilon^{\frac{n}{2}} / (2C_{\mathcal{M}})}$ for each $j \in [M]$. Hence, by a union bound, there is at least one sample point in each B_j with probability at least $1 - M e^{-N \epsilon^{\frac{n}{2}} / (2C_{\mathcal{M}})}$. The Bishop–Günther inequality then tells that there is a constant $C'_{\mathcal{M}} > 0$ such that for $0 < \epsilon \leq C'_{\mathcal{M}}$, $M \lesssim \epsilon^{-\frac{n}{2}}$. Assuming this event it follows that for any $\ell, \ell' \in [N]$, there are $j, j' \in [M]$ such that $d_g(x_\ell, x_j^*), d_g(x_{\ell'}, x_{j'}^*) \leq \sqrt{r_k \epsilon} / 8$ and there are $1 \leq j_1 \leq \dots \leq j_m \leq M$ with $m \leq M - 2$ such that $d_g(x_{j_{\gamma_1}}^*, x_{j_{\gamma_2}}^*) \leq \sqrt{r_k \epsilon} / 4$ for all $1 \leq \gamma_1 \leq \gamma_2 \leq m$ and $d_g(x_j^*, x_{j_1}^*), d_g(x_{j'}^*, x_{j_m}^*) \leq \sqrt{r_k \epsilon} / 4$. Furthermore, for each $1 \leq \gamma \leq m$, there is ℓ_γ such that $d_g(x_{\ell_\gamma}, x_{j_\gamma}^*) \leq \sqrt{r_k \epsilon} / 8$. Therefore, for all $1 \leq \gamma_1 \leq \gamma_2 \leq m$, $d_g(x_{\ell_{\gamma_1}}, x_{\ell_{\gamma_2}}) \leq \sqrt{r_k \epsilon} / 2$ and $d_g(x_\ell, x_{\ell_1}), d_g(x_{\ell'}, x_{\ell_m}) \leq \sqrt{r_k \epsilon} / 2$. By the assumption on the kernel function k and the Assumptions on $\mathcal{M}$ and Λ , whenever $\epsilon < \kappa$ we have that $k(|\iota(x_{\ell_1}) - \iota(x_{\ell_2})|^2 / \epsilon) > \|k\|_\infty / 2$. Hence altogether we have a path $x_\ell \rightarrow x_{\ell_1} \rightarrow \dots \rightarrow x_{\ell_m} \rightarrow x_{\ell'}$ such that the entries of $A_{\lambda, \epsilon, N}$ corresponding to neighbouring points along this path are bounded below by $\|k\| / 2 > 0$, which gives that the underlying graph is connected.

Now together with the holomorphic functional calculus, properties (1)–(3) imply property (4). $\square$

A summary of the notation introduced here is provided in Appendix B.4.

⁽⁴⁾We use the notation, $[M] := \{1, \dots, M\}$.

2.2.1. Consistency bounds redux

The relationship among the discrete and continuum operators is that the discrete averaging operators are naturally accessed from samples of Λ and these are shown to converge, in the $N \rightarrow \infty$ limit to the continuum averaging operators; the residual coming from the difference of the two operators is deemed the *variance term*. Then, a sequence of Taylor expansions shows that the (λ -renormalized) continuum graph Laplacians, derived from the continuum averaging operators, converge to $\Delta_{\mathcal{M}} +$ (lower order differential terms) in the $\epsilon \rightarrow 0$ limit and the corresponding residuals are deemed the *bias terms*. A general treatment of the convergence of both terms, simultaneously, is given in [HAVL05]. We will draw upon these results throughout the forthcoming analyses, so we record the precise forms of the particular theorems here.

In regards to the bias term, our requirements are modest: for the most part, we will need a semiclassical expansion of the operator, which in this case is similar to the Taylor series type expansions given, for example in [HAVL05], but requires an essentially different approach. These expansions will be carried out in Section 4.1. Nevertheless, the *degree functions* $p_{\lambda,\epsilon}$ have an important role in making the approximation procedures agnostic to a priori knowledge of the intrinsic dimensionality n of the manifold and controlling the effect of lower-order error terms in the approximation to the Laplace–Beltrami operator, primarily in as far as the effect of the non-uniform sampling density p is concerned. This is carried out essentially through their Taylor expansions about a given point $x \in \mathcal{M}$; the following is recorded here for use in later sections:

LEMMA 2.13. — *Let $\lambda \geq 0$ and $\epsilon > 0$. Then, there exists $q_\lambda \in C^\infty(\mathcal{M})$ depending only on k, p, λ and $\mathcal{M}$ such that for all $x \in \mathcal{M}$,*

$$p_{\lambda,\epsilon}(x) = (c_0 p(x))^{1-2\lambda} + \epsilon \frac{c_2}{2} p(x)^{1-2\lambda} q_\lambda(x) + O(\epsilon^2).$$

Proof. — The proof of this expansion is contained in the proof of [Hei05, Proposition 2.33]. $\square$

As for the variance term, we now recount some of the prior results, with small modifications that we will use for the convergence of quantum dynamics from graphs to manifolds. In particular, prior works have left out the explicit dependence on $\|u\|_\infty$ in the probabilistic convergence bounds for consistency. Since we ultimately wish to drive localized, L^2 bounded states according to Schrödinger-type dynamics, their L^∞ norms depend on ϵ , hence it is useful for the convergence theory to make this dependence explicit. Therefore, we proceed with the essential convergence results from the thesis [Hei05], while making the small adjustments necessary to *unpack* the uniform norm dependence from the constants. The primary cases that concern us are for the averaging operators.

Since constants bounding the kernel, probability and geometric quantities appear abundantly in these considerations, we record the useful

Notation 2.14 (*Bounds on degree functions*). — See [Hei05, Lemma 2.32] for more detailed bounds:

- $\underline{C}_p := \inf p_\epsilon \gtrsim \|k\|_\infty (\inf p) \inf_x \text{vol}(B(x, \epsilon^{1/2} R_k))$

- $\bar{C}_p := \sup p_\epsilon \lesssim_{\mathcal{M}} R_k^n \|k\|_\infty \|p\|_\infty$
- $\underline{C}_{p,\lambda} := \inf p_{\lambda,\epsilon} \geq \underline{C}_p / \bar{C}_p^{2\lambda}$, $\bar{C}_{p,\lambda} := \|p_{\lambda,\epsilon}\|_\infty \leq \bar{C}_p / \underline{C}_p^{2\lambda}$
- $\underline{C}_{k,p} := \|k\|_\infty / (\inf p)$.

Let the subscripted variables $X_1, \dots, X_j, \dots, X_N$ denote i.i.d. random vectors in $\mathbb{R}^D$ with law P that has positive $C^\infty(\Lambda)$ density $\tilde{p}$ with respect to the volume element dV on $\Lambda = \iota(\mathcal{M}) \subset \mathbb{R}^D$; we denote by $x_j := \iota^{-1}(X_j)$ the pull-back of X_j and by p the pull-back of $\tilde{p}$ to $\mathcal{M}$, which gives a density with respect to $d\nu_g$. For simplicity, we assume k has compact support on $[0, R_k^2]$ (but this can be generalized to *essential support* so that $t^N k(t) < C_N$ for all $t > R_k^2$, $N \geq 0$). Then, Hein has shown,

LEMMA 2.15 ([Hei05, Lemma 2.30]). — *There exists a constant $K_{\mathcal{M},k,p}$ depending on the curvature and injectivity radius of $\mathcal{M}$, $\|p\|_\infty$, $\|k\|_\infty$ and R_k such that for all $u \in L^\infty(\mathcal{M})$ and $x \in \mathcal{M}$, given any $\delta > 0$,*

$$\Pr \left[\left| \frac{1}{N} \sum_{j=1}^N k_\epsilon(x, x_j) u(x_j) - \int_{\mathcal{M}} k_\epsilon(x, y) u(y) p(y) d\nu_g(y) \right| > \delta \right] \leq 4 \exp \left(- \frac{N \epsilon^{\frac{n}{2}} \delta^2}{2 \|u\|_\infty (K_{\mathcal{M},k,p} \|u\|_\infty + \|k\|_\infty \delta / 3)} \right).$$

Proof. — The proof is exactly as in [Hei05, Lemma 2.30], with the only change that we allow u to be complex-valued, which gives another factor of 2 for the probability, due to either applying the real-valued version in two parts, or the two-dimensional Matrix Bernstein inequality via the matrix representation of complex numbers. $\square$

On extending this to the consistency of normalized averaging operators, one must account for the factors of $p_{\epsilon,N}, p_\epsilon$ appearing in $A_{\epsilon,N}[u], A_\epsilon[u]$ respectively. As random variables, the $k_\epsilon(x, x_j)/p_{\epsilon,N}(x)$ are now coupled, so the application of Bernstein's inequality requires a decoupling step. This comes in the form of the assumption that $p_{\epsilon,N}(x_j) - p_\epsilon(x_j)$ is small for every $j \in [N]$, which upon taking a union bound introduces a factor of N in the probability. Since this gives the same bound for all $\lambda \geq 0$, Hein has shown altogether a Bernstein-type bound for the probabilistic consistency between $A_{\lambda,\epsilon,N}[u](x)$ and $A_{\lambda,\epsilon}[u](x)$ for all $\lambda \geq 0$, $u \in L^\infty$ and $x \in \mathcal{M}$. However, the bounds have implicitly rolled up the dependence on $\|u\|_\infty$ into constants, while in Section 6 we will use this dependence explicitly so that we have a clear view of the convergence rates when applied to localized states. Therefore, we reproduce the proof of consistency while pulling out the relevant pieces of the constants and record it as,

LEMMA 2.16 ([Hei05, Proposition 2.38]). — *Given $\lambda \geq 0$, there is a constant $K_\lambda > 1$ depending only on $\|k\|_\infty$, $\underline{C}_p$, $\bar{C}_p$ and λ such that given $u \in L^\infty$ and $x \in \mathcal{M}$, we have for all $\epsilon > 0$, and $2\|k\|_\infty \epsilon^{-\frac{n}{2}}/N < \delta \leq \underline{C}_p/2$,*

$$\Pr \left[|A_{\lambda,\epsilon,N}[u](x) - A_{\lambda,\epsilon}[u](x)| > \delta \right] \leq (4 + 2N) \exp \left(- \frac{N \epsilon^{\frac{n}{2}} \delta^2}{2 K_\lambda \underline{C}_p^{-\lambda} \|u\|_\infty (K_{\mathcal{M},k,p} K_\lambda \|u\|_\infty \underline{C}_p^{-\lambda} + \|k\|_\infty \delta / 3)} \right).$$

Remark 2.17. — The choice of $\delta < \underline{C}_p/2$ was made for simplicity; a different choice of $\delta < \underline{C}_p$ changes only K_λ (in the proof, $K_{\lambda,k,p}$) as a rational function of δ . For states that are localized in tandem with the operators — as will be our case — only the first bound is useful, since $\|u\|_\infty$ will grow as ϵ decreases and the condition would then have δ growing as well.

Proof of Lemma 2.16. — We follow the proof of [Hei05, Proposition 2.38], paying close attention to the dependency of the constants on $\|u\|_\infty$. As shown there, using that for all $\lambda \geq 0$ and $a, b \geq \beta \geq 0$, $|1/a^\lambda - 1/b^\lambda| \leq \lambda|a - b|/\beta^{\lambda+1}$ gives,

$$\begin{aligned} & \left| \mathcal{A}_{\epsilon,N} \left[u/p_\epsilon^\lambda \right] (x) - \mathcal{A}_\epsilon \left[u/p_\epsilon^\lambda \right] (x) \right| \\ & \leq \left| \mathcal{A}_{\epsilon,N} \left[u \left(1/p_{\epsilon,N}^\lambda - 1/p_\epsilon^\lambda \right) \right] \right| + \left| \mathcal{A}_{\epsilon,N} \left[u/p_\epsilon^\lambda \right] - \mathcal{A}_\epsilon \left[u/p_\epsilon^\lambda \right] \right| \\ & \leq \|u\|_\infty \lambda \mathcal{A}_{\epsilon,N} \left[\frac{|p_\epsilon - p_{\epsilon,N}|}{(\min\{\inf p_{\epsilon,N}, \inf p_\epsilon\})^{\lambda+1}} \right] + \left| (\mathcal{A}_\epsilon - \mathcal{A}_{\epsilon,N}) \left[u/p_\epsilon^\lambda \right] \right| \\ & =: \mathcal{E}_{\lambda,1}[u]. \end{aligned}$$

and using that for all a, b , $|a - b|^\lambda \leq \lambda \max\{|a|, |b|\}^{\lambda-1} |a - b|$, we have,

$$\begin{aligned} & \left| \frac{\mathcal{A}_{\epsilon,N} \left[u/p_{\epsilon,N}^\lambda \right]}{p_{\epsilon,N}^\lambda} - \frac{\mathcal{A}_\epsilon \left[u/p_\epsilon^\lambda \right]}{p_\epsilon^\lambda} \right| \\ & \leq \frac{\left| \mathcal{A}_{\epsilon,N} \left[u/p_{\epsilon,N}^\lambda \right] - \mathcal{A}_\epsilon \left[u/p_\epsilon^\lambda \right] \right|}{p_{\epsilon,N}^\lambda} + \left| \mathcal{A}_\epsilon \left[u/p_\epsilon^\lambda \right] \right| \frac{|p_{\epsilon,N}^\lambda - p_\epsilon^\lambda|}{p_\epsilon^\lambda p_{\epsilon,N}^\lambda} \\ & \leq \mathcal{E}_{\lambda,1}[u]/p_{\epsilon,N}^\lambda + \|u\|_\infty \lambda \max\{\sup p_{\epsilon,N}, \sup p_\epsilon\}^{\lambda-1} \frac{\bar{C}_p |p_{\epsilon,N} - p_\epsilon|}{\underline{C}_p^\lambda (p_\epsilon p_{\epsilon,N})^\lambda} \\ & =: \mathcal{E}_{\lambda,2}[u]. \end{aligned}$$

Taking the normalizations by the λ -degree functions into account, we have

$$\begin{aligned} |A_{\lambda,\epsilon,N}[u] - A_{\lambda,\epsilon}[u]| &= \left| \frac{\mathcal{B}_N}{p_{\lambda,\epsilon,N}} - \frac{\mathcal{B}}{p_{\lambda,\epsilon}} \right| \\ &\leq \frac{|\mathcal{B}_N - \mathcal{B}|}{p_{\lambda,\epsilon,N}} + |\mathcal{B}| \frac{|p_{\lambda,\epsilon,N} - p_{\lambda,\epsilon}|}{p_{\lambda,\epsilon,N} p_{\lambda,\epsilon}} \\ &\leq \frac{\mathcal{E}_{\lambda,2}[u]}{p_{\lambda,\epsilon,N}} + |\mathcal{B}| \frac{\mathcal{E}_{\lambda,2}[1]}{p_{\lambda,\epsilon,N} p_{\lambda,\epsilon}}, \end{aligned}$$

with

$$\mathcal{B}_N := \frac{\mathcal{A}_{\epsilon,N} \left[u/p_{\epsilon,N}^\lambda \right]}{p_{\epsilon,N}^\lambda}, \quad \mathcal{B} := \frac{\mathcal{A}_\epsilon \left[u/p_\epsilon^\lambda \right]}{p_\epsilon^\lambda}.$$

In the event that $|p_{\epsilon,N}(y) - p_\epsilon(y)| \leq \delta$, for the deterministic choice $y = x$ along with all random variables $y = x_j$ for all $j \in [N]$, we have that $\underline{C}_p - \delta < p_{\epsilon,N}(y) < \bar{C}_p + \delta$. Call this event $\mathcal{A}_1$ and call $\mathcal{A}_2$ the event that $|\mathcal{A}_{\epsilon,N} \left[u/p_\epsilon^\lambda \right] - \mathcal{A}_\epsilon \left[u/p_\epsilon^\lambda \right]| \leq \delta \|u\|_\infty$. Then,

$$\mathcal{E}_{\lambda,1}[u] \leq \delta \|u\|_\infty \left\{ \lambda(\bar{C}_p + \delta)/(\underline{C}_p - \delta)^{\lambda+1} + 1 \right\},$$

$$\begin{aligned}
(\underline{C}_p - \delta)/(\overline{C}_p + \delta)^{2\lambda} &\leq p_{\lambda,\epsilon,N} = \mathcal{A}_{\epsilon,N}[1/p_{\epsilon,N}^\lambda]/p_{\epsilon,N}^\lambda \\
&\leq (\overline{C}_p + \delta)/(\underline{C}_p - \delta)^{2\lambda}, \\
|\mathcal{A}_\epsilon[u/p_\epsilon^\lambda]| &\leq \|u\|_\infty \overline{C}_p / \underline{C}_p^\lambda, \\
\underline{C}_p / \overline{C}_p^{2\lambda} &\leq p_{\lambda,\epsilon} \leq \overline{C}_p / \underline{C}_p^{2\lambda},
\end{aligned}$$

wherein we've used the occurrence of the joint event $\mathcal{A} := \mathcal{A}_1 \wedge \mathcal{A}_2$ for the first inequality and that of $\mathcal{A}_1$ for the second inequality. The event $\mathcal{A}_1$ further supplies,

$$\mathcal{E}_{\lambda,2}[u] \leq \frac{\mathcal{E}_{\lambda,1}[u]}{(\underline{C}_p - \delta)^\lambda} + \delta \lambda \|u\|_\infty \frac{(\overline{C}_p + \delta)^{\lambda-1} \overline{C}_p}{\underline{C}_p^{2\lambda} (\underline{C}_p - \delta)^\lambda}.$$

Now, working in event $\mathcal{A}$ together with the assumption that $\delta \leq \underline{C}_p/2$ we find,

$$\begin{aligned}
|A_{\lambda,\epsilon,N}[u](x) - A_{\lambda,\epsilon}[u](x)| &\leq \mathcal{E}_{\lambda,2}[u] \frac{(\overline{C}_p + \delta)^{2\lambda}}{\underline{C}_p - \delta} + \|u\|_\infty \mathcal{E}_{\lambda,2}[1] \frac{\overline{C}_p^{2\lambda+1}}{\underline{C}_p^{2\lambda+1}} \frac{(\overline{C}_p + \delta)^{2\lambda}}{\underline{C}_p - \delta} \\
&\leq \delta \|u\|_\infty \left[(\overline{C}_p + \delta)^{2\lambda} (\underline{C}_p - \delta)^{-\lambda-1} + \tilde{C}_{\lambda,k,p}(\delta) + \lambda C_{k,p}(\lambda, \delta) \right] \\
&\leq 2(9/2)^\lambda \delta \|u\|_\infty \left(\overline{C}_p^{2\lambda} \underline{C}_p^{-\lambda-1} + 2^{-\lambda} \overline{C}_p^{4\lambda+1} \underline{C}_p^{-2(\lambda+1)} + \lambda C_{\lambda,k,p} \right), \\
&:= K_{\lambda,k,p} \|u\|_\infty \delta,
\end{aligned}$$

wherein $\tilde{C}_{\lambda,k,p}(\delta) := \overline{C}_p^{2\lambda+1} (\overline{C}_p + \delta)^{2\lambda} \underline{C}_p^{-2\lambda-1} (\underline{C}_p - \delta)^{-1}$, $C_{k,p}(\lambda, \delta) > 0$ is monotonically increasing in δ , $\lambda \geq 0$ that is rational and bounded in $\delta < \underline{C}_p$ and has coefficients that depend only on $\underline{C}_p, \overline{C}_p$. The final inequality follows upon assuming that $\delta \leq \underline{C}_p/2$ and setting $C_{\lambda,k,p} := C_{k,p}(\lambda, \underline{C}_p/2)$.

Concerning the probabilities governing the event $\mathcal{A}$, since $p_\epsilon = \mathcal{A}_\epsilon[1]$ and $p_{\epsilon,N} = \mathcal{A}_{\epsilon,N}[1]$, an application of Lemma 2.15 along with a union bound gives that whenever $\delta > 2\|k\|_\infty \epsilon^{-\frac{n}{2}}/N$, we have that

$$\Pr[(\forall) j \in [N], |p_{\epsilon,N}(x_j) - p_\epsilon(x_j)| \leq \delta] > 1 - 2N \exp\left(-\frac{(N-1)\epsilon^{\frac{n}{2}}\delta^2}{4(2K_{\mathcal{M},k,p} + \|k\|_\infty \delta/3)}\right).$$

Another application of Lemma 2.15 gives,

$$\begin{aligned}
\Pr\left[|\mathcal{A}_{\epsilon,N}[u/p_\epsilon^\lambda](x) - \mathcal{A}_\epsilon[u/p_\epsilon^\lambda](x)| \leq \|u\|_\infty \delta\right] \\
> 1 - 4 \exp\left(-\frac{N\epsilon^{\frac{n}{2}}\delta^2}{2\underline{C}_p^{-\lambda}(K_{\mathcal{M},k,p}\underline{C}_p^{-\lambda} + \|k\|_\infty \delta/3)}\right).
\end{aligned}$$

Therefore, a union bound gives the bound in the statement of Lemma 2.16. $\square$

On the other hand, Hein has given a simpler argument for the $\lambda = 0$ case that is related to the *random walk* graph Laplacian:

LEMMA 2.18 ([Hei05, Theorem 2.37]). — *For all $u \in C^\infty$ and $x \in \mathcal{M}$, given any $\delta > 0$,*

$$\Pr[|A_{\epsilon,N}[u](x) - A_\epsilon[u](x)| > \delta] \leq 6 \exp\left(-\frac{N\epsilon^{\frac{n}{2}}\delta^2}{8\|u\|_\infty(K_{\mathcal{M},k,p}\|u\|_\infty + \|k\|_\infty \delta/6)}\right).$$

Proof. — The proof in [Hei05, Theorem 2.37] and [HAVL05, Theorem 2] is based on a rewriting of $A_{\epsilon,N}[u]$ following [GKP84] as,

$$\begin{aligned} A_{\epsilon,N}[u](x) &= \frac{A_\epsilon[u](x) - \mathcal{B}_{1,N}}{1 + \mathcal{B}_{2,N}}, \\ \mathcal{B}_{1,N} &:= \frac{1}{p_\epsilon(x)} \mathcal{A}_{\epsilon,N}[u](x) - A_\epsilon[u](x), \\ \mathcal{B}_{2,N} &:= \frac{p_{\epsilon,N}(x)}{p_\epsilon(x)} - 1. \end{aligned}$$

On applying Lemma 2.15 twice while noting $p_\epsilon(x) = \mathcal{A}_\epsilon[1](x)$ and $p_{\epsilon,N}(x) = \mathcal{A}_{\epsilon,N}[1](x)$, we have that

$$\begin{aligned} \Pr[\mathcal{B}_{1,N} > \delta/2] &\leq 4 \exp\left(-\frac{N\epsilon^{\frac{n}{2}}\delta^2}{8\|u\|_\infty(K_{\mathcal{M},k,p}\|u\|_\infty + \|k\|_\infty\delta/6)}\right), \\ \Pr\left[\mathcal{B}_{2,N} > \frac{\delta}{2\|u\|_\infty}\right] &\leq 2 \exp\left(-\frac{N\epsilon^{\frac{n}{2}}\delta^2}{8\|u\|_\infty(K_{\mathcal{M},k,p}\|u\|_\infty + \|k\|_\infty\delta/6)}\right). \end{aligned}$$

We also see,

$$|A_{\epsilon,N}[u](x) - A_\epsilon[u](x)| \leq \left(\left|\frac{\mathcal{B}_{1,N}}{1 + \mathcal{B}_{2,N}}\right| + \|u\|_\infty \left|\frac{\mathcal{B}_{2,N}}{1 + \mathcal{B}_{2,N}}\right|\right).$$

Thus taking a union bound gives,

$$\begin{aligned} \Pr[|A_{\epsilon,N}[u](x) - A_\epsilon[u](x)| > \delta] \\ \leq 6 \exp\left(-\frac{N\epsilon^{\frac{n}{2}}\delta^2}{8\|u\|_\infty(K_{\mathcal{M},k,p}\|u\|_\infty + \|k\|_\infty\delta/6)}\right). \quad \square \end{aligned}$$

Remark 2.19. — In our application, when $u = \psi_h$ is a state localized to an $O(\sqrt{h})$ -ball with unit L^2 norm, we will have that $\|\psi_h\|_\infty \geq h^{-\frac{n}{2}}$, so this will give a convergence rate of $e^{-\Omega(N\epsilon^{\frac{n}{2}}h^n\delta^2)}$ for $A_{\epsilon,N}\psi_h(x) \rightarrow A_\epsilon\psi_h(x)$ as $N \rightarrow \infty$ and $\epsilon, h \rightarrow 0$.

2.3. Quantization and Symbol classes

The study of pseudodifferential calculus is rooted in the relationships between certain classes of smooth functions on phase space and linear operators acting on smooth functions on configuration space, called *pseudodifferential operators* (Ψ DOs) and in relation to the phase space functions, often called their *quantizations*. The classes of functions under study are called *symbols* and they are typically bounded on configuration space with well-behaved (e.g., polynomially bounded) momentum space asymptotics. Then, of interest are the relationships between Ψ DOs and the symbols they quantize. An additional *small parameter* $h \in (0, 1]$ enters the picture when we work in the *semiclassical* regime and serves essentially to rescale the unit length in momentum space, so the asymptotics we are concerned with happen simultaneously at scales of vanishing h and increasing momentum variable.

The formal classes of functions that we quantize, as well as the exact quantization procedures, are standard and described, for example, in [Zwo12, Section 14.2]. These procedures amount to locally pushing the symbols onto Euclidean space by charts and seeing these local pieces as quantizations on open balls in $\mathbb{R}^n$, then gluing them together through an atlas. Hence, the key definitions are specified on $\mathbb{R}^n$. To summarize the idea briefly, we make

DEFINITION 2.20 (Symbols & quantization on $\mathbb{R}^n$ [Zwo12, Section 4]). — *Let $h_0 \in (0, 1]$. A smooth function $a \in C^\infty(\mathbb{R}^{2n} \times (0, h_0])$ belongs to the h -symbol class of order $(\ell, m; \rho) \in \mathbb{N}_0 \times \mathbb{Z} \times [0, 1/2)$ on $\mathbb{R}^n$, $h^{\ell(1-2\rho)} S_\rho^m(\mathbb{R}^{2n})$ if for all $\alpha, \beta \in \mathbb{N}_0^n$, $|\partial_x^\alpha \partial_\xi^\beta a(x, \xi; h)| \lesssim_{\alpha, \beta} h^{\ell(1-2\rho) - \rho(|\alpha| + |\beta|)} \langle \xi \rangle^{m - |\beta|}$. Then, a quantization of $a \in h^{\ell(1-2\rho)} S_\rho^m$ is an operator acting on $u \in \mathcal{S}(\mathbb{R}^n)$ given by,*

$$\text{Op}_h^t(a) := \frac{1}{(2\pi h)^n} \int_{\mathbb{R}^{2n}} e^{\frac{i}{h} \langle x-y, \xi \rangle} a(tx + (1-t)y, \xi; h) u(y) d\xi dy,$$

for any $t \in [0, 1]$. We will denote $h_\rho := h^{1-2\rho}$. In the case that $\rho = 0$, we simplify the notation of the symbol class to $h^\ell S^m$ and its order to (ℓ, m) . We call the quantization with $t = 0$ the adjoint quantization, which we will primarily use and hence we denote it simply as $\text{Op}_h := \text{Op}_h^0$, while the case $t = 1$ is called the Kohn–Nirenberg (or standard) quantization and we will denote it $\text{Op}_h^{KN} := \text{Op}_h^1$. A highly used case is $t = 1/2$ and called the Weyl quantization; while it is very useful in proving various properties of pseudodifferential operators, we will not make explicit use of this.

An operator of the form $\text{Op}_h^t(a)$ is called a (semiclassical) pseudodifferential operator of order $(\ell, m; \rho)$ and sometimes (to evoke a physical interpretation) a quantum observable, while its symbol a is sometimes called a classical observable. We also say that $a \in h^\ell S_\rho^m$ is a symbol of order $(\ell, m; \rho)$ and both, for symbols and their quantizations, we simplify the order notation to $(\ell, m) := (\ell, m; 0)$.

We quantize symbols whose higher order derivatives are allowed to become increasingly singular as $h \rightarrow 0$, controlled by the index $\rho \in [0, 1/2)$. These enter naturally as for example, a smoothly parameterized family of symplectic transformations $\Phi^t : T^*\mathbb{R}^n \rightarrow T^*\mathbb{R}^n$ may locally *stretch* space increasingly in $t \rightarrow \infty$ so that given $a \in C^\infty$, taking t to be strictly increasing with $1/h$, the derivatives of $a \circ \Phi^t$ become increasingly singular with $h \rightarrow 0$. The endpoint $\rho = 1/2$ is *critical* in the sense that the first and higher order terms of stationary phase asymptotics decay with $h \rightarrow 0$ only for $\rho \in [0, 1/2)$ (see [Zwo12, Theorem 3.16]). Such expansions are the life force of semiclassical calculus and while certain aspects remain intact at $\rho = 1/2$ without the decay in small h , our study will focus on increasing the resolution of dominating terms with decaying h .

A key property in the definition of the symbol class is that under a *symplectic* change of variables $\tilde{\gamma} := (\gamma, [D\gamma^{-1}|_\gamma]^T)$ on $\mathbb{R}^{2n}$ for any diffeomorphism $\gamma : \mathbb{R}^n \rightarrow \mathbb{R}^n$, the symbol class $h^{\ell(1-2\rho)} S_\rho^m$ is invariant *to top order*, meaning that if $a \in h_\rho^\ell S_\rho^m$

then $a \circ \tilde{\gamma} \in h_\rho^\ell S_\rho^m$ and $u \mapsto \text{Op}_h^t(a)[u \circ \gamma] \circ \gamma^{-1} = \text{Op}_h^t(a_\gamma)[u]$ with $a_\gamma(\gamma(x), \xi) = a(x, [D\gamma|_x]^T \xi) + b(x, \xi)$ for $b \in h_\rho^{\ell+1} S_\rho^{m-1}$ (see⁽⁵⁾ [Zwo12, Section 9]). While the asymptotic behaviour required in ξ is simple to understand, we offer the notion about the joint asymptotics with h that a symbol should have, asymptotically, at most polynomial variation in cubes of side-length h in phase space.

The basic calculus of pseudodifferential operators and symbols on $\mathbb{R}^n$ is exposed in detail in [Zwo12] and [DS99]. Now using this, we can give meaning to quantization on a compact manifold $\mathcal{M}$, following [Zwo12]:

DEFINITION 2.21 (Symbols & quantization on $\mathcal{M}$ [Zwo12, Section 14.2.2]). — *A linear operator $A : C^\infty(\mathcal{M}) \rightarrow C^\infty(\mathcal{M})$ is a pseudodifferential operator on $\mathcal{M}$ if*

- (1) *given an atlas $\{(\gamma : \mathcal{M} \supset U_\gamma \rightarrow V_\gamma \subset \mathbb{R}^n, U_\gamma) \mid \gamma \in \mathcal{F}\}$, there is $(\ell, m; \rho) \in \mathbb{N}_0 \times \mathbb{Z} \times [0, 1/2)$ and $t \in \mathbb{R}$ such that for each $\gamma \in \mathcal{F}$, there is $a_\gamma \in h_\rho^\ell S_\rho^m$ so that we may write, given any $\chi_1, \chi_2 \in C_c^\infty(U_\gamma)$ and $u \in C^\infty(\mathcal{M})$,*

$$\chi_1 A[\chi_2 u] = \chi_1 \gamma^* \text{Op}_h^t[a_\gamma] \circ (\gamma^{-1})^* [\chi_2 u],$$

wherein $(\gamma^{-1})^* : C^\infty(U_\gamma) \rightarrow C^\infty(V_\gamma)$ denotes the pullback, $(\gamma^{-1})^* : u \mapsto u \circ \gamma^{-1}$ and similarly γ^* the pullback from V_γ to U_γ and

- (2) *A is pseudolocal, meaning: given any $\chi_1, \chi_2 \in C^\infty(\mathcal{M})$ with $\text{supp } \chi_1 \cap \chi_2 = \emptyset$ and any $N \in \mathbb{N}$, we have $\|\chi_1 A \chi_2\|_{H^{-N}(\mathcal{M}) \rightarrow H^N(\mathcal{M})} = O(h^\infty)$, wherein $H^{\pm N}(\mathcal{M})$ Sobolev spaces as defined in [Zwo12, Section 14.2.1].*

We say then that the pseudodifferential operator A is of order $(\ell, m; \rho)$ and belongs to $h_\rho^\ell \Psi_\rho^m$ and for brevity, we call it a Ψ DO. In the case that $\rho = 0$, we denote the order and class of such an operator simply by (ℓ, m) and $h^\ell \Psi^m$, respectively.

A function $a \in C^\infty(T^*\mathcal{M})$ belongs to the h -symbol class of order $(\ell, m; \rho) \in \mathbb{N}_0 \times \mathbb{Z} \times [0, 1/2)$ on $\mathcal{M}$, $h_\rho^\ell S_\rho^m(T^*\mathcal{M})$ if given an atlas $\mathcal{F}$, for each $\gamma \in \mathcal{F}$ and $\chi \in C_c^\infty(U_\gamma)$ the pullback $a_\gamma \in C^\infty(V_\gamma \times \mathbb{R}^n)$ of $a\chi$ under the induced change of coordinates $V_\gamma \times \mathbb{R}^n \rightarrow T^*(U_\gamma)$ belongs to $h_\rho^\ell S_\rho^m(\mathbb{R}^{2n})$. In short, we say that a is a symbol of order $(\ell, m; \rho)$ and if $\rho = 0$, then we denote its order by (ℓ, m) and its symbol class by $h^\ell S^m$.

The facts that $h_\rho^\ell \Psi_\rho^m$ forms a bi-filtered algebra in the order (ℓ, m) , which respects the properties of a *quantization map*, and that quantized operators extend to Sobolev spaces, mapping $A : H_h^s \rightarrow H_h^{s-m}$ continuously whenever $A \in h^0 \Psi_\rho^m$ and $A : L^2 \rightarrow L^2$ whenever $A \in h^0 \Psi_\rho^0$, are standard results from pseudodifferential calculus [DS99, Zwo12]. We will make liberal use of these properties along with the following basic *symbol calculus*:

FACT 2.22 ([Zwo12, Theorem 14.1]). — *There are linear maps*

$$\text{Sym} : h_\rho^\ell \Psi_\rho^m \longrightarrow h_\rho^\ell S_\rho^m(T^*\mathcal{M})/h_\rho^{\ell+1} S_\rho^{m-1}(T^*\mathcal{M})$$

and for all $t \in [0, 1]$,

$$\text{Op}_h^t : h_\rho^\ell S_\rho^m \longrightarrow h_\rho^\ell \Psi_\rho^m$$

⁽⁵⁾The version suitable for the symbol class $h^\ell S_\rho^m$ follows from accounting for powers of $h^{-\rho}$ in the stationary phase expansion as in [Zwo12, Theorem 3.16] applied to the symbol under change of coordinates in the proof of [Zwo12, Theorem 9.9].

such that

$$\mathrm{Sym}(A_1 A_2) = \mathrm{Sym}(A_1) \mathrm{Sym}(A_2)$$

and

$$\mathrm{Sym}[\mathrm{Op}_h^t(a)] = [a] \in h^\ell S_\rho^m(T^*\mathcal{M})/h^{\ell+1} S_\rho^{m-1}(T^*\mathcal{M}),$$

wherein $[a]$ denotes the equivalence class of a in the quotient space $h^\ell S_\rho^m/h^{\ell+1} S_\rho^{m-1}$.

We often call $\mathrm{Sym}(A)$ the *principal symbol* of A and note that by the invariance properties of $h^\ell S_\rho^m$ under changes of coordinates as discussed above, this equivalence class is defined invariantly of the choice of coordinates. In fact, this is independent of the particular quantization $t \in [0, 1]$ as well (see [Zwo12, Theorem 9.10]).

A useful sub-class of $h^\ell S^m$ is the class of semiclassical *polyhomogeneous* symbols. The quantizations of these symbols are more direct generalizations of partial differential operators, whose symbols can be seen to behave like polynomials in the momentum ξ variable. The polyhomogeneous symbols enjoy many nice properties through their asymptotic expansions, including that we can specify an exact principal symbol. We restrict to this class primarily when dealing with the phases and amplitudes appearing in the FBI transform, following [WZ01] (discussed below, in Section 3). In particular, we will use such symbols in the phases defining coherent states, for then we have a good interaction between them and the FBI transform. Assuming the definitions of *classical* polyhomogeneous symbols, as given in [Hör07], the definitions of their semiclassical counterparts are as follows:

DEFINITION 2.23 (following [WZ01]). — *A smooth function $a \in C^\infty(T^*\mathcal{M} \times \mathcal{M} \times [0, h_0))$ for some $h_0 > 0$ belongs to the h -polyhomogeneous symbol class of order (ℓ, m) , $h^\ell S_{\mathrm{phg}}^m(T^*\mathcal{M} \times \mathcal{M}) \subset C^\infty(T^*\mathcal{M} \times \mathcal{M} \times [0, h_0))$, if for every $j \geq 0$, there exists a polyhomogeneous symbol $a_j(x, \xi, y)$ of degree j in ξ and a constant $C_j > 0$ such that for all $|\xi| > 1$ and $h \in [0, h_0)$, the following asymptotic expansion holds:*

$$\left| a(x, \xi, y; h) - h^\ell (a_m + h a_{m-1} + \cdots + h^\ell a_{m-j}) \right| \leq C_j h^{\ell+j+1} |\xi|^{m-j-1}.$$

We abbreviate this as,

$$a(x, \xi, y; h) \sim h^\ell (a_m(x, \xi, y) + h a_{m-1}(x, \xi, y) + \cdots)$$

and call a_m the principal part of a . Similarly, we define the h -symbol class

$$h^\ell S_{\mathrm{phg}}^m(T^*\mathcal{M}) \subset h^\ell S_{\mathrm{phg}}^m(T^*\mathcal{M} \times \mathcal{M})$$

as the subset of the above class without dependence on the y variable. When ambiguity is not an issue, we drop the explicit dependence on the space and use simply the notation $h^\ell S_{\mathrm{phg}}^m$ to denote either of the two classes of symbols.

The quantization of $a \in h^\ell S_{\mathrm{phg}}^m(T^*\mathcal{M} \times \mathcal{M})$ is the operator $\mathrm{Op}_h(a) : C^\infty(\mathcal{M}) \rightarrow C^\infty(\mathcal{M})$ given by

$$(2.2) \quad \mathrm{Op}_h(a)[u](x) := \frac{1}{(2\pi h)^n} \int_{T^*\mathcal{M}} e^{\frac{i}{h} \langle \exp_y^{-1}(x), \xi \rangle_{g_y}} a(y, \xi, x; h) \chi(x, y) u(y) dy d\xi,$$

wherein χ is a smooth cut-off near $x = y$. We denote by $h^\ell \Psi_{\mathrm{phg}}^m(\mathcal{M})$ the algebra of all operators quantizing symbols modulo h^∞ , viz., $A \in h^\ell \Psi_{\mathrm{phg}}^m(\mathcal{M})$ iff. $A = \mathrm{Op}_h(a) + R$ for some $a \in h^\ell S_{\mathrm{phg}}^m(T^*\mathcal{M} \times \mathcal{M})$ and $R : C^{-\infty}(\mathcal{M}) \rightarrow C^\infty(\mathcal{M})$ of order $O(h^\infty)$. When

the polyhomogeneous and space contexts are clear, we will shorten the notation to just $h^\ell \Psi_{\text{phg}}^m$.

The symbol map of order (ℓ, m) is the linear operator

$$\text{Sym}_{\ell, m} : h^\ell \Psi_{\text{phg}}^m \longrightarrow h^\ell S_{\text{phg}}^m / h^{\ell-1} S_{\text{phg}}^{m-1}$$

such that the principal symbol of an operator $A = \text{Op}_h(a) \in h^\ell \Psi_{\text{phg}}^m$ is given by $\text{Sym}_{\ell, m}(A) = [a]$. This gives a short exact sequence,

$$0 \longrightarrow h^{\ell-1} \Psi_{\text{phg}}^{m-1} \hookrightarrow h^\ell \Psi_{\text{phg}}^m \xrightarrow{\text{Sym}_{\ell, m}} h^\ell S_{\text{phg}}^m / h^{\ell-1} S_{\text{phg}}^{m-1} \longrightarrow 0.$$

An elliptic symbol is a symbol $a \in h^\ell S_{\text{phg}}^m$ whose principal part follows $|a_k| \sim \langle \xi \rangle$ uniformly in all other variables.

Symbols that are functions of both, the integrand as well as the output parameter with respect to quantization, such as $a \in h^\ell S_{\text{phg}}^m(T^*\mathcal{M} \times \mathcal{M})$ are sometimes called *amplitudes* (see e.g., [Tay81]). The phases appearing in coherent states (as in Section 3) are naturally of this sort. However, the notation for the quantization of amplitudes in (2.2) is a slight abuse of the short-hand for the adjoint quantization in Definition 2.20. Nevertheless, this is consistent in the sense that quantizations of amplitudes that are constant in the output parameter reduce to standard quantizations of the corresponding symbols on the cotangent bundle.

We aim to bring graph Laplacians into the context of pseudodifferential operators and by their basic characteristics, we find that they must belong to a more general class than the polyhomogeneous. Indeed, the polyhomogeneous class is too restrictive to support symbols localized in phase-space $T^*\mathcal{M}$, which is a stepping-stone since we go through the diffusive averaging operators $\mathcal{A}_{\lambda, \epsilon}$; nevertheless, we will have solace in the class $h^\ell S^m$, which is able to support this while remaining invariant to coordinate transformations.

2.4. FBI Transform

We follow [WZ01] to state the fundamental results about FBI transforms on smooth, compact manifolds. They define the following:

DEFINITION 2.24 (Admissible Phase & FBI Transform). — *A smooth function $\phi : T^*\mathcal{M} \times \mathcal{M} \rightarrow \mathbb{C}$ is an admissible phase if it satisfies all of the properties:*

- (1) $\phi(x, \xi, y)$ is an elliptic polyhomogeneous symbol of order one in ξ ,
- (2) $\Im(\phi) \geq 0$,
- (3) $D_y \phi|_{(x, \xi, x)} = -\xi dy$,
- (4) $D_y^2 \Im(\phi)|_{(x, \xi, x)} \sim \langle \xi \rangle$,
- (5) and $\phi|_{(x, \xi, x)} = 0$;

herein we have denoted by $\varphi|_{(x, \xi, x)}$ the restriction of a function φ with co-domain $T^*\mathcal{M} \times \mathcal{M}$ to the set $\{(x, \xi, y) \mid x = y\}$.

An FBI transform is a map $T_h[\cdot; \phi, a] : C^\infty(\mathcal{M}) \rightarrow C^\infty(T^*\mathcal{M})$ given by,

$$T_h[u; \phi, a](x) := \int_{\mathcal{M}} e^{\frac{i}{h}\phi(x, \xi, y)} a(x, \xi, y; h) \chi(x, \xi, y) u(y) dy,$$

with ϕ a fixed admissible phase function, $a \in h^{-\frac{3n}{4}} S_{\text{phg}}^{\frac{n}{4}}$ is elliptic and χ is a cut-off function near $\{(x, \xi, y) \mid x = y\}$.

We will need the following basic properties of the FBI transform, as it relates to quantization:

THEOREM 2.25 ([WZ01]). — Let $q \in h_{\rho}^{\ell} S_{\rho}^m(T^*\mathcal{M})$ and fix both, an admissible phase function ϕ and an elliptic symbol $a \in h^{-\frac{3n}{4}} S_{\text{phg}}^{\frac{n}{4}}(T^*\mathcal{M} \times \mathcal{M})$. Denote $T_h := T_h[\cdot; \phi, a]$. Then, there exists $b_0 \in h^{\frac{3n}{2}} S_{\text{phg}}^{-\frac{n}{2}}(T^*\mathcal{M} \times \mathcal{M})$ positive, elliptic and depending only on ϕ , such that $T_h^* q T_h \in h_{\rho}^{\ell} \Psi_{\rho}^m$ and

$$T_h^* q T_h - \text{Op}_h(|a|^2 b_0 q) \in h_{\rho}^{\ell+1} \Psi_{\rho}^{m-1}.$$

Furthermore, b_0 is determined explicitly through ϕ so that on specializing to $a = b_0^{-\frac{1}{2}}$, there exists an elliptic $b \in h^{\frac{3n}{2}} S_{\text{phg}}^{-\frac{n}{2}}$ depending only on ϕ with a positive principal symbol such that setting $T_h := T_h[\cdot; \phi, b^{-\frac{1}{2}}]$ gives

$$\begin{aligned} T_h^* q T_h - \text{Op}_h(q) &\in h_{\rho}^{\ell+1} \Psi_{\rho}^{m-1}, \\ T_h^* T_h - I &\in h^{\infty} \Psi_{\text{phg}}^{-\infty}. \end{aligned}$$

Whenever q is polyhomogeneous, then so is the symbol being quantized by the FBI transform, above. The operator $T_h : L^2(\mathcal{M}) \rightarrow L^2(T^*\mathcal{M})$ is bounded for all $h \in [0, h_0]$.

Remark 2.26. — The proof given in [WZ01, Proposition 3.1] goes through for q taken to be a symbol belonging to the more general class we consider here, $h_{\rho}^{\ell} S_{\rho}^m$, with $\text{Op}_h(|a|^2 b_0 q)$ understood as the right-hand side of (2.2). In regards to the increasing singularity of derivatives controlled by ρ , it is in the application of the method of complex stationary phase, namely [Hör03, Theorem 7.7.12], during the course of the proof, where we find that the symbol of $T_h^* q T_h$ has an asymptotic expansion in powers of h_{ρ} .

3. Semi-classical measures of coherent states

The basic properties of FBI transforms, as in Theorem 2.25 show that much like the Fourier transform in flat space, they give a *diagonal* representation of pseudo-differential operators through their principal symbols on phase space. On the other hand, as a map, T_h also *lifts* an $L^2(\mathcal{M})$ element to $L^2(T^*\mathcal{M})$. These lifts allow us to access certain *statistics* on phase space through inner products of the original (configuration-space) functions with quantized operators. To give some concreteness, let $u_h \in L^2(\mathcal{M})$ for every $h \in (0, h_0)$. Then, the *Husimi function* for u_h is $|T_h[u_h]|^2 \in L^2(T^*\mathcal{M})$ and clearly, $\mu_h[u_h] := |T_h[u_h]|^2 dx d\xi$ defines a sequence of measures on the cotangent bundle in the parameter $h \in (0, h_0)$. If $\sup_{0 \leq h < h_0} \|u_h\|_{L^2}^2 < \infty$, then also $\sup_{0 \leq h < h_0} \|T_h[u_h]\|_{L^2(T^*\mathcal{M})} < \infty$ so by a diagonal argument, given any sequence $h_j \rightarrow 0$, there exists a subsequence $h_{j_k} \rightarrow 0$ and a non-negative finite Borel measure μ on $L^2(T^*\mathcal{M})$ such that $\mu_{h_{j_k}}[u_{h_{j_k}}] \rightarrow \mu$ weakly; this is often called

a *semi-classical (defect) measure* [Zwo12]. Therefore, Theorem 2.25 allows us to take expectations of symbols with respect to Husimi functions in a simple way:

$$\begin{aligned}
 (3.1) \quad \langle u_h | \text{Op}_h(q) | u_h \rangle_{L^2(\mathcal{M})} &= \langle u_h | T_h^*[\cdot; \phi, b^{-\frac{1}{2}}] q T_h[\cdot; \phi, b^{-\frac{1}{2}}] | u_h \rangle + O(h^{1-2\rho}) \\
 &= \langle T_h[u_h] | q | T_h[u_h] \rangle_{L^2(T^*\mathcal{M})} + O(h^{1-2\rho}) \\
 &= \int_{T^*\mathcal{M}} q(x, \xi) |T_h[u_h]|^2(x, \xi) dx d\xi + O(h^{1-2\rho}), \\
 \text{hence, } \langle u_{h_{j_k}} | \text{Op}_h(q) | u_{h_{j_k}} \rangle_{L^2(\mathcal{M})} &\xrightarrow{h_{j_k} \rightarrow 0} \int_{T^*\mathcal{M}} q(x, \xi) d\mu(x, \xi).
 \end{aligned}$$

Now, of particular interest as a step towards *quantum-classical correspondence* is if a state u_h could have a Dirac mass as semi-classical measure, for then we could access the *classical* space of symbols by probing pseudodifferential operators via inner products. There are in fact many such candidate states and we can construct and understand them through stationary phase analysis of the FBI transform. Indeed, a particularly simple case is essentially to use the kernel itself: that is, to consider the interaction between the state

$$\psi_h(x; x_0, \xi_0) := e^{-\frac{i}{h}\bar{\phi}(x_0, \xi_0, x)}$$

with a fixed admissible phase ϕ and *localization* $(x_0, \xi_0) \in T^*\mathcal{M}$ and the FBI transform $T_h := T_h[\cdot; \phi, a]$ with the same phase and some fixed elliptic $a \in h^{-\frac{3n}{4}} S^{\frac{n}{4}}$. Then, we would like to know the Husimi function for ψ_h and the *ansatz* from looking at the flat case is that this is indeed a Dirac mass at (x_0, ξ_0) , weighted by an order zero symbol. In fact, the Husimi function is just the modulus square of the Schwartz kernel for the projection operator $T_h T_h^*$, up to an amplitude factor: indeed,

$$\begin{aligned}
 T_h T_h^*(x, \xi, x', \eta) dx' d\eta \\
 = \int_{\mathcal{M}} e^{\frac{i}{h}(\phi(x, \xi; y) - \bar{\phi}(x', \eta; y))} a(x, \xi, y; h) \bar{a}(x', \eta, y; h) \chi(x, \xi, y) \bar{\chi}(x', \eta, y) dy dx' d\eta,
 \end{aligned}$$

while

$$T_h[\psi_h(\cdot; x_0, \xi_0)](x, \xi) = \int_{\mathcal{M}} e^{\frac{i}{h}(\phi(x, \xi; y) - \bar{\phi}(x_0, \xi_0; y))} a(x, \xi, y; h) \chi(x, \xi, y) dy.$$

The computation of the Schwartz kernel for $T_h T_h^*$ is carried out in [WZ01, Theorem 4.4] and the corresponding stationary phase analysis yields also $T_h[\psi_h]$. The proof of [WZ01, Theorem 4.4] goes on to elucidate the real (oscillatory) part of the resulting phase, which is more than what's necessary to understand the Husimi function $|T_h[\psi_h]|^2$; therefore, although the changes are straight-forward, for completeness we will recount their proof, with the necessary modifications, stopping just at the relevant outcome for our context and record the resulting characterization as,

LEMMA 3.1 ([WZ01, Theorem 4.4.]). — *Let ϕ be an admissible phase function and $a \in h^{-\frac{3n}{4}} S^{\frac{n}{4}}_{\text{phg}}$ be an elliptic amplitude such that $h^{\frac{3n}{4}} a(x_0, \xi_0, x_0; h)|_{h=0} \neq 0$. Then, there exist $\Phi \in C^\infty(T^*\mathcal{M} \times T^*\mathcal{M}_{(x_0, \xi_0)})$ and $c \in C^\infty(T^*\mathcal{M} \times T^*\mathcal{M}_{(x_0, \xi_0)} \times [0, h_0])$ such that*

- (1) $c(x, \xi; x_0, \xi_0; h)$ is order zero in h , supported in a neighbourhood of (x_0, ξ_0) in the first variable and $c(x_0, \xi_0; x_0, \xi_0; 0) \neq 0$,

(2) there is a positive-definite matrix H depending only on x_0, ξ_0 such that

$$\Im \Phi = \frac{1}{2} \langle (x - x_0, \xi - \xi_0) | H | (x - x_0, \xi - \xi_0) \rangle + O(|x - x_0|^4 + |\xi - \xi_0|^4)$$

and

$$T_h[\psi_h](x, \xi) = h^{-\frac{n}{4}} c(x, \xi; x_0, \xi_0; h) e^{\frac{i}{h} \Phi(x, \xi; x_0, \xi_0)} + O(h^\infty).$$

Proof. — We follow closely the proof of [WZ01, Theorem 4.4] to compute

$$T_h[\psi_h(\cdot; x_0, \xi_0)](x, \xi) = \int_{\mathcal{M}} e^{\frac{i}{h} [\phi(x, \xi; y) - \bar{\phi}(x_0, \xi_0; y)]} a(x, \xi, y; h) dy,$$

wherein we have absorbed the cut-off χ into the symbol a . The conditions of an admissible phase allow us to write locally, by Taylor expansion in y near $\{(x, \xi, y) \in T^*\mathcal{M} \times \mathcal{M} \mid x = y\}$,

$$\phi(x, \xi; y) = \xi \cdot (y - x) + \frac{1}{2} \langle Q(y; x, \xi)(x - y), x - y \rangle + O(|x - y|^3),$$

wherein Q is a complex-symmetric matrix symbol of degree one in ξ such that $\Im Q|_{x=y} \sim \langle \xi \rangle I$ and $\langle \cdot, \cdot \rangle$ denotes the *real* inner product. Since T_h localizes to a neighbourhood of x , we can therefore write (up to $O(|x - y|^3)$ terms),

$$\begin{aligned} \varphi_0(x, \xi, x_0, \xi_0; y) &:= \phi(x, \xi; y) - \bar{\phi}(x_0, \xi_0; y) \\ &= (x_0 - y) \cdot \xi_0 - (x - y) \cdot \xi \\ &\quad + \frac{1}{2} \langle Q(y; x_0, \xi_0)(x_0 - y), (x_0 - y) \rangle \\ &\quad - \frac{1}{2} \langle \bar{Q}(y; x, \xi)(x - y), (x - y) \rangle. \end{aligned}$$

The integrand is localized near $x = x_0 = y$, and since the integral decays rapidly as $O(h^\infty)$ away from the neighbourhood of points where the phase is real and stationary, we also reduce to localization about $\xi = \xi_0$. Hence, we switch to the coordinates,

$$\vartheta := x_0 - y, \quad \omega := x_0 - x, \quad \zeta := \xi_0 - \xi,$$

giving

$$\begin{aligned} \tilde{\varphi}_0(\vartheta, \omega, \zeta; x_0, \xi_0) &:= \varphi_0(x_0 - \omega, \xi_0 - \zeta, x_0, \xi_0; x_0 - \vartheta) \\ &= \vartheta \cdot \xi_0 - (\vartheta - \omega) \cdot (\xi_0 - \zeta) + \frac{1}{2} \langle Q(x_0 - \vartheta; x_0, \xi_0) \vartheta, \vartheta \rangle \\ &\quad - \frac{1}{2} \langle \bar{Q}(x_0 - \vartheta; x_0 - \omega, \xi_0 - \zeta) (\vartheta - \omega), \vartheta - \omega \rangle. \end{aligned}$$

We wish to apply the method of complex stationary phase, as per [Hör03, Theorem 7.7.12]. To see that this can be done, just note that the change of variables $y \mapsto \vartheta$ along with the admissibility conditions on φ and $\bar{\varphi}$ imply that $\tilde{\varphi}_0$ satisfies the hypotheses of that theorem around $\{\vartheta = \omega = \zeta = 0\}$. The result is determined up to the ideal $I_{\tilde{\varphi}_0} := \langle \partial_{\vartheta_1} \tilde{\varphi}_0, \dots, \partial_{\vartheta_n} \tilde{\varphi}_0 \rangle$ — the generators of which, if we expand in Taylor series about $\vartheta = \omega = \zeta = 0$, are given by the components of the vector,

$$D_{\vartheta} \tilde{\varphi}_0 = \zeta + Q(x_0; x_0, \xi_0) \cdot \vartheta - \bar{Q}(x_0; x_0, \xi_0) \cdot (\vartheta - \omega) + O(|\vartheta|^2 + |\omega|^2).$$

Thus, we can proceed to apply the Malgrange preparation theorem, which allows us to divide $\partial_{\vartheta_1}\tilde{\varphi}_0, \dots, \partial_{\vartheta_n}\tilde{\varphi}_0$ by each of the coordinates $\vartheta_1, \dots, \vartheta_n$ to yield (complex-valued) smooth remainder functions $X_{\vartheta_1}, \dots, X_{\vartheta_n}(\omega, \zeta, x_0, \xi_0)$ in a neighbourhood of $\omega = \zeta = 0$; *viz.*,

$$\vartheta \equiv X_{\vartheta} \pmod{I_{\tilde{\varphi}_0}}.$$

We now work modulo the ideal $I_{\tilde{\varphi}_0}$. We can resolve X_{ϑ} via the Taylor expansion of $D_{\vartheta}\tilde{\varphi}_0$ in a neighbourhood of $\vartheta = \omega = \zeta = 0$: set $Q_0 := Q(x_0; x_0, \xi_0)$, then

$$0 \equiv D_{\vartheta}\tilde{\varphi}_0 \equiv \zeta + 2i\Im Q_0 \cdot X_{\vartheta} + \bar{Q}_0 \cdot \omega + O(|X_{\vartheta}|^2 + |\omega|^2),$$

hence,

$$X_{\vartheta}(\omega, \zeta; x_0, \xi_0) \equiv \frac{i}{2}(\Im Q_0)^{-1}(\zeta + \bar{Q}_0 \cdot \omega + O(|\zeta|^2 + |\omega|^2))$$

(wherein, the $O(|\zeta|^2 + |\omega|^2)$ term comes from recursively substituting the expression for X_{ϑ} in the higher order term). Now, we may expand $\tilde{\varphi}_0$ in Taylor series about $\{\vartheta = \omega = \zeta = 0\}$ and substitute X_{ϑ} for ϑ , to find the phase resulting from the integration:

$$\begin{aligned} \Phi_0(\omega, \zeta; x_0, \xi_0) &:= X_{\vartheta} \cdot \zeta + \omega \cdot (\xi_0 - \zeta) + \frac{1}{2}\langle Q_0 X_{\vartheta}, X_{\vartheta} \rangle - \frac{1}{2}\langle \bar{Q}_0(X_{\vartheta} - \omega), X_{\vartheta} - \omega \rangle \\ &\quad + O(|\omega|^2 + |\zeta|^2)^2 \equiv \tilde{\varphi}_0 \pmod{I_{\tilde{\varphi}_0}} \end{aligned}$$

(wherein, $|X_{\vartheta}|^2 \lesssim |\omega|^2 + |\zeta|^2$ gives size of the higher order terms).

We elucidate this phase a bit: note that

$$X_{\vartheta} - \omega = \frac{i}{2}(\Im Q_0)^{-1}(\zeta + \Re Q_0 \cdot \omega) - \frac{1}{2}\omega = \bar{X}_{\vartheta}.$$

Letting $S := \Re Q_0$ and $T := \Im Q_0$, this gives

$$\begin{aligned} \Im \Phi_0(\omega, \zeta; x_0, \xi_0) &= \frac{1}{2}\langle T^{-1}\zeta, \zeta \rangle + \frac{1}{2}\langle T^{-1}S\omega, \zeta \rangle \\ &\quad - \frac{1}{4}\Im \langle T^{-1}Q_0 T^{-1}(\zeta + \bar{Q}_0\omega), \zeta + \bar{Q}_0\omega \rangle + O(|\omega|^2 + |\zeta|^2)^2 \end{aligned}$$

and after expanding fully, we find that the Hessian of $\Im \Phi_0$ at $(\omega, \zeta) = (0, 0)$ is,

$$\frac{1}{4} \begin{pmatrix} T^{-1} & T^{-1}S \\ ST^{-1} & T + ST^{-1}S \end{pmatrix} = \frac{1}{4} \begin{pmatrix} I & 0 \\ S & I \end{pmatrix} \begin{pmatrix} T^{-1} & 0 \\ 0 & T \end{pmatrix} \begin{pmatrix} I & S \\ 0 & I \end{pmatrix}.$$

By the admissible phase assumption, $T \sim \langle \xi_0 \rangle I$ at $(\omega, \zeta) = (0, 0)$, therefore this decomposition shows that this Hessian H_0 of $\Im \Phi_0$ is also positive definite, whence, there exists a constant $C > 1$ such that

$$C^{-1}(|\omega|^2 + |\zeta|^2) \leq \Im \Phi_0 = \langle (\omega, \zeta) | H_0 | (\omega, \zeta) \rangle + O(|\omega|^2 + |\zeta|^2)^2 \leq C(|\omega|^2 + |\zeta|^2).$$

This proves part (2) with $H := 2H_0$.

By [Hör03, Theorem 7.7.12], there are differential operators L_j of order $2j$ acting in the ω, ζ variables, with coefficients that are dependent only on $\tilde{\varphi}_0$ such that

$$\left| T_h[\psi_h] - e^{\frac{i}{h}\Phi_0(\omega, \zeta; x_0, \xi_0)} \sum_{j=0}^{N-1} \tilde{b}^0(L_j[a])^0(\omega, \zeta; x_0, \xi_0; h) h^j \right| \lesssim_N h^{N+n/2}.$$

Here, $\tilde{b} := (\det[\partial_{\vartheta}^2 \tilde{\varphi}_0 / (2\pi i h)])^{-\frac{1}{2}}$ and (following Hörmander) we denote for a function $G(x, \xi, y; x_0, \xi_0)$, its reduction modulo $I_{\tilde{\varphi}_0}$ by $G^0 \equiv G \pmod{I_{\tilde{\varphi}_0}}$, which can be determined by a change of variables to $G(\vartheta, \omega, \zeta; x_0, \xi_0; h) := G(x_0 - \omega, \xi_0 - \zeta, x_0 - \vartheta; x_0, \xi_0; h)$, followed by Taylor expansion about $(\vartheta, \omega, \zeta) = 0$ and substitution of X_{ϑ} for ϑ . We note that $\tilde{b}^0 \equiv (h/\pi)^{\frac{n}{2}} [(\det H_0)^{-\frac{1}{2}} + O(|\omega|^2 + |\zeta|^2)]$. Then, the series can be summed, upon taking $N \rightarrow \infty$, to $h^{-\frac{n}{4}}$ times a smooth function $c_0(\omega, \zeta; x_0, \xi_0; h)$ of order zero in h in a neighbourhood of $(\omega, \zeta) = (0, 0)$, which is non-vanishing at $\{(\omega, \zeta, x, \xi, h) \mid \omega = \zeta = 0, h = 0\}$ due to the non-vanishing of a and the Hessian of $\tilde{\varphi}_0$ there. After re-labelling the variables to give $\Phi(x, \xi; x_0, \xi_0) := \Phi_0(\omega, \zeta; x, \xi)$ and $c(x, \xi, x_0, \xi_0; h) := c_0(\omega, \zeta; x_0, \xi_0; h)$, altogether this brings us to

$$T_h[\psi_h] = h^{-\frac{n}{4}} c(x, \xi; x_0, \xi_0; h) e^{\frac{i}{h} \Phi(x, \xi; x_0, \xi_0)} + O(h^\infty). \quad \square$$

Remark 3.2. — The statement of the theorem expresses the phase and symbol of the result of $T_h[\psi_h]$ in terms of $(x, \xi; x_0, \xi_0)$, but since we know that the functions are localized to a neighbourhood of (x_0, ξ_0) in the variable (x, ξ) , we can just as well switch to local coordinates and write these as functions of $(\omega, \zeta; x_0, \xi_0)$ localized at $(\omega, \zeta) = (0, 0)$ as in the proof. This will be useful at times in the forthcoming calculations.

We now have quite precise information about the *localization* of $T_h[\psi_h]$, but we are left with the symbol c as a factor, which persists when trying to access the value of the symbol of a Ψ DO at $(x_0, \xi_0) \in T^*\mathcal{M}$ through (3.1); this would later be obstructive to locating geodesic points through operator expectations. To alleviate this, it is sufficient to use L^2 -normalized states $\psi_h/\|\psi_h\|$: by Theorem 2.25 and the lemma just proved, using $T_h := T_h[\cdot; \phi, b^{-\frac{1}{2}}]$ gives,

$$(3.2) \quad \langle \psi_h | \psi_h \rangle = \langle \psi_h | T_h^* T_h | \psi_h \rangle + O(h^\infty) = h^{-\frac{n}{2}} \|c e^{\frac{i}{h} \Phi}\|_{(x, \xi)}^2(x_0, \xi_0; h) + O(h^\infty),$$

where $\|\cdot\|_{(x, \xi)}$ denotes the norm in $L^2(T^*\mathcal{M})$ in the variables (x, ξ) and the form on the right-hand side leads to the following,

THEOREM 3.3 (Symbol from C-S expectation). — *Let ϕ be an admissible phase, and $\psi_h(x; x_0, \xi_0) := C_h(x_0, \xi_0) e^{-\frac{i}{h} \bar{\phi}(x_0, \xi_0; x)}$ be normalized to $\|\psi_h\|_{L^2(\mathcal{M})} = 1$. Then, for all $m \in \mathbb{Z}$ and $a \in h^0 S_\rho^m(T^*\mathcal{M})$,*

$$\langle \psi_h | \text{Op}_h(a) | \psi_h \rangle = a(x_0, \xi_0; h) + O(h^{1-2\rho}).$$

Proof. — The preceding theorem tells that on Taylor expanding in a neighbourhood of $x = x_0$, $\xi = \xi_0$,

$$\begin{aligned} T_h[\psi_h]^2 &= e^{-\frac{2}{h} \Im \Phi} \\ &= e^{-\frac{1}{h} \|(x-x_0, \xi-\xi_0)\|_H^2} \left(1 + \sum_{j=1}^{\infty} O(|x-x_0|^4 + |\xi-\xi_0|^4)^j / h^j \right). \end{aligned}$$

This, together with (3.2), Taylor expansion of $|c|^2$ about $(x, \xi) = (x_0, \xi_0)$ and $d[(s_{x_0}^{-1})^* \nu_g](v) = \sqrt{|g_{s_{x_0}^{-1}(v)}|} dv$ (see [BGM71, Proposition C.III.2]) along with $d\xi dx =$

$(d\xi/\sqrt{|g_x|}) d\nu_g(x)$ gives,

$$\begin{aligned}
h^{\frac{n}{2}} C_h(x_0, \xi_0)^{-2} &= \left\| c e^{\frac{i}{h} \Phi} \right\|^2(x_0, \xi_0) \\
&= \int |c|^2(x, \xi; x_0, \xi_0; h) e^{-\frac{2}{h} \Im \Phi(x-x_0, \xi-\xi_0)} dx d\xi \\
&= \int e^{-\frac{1}{h} \|(x-x_0, \xi-\xi_0)\|_H^2} \left[1 + \sum_{j=1}^{\infty} O(|x-x_0|^4 + |\xi-\xi_0|^4)^j / h^j \right] \\
&\quad \times \left[|c|^2(x_0, \xi_0; x_0, \xi_0; h) + O(|x-x_0| + |\xi-\xi_0|) \right] dx d\xi \\
&= \int_{\mathbb{R}^n} \int_{V_{x_0}} e^{-\frac{1}{h} \|(v, \zeta)\|_H^2} \left[1 + \sum_{j=1}^{\infty} O(|v|^4 + |\zeta|^4)^j / h^j \right] \\
&\quad \times \left[|c|^2(x_0, \xi_0; x_0, \xi_0; h) + O(|v| + |\zeta|) \right] dv d\zeta + O(h^\infty) \\
&= h^n \left[m_\Phi |c|^2(x_0, \xi_0; x_0, \xi_0; h) + O(h) \right], \\
m_\Phi &:= \int_{\mathbb{R}^{2n}} e^{-\|(v, \zeta)\|_H^2} dv d\zeta.
\end{aligned}$$

Therefore, another application of the preceding theorem and the same method of Taylor expansions gives, for any $a \in h^0 S^m$,

$$\begin{aligned}
\langle \psi_h | T_h^* a T_h | \psi_h \rangle &= h^{-\frac{n}{2}} \int_{T^* \mathcal{M}} a(x, \xi) C_h(x_0, \xi_0)^2 |c|^2(x, \xi; x_0, \xi_0; h) e^{-\frac{2}{h} \Im \Phi(x-x_0, \xi-\xi_0)} dx d\xi \\
&= h^{-\frac{n}{2}} \int a e^{-\frac{2}{h} \Im \Phi} \frac{|c|^2(x_0, \xi_0; x_0, \xi_0; h) + O(|x-x_0| + |\xi-\xi_0|)}{h^{\frac{n}{2}} [m_\Phi |c|^2(x_0, \xi_0; x_0, \xi_0; h) + O(h)]} dx d\xi \\
&= h^{-n} \int a e^{-\frac{2}{h} \Im \Phi} [1/m_\Phi + O(|x-x_0| + |\xi-\xi_0|) + O(h)] dx d\xi \\
&= h^{-n} \int e^{-\frac{1}{h} \|(x-x_0, \xi-\xi_0)\|_H^2} \\
&\quad \times [a(x, \xi)/m_\Phi + O(|x-x_0| + |\xi-\xi_0|) + O(h)] \\
&\quad \times \left[1 + \sum_{j=1}^{\infty} O(|x-x_0|^4 + |\xi-\xi_0|^4)^j / h^j \right] dx d\xi \\
&= h^{-n} \int_{\mathbb{R}^{2n}} [a(x_0, \xi_0)/m_\Phi + p_a(v, \zeta; h) + r_a(v, \zeta; h) + O(|v| + |\zeta|)] \\
&\quad \times e^{-\frac{1}{h} \|(v, \zeta)\|_H^2} \left[1 + \sum_{j=1}^{\infty} h^{-j} O(|v|^4 + |\zeta|^4)^j \right] \\
&\quad \times [1 + O(|v| + |\zeta|) + O(h)] dv d\zeta \\
&= a(x_0, \xi_0) + O(h^{1-2\rho}).
\end{aligned}$$

The domains of integration have been localized and expanded (as in the fourth equality) at will, due to the fact that a symbol $a \in h^0 S^m$ has at most polynomial growth in the cotangent fibres, so $|T_h[\psi_h]|^2$ localizes the integrand to an $O(\sqrt{h})$ ball around $(x_0, \xi_0) \in T^* \mathcal{M}$. The terms p_a and r_a on the right-hand side of the fifth equality denote the first-order polynomial and second-order term with remainder,

in the Taylor expansion of a about (x_0, ξ_0) , respectively. The linear function p_a has coefficients of order $h^{-\rho}$ and the integral of $p_a e^{-\frac{1}{h}\|(v, \zeta)\|_H^2}$ vanishes since it is odd, while r_a decays as $h^{-2\rho}O(|v|^2 + |\zeta|^2)$ near the origin. By applying Theorem 2.25, we have the last part of the statement of the theorem. $\square$

Having seen the utility of the function ψ_h , we now dignify it with its own,

DEFINITION 3.4 (Coherent states). — *With ϕ an admissible phase and $h > 0$, we call $\psi_h(x; x_0, \xi_0) := C_h(x_0, \xi_0)e^{-\frac{i}{h}\bar{\phi}(x_0, \xi_0; x)}$, with $C_h := \|e^{\frac{i}{h}\phi}\|_{L^2(\mathcal{M})}$, a coherent state localized at $(x_0, \xi_0) \in T^*\mathcal{M}$, or simply a coherent state for brevity. At times, we will also use the un-normalized coherent state, $\tilde{\psi}_h := e^{-\frac{i}{h}\bar{\phi}(x_0, \xi_0; x)}$.*

3.1. State preparation

We discuss briefly some considerations in practically constructing coherent states. At the outset, when the isometry $\iota : \mathcal{M} \rightarrow \mathbb{R}^D$ is available, a simple prescription for a phase is $\phi_\iota := \langle \Pi_\iota^T(x) \cdot \xi, \iota(x) - \iota(y) \rangle_{\mathbb{R}^D} + \frac{i}{2} \frac{\langle \xi \rangle}{\langle \xi_0 \rangle} |\iota(y) - \iota(x)|_{\mathbb{R}^D}^2$, with $\Pi_\iota(x) \cong D\iota|_x^T : \mathbb{R}^D \supset T_{\iota(x)}^*\Lambda \rightarrow T_x^*\mathcal{M} \cong \mathbb{R}^n$ and a fixed $(x_0, \xi_0) \in T^*\mathcal{M}$. Then,

$$D\phi_\iota|_{y=x} = -\xi dx, \quad D^2\Im(\phi)|_{y=x} = \frac{\langle \xi \rangle}{\langle \xi_0 \rangle} D\iota|_x^T D\iota|_x \sim \langle \xi \rangle,$$

so ϕ_ι is an admissible phase and $\phi_\iota(x_0, \xi_0; y) = \langle \Pi_\iota^T(x_0) \cdot \xi_0, \iota(x_0) - \iota(y) \rangle_{\mathbb{R}^D} + \frac{i}{2} |\iota(y) - \iota(x_0)|_{\mathbb{R}^D}^2$. Hence, if $\psi_{\iota, h}$ is a coherent state localized at (x_0, ξ_0) with phase ϕ_ι , then for any $a \in h^0 S^m$ we have by Theorem 3.3,

$$\langle \psi_{\iota, h} | \text{Op}_h(a) | \psi_{\iota, h} \rangle = a(x_0, \xi_0; h) + O(h).$$

The vector $\xi_{\iota, 0} := \Pi_\iota^T(x_0) \cdot \xi_0$ is just the coordinate representation of ξ_0 in the hyperplane tangent to Λ with center $\iota(x_0)$. If normal coordinates are placed at x_0 and x_* is in a normal neighbourhood of x_0 , then we understand that $\xi_0 := s_{x_0}(x_*)/|s_{x_0}(x_*)|_{\mathbb{R}^n}$ is the direction in which a geodesic originating at x_0 must emanate, to reach x_* . Then, given $\iota(x_*) \in \Lambda$ in a small neighbourhood of $\iota(x_0)$, a reasonable approximation to $\xi_{\iota, 0}$ is given by

$$\begin{aligned} \xi_* &:= \frac{\iota(x_*) - \iota(x_0)}{|\iota(x_*) - \iota(x_0)|_{\mathbb{R}^D}} = D\iota|_{x_0} \cdot \frac{s_{x_0}(x_*)}{|s_{x_0}(x_*)|_{\mathbb{R}^n}} + O(|\iota(x_*) - \iota(x_0)|_{\mathbb{R}^D}) \\ &= \Pi_\iota^T(x_0) \cdot \xi_0 + O(|\iota(x_*) - \iota(x_0)|_{\mathbb{R}^D}), \end{aligned}$$

wherein the first equality follows from Lemma 2.5 and Taylor's theorem upon expanding $\iota \circ s_{x_0}^{-1}$ in a neighbourhood of the origin. Now, supposing $|\iota(x_*) - \iota(x_0)|_{\mathbb{R}^D} \lesssim h^{\frac{n}{4}+2}$ and setting $\hat{\phi}_\iota := \langle \xi, \iota(x) - \iota(y) \rangle_{\mathbb{R}^D} + \frac{i}{2} |\iota(y) - \iota(x)|_{\mathbb{R}^D}^2$, another application of Taylor's theorem gives,

$$\begin{aligned} e^{-\frac{i}{h}\bar{\phi}_\iota(x_0, \xi_*; x)} &= e^{-\frac{i}{h}[\Re(\hat{\phi}_\iota)(x_0, \xi_{\iota, 0} + O(h^2); x) - i\Im(\phi_\iota)(x_0, \xi_0; x)]} \\ &= e^{-\frac{i}{h}\bar{\phi}_\iota(x_0, \xi_{\iota, 0}; x)} + O_{L^\infty}(h^{\frac{n}{4}+1}), \end{aligned}$$

wherein we've expanded in a neighbourhood of $\xi_{\iota,0}$ in increments of the error term coming from the Taylor expansion of ξ_* . Then, $\hat{\psi}_{\iota,h} := e^{-\frac{i}{h}\hat{\phi}_{\iota}(x_0,\xi_*;x)} / \|e^{\frac{i}{h}\hat{\phi}_{\iota}(x_0,\xi_*;\cdot)}\|_{L^2}$ satisfies $\|\hat{\psi}_{\iota,h} - \psi_{\iota,h}\|_{\infty} = O(h)$, from which we recover,

$$\langle \hat{\psi}_{\iota,h} | \text{Op}_h(a) | \hat{\psi}_{\iota,h} \rangle = a(x_0, \xi_0; h) + O(h^{1-2\rho}).$$

This means that we can use points in a sufficiently small neighbourhood of $\iota(x_0)$ to determine unit momentum vectors at which to recover, to order $O(h^{1-2\rho})$, the value of the symbol of a given Ψ DO.

The specifications of an admissible phase make coherent states particularly well-suited for a description in local coordinate patches. Let $u: \mathcal{O} \rightarrow V \subset \mathbb{R}^n$ be a diffeomorphism providing local coordinates in a neighbourhood $\mathcal{O}$ of $x_0 \in \mathcal{M}$. Then, for a fixed $\xi_0 \in T_{x_0}^* \mathcal{M}$, a simple construction of a phase is of the sort,

$$\phi_u(x, \xi; y) := \langle Du|_x^T \xi, u(x) - u(y) \rangle_{\mathbb{R}^n} + \frac{i}{2} \frac{\langle \xi \rangle}{\langle \xi_0 \rangle} |u(y) - u(x)|_{\mathbb{R}^n}^2$$

and we have,

$$D_y \phi_u|_{y=x} = -\xi, \quad D_y^2 \Im(\phi_u)|_{y=x} = \frac{\langle \xi \rangle}{\langle \xi_0 \rangle} Du|_x^T Du|_x,$$

so ϕ_u is admissible in $\mathcal{O}$. Also suppose $\chi \in C^\infty$ is a cut-off in $\text{supp } \chi \subset \mathcal{O}$ such that $\chi \equiv 1$ on $\bar{\mathcal{O}}_0 \subset \mathcal{O}$ with $\mathcal{O}_0$ an open neighbourhood of x_0 . Letting $\psi_{u,h}$ be the coherent state localized at (x_0, ξ_0) with phase ϕ_u , we find that Lemma 3.1 holds also for $T_h[\chi\psi_{u,h}]$ since χ cuts off the integration domain, with a slightly different symbol c that still satisfies all of the properties stated in the lemma. Further, $\|\psi_{u,h}\chi\|_{L^2} = 1 + O(h^\infty)$, so by Theorem 3.3, we have,

$$(3.3) \quad \langle \psi_{u,h}\chi | \text{Op}_h(a) | \chi\psi_{u,h} \rangle = a(x_0, \xi_0) + O(h^{1-2\rho}).$$

Now suppose $u(x_0) = 0$ and let $\eta_0 \in T_{x_0}^* \mathbb{R}^n$. Then, $\xi_{u,0} := Du|_{x_0}^T \eta_0 \in T_{x_0}^* \mathcal{M}$ is the corresponding cotangent vector in the dual to standard basis. A practical phase to construct, a priori, is simply $\hat{\phi}_u := \langle \eta_0, u(x_0) - u(x) \rangle_{\mathbb{R}^n} + \frac{i}{2} |u(x) - u(x_0)|_{\mathbb{R}^n}^2$. Since $|\xi_{u,0}|_{g_{x_0}} = |\eta_0|_{\mathbb{R}^n}$, we have that $\hat{\phi}_u = \phi_u(x_0, \xi_{u,0}; x)$ and the implementation of $\psi_{u,h}(x_0, \xi_{u,0}; x)$ is straight-forward. Therefore, with $\xi_0 = \xi_{u,0}$, (3.3) observes the value of the symbol of a Ψ DO at the momentum vector that is specified in coordinates by η_0 .

We have described how to construct approximations of coherent states in the sense of Definition 3.4 using extrinsic coordinates or local coordinate patches. Their position localizations are given by the coordinates of x_0 . However, the direction vector is given by an approximation to the differential map sending coordinates to tangent vectors. We've shown that to have a good approximation in order to achieve quantum-classical correspondence to order $O(h)$ error, with unit momentum vectors, it suffices to choose the direction with a small vector given by $\iota(x_*) - \iota(x_0)$, for $x_* \in \mathcal{M}$ sufficiently close to x_0 , then normalize it to a unit vector. The same schema applies to approximations using a local coordinate patch around x_0 . This analysis leaves out the finite sampling effects of the probability of choosing such sufficiently close vectors and normalising them, then applying these in concert with

the finite sampling propagation results of Section 6. This is carried out in detail in the companion [KS22] and completes the picture for a statistical estimator of the geodesic flow from finite sampled data points.

4. Graph Laplacians as Ψ DOs

As discussed in the Introduction, there is now a wide collection of results on the convergence of graph Laplacians to Laplace–Beltrami operators (modulo lower order terms) on manifolds. These take the following form: starting from a collection of N samples, they approximate $\Delta_{\lambda,\epsilon}$ in the $N \rightarrow \infty$ limit and in turn, $\Delta_{\lambda,\epsilon}$ approximates $\Delta_{\mathcal{M}} + O(\partial^1)$ in the sense that for each $u \in C^\infty$, $\|\Delta_\epsilon u - [\Delta_{\mathcal{M}} + O(\partial^1)]u\|_\infty = O(\epsilon)$ (we denote by $O(\partial^1)$ a partial differential operator of order at most one). These are results along the lines of those displayed in Section 2.2 and they are closely related to diffusion processes [NLCK06]. We now wish to bring a *quantum* perspective to graph Laplacians. Methods of semi-classical analysis enable us to instantiate a quantum-classical correspondence via semiclassical Ψ DOs. Namely, as discussed in Section 2.3, a *quantization procedure* assigns a linear operator $\text{Op}_h(a) : C^\infty(\mathcal{M}) \rightarrow C^\infty(\mathcal{M})$ to a function $a \in C^\infty(T^*\mathcal{M} \times (0, h_0])$ (for some $h_0 < 1$) belonging to a class of *symbols* (*classical observables*); these are, roughly speaking, functions that have controlled variation in regions of phase space $T^*\mathcal{M}$ of unit volume, uniformly with scaling the unit length in each fibre $T_x^*\mathcal{M}$ as $1/h$ for $h \in (0, h_0]$. If a symbol q is real-valued, then we may treat it as a Hamiltonian that generates a flow Θ_q^t with respect to time $|t| \leq T$ on $T^*\mathcal{M}$. By Egorov’s theorem, we can relate, or *quantize*, the Hamiltonian flow Θ_q^t with respect to a real-valued symbols q to *Heisenberg dynamics* $A(t) := U_q^{-t} A U_q^t$ of $A := \text{Op}_h(a)$ for $U_q^t := e^{-\frac{i}{h}t \text{Op}_h(q)}$, in the sense that the theorem gives conditions on q and a such that $A(t)$ has principal symbol $a \circ \Theta_q^t$. In particular, using $q := |\xi|_x$ gives the quantization of the geodesic flow Γ^t . Our first aim is to give light to the conjugate flow on Ψ DOs by $U_{\lambda,\epsilon}^t := e^{-it\sqrt{\Delta_{\lambda,\epsilon}}}$ as the quantization of a flow on symbols $a \circ \Theta_q^t$ for an appropriate q . To this end, we will find that when $\epsilon = h^{2+\alpha}$ with $\alpha > 0$, we have $h^2 \Delta_{\lambda,\epsilon} = \text{Op}_h(q_{\lambda,\alpha})$ with $q_{\lambda,\alpha}$ a symbol of *order two* and to order⁽⁶⁾ $O_s(h)$, this agrees with $|\xi|_x^2$ on compact neighbourhoods of the origin in $T^*\mathcal{M}$ whenever $\alpha > 1$. In terms of quantization, the scaling $\epsilon = h^{2+\alpha}$ has a simple interpretation: since the kernel $k(x, y; \epsilon)$ is localized to $\sqrt{\epsilon}$ -balls on $\mathcal{M}$, the corresponding symbol must be localized to an $h/\sqrt{\epsilon}$ -ball in phase space, which is above unit volume (*viz.*, the uncertainty principle) when $\epsilon \in o(h^2)$.

The next task is to extract the geodesic flow: once we have quantized it near a cosphere bundle $S_r^*\mathcal{M}$ for $r > 0$, we can use coherent states localized at $(x_0, \xi_0) \in S_r^*\mathcal{M}$ to retrieve $a \circ \Gamma^t(x_0, \xi_0)$ up to $O(h)$ error. This works because the localization of a coherent state restricts the action of $\text{Op}_h(a)$ to that of another whose symbol agrees with a on an $O(\sqrt{h})$ neighbourhood of (x_0, ξ_0) and vanishes outside this. Since, as we will see, $q_{\lambda,\alpha} = |\xi|_x^2 + O_s(h)$ on a fixed size neighbourhood of $S_r^*\mathcal{M}$,

⁽⁶⁾We write for $a \in C^\infty$ that $a = O_s(h)$ whenever there is a constant $h_0 > 0$ such that for each β , there is a constant $C_\beta > 0$ such that for $h \in [0, h_0)$, $|\partial^\beta a| \leq C_\beta h$.

this allows us to reduce to $U_{\lambda,\epsilon}^{-t} \text{Op}_h(a) U_{\lambda,\epsilon}^t |\psi_h\rangle = U_{|\xi|\chi}^{-t} \text{Op}_h(a) U_{|\xi|\chi}^t |\psi_h\rangle + O_{L^2}(h)$ with χ an appropriate cut-off equal to one in part of the neighbourhood. Tying this together with Egorov's theorem and the results of Section 3 leads to the desired propagation result: $\langle \psi_h | U_{\lambda,\epsilon}^{-t} \text{Op}_h(a) U_{\lambda,\epsilon}^t | \psi_h \rangle = a \circ \Gamma^t(x_0, \xi_0) + O(h)$.

4.1. Symbol of a graph Laplacian

We now compute the symbol of a graph Laplacian operator. An important aspect of this is that in order to *see* the symbol of a graph Laplacian, the quantization must be done at lengths h *above* the *sampling density* $\sqrt{\epsilon}$. We proceed with an *intrinsic* version of the averaging operator, which readily exposes this basic facet of the application of semiclassical analysis: namely, define

$$(4.1) \quad \mathcal{A}_{g,\epsilon} : C^\infty \ni u \longmapsto \epsilon^{-\frac{n}{2}} \int_{\mathcal{M}} k(d_g(\cdot, y)^2/\epsilon) u(y) p(y) d\nu_g(y) \in C^\infty.$$

This operator takes on the form (2.2) in the following way,

$$\begin{aligned} \mathcal{A}_{g,\epsilon}[u](x) &\equiv \int_{\mathbb{R}^n} \int_{\mathbb{R}^n} e^{-\frac{i}{h} v \cdot \xi} \mathcal{F}_h^{-1}[k(|z|^2/\epsilon)]_{z \rightarrow \xi}(\xi) (u \cdot p \cdot \chi_x) \circ s_x^{-1}(v) \sqrt{|g_{s_x^{-1}(v)}|} d\xi dv \\ &\equiv \frac{1}{(2\pi h)^n} \int_{\mathcal{M}} \int_{T_x^* \mathcal{M}} e^{-\frac{i}{h} \langle s_x(y), \xi \rangle_{g_x}} \left(\epsilon^{-\frac{n}{2}} \int_{T_x^* \mathcal{M}} e^{\frac{i}{h} \langle z, \xi \rangle_{g_x}} k(|z|_{g_x}^2/\epsilon) \frac{dz}{\sqrt{|g_x|}} p(y) \right) \\ &\quad \times u(y) \chi_x(y) \frac{d\xi}{\sqrt{|g_x|}} d\nu_g(y) \\ &\equiv \frac{1}{(2\pi h)^n} \int_{T^* \mathcal{M}} e^{\frac{i}{h} \langle s_y(x), \eta \rangle_{g_y}} \left(\epsilon^{-\frac{n}{2}} \int_{T_y^* \mathcal{M}} e^{\frac{i}{h} \langle \zeta, \eta \rangle_{g_y}} k(|\zeta|_{g_y}^2/\epsilon) \frac{d\zeta}{\sqrt{|g_y|}} p(y) \right) \\ &\quad \times u(y) \chi_x(y) dy d\eta \\ &\equiv \frac{1}{(2\pi h)^n} \int_{T^* \mathcal{M}} e^{\frac{i}{h} \langle s_y(x), \eta \rangle_{g_y}} H_{g,h,\epsilon}(y, \eta) u(y) \chi_x(y) d\eta dy, \end{aligned}$$

with

$$\begin{aligned} (4.2) \quad H_{g,h,\epsilon}(x, \xi) &:= \epsilon^{-\frac{n}{2}} \int_{T_x^* \mathcal{M}} e^{\frac{i}{h} \langle \zeta, \xi \rangle_{g_x}} k(|\zeta|_{g_x}^2/\epsilon) \frac{d\zeta}{\sqrt{|g_x|}} p(x) \\ &= \epsilon^{-\frac{n}{2}} \int_{\mathbb{R}^n} e^{\frac{i}{h} \langle \zeta, \xi \rangle} k\left(\left|g_x^{\frac{1}{2}} \zeta\right|^2/\epsilon\right) d\zeta \sqrt{|g_x|} p(x), \end{aligned}$$

and wherein $\equiv$ denotes equality up to a term of order $O(\epsilon^\infty) \in C^\infty$, $\chi_x(y)$ is a smooth cut-off within the normal neighbourhood of x such that $\chi_x(y) = 1$ on a fixed, open neighbourhood of x , $\mathcal{F}_h^{-1}[\cdot](\xi)$ is the inverse h -Fourier transform in $\mathbb{R}^n$ with kernel $(2\pi h)^{-n} e^{\frac{i}{h} z \cdot \xi}$ and we have used the parallel transport operator $\mathcal{T}_{y \rightarrow x} : T_y^* \mathcal{M} \rightarrow T_x^* \mathcal{M}$ along the unit speed geodesic from y to x to make the changes of variables $\eta := \mathcal{T}_{y \rightarrow x}^* \xi$ and $\zeta := \mathcal{T}_{y \rightarrow x} z$. The features of parallel transport used here are that it is an isometry

with $\mathcal{T}_{y \rightarrow x}^* = \mathcal{T}_{x \rightarrow y}$, $\mathcal{T}_{y \rightarrow x} s_y(x) = -s_x(y)$ and $d\mathcal{T}_{x \rightarrow y}(\cdot) = (|g_x|/|g_y|)^{\frac{1}{2}} d(\cdot)$. The fact that $d[(s_x^{-1})^* \nu_g](v) = \sqrt{|g_{s_x^{-1}(v)}|} dv$ is another consequence of parallel transport we've used and its justification can be found in [BGM71, Proposition C.III.2].

The formal symbol $H_{g,h,\epsilon}$ has

$$\begin{aligned} & \langle \xi \rangle^{|\beta|-m} \left| \partial_x^\gamma \partial_\xi^\beta H_{g,h,\epsilon} \right| \\ &= \langle \xi \rangle^{|\beta|-m} \left| \partial_x^\gamma \int_{\mathbb{R}^n} \left(i\epsilon^{\frac{1}{2}}/h \right)^{|\beta|} z^\beta e^{i\frac{\sqrt{\epsilon}}{h} \langle z, \xi \rangle} k \left(\left| g_x^{\frac{1}{2}} z \right|^2 \right) dz \left| g_x^{\frac{1}{2}} \right| p(x) \right| \\ &= \left(\frac{\epsilon}{h^2} \right)^{\frac{m}{2}} \left| \int_{\mathbb{R}^n} e^{i\frac{\sqrt{\epsilon}}{h} \langle z, \xi \rangle} \left(\epsilon/h^2 + \Delta_z \right)^{\frac{|\beta|-m}{2}} \left(z^\beta \partial_x^\gamma \left[k \left(\left| g_x^{\frac{1}{2}} z \right|^2 \right) \left| g_x^{\frac{1}{2}} \right| p(x) \right] \right) dz \right|, \end{aligned}$$

which is uniformly bounded in $(0, 1]_h \times T^*\mathcal{M}$ for $\epsilon = h^{2+\alpha}$ with $\alpha \geq 0$ and each $m, |\gamma|, |\beta| \geq 0$, while taking $\beta = 0$ with $m < 0$ and evaluating the right-hand side at $\xi = 0$ shows that this quantity grows as $\Omega(h^{m\alpha/2})$ whenever $\alpha > 0$ and is uniformly bounded when $\alpha = 0$. Thus, $H_{g,h^\alpha} := H_{g,h,h^{2+\alpha}} \in h^0 S^0$ for $\alpha > 0$ and $H_{g,h^0} \in h^0 S^{-\infty}$. On the other hand if $\alpha < 0$, then for any $m > 0, \delta < 0$, taking $|\beta| = m$ gives

$$\sup_{(x,\xi) \in T^*\mathcal{M}} h^\delta \left| \partial_\xi^\beta H_{g,h,h^{2+\alpha}} \right| \gtrsim_p h^{\alpha \frac{m}{2} + \delta} \left| \int_{\mathbb{R}^n} z^\beta k \left(\left| g_x^{\frac{1}{2}} z \right|^2 \right) dz \right| \gtrsim_{p,\beta} h^{\alpha \frac{m}{2} + \delta},$$

hence $H_{g,h,h^{2+\alpha}} \notin h^k S^m$ for any $k, m \in \mathbb{Z}$. This shows,

LEMMA 4.1. — Let $\epsilon, h \in (0, 1]$, $\mathcal{A}_{g,\epsilon}$ be given by (4.1) and $H_{g,h,\epsilon}$ be given by (4.2). Then, $\mathcal{A}_{g,\epsilon}$ with $\epsilon = h^{2+\alpha}$ for $\alpha \in \mathbb{R}$ is a Ψ DO if and only if $\alpha \geq 0$, in which case $\mathcal{A}_{g,h^{2+\alpha}} = \text{Op}_h(H_{g,h^\alpha})$ with $H_{g,h^\alpha} := H_{g,h,h^{2+\alpha}} \in h^0 S^0$ for $\alpha > 0$ and $H_{g,h^\alpha} \in h^0 S^{-\infty}$ whenever $\alpha = 0$.

The *extrinsically defined* averaging operator $\mathcal{A}_\epsilon$ given by (2.1) has small deformations from an isotropic kernel in normal coordinates that must be accounted for in its description as a Ψ DO. Even so, the regime for ϵ and h giving pseudodifferentiability is the same as in the intrinsic case and the extrinsic deviations only give lower-order terms in the symbol: this we now see in,

LEMMA 4.2. — Let $\epsilon, h \in (0, 1]$. Then, $\mathcal{A}_\epsilon$ with $\epsilon = h^{2+\alpha}$ for $\alpha \in \mathbb{R}$ is a Ψ DO if and only if $\alpha \geq 0$, in which case $\mathcal{A}_{h^{2+\alpha}} \equiv \text{Op}_h(H_{g,h^\alpha}) \pmod{h^\ell \Psi^{-m}}$ with $(\ell, m) = (2 + \alpha(1 - m/2), m)$ for $1 \leq m \leq 2(1 + 1/\alpha)$.

Remark 4.3. — We note the following cases of the order of the sub-principal symbol of $\mathcal{A}_{h^{2+\alpha}}$: we have the extremes $(\ell, m) = (1, 2(1 + 1/\alpha))$ and $(\ell, m) = (2 + \alpha/2, 1)$ and the *balanced case*, $(\ell, m) = (2, 2)$.

Proof. — We begin with a series expansion of the kernel of $\mathcal{A}_\epsilon$: by Lemma 2.5 and Taylor's formula,

$$\begin{aligned} & \left| \iota(x) - \iota \circ s_x^{-1}(v) \right|^2 = |v|^2 + \sum_{|\beta|=4} v^\beta \tilde{E}_{\iota,\beta}(x, v), \\ & \tilde{E}_{\iota,\beta}(x, v) := \frac{1}{6} \int_0^1 (1-t)^3 D_v^\beta \left[\left| \iota(x) - \iota \circ s_x^{-1}(\cdot) \right|^2 \right] \Big|_{\cdot=tv} dt, \end{aligned}$$

hence denoting $k^{(1)}(t) := \partial_t k(t)$ and $E_\iota(x, y) := \sum_{|\beta|=4} s_x(y)^\beta \tilde{E}_{\iota, \beta}(x, s_x(y))$ we have,

$$k\left(|\iota(x) - \iota(y)|^2/\epsilon\right) - k\left(d_g(x, y)^2/\epsilon\right) = k_{\iota, \epsilon}(x, y),$$

$$k_{\iota, \epsilon}(x, y) := \frac{E_\iota(x, y)}{\epsilon} \int_0^1 k^{(1)}\left(d_g(x, y)^2/\epsilon + tE_\iota(x, y)/\epsilon\right) dt.$$

There is a constant $C_{\mathcal{M}, \iota} > 0$ depending only on the geometry of $\mathcal{M}$ and embedding ι so that for all pairs $(x, y) \in \mathcal{M}^2$ in a geodesically convex neighbourhood, $|E_\iota(x, y)| \leq C_{\mathcal{M}, \iota} d_g(x, y)^4$ and by the defining assumptions on k , there is $R_k > 0$ such that k and $k^{(1)}$ decay exponentially outside of $[0, R_k]$. Therefore, if $\chi : \mathbb{R} \rightarrow \mathbb{R}$ is an even, non-negative smooth cut-off supported in $[-2R_k, 2R_k]$ and such that $\chi(t) = 1$ on $|t| \leq R_k$, then

$$k\left(|\iota(x) - \iota(y)|^2/\epsilon\right) - k\left(d_g(x, y)^2/\epsilon\right) = \tilde{k}_{\iota, \epsilon}(x, y) + O_S(\epsilon^\infty),$$

$$\tilde{k}_{\iota, \epsilon}(x, y) := k_{\iota, \epsilon}(x, y) \chi\left(d_g(x, y)^2/\epsilon - C_{\mathcal{M}, \iota} d_g(x, y)^4/\epsilon\right)$$

and there is a constant $C > 0$ depending only on $C_{\mathcal{M}, \iota}$ such that $\text{supp}[\tilde{k}_{\iota, \epsilon}(x, \cdot)] \subseteq B_{C\sqrt{\epsilon}}(x) =: \tilde{B}_{\sqrt{\epsilon}}(x) \subset \mathcal{M}$.

Now consider the operator

$$\mathcal{A}_\epsilon - \mathcal{A}_{g, \epsilon} \equiv \mathcal{A}_\epsilon^{(1)} : C^\infty \longrightarrow C^\infty$$

$$u \longmapsto \epsilon^{-\frac{n}{2}} \int_{\mathcal{M}} \tilde{k}_{\iota, \epsilon}(\cdot, y) u(y) p(y) d\nu_g(y) \pmod{h^\infty \Psi^{-\infty}}.$$

We wish to see that this is a Ψ DO with symbol belonging to $h^\ell S^{-m}$ for some $\ell, m \geq 1$, which would establish $\mathcal{A}_\epsilon$ as a Ψ DO with h -principal symbol $H_{g, \epsilon}$. By the definition of Ψ DOs on a manifold, we must thus establish that $\mathcal{A}_\epsilon^{(1)}$ is *pseudolocal* and locally resembles a Ψ DO on an open subset of Euclidean space. We begin with the former property: suppose $\chi_1, \chi_2 \in C^\infty$ with $\text{supp } \chi_1 \cap \text{supp } \chi_2 = \emptyset$. Since $\tilde{k}_{\iota, \epsilon}(x, \cdot) \chi_1(\cdot) = 0$ whenever $\text{supp } \chi_2 \cap \tilde{B}_{\sqrt{\epsilon}}(x) = \emptyset$, in order for $\chi_1(x) \tilde{k}_{\iota, \epsilon}(x, \cdot) \chi_1(\cdot) \neq 0$ we must have $\text{supp } \chi_2 \cap \tilde{B}_{\sqrt{\epsilon}}(x) \neq \emptyset$ and $x \in \text{supp } \chi_1 \cap \tilde{B}_{\sqrt{\epsilon}}(x) \neq \emptyset$, but when $\epsilon > 0$ is sufficiently small, $\tilde{B}_{\sqrt{\epsilon}}(x) \subset \text{supp } \chi_1$, so uniformly over $(0, 1]_\epsilon \times \mathcal{M}^2$ we have $|\chi_1(x) \tilde{k}_{\iota, \epsilon}(x, y) \chi_2(y)| \in O(\epsilon^\infty)$. The same holds for all derivatives of $\chi_1(x) \tilde{k}_{\iota, \epsilon}(x, y) \chi_2(y)$ since the support is stable under differentiation; furthermore, due to smoothness of this kernel, we have that $\chi_1 \mathcal{A}_\epsilon^{(1)}[\chi_2 \cdot] \in h^\infty \Psi^{-\infty}$, viz., $\mathcal{A}_\epsilon^{(1)}$ is *pseudolocal*.

We wish to see now that $\mathcal{A}_\epsilon^{(1)}$ gives, under a change of coordinates within a given patch, a Ψ DO on the corresponding open set in $\mathbb{R}^n$. So fix an atlas for $\mathcal{M}$ with $\gamma : \mathcal{M} \supset U \rightarrow V \subset \mathbb{R}^n$ providing local coordinates on the patch U and let $\chi_1, \chi_2 \in C^\infty$ with $\text{supp } \chi_1, \text{supp } \chi_2 \subset U$. Then,

$$\mathcal{A}_\epsilon^{(1)}[\chi_2 u](x) \equiv \epsilon^{-\frac{n}{2}} \int_V \tilde{k}_{\iota, \epsilon}(x, \gamma^{-1}(v)) \left[(\chi_2 \cdot p \cdot u) \circ \gamma^{-1} \right](v) |\det D\gamma^{-1}(v)| \sqrt{|g_{\gamma^{-1}(v)}|} dv$$

$$\equiv \frac{1}{(2\pi h)^n} \int_{\mathbb{R}^n} \int_{\mathbb{R}^n} e^{\frac{i}{h} \langle \gamma(x) - v, \xi \rangle} a_\gamma(\gamma(x), \xi) (\chi_2 \cdot u) \circ \gamma^{-1}(v) dv d\xi,$$

with

$$a_\gamma(\tilde{w}, \xi) := \epsilon^{-\frac{n}{2}} \int_{\mathbb{R}^n} e^{\frac{i}{h} \langle \xi, w - \tilde{w} \rangle} b_{\gamma, \epsilon}(\tilde{w}, w) dw,$$

$$b_{\gamma, \epsilon}(\tilde{w}, w) := \tilde{k}_{\iota, \epsilon}(\gamma^{-1}(\tilde{w}), \gamma^{-1}(w)) p \circ \gamma^{-1}(w) |\det D\gamma^{-1}(w)| \sqrt{|g_{\gamma^{-1}(w)}|}$$

and wherein $\equiv$ denotes equality up to a term $O_S(\epsilon^\infty)$ that is given by the action of a smoothing operator. The definition of a_γ is sensible because whenever $x \in U$, with ϵ sufficiently small we have $\text{supp}[\tilde{k}_{\iota, \epsilon}(x, \cdot)] \subset \tilde{B}_{\sqrt{\epsilon}}(x) \subset U$.

We now have $\chi_1 \mathcal{A}_\epsilon^{(1)}[\chi_2 u] = \chi_1 \gamma^* \text{Op}_h^{KN}(a_\gamma)(\gamma^{-1})^*[\chi_2 u]$ in the formal sense of quantizing a smooth scalar-valued function; we wish to see that for a certain regime of ϵ with respect to h , a_γ indeed belongs to an appropriate symbol class. We first switch to normal coordinates, wherein homothetic rescalings apply cleanly so that contracting by $\epsilon^{\frac{1}{2}}$ in these coordinates exposes the decay of a_γ in ϵ . On a change of variables $w = \gamma \circ s_x^{-1}(v)$ with $x = \gamma^{-1}(\tilde{w})$, we have

$$a_\gamma(\tilde{w}, \xi) = \epsilon^{-\frac{n}{2}} \int_{\mathbb{R}^n} e^{\frac{i}{h} \langle \xi, \gamma \circ s_x^{-1}(v) - \gamma \circ s_x^{-1}(0) \rangle} b_{\iota, \epsilon}(\tilde{w}, v) dv,$$

$$b_{\iota, \epsilon}(\tilde{w}, v) := \tilde{k}_{\iota, \epsilon}(s_x^{-1}(0), s_x^{-1}(v)) p \circ s_x^{-1}(v) |\det Ds_x^{-1}(v)| \sqrt{|g_{s_x^{-1}(v)}|}.$$

We may now apply the Kuranishi trick to the phase appearing in the representation of a_γ by way of the Taylor expansion

$$\gamma \circ s_x^{-1}(v) - \gamma \circ s_x^{-1}(0) = D[\gamma \circ s_x^{-1}]|_{v=0} \cdot v + E_\gamma(\tilde{w}, v),$$

$$E_\gamma(\tilde{w}, v) := \sum_{|\beta|=2} v^\beta \int_0^1 D_v^2[\gamma \circ s_x^{-1}](tv) dt$$

with $F(\tilde{w}) := D[\gamma \circ s_x^{-1}]|_{v=0}$ a smooth matrix-valued function, invertible at all $\tilde{w} \in V$. Since

$$E_\gamma(\tilde{w}, \epsilon^{\frac{1}{2}}v) = \epsilon E_{\gamma, \epsilon}(\tilde{w}, v),$$

$$E_{\gamma, \epsilon}(\tilde{w}, v) := \sum_{|\beta|=2} v^\beta \int_0^1 D_v^2[\gamma \circ s_x^{-1}](t\epsilon^{\frac{1}{2}}v) dt,$$

another Taylor expansion then gives,

$$e^{\frac{i}{h} \langle \xi, F(\tilde{w}) \cdot \epsilon^{\frac{1}{2}}v + E_\gamma(\tilde{w}, \epsilon^{\frac{1}{2}}v) \rangle} = e^{i\frac{\sqrt{\epsilon}}{h} \langle \xi, F(\tilde{w}) \cdot v \rangle} (1 + \epsilon^{\frac{1}{2}} \Theta_h(\tilde{w}, v, \xi, \epsilon)),$$

$$\Theta_h(\tilde{w}, v, \xi, \epsilon) := \sum_{j=1}^{\infty} \frac{\epsilon^{\frac{j-1}{2}}}{j!} \langle E_{\gamma, \epsilon}(\tilde{w}, v), (\epsilon^{\frac{1}{2}}/h) i\xi \rangle^j.$$

We also have,

$$\tilde{k}_{\iota, \epsilon}(x, s_x^{-1}(\epsilon^{\frac{1}{2}}v)) = \epsilon \tilde{b}_{\iota, \epsilon}(x, v),$$

$$\tilde{b}_{\iota, \epsilon}(x, v) := \chi(|v|^2 - \epsilon C_{\mathcal{M}, \iota} |v|^4) E_\iota(x, s_x^{-1}(v)) \int_0^1 k^{(1)}(|v|^2 + \epsilon t E_\iota(x, s_x^{-1}(v))) dt.$$

Therefore,

$$\begin{aligned} a_\gamma(\tilde{w}, \xi) &= \epsilon \int_{\mathbb{R}^n} e^{i\frac{\sqrt{\epsilon}}{h}\langle \xi, v \rangle} \left(1 + \epsilon^{\frac{1}{2}} \Theta_h(\tilde{w}, \tilde{v}, \xi, \epsilon)\right) \tilde{b}_{\iota, \epsilon}(\gamma^{-1}(\tilde{w}), \tilde{v}) \\ &\quad \times p \circ s_x^{-1}(\epsilon^{\frac{1}{2}} \tilde{v}) \left| \det Ds_x^{-1}(\epsilon^{\frac{1}{2}} \tilde{v}) \right| \left| g_{s_x^{-1}(\epsilon^{\frac{1}{2}} \tilde{v})} \right|^{\frac{1}{2}} d\tilde{v}, \\ \tilde{v} &:= F(\tilde{w})^{-1} \cdot v \end{aligned}$$

and an integration by parts gives,

$$\begin{aligned} a_\gamma(\tilde{w}, \xi) &= \epsilon \int_{\mathbb{R}^n} e^{i\frac{\sqrt{\epsilon}}{h}\langle \xi, v \rangle} \left(B_{\iota, \epsilon}(\tilde{w}, \tilde{v}) + \epsilon^{\frac{1}{2}} \tilde{B}_{\iota, \epsilon}(\tilde{w}, \tilde{v}) \right) d\tilde{v}, \\ B_{\iota, \epsilon}(\tilde{w}, \tilde{v}) &:= \tilde{b}_{\iota, \epsilon}(x, \tilde{v}) p \circ s_x^{-1}(\epsilon^{\frac{1}{2}} \tilde{v}) \left| \det Ds_x^{-1}(\epsilon^{\frac{1}{2}} \tilde{v}) \right| \left| g_{s_x^{-1}(\sqrt{\epsilon} \tilde{v})} \right|^{\frac{1}{2}}, \end{aligned}$$

wherein $\text{supp } B_{\iota, \epsilon}(\tilde{w}, \cdot) \subset \{|\tilde{v}| \leq C\}$ and $\tilde{B}_{\iota, \epsilon}(\tilde{w}, \tilde{v}) \in C_c^\infty(V \times \{|\tilde{v}| \leq C\})$ has the asymptotic expansion,

$$\tilde{B}_{\iota, \epsilon}(\tilde{w}, \tilde{v}) \sim \sum_{j=1}^{\infty} \frac{\epsilon^{\frac{j-1}{2}}}{j!} \langle E_{\gamma, \epsilon}(\tilde{w}, \tilde{v}), \nabla_v \rangle^j [B_{\iota, \epsilon}(\tilde{w}, \cdot)](\tilde{v}).$$

Now we proceed as we've done before:

$$\begin{aligned} &\langle \xi \rangle^{|\beta|-m} |\partial_{\tilde{w}}^\vartheta \partial_\xi^\beta a_\gamma| \\ &= \epsilon \langle \xi \rangle^{|\beta|-m} \left| \partial_{\tilde{w}}^\vartheta \int_{\mathbb{R}^n} \left(i\epsilon^{\frac{1}{2}}/h \right)^{|\beta|} v^\beta e^{i\frac{\sqrt{\epsilon}}{h}\langle \xi, v \rangle} \left(B_{\iota, \epsilon}(\tilde{w}, \tilde{v}) + \epsilon^{\frac{1}{2}} \tilde{B}_{\iota, \epsilon}(\tilde{w}, \tilde{v}) \right) d\tilde{v} \right| \\ &= \frac{\epsilon^{1+\frac{m}{2}}}{h^m} \left| \int_{\mathbb{R}^n} e^{i\frac{\sqrt{\epsilon}}{h}\langle \xi, v \rangle} \left(\epsilon/h^2 + \Delta_v \right)^{\frac{|\beta|-m}{2}} \right. \\ &\quad \left. \times \left(v^\beta \partial_{\tilde{w}}^\vartheta \left[\left(B_{\iota, \epsilon}(\tilde{w}, \tilde{v}) + \epsilon^{\frac{1}{2}} \tilde{B}_{\iota, \epsilon}(\tilde{w}, \tilde{v}) \right) / |\det F(\tilde{w})| \right] \right) dv \right| \end{aligned}$$

so that using $\epsilon = h^{2+\alpha}$ gives $\epsilon^{1+\frac{m}{2}}/h^m = h^{2+\alpha(1+m/2)}$. The Fourier transform is of a smooth, compactly supported function, hence it is uniformly bounded in $(0, 1]_h \times T^*\mathcal{M}$. Thus, if $\alpha > 0$ then $a_\gamma \in h^\ell S^{-m}$ for $(\ell, m) = (2 + \alpha(1 - m/2), m)$ with $m \in \mathbb{N}$, $m \leq 2(1 + 1/\alpha)$ and we may change quantizations to the adjoint form by a transformation of the symbol [Zwo12, Theorem 4.13], which retains its order. $\square$

Example. — The simplest case is to take for $\mathcal{A}_{g, \epsilon}$ the operator with Schwartz kernel $k_{g, \epsilon}(x, y) := \epsilon^{-\frac{n}{2}} e^{-d_g(x, y)^2/\epsilon}$ and uniform density $p \equiv 1$. Then, an h -Fourier transformation shows that $H_{g, h, \epsilon} := \pi^{\frac{3n}{2}} e^{-\frac{\epsilon}{4h^2} |\xi|_{g_x}^2} |g_x|^{-\frac{1}{2}}$. Recall that due to the uncertainty principle, a semiclassical Ψ DO is defined for symbols with small variation in regions of phase space with unit volume. This symbol $H_{g, h, \epsilon}$ varies polynomially within a ball of radius $O(h/\sqrt{\epsilon})$ in each cotangent fibre $T_x^*\mathcal{M}$ and decays exponentially outside of this ball. When $\epsilon = h^{2+\alpha}$, this symbol has exponential decay within a ball of radius $h^{-\alpha/2-\delta}$ for $\delta > 0$, so for $\alpha < 0$ this amounts to large variation in sub-unit volume regions of phase space. Another (*dual*) perspective is that in order for $\mathcal{A}_{g, \epsilon}$ to be regarded as a semiclassical Ψ DO in quantization scale h , by pseudolocality it must have Schwartz kernel $k_{g, \epsilon}$ that decays, along with all derivatives, as $O(h^\infty |x - y|^{-\infty})$ outside of the diagonal. The critical rate here is $\sqrt{\epsilon}$, in the sense

that for points with $0 < d_g(x, y) < \sqrt{\epsilon}$, the Schwartz kernel $k_{g,\epsilon}$ follows this decay rate if and only if $h > \sqrt{\epsilon}$. Effectively, if h remains below this rate, then all of the *content* of the symbol is lost and hence the quantum-classical correspondence breaks down: quantization forces such a symbol to be essentially zero (an impulse at the zero section of the cotangent bundle), while $\mathcal{A}_{g,\epsilon}$ behaves as $\epsilon \rightarrow 0$ like an operator with symbol having support in all of the cotangent bundle and moreover, going to a constant as $h \rightarrow 0$.

We may now employ symbol calculus to express graph Laplacians as Ψ DOs:

THEOREM 4.4. — *Let $\lambda \geq 0$, $\epsilon, h \in (0, 1]$ with $\epsilon = h^{2+\alpha}$ and $\alpha > 0$. Then,*

$$\mathcal{L}_{g,\lambda,h^\alpha} := \frac{2c_0}{c_2} \frac{1 - H_{g,h^\alpha} / (p_\epsilon^{2\lambda} p_{\lambda,\epsilon})}{h^\alpha} \in h^0 S^2$$

and $h^2 \Delta_{\lambda,\epsilon} \in h^0 \Psi^2$ with

$$h^2 \Delta_{\lambda,\epsilon} \equiv \text{Op}_h(\mathcal{L}_{g,\lambda,h^\alpha}) \pmod{h\Psi^1}.$$

Moreover, if we fix $0 \leq \delta \leq 1$ and $C > 0$ and let $\chi_C : \mathbb{R} \rightarrow \mathbb{R}$ be a smooth function with $\text{supp } \chi_C \subseteq [-C, C]$, then for all pairs $(m, \alpha) \in \mathbb{Z} \times [1, \infty)$ that satisfy $\alpha \geq 1 + \delta(4 + m)$, we have

$$\text{Op}_h(\mathcal{L}_{g,\lambda,h^\alpha} \chi_C(h^{2\delta} |\xi|_{g_x}^2)) \equiv \text{Op}_h(|\xi|_{g_x}^2 \chi_C(h^{2\delta} |\xi|_{g_x}^2)) \pmod{h\Psi^{-m}}$$

and in particular, when $\delta = 0$, this holds with $m = \infty$ for all $\alpha \geq 1$.

Remark 4.5. — The picture to keep in mind for the symbol is, for example, given in Figure 4.1 for the kernel $k(d_g(x, y)^2/\epsilon) := \exp(-d_g(x, y)^2/\epsilon)$ with $\epsilon = h^{2+\alpha}$. The function $\mathcal{L}_{g,\lambda,h^\alpha}$ approximates $|\xi|_{g_x}^2$ within a neighbourhood of $0 \in T^*\mathcal{M}$ that grows as $h \rightarrow 0$. The rate of this approximation governs simultaneously, the symbol class and the momentum magnitude within which we can recover $|\xi|_{g_x}^2$, set by m and δ , respectively. As the figure shows, $\mathcal{L}_{g,\lambda,h^\alpha}$ is clearly not principal in $h^0 S^2$; hence, as we will see later, dynamics generated by the graph Laplacian connect well to Hamiltonian dynamics on $T^*\mathcal{M}$ when we can take $m = \infty$.

Proof. — Since Lemma 4.2 gives $\mathcal{A}_\epsilon$ as a Ψ DO and the operators of multiplication by $p_{\lambda,\epsilon}^{-1}, p_\epsilon^{-\lambda} \in C^\infty$ are readily seen to be Ψ DOs with symbols $p_{\lambda,\epsilon}^{-1}, p_\epsilon^{-\lambda} \in h^0 S^0$ respectively, we may employ the symbol calculus upon writing $\mathcal{A}_{\lambda,\epsilon}$ as a product of these operators to get:

$$\begin{aligned} A_{\lambda,\epsilon}^{(1)} &:= \mathcal{A}_{\lambda,\epsilon} - A_{g,\lambda,\epsilon} = p_{\lambda,\epsilon}^{-1} p_\epsilon^{-\lambda} \mathcal{A}_\epsilon^{(1)} p_\epsilon^{-\lambda} \in h^\ell \Psi^{-m}, \\ A_{g,\lambda,\epsilon}[\cdot] &:= p_{\lambda,\epsilon}^{-1} p_\epsilon^{-\lambda} \mathcal{A}_{g,\epsilon}[p_\epsilon^{-\lambda} \cdot] \in h^0 \Psi^0 \end{aligned}$$

with $(\ell, m) \in \mathbb{R} \times \mathbb{Z}$ as in Lemma 4.2 and

$$\tilde{\Delta}_{\lambda,h,\alpha} := h^2 \frac{c_2}{2c_0} \Delta_{\lambda,\epsilon} = \frac{I - A_{\lambda,\epsilon}}{h^\alpha} = \frac{I - A_{g,\lambda,\epsilon}}{h^\alpha} - h^{-\alpha} A_{\lambda,\epsilon}^{(1)}.$$

Since $h^{-\alpha} A_{\lambda,\epsilon}^{(1)} \in h^{\ell'} \Psi^{-m}$ with $(\ell', m) = (2 - \alpha m/2, m)$ and

$$\text{Op}_h(H_{g,h^\alpha} / (p_\epsilon^{2\lambda} p_{\lambda,\epsilon})) \equiv \mathcal{A}_{g,\epsilon} \circ \frac{1}{p_\epsilon^{2\lambda} p_{\lambda,\epsilon}} \pmod{h^\infty \Psi^{-\infty}},$$

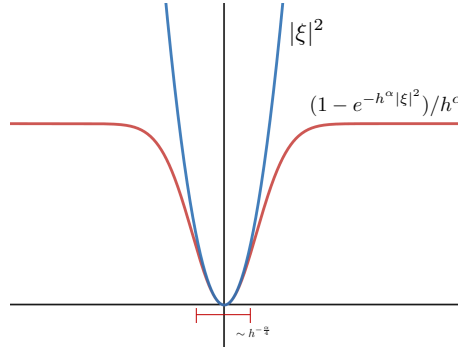


Figure 4.1. The symbol $\mathcal{L}_{g,\lambda,h^\alpha}$ for $k(d_g(x,y)^2/h^{2+\alpha}) := \exp(-d_g(x,y)^2/h^{2+\alpha})$ (modulo normalization factors) in comparison with the symbol $|\xi|_{g_x}^2$, depicted in terms of momentum magnitudes $|\xi|$ along the horizontal axis. Note that the modulus of the symbol of the graph Laplacian grows as $\Theta(h^{-\alpha})$ outside of a sufficiently large neighbourhood of $0 \in T^*\mathcal{M}$, which means it is not principal in h^0S^2 , but cutting off to a neighbourhood is sufficient for connecting with Hamiltonian mechanics via Egorov's theorem.

we have

$$(4.3) \quad \begin{aligned} \tilde{\Delta}_{\lambda,h,\alpha} &\equiv (p_\epsilon^\lambda p_{\lambda,\epsilon})^{-1} \tilde{\Delta}_{g,\lambda,h^\alpha} p_\epsilon^\lambda p_{\lambda,\epsilon} - h^{-\alpha} A_{\lambda,\epsilon}^{(1)} \pmod{h^\infty \Psi^{-\infty}}, \\ \tilde{\Delta}_{g,\lambda,h^\alpha} &:= (I - \text{Op}_h(H_{g,h^\alpha}/p_\epsilon^{2\lambda} p_{\lambda,\epsilon}))/h^\alpha, \end{aligned}$$

hence to see the first part of the theorem, it suffices to show that

$$L_{g,\lambda,h^\alpha} := \frac{1 - H_{g,h^\alpha}/p_\epsilon^{2\lambda} p_{\lambda,\epsilon}}{h^\alpha} \in h^0S^2.$$

A change of variables in the representation (4.2) shows the form,

$$H_{g,h^\alpha}(x, \xi) = p(x) \int_{\mathbb{R}^n} e^{ih^{\alpha/2} \langle z, g_x^{-1/2} \xi \rangle} k(|z|^2) dz$$

and combining this with the defining assumption that k decays at least as fast as an exponential implies that H_{g,h^α} is analytic in ξ . Thus, by a Taylor series at $\xi = 0$ we have the expansion

$$\begin{aligned} (H_{g,h^\alpha}/(p_\epsilon^{2\lambda} p_{\lambda,\epsilon}))(x, \xi) &= \frac{p(x)}{p_\epsilon^{2\lambda} p_{\lambda,\epsilon}(x)} \sum_{|\kappa| \geq 0} \frac{(-1)^{|\kappa|} h^{|\kappa|}}{(2\kappa)!} (g_x^{-1/2} \xi)^{2\kappa} c_{2\kappa}, \\ c_{2\kappa} &:= \int z^{2\kappa} k(|z|^2) dz. \end{aligned}$$

By Lemma 2.13, there is a function $q_\lambda \in C^\infty$ depending only on p , $\mathcal{M}$, c_0 and λ such that

$$p_{\lambda,\epsilon} = (c_0 p)^{1-2\lambda} + \epsilon c_2 p^{1-2\lambda} q_\lambda + O(\epsilon^2).$$

Applying this to $p_\epsilon = p_{0,\epsilon}$ and taking a Taylor series shows

$$\begin{aligned} p_\epsilon^{2\lambda} &= (c_0 p)^{2\lambda} + \epsilon (c_0 p)^{2\lambda-1} \tilde{q}_\lambda + O(\epsilon^2), \\ \tilde{q}_\lambda &:= 2\lambda c_2 p q_0. \end{aligned}$$

Therefore,

$$p_{\lambda,\epsilon} p_\epsilon^{2\lambda} = c_0 p + \epsilon \tilde{q}_{\lambda,0} + O(\epsilon^2),$$

$$\tilde{q}_{\lambda,0} := \tilde{q}_\lambda + c_0^{2\lambda} c_2 p q_\lambda$$

and upon taking a geometric series expansion this leads to

$$p / (p_{\lambda,\epsilon} p_\epsilon^{2\lambda}) = c_0^{-1} [1 - \epsilon \tilde{q}_{\lambda,0} / (c_0 p) + O(\epsilon^2)].$$

Employing this expansion we now have,

$$(4.4) \quad \frac{1 - H_{g,h^\alpha} / (p_\epsilon^{2\lambda} p_{\lambda,\epsilon})}{h^\alpha}$$

$$= h^{-\alpha} \left(1 - \frac{c_0 p}{p_\epsilon^{2\lambda} p_{\lambda,\epsilon}} \right) + \frac{p}{p_\epsilon^{2\lambda} p_{\lambda,\epsilon}} \sum_{|\kappa| \geq 1} \frac{(-1)^{|\kappa|-1}}{(2\kappa)!} h^{\alpha(|\kappa|-1)} (g_x^{-1/2} \xi)^{2\kappa} c_{2\kappa}$$

$$= \frac{c_2}{2} \frac{p}{p_\epsilon^{2\lambda} p_{\lambda,\epsilon}} |\xi|_{g_x}^2 + h^2 \tilde{q}_{\lambda,0} / (c_0 p) + O_x(h^{4+\alpha})$$

$$+ \frac{p}{p_\epsilon^{2\lambda} p_{\lambda,\epsilon}} \sum_{|\kappa| \geq 2} \frac{(-1)^{|\kappa|-1}}{(2\kappa)!} h^{\alpha(|\kappa|-1)} (g_x^{-1/2} \xi)^{2\kappa} c_{2\kappa}$$

$$= \frac{c_2}{2c_0} |\xi|_{g_x}^2 + O_x(h^2) + \frac{p}{p_\epsilon^{2\lambda} p_{\lambda,\epsilon}} \sum_{|\kappa| \geq 2} \frac{(-1)^{|\kappa|-1}}{(2\kappa)!} h^{\alpha(|\kappa|-1)} (g_x^{-1/2} \xi)^{2\kappa} c_{2\kappa},$$

wherein the $O_x(h^2)$ term denotes that it is a function only of x and h and is uniformly bounded (due to compactness of $\mathcal{M}$) by a constant multiple of h^2 . Denoting $L_{g,\lambda,h^\alpha} := (1 - H_{g,h^\alpha} / (p_\epsilon^{2\lambda} p_{\lambda,\epsilon})) / h^\alpha$, we see from this, that for small $|\xi| \leq h^{-\alpha/2}$, $m \geq 2$, $0 \leq |\beta| \leq m$ and all $\gamma \geq 0$,

$$\begin{aligned} & |\langle \xi \rangle^{|\beta|-m} \partial_x^\gamma \partial_\xi^\beta L_{g,\lambda,h^\alpha}| \\ & \lesssim_\gamma \langle \xi \rangle^{2-m} + h^2 \langle \xi \rangle^{-m} + \langle \xi \rangle^{|\beta|-m} \sum_{|\kappa| \geq \max\{2, |\beta|/2\}} h^{\alpha(|\kappa|-1)} \frac{c_{2\kappa}}{(2\kappa - \beta)!} |\xi^{2\kappa - \beta}| \\ & \lesssim_{\gamma,\beta} (1 + h^{-\alpha})^{(|\beta|-2-(m-2))/2} (h^\alpha)^{|\beta|/2-1} \sum_{|\kappa| \geq 2} \frac{c_{2\kappa}}{(2\kappa - \beta)!} \\ & \lesssim_{\gamma,\beta} (h^\alpha + 1)^{|\beta|/2-1} (1 + h^{-\alpha})^{-(m-2)/2} \lesssim_{\gamma,\beta} 1, \end{aligned}$$

while for large $|\xi| > h^{-\frac{\alpha}{2}}$,

$$\begin{aligned} & |\langle \xi \rangle^{|\beta|-m} \partial_x^\gamma \partial_\xi^\beta L_{g,\lambda,h^\alpha}| \\ & \lesssim (1 + h^{-\alpha})^{\frac{|\beta|-m}{2}} (h^\alpha)^{\frac{|\beta|}{2}-1} \\ & \quad \times \left| \int_{\mathbb{R}^n} e^{ih^{\alpha/2} \langle z, \xi \rangle} z^\beta \partial_x^\gamma \left(\delta_0(z) - k(|g_x^{1/2} z|^2) |g_x|^{1/2} \frac{p(x)}{p_\epsilon^{2\lambda}(x) p_{\lambda,\epsilon}(x)} \right) dz \right| \\ & \lesssim_{\gamma,\beta} (h^\alpha + 1)^{|\beta|/2-1} (1 + h^{-\alpha})^{-(m-2)/2} \end{aligned}$$

so together this implies $\langle \xi \rangle^{|\beta|-m} |\partial_x^\gamma \partial_\xi^\beta L_{g,\lambda,h^\alpha}|$ is uniformly bounded in $(0, 1]_h \times T^* \mathcal{M}$. Further, for $|\beta| \geq m$ we have

$$\begin{aligned}
& \left| \langle \xi \rangle^{|\beta|-m} \partial_x^\gamma \partial_\xi^\beta L_{g,\lambda,h^\alpha} \right| \\
&= \left| \int e^{ih^{\alpha/2} \langle z, \xi \rangle} (h^\alpha)^{m/2-1} (h^\alpha + \Delta_z)^{(|\beta|-m)/2} \right. \\
&\quad \left. \left(z^\beta \partial_x^\gamma \left[k \left(|g_x^{1/2} z|^2 \right) |g_x|^{1/2} \frac{p(x)}{p_\epsilon^{2\lambda}(x) p_{\lambda,\epsilon}(x)} \right] \right) dz \right| < \infty,
\end{aligned}$$

so altogether we find that $L_{g,\lambda,h^\alpha} \in h^0 S^2$. This is the minimal order for this symbol because if we follow the expansion (4.4) along $\langle \xi \rangle \sim h^{-\beta}$ for $\beta < \alpha/2$, then we find that $L_{g,\lambda,h^\alpha}(\cdot, \xi)/\langle \xi \rangle \sim h^{-\beta}$, hence through its scaling with h , the symbol L_{g,λ,h^α} escapes the lower order classes.

Now an application of symbol calculus to (4.3) shows that for $\alpha > 0$,

$$h^2 \Delta_{\lambda,\epsilon} \equiv \text{Op}_h \left(\frac{2c_0}{c_2} L_{g,\lambda,h^\alpha} \right) \pmod{h\Psi}.$$

If we introduce a smooth cut-off $\chi_{C,h^{-\delta}}(\cdot) := \chi_C(h^{2\delta} \cdot)$ with $\text{supp } \chi_C \subseteq [-C, C]$ for $0 < \delta < 1$ and $C > 0$, then from (4.4) we see that for each $m \in \mathbb{R}$,

$$\begin{aligned}
& h^{-1} \langle \xi \rangle^{|\beta|+m} \left| \chi_{C,h^{-\delta}}(|\xi|_{g_x}^2) \partial_x^\gamma \partial_\xi^\beta \left[L_{g,\lambda,h^\alpha} - \frac{c_2}{2c_0} |\xi|_{g_x}^2 \right] \right| \\
& \lesssim_\gamma h^{-1} (1 + C^2 h^{-2\delta})^{(|\beta|+m)/2} \sum_{|\kappa| \geq \max\{2, |\beta|/2\}} h^{\alpha(|\kappa|-1) - \delta(2|\kappa|-|\beta|)} \frac{c_{2\kappa}}{(2\kappa - \beta)!} \\
& \lesssim_{\gamma,\beta} \sum_{|\kappa| \geq \max\{2, |\beta|/2\}} h^{-\delta(m+|\beta|)} h^{-1} h^{\alpha(|\kappa|-1) - \delta(2|\kappa|-|\beta|)} \frac{c_{2\kappa}}{(2\kappa - \beta)!} \\
& \lesssim_{\gamma,\beta} \sum_{|\kappa| \geq 2} h^{(|\kappa|-1)(\alpha - [\delta(2|\kappa|+m)+1]/(|\kappa|-1))} \frac{c_{2\kappa}}{(2\kappa)!} \\
& \lesssim_{\gamma,\beta} h^{\alpha - (1+\delta(4+m))}.
\end{aligned}$$

Since the partial derivatives of $\chi_{C,h^{-\delta}}(|\xi|_{g_x}^2)$ are also cut-offs of $|\xi|_{g_x}^2$ in the same region and the above bound holds with the factor $\chi_{C,h^{-\delta}}$ replaced by any such cut-off, we find that upon summing up via the triangle inequality, we have the same bound up to (new) constants depending on γ and β . Therefore,

$$\text{Op}_h \left((2c_0/c_2) L_{g,\lambda,h^\alpha} \chi_{C,h^{-\delta}}(|\xi|_{g_x}^2) \right) \equiv \text{Op}_h \left(|\xi|_{g_x}^2 \chi_{C,h^{-\delta}}(|\xi|_{g_x}^2) \right) \pmod{h\Psi^{-m}}$$

whenever $\alpha \geq 1 + \delta(4+m)$ so in particular, we may take $m = \infty$ when $\delta = 0$. $\square$

Remark 4.6. — The second part of this theorem can be generalized to give a lower bound $\rho + \delta(4+m)$ on α if instead of using the unit step size for orders of h in the pseudodifferential calculus, we take steps of size $\rho > 0$. In any case, while $\alpha = 0$ is applicable to the first part of the theorem (and then we actually have $h^2 \Delta_{\lambda,\epsilon} \in h^0 \Psi^{-\infty}$) as the second part shows, this would not be able to extract the *kinetic term* $|\xi|_{g_x}^2$ (for any step size $\rho > 0$).

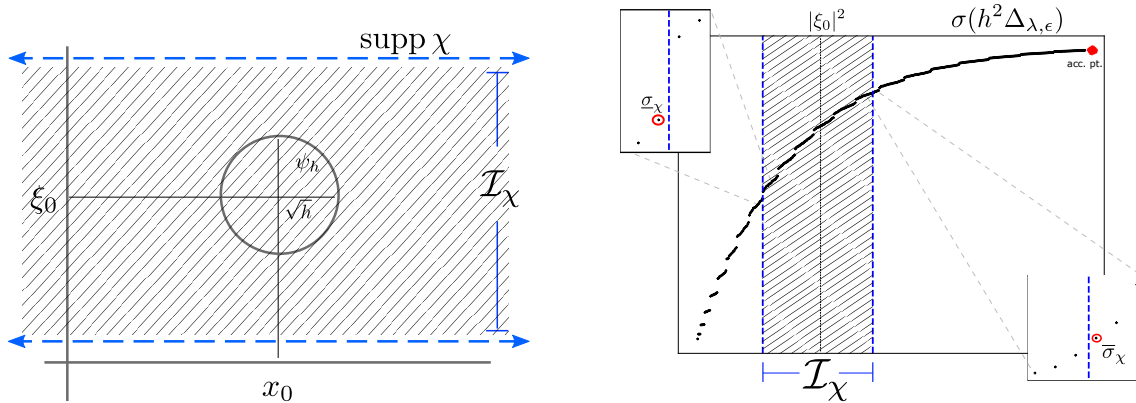


Figure 4.2. The cut-off χ on phase-space (left) and on the spectrum⁽⁷⁾ (right). The accumulation point of the spectrum sits at $1/\epsilon$ and as the shape along with the spectral gaps indicate, the spectrum approximates that of $\Delta_{\mathcal{M}}$ in a scaling $\ll 1/\sqrt{\epsilon}$ below the reciprocal of the kernel bandwidth. Note the similarity of structure, even to the high end of the spectrum, with the approximation of the symbol $|\xi|_{g_x}^2$ by the symbol of the graph Laplacian in Figure 4.1. The points $\sigma_\chi, \bar{\sigma}_\chi$ mark the nearest eigenvalues outside of $\mathcal{I}_\chi$.

4.2. Semiclassical spectral calculus for graph Laplacians

In light of the semiclassical analysis of graph Laplacians, we may apply microlocal methods to discern frequency space behaviour of their higher spectral components, following the methods of [DS99, Section 8]. Broadly, the notion is that once the pseudodifferential calculus is turned to spectral functions $f(h^2 \Delta_{\lambda, \epsilon})$ for $f \in C_0^\infty(\mathbb{R})$, the resulting symbol calculus reveals phase space properties such as localization and growth of the spectrum of $\Delta_{\lambda, \epsilon}$ at eigenvalue scales $\sim 1/h^2 = \epsilon^{-\frac{2}{2+\alpha}}$. This is supported by the machinery of the Helffer–Sjöstrand functional calculus that gives symbol estimates through an almost-analytic continuation of f combined with a priori semiclassical estimates for resolvents. Our main application will be to see that the spectral localizations of graph Laplacians at such *semiclassical* scales are microlocalized to balls of constant radius in semiclassical⁽⁸⁾ phase space.

The symbol calculus of Theorem 4.4 and remarks thereafter point out a caveat in the application of the Helffer–Sjöstrand functional calculus, however: the graph Laplacian $h^2 \Delta_{\lambda, \epsilon}$ is not elliptic in its class, $h^0 \Psi^2$. This reflects that at sufficiently high frequencies, the symbol $L_{\lambda, \epsilon}$ stops providing a good approximation of $|\xi|_{g_x}^2$, as depicted in Figure 4.1. In that regime, then, the graph Laplacian behaves more like a scalar operator rather than the Laplace–Beltrami operator. Furthermore, if $\chi \in C_c^\infty(\mathbb{R})$, then $\epsilon \Delta_{\lambda, \epsilon} \in h^\alpha S^0$ is elliptic of zeroth order only when $\alpha = 0$. As we have remarked already following Theorem 4.4, at this scaling we are not able to extract

⁽⁷⁾ The plot is actually of the first 480 eigenvalues of $\Delta_{1, \epsilon, N}$ for $N = 6000$ uniformly random samples from the unit sphere in $\mathbb{R}^3$ with $\epsilon = e^{-3.4}$.

⁽⁸⁾ We refer to the scaling of momentum ξ , or effectively the cotangent space $T_x^*(\mathcal{M})$, at the rate ξ/h , as the *semiclassical phase space*. Hence, a ball of constant radius in this scaling is a ball of radius $\Theta(1/h)$ at momentum magnitudes $\Theta(1/h)$.

the *kinetic term* $|\xi|_{g_x}^2$ of the classical Hamiltonian from the principal symbol of $h^2\Delta_{\lambda,\epsilon}$. We mention a relationship with the spectral convergence of graph Laplacians to the Laplace–Beltrami operator $\Delta_{\mathcal{M}}$: the convergence of eigenvectors is based on the presence of spectral gaps in $\Delta_{\lambda,\epsilon}$ of roughly the same sizes as present in $\Delta_{\mathcal{M}}$, established through the Davis–Kahan method, for example as in [CGT22, proof of Theorem 2.7(2)] or [BN06]. Interestingly, Weyl asymptotics yield that the threshold for this at the semiclassical eigenvalue scales $\sim 1/h^2$ is the condition $h \gg \epsilon^{1/(2n-4)}$, with rates that depend directly on the bias error discrepancy, requiring $\epsilon^{1/6}/h \ll 1$ for stability.

Should a *clean* application of the Helffer–Sjöstrand formalism be possible, we would obtain global phase space information about the eigenfunctions of graph Laplacians as follows: if $\chi(h^2\Delta_{\lambda,\epsilon})$ would be a Ψ DO with a symbol expansion given by that method (specifically, [DS99, Theorem 8.7 & following remarks]) with $\mathcal{I}_\chi := \{\chi \equiv 1\}$ an interval, then we would have for any $\tilde{\chi} \in C_c^\infty(\mathbb{R})$ with $\text{supp } \tilde{\chi} \subset \mathcal{I}_\chi$ that for all sufficiently small $h > 0$, $\text{Op}_h(\tilde{\chi}(|\xi|_{g_x}^2))[I - \chi(h^2\Delta_{\lambda,\epsilon})] \in h^\infty\Psi^{-\infty}$. This means that given any eigenfunction φ with corresponding eigenvalue $\lambda \notin \text{supp } \chi$, we would find $\text{Op}_h(\tilde{\chi}(|\xi|_{g_x}^2))\varphi = O_s(h^\infty)$. In turn, given any coherent state ψ_h^ζ with $\zeta := (x, \xi)$ such that the essential support of $T_h\psi_h^\zeta$ resides in $\text{supp } \tilde{\chi}(|\xi|_{g_x}^2)$, we would have that $|\langle \psi_h^\zeta | \varphi \rangle| = O(h^\infty)$. The schematics in Figure 4.2 show a cut-off applied to the true spectrum of a numerical graph Laplacian and a depiction of the corresponding action of the cut-off in phase space, relative to the localization of ψ_h^ζ . Altogether, in as far as the quantization of $\tilde{\chi}(|\xi|_{g_x}^2)$ is seen as a frequency cut-off or the inner products of a function with coherent states (effectively the function’s FBI transform) gives its phase space content, we would find that *only* the eigenfunctions with eigenvalues in $\mathcal{I}_\chi$ have frequency content at scales $|\xi|_{g_x} \sim \sqrt{\mathcal{I}_\chi}/h$. As mentioned, the Ψ DO calculus and hence, this analysis, go through for $\alpha = 0$, modulo χ being a spectral projector. This tells that the eigenfunctions at the *extreme end* of the spectrum, with eigenvalues $\sim 1/\epsilon$ are localized in frequency space in balls of radius $\sim 1/\sqrt{\epsilon}$ at frequencies of magnitude $\sim 1/\sqrt{\epsilon}$. Moreover, eigenfunctions corresponding to eigenvalues σ with $0 < \sigma \ll 1/\epsilon$ must have frequency content $\ll 1/\sqrt{\epsilon}$.

The spectral asymptotics may be pushed further by using h -dependent cut-offs $\chi_{h^\delta}(\cdot) := \chi(h^{-\delta}\cdot)$ for $0 \leq \delta < 1/2$, following the extension of the Helffer–Sjöstrand approach to this case given in [Küs17]. Continuing with $\alpha = 0$, this leads to the frequency concentration of eigenfunctions in the spectral regime $\sigma \sim 1/\epsilon^{1-\delta/2}$ to within balls of radius $\sim 1/\epsilon^{1/2-\delta/4}$ at frequency magnitudes $\sim 1/\epsilon^{1/2-\delta/4}$. All eigenfunctions outside of this spectral scaling must then also be localized away from the corresponding *strips* of phase space. If we switch to $h^2 = \epsilon^{1-\delta/2}$, then $\alpha = 2\delta/(2-\delta)$ sets $h := \epsilon^{1/(2+\alpha)} = \epsilon^{1/2-\delta/4}$, so this approach in fact gives semiclassical estimates for $\Theta(h^0)$ -localized spectral functions of $h^2\Delta_{\lambda,\epsilon}$ in the regime $0 \leq \alpha < 2/3$. This means we are able to extract the principal symbol $f(\mathcal{L}_{g,\lambda,h^\alpha})$, hence also the approximation $f(|\xi|_{g_x}^2)$ corresponding to the kinetic term, from $f(h^2\Delta_{\lambda,\epsilon})$, to order $\epsilon^{\min\{\delta/2, 1-2\delta\}}$. Such direct applications of these techniques only reach as low as the spectral regime $\sigma \sim \epsilon^{-3/4}$, and we must apply some restrictions in the frequency domain to peer lower.

We study spectral regimes of graph Laplacians at $\sigma \sim \epsilon^{-2/(2+\alpha)}$ for $\alpha \geq 1$ by localizing the analysis in frequency space. Rather than providing direct information about the frequency localization of eigenfunctions within some spectral window, this approach reveals that those lying *outside* of the spectral regime fixed by α must have frequency content *disjoint* from momentum shells of scale $\sim 1/h$. Specifically, we develop semiclassical estimates for $f(h^2\Delta_{\lambda,\epsilon})\hat{\chi}$ where $\hat{\chi} \in \Psi^{-\infty}$ is a frequency cutoff in some phase space strip $\mathcal{K} \subset T^*\mathcal{M}$. By choosing f to act *locally* as an identity in a spectral window larger than the width of $\mathcal{K}$, we ensure that $O(h^0)$ -localized frequency strips are occupied exclusively by eigenfunctions at spectral scales $\Theta(h^0)$.

THEOREM 4.7. — *Let $\lambda \geq 0$, $\epsilon, h \in (0, 1]$ with $\epsilon = h^{2+\alpha}$ and $\alpha \geq 1$. Then, given $\chi, \tilde{\chi} \in C_c^\infty(\mathbb{R})$, there is $h_0 \in (0, 1]$ such that for all $h \in (0, h_0]$, we have for $\hat{\chi} := \text{Op}_h(\tilde{\chi}(|\xi|_{g_x}^2))$ and $P_\chi := \chi(h^2\Delta_{\lambda,\epsilon})$ that*

$$P_\chi \hat{\chi}, \hat{\chi} P_\chi \in h^0 \Psi^{-\infty}, \quad \text{Sym}[P_\chi \hat{\chi}] = \text{Sym}[\hat{\chi} P_\chi] = \chi(|\xi|_{g_x}^2) \tilde{\chi}(|\xi|_{g_x}^2)$$

and in particular if $\text{supp } \tilde{\chi} \subset \{\chi \equiv 1\}$ then,

$$\chi(h^2\Delta_{\lambda,\epsilon})\hat{\chi} \equiv \hat{\chi} \pmod{h^\infty \Psi^{-\infty}}, \quad [\chi(h^2\Delta_{\lambda,\epsilon}), \hat{\chi}] \in h^\infty \Psi^{-\infty}.$$

Proof. — We will switch temporarily to the symmetric graph Laplacian $\Delta_{\lambda,\epsilon}^{(s)}$ by conjugating $\Delta_{\lambda,\epsilon}$ with $\sqrt{p_{\lambda,\epsilon}}$ as per Lemma 2.12 and utilize the Weyl quantization $\text{Op}_h^w := \text{Op}_h^{1/2}$. We will use the notation $\sharp_h$ to denote the corresponding composition formula for symbols in the context of Weyl quantization: $\text{Op}_h^w(a) \text{Op}_h^w(b) = \text{Op}_h^w(a \sharp_h b)$. This guarantees that the symbol $L_{\lambda,\epsilon}^{(s)} \in h^0 S^2$ such that $\Delta_{\lambda,\epsilon}^{(s)} = \text{Op}_h^w(L_{\lambda,\epsilon}^{(s)})$ is real-valued. Moreover, since $L_{\lambda,\epsilon}^{(s)} \equiv \mathcal{L}_{g,\lambda,h^\alpha} \pmod{hS^1}$, the local approximation of $\mathcal{L}_{g,\lambda,h^\alpha}$ by $|\xi|_{g_x}^2$ given in Theorem 4.4 shows that if $\chi_0 \in C_c^\infty(\mathbb{R})$ and $\text{supp } \tilde{\chi} \subset \{\chi_0 \equiv 1\}$, then there is $h_0 \in (0, 1]$ such that for all $h \in (0, h_0]$ we have $\text{supp } \tilde{\chi}(|\xi|_{g_x}^2) \subset \{\chi_0 \circ L_{\lambda,\epsilon}^{(s)} \equiv 1\}$. We now proceed in this regime and just note that by changing quantizations and conjugating with $1/\sqrt{p_{\lambda,\epsilon}}$, we will have the results for the graph Laplacian and adjoint quantization, up to the sub-principal symbols.

Step 1. — The almost-analytic functional calculus developed by Helffer and Sjöstrand in [HS89] shows that for χ_{an} the almost-analytic extension of χ ,

$$P_\chi := \chi(h^2\Delta_{\lambda,\epsilon}^{(s)}) = -\frac{1}{\pi} \int_{\mathbb{C}} \bar{\partial} \chi_{\text{an}}(z) \left(z - h^2\Delta_{\lambda,\epsilon}^{(s)} \right)^{-1} dz.$$

Now let $E_{\lambda,\epsilon,h} := [I - (z - h^2\Delta_{\lambda,\epsilon}^{(s)}) \text{Op}_h^w(1/(z - L_{\lambda,\epsilon}^{(s)}))]/h = \text{Op}_h^w(\tilde{r}_{\lambda,\epsilon}(\cdot; z))$ with $\tilde{r}_{\lambda,\epsilon}(\cdot; z) := \frac{1}{h} [1 - (z - L_{\lambda,\epsilon}^{(s)}) \sharp_h 1/(z - L_{\lambda,\epsilon}^{(s)})]$. By following the shape of L_{g,λ,h^α} and arguing along the lines of the exactness of its order in the proof of Theorem 4.4, we find that in the region of frequency space (modulated by the semiclassical parameter, namely $|\xi|_{g_x} \sim h^{-\alpha/2}$) where that symbol is of order $(0, 2)$, the symbol $1/(z - L_{\lambda,\epsilon}^{(s)})$ is of order $(0, -2)$. Likewise, at higher frequencies where L_{g,λ,h^α} behaves of order $(0, 0)$, we find that so does $1/(z - L_{\lambda,\epsilon}^{(s)})$. Thus working locally, we find that in fact

$\tilde{r}_{\lambda,\epsilon}(\cdot; z) \in h^0 S^{-1}$. Then,

$$\mathrm{Op}_h^w\left(\frac{1}{z - L_{\lambda,\epsilon}^{(s)}}\right) \sum_{j=0}^N h^j E_{\lambda,\epsilon,h}^j = \left(z - h^2 \Delta_{\lambda,\epsilon}^{(s)}\right)^{-1} \left(I - h^{N+1} E_{\lambda,\epsilon,h}^{N+1}\right)$$

and the left-hand side along with $(I - h^{N+1} E_{\lambda,\epsilon,h}^{N+1})^{-1}$ are Ψ DOs, so that $(z - h^2 \Delta_{\lambda,\epsilon}^{(s)})^{-1}$ is as well. Hence, $R_N(z) := (z - h^2 \Delta_{\lambda,\epsilon}^{(s)})^{-1} E_{\lambda,\epsilon,h}^{N+1} \in h^0 \Psi^{-N-1}$ and continuing this way we have,

$$(4.5) \quad P_\chi = -\frac{1}{\pi} \int_{\mathbb{C}} \bar{\partial} \chi_{\mathrm{an}}(z) \left[\mathrm{Op}_h^w(r_{\lambda,\epsilon}(\cdot; z)) + R(z) \right] dz,$$

with $R(z) \in h^\infty \Psi^{-\infty}$ and

$$r_{\lambda,\epsilon} \sim \sum_{j=0}^{\infty} h^j \left(z - L_{\lambda,\epsilon}^{(s)}\right)^{-1} \underbrace{\sharp_h \tilde{r}_{\lambda,\epsilon}(\cdot; z) \sharp_h \dots \sharp_h \tilde{r}_{\lambda,\epsilon}(\cdot; z)}_{j \text{ times}}.$$

This gives an integral representation for P_χ through a family of Ψ DOs, which yields a symbol expansion upon microlocalization to a compact part of phase space.

Step 2. — We introduce a frequency cut-off by forming the product $P_\chi \hat{\chi}$. Then for the family of operators in the integrand on the right-hand side of (4.5) we have that

$$r_{\lambda,\epsilon} \sharp_h \tilde{\chi}(|\xi|_{g_x}^2) \sim \sum_{j=0}^{\infty} h^j (z - L^0)^{-1} \underbrace{\sharp_h \tilde{r}_{\lambda,\epsilon}^0(\cdot; z) \sharp_h \dots \sharp_h \tilde{r}_{\lambda,\epsilon}^0(\cdot; z)}_{j \text{ times}} \sharp_h \tilde{\chi}(|\xi|_{g_x}^2),$$

wherein $L^0 := L_{\lambda,\epsilon}^{(s)} \chi_0 \circ L_{\lambda,\epsilon}^{(s)}$ and $\tilde{r}_{\lambda,\epsilon}^0(\cdot; z) \sim \frac{1}{h} [1 - (z - L^0) \sharp_h 1 / (z - L^0)]$. Indeed, this follows from the fact that for $h \in (0, h_0]$, $L^0 \equiv L_{\lambda,\epsilon}^{(s)}$ on $\mathrm{supp} \tilde{\chi}(|\xi|_{g_x}^2)$ and for the same reason, if any partial derivatives in the expansion of the $\sharp_h$ operator land on $\chi_0 \circ L_{\lambda,\epsilon}^{(s)}$, then the corresponding term vanishes. Thus setting $\hat{\chi}^w := \mathrm{Op}_h^w(\tilde{\chi}(|\xi|_{g_x}^2))$ we have,

$$P_\chi \hat{\chi}^w \equiv \left(-\frac{1}{\pi} \int_{\mathbb{C}} \bar{\partial} \chi_{\mathrm{an}}(z) \mathrm{Op}_h^w(r_{\lambda,\epsilon}^0(\cdot; z)) dz \right) \hat{\chi}^w \pmod{h^\infty \Psi^{-\infty}}$$

and on applying the foregoing discussion to L^0 in place of $L_{\lambda,\epsilon}^{(s)}$, we recognize the left-most factor on the right-hand side to be the application of the Helffer–Sjöstrand formula to $P_\chi^0 := \chi(\mathrm{Op}_h^w(L^0))$. Since $L^0 \in h^0 S^{-\infty}$, the semiclassical estimates of [DS99, Section 8] apply directly to give $P_\chi^0 \in h^0 \Psi^{-\infty}$. Hence also $P_\chi \hat{\chi}^w \in h^0 \Psi^{-\infty}$ and we compute its symbol modulo $h \Psi^{-\infty}$ to be $\chi \circ \mathcal{L}_{g,\lambda,h^\alpha}(x, \xi) \tilde{\chi}(|\xi|_{g_x}^2)$, from which a local Taylor expansion further refines this to the symbol as in the statement of the present theorem. On running the previous steps starting with $\tilde{\chi}(|\xi|_{g_x}^2) \sharp_h r_{\lambda,\epsilon}$, we find $\hat{\chi}^w P_\chi \in h^0 \Psi^{-\infty}$ with the same symbol properties.

Step 3. — In the case that $\mathrm{supp} \tilde{\chi} \subset \{\chi \equiv 1\}$, it suffices to choose the auxiliary cutoff above to be $\chi_0 \equiv \chi$. We may now apply the symbol expansion given in the remarks following [DS99, Theorem 8.7] to P_χ^0 . In this expansion, each term of order h^j for $j \geq 1$ contains a factor with at least one derivative of χ evaluated at

$L^0(x, \xi)$. Hence, the inclusion $\text{supp } \tilde{\chi}(|\xi|_{g_x}^2) \subset \{\chi \circ L_{\lambda, \epsilon}^{(s)} \equiv 1\}$ for all $h \in (0, h_0]$ implies $(I - P_\chi^0)\hat{\chi}^w, \hat{\chi}^w(I - P_\chi^0) \in h^\infty\Psi^{-\infty}$. Thus, we obtain

$$P_\chi \hat{\chi}^w \equiv P_\chi^0 \hat{\chi}^w \equiv \hat{\chi}^w \pmod{h^\infty\Psi^{-\infty}},$$

along with the desired commutation relation $[\chi(h^2\Delta_{\lambda, \epsilon}^{(s)}), \hat{\chi}^w] \in h^\infty\Psi^{-\infty}$.

Step 4. — The preceding remarks regarding the similarity of graph Laplacians and moving between quantizations, all up to a lower order symbol, now apply. On noting that the supports and flat regions of the symbols are preserved (modulo $h^\infty\Psi^{-\infty}$) under changes of quantization, we conclude the statement of Theorem 4.7. $\square$

5. Propagation of coherent states

The inclusion of graph Laplacians in the framework of semiclassical pseudodifferential operators greatly facilitates a central theme of our study: the behaviour of a coherent state as it propagates according to the dynamics $U_{\lambda, \epsilon}^t := e^{-it\sqrt{\Delta_{\lambda, \epsilon}}} : L^2(\mathcal{M}) \rightarrow L^2(\mathcal{M})$. Since we have seen that $h^2\Delta_{\lambda, \epsilon}$ *microlocally resembles* $h^2\Delta_{\mathcal{M}}$ and detailed descriptions of coherent state evolution under the quantum dynamics generated by $h\sqrt{\Delta_{\mathcal{M}}}$ are well-known, for example by Fourier integral operator methods [PU96], we expect that $U_{\lambda, \epsilon}^t \psi_h$ is roughly another coherent state, with a different amplitude, centered at (x_t, ξ_t) . On Euclidean space, rather explicit forms for propagated coherent states can be obtained for real-valued Hamiltonians in $S^m(\mathbb{R}^n)$ through the application of metaplectic operators to the second order Taylor approximation of the Hamiltonian along the classical trajectory [RC21, Section 4.1]. In fact, this relates to the WKB method for the propagation of *Lagrangian states* [SVT12]. While these techniques may be adapted to Ψ DOs on manifolds by working in local patches along the classical trajectory, the application to $U_{\lambda, \epsilon}^t$ additionally requires dealing with principal symbols and the square root function being applied spectrally to the non-elliptic operator $h^2\Delta_{\lambda, \epsilon}$. Such descriptions can be likened to the *Schrödinger picture* of quantum dynamics, where one is concerned with the explicit description of propagated states $|\psi_h(t)\rangle$ according to the dynamics $ih\partial_t|\psi_h(t)\rangle = Q_h|\psi_h(t)\rangle$ given by a quantum Hamiltonian Q_h .

Our approach is through the *quantum statistical* or *Heisenberg* framework, using the correspondence between the evolution of symbols under the Hamiltonian flow and the evolutions of their corresponding quantized operators under conjugation by the dynamics $U_{\lambda, \epsilon}^t$. We will ultimately arrive at a middle-ground with regards to the Schrödinger picture: the quantity $|U_{\lambda, \epsilon}^t \psi_h(x)|^2$ is physically interpreted (as per the *Born rule*) as the probability that at time t , the particle whose quantum state is described by $|\psi_h(t)\rangle$ can be found at the position x , while in the following we use quantum-classical correspondence in the Heisenberg picture to turn this quantity into a description about the location of x_t . This is driven by Egorov's theorem, which states roughly that if Q is a Ψ DO with principal symbol q_0 , then the *operator dynamics* $A(t) = e^{-\frac{i}{h}tQ} \text{Op}_h(a) e^{\frac{i}{h}tQ}$ preserves pseudodifferentiability, meaning that up to *Ehrenfest time* $T_E(h, \rho; q_0)$ that increases at a controlled rate in $1/h^\rho$ for $\rho \in [0, 1/2)$, $A(0) \in \Psi^m \Rightarrow A(t) \in \Psi_\rho^m$ for all $|t| \leq T_E$ and furthermore,

$A(t) \equiv \text{Op}_h(a \circ \Phi_{q_0}^t) \bmod h^{1-2\rho} \Psi_\rho^{m-1}$. The growth rate of T_E is determined by the local expansion rates of the classical flow⁽⁹⁾, which induce time-dependent *roughness* in the derivatives of the symbol $a \circ \Phi_{q_0}^t$ and thus necessitate the ρ -dependent symbol classes.

On adapting this and utilising the broader semiclassical framework, we will arrive at a sufficiently descriptive picture of the propagated coherent state $U_{\lambda,\epsilon}^t \psi_h$ for our needs: namely, that it is localized in an $O(h^{1/2-\delta})$ neighbourhood of $(x_t, \xi_t) := \Gamma^t(x_0, \xi_0)$, for all $\delta > 0$, and that the coordinate *mean* of the probability density $|U_{\lambda,\epsilon}^t \psi_h|^2 / \|U_{\lambda,\epsilon}^t \psi_h\|_{L^2}^2$ is within $O(h^{1-2\rho})$ distance from x_t for times up to $|t| \leq T_E$. We will revisit the latter interpretation in Section 5.2. Presently, we will develop a version of Egorov's theorem that applies to quantum dynamics generated by a *cut-off* of $h\sqrt{\Delta_{\lambda,\epsilon}}$ in phase space at appropriate frequency scales. Then, we will show essentially that the application of ψ_h to the propagator $U_{\lambda,\epsilon}^t$ implicitly performs this cut-off. The techniques involve mainly asymptotic expansions of the symbol calculus and spectral properties of the graph Laplacian.

5.1. Geodesic flows of symbols

We have seen in Section 4 that the principal symbol of a graph Laplacian is locally equal to $|\xi|_{g_x}^2$. So, for a fixed $(x_0, \xi_0) \in T^*\mathcal{M}$ and h sufficiently small, we expect that the Hamiltonian flow given by the square root of (the principal part of) the symbol of a graph Laplacian coincides with the co-geodesic flow in a neighbourhood of this point. An issue, however, is that graph Laplacians are not elliptic, which obstructs directly applying certain bounds on symbol propagations and utilising their square roots. Our way out goes back to the application of coherent states: since ψ_h is localized at (x_0, ξ_0) in phase space, by going through the FBI transform as in Lemma 3.1, we can approximate it with the application of the quantization of a phase space localized symbol. Upon enlarging this symbol to a frequency space cut-off in a strip containing ξ_0 that includes the essential support in phase space of ψ_h (as depicted in the left of Figure 4.2), we get in concert with Theorem 4.7, a spectral and frequency-space cut-off of the graph Laplacian. Finally, we will use this to bring a cut-off into the generator Q , for which we have the following version of Egorov's theorem:

THEOREM 5.1 (Egorov). — *Let $q \in C_c^\infty(T^*\mathcal{M} \times [0, h_0)) \cap h^0 S^{-\infty}$ for some $h_0 > 0$ have a real principal symbol q_0 that generates the Hamiltonian flow $\Phi_{q_0}^t$ on $T^*\mathcal{M}$ with maximal Lyapunov exponent $\Lambda_{q_0} \geq 0$. Then, given $a \in S_\rho^m$, $\tilde{\rho} \in [0, 1/2 - \rho)$, $\tilde{\Lambda} > \Lambda_{q_0}$ and $T > 0$, we have for all*

$$|t| \leq T_E(h; \tilde{\rho}, q_0) := T + \frac{\tilde{\rho}}{\tilde{\Lambda}} \log\left(\frac{1}{h}\right)$$

⁽⁹⁾Regions of negative curvature on $\mathcal{M}$ naturally lead to exponential stretching with respect to t , so in this case we expect $T_E \lesssim \log(1/h^\rho)$. When the geodesic flow is not so chaotic, the Ehrenfest time may be a power law in $1/h^\rho$.

that with $Q := \text{Op}_h(q)$ and $U^t := e^{-\frac{i}{h}tQ}$,

$$A(t) := U^{-t} \text{Op}_h(a) U^t \in \Psi_{\bar{\rho}}^m, \quad \bar{\rho} := \rho + \tilde{\rho}.$$

On the symbol side, there is $a_t \in \Psi_{\bar{\rho}}^m$ with $\text{supp } a_t \subseteq \Phi_{q_0}^{-t}(\text{supp } a)$ such that

$$A(t) \equiv \text{Op}_h(a_t) \pmod{h^\infty \Psi^{-\infty}}$$

and this has the principal symbol $a \circ \Phi_{q_0}^t \in S_{\bar{\rho}}^m$ that satisfies,

$$A(t) \equiv \text{Op}_h(a \circ \Phi_{q_0}^t) \pmod{h_{\bar{\rho}} \Psi^{-\infty}}.$$

Proof of Theorem 5.1. — The main differences from standard treatments are that we use the full symbol to generate the operator dynamics, while we give the correspondence with the flow generated by the principal part and we are using the *standard* quantization as opposed to the Weyl quantization for Q . Thus, while the propagator $e^{\frac{i}{h}tQ}$ solves an operator equation of the same form, it need not be unitary. Other minor differences are that typically $\rho = 0$ and Egorov's theorem is given for polyhomogeneous symbols when the operator dynamics uses the full symbol and the correspondence is to a classical flow with only the principal symbol. Nevertheless, the statement holds following the arguments in the proof of [Tay81, *Egorov's Theorem* in Section 1, Chapter 8] and importing them into the semiclassical calculus; we carry this out presently.

Let $A := \text{Op}_h(a)$ so that $A(t)$ is a solution to the system,

$$\partial_t A(t) = \frac{i}{h} [Q, A(t)], \quad A(0) = A.$$

We wish to construct a solution $\tilde{A}(t)$ to this system with principal symbol $a \circ \Phi_{q_0}^t$ such that $\tilde{A}(t) - A(t) \in h^\infty \Psi^{-\infty}$. That is, we look for $\tilde{A}(t) = \text{Op}_h(\tilde{a}(t, x, \xi; h))$ that satisfies

$$\partial_t \tilde{A}(t) = \frac{i}{h} [Q, \tilde{A}(t)] + R(t), \quad \tilde{A}(0) = A,$$

with $R(t) \in h^\infty \Psi^{-\infty}$. On the symbol side, we look for $\tilde{a}(t, x, \xi; h)$ with asymptotic expansion

$$\tilde{a}(t, x, \xi; h) \sim \sum_{j=0}^{\infty} \tilde{a}_j(t, x, \xi; h)$$

such that $\tilde{a}_j \in h_{\bar{\rho}}^j S_{\bar{\rho}}^{m-j}$. We will use the notation $\overline{\text{Sym}}[\cdot]$ to denote the *full* symbol of a Ψ DO. Then by [Zwo12, Theorem 9.5], the symbol of $\frac{i}{h} [Q, \tilde{A}(t)]$ must have an asymptotic expansion in $S_{\bar{\rho}}^m$ given in local coordinates by,

$$\begin{aligned} & \overline{\text{Sym}} \left[\frac{i}{h} [Q, \tilde{A}(t)] \right] \\ & \sim \sum_{|\beta| \geq 0} \frac{h^{|\beta|-1}}{i^{|\beta|-1} \beta!} \left(\partial_\xi^\beta \tilde{a}(t, x, \xi; h) \partial_x^\beta q(x, \xi; h) - \partial_\xi^\beta q(x, \xi; h) \partial_x^\beta \tilde{a}(t, x, \xi; h) \right) \\ & = \{q_0, \tilde{a}\} + \{\tilde{q}_0, \tilde{a}\} + \sum_{|\beta| \geq 2} \frac{h^{|\beta|-1}}{i^{|\beta|-1} \beta!} \left(\partial_\xi^\beta \tilde{a} \partial_x^\beta q - \partial_\xi^\beta q \partial_x^\beta \tilde{a} \right), \end{aligned}$$

with $\tilde{q}_0 := q - q_0 \in hS^{-\infty}$. Since $\partial_t \tilde{A}_t = \text{Op}_h(\partial_t \tilde{a})$, it follows that $\text{Sym}[ih^{-1}[Q, \tilde{A}(t)]] = \partial_t \tilde{a}$, hence the asymptotic expansions would coincide. So let $\tilde{a}_0(t, x, \xi; h)$ be defined by the transport equation

$$\partial_t \tilde{a}_0 = \{q_0, \tilde{a}_0\}, \quad \tilde{a}_0(0, x, \xi) = a(x, \xi),$$

which is sensible as it is solved by $\tilde{a}_0 = a \circ \Phi_{q_0}^t$. This symbol is of order $(\ell, m; \bar{\rho})$: indeed, the discussions in [AN07, Section 5.2] and [DJN22, Section 5.2] (see also [Zwo12, Theorem 11.11] and the remarks thereafter) apply due to the generator q having compact support and show that for all $(\alpha, \beta) \in \mathbb{N}_0^{2n}$,

$$\|\partial^\beta \tilde{a}_0\| \lesssim_{\beta, \tilde{\Gamma}} e^{\tilde{\Lambda}|t| \cdot |\alpha + \beta|} \sup_{|\gamma| \leq |\beta|} \|\partial^\gamma a\|_{L^\infty(T^*\mathcal{M})} \lesssim e^{T|\beta|} h^{-\bar{\rho}|\alpha + \beta|} \langle \xi \rangle^{m - |\beta|}.$$

Hence, the operator $\tilde{A}_0(t) := \text{Op}_h(\tilde{a}_0)$ has

$$\begin{aligned} & \overline{\text{Sym}} \left[\frac{i}{h} [Q, \tilde{A}_0(t)] - \partial_t \tilde{A}_0(t) \right] \\ & \sim \{\tilde{q}_0, \tilde{a}_0\} + \sum_{|\beta| \geq 2} \frac{h^{|\beta| - 1}}{i^{|\beta| - 1} \beta!} (\partial_\xi^\beta \tilde{a}_0 \partial_x^\beta q - \partial_\xi^\beta q \partial_x^\beta \tilde{a}_0) =: r_0(t, x, \xi; h) \in h_{\bar{\rho}} S^{-\infty} \end{aligned}$$

and $\text{supp } r_0^t \subseteq \text{supp } \tilde{a}_0^t \cap (\text{supp } q \cup \text{supp } q_0)$, wherein we use the notation $\bullet^t(x, \xi) := \bullet(t, x, \xi)$. Now, $\tilde{a}_1(t, x, \xi; h)$ defined by the transport equation

$$\partial_t \tilde{a}_1 = \{q_0, \tilde{a}_1\} - r_0, \quad \tilde{a}_1(0, x, \xi) = 0$$

is a symbol of order $(1, -\infty; \bar{\rho})$ due to Duhamel's formula and the fact that r_0 and q_0 are smooth and compactly supported. Moreover, we read directly from the transport equation that $\text{supp } \tilde{a}_1^t \subseteq \text{supp } r_0^t$ at all times.

We thus have a recursive procedure to determine $\tilde{a}_j$ for $j \geq 1$ via transport equations: suppose that for all $0 \leq j \leq J - 1$ we have $\tilde{a}_j \in h_{\bar{\rho}}^j S^{-\infty}$ such that $\text{supp } \tilde{a}_j^t \subseteq \text{supp } r_0^t$, $\tilde{A}_{J-1}(t) := \sum_{j=0}^{J-1} \text{Op}_h(\tilde{a}_j)$ has $\sum_{j=0}^{J-1} \tilde{a}_j(0, x, \xi) = a(x, \xi)$ and

$$\begin{aligned} & \overline{\text{Sym}} \left[\frac{i}{h} [Q, \tilde{A}_{J-1}(t)] - \partial_t \tilde{A}_{J-1}(t) \right] \sim r_{J-1}, \\ & r_{J-1} := \{\tilde{q}_0, \tilde{a}_{J-1}\} + \sum_{|\beta| \geq 2} \frac{h^{|\beta| - 1}}{i^{|\beta| - 1} \beta!} (\partial_\xi^\beta \tilde{a}_{J-1} \partial_x^\beta q - \partial_\xi^\beta q \partial_x^\beta \tilde{a}_{J-1}) \in h_{\bar{\rho}}^J S^{-\infty}. \end{aligned}$$

Then, let $\tilde{a}_J(t, x, \xi; h)$ be defined by the transport equation

$$\partial_t \tilde{a}_J = \{q_0, \tilde{a}_J\} - r_{J-1}, \quad \tilde{a}_J(0, x, \xi) = 0.$$

Since r_{J-1} and q_0 are smooth and compactly supported, by Duhamel's formula this is solved with $\tilde{a}_J$ also of order $(J, -\infty; \bar{\rho})$. Moreover, $\text{supp } \tilde{a}_J^t \subseteq \text{supp } r_{J-1}^t \subseteq r_0^t$, $A_J(t) := A_{J-1}(t) + \text{Op}_h(\tilde{a}_J)$ has $\sum_{j=0}^J \tilde{a}_j(0, x, \xi) = a(x, \xi)$ and

$$\begin{aligned} & \overline{\text{Sym}} \left[\frac{i}{h} [Q, \tilde{A}_J(t)] - \partial_t \tilde{A}_J(t) \right] \sim r_J, \\ & r_J := \{\tilde{q}_0, \tilde{a}_J\} + \sum_{|\beta| \geq 2} \frac{h^{|\beta| - 1}}{i^{|\beta| - 1} \beta!} (\partial_\xi^\beta \tilde{a}_J \partial_x^\beta q - \partial_\xi^\beta q \partial_x^\beta \tilde{a}_J) \in h_{\bar{\rho}}^{J+1} S^{-\infty}. \end{aligned}$$

Continuing like this, we have for all $j \geq 1$, $\tilde{a}_j \in h_{\bar{\rho}}^j S^{-\infty}$ so by Borel's theorem there is $\tilde{a}^{(1)} \in h_{\bar{\rho}} S^{-\infty}$ such that

$$\tilde{a}^{(1)} \sim \sum_{j=1}^{\infty} \tilde{a}_j, \quad \tilde{a} := \tilde{a}_0 + \tilde{a}^{(1)} \in h_{\bar{\rho}} S^m$$

and therefore, $\tilde{A}(t) := \text{Op}_h(\tilde{a}(t, x, \xi; h))$ satisfies

$$\partial_t \tilde{A}(t) = \frac{i}{h} [Q, \tilde{A}] + R(t), \quad \tilde{A}(0) = A,$$

with $R(t) \in h^\infty \Psi^{-\infty}$.

Now we wish to see that $\tilde{R}(t) := A(t) - \tilde{A}(t) \in h^\infty \Psi^{-\infty}$. Since $U^{-t}: H_h^s \rightarrow H_h^s$ continuously for all $s \in \mathbb{R}$, it suffices to show that $U^{-t}A - \tilde{A}(t)U^{-t} = \tilde{R}(t)U^{-t} \in h^\infty \Psi^{-\infty}$. Let $u \in H_h^{-N}$ for $N \in \mathbb{N}$ and denote $v(t, x) := \tilde{A}(t)U^{-t}u$. Then v satisfies $v(0, x) = Au$ and

$$\begin{aligned} \partial_t v &= ((\partial_t \tilde{A}(t))U^{-t} + \tilde{A}(t)(\partial_t U^{-t}))u \\ &= \left(\frac{i}{h} [Q, \tilde{A}(t)] + R(t) \right) U^{-t}u + \frac{i}{h} \tilde{A}(t) Q U^{-t}u \\ &= \frac{i}{h} Q \tilde{A}(t) U^{-t}u + R(t) U^{-t}u \\ &= \frac{i}{h} Q v + R(t) U^{-t}u. \end{aligned}$$

Thus, $\tilde{v}(t, x) := v(t, x) - U^{-t}Au(x)$ satisfies

$$\partial_t \tilde{v} = \frac{i}{h} Q \tilde{v} + R(t) U^{-t}u, \quad \tilde{v}(0, x) = 0.$$

Since $w(t) := R(t)U^{-t}u \in C^\infty$ with $\|w(t)\|_{H_h^N} = O(h^\infty)$ and $U^s: C^\infty \rightarrow C^\infty$ for all $s \in \mathbb{R}$, by Duhamel's formula it follows that $\tilde{v} = \tilde{R}(t)U^{-t}u \in C^\infty$ with $\|\tilde{v}\|_{H_h^N} = O(h^\infty)$. Thus, $\|\tilde{R}(t)U^{-t}\|_{H_h^{-N} \rightarrow H_h^N} = O(h^\infty)$, whence $\tilde{R}(t)U^{-t} \in h^\infty \Psi^{-\infty}$. $\square$

The equivalence between the operator dynamics given by conjugation with $e^{-\frac{i}{h}tQ}$ and the dynamics on symbols given by composition with $\Phi_{q_0}^t$ as guaranteed by Egorov's theorem is a precise form of the physical notion of *quantum-classical correspondence*. This establishes an assurance of the correspondence for a Liouvillian flow on symbols when we use a smoothing generator Q the operator side, whose real principal symbol serves as a local Hamiltonian for the symbol dynamics. On one hand, the second part of Theorem 4.4 shows that smoothly cutting-off the principal symbol of $h^2 \Delta_{\lambda, \epsilon}$ in a sufficiently small region of phase space gives a symbol whose Hamiltonian flow is geodesic for initial points in that region. On the other hand, the first part of that theorem gives that this operator has order $(0, 2)$. Thus, to apply Egorov's theorem we must maintain the former property and simultaneously localize the symbol of our generator to an appropriately small part of the phase space.

We proceed as follows: we first see that when applied to a coherent state at (x_0, ξ_0) , the operator dynamics given by $U_{\lambda, \epsilon}^t$ is essentially generated by the quantization of $q_0 \in C_c^\infty(T^*\mathcal{M})$. More specifically, an application of Theorem 4.7 tells us that this is

the square root of a frequency-localized form of the graph Laplacian, in a momentum strip containing ξ_0 (as depicted in the left graphic of Figure 4.2). This also tells us that the Hamiltonian flow of its principal symbol is geodesic near the initial point (x_0, ξ_0) where the coherent state is localized. This puts us in a setting to apply Egorov's theorem, which gives the equivalence to the quantization of a symbol propagated along this flow. Immediately, taking an inner product with the same coherent state recovers, up to $O(h^{1-2\tilde{\rho}})$ error, the symbol propagated along the geodesic to within Ehrenfest time $T_E(h; \tilde{\rho}, q_0)$.

Further, we apply the propagation of supports part of Theorem 5.1 to microlocalize the propagation of coherent states in phase space. That is, we apply this aspect of Egorov's theorem to the quantum dynamics of a quantum observable microlocalized in a neighbourhood of a coherent state at (x_0, ξ_0) such that up to $O_s(h^\infty)$ error, it acts as the identity on the coherent state. Such an observable follows from the FBI transform's localization of coherent states in phase space along with asymptotic expansions that show the preservation of support of the symbol on switching between the FBI and adjoint quantizations. We find that the support of the full symbol of the propagated observable is transported by the geodesic flow to time t . This leads to the characterisation of the propagated coherent state $U_{\lambda, \epsilon}^t \psi_h$ that it is *essentially* microlocalized in an $O(h^\rho)$ neighbourhood of (x_t, ξ_t) for all $\rho \in [0, 1/2 - \tilde{\rho})$ and all times $|t| \leq T_E(h; \tilde{\rho}, q_0)$.

The recovery of the geodesic flows of symbols and the propagation of support of coherent states just discussed are the results of the following,

THEOREM 5.2. — *Let $\lambda \geq 0$, $\alpha \geq 1$, $\tilde{\rho} \in [0, 1/2)$ and $(x_0, \xi_0) \in T^*\mathcal{M} \setminus 0$. Given a cut-off $\tilde{\chi} \in C_c^\infty(\mathbb{R}, [0, 1])$ such that $\text{supp } \tilde{\chi} \subset \mathbb{R}_{>0}$ and $\tilde{\chi} \equiv 1$ on an interval $[|\xi_0|_{g_{x_0}}^2 - r, |\xi_0|_{g_{x_0}}^2 + r]$ for some $r > 0$, there exists $h_0 > 0$ such that, defining $q_0 := |\xi|_{g_x} \tilde{\chi}(|\xi|_{g_x}^2)$, for all $h \in (0, h_0]$, $a \in S^m$, and $|t| \leq T_E(h; \tilde{\rho}, q_0)$, with $\epsilon := h^{2+\alpha}$ and $\zeta_t := \Gamma^t(x_0, \xi_0)$, we have the symbol estimate*

$$(5.1) \quad \left\langle \psi_h(\cdot; x_0, \xi_0) \left| U_{\lambda, \epsilon}^{-t} \text{Op}_h(a) U_{\lambda, \epsilon}^t \right| \psi_h(\cdot; x_0, \xi_0) \right\rangle = a(\zeta_t) + O(h^{1-2\tilde{\rho}}).$$

In fact, for all $t \in \mathbb{R}$, the following holds on coherent states:

$$U_{\lambda, \epsilon}^{-t} \text{Op}_h(a) U_{\lambda, \epsilon}^t \psi_h = U_Q^{-t} \text{Op}_h(a) U_Q^t \psi_h + O_s(h^\infty),$$

where $U_Q := e^{\frac{i}{h}tQ}$ is the unitary propagator with effective Hamiltonian $Q = \text{Op}_h(q)$ for some $q \in C_c^\infty(T^*\mathcal{M} \times [0, h_0)) \cap h^0 S^{-\infty}$ satisfying $\text{Sym}[Q](x, \xi) = q_0(x, \xi)$.

Furthermore, if $\chi_{\zeta_0} \in C_c^\infty(T^*\mathcal{M} \times (0, h_0]) \cap S_\rho^{-\infty}$ with $\rho \in [0, 1/2 - \tilde{\rho})$, $\text{supp } \chi_{\zeta_0} \subset B_{h^\rho}(\zeta_0)$, and $\chi_{\zeta_0} \equiv 1$ on $B_{\frac{1}{2}h^\rho}(\zeta_0)$, then for all $h \in (0, h_0]$ and $|t| \leq T_E(h; \tilde{\rho}, q_0)$, there exists $\chi_{\zeta_0, t} \in S_{\tilde{\rho}}^{-\infty}$ with $\text{supp } \chi_{\zeta_0, t} \subset \Gamma^t(B_{h^\rho}(\zeta_0))$ such that

$$(5.2) \quad (I - \text{Op}_h(\chi_{\zeta_0, t})) U_{\lambda, \epsilon}^t \psi_h = O_s(h^\infty).$$

This implies the following concentration: for any $\chi^{x_t} \in C_c^\infty(\mathcal{M})$ satisfying $\|\chi^{x_t}\|_{C^k} \lesssim_k h^{-k\rho}$ for all $k \in \mathbb{N}$ and $\chi^{x_t} \equiv 1$ on $\pi_{\mathcal{M}}(\Gamma^t(B_{h^\rho}(\zeta_0)))$, we have

$$(1 - \chi^{x_t}) U_{\lambda, \epsilon}^t \psi_h = O_s(h^\infty),$$

with constants depending on the choices of $\tilde{\chi}$ and $\chi_{\zeta_0, t}$.

The above statements hold with $U_{\lambda,\epsilon}^{\pm(\epsilon)t} := e^{\mp it(\Delta_{\lambda,\epsilon} + (2c_0/c_2)(\epsilon/\epsilon)I)^{1/2}}$ in place of $U_{\lambda,\epsilon}^{\pm t}$, whenever $\epsilon \in O(h^{1+\alpha})$.

Proof of Theorem 5.2. — The quantum-classical correspondence underlying the dynamics of coherent states under $U_{\lambda,\epsilon}^t$ relies on the *model propagator* $U_Q^t := e^{-\frac{i}{h}tQ_\chi}$, where the effective Hamiltonian is defined by $Q_\chi := h\sqrt{\Delta_{\lambda,\epsilon}}\chi(h^2\Delta_{\lambda,\epsilon})\hat{\chi}$. Here, $\chi \in C_c^\infty(\mathbb{R})$ and $\hat{\chi} = \text{Op}_h(\tilde{\chi}(|\xi|_{g_x}^2))$ are chosen as in Theorem 4.7, satisfying the support nesting $\text{supp } \tilde{\chi} \subset \{\chi \equiv 1\}$. We further choose χ such that $\text{supp } \chi \subset \mathbb{R}_{>0}$, which guarantees the smoothness of the spectral function $\sqrt{\cdot}\chi(\cdot) \in C_c^\infty(\mathbb{R})$, as it vanishes with all derivatives in a neighbourhood of the origin. This ensures that Theorem 4.7 applies directly; in particular, we have $\text{Sym}[Q_\chi] = q_0$. We first observe that $U_Q^t\psi_h$ is microlocalized in phase space; this follows directly from the initial phase space localization of ψ_h and the transport of microsupport as per Theorem 5.1. Subsequently, we apply this result to show that the dynamics are well approximated by $U_{\lambda,\epsilon}^t\psi_h$. This specialization to coherent states allows for an appropriate frequency-space cut-off of the generator $h\sqrt{\Delta_{\lambda,\epsilon}}$, localizing it to a region where it provides a sufficient semiclassical approximation to $h\sqrt{\Delta_{\mathcal{M}}}$.

Step 1. — We first consider the microlocalization of $U_Q^t\psi_h$. Let $\chi_{\zeta_0} \in C_c^\infty(T^*\mathcal{M} \times (0, h_0]) \cap S_\rho^{-\infty}$ satisfy $\text{supp } \chi_{\zeta_0} \subset B_{h^\rho}(\zeta_0)$ and $\chi_{\zeta_0} \equiv 1$ on $B_{\frac{1}{2}h^\rho}(\zeta_0)$. By Theorem 2.25, there is a symbol $\chi_{\zeta_0}^{\text{op}} \in S_\rho^{-\infty}$ such that $T_h^*\chi_{\zeta_0}T_h \equiv \text{Op}_h(\chi_{\zeta_0}^{\text{op}}) \pmod{h^\infty\Psi^{-\infty}}$. Combining this with Theorem 3.1, there is $h_1 > 0$ such that for all $h \in (0, h_1]$,

$$\psi_h = T_h^*\chi_{\zeta_0}T_h\psi_h + O_s(h^\infty) = \text{Op}_h(\chi_{\zeta_0}^{\text{op}})\psi_h + O_s(h^\infty).$$

The proof of Theorem 2.25 ensures $\text{supp } \chi_{\zeta_0}^{\text{op}} = \text{supp } \chi_{\zeta_0}$. The evolution of the full symbol is tracked via Egorov's theorem: for $|t| \leq T_E(h; \rho, q_0)$, Theorem 5.1 ensures the existence of $\chi_{\zeta_0,t} \in S_\rho^{-\infty}$ with $\text{supp } \chi_{\zeta_0,t} \subseteq \Phi_{q_0}^t(\text{supp } \chi_{\zeta_0})$ such that

$$U_Q^t \text{Op}_h(\chi_{\zeta_0}^{\text{op}}) U_Q^{-t} \equiv \text{Op}_h(\chi_{\zeta_0,t}) \pmod{h^\infty\Psi^{-\infty}}.$$

Since q_0 is conserved under its own flow, and given that $q_0(x, \xi) = |\xi|_{g_x}$ on the momentum strip

$$\mathcal{N}_{\xi_0}(r) := \{(x, \xi) \mid |\xi|_{g_x}^2 \in [|\xi_0|_{g_{x_0}}^2 - r, |\xi_0|_{g_{x_0}}^2 + r]\},$$

the Hamiltonian flow coincides with the geodesic flow: $\Phi_{q_0}^t(x_0, \xi_0) = \Gamma^t(x_0, \xi_0)$. This implies $\text{supp } \chi_{\zeta_0,t} \subseteq \Gamma^t(\text{supp } \chi_{\zeta_0})$. Applying the preceding equivalence to $U_Q^t\psi_h$, we obtain

$$(I - \text{Op}_h(\chi_{\zeta_0,t}))U_Q^t\psi_h = O_s(h^\infty),$$

establishing the microlocalization of $U_Q^t\psi_h$ at scale $O(h^\rho)$ near ζ_t .

Step 2. — We establish the microlocalization of $U_{\lambda,\epsilon}^t\psi_h$ by showing that

$$(5.3) \quad X(t)\psi_h := U_{\lambda,\epsilon}^t\psi_h - U_Q^t\psi_h \in O_s(h^\infty).$$

By the Duhamel formula, the difference of operators satisfies

$$X(t) = \frac{i}{h} \int_0^t U_{\lambda,\epsilon}^{t-s} (Q_\chi - h\sqrt{\Delta_{\lambda,\epsilon}}) U_Q^s ds.$$

The frequency cut-off imposed by coherent states ensures the smallness of $Q_\chi - h\sqrt{\Delta_{\lambda,\epsilon}}$ via Theorem 4.7. Such estimates depend on the stability of $U_{\lambda,\epsilon}^t$ on the Schwartz space $\mathcal{S}$, derived from the decomposition (1.1).

Specifically, taking higher-order derivatives of the kernel $k_{\lambda,\epsilon}$, the modifications to the bound (6.11) with $\epsilon = h^{2+\alpha}$ imply the existence of $K(\alpha) \in \mathbb{N}$ such that for all $\beta \in \mathbb{N}_0^n$ and $u \in \mathcal{S}$,

$$\|\partial^\beta U_{\lambda,\epsilon}^t u\|_\infty \lesssim_\beta h^{-K(\alpha)|\beta|} \|\partial^\beta u\|_\infty.$$

In particular, the definition of the semiclassical Schwartz space implies that for $u = O_s(h^\infty)$ and any $N \in \mathbb{N}$, the bounds $\|\partial^\beta u\|_\infty \lesssim_{\beta,N} h^{N+K(\alpha)|\beta|}$ hold. Thus, for any $\beta \in \mathbb{N}_0^n$, we obtain $\|\partial^\beta U_{\lambda,\epsilon}^t u\|_\infty \lesssim_{\alpha,\beta,N} h^N$, which shows that $U_{\lambda,\epsilon}^t u \in O_s(h^\infty)$. (We note for later use in the propagation of symbols that this stability also implies $RU_{\lambda,\epsilon}^t \psi_h \in O_s(h^\infty)$ for any $R \in h^\infty \Psi^{-\infty}$.)

The microlocalization of $U_Q^t \psi_h$ observed in the previous step implies that $u_h(t) := (I - \chi(h^2 \Delta_{\lambda,\epsilon}) \hat{\chi}) U_Q^t \psi_h \in O_s(h^\infty)$, since $\text{supp } \chi_{\zeta_0,t} \subset \mathcal{N}_{\xi_0}(r)$. Applying the identity

$$(Q_\chi - h\sqrt{\Delta_{\lambda,\epsilon}}) \chi(h^2 \Delta_{\lambda,\epsilon}) \hat{\chi} = Q_\chi R,$$

where

$$R := \chi(h^2 \Delta_{\lambda,\epsilon}) \hat{\chi} - I \in h^\infty \Psi^{-\infty},$$

we obtain

$$U_{\lambda,\epsilon}^{t-s} (Q_\chi - h\sqrt{\Delta_{\lambda,\epsilon}}) U_Q^s \psi_h = U_{\lambda,\epsilon}^{t-s} Q_\chi R \psi_h + U_{\lambda,\epsilon}^{t-s} u_h(s).$$

Integrating in s and using the stability of $U_{\lambda,\epsilon}^t$ yields (5.3). The microlocalization of $U_{\lambda,\epsilon}^t \psi_h$ then follows from the triangle inequality:

$$\begin{aligned} (I - \text{Op}_h(\chi_{\zeta_0,t})) U_{\lambda,\epsilon}^t \psi_h &= (I - \text{Op}_h(\chi_{\zeta_0,t})) X(t) \psi_h + (I - \text{Op}_h(\chi_{\zeta_0,t})) U_Q^t \psi_h \\ &= O_s(h^\infty). \end{aligned}$$

Step 3. — The propagation of symbols follows from the control of the commutator in the Duhamel formula for observables. For $A \in \Psi^m$ and $\tilde{A}(s) := U_Q^{-s} A U_Q^s$, we define the operator

$$Y(t) := U_{\lambda,\epsilon}^{-t} A U_{\lambda,\epsilon}^t - U_Q^{-t} A U_Q^t = \frac{i}{h} \int_0^t U_{\lambda,\epsilon}^{s-t} [Q_\chi - h\sqrt{\Delta_{\lambda,\epsilon}}, \tilde{A}(s)] U_{\lambda,\epsilon}^{t-s} ds.$$

Using the remainder R from the previous step, Theorem 4.7 yields the commutator identity

$$\begin{aligned} [Q_\chi - h\sqrt{\Delta_{\lambda,\epsilon}}, \tilde{A}(s)] \chi(h^2 \Delta_{\lambda,\epsilon}) \hat{\chi} \\ = (Q_\chi - I) R \tilde{A}(s) \chi(h^2 \Delta_{\lambda,\epsilon}) \hat{\chi} - \tilde{A}(s) Q_\chi R \in h^\infty \Psi^{-\infty}. \end{aligned}$$

Since $RU_{\lambda,\epsilon}^{t-s} \psi_h = O_s(h^\infty)$ by the stability of $U_{\lambda,\epsilon}^t$ on $\mathcal{S}$, these observations combined with the integral representation above show that $Y(t) \psi_h \in O_s(h^\infty)$.

The recovery of symbols is then a direct consequence of Egorov's theorem. Applying Theorem 5.1 for $|t| < T_E(h; \tilde{\rho}, q_0)$ and Theorem 3.3, we obtain for all $A \in \Psi^m$:

$$\langle \psi_h | U_{\lambda,\epsilon}^{-t} A U_{\lambda,\epsilon}^t | \psi_h \rangle = a(\zeta_t) + O(h^{1-2\tilde{\rho}}).$$

Step 4. — We may extract position space localization from the phase space localization of $U_{\lambda,\epsilon}^t \psi_h$. Let χ^{x_t} be as in the statement of the theorem and define $\hat{\chi}_t := \text{Op}_h(\chi_{\zeta_0,t})$. Since the symbol $\chi^{x_t} \otimes 1(x, \xi) \in S_\rho^0(T^*\mathcal{M})$ quantizes to the multiplication operator χ^{x_t} , and since it is identically 1 on the support of $\chi_{\zeta_0,t}$, it follows from the semiclassical calculus that $\chi^{x_t} \hat{\chi}_t \equiv \hat{\chi}_t \pmod{h^\infty \Psi^{-\infty}}$. Hence, we have

$$(I - \chi^{x_t}) U_{\lambda,\epsilon}^t \psi_h = (I - \chi^{x_t}) \hat{\chi}_t U_{\lambda,\epsilon}^t \psi_h + O_s(h^\infty) = O_s(h^\infty).$$

The preceding arguments apply to $U_{\lambda,\epsilon}^{(\varepsilon)t}$ as well, since with $\varepsilon \in O(h^{1+\alpha})$, $h^2(\Delta_{\lambda,\epsilon} + \frac{2c_0}{c_2}(\varepsilon/\epsilon)I) = h^2\Delta_{\lambda,\epsilon} + \frac{2c_0}{c_2}hI$ has the same principal symbol as $h^2\Delta_{\lambda,\epsilon}$. This gives the final part of Theorem 5.2. $\square$

Remarks 5.3. —

- (1) The method of proof for applying Egorov's theorem to the microlocalization of the propagation of coherent states was generously suggested to the author by a referee. This of course extends to any U in place of U_Q to which Theorem 5.1 applies.
- (2) The proof of the preceding theorem shows that we may approximate the flow of classical observables along geodesics upon *smoothly* projecting onto any $\Theta(h^0)$ part of the spectrum of $h^2\Delta_{\lambda,\epsilon}$ in an interval $[|\xi_0|_{g_{x_0}}^2 - r, |\xi_0|_{g_{x_0}}^2 + r]$ with $r < |\xi_0|_{g_{x_0}}^2$. As $\epsilon \rightarrow 0$, the spectral convergence of $\Delta_{\lambda,\epsilon}$ to $\Delta_{\mathcal{M}} + O(\partial^1)$ and Weyl's law imply that the k^{th} eigenvalue $\sigma_{\epsilon,k} \in \text{Spec}(\Delta_{\lambda,\epsilon})$ satisfies the gap estimate $\sigma_{\epsilon,k+1} - \sigma_{\epsilon,k} \sim k^{(2/n)-1}$. For $h \sim k^{-1}$ and $|\xi_0|_{g_{x_0}}^2 = 1$, the spectral window $\text{Spec}(\Delta_{\lambda,\epsilon}) \cap k^2[1 - r, 1 + r]$ contains $O(h^{-n})$ eigenvalues as $h \rightarrow 0$.

5.2. Observing geodesics

The localization of a propagated coherent state informs the location of its maximum amplitude, which *observes* the geodesic flow in the sense that it gives an $O(h^{1/2-\delta})$ ball in configuration space where it can be found. Now, we borrow from quantum mechanics the *position operator*, which in the basis of Dirac mass distributions represents position statistics of a particle. In particular, taking the expectation of the position operator with $|\psi_h(t)\rangle$ gives the *mean position* of a particle with quantum state $|\psi_h(t)\rangle$. When U is unitary quantizing the geodesic flow in the sense of Theorem 5.1 and a position operator is given by a vector of multiplication operators by coordinate functions, then recalling the interpretation of $|U^t[\psi_h]|^2$ via the Born rule, we understand the mean position to be the mean of this probability density. On a submanifold of Euclidean space, the extrinsic coordinates can be used, but from a local perspective, in light of the first remark to Theorem 5.2, the concentration of $|U^t[\psi_h]|^2$ at scale $O(h^{1/2-\delta})$ near x_t can be used to identify a position operator given by local coordinates of intrinsic dimension. In either case, through Egorov's theorem and quantization of Ψ DOs by FBI transforms, the mean turns out to be located in an $O(h^{1-2\rho})$ ball around x_t for all times $|t| \leq T_E$. Thus, we have a quadratic improvement in the error term when going from the maximum to the mean. We now elaborate on this point of view.

In principle, working in coordinates given by fixing a smooth, injective map $u = (u_1, \dots, u_N) : \mathcal{M} \rightarrow \mathbb{R}^N$ with $u_j \in C^\infty(\mathcal{M})$, for any $N \in \mathbb{N}$, we'd like to compute

$$\bar{u}_j^t(x_0, \xi_0) := \int_{\mathcal{M}} u_j(x) |U^t \psi_h|^2(x) d\nu_g(x)$$

for each $j = 1, \dots, N$. Quantizing u_j gives a multiplication operator in $h^0\Psi^0$ and therefore by the remark to Theorem 5.2 we have for U_Q in the proof of that theorem replaced with U that

$$\langle \psi_h | U^{-t} \text{Op}_h(u_j) U^t | \psi_h \rangle = u_j \circ \Gamma^t(x_0, \xi_0) + O(h) = u_j(x_t) + O(h^{1-2\rho})$$

and when U is unitary so that $U^{-t} = (U^t)^*$ this gives,

$$(5.4) \quad \bar{u}_j^t(x_0, \xi_0) = u_j(x_t) + O(h^{1-2\rho}).$$

Hence, for the *mean coordinates*, $\bar{u}^t := (\bar{u}_1^t, \dots, \bar{u}_N^t)$ we have in the unitary case, $\|\bar{u}^t(x_0, \xi_0) - u(x_t)\|_{\mathbb{R}^N} \lesssim N^{\frac{1}{2}} h^{1-2\rho}$. One goal is then to turn this into a bound on $d_g(u^{-1}[\bar{u}^t(x_0, \xi_0)], x_t)$ so that we can be certain that taking the mean of $|U^t[\psi_h]|^2$ brings us close to the geodesic neighbour of x_0 at distance t in the direction ξ_0 , *viz.*, that we are *observing* the geodesic flow.

Another aspect is to see that this can work *locally*: we've seen already that for sufficiently small h , the geodesic neighbour x_t is within distance $O(h^{1/2-\delta})$ of the maximizer of $|U^t[\psi_h]|^2$, for $\delta \in (\rho, 1/2]$. Therefore, by (5.4), we can localize the mean of each coordinate to this neighbourhood. This is of practical importance because the computation, along with coefficients of error, can be reduced after setting up a local, dimensionally reduced coordinate system, as opposed to working in the extrinsic coordinates (which in some applications can be exceedingly large and might even grow as a function of h^{-1} !). Further, when needed to be done in extrinsic coordinates, it would be useful to compute the means within extrinsic neighbourhoods of the maximum and then take a nearest embedded point.

This is all feasible and the proof is now rather simple. It is facilitated by the following,

DEFINITION 5.4. — *Let ψ_h be a coherent state localized at $(x_0, \xi_0) \in T^*\mathcal{M}$ and $|t| \leq \text{inj}(x_0)$. The intrinsic maximizer of the propagated coherent state is,*

$$\hat{x}_t := \arg \max_{\mathcal{M}} |U^t[\psi_h]|^2.$$

(1) *Extrinsic case: The extrinsic maximizer of the propagated coherent state is,*

$$\hat{x}_{\iota, t} := \arg \max_{\Lambda} |U^t[\psi_h]|^2 \circ \iota^{-1}$$

and we call the extrinsic mean of the propagated coherent state to be $\bar{x}_{\chi_{\iota}, t} \in \Lambda$, defined with respect to a cut-off $\chi_{\iota} \in C_c^\infty(\mathbb{R}^D)$, as the closest point on Λ to

$$\bar{\iota}^t(x_0, \xi_0) := (\bar{\iota}_1^t(x_0, \xi_0), \dots, \bar{\iota}_D^t(x_0, \xi_0)),$$

with

$$\bar{\iota}_j^t(x_0, \xi_0) := \int_{\mathcal{M}} |U^t[\psi_h]|^2(x) (\chi_{\iota} \circ \iota)(x) \iota_j(x) d\nu_g(x).$$

- (2) Local coordinates: Let $\mathcal{O}_t \subset \mathcal{M}$ be an open neighbourhood of $\hat{x}_t$. Then, given a diffeomorphic coordinate mapping $u : \mathcal{O}_t \rightarrow V_t \subset \mathbb{R}^n$, and $\chi \in C_c^\infty(\mathbb{R}^n)$ a cut-off with $\text{supp } \chi \subset V_t$, the u -maximizer, or coordinate maximizer of the propagated coherent state is,

$$\hat{x}_{u,t} := \arg \max_{\mathcal{O}_t} |U^t[\psi_h]|^2 \circ u^{-1}$$

and we call

$$\bar{x}_{u,\chi,t} := (\bar{u}_1^t(x_0, \xi_0), \dots, \bar{u}_n^t(x_0, \xi_0)),$$

with

$$\bar{u}_j^t(x_0, \xi_0) := \int_{\mathcal{M}} |U^t[\psi_h]|^2(x) (\chi \circ u)(x) u_j(x) d\nu_g(x)$$

the u -mean with respect to χ .

It's clear that $\iota(\hat{x}_t) = \hat{x}_{\iota,t}$ and $u(\hat{x}_t) = \hat{x}_{u,t}$, so the notation is there just for brevity. With this at hand, assuming U is unitary, we may state,

PROPOSITION 5.5. — Let ψ_h be a coherent state localized at $(x_0, \xi_0) \in T^*\mathcal{M}$ and $U = e^{\frac{i}{h}tQ}$ with $Q \in C_c^\infty(T^*\mathcal{M} \times [0, 1)_h)$ with principal symbol q_0 as in the statement of Theorem 5.2. Then, for all $|t| < T_E(h; \rho, q_0)$, given any open neighbourhood $\mathcal{O}_t \subset \mathcal{M}$ of $\hat{x}_t$ with its diffeomorphic coordinate mapping $u : \mathcal{O}_t \rightarrow V_t \subset \mathbb{R}^n$, there are constants $h_{u,\max}, C_{u,\max} > 0$ such that if $h \in [0, h_{u,\max})$ and $\bar{\mathcal{B}}_t := \bar{B}_{C_{u,\max}h^{1/2-\delta}}(\hat{x}_{u,t}, \|\cdot\|_{\mathbb{R}^n}) \subset V_t$ for $\delta \in (\rho, 1/2]$, then for any smooth cut-off χ with $\text{supp } \chi \subset V_t$ that is $\chi \equiv 1$ on $\bar{\mathcal{B}}_t$, we have

$$d_g(u^{-1}(\bar{x}_{u,\chi,t}), x_t) \leq C_u h^{1-2\rho},$$

for $C_u > 0$ a constant.

Likewise, there are constants $h_{\iota,\max}, C_{\iota,\max} > 0$ such that for all $h \in [0, h_{\iota,\max})$, given any cut-off $\chi_\iota \in C_c^\infty(\mathbb{R}^D)$ such that $\chi_\iota \equiv 1$ on $\bar{\mathcal{B}}_{\iota,t} := \bar{B}_{C_{\iota,\max}h^{1/2-\delta}}(\hat{x}_{\iota,t}, \|\cdot\|_D)$, we have

$$d_g(\iota^{-1}(\bar{x}_{\chi_\iota,t}), x_t) \leq C_\iota h^{1-2\rho},$$

for $C_\iota > 0$ a constant.

Remark 5.6. — In both cases, if the cut-off is supported on a sufficiently large region that is of size $\Theta(1)$ with respect to h , then the $O(h^{1-2\rho})$ proximity of the coordinate means to the geodesics holds for $h \in [0, h_0]$ with h_0 given by Theorem 5.2.

Proof. — The localization of $U^t[\psi_h]$ as observed in (the proof of) Theorem 5.2 gives a constant $h_{\max} > 0$ such that $d_g(u^{-1}(\hat{x}_{u,t}), x_t) \leq h^{1/2-\delta}$ for $h \in (0, h_{\max}]$ and $\delta \in (\rho, 1/2]$. Indeed, we have a basic lower bound that $\|U^t[\psi_h]\|_\infty \geq C_{\mathcal{M}} h^{-(\frac{1}{2}-\delta)\frac{n}{2}}$ with $C_{\mathcal{M}} > 0$ a constant that depends only on the local geometry of $B_0 := B(x_t, g; h^{1/2-\delta})$. By the decay of the amplitude of $U^t[\psi_h]$ outside of B_t for $h \in (0, h_0]$, we have for all $N \in \mathbb{N}$ some constant $C_N > 0$ such that $C_N h^N \geq \sup_{x \in \mathcal{M} \setminus \bar{B}_t} |U^t[\psi_h]|(x_t)$. So we choose $h_{\max} \in (0, h_0]$ such that for some $N \geq (1/2 - \delta)n/2$ we have for all $h \in (0, h_{\max}]$ that $C_{\mathcal{M}} h^{\delta n/2 - n/4} > C_N h^N$.

We now give the steps to deduce a basic geometric fact for smooth, compact manifolds:

$$(5.5) \quad (\exists) h_{u,0} : (\forall) h \in [0, h_{u,0}], \\ \left[(\exists) C_1 > 0 : x_t \in B_{C_1 h^{1/2-\delta}}(u^{-1}(\hat{x}_{u,t}), g) \right. \\ \left. \implies (\exists) C_2 > 0 : u(x_t) \in B_{C_2 h^{1/2-\delta}}(\hat{x}_{u,t}, \|\cdot\|_{\mathbb{R}^n}) \right].$$

Since u is a diffeomorphism, there is a constant $h_u > 0$ such that for all $h \in [0, h_u]$,

$$|\det Du(x_t)| \operatorname{vol}(\tilde{\mathcal{B}}_t)/2 \leq \operatorname{vol}(\bar{\mathcal{B}}_{g,t}), \\ \bar{\mathcal{B}}_{g,t} := \bar{B}_{h^{1/2-\delta}}(u^{-1}(\hat{x}_{u,t}), g), \quad \tilde{\mathcal{B}}_t := u[\bar{\mathcal{B}}_{g,t}].$$

Moreover, there are constants $h_{\mathcal{M}} > 0$ and $S_2 > 0$ such that for all $h \in [0, h_{\mathcal{M}}]$, $\operatorname{vol}(\bar{\mathcal{B}}_{g,t}) \leq S_2 h^{n(\frac{1}{2}-\delta)}$. Since $\inf_{\mathcal{M}} |\det Du| > 0$, there is thus a constant $C_u > 0$ such that for all $h \in [0, \min\{h_{\max}, h_u, h_{\mathcal{M}}\}]$, we have $\operatorname{vol}(\tilde{\mathcal{B}}_t) \leq 2C_u \operatorname{vol}(\bar{\mathcal{B}}_{g,t}) \leq 2C_u S_2 h^{n(\frac{1}{2}-\delta)}$. Then, denoting $C_{u,\max} := (2C_u S_2)^{\frac{1}{n}} C_n$ for some constant $C_n > 0$ and $\mathcal{B}_t := B_{C_{u,\max} h^{1/2-\delta}}(\hat{x}_{u,t}, \|\cdot\|_{\mathbb{R}^n})$, we have $\hat{x}_{u,t}, u(x_t) \in \tilde{\mathcal{B}}_t \subset \bar{\mathcal{B}}_t$. Now if $\chi \in C_c^\infty(V_t)$ such that $\chi \equiv 1$ on $\bar{\mathcal{B}}_t$, then by (5.4) we have,

$$\bar{u}_j^t(x_0, \xi_0) = u_j(x_t) \chi(x_t) + O(h^{1-2\rho}) = u_j(x_t) + O(h^{1-2\rho}).$$

This means that $\|\bar{u}^t(x_0, \xi_0) - u(x_t)\|_{\mathbb{R}^n} \leq C' h^{1-2\rho}$ for some $C' > 0$. Going through essentially the same arguments as we just saw for (5.5), we have that there are $C, h_1 > 0$ such that for all $h \in [0, h_1]$, $d_g(u^{-1}(\bar{x}_{u,\chi,t}), x_t) \leq C h^{1-2\rho}$, so with $h_{u,\max} := \min\{h_{\max}, h_u, h_{\mathcal{M}}, h_1\}$, we have the first part of the statement of the proposition.

As for the second part, since $\iota^{-1}(\hat{x}_{\iota,t}) = \hat{x}_t$, as in the previous discussion we have that $d_g(\iota^{-1}(\hat{x}_{\iota,t}), x_t) \leq h^{1/2-\delta}$ for $h \in [0, h_{\max}]$. Then, the Assumptions imply (see the Remarks just following) that for $0 \leq h < \min\{h_{\max}, (\kappa/2)^{\frac{2}{1-2\delta}}\}$, $\|\hat{x}_{\iota,t} - \iota(x_t)\|_{\mathbb{R}^D} \leq h^{1/2-\delta}$ so that $\iota(x_t) \in \bar{\mathcal{B}}_{\iota,t}$. If $\chi_\iota \equiv 1$ on $\bar{\mathcal{B}}_{\iota,t}$, then we again have from (5.4) that $\bar{\iota}_j^t(x_0, \xi_0) = \iota_j(x_t) + O(h^{1-2\rho})$. This gives $\|\bar{\iota}^t(x_0, \xi_0) - \iota(x_t)\|_{\mathbb{R}^D} \leq C'_\iota D^{\frac{1}{2}} h^{1-2\rho}$ for some $C'_\iota > 0$. Now for any $x_\iota^* \in B(\bar{\iota}^t(x_0, \xi_0), \|\cdot\|_{\mathbb{R}^D}; C'_\iota D^{\frac{1}{2}} h^{1-2\rho}) \cap \Lambda$, we have $\|x_\iota^* - \iota(x_t)\|_{\mathbb{R}^D} \leq 2C'_\iota D^{\frac{1}{2}} h^{1-2\rho}$. Thus, by the Assumptions, if $0 \leq h < \min\{h_{\max}, (\kappa/2)^{\frac{2}{1-2\delta}}, [\kappa/(4C'_\iota D^{\frac{1}{2}})]^{\frac{1}{1-2\rho}}\}$, then $d_g(\iota^{-1}(x_\iota^*), x_t) \leq 4C'_\iota D^{\frac{1}{2}} h^{1-2\rho}$, which gives the second part of the statement of the proposition. $\square$

6. From graphs to manifolds

We wish to develop consistency between the discrete semigroup $U_{\lambda,\epsilon,N}^t$ that solves a finite-dimensional linear differential equation and the propagator $U_{\lambda,\epsilon}^t$. We proceed by first establishing this for short times, $t \sim \sqrt{\epsilon}$ and then extending by splitting the time into an integer sum of smaller times. For the former part, we need two constructions: first, the consistency of the analytic functional calculus follows almost

immediately from the consistency between the averaging operators $A_{\lambda,\epsilon,N}$ and $A_{\lambda,\epsilon}$. This supplies us with consistency for

$$(6.1) \quad \begin{aligned} \mathcal{C}_N &:= f_e(1 - A_{\lambda,\epsilon,N}; c_{2,0}t\sqrt{\epsilon}) \xrightarrow{N \rightarrow \infty} \mathcal{C} := f_e(1 - A_{\lambda,\epsilon}; c_{2,0}t\sqrt{\epsilon}), \\ \mathcal{S}_N &:= f_o(1 - A_{\lambda,\epsilon,N}; c_{2,0}t\sqrt{\epsilon}) \xrightarrow{N \rightarrow \infty} \mathcal{S} := f_o(1 - A_{\lambda,\epsilon}; c_{2,0}t\sqrt{\epsilon}) \end{aligned}$$

(in the probabilistic sense that we will discuss shortly), wherein we define $c_{2,0} := \sqrt{2c_0/c_2}$ and

$$\begin{aligned} f_e(1 - z; c_{2,0}t\sqrt{\epsilon}) &:= \cos\left(c_{2,0}t\sqrt{\frac{1-z}{\epsilon}}\right), \\ f_o(1 - z; c_{2,0}t\sqrt{\epsilon}) &:= \sin\left(c_{2,0}t\sqrt{\frac{1-z}{\epsilon}}\right) / \sqrt{1-z}. \end{aligned}$$

Thereafter, we construct $\frac{\sqrt{\epsilon}}{c_{2,0}}\sqrt{\Delta_{\lambda,\epsilon,N}} = \sqrt{I - A_{\lambda,\epsilon,N}}$ in order to recover $U_{\lambda,\epsilon,N}^t = \mathcal{C}_N - i\frac{\sqrt{\epsilon}}{c_{2,0}}\sqrt{\Delta_{\lambda,\epsilon,N}}\mathcal{S}_N$. The square root needs more care due to the branch point of $\sqrt{1-z}$ at $z = 1$ that poses an obstruction to the direct application of the consistency for the functional calculus.

Since we are concerned with the functional calculus of averaging operators, we note that in the same way that $A_{\lambda,\epsilon,N}$ extends to a finite-rank operator globally defined on $L^2(\mathcal{M})$, we can also define functions of $A_{\lambda,\epsilon,N}$ as operators on $L^2(\mathcal{M})$ via essentially a form of *Nyström extension*. The general situation is as follows: given $f : \mathcal{D} \rightarrow \mathbb{C}$ analytic on a disk $\mathcal{D} \subset \mathbb{C}$ with $[-1, 1] \subset \overline{\mathcal{D}}$ and having an absolutely convergent Taylor series on $z \in [-1, 1]$, the *derived function relative to f* given by

$$Df(z) := \frac{f(z) - f(0)}{z}$$

is also analytic on $\mathcal{D}$ with absolutely convergent Taylor series on $[-1, 1]$, hence we have $Df(A_{\lambda,\epsilon,N})[u] \in L^\infty$ and

$$(6.2) \quad (\forall)x \in \mathcal{M}, \quad f(A_{\lambda,\epsilon,N})[u](x) = f(0)u(x) + A_{\lambda,\epsilon,N}[Df(A_{\lambda,\epsilon,N})[u]](x);$$

the case for $A_{\lambda,\epsilon,N}$ replaced with $A_{\lambda,\epsilon}$ above is clear. Since $A_{\lambda,\epsilon,N}, A_{\lambda,\epsilon} : L^\infty \rightarrow C^\infty$ are smoothing, this further implies that $(f(A_{\lambda,\epsilon}) - f(A_{\lambda,\epsilon,N})) : L^\infty \rightarrow C^\infty$ and $f(A_{\lambda,\epsilon,N}), f(A_{\lambda,\epsilon}) : C^\infty \rightarrow C^\infty$. A particularly useful consequence is that

$$(6.3) \quad \begin{aligned} &|f(A_{\lambda,\epsilon,N})[u](x)| \\ &\leq |f(0)||u(x)| + \frac{\|k_{\lambda,\epsilon,N}(x, \cdot)\|_{N,\infty}}{p_{\lambda,\epsilon,N}(x)} \frac{1}{N} \sum_{j=1}^N |Df(A_{\lambda,\epsilon,N})[u](x_j)| \\ &\leq |f(0)||u(x)| \\ &\quad + \frac{\|k_{\lambda,\epsilon,N}(x, \cdot)\|_{N,\infty}}{p_{\lambda,\epsilon,N}(x)} \|p_{\lambda,\epsilon,N}\|_{N,\infty}^{\frac{1}{2}} \|p_{\lambda,\epsilon,N}^{-1}\|_{N,2}^{\frac{1}{2}} \sup_{z \in [-1,1]} |Df(z)| \|u\|_{N,2}, \end{aligned}$$

wherein $\|\cdot\|_{N,q} := (\frac{1}{N} \langle |\cdot|^{\frac{q}{2}}, |\cdot|^{\frac{q}{2}} \rangle_{\mathcal{H}_N})^{\frac{1}{q}}$ is the generalized mean q -norm on the space $\mathcal{H}_N := \{u|_{\mathcal{X}_N} : u \in L^\infty(\mathcal{M})\} \cong \mathbb{C}^N$ of the restriction of bounded functions on $\mathcal{M}$

to the set of samples $\mathcal{X}_N := \{x_1, \dots, x_N\}$. The second inequality follows from the symmetric and spectral relations given in Lemma 2.12.

In the following, we will be building on the basic probabilistic bounds from Lemmas 2.16 and 2.18 to develop bounds that give consistency of solutions to wave equations and ultimately, a quantum-classical correspondence. Thus, along the way, we will have several other probabilistic bounds that will depend on previous ones and the notations will pack several functions of N, ϵ, λ , bounds of $p_{\lambda, \epsilon}$, norms of u , etc., so we record here for quick reference the primary bounds and where they are defined or make their first appearance:

Notation 6.1 (Probability bounds). —

- $\gamma_N^{\text{pw}}, \gamma_{\lambda, N}^{\text{pw}}, \gamma_{\lambda, N}, \gamma_{\lambda, N}^*$ are introduced in the beginning of Section 6.1 and the Notation following Lemma 6.3,
- $\tilde{\gamma}_N$ is defined in the statement of Theorem 6.6,
- $\gamma_{\lambda, N, v}, \gamma_{\lambda, N, v}^*$ are defined in the Notation following Lemma 6.8,
- $\omega_{\lambda, N}, \omega_{\lambda, N}^*$ are defined in the Notation following Lemma 6.12,
- $\Omega_{\lambda, t, N}, \Omega_{\lambda, t, N}^*$ are defined in the statement of Theorem 6.14,
- $\rho_N, \rho_{N, 2}$ are defined in the statement of Lemma 6.21,
- $\Xi_{\lambda, N}$ is defined in the statement of Lemma 6.23 and
- $\tilde{\Omega}_{\lambda, t, N}, \tilde{\Omega}_{\lambda, t, N}^*$ are defined in the statement of Lemma 6.24.

We briefly remark on the sequence of convergence results to follow and the nature⁽¹⁰⁾ of the arguments. In Section 6.1 we establish *uniform* consistency of a functional calculus for $A_{\lambda, \epsilon, N}$ with respect to holomorphic functions admitting a uniform bound over derivatives of all orders, along with the consistency of $\sqrt{I - A_{\lambda, \epsilon, N}}$ and combine these to give consistency of $U_{\lambda, \epsilon, N}^t[u]$ for $t \lesssim \sqrt{\epsilon}$ and $u \in L^\infty$, in Lemma 6.12. Then, in Section 6.2 we extend this via a time splitting argument using the semigroup property for the propagator, to $t \lesssim \epsilon^{-\frac{n}{16}}$ in Theorem 6.14. We remark that while the proofs rely on Lemma 2.12 establishing the spectral properties of $A_{\lambda, \epsilon, N}$ due to the connectedness of its graph and on Lemma 2.15 for its pointwise consistency (used in Lemmas 2.16 and 2.18), which involve probabilistic arguments (namely, Chernoff and Bernstein bounds, respectively), the forthcoming arguments using these, until Theorem 6.14 are themselves deterministic. Then, using the control on $\|U_{\lambda, \epsilon}^t[\psi_h]\|_\infty$ we arrive at a Bernstein-type probabilistic bound for the consistency of the discrete propagation of coherent states in the first part of Proposition 6.18, which is again a deterministic argument. In the rest of that proposition we find by an application of the localization of $U_{\lambda, \epsilon}^t[\psi_h]$ established in Theorem 5.2 that for dynamics to time $T_E(h; \rho, q_0)$ and ψ_h localized at (x_0, ξ_0) , $\arg \max_{x \in \mathcal{X}_N} |U_{\lambda, \epsilon, N}^t[\psi_h]|$ is located within an $O(h^{1/2-\tilde{\rho}})$ ball of $x_t := \pi_{\mathcal{M}} \Gamma^{t(x_0, \xi_0)}$ for $\tilde{\rho} \in (\rho, 1/2]$. Then Section 6.4 gives a Bernstein-type bound for the approximation of $u(x_t)$ with $\sum_{j=1}^N u(x_j) |U_{\lambda, \epsilon, N}^t[\psi_h](x_j)|^2 / \|U_{\lambda, \epsilon, N}^t[\psi_h]\|_{N, 2}^2$ for $u \in C^\infty$, which is a discrete realisation of the quantum-classical correspondence (5.1). This follows again by deterministic

⁽¹⁰⁾The author thanks Nalini Anantharaman for bringing attention to the predominantly deterministic nature of the forthcoming arguments.

reasoning, modulo the consistency between discrete and L^2 inner products established in Lemma 6.21, which follows from a Bernstein inequality (similar to the proof of Lemma 2.15). Combining these, we arrive at a discrete analogue of Proposition 5.5: namely, in Proposition 6.29 we have the recovery of geodesics from samples through the coordinate means of propagated coherent states. In Section 6.7 we *unroll* several of these bounds to give the dominant convergence rates for the various discrete objects under study.

6.1. Uniform, short-time consistency

We have seen from Lemmas 2.16 and 2.18 that for each $\lambda \geq 0$ there are C_0, C_1, s, η so that

$$\Pr \left[|(A_{\lambda, \epsilon, N} - A_{\lambda, \epsilon})[u](x)| > \delta \right] \leq \gamma_N^{\text{pw}}(\delta, 1; s, \eta; C_0, C_1; u),$$

wherein we define

$$\gamma_N^{\text{pw}}(\delta, \sigma; s, \eta; C_0, C_1; u) := (C_0 + C_1 N) \exp \left(- \frac{(N - \eta) \epsilon^{n/2} \delta^2 \sigma}{2s \|u\|_\infty (K_{\mathcal{M}, k, p} s \|u\|_\infty + \|k\|_\infty \delta / 3)} \right).$$

We will often use a short-hand to denote this function with only the relevant arguments. The unspecified arguments will be understood to be set by the context, in view of the preceding lemmas and unless specified, we set by default $\sigma, s = 1$. That is to say, in the following arguments we will use the probabilistic consistency rates of the averaging operators on graphs as a black-box, so for brevity we will use the,

Notation 6.2. — The symbol $\gamma_{\lambda, N}^{\text{pw}}(\delta; u)$ denotes the minimal probability bound provided in Lemmas 2.16 and 2.18 for the data $(\mathcal{M}, k, p, \lambda, \epsilon, N, u, \delta)$. Specifically, this function gives the optimal bound when the parameters satisfy the statements of either lemma; otherwise, it yields 1. We further denote by $\eta_\lambda, s_\lambda, C_{0, \lambda}$ and $C_{j, \lambda}$ the structural constants such that

$$\gamma_N^{\text{pw}}(\delta, 1; \eta_\lambda, s_\lambda; C_{0, \lambda}, C_{1, \lambda}; u) = \gamma_{\lambda, N}^{\text{pw}}(\delta; u).$$

When the dependence on u is clear from the context, we will write simply $\gamma_{\lambda, N}^{\text{pw}}(\delta)$.

LEMMA 6.3. — Given $\lambda \geq 0, \epsilon > 0, u \in L^\infty$ and $\delta > 0$, there is a constant $C > 0$ depending only on k, p, λ and the geometry of $\mathcal{M}$ such that

$$(6.4) \quad \Pr \left[\left\| (A_{\lambda, \epsilon, N} - A_{\lambda, \epsilon})[u] \right\|_\infty > \delta \right] \leq C \varepsilon_{\mathcal{M}}^{-n} \left(\gamma_{\lambda, N}^{\text{pw}}(\delta; u) + \gamma_{\lambda, N}^{\text{pw}}(C; 1) \right) =: \gamma_{\lambda, N}(\delta; u)$$

with $\varepsilon_{\mathcal{M}} := \min \{ \text{inj}_{\mathcal{M}}, \epsilon^{\frac{n+1}{2}}, \epsilon^{n+\frac{1}{2}}, \delta \epsilon^{n+\frac{1}{2}} / \|u\|_\infty \}$. Thus, whenever $0 < \epsilon \leq 1$ and $0 < \delta \leq \text{inj}_{\mathcal{M}} \|u\|_\infty$, we have

$$\Pr \left[\left\| (A_{\lambda, \epsilon, N} - A_{\lambda, \epsilon})[u] \right\|_\infty > \delta \right] \leq C \left(\epsilon^{n+\frac{1}{2}} \delta / \|u\|_\infty \right)^{-n} (\gamma_N^{\text{pw}}(\delta; u) + \gamma_N^{\text{pw}}(C; 1)).$$

Proof. — Let $0 < \varepsilon < \text{inj}(\mathcal{M})$ and take $x_1^*, \dots, x_M^* \in \mathcal{M}$ such that $M = \mathcal{N}(\varepsilon)$ is the minimal covering number given by Bishop–Günther inequality and $\bigcup_{j=1}^M B(x_j^*, \varepsilon) = \mathcal{M}$. For each $j \in [M] := \{1, \dots, M\}$, let $\mathcal{U}_j \subset B_{\mathcal{M}}(x_j^*, \text{inj}(x_j^*)) \subset \mathcal{M}$

be a geodesically convex neighbourhood of x_j^* and let $s^{-1} : \mathcal{U}_j \rightarrow V_j \subset \mathbb{R}^n$ provide normal coordinates for this neighbourhood. Then, for any $v \in C^\infty$ and $x \in \mathcal{M}$, there is $j \in [M]$ such that $x \in B(x_j^*, \varepsilon)$ so by Taylor expansion centered at $0 \in V_j$ and evaluated at $s^{-1}(x) =: w \in V_j$, Taylor's theorem gives that

$$(6.5) \quad |v(x)| \leq |v(x_j^*)| + \varepsilon \max_{|\alpha|=1} \sup_{w \in \tilde{B}_j} |\partial^\alpha [v \circ s](w)|,$$

with $\tilde{B}_j := s(B(x_j^*, \varepsilon))$. We will use the following bound:

$$(6.6) \quad \begin{aligned} & |\partial_{w^{(i)}} k_\epsilon(s(w), y)| \\ &= 2\epsilon^{-\frac{n+2}{2}} \left| \left\langle \iota \circ s(w) - \iota(y), \partial_{w^{(i)}} [\iota \circ s(\cdot) - \iota(y)](w) \right\rangle_{\mathbb{R}^n} \times k'_\epsilon(s(w), y) \right| \\ &\leq \epsilon^{-\frac{n+2}{2}} \|\iota \circ s(w) - \iota(y)\| \|J_\iota[\partial_{w^{(i)}} s](w)\| |k'_\epsilon(s(w), y)| \\ &= \epsilon^{-\frac{n+2}{2}} \|\iota \circ s(w) - \iota(y)\| \|\partial_{w^{(i)}} s(w)\| |k'_\epsilon(s(w), y)| \\ &\leq C_{\mathcal{M}, k, 1} \epsilon^{-\frac{n+1}{2}}, \end{aligned}$$

wherein $k' : r \mapsto \partial_r k$ is localized to $[0, R_k^2]$ and $k'_\epsilon(x, y) := k'(\|\iota(x) - \iota(y)\|^2/\epsilon)$, which gives that $\|\iota(x) - \iota(y)\| \leq R_k \sqrt{\epsilon}$ and $C_{\mathcal{M}, k, 1} = C_{\mathcal{M}, 1} R_k \|k'\|_\infty$ with $C_{\mathcal{M}, 1} := \max_{i \in [n]} \|\partial_{w^{(i)}} s(w)\|_\infty$. Hence also, $|\partial_{w^{(i)}} [p_\epsilon \circ s](w)|, |\partial_{w^{(i)}} [p_{\epsilon, N} \circ s](w)| \leq C_{\mathcal{M}, k, 1} \epsilon^{-\frac{n+1}{2}}$.

Now let $\delta_1 > 0$ and assume we are in the event

$$\mathcal{A}(\varepsilon, \delta_1) : |p_{\lambda', \epsilon, N}(x_j^*) - p_{\lambda', \epsilon}(x_j^*)| \leq \delta_1/2 \quad \text{for all } j \in \{1, \dots, M\}, \lambda' \in \{0, \lambda\}.$$

Then for any $x \in \mathcal{M}$, there is $j \in [M]$ such that $d_g(x_j^*, x) \leq \varepsilon$, so that by (6.5) and (6.6),

$$\begin{aligned} |p_{\epsilon, N}(x) - p_\epsilon(x)| &\leq \frac{\delta_1}{2} + 2\varepsilon \max_{|\alpha|=1} \sup_{(w, y) \in \tilde{B}_j \times \mathcal{M}} |\partial^\alpha [k_\epsilon(s)](w, y)| \\ &\leq \frac{\delta_1}{2} + 2C_{\mathcal{M}, k, 1} \epsilon^{-\frac{n+1}{2}} \varepsilon. \end{aligned}$$

In the following, we will use the notation:

$$\min_{\mathcal{M}} : \mathbb{R}^S \ni \vec{a} \mapsto \min\{\text{inj}(\mathcal{M}), a_1, \dots, a_S\} \in \mathbb{R}$$

for any $S \geq 1$. Hence, with

$$\varepsilon \leq \min\{\text{inj}(\mathcal{M}), \epsilon^{\frac{n+1}{2}} \delta_1 / (4C_{\mathcal{M}, k, 1})\} = \min_{\mathcal{M}} \left(\epsilon^{\frac{n+1}{2}} \delta_1 / (4C_{\mathcal{M}, k, 1}) \right),$$

we have that $|p_{\epsilon, N}(x) - p_\epsilon(x)| \leq \delta_1$. Thus, assuming $\epsilon \leq 1$ we have the bound,

$$|\partial_{w^{(i)}} [p_{\lambda, \epsilon, N} \circ s](w)| \leq \epsilon^{-n-\frac{1}{2}} C_{\mathcal{M}, k, 1} C_{p, \lambda, 1, \delta_1},$$

with

$$C_{p, \lambda, 1, \delta_1} := \frac{\lambda(\overline{C}_p + \delta_1)^{2\lambda}}{(\underline{C}_p - \delta_1)^{4\lambda}} \left(\frac{1}{\lambda} + \frac{\|k\|_\infty}{\overline{C}_p + \delta_1} \right)$$

and further assuming that $\varepsilon \leq \min_{\mathcal{M}} (\delta_1 (\epsilon^{\frac{n+1}{2}}, \epsilon^{n+\frac{1}{2}}/C_{p, \lambda, 1, \delta_1}) / (4C_{\mathcal{M}, k, 1}))$ gives on another application of (6.5) and (6.6),

$$|p_{\lambda, \epsilon, N}(x) - p_{\lambda, \epsilon}(x)| \leq \delta_1.$$

Now let $x, y \in \mathcal{M}$ and s^{-1} be centered at x_j^* such that $x \in B(x_j^*, \varepsilon)$. Then, combining the above bounds gives,

$$\begin{aligned} & \left| \partial_{w^{(i)}} \left[\frac{k_{\lambda, \epsilon, N}(s(\cdot), y)}{p_{\lambda, \epsilon, N} \circ s(\cdot)} \right]_{(\cdot=w)} \right| \\ &= \left| \frac{(p_{\lambda, \epsilon, N} p_{\epsilon, N}^\lambda)(x) \partial_{w^{(i)}} [k_\epsilon(s, y)](w) - k_\epsilon(s, y) \partial_{w^{(i)}} [p_{\lambda, \epsilon, N} p_{\epsilon, N}^\lambda \circ s](w)}{p_{\epsilon, N}(y)^\lambda (p_{\lambda, \epsilon, N}(x) p_{\epsilon, N}^\lambda(x))^2} \right| \\ &\leq \epsilon^{-(n+\frac{1}{2})} \frac{C_{\mathcal{M}, k, 1}}{(\underline{C}_{p, \lambda} - \delta_1)^3 (\underline{C}_p - \delta_1)^{3\lambda}} \\ &\quad \times \left[\epsilon^{\frac{n}{2}} (\overline{C}_{p, \lambda} + \delta_1) (\overline{C}_p + \delta_1)^\lambda \right. \\ &\quad \left. + \|k\|_\infty (C_{p, \lambda, 1, \delta_1} (\overline{C}_p + \delta_1)^\lambda + \lambda (\overline{C}_{p, \lambda} + \delta_1) (\overline{C}_p + \delta_1)^{\lambda-1}) \right] \\ &\leq \epsilon^{-(n+\frac{1}{2})} C_{\mathcal{M}, k, 1} C_{k, p, \lambda, 1, \delta_1} \end{aligned}$$

with

$$\begin{aligned} C_{k, p, \lambda, 1, \delta_1} &:= ((\underline{C}_{p, \lambda} - \delta_1) (\underline{C}_p - \delta_1)^\lambda)^{-3} \left[(\overline{C}_{p, \lambda} + \delta_1) (\overline{C}_p + \delta_1)^\lambda \right. \\ &\quad \left. + \|k\|_\infty (C_{p, \lambda, 1, \delta_1} (\overline{C}_p + \delta_1)^\lambda + \lambda (\overline{C}_{p, \lambda} + \delta_1) (\overline{C}_p + \delta_1)^{\lambda-1}) \right]. \end{aligned}$$

In the continuum case, these bounds hold with $\delta_1 = 0$; so letting $\delta_1 = \min\{\underline{C}_{p, \lambda}, \underline{C}_p\}/2$ we have $C_{p, \lambda, 1, \delta_1} \leq 36^\lambda C_{p, \lambda, 1, 0} =: C_{p, \lambda, 1}$ and

$$\begin{aligned} & \left| \partial_{w^{(i)}} \left[\frac{k_{\lambda, \epsilon, N}(s(\cdot), y)}{p_{\lambda, \epsilon, N} \circ s(\cdot)} \right]_{(\cdot=w)} \right|, \quad \left| \partial_{w^{(i)}} \left[\frac{k_{\lambda, \epsilon}(s(\cdot), y)}{p_{\lambda, \epsilon} \circ s(\cdot)} \right]_{(\cdot=w)} \right| \leq \epsilon^{-(n+\frac{1}{2})} C_{\mathcal{M}, k, 1} C_{k, p, \lambda, 1}, \\ & \text{where } C_{k, p, \lambda, 1} := 12(432^\lambda C_{k, p, \lambda, 1, 0}). \end{aligned}$$

With this and the event

$$\mathcal{B}(\varepsilon, \delta) : |A_{\lambda, \epsilon, N}[u](x_j^*) - A_{\lambda, \epsilon}[u](x_j^*)| \leq \delta/2 \quad \text{for all } j \in \{1, \dots, M\},$$

gives upon Taylor expanding as in (6.5),

$$\begin{aligned} & |(A_{\lambda, \epsilon, N} - A_{\lambda, \epsilon})[u](x)| \leq \delta/2 + \varepsilon \max_{|\alpha|=1} \|\partial^\alpha (A_{\lambda, \epsilon, N} - A_{\lambda, \epsilon})[u] \circ s\|_\infty \\ & \leq \delta/2 + C' \varepsilon \epsilon^{-(n+\frac{1}{2})} \|u\|_\infty \end{aligned}$$

with $C' := 2C_{\mathcal{M}, k, 1} C_{k, p, \lambda, 1}$. Since the second inequality on the right-hand side is independent of x and the Bishop–Günther inequality tells that $M = C\varepsilon^{-n}$ for some constant $C > 0$, we have upon taking

$$\varepsilon = \min_{\mathcal{M}} \left(\frac{1}{4C_{\mathcal{M}, k, 1}} \left[\delta_1 \epsilon^{\frac{n+1}{2}}, \frac{\delta_1 \epsilon^{n+\frac{1}{2}}}{C_{p, \lambda, 1}}, \frac{\delta \epsilon^{n+\frac{1}{2}}}{\|u\|_\infty C_{k, p, \lambda, 1}} \right] \right)$$

and a union bound over the probability events $\mathcal{A}(\varepsilon, \delta_1)$ and $\mathcal{B}(\varepsilon, \delta)$ that

$$\Pr \left[\left\| (A_{\lambda, \epsilon, N} - A_{\lambda, \epsilon})[u] \right\|_{\infty} > \delta \right] \leq C\varepsilon^{-n} \left(\gamma_N^{\text{pw}}(\delta; u) + \gamma_N^{\text{pw}}(\delta_1; 1) \right).$$

□

Notation 6.4. — We will denote

$$\gamma_{\lambda, N}(\cdot) := C\varepsilon_{\mathcal{M}}^{-n} \left(\gamma_{\lambda, N}^{\text{pw}}(\delta; u) + \gamma_{\lambda, N}^{\text{pw}}(C; 1) \right)$$

with the notational simplifications for $\gamma_{\lambda, N}^{\text{pw}}$ being applied in the same way to $\gamma_{\lambda, N}$. Additionally, to allow variability, we will denote

$$\gamma_{\lambda, N}^*(\delta, \sigma; u) := C\varepsilon_{\mathcal{M}}^{-n} \left(\gamma_N^{\text{pw}}(\delta, \sigma; \eta_{\lambda}, s_{\lambda}; C_{0, \lambda}, C_{1, \lambda}; u) + \gamma_{\lambda, N}^{\text{pw}}(C; 1) \right)$$

and shorten this to $\gamma_N^*(\delta, \sigma)$ when the dependence on u is clear from context.

LEMMA 6.5. — Given $\lambda \geq 0$, $\epsilon > 0$, $u \in L^{\infty}$ and $m \in \mathbb{N}$, we have for all $\delta > 0$,

$$\Pr \left[\left\| A_{\lambda, \epsilon, N}^m[u] - A_{\lambda, \epsilon}^m[u] \right\|_{\infty} > m\delta \right] \leq m\gamma_{\lambda, N}(\delta; u).$$

Proof. — Since $\|A_{\lambda, \epsilon}[u]\|_{\infty} \leq \|u\|_{\infty}$, we have the same probabilistic bound for the event that $\|(A_{\lambda, \epsilon, N} - A_{\lambda, \epsilon})[A_{\epsilon}u]\|_{\infty} \leq \delta$ as for the event $\|(A_{\lambda, \epsilon, N} - A_{\lambda, \epsilon})[u]\|_{\infty} \leq \delta$. Moreover since $A_{\lambda, \epsilon, N}[1] = 1$ and the matrix has non-negative entries,

$$\begin{aligned} \left\| A_{\lambda, \epsilon, N}^2[u] - A_{\lambda, \epsilon}^2[u] \right\|_{\infty} &\leq \left\| (A_{\lambda, \epsilon, N} - A_{\lambda, \epsilon})[A_{\lambda, \epsilon}u] \right\|_{\infty} + \left\| A_{\lambda, \epsilon, N}[(A_{\lambda, \epsilon, N} - A_{\lambda, \epsilon})[u]] \right\|_{\infty} \\ &\leq \left\| (A_{\lambda, \epsilon, N} - A_{\lambda, \epsilon})[A_{\lambda, \epsilon}u] \right\|_{\infty} + \left\| (A_{\lambda, \epsilon, N} - A_{\lambda, \epsilon})[u] \right\|_{\infty} \end{aligned}$$

Therefore, applying a union bound over both events, we have,

$$\Pr \left[\left\| (A_{\lambda, \epsilon, N}^2 - A_{\lambda, \epsilon}^2)[u] \right\|_{\infty} > 2\delta \right] \leq 2\gamma_{\lambda, N}(\delta; u).$$

Now assume that for all $2 \leq m \leq M-1$,

$$\Pr \left[\left\| (A_{\lambda, \epsilon, N}^m - A_{\lambda, \epsilon}^m)[u] \right\|_{\infty} \leq m\delta \right] > 1 - m\gamma_{\lambda, N}(\delta; u).$$

Write similar to before,

$$\begin{aligned} \left\| A_{\lambda, \epsilon, N}^M[u] - A_{\lambda, \epsilon}^M[u] \right\|_{\infty} &\leq \left\| (A_{\lambda, \epsilon, N}^{M-1} - A_{\lambda, \epsilon}^{M-1})[A_{\lambda, \epsilon}u] \right\|_{\infty} + \left\| A_{\lambda, \epsilon, N}^{M-1}[(A_{\lambda, \epsilon, N} - A_{\lambda, \epsilon})[u]] \right\|_{\infty}. \end{aligned}$$

Since for any integer $m \geq 1$, $A_{\lambda, \epsilon, N}^m$ has non-negative entries and $A_{\lambda, \epsilon, N}^m[1] = 1$, we see that for any $v \in L^{\infty}$, $|A_{\lambda, \epsilon, N}^m[v](x)| \leq \|v\|_{\infty}$. Therefore, after a union bound we have that

$$\Pr \left[\left\| (A_{\lambda, \epsilon, N}^M - A_{\lambda, \epsilon}^M)[u] \right\|_{\infty} \leq M\delta \right] > 1 - M\gamma_{\lambda, N}(\delta; u),$$

whence having completed the induction step, we have the bound as given in the first part of the statement of Lemma 6.5. □

THEOREM 6.6. — *Let $f: \mathbb{C} \rightarrow \mathbb{C}$ be an entire function such that for $w \in \mathbb{C}$ there exists a constant $K_w > 0$ satisfying*

$$(\forall) m \geq 0, \quad |\partial_z^m f|_{z=w}| < K_w.$$

Then, given $\lambda \geq 0$, $\epsilon > 0$, $u \in L^\infty$ and $\delta > 0$,

$$\Pr \left[\left\| f(A_{\lambda, \epsilon, N} + wI)[u] - f(A_{\lambda, \epsilon} + wI)[u] \right\|_\infty > \delta \right] \leq \tilde{\gamma}_{\lambda, N}(\delta/(2eK_w)),$$

$$\text{with } \tilde{\gamma}_{\lambda, N} := \frac{\gamma_{\lambda, N}}{(1 - \gamma_{\lambda, N})^2}.$$

Proof. — Let $f: \mathbb{C} \rightarrow \mathbb{C}$ be an entire function with $|\partial_z^m f|_{z=w}| < K_w$ for some constant $K_w > 0$ and all $m \geq 0$. By Lemma 6.5 and a union bound, we have

$$\Pr \left[(\forall) m \in \{1, \dots, M\}, \left\| (A_{\lambda, \epsilon, N}^m - A_{\lambda, \epsilon}^m)[u] \right\|_\infty \leq m^2 \delta \right] > 1 - \sum_{m=1}^M m \gamma_{\lambda, N}(m\delta; u)$$

and since for all $m \geq 1$, $\gamma_{\lambda, N}(m\delta) \leq \gamma_{\lambda, N}^*(\delta, m)$, we can take all powers at once to have,

$$\begin{aligned} \Pr \left[(\forall) m \in \mathbb{N}, \left\| (A_{\lambda, \epsilon, N}^m - A_{\lambda, \epsilon}^m)[u] \right\|_\infty > m^2 \delta \right] \\ \leq \sum_{m=1}^{\infty} m \gamma_{\lambda, N}^*(\delta, m) \leq \frac{\gamma_{\lambda, N}(\delta)}{(1 - \gamma_{\lambda, N}(\delta))^2} =: \tilde{\gamma}(\delta). \end{aligned}$$

In this event, upon taking a Taylor series expansion of $f(z)$ at $z = w$,

$$\begin{aligned} \left| f(A_{\lambda, \epsilon, N} + wI)[u] - f(A_{\lambda, \epsilon} + wI)[u] \right| &\leq K_w \delta \sum_{m=1}^{\infty} \frac{m^2}{m!} \\ &< eK_w \delta \end{aligned}$$

hence,

$$\Pr \left[\left\| f(A_{\lambda, \epsilon, N})[u] - f(A_{\lambda, \epsilon})[u] \right\|_\infty > \delta \right] \leq \tilde{\gamma} \left(\frac{\delta}{2eK_w} \right). \quad \square$$

Remark 6.7. — The condition that all derivatives of f are bounded enforces that we take $t \sim \sqrt{\epsilon}$. While the class of f can be generalized by way of Hadamard's multiplication theorem, the condition on the short time-scales is not artificial: if we directly apply this to the approximation of $\mathcal{C}(t/\sqrt{\epsilon})$ from $\mathcal{C}_N(t/\sqrt{\epsilon})$, then the resulting error is $O(e^{\frac{t}{\sqrt{\epsilon}}} t^2 / \epsilon)$, which is only practical for asymptotically short times, $t \sim \sqrt{\epsilon}$ in any case.

LEMMA 6.8. — *Let $\lambda \geq 0$, $\epsilon > 0$, $u \in L^\infty$ and $\delta > 0$. Suppose $N \in \mathbb{N}$ is large enough so that*

$$\beta_\gamma := \log \left[\frac{C_{0, \lambda} + C_{1, \lambda} N}{\gamma_{\lambda, N}(\delta; u)} \right] > 1.$$

Then for $v := 8 \log(\beta_\gamma/2)/\beta_\gamma$ and any $0 < \varepsilon \leq 1$, we have

$$(6.7) \quad \Pr \left[\left\| B_{\lambda, \epsilon, N}^{(\varepsilon)}[u] - B_{\lambda, \epsilon}^{(\varepsilon)}[u] \right\|_\infty > \delta \right] \leq \gamma_{\lambda, N} \left(\frac{\delta \varepsilon^{\frac{1}{2} + v(\beta)}}{2\sqrt{\pi}}; u \right),$$

wherein $B_{\lambda,\epsilon,N}^{(\epsilon)} := \sqrt{(1+\epsilon)I - A_{\lambda,\epsilon,N}}$ and $B_{\lambda,\epsilon}^{(\epsilon)} := \sqrt{(1+\epsilon)I - A_{\lambda,\epsilon}}$.

Thus,

$$\Pr\left[\|B_{\lambda,\epsilon,N}^{(\delta^2)}[u] - B_{\lambda,\epsilon}^{(\delta^2)}[u]\|_\infty > \delta\right] \leq \gamma_{\lambda,N}\left(\frac{\delta^{2(1+v)}}{2\sqrt{\pi}}; u\right).$$

Proof. — Let $v > 0$ be variable for the moment and proceed as in the proof of Theorem 6.6, with the change that now we take for each $m \in \mathbb{N}$ an $m^v \delta$ error in $\|A_{\lambda,\epsilon,N}[u] - A_{\lambda,\epsilon}[u]\|_\infty$, so *mutatis mutandis* we have,

$$\Pr\left[(\forall)m \in \mathbb{N}, \|A_{\lambda,\epsilon,N}^m - A_{\lambda,\epsilon}^m[u]\|_\infty > m^{1+v}\delta\right] \leq \sum_{m=1}^{\infty} m\gamma_{\lambda,N}^*(\delta, m^v; u).$$

Suppressing all coefficients independent of m , the right-hand side has the form

$$\sum_{m=1}^{\infty} m\gamma_{\lambda,N}^*(\delta, m^v; u) = O\left(\sum_{m=1}^{\infty} m(\alpha e^{-\beta m^v})\right)$$

for some $\alpha > 0$ and $\beta = \beta_\gamma > 0$. We have,

$$\alpha \sum_{m=1}^{\infty} m e^{-\beta m^v} \leq \frac{1}{v} \int_1^{\infty} y^{\frac{2}{v}-1} e^{-\beta y} dy.$$

Letting $r := \lceil \frac{1}{v} \rceil$ then bounding the right-hand side with the substitution of $1/v$ with r and applying successive integration by parts gives,

$$\begin{aligned} \sum_{m=1}^{\infty} m e^{-\beta m^v} &\leq \frac{e^{-\beta}}{\beta} r \sum_{j=1}^{2(r-1)} \frac{(2r-1)!}{(2r-j)!} + r(2r)! \int_1^{\infty} y^{-1} e^{-\beta y} dy \\ &\leq \frac{2r(2r)!}{\beta} e^{-\beta}. \end{aligned}$$

By Stirling's approximation, [Rob55] gives the bound $(2r)! \leq e^{1-2r}(2r)^{2r+\frac{1}{2}}$ and therefore,

$$\sum_{m=1}^{\infty} m e^{-\beta m^v} \leq \frac{e(2r)^{\frac{3}{2}}}{\beta} e^{-\beta+2r(\log(2r)-1)}.$$

Setting $v(\beta) := 8 \log(\beta/2)/\beta$ and using that $\beta \geq 1$ for sufficiently large N then gives,

$$\begin{aligned} 2r(\log(2r)-1) &= 2 \left\lceil \frac{\beta}{8 \log(\beta/2)} \right\rceil \left(\log \left(2 \left\lceil \frac{\beta}{8 \log(\beta/2)} \right\rceil \right) - 1 \right) \\ &\leq \frac{\beta}{2 \log(\beta/2)} \left(\log \left(\frac{\beta/2}{\log(\beta/2)} \right) - 1 \right), \end{aligned}$$

hence,

$$\begin{aligned} \sum_{m=1}^{\infty} m e^{-\beta m^{v(\beta)}} &\leq e \left(\frac{\beta}{2 \log(\beta/2)} \right)^{\frac{1}{2}} e^{-\frac{\beta}{2} \left(1 + \frac{1}{\log(\beta/2)} \right)} \\ &\leq e^{-\frac{\beta}{2}}. \end{aligned}$$

On recovering the original form of the probability upper bound, we have,

$$\Pr\left[(\forall)m \in \mathbb{N}, \left\| (A_{\lambda,\epsilon,N}^m - A_{\lambda,\epsilon}^m)[u] \right\|_{\infty} > m^{1+v(\beta)}\delta\right] \leq \gamma_{\lambda,N}(\delta/\sqrt{2}; u).$$

Next, given the event that for all $m \in \mathbb{N}$, $|(A_{\lambda,\epsilon,N}^m - A_{\lambda,\epsilon}^m)[u]| \leq m^{1+v(\beta)}\delta$, we compare the applications of the Taylor series expansion of $f := \sqrt{z}$ at $1+\varepsilon$ to $(1+\varepsilon)I - A_{\lambda,\epsilon,N}$ and $(1+\varepsilon)I - A_{\lambda,\epsilon}$, for a *perturbation parameter* $\varepsilon > 0$, with this term-wise absolute error rate: assuming N is sufficiently large that $v(\beta) \leq 1$, we have,

$$\begin{aligned} \left\| B_{\lambda,\epsilon,N}^{(\varepsilon)}[u] - B_{\lambda,\epsilon}^{(\varepsilon)}[u] \right\|_{\infty} &\leq \delta \sum_{m=1}^{\infty} \left| \binom{\frac{1}{2}}{m} \right| \frac{m^{1+v(\beta)}}{(1+\varepsilon)^{m-\frac{1}{2}}} \\ &\leq \delta \sum_{m=1}^{\infty} \frac{m^{v(\beta)-\frac{1}{2}}}{(1+\varepsilon)^{m-\frac{1}{2}}} = \delta \sqrt{1+\varepsilon} \operatorname{Li}\left(\frac{1}{2} - v(\beta), \frac{1}{1+\varepsilon}\right) \\ &\leq \delta \Gamma\left[\frac{1}{2} + v(\beta)\right] \varepsilon^{-(\frac{1}{2}+v(\beta))} \sqrt{1+\varepsilon} \\ &\leq \sqrt{2\pi} \varepsilon^{-(\frac{1}{2}+v(\beta))} \delta. \end{aligned}$$

The second inequality comes from $\left| \binom{1/2}{m} \right| \leq m^{-\frac{3}{2}}$ and the following one is due to the observation that

$$\begin{aligned} \varepsilon^{s+1/2} \operatorname{Li}\left(\frac{1}{2} - s, \frac{1}{1+\varepsilon}\right) &= \frac{1}{\Gamma\left(\frac{1}{2} - s\right)} \int_0^{\infty} \frac{\varepsilon^{s+1/2} t^{-(s+1/2)}}{e^t(1+\varepsilon) - 1} dt \\ &= \frac{1}{\Gamma\left(\frac{1}{2} - s\right)} \int_0^{\infty} \frac{\varepsilon}{e^{\varepsilon t}(1+\varepsilon) - 1} t^{-(s+1/2)} dt \\ &\xrightarrow{\varepsilon \rightarrow 0} \frac{1}{\Gamma\left(\frac{1}{2} - s\right)} \int_0^{\infty} \frac{t^{-(s+1/2)}}{1+t} dt \\ &= \frac{B\left(\frac{1}{2} - s, \frac{1}{2} + s\right)}{\Gamma\left(\frac{1}{2} - s\right)} = \Gamma\left(\frac{1}{2} + s\right), \end{aligned}$$

(wherein $B(x, y) = \Gamma(x)\Gamma(y)/\Gamma(x+y)$ is the Beta function) together with the monotonicity of $\operatorname{Li}\left(\frac{1}{2} - v(\beta), \frac{1}{1+\varepsilon}\right)$ in ε . The fourth (final) inequality uses that $\Gamma\left(\frac{1}{2} + s\right)$ is maximized at $s = 0$ when $0 \leq s \leq 1$, *viz.*, we employ the assumption that N is sufficiently large that $v(\beta) \leq 1$. Altogether,

$$\Pr\left[\left\| B_{\lambda,\epsilon,N}^{(\varepsilon)}[u] - B_{\lambda,\epsilon}^{(\varepsilon)}[u] \right\|_{\infty} > \delta\right] \leq \gamma_{\lambda,N}(\delta \varepsilon^{\frac{1}{2}+v(\beta)} / (2\sqrt{\pi}); u),$$

which upon setting $\varepsilon = \delta^2$ gives both of the probability bounds in the statement of the lemma. $\square$

Notation 6.9. — We will use the symbol v to denote the function given by Lemma 6.8 and we define the functions

$$\gamma_{\lambda,N,v}^*(\delta, \varepsilon; u) := \gamma_{\lambda,N}(\delta \varepsilon^{\frac{1}{2}+v(\beta)} / (2\sqrt{\pi}); u)$$

and

$$\gamma_{\lambda,N,v}(\delta; u) := \gamma_{\lambda,N}(\delta^{2(1+v)}/(2\sqrt{\pi}); u)$$

to denote the corresponding probability bounds for the consistency of the square root of the perturbed operators.

An application of the relations in Lemma 2.12 is to transfer consistency between the pair $B_{\lambda,\epsilon,N}^{(\varepsilon)}, B_{\lambda,\epsilon}^{(\varepsilon)}$ to that between the pair of square roots of the unperturbed operators: namely we have,

THEOREM 6.10. — *Let $\lambda \geq 0$ and $u \in L^\infty$. Then, there are constants $C_1, C_2 > 0$ depending only on k and the geometry of $\mathcal{M}$ such that for all $\epsilon \in (0, C_1]$ and $\delta > 0$,*

$$(6.8) \quad \Pr \left[\|B_{\lambda,\epsilon,N}[u] - B_{\lambda,\epsilon}[u]\|_\infty > \delta \right] \leq \gamma_{\lambda,N,v}(\delta/3; u) + e^{-\frac{N\epsilon^{\frac{N}{2}}\delta^2}{C_2}},$$

with $B_{\lambda,\epsilon,N} := \sqrt{I - A_{\lambda,\epsilon,N}}$ and $B_{\lambda,\epsilon} := \sqrt{I - A_{\lambda,\epsilon}}$.

Proof. — Let $\varepsilon \geq 0$ and set $B_{\lambda,\epsilon,N}^{(\varepsilon)}$ and $B_{\lambda,\epsilon}^{(\varepsilon)}$ as in the proof of Lemma 6.8. Assume throughout the event that $A_{\lambda,\epsilon,N}$ gives a connected graph, as per part (2) of Lemma 2.12. Then, the matrix $(1 + \varepsilon)I - A_{\lambda,\epsilon,N}$ is an M-matrix and (in modulus) the largest eigenvalue of $A_{\lambda,\epsilon,N}$ is one, which is also simple. Therefore, it follows from [AS82, Theorem 4] that $B_{\lambda,\epsilon,N}^{(\varepsilon)} = (1 + \varepsilon)^{\frac{1}{2}}(I - \mathcal{B}_{\lambda,\epsilon,N}^{(\varepsilon)})$ is also an M-matrix for $\mathcal{B}_{\lambda,\epsilon,N}^{(\varepsilon)}$ some matrix with non-negative entries and spectral radius $r_{\varepsilon,N} < ((2 + \varepsilon)/(1 + \varepsilon))^{\frac{1}{2}} - 1 < 1$.

Let $L_{\mathbb{R}}^2(\mathcal{M}) := L^2(\mathcal{M} \rightarrow \mathbb{R})$ be the real Hilbert space of real-valued functions on $\mathcal{M}$. Then, $(B_{\lambda,\epsilon}^{(\varepsilon)})^2_{\lambda,\epsilon} : L_{\mathbb{R}}^2(\mathcal{M}) \rightarrow L_{\mathbb{R}}^2(\mathcal{M})$ is an *M-operator* (an infinite-dimensional generalization of M-matrices) with respect to the cone $\mathcal{K}$ of non-negative functions and satisfies the conditions of [Mar95, Theorem 3]. Therefore, by that theorem, $B_{\lambda,\epsilon}^{(\varepsilon)} = (1 + \varepsilon)^{\frac{1}{2}}(I - \mathcal{B}_{\lambda,\epsilon}^{(\varepsilon)})$ is also an M-operator for some $\mathcal{B}_{\lambda,\epsilon}^{(\varepsilon)} : L_{\mathbb{R}}^2 \rightarrow L_{\mathbb{R}}^2$ with spectral radius $r_\varepsilon < 1$ (in the same way as for the discrete counterpart) and such that $\mathcal{B}_{\lambda,\epsilon}^{(\varepsilon)}[\mathcal{K}] \subset \mathcal{K}$.

As per Lemma 2.12, $B_{\lambda,\epsilon,N}^{(\varepsilon)}$ and $B_{\lambda,\epsilon}^{(\varepsilon)}$ are symmetrized via conjugation by $\sqrt{p_{\lambda,\epsilon,N}}$ and $\sqrt{p_{\lambda,\epsilon}}$, respectively, hence $\mathcal{B}_{\lambda,\epsilon,N}^{(\varepsilon)}$ and $\mathcal{B}_{\lambda,\epsilon}^{(\varepsilon)}$ are as well, so it follows from spectral theory that the symmetrizations of each of the latter operators have spectral radius less than one. Therefore, the spectral radius of $\mathcal{B}_{\lambda,\epsilon,N}^{(\varepsilon)} + \mathcal{B}_{\lambda,\epsilon,N}^{(0)}$ and $\mathcal{B}_{\lambda,\epsilon}^{(\varepsilon)} + \mathcal{B}_{\lambda,\epsilon}^{(0)}$ is less than two. We may write,

$$\begin{aligned} B_{\lambda,\epsilon,N}^{(\varepsilon,0)} &:= B_{\lambda,\epsilon,N}^{(\varepsilon)} + B_{\lambda,\epsilon,N}^{(0)} = 2(1 + \varepsilon)^{\frac{1}{2}} \left(I - \frac{1}{2}(\mathcal{B}_{\lambda,\epsilon,N}^{(\varepsilon)} + \mathcal{B}_{\lambda,\epsilon,N}^{(0)}) \right), \\ B_{\lambda,\epsilon}^{(\varepsilon,0)} &:= B_{\lambda,\epsilon}^{(\varepsilon)} + B_{\lambda,\epsilon}^{(0)} = 2(1 + \varepsilon)^{\frac{1}{2}} \left(I - \frac{1}{2}(\mathcal{B}_{\lambda,\epsilon}^{(\varepsilon)} + \mathcal{B}_{\lambda,\epsilon}^{(0)}) \right), \end{aligned}$$

that is, each of these operators are in the form $t(I - B)$ with $t > 0$ and B having a spectral radius less than one and either having non-negative entries in the matrix case or preserving the non-negative cone $\mathcal{K}$ in the infinite dimensional case. This means that the first sum is an M-matrix and the second is an M-operator. Moreover, whenever $\varepsilon > 0$, both operators are non-singular. In the non-singular M-operator case,

[Mar95, Theorem 1] tells that $(B_{\lambda,\epsilon}^{(\varepsilon,0)})^{-1}$ preserves $\mathcal{K}$. We may express $(B_{\lambda,\epsilon}^{(\varepsilon,0)})^{-1}$ as the spectral application of the function $f(z) := (\sqrt{1+\varepsilon-z} + \sqrt{1-z})^{-1}$ to $z = A_{\lambda,\epsilon}$. Then, the decomposition (6.2) applies since f is analytic on the unit disc and has absolutely convergent Taylor series on $[-1, 1]$. Using this, we see that $(B_{\lambda,\epsilon}^{(\varepsilon,0)})^{-1}(x, y)$ is smooth for $x \neq y$ and due to the preservation of $\mathcal{K}$ we also have that given any $(x, y) \in \mathcal{M}^2$, for all $\epsilon_0 > 0$,

$$A_{\epsilon_0} \left[(B_{\lambda,\epsilon}^{(\varepsilon,0)})^{-1}(\cdot, y) \right](x) \geq 0.$$

Combining these properties, we have by continuity off the diagonal that on letting $\epsilon_0 \rightarrow 0$, we find that for all $x \neq y$, $(B_{\lambda,\epsilon}^{(\varepsilon,0)})^{-1}(x, y) \geq 0$. Thus by (6.2), $(B_{\lambda,\epsilon}^{(\varepsilon,0)})^{-1} - f(0)I$ has a smooth kernel that is non-negative off the diagonal, hence by continuity the kernel is also non-negative on the diagonal. Moreover, by Lemma 2.12, $((B_{\lambda,\epsilon}^{(\varepsilon,0)})^{-1} - f(0)I)[1] = \varepsilon^{-1/2} - f(0) > 0$, so for any $u \in C^\infty$ and $x \in \mathcal{M}$,

$$\begin{aligned} \left| (B_{\lambda,\epsilon}^{(\varepsilon,0)})^{-1}[u](x) \right| &\leq f(0)|u(x)| + \left| \left((B_{\lambda,\epsilon}^{(\varepsilon,0)})^{-1} - f(0)I \right)[u](x) \right| \\ &\leq \varepsilon^{-1/2} \|u\|_\infty. \end{aligned}$$

Further applications of Lemma 2.12 give that $(B_{\lambda,\epsilon,N}^{(\varepsilon,0)})^{-1}$ also maps $1 \mapsto \varepsilon^{-1/2}$ and due to commutativity under spectral mapping, we have,

$$B_{\lambda,\epsilon,N}^{(\varepsilon)} - B_{\lambda,\epsilon,N}^{(0)} = \varepsilon (B_{\lambda,\epsilon,N}^{(\varepsilon,0)})^{-1}, \quad B_{\lambda,\epsilon}^{(\varepsilon)} - B_{\lambda,\epsilon}^{(0)} = \varepsilon (B_{\lambda,\epsilon}^{(\varepsilon,0)})^{-1}.$$

Therefore, in the event that $|B_{\lambda,\epsilon,N}^{(\varepsilon)}[u](x) - B_{\lambda,\epsilon}^{(\varepsilon)}[u](x)| \leq \|u\|_\infty \delta$, we get

$$\begin{aligned} &\left| B_{\lambda,\epsilon,N}[u](x) - B_{\lambda,\epsilon}[u](x) \right| \\ &\leq \left| B_{\lambda,\epsilon,N}[u](x) - B_{\lambda,\epsilon,N}^{(\varepsilon)}[u](x) \right| + \left| B_{\lambda,\epsilon,N}^{(\varepsilon)}[u](x) - B_{\lambda,\epsilon}^{(\varepsilon)}[u](x) \right| \\ &\quad + \left| B_{\lambda,\epsilon}^{(\varepsilon)}[u](x) - B_{\lambda,\epsilon}^{(0)}[u](x) \right| \\ &\leq \varepsilon \left(\left| (B_{\lambda,\epsilon,N}^{(\varepsilon,0)})^{-1}[u](x) \right| + \left| (B_{\lambda,\epsilon}^{(\varepsilon,0)})^{-1}[u](x) \right| \right) + \|u\|_\infty \delta \\ &\leq 2\varepsilon^{1/2} \|u\|_\infty + \|u\|_\infty \delta, \end{aligned}$$

whence upon setting $\varepsilon = \delta^2$ and applying Lemma 6.8 along with a union bound over the probability in part (2) of Lemma 2.12 that $A_{\lambda,\epsilon,N}$ gives a connected graph, we arrive at the probability bound in the statement of Theorem 6.10. $\square$

The consistency of the square root of the graph Laplacian and the quantum dynamics according to it are of interest in their own right, so we will carry out that theory below. Along with it, we will also state the consistency theorems for the dynamics given by the perturbed operator $B_{\lambda,\epsilon,N}^{(\varepsilon)}$. This can be seen as a kind of *Tikhonov regularization* with the parameter ε : by tuning this to the noise variance δ^2 , we recover consistency of the unperturbed model, while as we will see in Theorem 6.14 and onwards, the decoupled form enjoys tighter consistency rates. This yields a concurrent path to recovering the geodesic flow when we scale ε with respect

to a power law in h , *independently* of the dimensions n or D . Therefore, alongside our propagators we will also consider the perturbed ones, which we will write as,

Notation 6.11. — Let $\lambda \geq 0$ and $\epsilon > 0$. Then, with $\varepsilon \in [0, 1]$, we denote

$$\begin{aligned}\Delta_{\lambda,\epsilon,N}^{(\varepsilon)} &:= \left(\Delta_{\lambda,\epsilon,N} + c_{2,0}(\varepsilon/\epsilon)I\right)^{1/2}, & \Delta_{\lambda,\epsilon}^{(\varepsilon)} &:= \left(\Delta_{\lambda,\epsilon} + c_{2,0}(\varepsilon/\epsilon)I\right)^{1/2}, \\ U_{\lambda,\epsilon,N}^{(\varepsilon)t} &:= \exp\left(-it\Delta_{\lambda,\epsilon,N}^{(\varepsilon)}\right), & U_{\lambda,\epsilon}^{(\varepsilon)t} &:= \exp\left(-it\Delta_{\lambda,\epsilon}^{(\varepsilon)}\right),\end{aligned}$$

which for $\varepsilon > 0$ we call $\Delta_{\lambda,\epsilon,N}^{(\varepsilon)}$ and $\Delta_{\lambda,\epsilon}^{(\varepsilon)}$ the (ε) -perturbed graph Laplacians and $U_{\lambda,\epsilon,N}^{(\varepsilon)t}$ and $U_{\lambda,\epsilon}^{(\varepsilon)t}$ the (ε) -perturbed propagators, while for $\varepsilon = 0$ we have the usual, unperturbed graph Laplacians and propagators, respectively.

Now we are ready to state the consistency of both, the unperturbed and perturbed propagators for short-times:

LEMMA 6.12. — Let $\tau \in [-1/c_{2,0}, 1/c_{2,0}]$. Then, given $\lambda \geq 0$, $\epsilon \in (0, C_1]$, $u \in L^\infty$ and $\delta > 0$, we have,

$$\Pr\left[\left\|U_{\lambda,\epsilon,N}^{\tau\sqrt{\epsilon}}[u] - U_{\lambda,\epsilon}^{\tau\sqrt{\epsilon}}[u]\right\|_\infty > \delta\right] \leq \gamma_{\lambda,N,v}\left(\frac{\delta}{12e}; u\right) + 2\tilde{\gamma}_{\lambda,N}\left(\frac{\delta}{8e}; u\right) + e^{-\frac{N\epsilon^{n/2}\delta^2}{C_2}},$$

wherein

$$U_{\lambda,\epsilon,N}^t := \exp(it\sqrt{\Delta_{\lambda,\epsilon,N}}) \quad \text{and} \quad U_{\lambda,\epsilon}^t := \exp(it\sqrt{\Delta_{\lambda,\epsilon}})$$

for $t \in \mathbb{R}$ and $C_1, C_2 > 0$ are constants as in Lemmas 2.12 and 6.10.

Moreover, for $\varepsilon > 0$ we have for all $\epsilon > 0$,

$$\Pr\left[\left\|U_{\lambda,\epsilon,N}^{(\varepsilon)\tau\sqrt{\epsilon}}[u] - U_{\lambda,\epsilon}^{(\varepsilon)\tau\sqrt{\epsilon}}[u]\right\|_\infty > \delta\right] \leq \gamma_{\lambda,N,v}^*\left(\frac{\delta}{4e}, \varepsilon; u\right) + 2\tilde{\gamma}_{\lambda,N}\left(\frac{\delta}{8e}; u\right).$$

Proof. — We start with the application of Theorem 6.6 to the pairs $(\mathcal{C}_N, \mathcal{C})$ and $(\mathcal{S}_N, \mathcal{S})$ of (6.1) at time $t = \tau\sqrt{\epsilon}$. More generally, Let $f_{e,w} := f_e(z - w)$ and $f_{o,w} := f_o(z - w)$, so we may write

$$f_{e,w}(z) = \sum_{j=0}^{\infty} \frac{(-1)^j}{(2j)!} \partial_z^{2j} \left[\cos(tc_{2,0}\epsilon^{-1/2} \cdot) \right]_{(\cdot=1+w)} z^j$$

and similarly for $f_{o,w}$. Hence, using the notation of that theorem, we have that $K_{1+w} = 1$ for $f_{e,w}$ and $f_{o,w}$, so we can apply it to get that

$$(6.9) \quad \Pr\left[\left\|\mathcal{C}_{w,N}[u] - \mathcal{C}_w[u]\right\|_\infty > \delta, \quad \left\|\mathcal{S}_{w,N}[u] - \mathcal{S}_w[u]\right\|_\infty > \delta\right] \leq 2\tilde{\gamma}_{\lambda,N}(\delta/(2e); u),$$

for $\mathcal{C}_w := f_{e,w}(A_{\lambda,\epsilon})$, $\mathcal{C}_{w,N} := f_{e,w}(A_{\lambda,\epsilon,N})$, $\mathcal{S}_w := f_{o,w}(A_{\lambda,\epsilon})$ and $\mathcal{S}_{w,N} := f_{o,w}(A_{\lambda,\epsilon,N})$.

Now suppose the event that

$$\|\mathcal{S}_N[u] - \mathcal{S}[u]\|_\infty \leq \delta \quad \text{and} \quad \|B_{\lambda,\epsilon,N}[\mathcal{S}[u]] - B_{\lambda,\epsilon}[\mathcal{S}[u]]\|_\infty \leq \delta$$

and note that through the spectral mapping properties we have

$$\sin(t\sqrt{\Delta_{\lambda,\epsilon,N}}) = B_{\lambda,\epsilon,N}\mathcal{S}_N \quad \text{and} \quad \sin(t\sqrt{\Delta_{\lambda,\epsilon}}) = B_{\lambda,\epsilon}\mathcal{S}.$$

Further, recall from the proof of Theorem 6.10 that $B_{\lambda,\epsilon,N}$ is an M-matrix so that $b_{\lambda,\epsilon,N} := I - B_{\lambda,\epsilon,N}$ has all entries non-negative and $b_{\lambda,\epsilon,N}[1] = 1$. Then,

$$\begin{aligned} & \left\| \sin\left(t\sqrt{\Delta_{\lambda,\epsilon,N}}\right)[u] - \sin\left(t\sqrt{\Delta_{\lambda,\epsilon}}\right)[u] \right\|_{\infty} \\ & \leq \left\| b_{\lambda,\epsilon,N}[(\mathcal{S}_N - \mathcal{S})[u]] \right\|_{\infty} + \left\| (\mathcal{S}_N - \mathcal{S})[u] \right\|_{\infty} + \left\| (B_{\lambda,\epsilon,N} - B_{\lambda,\epsilon})[\mathcal{S}[u]] \right\|_{\infty} \leq 3\delta. \end{aligned}$$

On including the event that $|\mathcal{C}_N[u](x) - \mathcal{C}[u](x)| \leq \delta$, we have

$$\left\| U_{\lambda,\epsilon,N}^t[u] - U_{\lambda,\epsilon}^t[u] \right\|_{\infty} \leq 4\delta.$$

By a Taylor series expansion we have that for any $u \in L^{\infty}$,

$$|\mathcal{S}[u]| \leq \sum_{m=0}^{\infty} \frac{|A_{\lambda,\epsilon}^m[u]|}{m!} \leq e \|u\|_{\infty}.$$

Therefore, taking a union bound over all events and applying Theorem 6.10 we arrive at,

$$\Pr \left[\left\| U_{\lambda,\epsilon,N}^t[u] - U_{\lambda,\epsilon}^t[u] \right\|_{\infty} > \delta \right] \leq \gamma_{\lambda,N,v} \left(\frac{\delta}{12e}; u \right) + 2\tilde{\gamma}_{\lambda,N} \left(\frac{\delta}{8e}; u \right) + e^{-\frac{N\epsilon^{n/2}\delta^2}{C_2}}.$$

For the second part of the statement of the theorem, (6.9) already gives the probabilistic consistency bound for $\mathcal{C}_{\varepsilon,N}$ and $\mathcal{S}_{\varepsilon,N}$. Then, the above statements go through essentially in the same way, modulo that in place of $b_{\lambda,\epsilon,N}$ we use $b_{\lambda,\epsilon,N}^{(\varepsilon)} := (1+\varepsilon)^{\frac{1}{2}}I - B_{\lambda,\epsilon,N}^{(\varepsilon)}$, which also has all non-negative entries, since $B_{\lambda,\epsilon,N}^{(\varepsilon)}$ is an M-matrix with spectral radius $(1+\varepsilon)^{\frac{1}{2}}$. Then due to $b_{\lambda,\epsilon,N}^{(\varepsilon)}[1] = \sqrt{1+\varepsilon}$, we have under the analogous events,

$$\begin{aligned} & \left| \sin\left(t\sqrt{\Delta_{\lambda,\epsilon,N}^{(\varepsilon)}}\right)[u] - \sin\left(t\sqrt{\Delta_{\lambda,\epsilon}^{(\varepsilon)}}\right)[u] \right| \\ & \leq \left| b_{\lambda,\epsilon,N}^{(\varepsilon)}[(\mathcal{S}_{N,\varepsilon} - \mathcal{S}_{\varepsilon})[u]] \right| + (1+\varepsilon)^{1/2} |(\mathcal{S}_{N,\varepsilon} - \mathcal{S}_{\varepsilon})[u]| + |(B_{\lambda,\epsilon,N}^{(\varepsilon)} - B_{\lambda,\epsilon}^{(\varepsilon)})[\mathcal{S}[u]]| \\ & \leq 4\delta. \end{aligned}$$

On invoking the probabilistic consistency bound from Lemma 6.8 for the square root of the ε -perturbed graph Laplacian, we arrive at the bound in the second part of Lemma 6.12. $\square$

Notation 6.13. — We denote the pointwise convergence rate for the short-time solution to the half-wave equation by

$$\omega_{\lambda,N}(\delta, v; u) := \gamma_{\lambda,N,v} \left(\frac{\delta}{12e}; u \right) + 2\tilde{\gamma}_{\lambda,N} \left(\frac{\delta}{8e}; u \right) + e^{-\frac{N\epsilon^{n/2}\delta^2}{C_2}},$$

while absorbing the condition $\epsilon \in (0, C_1]$ in the notation; in the perturbed case we denote,

$$\omega_{\lambda,N}^*(\delta, \varepsilon, v; u) := \gamma_{\lambda,N,v}^* \left(\frac{\delta}{4e}, \varepsilon; u \right) + 2\tilde{\gamma}_{\lambda,N} \left(\frac{\delta}{8e}; u \right).$$

The explicit dependence on v will often be suppressed in the usage of this notation and we will write simply, $\omega_{\lambda,N}(\delta; u)$ and $\omega_{\lambda,N}^*(\delta, \varepsilon; u)$ with the exact meaning understood to be as given above.

6.2. Uniform consistency at longer times

We wish to extend the consistency between the discretized solution $u_N^t := U_{\lambda,\epsilon,N}^t[u]$ and the continuum solution $u^t := U_{\lambda,\epsilon}^t[u]$ to longer times. For this purpose, we see that u_N^t is defined on $\mathcal{M}$ through the form of *Nyström extension* via $A_{\lambda,\epsilon,N}$ as discussed in the beginning of Section 6. The inequality (6.3) gives for all $u \in L^\infty$ and $t \in \mathbb{R}$,

$$(6.10) \quad \left| U_{\lambda,\epsilon,N}^t[u](x) \right| \leq \left(1 + c_{2,0} t \epsilon^{-1/2} \frac{\|k_{\lambda,\epsilon,N}(x, \cdot)\|_{N,\infty} \|p_{\lambda,\epsilon,N}\|_{N,\infty}^{1/2}}{\min_{j \in [N]} p_{\lambda,\epsilon,N}^{3/2}(x_j)} \right) \|u\|_{N,\infty}$$

since in this case $Df(z) = (\exp(-i\tau\sqrt{1-z}) - \exp(-i\tau))/z$ for $f = \exp(-i\tau\sqrt{1-z})$ and $\tau := c_{2,0} t \epsilon^{-1/2}$ and setting $w := 1 - \sqrt{1-z}$ then taking a Taylor series expansion at $w = 0$ of $|Df|(w)^2 = 2(1 - \cos(\tau w))/(w(2-w))^2$ shows that its maximum is achieved near the inverse of the second order coefficient, $w = \sqrt{48/(\tau^2 - 9)}/\tau$, which then applied to its first order Taylor approximation gives that $|Df|$ gives a maximum less than $\tau/2 + 1 < \tau$. Since (6.2) applies to the case with $A_{\lambda,\epsilon}$ in place of $A_{\lambda,\epsilon,N}$, we also have the bound for $|f(A_{\lambda,\epsilon})[u](x)|$ given by the ultimate inequality in (6.3) with $\|\cdot\|_q$ in place of $\|\cdot\|_{N,q}$. Hence,

$$(6.11) \quad \|U_{\lambda,\epsilon}^t[u]\|_\infty \leq \|u\|_\infty + c_{2,0} t \epsilon^{-1/2} \|k_{\lambda,\epsilon}\|_\infty \frac{\|p_{\lambda,\epsilon}\|_\infty^{1/2}}{\inf(p_{\lambda,\epsilon}^{3/2})} \|u\|_2$$

will be useful for bounding probabilities for pointwise consistency.

The bounds (6.10) and (6.11) hold also for $U_{\lambda,\epsilon,N}^{(\epsilon)t}[u]$ and $U_{\lambda,\epsilon}^{(\epsilon)t}[u]$, respectively. This, along with Lemma 6.12 is sufficient to establish consistency for the perturbed case through the same arguments as the *unperturbed* $\varepsilon = 0$ case. Indeed, in the following, we will use the short-time probabilistic consistency bounds given by Lemma 6.12 as a black-box while extending to long-time (that is, $O(1)$ in ϵ) probabilistic consistency. We will work through the unperturbed case, mainly to keep the notation simple, but since the arguments essentially rely on Lemma 6.12 in a simple way, they apply directly to the perturbed case with $\omega_{\lambda,N}^*$ in place of $\omega_{\lambda,N}$ as well, with the only thing to keep track of being that δ (i.e., error) multipliers are decoupled from ε , but the notation makes this clear.

We proceed by splitting time $t \in \mathbb{R}$ into *chunks* of length $\sim \sqrt{\epsilon}$ and combining the short-time consistency Lemma 6.12 with the semigroup structure of $U_{\lambda,\epsilon}^t$. This leads to Bernstein-type exponential probabilistic bounds for long-time, uniform consistency, as in the following,

THEOREM 6.14. — *Let $\lambda \geq 0$, $\epsilon > 0$, $t \in \mathbb{R}$ and $u \in L^\infty$ such that there exists $K_u > 0$ so that $\|U_{\lambda,\epsilon}^s[u]\|_\infty \leq K_u$ for all $|s| \leq |t|$. Then with $\kappa := \lceil |t| c_{2,0} / \sqrt{\epsilon} \rceil$, for all $\delta > 0$,*

$$(6.12) \quad \Pr \left[\left\| (U_{\lambda,\epsilon,N}^t - U_{\lambda,\epsilon}^t)[u] \right\|_\infty > \delta \right] \\ \leq \kappa \omega_{\lambda,N} \left(\frac{\delta \epsilon^{n/2}}{\kappa^2 \tilde{C}_{p,\lambda}}; K_u \right) + \gamma_{\lambda,N}(\underline{K}_{p,\lambda}; 1) + \gamma_{0,N}(\underline{K}_{p,\lambda}; 1) \\ =: \Omega_{\lambda,t,N}(\delta, \epsilon, K_u),$$

wherein $K_{p,\lambda} := \min\{\underline{C}_p, \underline{C}_{p,\lambda}\}/2$ and $\tilde{C}_{p,\lambda} > 0$ is a constant depending only on λ , $\bar{C}_{p,\lambda}$, $\underline{C}_{p,\lambda}$ and $\underline{C}_p$.

In the perturbed case, let $\tilde{\varepsilon} > 0$. Then, we have with a $K_u > 0$ satisfying $\|U_{\lambda,\epsilon}^{(\tilde{\varepsilon})s}[u]\|_\infty \leq K_u$ for all $|s| \leq |t|$,

$$(6.13) \quad \Pr \left[\left\| \left(U_{\lambda,\epsilon,N}^{(\tilde{\varepsilon})t} - U_{\lambda,\epsilon}^{(\tilde{\varepsilon})t} \right) [u] \right\|_\infty > \delta \right] \leq \Omega_{\lambda,t,N}^*(\delta, \tilde{\varepsilon}, \epsilon, K_u)$$

with $\Omega_{\lambda,t,N}^*$ defined in the same way as $\Omega_{\lambda,t,N}$, except with the instance of $\omega_{\lambda,N}(\cdot; \cdot)$ replaced with $\omega_{\lambda,N}^*(\cdot, \tilde{\varepsilon}; \cdot)$.

Remark 6.15. — We call attention to the discrepancy between the scalings of consistency rates for the propagators of the square root graph Laplacian and its regularization $\Delta_{\lambda,\epsilon,N}^{(\tilde{\varepsilon})}$. By decoupling $\tilde{\varepsilon}$ from the noise variance δ^2 , the spectral shift introduces a *bias floor*, but regularizes large variances arising from the singular part of the spectrum of the graph Laplacian. We have simplified the concentration bounds in Section 6.7 to the dominating order, wherein it's visible that the factor $\epsilon^{\frac{n}{2}}/\kappa^2 \sim \epsilon^{\frac{n}{2}+1}$ in (6.12) is amplified to a bias term dependence of ϵ^{2n+4} in the consistency rate due to the tuning $\tilde{\varepsilon} = \delta^2$ in Theorem 6.10. The perturbed propagator, on the other hand, enjoys a quadratically tighter concentration bound in this regard.

Proof. — We set $\kappa := \lceil |t|c_{2,0}/\sqrt{\epsilon} \rceil$ and $\tau := t/\kappa$ so that $|\tau| \leq \sqrt{\epsilon}/c_{2,0}$. Let $\epsilon, \delta_0 > 0$ and let us begin in the following events:

$$\begin{aligned} \mathcal{A}_{\lambda'}(\epsilon) : \|p_{\lambda',\epsilon,N} - p_{\lambda',\epsilon}\|_\infty &\leq \epsilon & (\forall) \lambda' \in \{0, \lambda\} \\ \mathcal{A}(\delta_0) : \left\| \left(U_{\lambda,\epsilon,N}^\tau - U_{\lambda,\epsilon}^\tau \right) U_{\lambda,\epsilon}^{m\tau} [u] \right\|_\infty &\leq \delta_0 & (\forall) 0 \leq m \leq \kappa - 1. \end{aligned}$$

Then we have due to (6.10),

$$\left\| U_{\lambda,\epsilon,N}^{m\tau} [u] \right\|_\infty \leq (1 + mC(\epsilon, \epsilon)) \|u\|_{N,\infty}$$

with

$$C(\epsilon, \epsilon) := \epsilon^{-\frac{n}{2}} \frac{\|k\|_\infty}{(\underline{C}_p - \epsilon)^{2\lambda}} \frac{(\bar{C}_{p,\lambda} + \epsilon)^{\frac{1}{2}}}{(\underline{C}_{p,\lambda} - \epsilon)^{\frac{3}{2}}}.$$

Define for each $m \in \mathbb{N}$, $v_m := U_{\lambda,\epsilon}^{m\tau} [u]$ so that in the current event we have for all $\kappa \geq 2$ and $0 \leq m \leq \kappa - 2$,

$$\begin{aligned} \left\| \left(U_{\lambda,\epsilon,N}^{2\tau} - U_{\lambda,\epsilon}^{2\tau} \right) [v_m] \right\|_\infty &\leq \left\| U_{\lambda,\epsilon,N}^\tau \left(U_{\lambda,\epsilon,N}^\tau - U_{\lambda,\epsilon}^\tau \right) [v_m] \right\|_\infty + \left\| \left(U_{\lambda,\epsilon,N}^\tau - U_{\lambda,\epsilon}^\tau \right) [v_{m+1}] \right\|_\infty \\ &\leq (2 + C(\epsilon, \epsilon)) \delta_0. \end{aligned}$$

Supposing that for all $2 \leq \kappa' \leq \kappa - 1$, each $s \in [\kappa']$ and $0 \leq m \leq \kappa' - s$,

$$\left\| \left(U_{\lambda,\epsilon,N}^{s\tau} - U_{\lambda,\epsilon}^{s\tau} \right) [v_m] \right\|_\infty \leq s \left(\frac{s-1}{2} C(\epsilon, \epsilon) + 1 \right) \delta_0$$

leads to,

$$\begin{aligned} \left\| \left(U_{\lambda,\epsilon,N}^{\kappa\tau} - U_{\lambda,\epsilon}^{\kappa\tau} \right) [u] \right\|_\infty &\leq \left\| U_{\lambda,\epsilon,N}^{(\kappa-1)\tau} \left(U_{\lambda,\epsilon,N}^\tau - U_{\lambda,\epsilon}^\tau \right) [u] \right\|_\infty + \left\| \left(U_{\lambda,\epsilon,N}^{(\kappa-1)\tau} - U_{\lambda,\epsilon}^{(\kappa-1)\tau} \right) [v_1] \right\|_\infty \\ &\leq \kappa \left(\frac{\kappa-1}{2} C(\epsilon, \epsilon) + 1 \right) \delta_0. \end{aligned}$$

Therefore, having satisfied the induction hypothesis, we have that for each $\kappa \in \mathbb{N}$, if for all $0 \leq m \leq \kappa - 1$, $\|(U_{\lambda,\epsilon,N}^\tau - U_{\lambda,\epsilon}^\tau)U_{\lambda,\epsilon}^{m\tau}[u]\|_\infty \leq \delta_0$ then

$$\|(U_{\lambda,\epsilon,N}^{\kappa\tau} - U_{\lambda,\epsilon}^{\kappa\tau})[u]\|_\infty \leq \kappa^2 C(\epsilon, \epsilon) \delta_0.$$

Now set $\varepsilon = \min\{\underline{C}_p, \underline{C}_{p,\lambda}\}/2$ and $\tilde{C}_{p,\lambda} := \sqrt{12}(2^\lambda) \bar{C}_{p,\lambda}^{\frac{1}{2}} / (\underline{C}_{p,\lambda}^{\frac{3}{2}} \underline{C}_p^{2\lambda})$ so that $C(\epsilon, \epsilon) \leq \epsilon^{-\frac{n}{2}} \tilde{C}_{p,\lambda}$. Moreover, by Lemma 6.3, the event $\mathcal{A}_{\lambda'}(\varepsilon)$ happens with probability at least $1 - \gamma_{\lambda',N}(\varepsilon; 1)$ for each $\lambda' \in \{0, \lambda\}$. Then, upon setting $\delta_0 = \delta(\epsilon^{\frac{n}{2}}/\kappa^2)/\tilde{C}_{p,\lambda}$ and taking a union bound with respect to Lemma 6.12, we find that the event $\mathcal{A}(\delta_0)$ happens with probability at least $1 - \kappa\omega_{\lambda,N}(\delta(\epsilon^{\frac{n}{2}}/\kappa^2)/\tilde{C}_{p,\lambda}; K_u)$. A union bound for the occurrence of all assumed events then gives the statement of the lemma. $\square$

A generic bound to be used in place of K_u in the conditions satisfying Theorem 6.14 is given by (6.11). We record this as,

COROLLARY 6.16. — *Let $\lambda \geq 0$, $\epsilon > 0$, $t \in \mathbb{R}$ and $u \in L^\infty$. Then, there exists a constant $C > 0$ depending only on k, p, λ and geometry of $\mathcal{M}$ such that for all $\delta > 0$,*

$$\Pr\left[\|(U_{\lambda,\epsilon,N}^t - U_{\lambda,\epsilon}^t)[u]\|_\infty > \delta\right] \leq \Omega_{\lambda,t,N}(\delta, \epsilon, C_{\epsilon,t,u}),$$

wherein

$$C_{\epsilon,t,u} := \|u\|_\infty + c_{2,0}|t|\epsilon^{-(n+1)/2}\|k\|_\infty \frac{\bar{C}_{p,\lambda}^{1/2}}{\underline{C}_p^{2\lambda} \underline{C}_{p,\lambda}^{3/2}} \|u\|_2$$

and $\Omega_{\lambda,t,N}$ is as defined in Theorem 6.14.

6.3. Propagation of coherent states on graphs

We now have the bridge to bring semiclassical analysis to discrete graph Laplacians. As a small preparatory step, we apply the continuum results to achieve a super-quadratic improvement on the generic norm bound $K_u \lesssim \|u\|_\infty + |t|\epsilon^{-(n+1)/2}$ for the propagation of coherent states, through an application of Theorem 5.2 along with Sobolev embedding. Indeed, the localization in phase space (5.2) tells that in fact $U_{\lambda,\epsilon}^t \psi_h$ is localized in (classical) frequency space to a *cubical annulus* of length $1/h^{3/2-\tilde{\rho}}$ in terms of its Littlewood–Paley decomposition, for all $|t| \leq T_E(h; \rho, q_0)$ with Ehrenfest time T_E , ρ and q_0 as in the statement of Theorem 5.2 and $\tilde{\rho} \in (\rho, 1/2]$. Hence, applying a semiclassical Ψ DO to $U_{\lambda,\epsilon}^t[\psi_h]$ that cuts off in frequency to within distance $O(h^{1/2-\tilde{\rho}})$ of ξ_0 gives on following the computation in [Zwo12, Theorem 7.15],

$$\|U_{\lambda,\epsilon}^t \psi_h\|_\infty \leq C \|U_{\lambda,\epsilon}^t \psi_h\|_{L^2} h^{-(\frac{1}{2}+\tilde{\rho})n/2} + O(h^\infty),$$

with the constant $C > 0$ depending only on $\mathcal{M}$ and the choice of frequency cut-off implicitly being applied. We may bound the L^2 norm using the similarity relation given by Lemma 2.12 in $L^2(\mathcal{M}, p d\nu_g)$ transported to $L^2(\mathcal{M})$ on conjugating by p , to find that there is a constant $K_\psi > 0$ such that

$$\|U_{\lambda,\epsilon}^t \psi_h\|_{L^2} \leq \frac{\|\sqrt{p}_{\lambda,\epsilon} p\|_\infty}{\inf(\sqrt{p}_{\lambda,\epsilon} p)}$$

implies that for all $|t| \leq T_E(h; \rho, q_0)$,

$$(6.14) \quad \|U_{\lambda, \epsilon}^t \psi_h\|_\infty \leq K_\psi h^{-(\frac{1}{2} + \tilde{\rho})n/2}.$$

Since the Ehrenfest time for the localized geodesic flow given by q_0 will be pertinent to us, we standardize the following,

Notation 6.17. — We will denote by $T_E^\rho := T_E(h; \rho, q_0)$ the Ehrenfest time for q_0 , both as given in the statement of Theorem 5.2. The parameter $\rho \in [0, 1/2)$ sets the duration into the Ehrenfest time regime and when dealing with the localization properties, we will denote $\tilde{\rho} \in (\rho, 1/2]$.

Now, to connect Theorem 6.14 with the propagation of coherent states, Theorem 5.2 also gives the position space localization that allows us to find the geodesic to within distance $O(h^{1/2-\tilde{\rho}})$ of the maximizer of the modulus of the propagated state, for $\tilde{\rho} \in (\rho, 1/2]$. Therefore, we may approximate the geodesic flow using the max observable; in doing so, we account for the fact that while the *un-normalized* coherent state $\tilde{\psi}_h := \psi_h / C_h(x_0, \xi_0)$ is readily interpolatable through the graph structure, its normalization is a matter of probabilistic L^2 convergence and not necessary to handle the max observable. For this reason, we use the un-normalized coherent state at present, to establish the consistency for this observation of the geodesic flow, in

PROPOSITION 6.18. — Let $\lambda \geq 0$, $\alpha \geq 1$, $h \in (0, h_0]$ for h_0 given by Theorem 5.2 and $(x_0, \xi_0) \in T^*\mathcal{M}$. Then, for $\tilde{\psi}_h := e^{-\frac{i}{h}\tilde{\phi}(x_0, \xi_0; \cdot)}$ an un-normalized coherent state localized at (x_0, ξ_0) and $|t| \leq T_E^\rho$, we have with $K_{\tilde{\psi}} \geq (h^{-n/4} / C_h(x_0, \xi_0)) K_\psi = O(h^0)$, K_ψ as in (6.14), $\epsilon := h^{2+\alpha}$ and for all $\delta > 0$,

$$\Pr \left[\left| \|U_{\lambda, \epsilon, N}^t \tilde{\psi}_h\|^2 - \|U_{\lambda, \epsilon}^t \tilde{\psi}_h\|^2 \right|_\infty > \delta \right] \leq \Omega_{\lambda, t, N} \left(\frac{\delta}{2K_{\tilde{\psi}} h^{-\tilde{\rho}n/2} + 1 + \delta}, \epsilon, K_{\tilde{\psi}} h^{-\tilde{\rho}n/2} \right).$$

Furthermore, defining the estimator $\hat{x}_{N, t} := \arg \max_{\mathcal{X}_N} |U_{\lambda, \epsilon, N}^t \tilde{\psi}_h|^2$ with $\mathcal{X}_N := \{x_1, \dots, x_N\}$, there exists a constant $h'_{\max} > 0$ such that for all $\tilde{\rho} \in (\rho, 1/2]$ and $h \in (0, h'_{\max}]$ we have,

$$(6.15) \quad \Pr \left[d_g(\hat{x}_{N, t}, x_t) > h^{1/2-\tilde{\rho}} \right] \leq \Omega_{\lambda, t, N} \left(\underline{K}_{\tilde{\psi}} h^{\tilde{\rho}n} / 4, \epsilon, K_{\tilde{\psi}} h^{-\tilde{\rho}n/2} \right),$$

provided $\underline{K}_{\tilde{\psi}} > 0$ satisfies $\underline{K}_{\tilde{\psi}} h^{\tilde{\rho}n} \geq \sup_{|t| \leq T_E^\rho} \|U_{\lambda, \epsilon}^t \tilde{\psi}_h\|_\infty$. In the perturbed case, we set $\varepsilon \in O(h^{1+\alpha})$ and define $\hat{x}_{N, t}^{(\varepsilon)} := \arg \max_{\mathcal{X}_N} |U_{\lambda, \epsilon, N}^{(\varepsilon)t} \tilde{\psi}_h|^2$. Then, there exist new constants $h'_{\max} > 0$,

$$K_\psi^{(\varepsilon)} := h^{\tilde{\rho}n/2} \sup_{|t| \leq T_E^\rho} \sup_{h \in (0, h'_{\max}]} \|U_{\lambda, \epsilon}^{(\varepsilon)t} \tilde{\psi}_h\|_\infty$$

and

$$\underline{K}_{\tilde{\psi}}^{(\varepsilon)} h^{\tilde{\rho}n} \geq \sup_{|t| \leq T_E^\rho} \|U_{\lambda, \epsilon}^{(\varepsilon)t} \tilde{\psi}_h\|_\infty$$

such that

$$(6.16) \quad \Pr \left[d_g(\hat{x}_{N, t}^{(\varepsilon)}, x_t) > h^{1/2-\tilde{\rho}} \right] \leq \Omega_{\lambda, t, N}^* \left(\underline{K}_{\tilde{\psi}}^{(\varepsilon)} h^{\tilde{\rho}n} / 4, \varepsilon, \epsilon, K_\psi^{(\varepsilon)} h^{-\tilde{\rho}n/2} \right).$$

Remark 6.19. — We remarked earlier (following Theorem 6.14) that the regularization parameter ε introduced a bias-variance tradeoff in the estimator for the propagation with respect to $U_{\lambda,\epsilon}^t$. Now when we combine with the semiclassical analysis of the preceding sections, we find that the *principal symbol* (and therefore the quantum-classical correspondence for the graph Laplacian) is invariant to spectral shifts of the order $\varepsilon \in O(h^{1+\alpha})$. At these rates, the regularization is tuned to the semiclassical scaling and the bias floor is replaced by the semiclassical resolution. This results in tighter concentration bounds for the regularized estimator than the unperturbed one (especially with respect to dimension) while maintaining the same bias rates.

Proof of Proposition 6.18. — We apply the preceding discussion (we give the arguments for the unperturbed case, but they follow in the same way for the perturbed case) to find that we have a constant $K_{\tilde{\psi}} > 0$ that satisfies

$$\|U_{\lambda,\epsilon}^t \tilde{\psi}_h\|_{\infty} \leq \frac{K_{\tilde{\psi}} h^{-n/4-\tilde{\rho}n/2}}{C_h(x_0, \xi_0)} \leq K_{\tilde{\psi}} h^{-\tilde{\rho}n/2}$$

for all $|t| \leq T_E^{\rho}$ and $h \in [0, h_0)$. Therefore, for all $\delta_0 > 0$,

$$(6.17) \quad \Pr\left[\|U_{\lambda,\epsilon,N}^t \tilde{\psi}_h - U_{\lambda,\epsilon}^t \tilde{\psi}_h\|_{\infty} > \delta_0\right] \leq \Omega_{\lambda,t,N}(\delta_0, \epsilon, h^{-\tilde{\rho}n/2} K_{\tilde{\psi}}).$$

To ease the notation, we will denote $K_{\psi,h} := h^{-\tilde{\rho}n/2} K_{\tilde{\psi}}$. Now suppose the event that $\|U_{\lambda,\epsilon,N}^t \tilde{\psi}_h - U_{\lambda,\epsilon}^t \psi_h\|_{\infty} \leq \delta/(2K_{\psi,h} + 1 + \delta)$ holds. Then,

$$\begin{aligned} \left| |U_{\lambda,\epsilon,N}^t \tilde{\psi}_h|^2 - |U_{\lambda,\epsilon}^t \tilde{\psi}_h|^2 \right| &= \left| |U_{\lambda,\epsilon,N}^t \tilde{\psi}_h| - |U_{\lambda,\epsilon}^t \tilde{\psi}_h| \right| \left(|U_{\lambda,\epsilon,N}^t \tilde{\psi}_h| + |U_{\lambda,\epsilon}^t \tilde{\psi}_h| \right) \\ &\leq \frac{\delta}{2K_{\psi,h} + 1 + \delta} \left(2K_{\psi,h} + \frac{\delta}{2K_{\psi,h} + 1 + \delta} \right) \\ &\leq \delta \frac{2K_{\psi,h} + 1}{2K_{\psi,h} + 1 + \delta} \leq \delta. \end{aligned}$$

This establishes the first part of the statement of Proposition 6.18.

The second part is a direct consequence of this, since on continuing under the foregoing presumed event, by L^{∞} comparison over $\mathcal{X}_N$ we have that for all $N \in \mathbb{N}$ there is a constant $C_N > 0$ such that if $\delta < \frac{1}{2}(\underline{K}_{\tilde{\psi}} h^{\tilde{\rho}n} - C_N h^N)$ for a constant $\underline{K}_{\tilde{\psi}} > 0$, then $\hat{x}_{N,t} \in B_t := B(x_t, g; h^{1/2-\tilde{\rho}})$. Indeed, the presumed event gives on the one hand,

$$|U_{\lambda,\epsilon,N}^t \tilde{\psi}_h|^2(\hat{x}_{N,t}) \geq \|U_{\lambda,\epsilon}^t \tilde{\psi}_h\|_{\infty}^2 - \delta.$$

The L^{∞} norm of the propagated state is lower-bounded through its localization:

$$\|U_{\lambda,\epsilon}^t \tilde{\psi}_h\|_{\infty}^2 \geq \frac{C_{\mathcal{M}} h^{-n/2+\tilde{\rho}n}}{C_h(x_0, \xi_0)^2} \|U_{\lambda,\epsilon}^t[\psi_h]\|_{L^2}^2,$$

with $C_{\mathcal{M}} > 0$ a constant depending only on the local geometry of B_t . Similar to (6.14), we have a lower-bound on the $L^2(\mathcal{M})$ norm of the propagated coherent state through

unitarity up to conjugation by $\sqrt{p}_{\lambda,\epsilon} \cdot p$: this gives,

$$\|U_{\lambda,\epsilon}^t \psi_h\|_{L^2} \geq \frac{\inf(\sqrt{p}_{\lambda,\epsilon} p)}{\|\sqrt{p}_{\lambda,\epsilon} p\|_\infty} \implies \|U_{\lambda,\epsilon}^t \tilde{\psi}_h\|_\infty^2 \geq \underline{K}_{\tilde{\psi}} h^{\tilde{\rho}n},$$

with $\underline{K}_{\tilde{\psi}} > 0$ a constant. On the other hand, the event of L^∞ consistency over $\mathcal{X}_N$ along with the localization of $\tilde{\psi}_h$ together imply that

$$K(h, \rho) := \sup_{x \in \mathcal{X}_N \setminus \overline{B_t}} |U_{\lambda,\epsilon,N}^t \tilde{\psi}_h|^2 \leq \delta + C_N h^N.$$

Thus, we have for δ as above,

$$|U_{\lambda,\epsilon,N}^t \tilde{\psi}_h(\hat{x}_{N,t})|^2 \geq \underline{K}_{\tilde{\psi}} h^{\tilde{\rho}n} - \delta > \delta + C_N h^N \geq K(h, \rho),$$

which tells that there is $h'_{\max} > 0$ such that for all $h \in (0, h'_{\max}]$, if we take $\delta = \frac{1}{4} \underline{K}_{\tilde{\psi}} h^{\tilde{\rho}n}$, then we have $d_g(\hat{x}_{N,t}, x_t) < h^{1/2-\tilde{\rho}}$. $\square$

6.4. Interlude: L^2 consistency

We discuss now an intermediary step to recovering the geodesic flow through the graph structure using the mean position observables. These observables, as discussed in Section 5.2, can be expressed as L^2 inner products, so to implement them we need a way to go from inner products on graphs to inner products on the manifold. The treatment in [Hei05, Sections 2.3.5-6] shows that if a complex vector space over the graph structure is endowed with an inner product given by $\langle \cdot, \cdot \rangle / N$ or $\langle \cdot, p_{\lambda,\epsilon,N} \cdot \rangle / N$, then on the continuum side, these converge as $N \rightarrow \infty$ and $\epsilon \rightarrow 0$ to the inner products $\langle \cdot, \cdot \rangle_p$ and $\langle \cdot, c_2^{1-2\lambda} p^{2-2\lambda} \cdot \rangle$, respectively. Hence, among these only the case $\lambda = 1$ converges to $\langle \cdot, \cdot \rangle_{L^2(\mathcal{M}, d\nu_g)}$, while by Theorem 5.2, for all other weights, the (classically) propagated continuum weight, namely $c_2^{1-2\lambda} p^{2-2\lambda} \circ \Gamma^t$ will show up as a multiplier to top order in the expectation of a propagated quantum observable against a coherent state. Since this also means that the propagated weight must show up by itself when taking the norm of the propagated coherent state, it suggests that in order to recover the flow of symbols along geodesics through the coherent states, we must normalize their propagations. It so happens that we may do this with *any* choice of the weights, so we proceed with the simplest choice that is sufficient for our needs: the corresponding picture on the continuum side is given by,

LEMMA 6.20. — *Let $\lambda \geq 0$, $h \in (0, h_0]$, $\alpha \geq 1$ and ψ_h be a coherent state localized at $(x_0, \xi_0) \in T^*\mathcal{M}$. Then, for all $|t| \leq T_E^\rho$ and $\varepsilon \in O(h^{1+\alpha})$, with $\epsilon := h^{2+\alpha}$, we have,*

$$\|U_{\lambda,\epsilon}^{(\varepsilon)t} \psi_h\|_p^2 = c_0^{2\lambda-1} p_{\lambda,\epsilon}(x_0) p(x_t)^{2\lambda} + O(h^{1-2\rho}),$$

wherein $x_t := \pi_{\mathcal{M}} \Gamma^t(x_0, \xi_0)$ and if $v \in C^\infty$, then

$$\left\langle \psi_{h,t,\varepsilon} \left| \left(U_{\lambda,\epsilon}^{(\varepsilon)t} \right)^* v U_{\lambda,\epsilon}^{(\varepsilon)t} \right| \psi_{h,t,\varepsilon} \right\rangle_p = v(x_t) + O(h^{1-2\rho})$$

with $\psi_{h,t,\varepsilon} := \psi_h / \|U_{\lambda,\epsilon}^{(\varepsilon)t}[\psi_h]\|_p$.

Proof. — This is a straightforward application of Theorem 5.2, which goes through for $U_{\lambda,\epsilon}^{(\epsilon)t}$ because $h^2\Delta_{\lambda,\epsilon}^{(\epsilon)} = h^2\Delta_{\lambda,\epsilon} + h^2c_{2,0}\epsilon/\epsilon I$ and $h^2\epsilon/\epsilon = O(h)$ so $\text{Sym}[h^2\Delta_{\lambda,\epsilon}^{(\epsilon)}] = \text{Sym}[h^2\Delta_{\lambda,\epsilon}]$. By Lemma 2.12,

$$\left(\frac{1}{p_{\lambda,\epsilon}}(U_{\lambda,\epsilon}^{(\epsilon)t})^* \circ p_{\lambda,\epsilon}\right)U_{\lambda,\epsilon}^{(\epsilon)t} = I,$$

with the adjoint being taken on $L^2(\mathcal{M}, p d\nu_g)$. Since the quantization of vp gives the multiplication operator by vp , we then have,

$$\begin{aligned} \langle \psi_h | (U_{\lambda,\epsilon}^{(\epsilon)t})^* vp U_{\lambda,\epsilon}^{(\epsilon)t} | \psi_h \rangle &= \left\langle \psi_h \left| p_{\lambda,\epsilon} (U_{\lambda,\epsilon}^{(\epsilon)t})^{-1} v \frac{p}{p_{\lambda,\epsilon}} U_{\lambda,\epsilon}^{(\epsilon)t} \right| \psi_h \right\rangle \\ &= \left\langle \psi_h \left| p_{\lambda,\epsilon} \text{Op}_h \left(v \frac{p}{p_{\lambda,\epsilon}} \circ \Gamma^t \right) \right| \psi_h \right\rangle + O(h^{1-2\rho}) \\ &= p_{\lambda,\epsilon}(x_0) v(x_t) \frac{p}{p_{\lambda,\epsilon}}(x_t) + O(h^{1-2\rho}) \\ &= c_0^{2\lambda-1} p_{\lambda,\epsilon}(x_0) p(x_t)^{2\lambda} v(x_t) + O(h^{1-2\rho}), \end{aligned}$$

wherein the ultimate equality follows from (2.13). Thus,

$$\langle \psi_{h,t,\epsilon} | (U_{\lambda,\epsilon}^{(\epsilon)t})^* vp U_{\lambda,\epsilon}^{(\epsilon)t} | \psi_{h,t,\epsilon} \rangle = v(x_t) + O(h^{1-2\rho}).$$

□

We turn now to the consistency between the Hilbert space on the graph, given by the inner product $\langle \cdot, \cdot \rangle_N := \langle \cdot, \cdot \rangle / N$ and the space $L^2(\mathcal{M}, p d\nu_g)$. The primary step is to establish the error in

$$\left| \langle \psi_{h,t,\epsilon,N} | (U_{\lambda,\epsilon,N}^{(\epsilon)t})^* v U_{\lambda,\epsilon,N}^{(\epsilon)t} | \psi_{h,t,\epsilon,N} \rangle_N - \langle \psi_{h,t,\epsilon} | (U_{\lambda,\epsilon}^{(\epsilon)t})^* v U_{\lambda,\epsilon}^{(\epsilon)t} | \psi_{h,t,\epsilon} \rangle_p \right|,$$

with

$$\psi_{h,t,\epsilon,N} := \psi_h / \|U_{\lambda,\epsilon,N}^{(\epsilon)t}[\psi_h]\|_N,$$

whereafter we can employ Lemma 6.20 to give the consistency of flows of position-space observables. In anticipation of specifying to coherent states, we state the L^2 inner product consistency bounds in terms that respect a class of *local* functions. The point of this is that when we apply a Bernstein bound for the consistency of the inner product between two functions, at least one of which is localized to roughly an $O(h^{\frac{\varsigma}{n}})$ radius ball with respect to $h \in (0, h_0]$ for some $h_0 > 0$, then we can use the dependence of the bound on the variance to get a better convergence rate by a factor of roughly h^ς in the exponential. This trick was used in [Hei05] to give a quadratic improvement of the rate of convergence in the bias term (*viz.*, the density parameter ϵ) for the graph Laplacian and we simply state it here in a somewhat more general and convenient form. More precisely, we have,

LEMMA 6.21. — *Let $\varsigma \in \mathbb{R}$ and $0 < h_0 \leq 1$ be fixed and let $u_{h,\varsigma} \in L^\infty$ be a family of functions over $h \in (0, h_0]$ satisfying: there are constants $\bar{K}_u, K_{u,2} > 0$ so*

that uniformly in h , $h^\varsigma \|u_{h,\varsigma}\|_\infty \leq \bar{K}_u$ and $\|u_{h,\varsigma}\|_{L^2}^2 \leq K_{u,2}$. Then, given any $v \in L^\infty$, for all $\delta > 0$, we have

$$\begin{aligned} \Pr \left[\left| \langle u_{h,\varsigma}, v \rangle_N - \langle u_{h,\varsigma}, v \rangle_p \right| > \delta \right] &\leq 4 \exp \left(- \frac{N h^\varsigma \delta^2}{2 \|v\|_\infty (h^\varsigma K_{u,2} \|v\|_\infty \|p\|_\infty + \bar{K}_u \delta / 3)} \right) \\ &=: \rho_N(\delta, h^\varsigma, \bar{K}_u, K_{u,2}, \|v\|_\infty). \end{aligned}$$

In case that $v = \tilde{u}_{h,\varsigma}$ is another such family, then

$$\begin{aligned} \Pr \left[\left| \langle u_{h,\varsigma}, \tilde{u}_{h,\varsigma} \rangle_N - \langle u_{h,\varsigma}, \tilde{u}_{h,\varsigma} \rangle_p \right| > \delta \right] &\leq 4 \exp \left(- \frac{N h^{2\varsigma} \delta^2}{2 \bar{K}_{\tilde{u}} (K_{u,2} \bar{K}_{\tilde{u}} \|p\|_\infty + \bar{K}_u \delta / 3)} \right) \\ &=: \rho_{N,2}(\delta, h^{2\varsigma}, \bar{K}_u, K_{u,2}, \bar{K}_{\tilde{u}}). \end{aligned}$$

Proof. — We first compute the maximum and variance in order to apply Bernstein's inequality:

$$\begin{aligned} \max_{1 \leq j \leq N} |u_{h,\varsigma}(x_j) \overline{v(x_j)}| &\leq h^{-\varsigma} \bar{K}_u \|v\|_\infty, \\ \text{Var}(u_{h,\varsigma} \bar{v}) &= \int_{\mathcal{M}} |u_{h,\varsigma} \bar{v}|^2 p \, d\nu_g \leq \|v\|_\infty^2 \|p\|_\infty \int_{\mathcal{M}} |u_{h,\varsigma}|^2 \, d\nu_g \\ &\leq K_{u,2} \|v\|_\infty^2 \|p\|_\infty. \end{aligned}$$

The probabilistic bounds in the statement of Lemma 6.21 now follows from Bernstein's inequality. $\square$

Remark 6.22. — The coefficient $K_{u,2}$ can be elaborated into more precise constants regarding the geometry of small balls in $\mathcal{M}$, if the localization of $u_{h,\varsigma}$ were explicitly utilised. The simpler form is sufficient for the essential purposes of the following applications.

From here onwards, we will specify to the application to coherent states, simply to have explicit bounds and keep the discussion concrete. An immediate application is that we can recover the $L^2(\mathcal{M}, p \, d\nu_g)$ norm of $U_{\lambda,\epsilon}^t[\psi_h]$:

LEMMA 6.23. — *Let $\lambda \geq 0$, $h \in (0, h_0]$ as in Proposition 6.18, $\alpha \geq 1$, $\epsilon = h^{2+\alpha}$, $\varepsilon \in O(h^{1+\alpha})$, $|t| \leq T_E^p$ and $(x_0, \xi_0) \in T^*\mathcal{M}$. Then, for $\tilde{\psi}_h$ an un-normalized coherent state localized at (x_0, ξ_0) , there is a constant $K_{\psi,2} > 0$ depending on ψ_h and $O(1)$ in h such that with $K_{\tilde{\psi}}$ and $\underline{K}_{\tilde{\psi}}$ given by Proposition 6.18, we have for all $\delta > 0$,*

$$\begin{aligned} \Pr \left[\left| \left\| U_{\lambda,\epsilon,N}^{(\varepsilon)t} \tilde{\psi}_h \right\|_N^2 - \left\| U_{\lambda,\epsilon}^{(\varepsilon)t} \tilde{\psi}_h \right\|_p^2 \right| > \delta \right] \\ \leq \rho_{N,2}(\delta/2, h^{\tilde{\rho}n}, K_{\tilde{\psi}}, K_{\psi,2}, K_{\tilde{\psi}}) \\ + \begin{cases} \Omega_{\lambda,t,N} \left(\frac{\delta}{4 K_{\tilde{\psi}} h^{-\tilde{\rho}n/2+2+2\delta}}, \epsilon, K_{\tilde{\psi}} h^{-\tilde{\rho}n/2} \right) & \text{if } \varepsilon = 0, \\ \Omega_{\lambda,t,N}^* \left(\frac{\delta}{4 K_{\tilde{\psi}} h^{-\tilde{\rho}n/2+2+2\delta}}, \varepsilon, \epsilon, K_{\tilde{\psi}} h^{-\tilde{\rho}n/2} \right) & \text{if } \varepsilon > 0 \end{cases} \\ =: \Xi_{\lambda,N}(\delta, \psi_h). \end{aligned}$$

Proof. — Assume the events $\mathcal{A}_1$ and $\mathcal{A}_2$ that

$$\left\| \left| U_{\lambda,\epsilon}^{(\epsilon)t} \tilde{\psi}_h \right|^2 - \left| U_{\lambda,\epsilon,N}^{(\epsilon)t} \tilde{\psi}_h \right|^2 \right\|_{\infty} \leq \frac{\delta}{2} \quad \text{and} \quad \left\| \left\| U_{\lambda,\epsilon}^{(\epsilon)t} \tilde{\psi}_h \right\|_N^2 - \left\| U_{\lambda,\epsilon,N}^{(\epsilon)t} \tilde{\psi}_h \right\|_N^2 \right\| \leq \frac{\delta}{2},$$

respectively. Then,

$$\begin{aligned} \left| \left\| U_{\lambda,\epsilon,N}^{(\epsilon)t} \tilde{\psi}_h \right\|_N^2 - \left\| U_{\lambda,\epsilon}^{(\epsilon)t} \tilde{\psi}_h \right\|_p^2 \right| \\ \leq \left| \left\| U_{\lambda,\epsilon,N}^{(\epsilon)t} \tilde{\psi}_h \right\|_N^2 - \left\| U_{\lambda,\epsilon}^{(\epsilon)t} \tilde{\psi}_h \right\|_N^2 \right| + \left| \left\| U_{\lambda,\epsilon}^{(\epsilon)t} \tilde{\psi}_h \right\|_N^2 - \left\| U_{\lambda,\epsilon}^{(\epsilon)t} \tilde{\psi}_h \right\|_p^2 \right| \\ \leq \delta. \end{aligned}$$

Now, we use Lemma 6.21 to establish a lower bound on the probability that $\mathcal{A}_2$ occurs. Since $U_{\lambda,\epsilon}^{(\epsilon)t}$ is similar to a unitary operator by the diagonal $\sqrt{p_{\lambda,\epsilon}}$, we have that

$$(6.18) \quad \left\| U_{\lambda,\epsilon}^{(\epsilon)t} \tilde{\psi}_h \right\|_p^2 \leq \frac{\|p_{\lambda,\epsilon}\|_{\infty}}{\inf p_{\lambda,\epsilon}} \|\tilde{\psi}_h\|_p^2 \leq h^{n/2} \bar{C}_{\psi,2} \|p\|_{\infty} \frac{\bar{C}_{p,\lambda}}{\underline{C}_{p,\lambda}}$$

for a constant $\bar{C}_{\psi,2} > 0$. Therefore, by adapting (6.14) to the perturbed case and applying Lemma 6.21 we have,

$$\Pr[\mathcal{A}_2] \geq 1 - \rho_{N,2}(\delta/2, h^{\tilde{\rho}n}, K_{\tilde{\psi}}, K_{\psi,2}, K_{\tilde{\psi}})$$

with $K_{\psi,2} := \bar{C}_{\psi,2} \bar{C}_{p,\lambda} / \underline{C}_{p,\lambda}$. As for the event $\mathcal{A}_1$, Proposition 6.18 gives a lower bound for the probability that this occurs; then, a union bound gives the probability as in the statement of the present Lemma 6.23. $\square$

The consistency of propagations given in Theorem 6.14 applies readily to ψ_h , as can be seen from a slight modification to account for the norm in the proof of Proposition 6.18. However, in practice, it is only reasonable to expect that we can construct $\psi_{h,t,\varepsilon,N} := \psi_h / \|U_{\lambda,\epsilon,N}^{(\varepsilon)t}[\psi_h]\|_N$. By combining Theorem 6.14 and Lemma 6.23, we have the consistency between $\psi_{h,t,\varepsilon,N}$ and $\psi_{h,t,\varepsilon}$. Now we use this to see the probabilistic consistency between the graph and manifold versions of the inner product of (the modulus squared of) a propagated, normalized coherent state with an arbitrary smooth function, in:

LEMMA 6.24. — *Let $\lambda \geq 0$, $h_0 \in (0, 1]$ be given by Theorem 5.2, $\alpha \geq 1$, and $(x_0, \xi_0) \in T^*\mathcal{M}$. Then, for ψ_h a coherent state localized at (x_0, ξ_0) , $|t| \leq T_E^{\rho}$, $\tilde{\rho} \in (\rho, 1/2]$ and given $u \in C^{\infty}$, there are constants $C_{\psi,\lambda,p,u}, C'_{\psi,\lambda,p,u} > 0$ and $\bar{K}_{\psi}, K_{\psi,2}, \bar{\underline{K}}_{\psi,2}, \underline{\bar{K}}_{\psi,2}, \bar{\bar{K}}_{\psi} > 0$ depending on ψ_h and independent of h with $C_{\psi,\lambda,p,u}, C'_{\psi,\lambda,p,u} > 0$ additionally depending on u such that for all $h \in (0, h_0]$ and $\delta \in (0, 4\|u\|_{\infty}]$,*

$$\begin{aligned} \Pr \left[\left| \left\langle \left| U_{\lambda,\epsilon,N}^t \psi_{h,t,N} \right|^2, u \right\rangle_N - \left\langle \left| U_{\lambda,\epsilon}^t [\psi_{h,t}] \right|^2, u \right\rangle_p \right| > \delta \right] \\ \leq \Omega_{\lambda,t,N} \left(C'_{\psi,\lambda,p,u} h^{n/2} \delta, \epsilon, h^{-\tilde{\rho}n} \bar{\bar{K}}_{\psi} \right) + \rho_N \left(\delta, h^{(1+2\tilde{\rho})n/2}, \bar{K}_{\psi}, K_{\psi,2}, \bar{K}_{\psi} \|u\|_{\infty} \right) \end{aligned}$$

$$\begin{aligned}
& + \rho_{N,2} \left(h^{(1+2\tilde{\rho})n/4} \widetilde{K}_{\psi,2}, 1, \widetilde{K}_{\psi}^{-1/2}, \widetilde{K}_{\psi,2}, \widetilde{K}_{\psi}^{-1/2} \right) + \Xi_{\lambda,N} \left(C_{\psi,\lambda,p,u} h^{n/2} \delta, \psi_h \right) \\
& =: \widetilde{\Omega}_{\lambda,t,N}(\delta, \epsilon, \psi_h, u),
\end{aligned}$$

wherein

$$\psi_{h,t,N} := \psi_h / \|U_{\lambda,\epsilon,N}^t \psi_h\|_N \quad \text{and} \quad \psi_{h,t} := \psi_h / \|U_{\lambda,\epsilon}^t \psi_h\|_p.$$

This holds as well in the perturbed case, wherein we have for $\varepsilon \in O(h^{1+\alpha})$,

$$\begin{aligned}
& \Pr \left[\left| \langle |U_{\lambda,\epsilon,N}^{(\varepsilon)t} \psi_{h,t,\varepsilon,N}|^2, u \rangle_N - \langle |U_{\lambda,\epsilon}^{(\varepsilon)t} \psi_{h,t,\varepsilon}|^2, u \rangle_p \right| > \delta \right] \\
& \leq \Omega_{\lambda,t,N}^* \left(C'_{\psi,\lambda,p,u} h^{n/2} \delta, \varepsilon, \epsilon, h^{-\tilde{\rho}n} \widetilde{K}_{\psi} \right) + \rho_N \left(\delta, h^{(1+2\tilde{\rho})n/2}, \bar{K}_{\psi}, K_{\psi,2}, \bar{K}_{\psi} \|u\|_{\infty} \right) \\
& \quad + \rho_{N,2} \left(h^{(1+2\tilde{\rho})n/4} \widetilde{K}_{\psi,2}, 1, \widetilde{K}_{\psi}^{-1/2}, h^{n/2} \widetilde{K}_{\psi,2}, \widetilde{K}_{\psi}^{-1/2} \right) + \Xi_{\lambda,N} \left(C_{\psi,\lambda,p,u} h^{n/2} \delta, \psi_h \right) \\
& =: \widetilde{\Omega}_{\lambda,t,N}^*(\delta, \varepsilon, \epsilon, \psi_h, u)
\end{aligned}$$

with new constants and

$$\psi_{h,t,\varepsilon,N} := \psi_h / \|U_{\lambda,\epsilon}^{(\varepsilon)t} \psi_h\|_N \quad \text{and} \quad \psi_{h,t,\varepsilon} := \psi_h / \|U_{\lambda,\epsilon}^{(\varepsilon)t} \psi_h\|_p.$$

Proof of Lemma 6.24. — We write,

$$\begin{aligned}
& \left| \langle |U_{\lambda,\epsilon,N}^t \psi_{h,t,N}|^2, u \rangle_N - \langle |U_{\lambda,\epsilon}^t \psi_{h,t}|^2, u \rangle_p \right| \\
& \leq \left| \langle |U_{\lambda,\epsilon,N}^t \psi_{h,t,N}|^2, u \rangle_N - \langle |U_{\lambda,\epsilon}^t \psi_{h,t}|^2, u \rangle_N \right| \\
& \quad + \left| \langle |U_{\lambda,\epsilon}^t \psi_{h,t}|^2, u \rangle_N - \langle |U_{\lambda,\epsilon}^t \psi_{h,t}|^2, u \rangle_p \right| \\
& =: \text{I} + \text{II}
\end{aligned}$$

and recalling that $\tilde{\psi}_h = e^{\frac{i}{\hbar}\phi}$ is the *un-normalized* coherent state,

$$\begin{aligned}
\text{I} & = \left| \langle |U_{\lambda,\epsilon,N}^t \psi_{h,t,N}|^2 - |U_{\lambda,\epsilon}^t \psi_{h,t}|^2, u \rangle_N \right| \\
& = \frac{1}{c_N c} \left| \langle c |U_{\lambda,\epsilon,N}^t \tilde{\psi}_h|^2 - (c + c_N - c) |U_{\lambda,\epsilon}^t \tilde{\psi}_h|^2, u \rangle_N \right| \\
& \leq \frac{1}{c_N} \left| \langle |U_{\lambda,\epsilon,N}^t \tilde{\psi}_h|^2 - |U_{\lambda,\epsilon}^t \tilde{\psi}_h|^2, u \rangle_N \right| + \frac{|c_N - c|}{c_N c} \left| \langle |U_{\lambda,\epsilon}^t \tilde{\psi}_h|^2, u \rangle_N \right| \\
& \leq \|\iota\|_{\infty} \left(c_N^{-1} \left\| (U_{\lambda,\epsilon,N}^t - U_{\lambda,\epsilon}^t) \tilde{\psi}_h \right\|_{\infty} \left\| (U_{\lambda,\epsilon,N}^t + U_{\lambda,\epsilon}^t) \tilde{\psi}_h \right\|_N + \frac{|c_N - c|}{c_N c} \left\| U_{\lambda,\epsilon}^t \tilde{\psi}_h \right\|_N^2 \right),
\end{aligned}$$

where

$$c := \|U_{\lambda,\epsilon}^t \tilde{\psi}_h\|_p^2 \quad \text{and} \quad c_N := \|U_{\lambda,\epsilon,N}^t \tilde{\psi}_h\|_N^2.$$

Suppose the occurrence of the following events:

$$\mathcal{A}_1: \left\| (U_{\lambda,\epsilon,N}^t - U_{\lambda,\epsilon}^t) \tilde{\psi}_h \right\|_{\infty} \leq \delta_1,$$

$$\begin{aligned}\mathcal{A}_2: & |c_N - c| \leq \delta_1, \\ \mathcal{A}_3: & \left| \left\| U_{\lambda,\epsilon}^t \tilde{\psi}_h \right\|_N^2 - c \right| \leq c', \\ \mathcal{A}_4: & \left| \left\langle \left| U_{\lambda,\epsilon}^t \psi_{h,t} \right|^2, u \right\rangle_N - \left\langle \left| U_{\lambda,\epsilon}^t \psi_{h,t} \right|^2, u \right\rangle_p \right| \leq \delta/2\end{aligned}$$

for some $0 < \delta_1 \leq c/2$ and $0 < c' \leq c$. Then,

$$\text{I} \leq \delta_1 \|u\|_\infty c^{-1} (4 + 6\sqrt{c}).$$

and $\text{II} \leq \delta/2$. So letting $\delta_1 = \delta c [2\|u\|_\infty (4 + 6\sqrt{c})]^{-1}$ then gives for $\delta \leq \|u\|_\infty (4 + 6\sqrt{c}) \in 4\|u\|_\infty + O(h^{\frac{n}{4}})$,

$$(6.19) \quad \text{I} + \text{II} \leq \delta.$$

We wish to apply the foregoing probabilistic bounds from the lemmas of this section and from the first part of Proposition 6.18 to bound the probabilities of the events $\mathcal{A}_1, \dots, \mathcal{A}_4$. In light of Lemma 6.21, we will have probabilistic bounds on the events $\mathcal{A}_3$ and $\mathcal{A}_4$ if we have L^2 and L^∞ bounds on $U_{\lambda,\epsilon}^t \tilde{\psi}_h$ and $U_{\lambda,\epsilon}^t \psi_{h,t}$. These are as follows: by (6.18), $c \leq h^{\frac{n}{2}} \bar{C}_{\psi,2} \|p\|_\infty \bar{C}_{p,\lambda} / \underline{C}_{p,\lambda}$. Likewise, by the proof of Theorem 3.3 we have a constant $\underline{C}_{\psi,2} > 0$ also $O(1)$ in h such that $C_h(x_0, \xi_0)^{-2} \geq h^{\frac{n}{2}} \underline{C}_{\psi,2}$, so

$$c \geq \frac{\inf p_{\lambda,\epsilon}}{\|p_{\lambda,\epsilon}\|_\infty} \left\| \tilde{\psi}_h \right\|_p^2 \geq h^{n/2} \underline{C}_{\psi,2} \underline{C}_p \frac{\underline{C}_{p,\lambda}}{\bar{C}_{p,\lambda}}.$$

Since $|U_{\lambda,\epsilon}^t[\psi_{h,t}]|^2 = |U_{\lambda,\epsilon}^t \tilde{\psi}_h|^2 / c$ and as in the proof of Proposition 6.18, there is a constant $K_{\tilde{\psi}} > 0$ such that $\|U_{\lambda,\epsilon}^t \tilde{\psi}_h\|_\infty^2 \leq h^{-\tilde{\rho}n} K_{\tilde{\psi}}^2$, we have,

$$\left\| U_{\lambda,\epsilon}^t \psi_{h,t} \right\|_\infty^2 \leq \frac{\left\| U_{\lambda,\epsilon}^t \tilde{\psi}_h \right\|_\infty^2}{c} \leq h^{-(1+2\tilde{\rho})n/2} \frac{K_{\tilde{\psi}}^2 \bar{C}_{p,\lambda}}{\underline{C}_{\psi,2} \underline{C}_{p,\lambda} \underline{C}_p} =: h^{-(1+2\tilde{\rho})n/2} \bar{K}_{\tilde{\psi}}^2$$

and there is a constant $K_{\psi,2} > 0$ such that

$$\begin{aligned}\left\| U_{\lambda,\epsilon}^t \psi_{h,t} \right\|_{L^2}^2 &= c^{-1} \left\| U_{\lambda,\epsilon}^t \tilde{\psi}_h \right\|_{L^2}^2 \\ &= c^{-1} \left\langle \tilde{\psi}_h \left| p p_{\lambda,\epsilon} U_{\lambda,\epsilon}^{-t} (p p_{\lambda,\epsilon})^{-1} U_{\lambda,\epsilon}^t \right| \tilde{\psi}_h \right\rangle \\ &\leq \frac{\bar{C}_{\psi,2} (1 + O(h^{1-2\rho})) \bar{C}_{p,\lambda}}{\underline{C}_{\psi,2} \underline{C}_{p,\lambda} \underline{C}_p} \\ &\leq K_{\psi,2},\end{aligned}$$

wherein the second equality follows from the fact that the adjoint of $U_{\lambda,\epsilon}^t$ over $L^2(\mathcal{M}, d\nu_g)$ is given by $p \circ (U_{\lambda,\epsilon}^t)^* \circ 1/p$ with $(U_{\lambda,\epsilon}^t)^*$ the adjoint on $L^2(\mathcal{M}, p d\nu_g)$. With this, we find on writing

$$\left\langle \left| U_{\lambda,\epsilon}^t \psi_{h,t} \right|^2, u \right\rangle_N - \left\langle \left| U_{\lambda,\epsilon}^t \psi_{h,t} \right|^2, u \right\rangle_p = \left\langle \left| U_{\lambda,\epsilon}^t \psi_{h,t} \right|, v \right\rangle_N - \left\langle \left| U_{\lambda,\epsilon}^t \psi_{h,t} \right|, v \right\rangle_p,$$

with

$$v(\cdot) := \left| U_{\lambda,\epsilon}^t \psi_{h,t}(\cdot) \right| u(\cdot)$$

and applying Lemma 6.21 that the event $\mathcal{A}_4$ happens with probability at least $1 - \rho_N(\delta/2, h^{(1+2\tilde{\rho})n/2}, \bar{K}_{\tilde{\psi}}, K_{\psi,2}, \bar{K}_{\tilde{\psi}} \|u\|_\infty)$ and the event $\mathcal{A}_3$ with probability at least

$1 - \rho_{N,2}(h^{n/4+\tilde{\rho}n/2}\widetilde{K}_{\psi,2}, 1, K_{\tilde{\psi}}, \widetilde{K}_{\psi,2}, K_{\tilde{\psi}})$ with $\widetilde{K}_{\psi,2} := \underline{C}_{\psi,2}\underline{C}_p\underline{C}_{p,\lambda}/\overline{C}_{p,\lambda}$ and $\widetilde{K}_{\psi,2} := \overline{C}_{\psi,2}\|p\|_{\infty}\overline{C}_{p,\lambda}/\underline{C}_{p,\lambda}$.

As for event $\mathcal{A}_2$, we may apply Lemma 6.23 while noting that in that notation, $C_{\psi} := \overline{C}_{\psi,2}$ and

$$\begin{aligned}\delta_1 &\geq \delta h^{n/2} \frac{\widetilde{K}_{\psi,2}}{2\|u\|_{\infty}(4+6\sqrt{c})} \\ &\geq \delta h^{n/2} \frac{\widetilde{K}_{\psi,2}}{2\|u\|_{\infty}(4+6\widetilde{K}_{\psi,2}^{1/2})} \\ &=: C_{\psi,\lambda,p,u} h^{n/2} \delta,\end{aligned}$$

so that

$$\Pr[\mathcal{A}_2] \geq 1 - \Xi_{\lambda,N}(h^{n/2}C_{\psi,\lambda,p,u}\delta, \psi_h).$$

Further, (6.17) gives a lower bound for the probability of event $\mathcal{A}_1$ happening. Thus, after taking into account the condition that $\delta \leq 4\|u\|_{\infty}$, which suffices to achieve (6.19), we have a constant $C'_{\psi,\lambda,p,u} > 0$ such that

$$\Pr[\mathcal{A}_1] \geq 1 - \Omega_{\lambda,t,N}(C'_{\psi,\lambda,p,u}h^{n/2}\delta, \epsilon, h^{-\tilde{\rho}n}K_{\tilde{\psi}}^2).$$

Hence, the probabilistic bounds in the statement of the present Lemma 6.24 follow from taking a union bound and noting that the analogous statements follow for the perturbed case. $\square$

Combined with Lemma 6.20, this tells that we may observe the propagation of classical configuration-space observables along the geodesic flow of $\mathcal{M}$ through their means with propagated coherent states on the graph approximating its structure:

THEOREM 6.25. — *Let $\lambda \geq 0$, $\alpha \geq 1$, $(x_0, \xi_0) \in T^*\mathcal{M}$ and $|t| \leq T_E^{\rho}$. Then, for ψ_h a coherent state localized at (x_0, ξ_0) and given $u \in C^{\infty}$, there is a constant $C > 0$ such that we have for all $h \in (0, \min\{h_0, 4\|u\|_{\infty}\})$ with $h_0 \in (0, 1]$ from Theorem 5.2 and $\epsilon := h^{2+\alpha}$,*

$$(6.20) \quad \Pr\left[\left|\left\langle |U_{\lambda,\epsilon,N}^t \psi_{h,t,N}|^2, u \right\rangle_N - u(x_t) \right| > Ch^{1-2\rho}\right] \leq \tilde{\Omega}_{\lambda,t,N}(h, \epsilon, \psi_h, u).$$

Letting $\varepsilon \in O(h^{1+\alpha})$, we also have

$$(6.21) \quad \Pr\left[\left|\left\langle |U_{\lambda,\epsilon,N}^{(\varepsilon)t} \psi_{h,t,N}|^2, u \right\rangle_N - u(x_t) \right| > Ch^{1-2\rho}\right] \leq \tilde{\Omega}_{\lambda,t,N}^*(h, \varepsilon, \epsilon, \psi_h, u).$$

Proof. — Suppose we are in the event that

$$\left| \left\langle |U_{\lambda,\epsilon,N}^t [\psi_{h,t,N}]|^2, u \right\rangle_N - \left\langle |U_{\lambda,\epsilon}^t [\psi_{h,t}]|^2, u \right\rangle_p \right| \leq h^{1-2\rho}.$$

Then by Lemma 6.20 there is a constant $C' > 0$ such that,

$$\begin{aligned} & \left| \left\langle \left| U_{\lambda,\epsilon,N}^t \psi_{h,t,N} \right|^2, u \right\rangle_N - u(x_t) \right| \\ & \leq \left| \left\langle \left| U_{\lambda,\epsilon,N}^t \psi_{h,t,N} \right|^2, u \right\rangle_N - \left\langle \left| U_{\lambda,\epsilon}^t [\psi_{h,t}] \right|^2, u \right\rangle_p \right| + \left| \left\langle \left| U_{\lambda,\epsilon}^t [\psi_{h,t}] \right|^2, u \right\rangle_p - u(x_t) \right| \\ & \leq (1 + C') h^{1-2\rho}. \end{aligned}$$

Now, Lemma 6.24 gives a lower bound on the occurrence of this event, under the condition that $h \in (0, \min\{h_0, 4\|u\|_\infty\}]$, as $1 - \tilde{\Omega}_{\lambda,t,N}(h, \epsilon, \psi_h, u)$.

The perturbed case follows along the same lines upon applying Lemmas 6.20 and 6.24 with $\varepsilon \in O(h^{1+\alpha})$. $\square$

6.5. Observing geodesics on graphs

We are now in the position to implement Proposition 5.5 on the graph holding an approximative structure of $\mathcal{M}$ and to give its probabilistic rate of consistency: to summarize the procedure, we give the example of an,

ALGORITHM 6.26 (Geodesic flow reconstruction). — Having constructed $\Delta_{\lambda,\epsilon,N}$ and $\tilde{\psi}_h$ localized at (x_0, ξ_0) on Λ_N with $\epsilon = h^{2+\alpha}$ and $\alpha \in [1, 2]$, the estimation of the geodesic flow proceeds as follows:

- (1) Construct $U_{\lambda,\epsilon,N}^t := e^{-it\sqrt{\Delta_{\lambda,\epsilon,N}}}$ by spectral methods.
- (2) Identify the local peak $\hat{x}_{N,t} = \arg \max_{\mathcal{X}_N} |U_{\lambda,\epsilon,N}^t \tilde{\psi}_h|$.
- (3) Form the normalized state $\psi_{h,t,N} := \tilde{\psi}_h / \|U_{\lambda,\epsilon,N}^t \tilde{\psi}_h\|_N$. Set the localization scale $\bar{\varepsilon}_t \sim h^{1/2-\tilde{\rho}}$ for $\tilde{\rho} \in (\rho, 1/2)$ and compute the coordinate-wise mean:

$$\bar{t}_{N,j}^t := \left\langle \left| U_{\lambda,\epsilon,N}^t \psi_{h,t,N} \right|^2, \chi_t \left(\|\iota(\cdot) - \iota(\hat{x}_{N,t})\|_{\mathbb{R}^D} \right) \iota_j \right\rangle_N$$

for each $j \in [D]$, where $\chi_t \in C_c^\infty(\mathbb{R})$ satisfies $\text{supp } \chi_t \subset [-R_t, R_t]$ such that $R_t > \bar{\varepsilon}_t$ and $\chi_t \equiv 1$ on $[-\bar{\varepsilon}_t, \bar{\varepsilon}_t]$.

- (4) Identify the reconstructed point $\bar{x}_{N,\iota,t} := \arg \min_{x \in \mathcal{X}_N} \|\iota(x) - \bar{t}_{N,j}^t\|_{\mathbb{R}^D}$.

The algorithm outputs $\bar{x}_{N,\iota,t} \in \Lambda_N$.

Remarks 6.27. —

- (1) We can simply take $\chi_t \equiv 1$ when working with extrinsic coordinates, since they are globally defined. This can be preferable in situations where using the cut-off χ_t increases uncertainty without significant cost benefit.
- (2) We have assumed that an un-normalized coherent state has been given; however, the definition of such states a priori relies on intrinsic information about $\mathcal{M}$. In Section 3.1 we have pointed out how to approximate coherent states with just extrinsic data and that discussion, combined with the results of Section 5, shows that the approximate coherent states are appropriate surrogates to affect quantum-classical correspondence. The construction of these approximate states from data Λ_N follows from further applications of concentration inequalities and our a priori $L^\infty \rightarrow L^\infty$ bound on $U_{\lambda,\epsilon,N}^t$. We

will remark on this further and note that this has been carried out in detail in [KS22].

Anticipating applications such as this Algorithm, implemented in detail for example in [KS22] (with data-driven approximations to coherent states), we make the following,

DEFINITION 6.28. — *Let ψ_h be a coherent state localized at $(x_0, \xi_0) \in T^*\mathcal{M}$ and consider its propagation with respect to $U_{\lambda, \epsilon, N}^t$. The intrinsic sample maximizer of the propagated coherent state is,*

$$\hat{x}_{N,t} := \arg \max_{\mathcal{X}_N} |U_{\lambda, \epsilon, N}^t \tilde{\psi}_h|^2.$$

- (1) *Extrinsic case. The extrinsic sample mean of the propagated coherent state is $\bar{x}_{N, \chi_t, t} \in \Lambda$, defined with respect to a cut-off $\chi_t \in C_c^\infty(\mathbb{R}^D)$, as the closest point on Λ_N to*

$$\iota_N^t(x_0, \xi_0) := (\iota_{N,1}^t(x_0, \xi_0), \dots, \iota_{N,D}^t(x_0, \xi_0)),$$

with

$$\iota_{N,j}^t(x_0, \xi_0) := \left\langle |U_{\lambda, \epsilon, N}^t \psi_{h,t,N}|^2, (\chi_t \circ \iota) \iota_j \right\rangle_N.$$

That is, $\bar{x}_{N, \chi_t, t} := \arg \min_{X \in \Lambda_N} \|X - \iota_N^t(x_0, \xi_0)\|_{\mathbb{R}^D}$.

- (2) *Local coordinates. Let $\mathcal{O}_t \subset \mathcal{M}$ be an open neighbourhood of $\hat{x}_t$. Then, given a diffeomorphic coordinate mapping $u : \mathcal{O}_t \rightarrow V_t \subset \mathbb{R}^n$ and $\chi \in C_c^\infty(\mathbb{R}^n)$ a cut-off with $\text{supp } \chi \subset V_t$, the u -sample mean with respect to χ of the propagated coherent state is $\bar{x}_{N, u, \chi, t} \in V_t$ that is the closest point on $\mathcal{V}_N := u[\mathcal{X}_N \cap \mathcal{O}_t]$ to*

$$\bar{u}_N^t(x_0, \xi_0) := (\bar{u}_{N,1}^t(x_0, \xi_0), \dots, \bar{u}_{N,n}^t(x_0, \xi_0)),$$

with

$$\bar{u}_{N,j}^t(x_0, \xi_0) := \left\langle |U_{\lambda, \epsilon, N}^t \psi_{h,t,N}|^2, (\chi \circ u) u_j \right\rangle_N.$$

That is, $\bar{x}_{N, u, \chi, t} := \arg \min_{X \in \mathcal{V}_N} \|X - \bar{u}_N^t(x_0, \xi_0)\|_{\mathbb{R}^n}$.

That the preceding Algorithm outputs, with high probability, a point within an *intrinsic* distance of $O(h^{1-2\rho})$ from x_t for $|t| \leq T_E^\rho \sim \log(1/h)$ is an application of the following,

PROPOSITION 6.29. — *Let $\lambda \geq 0$, $\alpha \geq 1$, $(x_0, \xi_0) \in T^*\mathcal{M}$ and $|t| \leq T_E^\rho$. Then, for ψ_h a coherent state localized at (x_0, ξ_0) , given any open neighbourhood $\mathcal{O}_t \subset \mathcal{M}$ of $\hat{x}_{N,t}$ with its diffeomorphic coordinate mapping $u : \mathcal{O}_t \rightarrow V_t \subset \mathbb{R}^n$, there are constants $h_{u, \max}, C_{u, \max} > 0$ such that if $h \in (0, h_{u, \max})$ and $\bar{\mathcal{B}}_t := \bar{B}(u(\hat{x}_{N,t}), \|\cdot\|_{\mathbb{R}^n}; C_{u, \max} h^{1/2-\tilde{\rho}}) \subset V_t$ with $\tilde{\rho} \in (\rho, 1/2)$, then for any smooth cut-off $\chi \in C_c^\infty(\mathbb{R}^n, [0, 1])$ with $\text{supp } \chi \subset V_t$ that is $\chi \equiv 1$ on $\bar{\mathcal{B}}_t$, we have*

$$\begin{aligned} & \Pr \left[d_g \left(u^{-1}(\bar{x}_{N, u, \chi, t}), x_t \right) > C_u h^{1-2\rho} \right] \\ & \leq n \tilde{\Omega}_{\lambda, t, N} \left(h, \epsilon, \psi_h, K_{\chi, u} \right) + \Omega_{\lambda, t, N} \left(\underline{K}_{\tilde{\psi}} h^{\tilde{\rho}n} / 4, \epsilon, K_{\tilde{\psi}} h^{-\tilde{\rho}n/2} \right) + \exp \left(-2NC'' h^{2(1-2\rho)n} \right), \end{aligned}$$

for constants $C_u, C'' > 0$, uniform constants $\underline{K}_{\tilde{\psi}}, K_{\tilde{\psi}} > 0$ provided in Proposition 6.18 and the coordinate-dependent bound $K_{\chi,u} := \max_{j \in [n]} \|1 + (\chi \circ u) u_j\|_\infty$.

Likewise, there are constants $h_{\iota,\max}, C_{\iota,\max} > 0$ such that for all $h \in [0, h_{\iota,\max})$, given any cut-off $\chi_\iota \in C_c^\infty(\mathbb{R}^D, [0, 1])$ such that $\chi_\iota \equiv 1$ on

$$\bar{\mathcal{B}}_{\iota,t} := \bar{B}(\iota(\hat{x}_{N,t}), \|\cdot\|_D; C_{\iota,\max} h^{1/2-\tilde{\rho}}),$$

we have

$$\begin{aligned} \Pr \left[d_g \left(\iota^{-1}(\bar{x}_{N,\chi_\iota,t}), x_t \right) > C_\iota h^{1-2\rho} \right] \\ \leq D\tilde{\Omega}_{\lambda,t,N}(h, \epsilon, \psi_h, K_{\chi_\iota}) + \Omega_{\lambda,t,N}(Ch^{\frac{n}{2}}, \epsilon, K_\psi) \\ + \exp(-2NC'h^{2n}) + \exp(-2NC'h^n), \end{aligned}$$

for $C_\iota > 0$ a constant and $K_{\chi,u} := \max_{j \in [n]} \|1 + (\chi_\iota \circ \iota) \iota_j\|_\infty$.

Proof. — We have by Proposition 6.18 constants $h'_{\max}, K_{\tilde{\psi}}, \underline{K}_{\tilde{\psi}} > 0$ such that for all $h \in (0, h'_{\max})$, $d_g(\hat{x}_{N,t}, x_t) \leq h^{1/2-\tilde{\rho}}$ with probability at least

$$1 - \Omega_{\lambda,t,N}(\underline{K}_{\tilde{\psi}} h^{\tilde{\rho}n}/4, \epsilon, K_{\tilde{\psi}} h^{-\tilde{\rho}n/2}).$$

Assume this event throughout and call it $\mathcal{A}_0$.

Step 1. — Following the arguments in the proof of the first part of Proposition 5.5, we have constants $h_{u,0} \in (0, h'_{\max}]$ and $C_{u,\max} > 0$ such that for all $h \in (0, h_{u,0})$, $\|u(\hat{x}_{N,t}) - u(x_t)\|_{\mathbb{R}^n} \leq C_{u,\max} h^{1/2-\tilde{\rho}}$.

Step 2. — By Theorem 6.25 we have for each $j \in [n]$, a constant $C_j > 0$ such that for all $h \in (0, \min\{h_0, 4\|u_{\chi,j}\|_\infty\})$, with $u_{\chi,j} := (\chi \circ u)u$, $|\bar{u}_{N,j}^t - u_{\chi,j}(x_t)| \leq C_j h^{1-2\rho}$ with probability at least $1 - \tilde{\Omega}_{\lambda,t,N}(h, \epsilon, \psi_h, u_{\chi,j})$. Assuming also these events, say $\mathcal{A}_1, \dots, \mathcal{A}_n$ and that for each $h \in (0, \min\{h_{u,0}, 4(\|u_{\chi,1}\|_\infty, \dots, \|u_{\chi,n}\|_\infty)\})$,

$$\bar{\mathcal{B}}_t \subset V_t \quad \text{and} \quad \chi \equiv 1 \text{ on } \bar{\mathcal{B}}_t,$$

we have that $|\bar{u}_{N,j}^t - u_j(x_t)| \leq C_j h^{1-2\rho}$ and hence,

$$\|\bar{u}_{N,\chi}^t(x_0, \xi_0) - u(x_t)\|_{\mathbb{R}^n} \leq (C_1^2 + \dots + C_n^2)^{1/2} h^{1-2\rho} =: C'_u h^{1-2\rho}.$$

Step 3. — Then, there are $C_u, h_{u,1} \in (0, 1]$ such that for all $h \in [0, h_{u,1}]$ and any $x_{u,\chi,N}^* \in B_{C'_u h}(\bar{u}_{N,\chi}^t(x_0, \xi_0), \|\cdot\|_{\mathbb{R}^n})$, $d_g(u^{-1}(x_{u,\chi,N}^*), x_t) \leq (C_u/2)h^{1-2\rho}$. Although the interval for h depends on χ , we may translate the coordinate mapping u to work with $\tilde{u} := I_n + u : \mathcal{O}_t \rightarrow \tilde{V}_t$ and $\tilde{\chi} := \chi(I_n - \cdot)$ so that $\tilde{V}_t \subset \mathbb{R}^n \setminus B_1(0, \|\cdot\|_{\mathbb{R}^n})$ and hence, $\|u_{\chi,1}\|_\infty \geq 1$ in the events $\mathcal{A}_j$. With this, we achieve the same result without affecting $h_{u,0}, h_{u,1}, C_{u,\max}$ and C_u : viz.,

$$\begin{aligned} \|u(\hat{x}_{N,t}) - u(x_t)\|_{\mathbb{R}^n} &= \|\tilde{u}(\hat{x}_{N,t}) - \tilde{u}(x_t)\|_{\mathbb{R}^n} \leq C_{u,\max} h^{1/2-\tilde{\rho}}, \\ d_g \left(u^{-1}[\bar{u}_{N,\chi}^t(x_0, \xi_0)], x_t \right) &= d_g \left(\tilde{u}^{-1}[\bar{\tilde{u}}_{N,\tilde{\chi}}^t(x_0, \xi_0)], x_t \right) \leq \frac{C_u}{2} h^{1-2\rho} \end{aligned}$$

and these are now valid over $h \in (0, \min\{h_{u,0}, h_{u,1}\})$.

Step 4. — The probability that

$$\{x_1, \dots, x_N\} \cap B_0 \neq \emptyset, \quad B_0 := B\left(u^{-1}\left[\bar{u}_{N,\chi}(x_0, \xi_0)\right], g; \frac{C_u}{2} h^{1-2\rho}\right),$$

may be lower bounded by a Chernoff bound applied to a Bernoulli process and this gives at least $1 - \exp(-2NC''h^{2(1-2\rho)n})$ success probability with $C'' > 0$ a constant. Indeed, let P_0 be the probability that a random vector x lies in B_0 , which with the aid of Lemma 2.6 is bounded below by,

$$P_0 = \int_{B_0} p(y) d\nu_g(y) \geq (\inf p) \text{vol}(B_0) \geq C_{\mathcal{M}}(\inf p) \left(\frac{C_u}{2} h^{1-2\rho}\right)^{n/2} =: \underline{P}_0.$$

Then a *sampler* $Y_0 : \mathcal{M} \rightarrow \{0, 1\}$ that maps $Y_0[B_0] = 1$ and $Y_0[B_0^c] = 0$ defines N i.i.d. random variables governed by a Bernoulli process with probability P_0 , when applied to the random vectors $x_1, \dots, x_N$. This process has mean $NP_0 \geq N\underline{P}_0$, so a Chernoff bound yields,

$$\Pr\left[\#(\mathcal{X}_N \cap B_j) \geq 1\right] \geq 1 - \exp(-2N\underline{P}_0^2),$$

giving the desired probabilistic bound with in fact $C'' = C_{\mathcal{M}}^2(\inf p)^2(C_u/2)^n$. Thus, possibly after translations and adjusting the probability for each $\mathcal{A}_j$ to at least $1 - \tilde{\Omega}_{\lambda,t,N}(h, \epsilon, \psi_h, \tilde{u}_{\chi,j})$, then taking a union bound and $h_{u,\max} := \min\{h_{u,0}, h_{u,1}\}$, we have the probabilistic bound in the first part of the statement of Proposition 6.29.

The second part of Proposition 6.29 follows the same line of arguments. —

Step 1. — By Theorem 6.25 we have for each $j \in [D]$, a constant $C_j > 0$ such that for all $h \in (0, \min\{h_0, 4\|\iota_{\chi,j}\|_\infty\})$, with $\iota_{\chi,j} := (\chi_\iota \circ \iota)\iota$, $|\bar{\iota}_{N,j}^t - \iota_{\chi,j}(x_t)| \leq C_j h^{1-2\rho}$ with probability at least $1 - \tilde{\Omega}_{\lambda,t,N}(h, \epsilon, \psi_h, \iota_{\chi,j})$.

Step 2. — Assuming these events, say $\mathcal{A}_1, \dots, \mathcal{A}_D$ along with the event $\mathcal{A}_0$, then due to the Assumptions we have that if for each $h \in (0, \min\{\underline{\kappa}, 4(\|\iota_{\chi,1}\|_\infty, \dots, \|\iota_{\chi,D}\|_\infty)\})$, with $\underline{\kappa} := (\kappa/C'_{\max})^2$, it holds that:

$$\bar{\mathcal{B}} := B\left(\iota(\hat{x}_{N,t}), \|\cdot\|_{\mathbb{R}^D}; C'_{\max}\sqrt{h}\right) \subset V_t \quad \text{and} \quad \chi_\iota \equiv 1 \text{ on } \bar{\mathcal{B}},$$

then $|\bar{\iota}_{N,j}^t - \iota_j(x_t)| \leq C_j h^{1-2\rho}$ and hence,

$$\left\|\bar{\iota}_N^t(x_0, \xi_0) - \iota(x_t)\right\|_{\mathbb{R}^D} \leq \left(C_1^2 + \dots + C_D^2\right)^{\frac{1}{2}} h^{1-2\rho} =: C'_\iota h^{1-2\rho}.$$

Step 3. — The Assumptions further imply that if

$$h < \kappa/C'_\iota \quad \text{and} \quad x_{\iota,N}^* \in B\left(\bar{\iota}_N^t(x_0, \xi_0), \|\cdot\|_{\mathbb{R}^D}; C'_\iota h^{1-2\rho}\right) \cap \Lambda,$$

then $d_g(\iota^{-1}(x_{\iota,N}^*), x_t) \leq 2C'_\iota h^{1-2\rho}$. As before, we have that with probability at least $1 - \exp(-2NC''h^{2(1-2\rho)n})$, there is $j \in [N]$ such that $d_g(x_j, \iota^{-1}(x_{\iota,N}^*)) \leq h^{1-2\rho}$, hence $d_g(x_j, x_t) \leq (1 + 2C'_\iota)h^{1-2\rho}$.

Step 4. — Now again we have the joint interval of h depending on χ , but as in the previous part, we can translate the isometry and χ_ι , so that upon taking $h_{\iota,\max} := \min\{h'_{\max}, (\kappa/C'_{\max})^2, \kappa/C'\}$ and a union bound (with respect to the shifted embedding), the probabilistic bound in the second part of the statement of the proposition follows. $\square$

Remark 6.30. — The preceding bounds hold also for the perturbed case with $\varepsilon \in O(h^{1+\alpha})$.

6.6. Statistical estimators

A *statistical estimator* is a procedure for estimating some quantity, or vector of quantities, from observed data. We have shown that the Algorithm outlined above is *nearly* a statistical estimator, modulo the construction of a coherent state, for the geodesic flow on $\mathcal{M}$ to long times. Importantly, this estimator has a high success probability to produce an estimate within an error that scales as a power law in $1/N$ with respect to the number of samples N . Crucial for applications, the exponent in this scaling depends *only* on the effective manifold dimension n and is independent of the extrinsic dimension D . We'll call estimators with these properties *asymptotically good estimators*.

In order to arrive at an asymptotically good estimator for the geodesic flow, we must construct an estimator for coherent states, whose definitions thus far have involved a priori knowledge of $\mathcal{M}$. To this effect, we have indicated in Section 3.1 the construction of approximate coherent states at a given $(x_0, \xi_0) \in S^*\mathcal{M}$ (the unit cosphere bundle: $|\xi_0|_{\mathbb{R}^n} = 1$) using only points on $\Lambda \subset \mathbb{R}^D$, which are suitable for recovering geodesics to time T_E^ρ and within error $O(h^{1-2\rho})$. Following that discussion, each sufficiently nearby point x^* to x_0 provides a direction $\tilde{p}_0 := \iota(x^*) - \iota(x_0)$, modulo a small angle, on the tangent space so that $p_0 := \tilde{p}_0 / |\tilde{p}_0|_{\mathbb{R}^D} \approx D\iota|_x \cdot \xi_0$. We find that for an estimator, the main requirement is to have such a sample point x^* in an $O(h^{n/4+1+\beta})$ neighbourhood of x_0 , for some $\beta \geq 0$, so that the vector

$$[\check{\psi}_h]_j := \left[\exp\left(\frac{i}{h} \langle \iota(x_j) - \iota(x_0), p_0 \rangle_{\mathbb{R}^D}\right) \exp\left(-\frac{1}{2h} |\iota(x_j) - \iota(x_0)|_{\mathbb{R}^D}^2\right) \right],$$

defined *on the sampled data*, has $O_{L^\infty(\mathcal{X}_N)}(h^{\frac{n}{4}+\beta})$ error from the evaluation of an unnormalized coherent state $\tilde{\psi}_h$ at (x_0, ξ_0) on data. An application of concentration inequalities using Chernoff bounds achieves this with high probability and the number of samples scaling polynomially in $1/h$ with the exponent depending only on n and independent of D [KS22, Lemma 2]. The choice of $\beta = (2 + \alpha)(n + 1) + 1$ comes from an application of the generic L^∞ bound (6.10) on $U_{\lambda, \epsilon, N}^t : \mathcal{H}_N \rightarrow \mathcal{H}_N$ and yields that the propagation $U_{\lambda, \epsilon, N}^t[\check{\psi}_h] / \|U_{\lambda, \epsilon, N}^t \check{\psi}_h\|_2$ approximates $U_{\lambda, \epsilon, N}^t \psi_{h, t, N}$ to within error $O_{L^\infty}(h)$ with similar probabilistic convergence rates [KS22, Proposition 2]. Hence, we arrive at a context wherein the preceding results apply directly. The results in [KS22, Lemma 2 & Proposition 2] further show that in place of this (asymptotically good) estimator of a coherent state, we may also use *local principal component analysis* [TVF13] (also [SW12, Theorem B.1]) to approximate cotangent vectors and form coherent state estimators, with similar convergence rates.

This completes the picture for an asymptotically good estimator for the geodesic flow to long times. Beyond such constructions, these coherent state estimators also yield asymptotically good estimators of FBI transforms on $\mathcal{M}$ (see [KS22, Proposition 3 & Figure 3]) and when used as asymptotically good estimators of the semiclassical relation $|\langle \psi_h | \Delta_{\lambda, \epsilon} | \psi_h \rangle - 1| = O(h)$ for ψ_h a coherent state at $(x_0, \xi_0) \in S^*\mathcal{M}$,

they provide efficient data-driven heuristics for good parameter choices ϵ and h . The latter has been an indispensable tool for applications [KS22, Sections II.D.6 & VI], since the choice of these parameter values is so crucial to producing good results and performing many runs of the full algorithm over the two-dimensional landscape of parameter choices is often computationally infeasible; in practice, we find optimal propagation results for parameters close to this heuristic. The algorithms resulting from these methods [KS22, Section VII] have been put to practice on samples from model manifolds with positive and negative curvatures to verify their accuracy in propagating coherent states and recovering the flow [KS22, Section III.A], as well as real-world datasets [KS22, Section III] for performing dimensionality reduction, clustering and statistical anomaly detection.

6.7. Summary of Convergence Rates

The foregoing discussions involve various inter-dependent probabilistic bounds. We now summarize them by giving their *unwrapped* dominant terms as closed-form Bernstein-type exponential bounds:

Approx.	Unperturbed	Perturbed	Bound functions
$A_N \sim_\delta A$: Lemma 6.3	(6.4) $\leq \exp[-\Omega(\bullet)]$ $\bullet := N\epsilon^{\frac{n}{2}}\delta^2$		$\gamma_{\lambda,N}(\delta; u)$
$B_N \sim_\delta B$: Theorem 6.10, Lemma 6.8	(6.8) $\leq \exp[-\Omega(\bullet)]$ $\bullet := N\epsilon^{\frac{n}{2}}\delta^{4(1+v)}$	(6.7) $\leq \exp[-\Omega(\bullet)]$ $\bullet := N\epsilon^{\frac{n}{2}}\delta^2\epsilon^{(1+2v)}$	$\gamma_{\lambda,N,v}(\delta; u) :=$ $\gamma_{\lambda,N}(\delta^{2(1+v(\beta))}; u)$ $\gamma_{\lambda,N,v}^*(\delta, \epsilon; u) :=$ $\gamma_{\lambda,N}(\delta\epsilon^{\frac{1}{2}+v(\beta)}; u)$
$U_N^t \sim_\delta U^t$: Theorem 6.14	(6.12) $\leq$ $ t \exp[-\Omega(\bullet)]$ $\bullet := \frac{N\delta^4\epsilon^{\frac{5}{2}n+4}}{(K_u^2 t ^8)^{\frac{1}{4}}}$, with $\delta > \frac{K_u^{\frac{1}{2}}\epsilon^{-(\frac{5}{8}n+1)}}{N^{\frac{1}{4}}}$, $ t \lesssim K_u^{\frac{1}{4}}\epsilon^{-\frac{n}{16}}$	(6.13) $\leq t $ $\exp[-\Omega(\bullet)\epsilon^\star]$ $\bullet := \frac{N\delta^2\epsilon^{\frac{3}{2}n+2}\epsilon}{K_u^2 t ^4}$, $\star := \tilde{O}(t ^4/N^\sigma)$, with $\delta > \frac{K_u\epsilon^{-(\frac{3}{4}n+1)}}{N^{\frac{1-\sigma}{2}}}$, $0 < \sigma < 1$	$\Omega_{\lambda,t,N}(\delta, \epsilon, K_u)$ $\Omega_{\lambda,t,N}^*$ $(\delta, \epsilon, \epsilon, K_u)$

Approx.	Unperturbed	Perturbed	Bound functions
$\mathbb{E}_t u \sim_{h^{1-2\rho}} u(x_t)$: Theorem 6.25	$(6.20) \leq \exp[-\Omega(\bullet)]$ $\bullet := \frac{Nh^{n(2+3\tilde{\rho})+4}\epsilon^{\frac{5}{2}n+4}}{ t ^8},$ with $ t \leq T_E^\rho$ (or $\lesssim h^{-\frac{\tilde{\rho}}{8}n}\epsilon^{-\frac{n}{16}}$), $\tilde{\rho} \in (\rho, 1/2]$, $\epsilon := h^{2+\alpha}$	$(6.21) \leq \exp[-\Omega(\bullet)]$ $\bullet := \frac{Nh^{n(1+2\tilde{\rho})+2}\epsilon^{\frac{3}{2}n+2}\epsilon^3}{ t ^4},$ with $ t \leq T_E^\rho$ (or $\lesssim N^{\frac{1}{4}}\epsilon^{\frac{3}{8}n+\frac{1}{4}}$), $\tilde{\rho} \in (\rho, 1/2]$, $\epsilon = h^{2+\alpha}$	$\tilde{\Omega}_{\lambda,t,N}(h, \epsilon, \psi_h, u)$ $\tilde{\Omega}_{\lambda,t,N}^*$ $(h, \epsilon, \epsilon, \psi_h, u)$ with $\epsilon \in \Theta(h^{1+\alpha+\beta})$, $\beta \geq 0$
$\hat{x}_{N,t} \sim_{h^{\frac{1}{2}-\tilde{\rho}}} x_t$: Proposition 6.18	$(6.15) \leq \exp[-\Omega(\bullet)]$ $\bullet := \frac{Nh^{5\tilde{\rho}n}\epsilon^{\frac{5}{2}n+4}}{ t ^8},$ with $ t , \tilde{\rho}, \epsilon$ as in (6.20)	$(6.16) \leq \exp[-\Omega(\bullet)]$ $\bullet := \frac{Nh^{3\tilde{\rho}n}\epsilon^{\frac{3}{2}n+2}\epsilon^3}{ t ^4},$ with $ t , \tilde{\rho}, \epsilon$ as in (6.21)	$\Omega_{\lambda,t,N}(h^{\frac{n}{2}}, \epsilon, K_\psi)$ $\Omega_{\lambda,t,N}^*$ $(h^{\frac{n}{2}}, \epsilon, \epsilon, K_\psi^{(\epsilon)})$ with $\epsilon \in \Theta(h^{1+\alpha+\beta})$, $\beta \geq 0$
$\bar{x}_{N,t} \sim_{h^{1-2\rho}} x_t$	Same as (6.20)	Same as (6.21)	(See the previous two rows)

The first column of the table indicates the approximation being considered, with a symbolic short-hand and the location of the precise statement. Here, A_N, A refer to the averaging operators, B_N, B the square roots, or ε -perturbed square roots of $I - A_N, I - A$ resp., as in Notation 6.11, U_N^t, U^t refer to the corresponding propagators and $\mathbb{E}_t u := \langle |U_N^t \psi_{h,t,N}|^2, u \rangle_N$ is short-hand for the *discrete expectation* of u with the density of the sample propagation of the coherent state. The notation $T_1 \sim_r T_2$ for $T_1, T_2 : L^\infty \rightarrow L^\infty$ and $r > 0$ means $\|(T_1 - T_2)[u]\|_\infty \lesssim r$ for any $u \in L^\infty$. The meaning when T_1, T_2 are scalars is clear by analogy and $x \sim_r x_t$ for $x \in \mathcal{M}$ and $r > 0$ refers to the condition $x \in B_r(x_t; g)$. The second and third columns give bounds for the corresponding probabilities in the $\varepsilon = 0$ (*unperturbed*) and $\varepsilon > 0$ (*perturbed*) cases, respectively. The fourth column gives, for reference, the dominant functions in the probability bounds for the unperturbed and perturbed cases that are being further bounded in the second and third columns, respectively.

We have borrowed from complexity theory the following,

Notation 6.31. — The following are asymptotic bounds of non-negative functions:

- (1) $f_0 = O(f(\Upsilon))$ means there is $\Upsilon^* > 0$ such that for all $\Upsilon \geq \Upsilon^*$, $f_0(\Upsilon) \lesssim f(\Upsilon)$;
- (2) $f_0 = \Omega(f(\Upsilon))$ means there is $\Upsilon^* > 0$ such that for all $\Upsilon \geq \Upsilon^*$, $f(\Upsilon) \lesssim f_0(\Upsilon)$;
- (3) $f_0 = \Theta(f(\Upsilon))$ means $f_0 = \Omega(f(\Upsilon))$ and $f_0 = O(f(\Upsilon))$ and
- (4) $f_0 = \hat{O}(f(\Upsilon))$ means there is $\Upsilon^* > 0$ and a polynomial with non-negative coefficients $q \in \mathbb{R}[\Upsilon]$ such that for all $\Upsilon \geq \Upsilon^*$, $f_0(\Upsilon) \lesssim q(\log \Upsilon)f(\Upsilon)$.

Sketch of how these bounds come about. —

Step 1. — By its definition in Lemma 6.8, $v \lesssim (\log N + N\delta^2\epsilon^{\frac{n}{2}})^{-1} \log(N\delta^2\epsilon^{\frac{n}{2}} + \log N)$, hence $v = \tilde{O}(N^{-1}\delta^{-2}\epsilon^{-\frac{n}{2}})$.

Step 2. — The dominant exponential term in $\Omega_{\lambda,t,N}(\delta, \epsilon, K_u)$ given by (6.12) is

$$\begin{aligned} \exp \left[- \left(\frac{N\delta^4 \epsilon^{\frac{5}{2}n+4}}{CK_u^2 |t|^8} \right) \left(\frac{\delta^4 \epsilon^{2n+4}}{|t|^8} \right)^{\tilde{O}\left(\frac{\epsilon^{\frac{n}{4}} |t|^4}{K_u \sqrt{N}}\right)} \right] &\leq \exp \left[- \left(\frac{N\delta^4 \epsilon^{\frac{5}{2}n+4}}{CK_u^2 |t|^8} \right) \left(\frac{K_u^2 \epsilon^{-\frac{n}{2}}}{N|t|^8} \right)^{\tilde{O}\left(\frac{\epsilon^{\frac{n}{4}} |t|^4}{K_u \sqrt{N}}\right)} \right] \\ &= \exp \left[- \left(\frac{N\delta^4 \epsilon^{\frac{5}{2}n+4}}{CK_u^2 |t|^8} \right) (Z/N)^{\tilde{O}\left(\frac{1}{\sqrt{NZ}}\right)} \right] \end{aligned}$$

with $Z := K_u^2 \epsilon^{-n/2} / |t|^8$. So assuming $|t| = O(K_u^{1/4} \epsilon^{-n/16})$ gives

$$Z \gtrsim 1 \quad \text{and} \quad (Z/N)^{\tilde{O}(1/\sqrt{NZ})} \gtrsim 1,$$

hence that factor can be replaced by a constant in the exponential.

Step 3. — We will use the preceding estimate in place of $\Omega_{\lambda,t,N}$ under the corresponding condition $|t| = O((h^{-2\tilde{\rho}n} \epsilon^{-n})^{1/16})$ (recall that $T_E^\rho \leq T + \rho \log(1/h)$ is a worst-case upper bound and the quantum-classical correspondence may be valid beyond this, so we use the generic condition from the preceding step). Then, examining $\Omega_{\lambda,t,N}(\underline{K}_{\tilde{\psi}} h^{\tilde{\rho}n}/4, \epsilon, K_{\tilde{\psi}} h^{-\tilde{\rho}n/2})$ gives the asymptotic bound,

$$(6.15) \leq \exp \left(-\Omega \left(N h^{5\tilde{\rho}n} \epsilon^{5n/2+4} / |t|^8 \right) \right).$$

Step 4. — We now bound the rate given by (6.20). The bound $\tilde{\Omega}_{\lambda,t,N}(\delta, \epsilon, \psi_h, u)$ is defined in Lemma 6.24 and its dominating term is $\Xi_{\lambda,N}(C_{\psi,\lambda,p,u} h^{n/2} \delta, \psi_h)$ with $\Xi_{\lambda,N}(\cdot)$ defined in Lemma 6.23. In turn, we may bound $\tilde{\Omega}_{\lambda,t,N}(h, \epsilon, \psi_h, u)$ in (6.20) using the bound in Step 2 applied to $\Omega_{\lambda,t,N}(h^{n(1+\tilde{\rho})/2+1}, \epsilon, h^{-\tilde{\rho}n/2})$. This gives the rate,

$$(6.20) \leq \exp \left(-\Omega \left(N h^{n(2+3\tilde{\rho})+4} \epsilon^{(5/2)n+4} / |t|^8 \right) \right).$$

Step 5. — In order to bound the rate (6.16) corresponding to the perturbed quantized propagator, we note that $\Omega_{\lambda,t,N}^*(\underline{K}_{\tilde{\psi}}^{(\varepsilon)} h^{\tilde{\rho}n}/4, \varepsilon, \epsilon, K_{\tilde{\psi}}^{(\varepsilon)} h^{-\tilde{\rho}n/2})$ is asymptotically dominated by

$$(6.22) \quad \gamma_{\lambda,N,v}^* \left(\delta \left(\epsilon^{n/2+1} / |t|^2 \right), \varepsilon; u \right) = \gamma_{\lambda,N} \left(\delta \left(\epsilon^{n/2+1} / |t|^2 \right) \varepsilon^{(1/2+v)}; u \right),$$

with $\delta = h^{\tilde{\rho}n}$ and $u = h^{-\tilde{\rho}n/2}$. Then, the dominating term gives

$$(6.16) \leq \exp \left(-\Omega \left(N h^{3\tilde{\rho}n} \epsilon^{3n/2+2} \varepsilon / |t|^4 \right) \varepsilon^{2v} \right)$$

and by Step 1,

$$v = \tilde{O} \left(N^{-1} \delta^{-2} \epsilon^{-3n/2-2} |t|^4 \right) = \tilde{O} \left(N^{-1} h^{-2\tilde{\rho}n} \epsilon^{-(3n/2+2)} |t|^4 \right).$$

Since we have assumed $\varepsilon \in \Theta(h^{1+\alpha+\beta})$ with $\beta \geq 0$ and we a priori require that $h \gtrsim (|t|^4 / (N \epsilon^{3n/2+2}))^{\frac{1}{3\tilde{\rho}n}}$ in order to have exponential decay of the rate, if we further assume that $N \geq |t|^4 \epsilon^{-3n/2-2}$, then this implies $v = \tilde{O}(1)$ and in fact, on expanding the log factors we have $v \leq 1$. Hence, the asymptotic bound becomes

$$(6.16) \leq \exp \left(-\Omega \left(N h^{3\tilde{\rho}n} \epsilon^{3n/2+2} \varepsilon^3 / |t|^4 \right) \right).$$

Step 6. — The asymptotics of the rate in (6.21) are governed, as noted in Step 4, by $\Xi_{\lambda,N}(C_{\psi,\lambda,p,u}h^{n/2}, \psi_h)$, so the definition in Lemma 6.23 gives,

$$(6.21) = O\left(\Omega_{\lambda,t,N}^*\left(h^{(1+\tilde{\rho})\frac{n}{2}+1}, \varepsilon, \epsilon, h^{-\tilde{\rho}\frac{n}{2}}\right)\right).$$

Now proceeding as in Step 5 with $\delta = h^{n(1+\tilde{\rho})/2+1}$ and $u = h^{-\tilde{\rho}n/2}$ applied to the right-hand side of the equality in (6.22), we have

$$(6.21) \leq \exp\left(-\Omega\left(Nh^{n(1+2\tilde{\rho})+2}\epsilon^{3n/2+2}\varepsilon/|t|^4\right)\varepsilon^{2v}\right).$$

As in the previous step, if we take $N \geq |t|^4\epsilon^{-3n/2-2}$, then $v \leq 1$ so that $\varepsilon \cdot \varepsilon^{2v} \geq \varepsilon^3$. $\square$

Appendix A. Why not the Schrödinger propagator?

The Schrödinger propagator $e^{ith\Delta_{\mathcal{M}}/2}$ on $\mathcal{M}$ quantizes the (co-)geodesic flow at all speeds. This makes the propagation of coherent states under this flow an attractive option for recovering the geometry of $\mathcal{M}$ from samples and our results transfer directly to this application. However, we have opted to study the quantization of the *unit speed* flow with respect to an approximation of the half-wave propagator generated by $h\sqrt{\Delta_{\mathcal{M}}}$ due to numerical stability issues. These issues appear in practical applications, showing the half-wave propagator to give higher quality approximations from fewer samples for the unit speed flow. A thorough investigation of this phenomenon is out of the scope of this work, but we will show a simple example in the context of the inverse problem we have studied here and make some remarks (mainly speculations) as to the possible origins of this discrepancy.

We will consider Schrödinger propagation of coherent states on the flat torus $\mathbb{T}^n$ because many objects under consideration have explicit forms. Following [AM12], we consider the coherent state at $(x_0, \xi_0) \in T^*\mathbb{T}^n$ to be given by,

$$\psi_h(x; x_0, \xi_0) := \frac{1}{h^{n/4}} \sum_{k \in \mathbb{Z}^n} e^{-\frac{1}{2h}|x-k-x_0|^2} e^{\frac{i}{h}\xi_0 \cdot (x-k)},$$

so that under the action of the Schrödinger propagator $e^{ith\Delta_{\mathbb{T}^n}/2}$ we have,

$$(A.1) \quad e^{\pi ith\Delta_{\mathbb{T}^n}} \psi_h = \frac{1}{h^{n/4}(1+it)^{n/2}} \sum_{k \in \mathbb{Z}^n} e^{-\frac{|x-k-x_0-t\xi_0|^2}{2h(1+t^2)} + \frac{i}{2h}\phi(t, x-k; x_0, \xi_0)},$$

with $\phi(t, x; x_0, \xi_0) := t|x-x_0-t\xi_0|^2/(1+t^2) - t|\xi_0|^2 + 2\xi_0 \cdot x$. This is just the periodization of the solution to Schrödinger's equation in $\mathbb{R}^n$ at time t with the initial state given by the usual coherent state at (x_0, ξ_0) . Meanwhile, the Schwartz kernel $K_{\Delta_{\mathbb{T}^n}}^t$ for $e^{it\Delta_{\mathbb{T}^n}/2}$ has the expansion,

$$(A.2) \quad K_{\Delta_{\mathbb{T}^n}}^t(x, y) = \frac{1}{(2\pi)^n} \sum_{k \in \mathbb{Z}^n} e^{2\pi i k \cdot (x+tk/2)} e^{-2\pi i k \cdot y}.$$

The dispersiveness of the Schrödinger propagator is visible in this expression, for it shows that any solution to Schrödinger's equation is a superposition of plane waves traveling at all velocities $k/2$ for each $k \in \mathbb{Z}^n$ that gives a non-zero Fourier coefficient

of the initial condition. The form (A.1) for the propagation of the coherent state may be seen as the result of having *exact* Fourier coefficients, so that modulo $O_s(h^\infty)$, only waves with velocities in a $\sim \sqrt{h}$ neighbourhood of ξ_0/h are picked up by the propagator. On the other hand, if we replace exact Fourier coefficients by *noisy* data coming from an approximate integration of the initial condition against the plane wave $e^{-2\pi i k \cdot y}$, then there may easily be many more plane waves traveling at different speeds with amplitudes decaying relatively slowly in h that appear in the propagation. In lieu of the Poisson summation formula, the approximation to the Fourier coefficients by sums over even small perturbations of the lattice may cause significant error terms to appear [Eps05]. Closer to our setting, the case of Monte Carlo integration is governed by concentration inequalities rather than smoothness properties. Moreover, even when the eigenvalues of the graph Laplacian are close to those of $\Delta_{\mathbb{T}^n}$ in the semiclassical range, the corresponding eigenfunctions may have support across various frequencies, again leading to the interaction of waves of many different speeds. Compare this with the situation for the half-wave propagator, whose Schwartz kernel takes the form,

$$K_{\sqrt{\Delta_{\mathbb{T}^n}}}^t(x, y) = \frac{1}{(2\pi)^n} \sum_{k \in \mathbb{Z}^n} e^{2\pi i k \cdot (x + tk/|k|)} e^{-2\pi i k \cdot y}$$

and therefore *implicitly homogenizes* all plane waves to unit speed. Although in higher dimensions the approximate Fourier coefficients may still cause some *directional pollution*, any interference from different wave speeds will be homogenized away, making the unit speed flow a natural candidate for reconstruction from random samples.

Related to the wave speed homogenization is the appearance of the semiclassical parameter h in the Schrödinger propagator. In dimension $n = 1$, the expression (A.2) is given by the boundary distribution on $\mathbb{R}$ of a Jacobi theta function in t on the upper half of the complex plane. When $t = p/q \in \mathbb{Q}$ in reduced form, the Schwartz kernel is a linear combination of point masses at translations of q^{th} roots of unity and when $t \in \mathbb{R} \setminus \mathbb{Q}$, this distribution resides in a Besov space of higher regularity determined by the properties of the continued fraction expansion of t [KR99]. This *microlocal smoothing* is another effect of dispersion in the Schrödinger propagator [Mac11]. We may see $K_{\Delta_{\mathbb{T}^1}}^t(x, \cdot) = e^{it\Delta_{\mathbb{T}^1}}|\delta_x\rangle$ as the solution to the Schrödinger equation with initial condition δ_x , which has a wavefront set with singularities in all directions and magnitudes. In that sense, the propagated coherent state $e^{iht\Delta_{\mathbb{T}^1/2}}\psi_h(x) = \langle \psi_h | K_{\Delta_{\mathbb{T}^1}}^{ht}(x, \cdot) \rangle$ gives effectively the FBI transform at (x_0, ξ_0) of the Schwartz kernel for the Schrödinger propagator in the second component. Since the regularity of the distribution changes suddenly with time, the modulation by h causes sudden changes in the detection of frequency content in the range $\sim 1/h$. On the discrete side, ϵ must scale according to the connectivity of the graph given by $\sqrt{\epsilon}$ -balls across samples and only oscillations slow enough to be *felt* by neighbourhoods on this graph will be detected. As regularity affects what is detected by ψ_h at the frequency scale $1/h$, this suggests an instability in the discrete approximation using the Schrödinger propagator, with regards to the choices of the interdependent parameters h and ϵ .

A.1. Random samples

We now show a simple numerical example where the discrepancy between these propagators is readily felt: let $\mathbb{T}^1$ be embedded in $\mathbb{R}^2$ as

$$\iota: \mathbb{T}^1 \hookrightarrow S^1 := \{(\cos \theta, \sin \theta) \mid \theta \in [0, 2\pi)\}$$

and let $\mathcal{X}_N$ be N uniform random samples from S^1 . By the discussion in Section 3.1, the state

$$\tilde{\psi}_{h,\iota}(x; x_0, \xi_0) := e^{-\frac{1}{2h}|\iota(x)-\iota(x_0)|_{\mathbb{R}^2}^2} e^{\frac{i}{h}\langle \iota(x)-\iota(x_0), D_\iota|_{x_0}\xi_0 \rangle_{\mathbb{R}^2}}$$

is an un-normalized coherent state, wherein $D_\iota|_{x_0} : T_{x_0}\mathbb{T}^1 \rightarrow T_{\iota(x_0)}S^1$ the differential map of the embedding at x_0 . In this case, given x_0 , we can explicitly calculate the unit norm tangent vectors to S^1 at $\iota(x_0)$, hence we have *exact* coherent states $\psi_{h,\iota}(x; x_0, \pm 1) := \tilde{\psi}_{h,\iota}(x; x_0, \pm 1)/\|\tilde{\psi}_{h,\iota}\|_{L^2}$ at $(x_0, \pm 1) \in T^*\mathbb{T}^1$. Using the state localized at $(x_0, +1)$, the top row of Figure A.1 shows the errors in approximations of the unit-speed geodesic flow $\Gamma^t(x_0, \xi_0)$ using the Schrödinger and half-wave propagators, across a landscape of (ϵ, h) parameters. In the region where ϵ and h are sufficiently small to affect reasonable approximations, we see that the half-wave propagator has a baseline error that is more than quadratically lower than that given by the Schrödinger propagator. Likewise, the bottom row of Figure A.1 shows the errors in geodesic distance approximations using the time t of the quantum dynamics along the flow. Corresponding to this, we see in Figure A.2 the profile of the initial coherent state in the top figure and in the bottom row we observe the spread of its propagation at the final time, under the action of each of the two propagators.

A.2. Lattice points

The convergence analysis for dynamics on the pointset

$$\mathcal{X}_N = \left\{ \left(\cos(2\pi j/N), \sin(2\pi j/N) \right) \mid j \in \{0, \dots, N-1\} \right\} \subset S^1 \subset \mathbb{R}^2$$

is greatly facilitated by the Poisson summation formula. For simplicity, we set $\lambda = 0$ and denote $\Delta_{\epsilon,N} := \Delta_{0,\epsilon,N}$. Then, this graph Laplacian matrix is given by,

$$\Delta_{\epsilon,N} = \frac{2c_0}{c_2 \epsilon} \left(I - \frac{\mathcal{A}_{\epsilon,N}}{\sigma_{\epsilon,N,0}} \right),$$

wherein by the identity $(\cos^2 x + \cos^2 y) - (\sin^2 x + \sin^2 y) = 2 - 2 \cos(x - y)$ we have,

$$[\mathcal{A}_{\epsilon,N}]_{j,j'} = k \left(\frac{2}{\epsilon} \left[1 - \cos(2\pi(j-j')/N) \right] \right)$$

and $\sigma_{\epsilon,N,0} := [\mathcal{A}_{\epsilon,N}[1]]_1$. We recognize that $\mathcal{A}_{\epsilon,N}$ is a circulant matrix, hence it is diagonalized by the (unitary) discrete Fourier transform DFT_N . The sequence of eigenvalues $[\sigma_{\epsilon,N}] \in \mathbb{C}^N$ is defined by the action of the transform on the first row:

$$[\sigma_{\epsilon,N}] := \sqrt{N} \text{DFT}_N [\mathcal{A}_{\epsilon,N}]_{0,\cdot}.$$

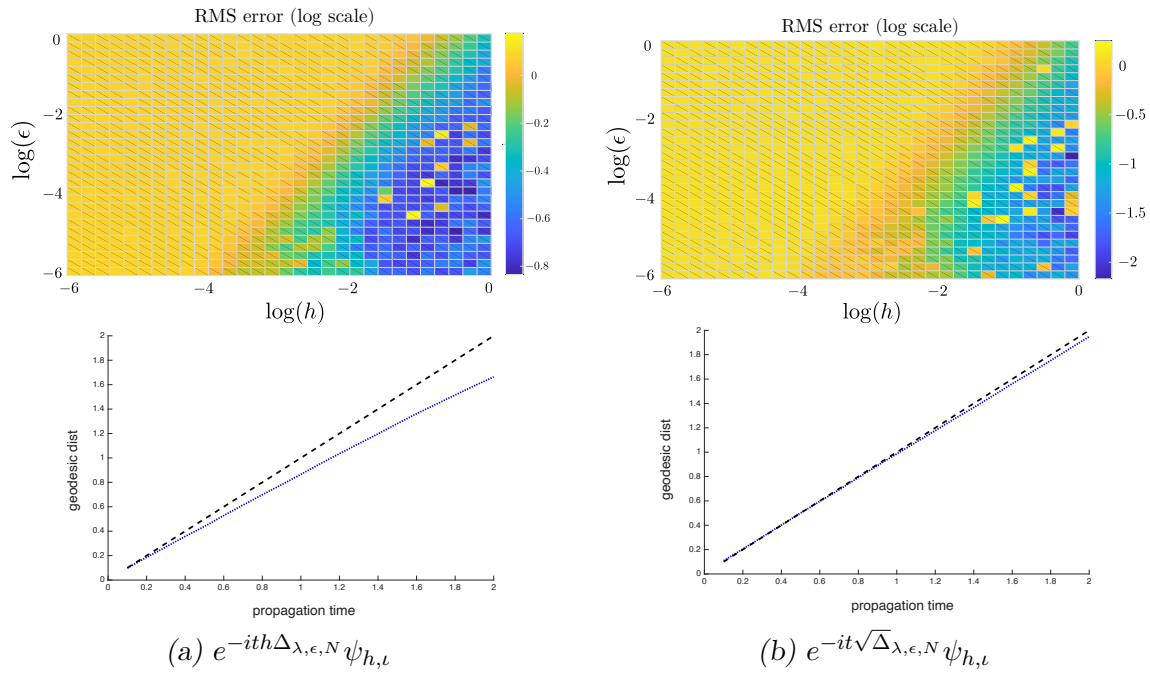


Figure A.1. Quality of propagation of the intrinsic coherent state $\hat{\psi}_{h,t}$ under the (a) Schrödinger and (b) half-wave propagators constructed from $N = 4000$ random samples on the unit circle in $\mathbb{R}^2$. The initial momenta of these states are fixed to $\xi_0 = +1$ by a simple tangent line computation. The basic strategy for quality testing is to compute the extrinsic mean coordinates of the propagated state at each of 20 time-steps in increments of $1/10$ units of time and compare the true distance of each mean to the initial point x_0 , with the corresponding time of the flow. The top row shows the log of the root mean square error from the true geodesic flow, across various combinations of ϵ and h values. For each pair of parameters, a new initial condition x_0 was chosen randomly from the sample set for the coherent state. The dotted lines in the bottom row are plots of time vs. recovered distances from the flows of coherent states, while the dashed lines show the ideal time vs distance lines.

Since the corresponding Schwartz kernel $\tilde{k}_\epsilon(\cdot) := \mathcal{A}_\epsilon(0, \cdot)$ for the averaging operator $\mathcal{A}_\epsilon$ is smooth and periodic, these eigenvalues rapidly approximate its scaled Fourier coefficients for $\sigma \in \{0, \dots, N-1\}$:

$$N\hat{\tilde{k}}_\epsilon(\sigma) = N \int_0^1 \tilde{k}_\epsilon(y) e^{-2\pi i \sigma y} dy.$$

Altogether, we have,

$$\Delta_{\epsilon,N} = \text{DFT}_N^* \text{diag} \left(\frac{2c_0}{c_2} \frac{[1] - [\sigma_{\epsilon,N}]/\sigma_{\epsilon,N,0}}{\epsilon} \right) \text{DFT}_N,$$

so in this case the eigenfunctions of $\Delta_{\epsilon,N}$ are just the restrictions of the eigenfunctions of $\Delta_{\mathbb{T}^1}$ on $\{j/N : j \in [0, N-1]\}$. The Poisson summation formula shows that for each $j \in \{0, \dots, N-1\}$, the eigenvalues satisfy $\sigma_{\epsilon,N,j} := [\sigma_{\epsilon,N}]_j = N\hat{\tilde{k}}_\epsilon(j) + O(N^{-\infty})$.

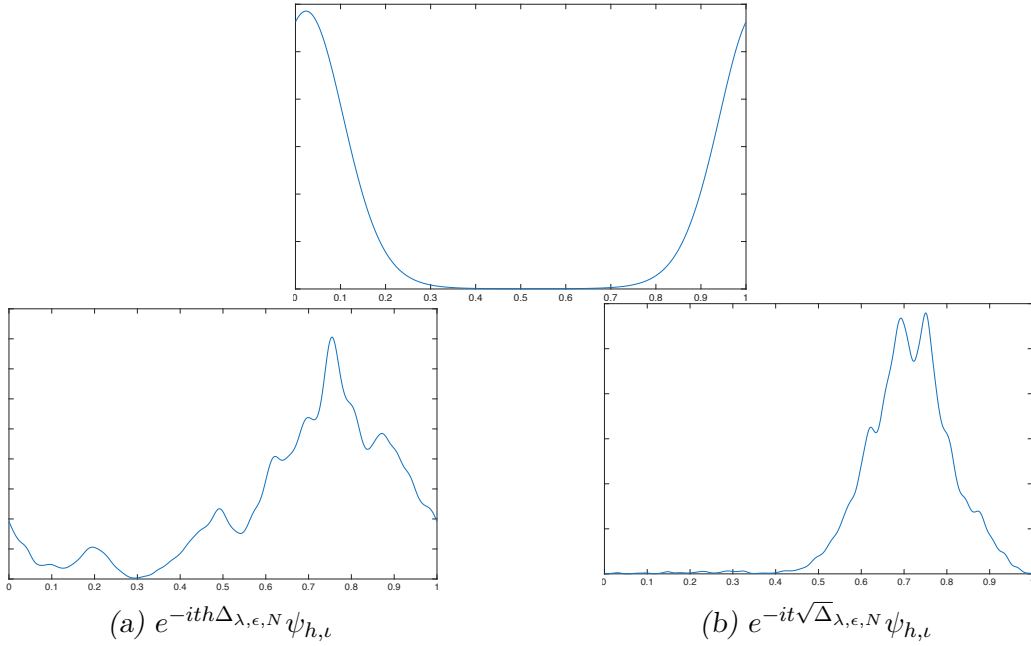


Figure A.2. Profile $|\psi_{h,t}|^2$ of the initial coherent state (top) used in the numerical experiment for the bottom row of Figure A.1. The bottom row shows the corresponding profiles of the propagated state under the (a) Schrödinger and (b) half-wave propagators; again, constructed from $N = 4000$ random samples on the unit circle in $\mathbb{R}^2$. The initial momenta of these states are fixed to $\xi_0 = +1$ by a simple tangent line computation. The final time is $t = 2.0$ and the initial state is fixed to be the angle $x_0 = 0.0235$.

Consequently, the discrete operators satisfy,

$$\|\Delta_{\epsilon,N} - \tilde{\Delta}_{\epsilon,N}\|_{\ell^2(\mathbb{C}^N) \rightarrow \ell^2(\mathbb{C}^N)} = O_{\ell^2 \rightarrow \ell^2}(N^{-\infty}),$$

wherein

$$\tilde{\Delta}_{\epsilon,N} := \text{DFT}_N^* \text{diag} \left(\frac{2c_0}{c_2} \frac{[1] - [\hat{k}_\epsilon(\cdot)]/\hat{k}_\epsilon(0)}{\epsilon} \right) \text{DFT}_N.$$

Then, taking a Taylor series expansion of $\cos(\cdot)$ along with that of the Fourier kernel, gives together with the evenness of $\tilde{k}_\epsilon$ that the eigenvalues $0 = \tilde{\sigma}_{\epsilon,0} < \tilde{\sigma}_{\epsilon,1} \leq \dots \leq \tilde{\sigma}_{\epsilon,N-1}$ of $\tilde{\Delta}_{\epsilon,N}$ follow $\tilde{\sigma}_{\epsilon,j} = j^2 + O(j^4\epsilon)$. Note that if we take $\sqrt{\epsilon} \ll h$ and suppose $|\xi_0| = O(1)$, then there is an $h_0 > 0$ such that for all $h \in (0, h_0]$ we have that if j_0 satisfies $|\tilde{\sigma}_{\epsilon,j_0} - \xi_0^2/h^2| \lesssim \sqrt{h}$, then

$$ht\tilde{\sigma}_{\epsilon,j_0} = htj_0^2 + O(t\xi_0^4\epsilon/h^3) = htj_0^2 + o(t/h).$$

Since the nearest eigenvalues to $[\xi_0^2/h^2 - \sqrt{h}, \xi_0^2/h^2 + \sqrt{h}]$ from the outside are at a distance $\Theta(1/h)$, we find that the application of a coherent state such as ψ_h or $\psi_{h,t}$ above, with this scaling of ϵ and h , localizes the action of $e^{ith\tilde{\Delta}_{\epsilon,N}}$ in frequency space to near ξ_0/h .

An application of the method of stationary phase along with the Poisson summation formula gives the localizations of the propagated states. When the coherent states oscillate at the frequency $h = 1/(2\pi N)$, there is a rapid localization in frequency space due to synchronisation with DFT_N . However, the requirement that $\sqrt{\epsilon} \ll h$ implies that this scaling of h is too strict: since $\sqrt{\epsilon}$ is the connectivity of the neighbourhood graph given by $\mathcal{A}_{\epsilon,N}$, a spacing below $1/N$ would mean that this matrix, along with $e^{iht\Delta_{\epsilon,N}}$, are both identities. This broader oscillation frequency for coherent states also means that the dispersive nature of Schrödinger dynamics allows waves at different speeds to rapidly develop in the propagation of the wavepacket, leading to a similar scenario as in Figures A.1 and A.2. Incidentally, we note in relation to the scaling of h that in order to apply the semiclassical quantizations of tori as in [CZ10, Vog20] to study the quantum-classical correspondence [BW23] in this setting, one must use a *rectangular* phase space that keeps the unit torus fixed in position and affords a larger width for the frequency space [BDB96].

Appendix B. Notation

We fix some general notation. Given a (complex) Hilbert space $\mathcal{H}$, $\langle \cdot | \cdot \rangle$ denotes its *complex* inner product that is anti-linear in the *first* component and we write the squared norm, $\|\cdot\|_{\mathcal{H}}^2 := \langle \cdot | \cdot \rangle$, which we often shorten to simply $\|\cdot\|^2$. Borrowing from physics, we use the following *Dirac notation*: if $A : \mathcal{H} \rightarrow \mathcal{H}$ is a linear operator and $\psi, \phi \in \mathcal{H}$ are vectors, then we identify $|\psi\rangle := \psi$ and $A|\psi\rangle \in \mathcal{H}$ denotes the application of A on ψ , while $\langle \phi |$ denotes the *dual* of $|\phi\rangle$ and we write, $\langle \phi | A | \psi \rangle := \langle \phi | A \psi \rangle$. The mathematically commonplace counterpart to this notation is denoted by $\langle \psi, \phi \rangle := \langle \phi | \psi \rangle$. In Section 3 we will also need a *bilinear* inner product that is a *complexification* of a real inner product: we denote this also by $\langle \cdot, \cdot \rangle$ and mark specifically that this is the form being used. Correspondingly, if M is a real symmetric matrix with $M > 0$, then we denote $\|\cdot\|_M^2 := \langle M \cdot, \cdot \rangle$. In the Euclidean case, we sometimes denote simply $|\cdot| := \|\cdot\|$, when the meaning is clear by context.

The operator A^* then denotes the adjoint to A with respect to the inner product on $\mathcal{H}$. Further, given $z \in \mathbb{C}$, we denote by $\Re z, \Im z$ its real and imaginary parts, respectively and when applied to $z = Z$ a bounded operator, these are the usual, $\Re Z := (Z + Z^*)/2$ and $\Im Z := (Z - Z^*)/(2i)$.

We have used various order notations: given some functions f_1, f_2 , we write $f_1 \sim f_2$ if there is some $c > 0$ such that $cf_1 \leq f_2 \leq f_1/c$ and we write $f_1 \lesssim f_2$ if $cf_1 \leq f_2$. Further, we have the asymptotic notations: for $N \geq 0$, we write $f = O_{L^2}(h^N)$ if there are constants $h_0 > 0$ and $C_N > 0$ such that for all $h \in (0, h_0]$, $\|f\|_{L^2} \leq C_N h^N$. Likewise, $f = O(h^N)$ means that $|f(h)| \leq C_N h^N$ and $f = O_s(h^N)$ means that for each α , there is a $C_{\alpha,N}$ such that $|\partial^\alpha f| \leq C_{\alpha,N} h^N$. When $N = \infty$ in these notations, we mean that these inequalities hold for all $N \geq 0$ with h_0 fixed.

At various times, we write $a \equiv b$ in different ways and hence, it is a blatant abuse of notation. Briefly, it means either that a, b belong to the same congruence class modulo some equivalence relation, or if a, b are functions then $a = b$ at all points on (a prescribed subset of) their domain of definition; the appropriate definition is clarified by the context.

B.1. Notation of fixed objects

Throughout this work, we have fixed a tuple $(\mathcal{M}, \iota, \Lambda, P)$ as per the Assumptions. These fixed objects and their relatives are denoted as follows:

Notation	Object
$\mathcal{M}$	manifold
g	Riemannian metric on $\mathcal{M}$
$d\nu_g(y)$	volume density on $\mathcal{M}$ with respect to the metric g
$n := \dim \mathcal{M}$	dimension of $\mathcal{M}$
Λ	Euclidean submanifold isometric to $\mathcal{M}$
D	dimension of ambient space of Λ
$\iota : \mathcal{M} \rightarrow \Lambda \subset \mathbb{R}^D$	isometry
P	sampling distribution with $\text{supp } P = \Lambda$
$p \in C^\infty(\mathcal{M})$	smooth density of $P \circ \iota^{-1}$ with respect to $d\nu_g$
$\Lambda_N = \{X_1, \dots, X_N\} \subset \Lambda$	set of N random vectors with law P
$\mathcal{X}_N = \{x_1, \dots, x_N\} \subset \mathcal{M}$	pull-back of Λ_N onto $\mathcal{M}$ by ι

B.2. Geometric notation

Generally, given a manifold $\mathcal{N}$ along with its metric g , we have used the following notation:

Notation	Meaning
$T^*\mathcal{N}$	cotangent bundle of $\mathcal{N}$
$dxd\xi$	short-hand for the measure induced by the canonical symplectic form on $T^*\mathcal{N}$
$ \xi _x, \xi _{g_x}$ (with $(x, \xi) \in T^*\mathcal{N}$)	norm of $\xi \in T_x^*\mathcal{N}$ according to the inner product given by g_x^{-1} on $T_x^*\mathcal{N}$
$\langle \zeta, \xi \rangle_x, \langle \zeta, \xi \rangle_{g_x}$ (with $(x, \xi), (x, \zeta) \in T^*\mathcal{N}$)	inner product between $\zeta, \xi \in T_x^*\mathcal{N}$ with respect to g_x^{-1}
$d_g(x, y)$	geodesic distance between the points $x, y \in \mathcal{N}$ w.r.t. g

Notation	Meaning
$\text{inj}(x), \text{inj}(\mathcal{N}) = \text{inj}(\mathcal{N}, g)$	injectivity radius at $x \in \mathcal{N}$ and its lower bound $\text{inj}(\mathcal{N}) := \inf_{x \in \mathcal{N}} \text{inj}(x)$, resp.
$s_{x_0} = \exp_{x_0}^{-1}$	normal coordinates at $x_0 \in \mathcal{N}$
$\gamma^*[dx]$	<i>pullback</i> of the density $\sqrt{\det g } dx_1 \wedge \cdots \wedge dx_n$ by the diffeomorphism $\gamma : \mathcal{N}_1 \rightarrow \mathcal{N}_2$ between manifolds $\mathcal{N}_1, \mathcal{N}_2$ of equal dimension
$ dv := \sqrt{\det g \circ u^{-1}(v) } dv$	the volume form in local coordinates $u : \mathcal{M} \supset U \rightarrow V \subset \mathbb{R}_v^n$
$B_r(x_0, g) = B(x_0, g; r)$	ball of radius r centered at $x_0 \in \mathcal{N}$ with respect to the metric g

B.3. Notation related to Ψ DOs

In Sections 2.3 and 2.4 we have introduced the following notation regarding pseudodifferential operators (Ψ DOs) and the FBI transform:

Notation	Meaning
$h^\ell S^m, h^\ell S_{\text{phg}}^m$	symbol classes of order (ℓ, m) and their polyhomogeneous subclasses, resp.
$h^\ell \Psi^m, h^\ell \Psi_{\text{phg}}^m$	classes of Ψ DOs of order (ℓ, m) and their subclasses of polyhomogeneous Ψ DOs, resp.
$\text{Op}_h(a)$	Ψ DO that is the (semiclassical) <i>right</i> (or <i>adjoint</i>) quantization of a symbol a
$T_h[u; \phi, a] = T[u; \phi/h, a]$	<i>FBI transform</i> of a smooth function u with <i>admissible phase</i> ϕ and symbol $a \in h^{-\frac{3n}{4}} S^{\frac{n}{4}}$
$b \in h^{\frac{3n}{2}} S^{-\frac{n}{2}}$	positive, elliptic symbol associated to T_h , depending on ϕ , such that the properties of $T_h[\cdot; \phi, b^{-\frac{1}{2}}]$ in Theorem 2.25 hold.

B.4. Notation related to graph Laplacians

In Section 2.2 we have introduced the following objects and notations related to the discrete and continuum graph Laplacian constructions:

Continuum / Discrete object	Name
$k : \mathbb{R}_+ \rightarrow \mathbb{R}_+$	kernel function
$p_\epsilon(x) := \int k_\epsilon(x, y)p(y)d\nu_g(g),$ $p_{\epsilon,N}(x) := \frac{1}{N} \sum_{j=1}^N k_\epsilon(x, y)$	degree functions
$k_{\lambda,\epsilon}(x, y) := k_\epsilon(x, y)/(p_\epsilon(x)p_\epsilon(y))^\lambda,$ $k_{\lambda,\epsilon,N}(x, y) := k_\epsilon(x, y)/(p_{\epsilon,N}(x)p_{\epsilon,N}(y))^\lambda$	sampling-dependent averaging kernels, or λ -averaging kernels
$\mathcal{A}_{\lambda,\epsilon} : u(\cdot) \mapsto \int k_{\lambda,\epsilon}(\cdot, y)u(y) d\nu_g(g),$ $(\mathcal{A}_{\lambda,\epsilon,N})_{j,m} := \frac{1}{N}k_{\lambda,\epsilon,N}(x_j, x_m)$	(sampling-dependent) λ -averaging operators
$p_{\lambda,\epsilon}(x) := \mathcal{A}_{\lambda,\epsilon}[1](x),$ $p_{\lambda,\epsilon,N}(x) := \mathcal{A}_{\lambda,\epsilon,N}[1](x)$	λ -degree functions
$A_{\lambda,\epsilon} : u(\cdot) \mapsto \mathcal{A}_{\lambda,\epsilon}[u]/p_{\lambda,\epsilon}(\cdot),$ $(A_{\lambda,\epsilon,N})_{j,m} := (\mathcal{A}_{\lambda,\epsilon,N})_{j,m}/p_{\lambda,\epsilon,N}(x_j)$	normalized λ -averaging operators
$\Delta_{\lambda,\epsilon} := \frac{2c_0}{c_2} \frac{1}{\epsilon}(I - A_{\lambda,\epsilon}),$ $\Delta_{\lambda,\epsilon,N} := \frac{2c_0}{c_2} \frac{1}{\epsilon}(I - A_{\lambda,\epsilon,N})$	(λ) -graph Laplacians

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