The Schrödinger propagator for scattering metrics

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Schrödinger equation for free particle:

$$\left(i^{-1}\partial_t + \frac{1}{2}\Delta\right)\psi = 0 \quad \psi\big|_{t=0} = \psi_0.$$

On curved space: $\Delta = \Delta_g = \nabla_g^* \nabla \geqslant 0$.

For example, on flat $\mathbb{R}^n$, the fundamental solution is

$$U(t, w, x) = (2\pi i t)^{-n/2} e^{i|x-w|^2/2t}.$$

- infinite speed of propagation
- lack of decay (unitarity)

Fix $t > 0, x$. Then

$$u(t, x, w) \text{ is smooth in } w, \text{ while}$$

$$u(0, x, w) = \delta(w - x) :$$

singularity disappears instantly.

Initial data $\psi_0 = e^{i(-\lambda x^2/2 + \xi\cdot x)}$: $\psi_0 \in \mathcal{C}^\infty$ but

$$\psi(t, w)|_{t=\lambda^{-1}} = C\delta(w + \xi/\lambda).$$

Singularity appears!

What happens on curved space?

Kapitanski-Safarov ('96):
If no trapped geodesics, $\psi_0 \in \mathcal{E}' \Longrightarrow$
$\boxed{\psi(t) \in \mathcal{C}^\infty \text{ for all } t > 0.}$

('98): Parametrix modulo $\mathcal{C}^\infty(\mathbb{R}^n)$, but no control at ∞.

Craig-Kappeler-Strauss ('95):
Regularity of the solution at all times, and in certain directions, under assumption of regularity of ψ_0 along all geodesics lying inside a given spatial cone near infinity.

Wunsch ('98):
Regularity along certain nontrapped geodesics at particular $t > 0$ described by "quadratic-scattering wavefront set" of ψ_0 :
specifies $\boxed{\text{Directions and times of singularities}}$
(location still mysterious).

Robbiano-Zuily ('02):
Analogue of Wunsch's result in analytic category.

Burq-Gérard-Tzvetkov ('01), Staffilani-Tataru ('02):
Strichartz estimates.

Flat $\mathbb{R}^n$ with a *potential* perturbation: various parametrix constructions: Fujiwara (1980), Zelditch (1983), Treves (1995), Yajima (1996),...

Contrast with well-developed theory for *wave equation.* Consider

$$(\partial_t - i\sqrt{\Delta})u = 0, \quad u(0) = u_0$$

on a compact, boundaryless Riemannian manifold M. Solution is $u(t) = e^{it\sqrt{\Delta}}u_0$. Let Φ_t be geodesic flow on S^*X at time t.

Theorem (Hörmander)

1. $e^{it\sqrt{\Delta}}$ is a *Fourier integral operator* which quantizes the contact transformation Φ_t.

2. $(x, \hat{\xi}) \in \mathrm{WF}u_0$ iff $\Phi_t(x, \hat{\xi}) \in \mathrm{WF}u(t)$.

- Φ_t is a contact transformation of the contact manifold S^*X with contact one-form $\hat{\xi}\, dx$.
- Singularities travel with unit speed along geodesics, and are neither created nor destroyed (time reversibility).
- Statement 2 follows immediately from statement 1.

Back to Schrödinger

Goal: construct parametrix, describe regularity of $\psi(t)$.

Specific questions:

(1) When and where can singularities appear in $\psi(t)$? (Describe in terms of initial data.)

(2) Where do singularities of initial data in $\mathcal{E}'$ disappear to?

(3) What is the structure of the fundamental solution with initial pole at x?

Questions (1) and (2) are dual. A strong enough answer to (3) will address both.

General geometric setup: (X, g) a Riemannian manifold with ends that look asymptotically like the large ends of cones $(1, \infty) \times Y$: (= 'manifold with scattering metric' as defined by Melrose):

$$g = dr^2 + r^2 h(r^{-1}, y, dy)$$

$$h \in \mathcal{C}^\infty,\ h_0 \equiv h(0, y, dy) \text{ a metric on } Y.$$

Key example: X = asymptotically Euclidian space; $r = |x|, y = \theta = x/|x| \in S^{n-1}$:

$$g = (1 + \frac{2m}{r}) dr^2 + r^2 d\theta^2 + O(r^{-2})(dr, r d\theta),\ r \to \infty$$

(*We stick with this example for remainder of talk.*)

Crucial geometric assumption:

$$\boxed{\text{no trapped geodesics}}$$

(Or, stay microlocally away from trapping region.)

Hamiltonian:

$$H \equiv \frac{1}{2}\Delta_g + V(x)$$

with $V(x) \in \mathcal{C}^\infty(\mathbb{R}^n;\mathbb{R})$ having asymptotic expansion:

$$\begin{aligned} V(x) &\sim \frac{c}{r} + r^{-2}V_{-2}(\theta) + r^{-3}V_{-3}(\theta) + \dots \\ &\in r^{-1}\mathcal{C}^\infty(r^{-1},\theta), \text{ for } r \geqslant r_0 > 0. \end{aligned}$$

- Newtonian gravity (the $1/r$ term in the potential) and Einsteinian gravity (the dr/r term in the metric) are both OK.

Schrödinger equation now reads

$$\boxed{(i^{-1}\partial_t + H)\psi = 0.}$$

and we are interested in the kernel of the fundamental solution, e^{-itH}.

Re-examine *Euclidean* fundamental solution (with $V = 0$):

Let $r = |w|$, $\theta = w/|w|$. Then

$$e^{-itH}\delta_x = (2\pi it)^{-n/2}e^{i|x-w|^2/2t}$$
$$= e^{ir^2/2t}\left(ae^{-i(rx\cdot\theta-|x|^2/2)/t}\right)$$

with $a = (2\pi t)^{-n/2}$.

We start at $t = 0$ with δ_x. Study later behavior of solution in r, θ variables ($x, t > 0$, fixed):

- The $e^{ir^2/2t}$ term is independent of x: loses all information about location of initial singularity.
- The $e^{-i(rx\cdot\theta-|x|^2/2)/t}$ term retains information about location of initial pole in its oscillation as $r \to \infty$.
- The time t appears in the phases in a very simple way.

Use this form as ansatz in more general geometric setting: divide by the explicit quadratic oscillatory factor $e^{ir^2/2t}$ and try to construct the resulting kernel, which is hopefully only *linearly* oscillatory.

Theorem. Let $\chi \in C_c^\infty(\mathbb{R}^n)$. The fundamental solution is of the form

$$e^{-itH}\chi = e^{ir^2/2t} W_t \chi,$$

where the kernel of W_t is a *scattering fibered Legendrian* (Melrose-Zworski, H.-Vasy).

- Inserting the function χ means that we only consider the asymptotics as $|w| \to \infty$, keeping x in a fixed (but arbitrary) compact set.

On $\mathbb{R}_t \times \mathbb{R}^n_{r,\theta} \times \mathbb{R}^n_x$, W is a finite sum of terms of the form

(0.1)

$$t^{-\frac{n}{2}-\frac{k}{2}} \int\limits_{U \Subset \mathbb{R}^k} a(t, r^{-1}, \theta, x, v) e^{i\phi(r^{-1}, \theta, x, v) r/t} \, dv.$$

We can state a slightly weaker version of the theorem more easily by composing with the Fourier transform $\mathcal{F}$:

Let $W_t = e^{-ir^2/2t}e^{-itH}$ for *fixed* $t > 0$. Then

$$\boxed{\mathcal{F} \circ W_t \text{ is a Fourier integral operator.}}$$

To analyze W_t further we recall the definition of the scattering wavefront set, which in $\mathbb{R}^n$ can be specified in terms of the usual wavefront set and the Fourier transform.

Let S^{n-1}_∞ denote the "sphere at infinity" of our asymptotically Euclidian space.

Can identify

$$S^*\mathbb{R}^n \equiv \mathbb{R}^n \times S^{n-1},$$

$$T^*_{S^{n-1}_\infty}\mathbb{R}^n \equiv S^{n-1} \times \mathbb{R}^n.$$

Hence exchanging coordinates

$$(\theta, \zeta) \to (\zeta, \theta)$$

gives diffeomorphism between these spaces (and gives $T^*_{S^{n-1}_\infty}\mathbb{R}^n$ a contact structure).

Definition. The *scattering wavefront set* of a distribution u is the subset of $T^*_{S^{n-1}_\infty}\mathbb{R}^n$ defined by

$$(\theta, \zeta) \in \mathrm{WF}_{sc}(u) \text{ iff } (\zeta, \theta) \in \mathrm{WF}(\mathcal{F}u).$$

(Definition originates with Melrose in more general setting (scattering metrics).)

WF_{sc} measures linear oscillation near infinity. For example, let $u(x) = e^{i\alpha\cdot x}$. Then

$$\mathrm{WF}_{sc}u = \{(\theta, \alpha) : \theta \in S^{n-1}_\infty\}.$$

Hence $e^{-ir^2/2t}e^{-itH}$ is a “scattering FIO” interchanging scattering wavefront set and ordinary wavefront set.

QUESTION: *what is the canonical relation of* $W_t = e^{-ir^2/2t} e^{-itH}$ *?*

Let $(x, \hat{\xi}) \in S^*\mathbb{R}^n$. Let $\gamma(t)$ be geodesic with

$$\gamma(0) = x, \quad \gamma'(0) = \hat{\xi}.$$

Define $\Phi : S^*\mathbb{R}^n \longrightarrow T^*_{S^{n-1}_\infty}\mathbb{R}^n$ by

$$\Phi(x, \hat{\xi}) = (\theta, \lambda\theta + \mu) \text{ with } \mu \perp \theta$$

given by

$$\theta = \lim_{t\to\infty} \frac{\gamma(t)}{|\gamma(t)|} \in S^{n-1}_\infty$$
$$\lambda = \lim_{t\to\infty} t - |\gamma(t)|$$
$$\mu = \lim_{t\to\infty} |\gamma| \left(\frac{\gamma(t)}{|\gamma(t)|} - \theta \right)$$

Thus

- θ is asymptotic direction;
- λ is "sojourn time" (cf. Guillemin) that a particle spends in finite region before heading out to ∞ (finite by assumption);
- μ measures angle of approach to S^{n-1}_∞.

Proposition. Φ is a *contact transformation* from $S^*\mathbb{R}^n$ to $T^*_{S^{n-1}_\infty}\mathbb{R}^n$.

THE CANONICAL RELATION FOR W:

The canonical relation parametrized by $W_t = e^{-ir^2/2t}e^{-itH}$ is $t^{-1}\Phi$

(scaling acts in fiber variable).

SPECIAL CASE: $x \in \mathbb{R}^n$, $\theta \in S^{n-1}_\infty$, and there exists a *unique geodesic* $\gamma(t)$ *from* x *to* θ (non-degenerate case). Then locally

$$W = ae^{irS(x,\theta)/t}$$

(no integral required), where

$$S(x,\theta) = \lim_{t\to\infty} t - |\gamma(t)|.$$

"*sojourn time.*"

EUCLIDEAN EXAMPLE once more:

$$e^{-ir^2/2t}e^{-itH}\delta_x = ae^{i(-x\cdot\theta+O(r^{-1}))r/t}.$$

Sojourn time in $\mathbb{R}^n$ for line through x in direction θ :

$$S(x,\theta) = \lim t - |x + t\theta| = -x \cdot \theta,$$

as appears in phase!

Egorov Theorem. Let A be a properly supported, zeroth order pseudo on $\mathbb{R}^n$. Then

$$\tilde{A} = W_t A W_t^*$$

is a zeroth order scattering pseudodifferential operator, and

$$\sigma_{sc}(\tilde{A})(\Phi(q)) = \sigma(A)(q).$$

Propagation Theorem. Let $\psi(t) = e^{-itH}\psi_0$. Fix a $t \neq 0$. Then

$$(x, \hat{\xi}) \in \mathrm{WF}\psi(t)$$

iff

$$-\frac{1}{t}\Phi(x, -\hat{\xi}) \in \mathrm{WF}_{sc}(e^{ir^2/2t}\psi_0).$$

Thus, we have a characterization of the singularities at nonzero time t in terms of the asymptotic behaviour of the initial data. Previous propagation results are immediate consequences.

Some words on the proof

A parametrix for e^{-itH} is constructed as a Legendrian distribution, starting at the diagonal near $t = 0$. Here it takes the form

$$U(w, x, t) = e^{i\Psi(w,x)/t} a(t, w, x), \quad a \text{ smooth},$$

with $\Psi(w, x)$ equal to $d(w, x)^2/2$. The function Ψ determines a Legendrian submanifold of $T^*\mathbb{R}^n \times T^*\mathbb{R}^n \times \mathbb{R}$, namely

$$L = \{(w, \zeta, x, \xi, \tau) \mid \zeta = d_w\Psi, \xi = d_x\Psi, \tau = \Psi\}$$

which is Legendrian with respect to the contact form $\zeta \cdot dw + \xi \cdot dx - d\tau$. This Legendrian becomes non-projectable outside the injectivity radius, meaning (w, x) are no longer coordinates on it, but it remains perfectly smooth. It may be defined by

$$(w, \zeta) = \exp_{sg/2}(x, \xi), \tau = s^2/2, \quad s \in (0, \infty).$$

We investigate the behaviour of L as $s \to \infty$. We see that $|\zeta|$ and $|\xi|$ grow linearly, and τ quadratically, as $s \to \infty$. Moreover, the form of the metric is such that $r = |w| \sim s$ as $s \to \infty$, provided the metric is nontrapping. So it makes sense to introduce scaled variables

$$\overline{\zeta} = \rho\zeta,\ \overline{\xi} = \rho\xi,\ \kappa = \rho^2\tau,$$

where $\rho \equiv r^{-1} \to 0$. We also write

$$\overline{\zeta} = \overline{\nu}\hat{w} + \overline{\mu} \ \text{ where } \ \overline{\mu} \perp \hat{w}.$$

If we do this, then we find that along every geodesic,

$$\overline{\nu} \to -1,\ \overline{\mu} \to 0,\ \kappa \to -1/2,\ \overline{\xi} \to \xi_0,$$

so the submanifold L is 'bounded' in terms of this scaling.

However, although bounded, L isn't smooth at $\rho = 0$; instead it has a conic singularity there. But this can be resolved by blowing up the set

$$\{\rho = 0, \overline{\nu} = -1, \overline{\mu} = 0\}.$$

This blowup desingularizes the submanifold L, which now meets the boundary of the blown-up space transversally. Moreover, the boundary of the blown-up space is a copy of $T^*_{S^{n-1}_\infty}\mathbb{R}^n$. So, we can start at any initial point $(x, \hat{\xi})$ and travel along the corresponding geodesic, eventually arriving at a point on the blown-up face which can identified with a point of $T^*_{S^{n-1}_\infty}\mathbb{R}^n$. This, by definition, is $\Phi((x, \hat{\xi}))$. Moreover, the symplectic nature of the construction implies that Φ is a contact transformation. The fact that Φ is contact in turn allows the application of the theory of Legendre distributions on manifolds with corners.

The operation of blowing up

$$\{\rho = 0, \overline{\nu} = -1, \overline{\mu} = 0\}$$

is the exact geometric analogue of removing the factor $e^{ir^2/2t}$ from the propagator. The boundary face created by blowup is 'one order better in ρ', and corresponds analytically to linear, rather than quadratic, oscillations. Indeed, parametrizing the submanifold L near the blowup gives us the phase function ϕ is in (0.1). The theory of fibred Legendre distributions then tells us that ϕ is independent of t (as in the free case) and gives us the very simple behaviour in t of singularity propagation for e^{-itH}.