FIO with quadratic complex phase, a mathematical justification of the semiclassical Herman-Kluk propagator

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collaboration with Torben SWART

- Semiclassical time-dependent Schrödinger equation

$$i\varepsilon\frac{\partial}{\partial t}\psi^\varepsilon = H^\varepsilon\psi^\varepsilon, \qquad \psi^\varepsilon(0) = \psi_0^\varepsilon \in L^2(\mathbb{R}^d;\mathbb{C})$$

$H^\varepsilon = Op^\varepsilon_{\text{Weyl}} h$ with $h(x,\xi)$ symbol in $\mathcal{C}^\infty(\mathbb{R}^{2d};\mathbb{C})$

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$$g^\varepsilon_{q,p}(x) = \frac{1}{(\pi\varepsilon)^{d/4}} e^{\frac{i}{\varepsilon}p.(x-q)} e^{-\frac{|x-q|^2}{2\varepsilon}}$$

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Overcomplete basis of $L^2(\mathbb{R}^d;\mathbb{C})$

$$\mathrm{Id}_{L^2} = \frac{1}{(2\pi\varepsilon)^d}\iint \left| g^\varepsilon_{q,p}\right\rangle \left\langle g^\varepsilon_{q,p}\right| \mathrm{d}q\mathrm{d}p$$

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Semiclassical propagation of Gaussian coherent states

(Hagedorn '80)

$$e^{\frac{i}{\varepsilon}tH^\varepsilon} g^\varepsilon_{q,p} = e^{\frac{i}{\varepsilon}S^{\kappa^t}(q,p)} \tilde{g}^\varepsilon_{\kappa^t(q,p)} + O(\varepsilon)$$

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- $\kappa^t = (X^{\kappa^t}, \Xi^{\kappa^t})$ given by Hamilton equation of motion in phase-space

$$\frac{\mathrm{d}}{\mathrm{d}t}\kappa^t = \begin{pmatrix} 0 & \mathrm{I} \\ -\mathrm{I} & 0 \end{pmatrix} \nabla_{(x,\xi)} h \circ \kappa^t, \qquad \kappa^0 = \mathrm{Id}$$

- S^{κ^t} classical action of motion

$$S^{\kappa^t}(q,p) = \int_0^t \left[\frac{\mathrm{d}}{\mathrm{d}t} X^{\kappa^\tau}(q,p).\Xi^{\kappa^\tau}(q,p) - h \circ \kappa^\tau(q,p)\right] \mathrm{d}\tau$$

Semiclassical approximation of the unitary propagator

- Thawed Gaussian Approximation *(Heller '75)*

$$U^{\varepsilon}_{\mathrm{TGA}}(t) = \frac{1}{(2\pi\varepsilon)^d} \iint \left| e^{\frac{i}{\varepsilon} S^{\kappa^t}(q,p)} \tilde{g}^{\varepsilon}_{\kappa^t(q,p)} \right\rangle \left\langle g^{\varepsilon}_{q,p} \right| \mathrm{d}q\mathrm{d}p$$

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- Herman-Kluk Propagator *(Herman and Kluk '84)*

$$U^{\varepsilon}_{\mathrm{HK}}(t) = \frac{1}{(2\pi\varepsilon)^d} \iint u^t(q,p) \left| e^{\frac{i}{\varepsilon} S^{\kappa^t}(q,p)} g^{\varepsilon}_{\kappa^t(q,p)} \right\rangle \left\langle g^{\varepsilon}_{q,p} \right| \mathrm{d}q \mathrm{d}p$$

Main result *(Swart R. '07)*

Assume that $h(x,\xi)$ is subquadratic *i.e.*

$$\|\partial^\alpha_{(x,\xi)} h\|_\infty < \infty, \qquad |\alpha| \geqslant 2$$

then, for $-T \leqslant t \leqslant T$,

$$\left\| e^{\frac{i}{\varepsilon} t H^\varepsilon} - U^\varepsilon_{\mathrm{HK}}(t) \right\|_{L^2 \to L^2} = O(\varepsilon^{N+1}|t|)$$

$$u^t_{HK}(q,p) = u^t_0(q,p) + \varepsilon u^t_1(q,p) + \cdots + \varepsilon^N u^t_N(q,p)$$

where u^t_k are solutions of transport equations with initial conditions

$$u^0_0 = 1, \qquad u^0_k = 0 \quad (1 \leqslant k \leqslant N)$$

Semiclassical FIO with complex quadratic phase associated to a canonical transformation

$$[I^\varepsilon(\kappa;u)\varphi](x) = \frac{2^{d/2}}{(2\pi\varepsilon)^{3d/2}} \iiint e^{\frac{i}{\varepsilon}\Phi^\kappa(x,y,q,p)} u(q,p)\varphi(y)\mathrm{d}y\mathrm{d}q\mathrm{d}p$$

with $$\Phi^\kappa(x,y,q,p) = S^\kappa + \Xi^\kappa.(x-X^\kappa) - p.(y-q) + \frac{i}{2}|x-X^\kappa|^2 + \frac{i}{2}|y-q|^2$$

$$\partial_q S^\kappa = -p + (\partial_q X^\kappa)\Xi^\kappa, \qquad \partial_p S^\kappa = (\partial_p X^\kappa)\Xi^\kappa$$

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for symbol u, $\quad I^\varepsilon(\kappa;u) : \mathcal{S}(\mathbb{R}^d;\mathbb{C}) \to \mathcal{S}(\mathbb{R}^d;\mathbb{C})$

Sketch of the proof

$$\left[i\varepsilon\frac{\partial}{\partial t} - H^\varepsilon\right] I^\varepsilon\left(\kappa^t; \sum_{k=0}^{N} \varepsilon^k u_k^t\right) =$$

$$I^\varepsilon\left(\kappa^t; \sum_{k=0}^{N} \varepsilon^k v_k^t + \varepsilon^{N+1} v_{[N+1,}^{t,\varepsilon}\right)$$

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as consequence of composition theorems *(Swart R. '07)*

$$[Op^\varepsilon_{\mathrm{Weyl}}h]\circ I^\varepsilon(\kappa; u) = I^\varepsilon\left(\kappa; \sum_{k=0}^{N}\varepsilon^k v_k + \varepsilon^{N+1} v^\varepsilon_{[N+1,}\right)$$

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where $v_0(q,p) = (h \circ \kappa)u$, $v_1 = \ldots$

$\ldots$ and $v^{\varepsilon}_{[N+1,}(x, y, q, p)$

- "eikonal" equation

$$v_0^t = \left[-\frac{\mathrm{d}}{\mathrm{d}t} S^{\kappa^t} + \frac{\mathrm{d}}{\mathrm{d}t} X^{\kappa^t} . \Xi^{\kappa^t} + h \circ \kappa^t \right] u_0^t$$

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- transport equations

$$v_1^t = i \frac{\mathrm{d}}{\mathrm{d}t} u_0^t - \frac{i}{2} \mathrm{Tr} \left[\left(\mathcal{Z}^{\kappa^t} \right)^{-1} \frac{\mathrm{d}}{\mathrm{d}t} \mathcal{Z}^{\kappa^t} \right] u_0^t$$

$$\mathcal{Z}^{\kappa^t} := (\partial_p + i \partial_q)(\Xi^{\kappa^t} - i X^{\kappa^t})$$

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$$v_{k+1}^t = i \frac{\mathrm{d}}{\mathrm{d}t} u_k^t - \frac{i}{2} \mathrm{Tr} \left[\left(\mathcal{Z}^{\kappa^t} \right)^{-1} \frac{\mathrm{d}}{\mathrm{d}t} \mathcal{Z}^{\kappa^t} \right] u_k^t + L_k^t(u_0^t, \ldots, u_{k-1}^t)$$

Final step of the proof

$$\left[i\varepsilon \frac{\partial}{\partial t} - H^\varepsilon \right] I^\varepsilon \left(\kappa^t; \sum_{k=0}^{N} \varepsilon^k u_k^t \right) = \varepsilon^{N+1} I^\varepsilon(\kappa^t; v^{t,\varepsilon}_{[N+1,})$$

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We combine Gronwall's lemma with
L^2-boundedness theorems *(Swart R. '07)*

$$\| I^\varepsilon(\kappa; u) \|_{L^2 \to L^2} \leqslant C \sum_{|\alpha| \leqslant 2d+1} \| \partial^\alpha_{(x,y)} u(x,y,q,p) \|_\infty$$