

Asymptotics of Wigner functions at high frequency and near caustics

EVANGELIA KALLIGIANNAKI^{(1),(3)} & GEORGE N. MAKRAKIS^{(2),(3)}

⁽¹⁾ Department of Mathematics, University of Crete

⁽²⁾ Department of Applied Mathematics, University of Crete

⁽³⁾ Institute of Applied & Computational Mathematics, FORTH, Crete
Greece

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ABSTRACT

Eigenfunction expansions of time-dependent Wigner functions are employed to motivate asymptotic expansions at high frequencies and near space-time caustics for the semiclassical Schrödinger equation with simple polynomial potentials and WKB initial data.

1 Schrödinger equation

Consider the semiclassical Schrödinger equation

$$i\varepsilon \frac{\partial \psi^\varepsilon}{\partial t} = \left(-\frac{\varepsilon^2}{2} \Delta + V(x) \right) \psi^\varepsilon(x, t), \quad x \in \mathbb{R}, t > 0$$

with oscillatory (WKB) initial data

$$\psi^\varepsilon(x, 0) = \psi_0^\varepsilon(x) = a_0(x) e^{iS_0(x)/\varepsilon}$$

Hypotheses for the potential :

$$\begin{aligned} &V(x) \text{ is analytic} \\ &\lim_{|x| \rightarrow \infty} V(x) = +\infty, \quad V \in C(\mathbb{R}) \\ &V \geq 0, \text{ for some } R > 0 \quad \inf_{|x| > R} V(x) > 0 \\ &V(0) = 0, V'(0) = 0 \quad \text{such that } V''(0) > 0 \\ &V \text{ is polynomially bounded } |V(x)| \leq c(1 + |x|^m) \text{ (or at least grows as fast as } e^{\beta x^2}) \end{aligned}$$

2 Phase space reformulation

Wigner function in phase space [Wigner, 1932]

$$W^\varepsilon(x, k, t) = W^\varepsilon[\psi^\varepsilon](x, k, t) = \frac{1}{\pi\varepsilon} \int_{\mathbb{R}} e^{-\frac{i}{2} 2k\xi} \psi^\varepsilon(x - \xi, t) \overline{\psi^\varepsilon}(x + \xi, t) d\xi$$

Wigner equation for the evolution of W^ε

$$\begin{cases} \frac{\partial}{\partial t} W^\varepsilon(x, k, t) + \mathcal{L}^\varepsilon W^\varepsilon(x, k, t) = 0, (x, k) \in \mathbb{R}^2, t > 0 \\ W^\varepsilon(x, k, t)|_{t=0} = W_0^\varepsilon(x, k) = W^\varepsilon[\psi_0^\varepsilon](x, k) \\ \mathcal{L}^\varepsilon \equiv k \frac{\partial}{\partial x} - V'(x) \frac{\partial}{\partial k} - \sum_{j=1}^{\infty} \varepsilon^{2j} \left(\frac{i}{2} \right)^{2j} \frac{V^{(2j+1)}(x)}{(2j+1)!} \frac{\partial^{2j+1}}{\partial k^{2j+1}} \end{cases}$$

Remark: For $\varepsilon \rightarrow 0$ quantum Liouville operator \mathcal{L}^ε , formally reduces to the corresponding stationary classical Liouville operator $\mathcal{L}_c \equiv k \frac{\partial}{\partial x} - V'(x) \frac{\partial}{\partial k}$, corresponding to the Hamiltonian $H(x, k) = k^2/2 + V(x)$.

3 Eigenfunction expansion of the Wigner function

W^ε admits of the eigenfunction expansion

$$W^\varepsilon(x, k, t) = \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} A_{nm}^\varepsilon(t) \Phi_{nm}^\varepsilon(x, k)$$

where

$$\Phi_{nm}^\varepsilon(x, k) = W^\varepsilon[u_n^\varepsilon, u_m^\varepsilon](x, k) = \frac{1}{\pi\varepsilon} \int_{\mathbb{R}} e^{-\frac{i}{2} 2k\xi} u_n^\varepsilon(x - \xi) \overline{u_m^\varepsilon}(x + \xi) d\xi$$

are the Wigner transforms of Schrödinger eigenfunctions (Moyal eigenfunctions; [Moyal, 1949])

$$\left(-\frac{\varepsilon^2}{2} \Delta + V(x) \right) u_n^\varepsilon(x) = E_n^\varepsilon u_n^\varepsilon(x)$$

Remark 3.1: $\Phi_{nm}^\varepsilon(x, k)$ are defined by the system of both eigenvalue equations

$$\mathcal{L}^\varepsilon \Phi_{nm}^\varepsilon(x, k) = \frac{i}{\varepsilon} (E_n^\varepsilon - E_m^\varepsilon) \Phi_{nm}^\varepsilon(x, k)$$

$$\mathcal{M}^\varepsilon \Phi_{nm}^\varepsilon(x, k) = \frac{1}{2} (E_n^\varepsilon + E_m^\varepsilon) \Phi_{nm}^\varepsilon(x, k)$$

where

$$\mathcal{M}^\varepsilon = -\frac{\varepsilon^2}{8} \Delta_{xk} + H(x, k) + \sum_{j=1}^{\infty} \varepsilon^{2j} \left(\frac{i}{2} \right)^{2j} \frac{V^{(2j)}(x)}{(2j)!} \partial_k^{2j} + \frac{\varepsilon^2}{8} \partial_k^2$$

Remark 3.2: Employing asymptotics of Schrödinger eigenfunctions u_n^ε about the eigenfunctions of the corresponding harmonic oscillator (potential $V_H(x) = x^2/2$) [Simon, 1983], we derive formal asymptotic expansions of the Moyal eigenfunctions

$$\Phi_{nm}^\varepsilon(x, k) \sim \Psi_{nm}^\varepsilon(x, k) + \sum_{l=1}^{\infty} \varepsilon^{\frac{l}{2}} Z_{nm}^{\varepsilon, (l)}(x, k)$$

where

$$\Psi_{nm}^\varepsilon(x, k) = W^\varepsilon[\psi_n^\varepsilon, \psi_m^\varepsilon](x, k),$$

$\{\psi_n^\varepsilon(x)\}_{n=0,1,\dots}$ being the eigenfunctions of the corresponding harmonic oscillator.

4 Asymptotics of the Wigner functions

4.1 Near Wigner functions of the harmonic oscillator

The eigenfunction expansion of $W^\varepsilon(x, k, t)$ and the asymptotic approximation of $\Phi_{nm}^\varepsilon(x, k)$, lead to the ansatz:

$$W^\varepsilon(x, k, t) \sim W_H^\varepsilon(x, k, t) + \sum_{l=1}^{\infty} \varepsilon^{l/2} Z^{\varepsilon, (l)}(x, k, t)$$

where $W_H^\varepsilon(\mathcal{X}, \mathcal{K}, t)$ and $Z^{\varepsilon, (l)}(\mathcal{X}, \mathcal{K}, t)$ ($\mathcal{X} = \frac{x}{\sqrt{\varepsilon}}$, $\mathcal{K} = \frac{k}{\sqrt{\varepsilon}}$) are solutions of

$$\begin{cases} \frac{\partial}{\partial t} W_H^\varepsilon(\mathcal{X}, \mathcal{K}, t) + L_H W_H^\varepsilon(\mathcal{X}, \mathcal{K}, t) = 0 \\ W_H^\varepsilon(\mathcal{X}, \mathcal{K}, t)|_{t=0} = W_0^\varepsilon(\mathcal{X}, \mathcal{K}) \end{cases}$$

$$\begin{cases} \frac{\partial}{\partial t} Z^{\varepsilon, (l)}(\mathcal{X}, \mathcal{K}, t) + L_H Z^{\varepsilon, (l)}(\mathcal{X}, \mathcal{K}, t) = D^{(l)}(\mathcal{X}, \mathcal{K}, t), l \geq 1 \\ Z^{\varepsilon, (l)}(\mathcal{X}, \mathcal{K}, t)|_{t=0} = 0 \end{cases}$$

where

$$L_H = \mathcal{K} \frac{\partial}{\partial \mathcal{X}} - \mathcal{X} \frac{\partial}{\partial \mathcal{K}}$$

$$D^{(l)}(\mathcal{X}, \mathcal{K}, t) = -B_l(\mathcal{X}, \frac{\partial}{\partial \mathcal{K}}) W_H^\varepsilon(\mathcal{X}, \mathcal{K}, t) - \sum_{\nu=1}^{l-1} B_\nu(\mathcal{X}, \frac{\partial}{\partial \mathcal{K}}) Z^{\varepsilon, (l-\nu)}(\mathcal{X}, \mathcal{K}, t)$$

$$B_\nu(\mathcal{X}, \frac{\partial}{\partial \mathcal{K}}) = -V^{(\nu+2)}(0) \sum_{j=0}^{[(\nu-1)/2]+1} \left(\frac{i}{2} \right)^{2j} \frac{1}{(2j+1)!} \frac{\mathcal{X}^{\nu+1-2j}}{\partial \mathcal{K}^{2j+1}}, \quad \nu \geq 1$$

Remark 4.1: Then initial value problem for W_H^ε , involving classical Liouville operator $\partial/\partial t + L_H$ can be integrated applying the method of characteristics.

Important observation 4.2: Such an expansion, valid for small times, is not appropriate near caustics, since L_H fails, in general, to produce the correct Lagrangian manifold due to linearization of Hamiltonian flow.

4.2 Near solutions of classical Liouville equation

Observe that

$$\mathcal{L}^\varepsilon = \mathcal{L}_c - \sum_{j=1}^{\infty} \varepsilon^{2j} \Theta_j(x, \frac{\partial}{\partial k}) \rightarrow \mathcal{L}_c, \text{ as } \varepsilon \rightarrow 0,$$

where

$$\mathcal{L}_c \equiv k \frac{\partial}{\partial x} - V'(x) \frac{\partial}{\partial k} \quad (\text{classical Liouville operator})$$

$$\Theta_j(x, \frac{\partial}{\partial k}) \equiv \left(\frac{i}{2} \right)^{2j} \frac{V^{(2j+1)}(x)}{(2j+1)!} \frac{\partial^{2j+1}}{\partial k^{2j+1}}$$

Then, for small ε , a natural expansion which respects the evolution of the Lagrangian manifold has the form

$$W^\varepsilon(x, k, t) \sim W_c^\varepsilon(x, k, t) + \sum_{l=1}^{\infty} \varepsilon^{2l} Z_c^{\varepsilon, (l)}(x, k, t)$$

where

$$\begin{cases} \frac{\partial}{\partial t} W_c^\varepsilon(x, k, t) + \mathcal{L}_c W_c^\varepsilon(x, k, t) = 0 \\ W_c^\varepsilon(x, k, t)|_{t=0} = W_0^\varepsilon(x, k) \end{cases}$$

and

$$\begin{cases} \frac{\partial}{\partial t} Z_c^{\varepsilon, (l)}(x, k, t) + \mathcal{L}_c Z_c^{\varepsilon, (l)}(x, k, t) = \Theta^{(l)}(x, k, t) = \sum_{j=1}^l \Theta_j(x, \frac{\partial}{\partial k}) Z_c^{\varepsilon, (l-j)}(x, k, t), l \geq 1 \\ Z_c^{\varepsilon, (l)}(x, k, t)|_{t=0} = 0 \end{cases}$$

Remark 4.3: See [Steinruck, 1990] for non-oscillatory initial data $\psi_0^\varepsilon(x)$, and [Pulvirenti, 2006] for oscillatory $\psi_0^\varepsilon(x)$ using asymptotics of $W_0^\varepsilon(x, k)$ in terms of Dirac functions.

5 Caustics

For simple Gaussian-Fresnel initial wave function

$$\psi_0^\varepsilon(x) = e^{-\frac{x^2}{2\varepsilon}} e^{i\frac{x^2}{2\varepsilon}},$$

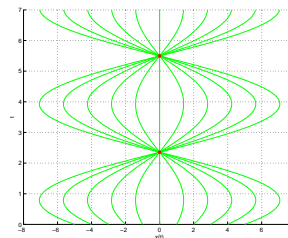
the initial Wigner function is Gaussian in phase space

$$W_0^\varepsilon(x, k) = \frac{1}{\sqrt{\pi\varepsilon}} e^{-x^2} e^{-\frac{(k-x)^2}{2\varepsilon}}$$

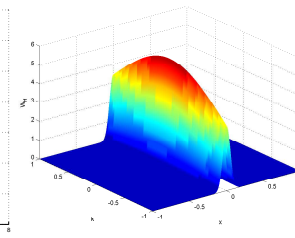
5.1 Harmonic Oscillator ($V_H(x) = \frac{x^2}{2}$). Focal points

Bicharacteristics $x(q, p, t) = q \cos(t) + p \sin(t)$, $k(q, p, t) = p \cos(t) - q \sin(t)$

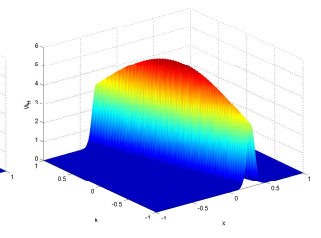
Focal points: $(x_\nu, t_\nu) = (0, \nu\pi - \frac{\pi}{4})$, $\nu = 1, 2, \dots$



Caustic & Rays



Harmonic Oscillator Wigner function (t=3π/4)

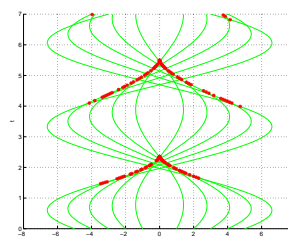


Harmonic Oscillator Wigner function (t=200)

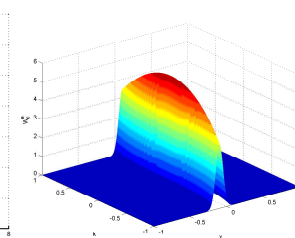
Amplitude computed approximately: $|\psi^\varepsilon(x, t)|^2 = \int_{\mathbb{R}} W^\varepsilon(x, k, t) dk \sim \int_{\mathbb{R}} W_H^\varepsilon(x, k, t) dk$

At the focal points: $|\psi^\varepsilon(x=0, t=t_\nu)| \sim 0(\varepsilon^{-1/2})$

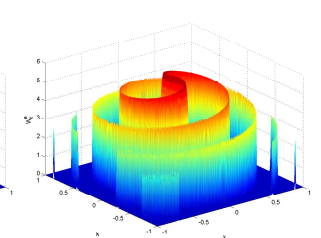
5.2 Quartic Oscillator ($V(x) = \frac{x^2}{2} + \mu \frac{x^4}{4}$, $\mu > 0$). Cusps



Caustic & Rays



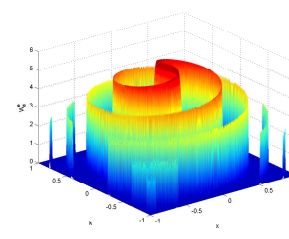
Wigner function (t=3π/4, μ=0.1)



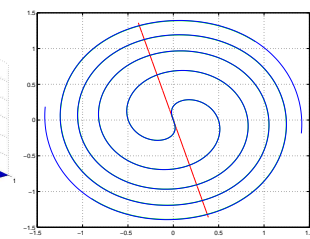
Wigner function (t=200, μ=0.1)

Approximate bicharacteristics via multiple scale asymptotics of the Hamiltonian system, for small μ .

Cusp points: $(x_\nu, t_\nu) = (0, \nu\pi - \frac{\pi}{4})$, $\nu = 1, 2, \dots$



Wigner function-Approximate bicharacteristics (t=200, μ=0.1)



Lagrangian manifolds (t=200, μ=0.1)

$|\psi^\varepsilon(x, t)|^2 \sim \int_{\mathbb{R}} W_a^\varepsilon(x, k, t) dk$

At the cusp points: $|\psi^\varepsilon(x=0, t=t_\nu)| \sim 0(\varepsilon^{-1/3})$

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