From generalized Gaussian wave packet dynamics to homoclinic orbits

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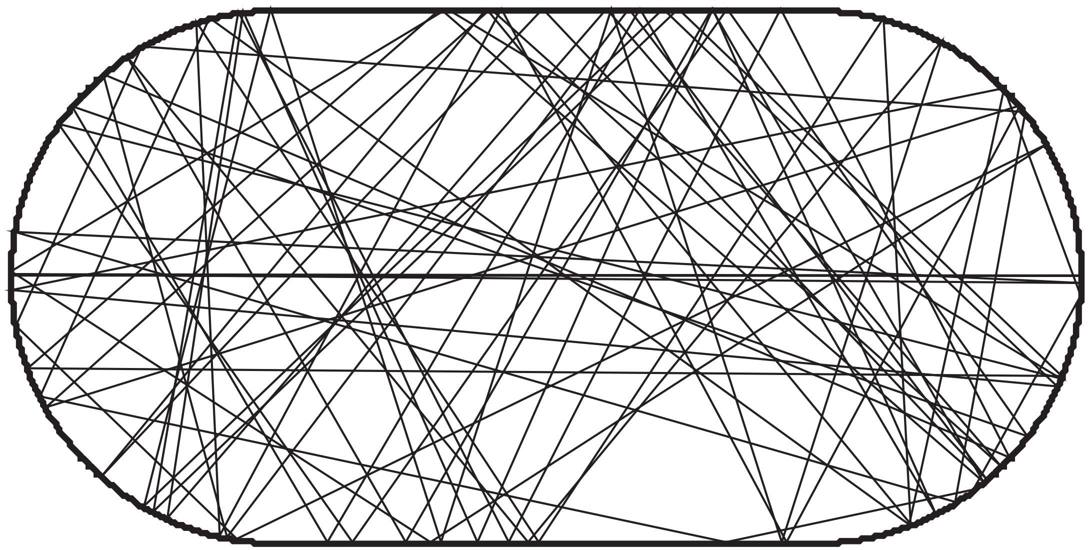
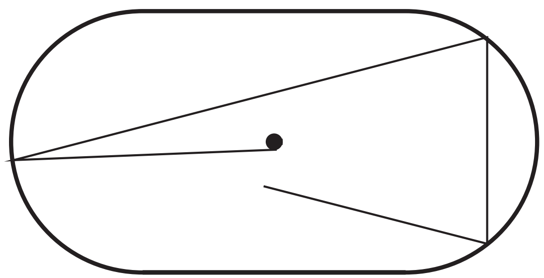
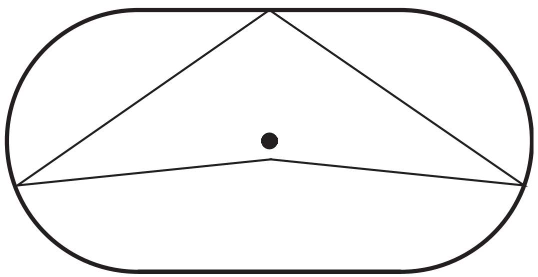






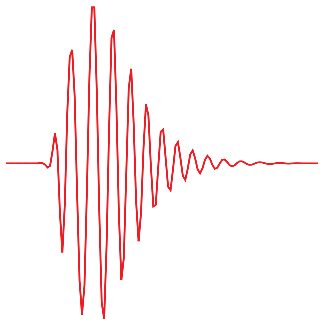
The general Gaussian integral

$$\left(\frac{\pi^N}{\mathrm{Det}\ \mathbf{A}}\right)^{\frac{1}{2}} \exp\left(\frac{\mathbf{p}^T \cdot \mathbf{A}^{-1} \cdot \mathbf{p}}{4}\right) = \int_{-\infty}^{\infty} \mathrm{d}\mathbf{x} \exp\left(-\mathbf{x}^T \cdot \mathbf{A} \cdot \mathbf{x} + \mathbf{p}^T \cdot \mathbf{x}\right)$$

where $(\mathbf{x}, \mathbf{p})$ are N-dimensional vectors and $\mathbf{A}$ is an $N \times N$ symmetric, generally complex, matrix.

General forms of Gaussian wave packets [3]

$$\begin{aligned}
\langle \mathbf{x} | \alpha \rangle &= \exp\left(\frac{i}{\hbar}\left[(\mathbf{x}-\mathbf{x}_0)^T \cdot \mathbf{A}_0 \cdot (\mathbf{x}-\mathbf{x}_0) + \mathbf{p}_0^T \cdot (\mathbf{x}-\mathbf{x}_0) + s_0\right]\right) \\
\langle \mathbf{x} | \alpha(t) \rangle &= \exp\left(\frac{i}{\hbar}\left[(\mathbf{x}-\mathbf{x}_t)^T \cdot \mathbf{A}_t \cdot (\mathbf{x}-\mathbf{x}_t) + \mathbf{p}_t^T \cdot (\mathbf{x}-\mathbf{x}_t) + s_t\right]\right) \\
\mathrm{Im}\ s_0 &= \frac{\hbar}{4} \ln\left(\mathrm{Det} \frac{2}{\pi\hbar} \mathrm{Im}\ \mathbf{A}_0\right)
\end{aligned}$$



The semiclassical time-dependent Green function [10, 2]

$$\begin{aligned}
\langle \mathbf{x} | \alpha(t) \rangle &= \int \mathrm{d}\mathbf{x}' \; \langle \mathbf{x} | \mathrm{e}^{-i\mathcal{H}t/\hbar} \mathbf{x}' \rangle \langle \mathbf{x}' | \alpha \rangle \\
\langle \mathbf{x} | \alpha(t) \rangle_{sc} &= \int \mathrm{d}\mathbf{x}' \; K_{sc}(\mathbf{x}, \mathbf{x}'; t) \langle \mathbf{x}' | \alpha \rangle \\
K_{sc}(\mathbf{x}, \mathbf{x}'; t) &= \left(\frac{1}{2\pi i \hbar} \right)^{\frac{N}{2}} \sum_j \left| \frac{\partial^2 \mathcal{S}_j(\mathbf{x}, \mathbf{x}'; t)}{\partial \mathbf{x} \partial \mathbf{x}'} \right|^{\frac{1}{2}} \exp \left[\frac{i}{\hbar} \mathcal{S}_j(\mathbf{x}, \mathbf{x}'; t) - \frac{i\pi}{2} \nu_j \right] \\
\mathcal{S}_j(\mathbf{x}, \mathbf{x}'; t) &= \int_0^t \mathrm{d}t' \mathcal{L}(\mathbf{x}, \mathbf{x}'; t')
\end{aligned}$$

- 1-D example

$$\begin{aligned}
\mathcal{S}(x, x'; t) \approx\; & \mathcal{S}(x_t, x_0; t) + (x - x_t) \left(\frac{\partial \mathcal{S}}{\partial x} \right)_{\substack{x_t \\ x_0}} + (x' - x_0) \left(\frac{\partial \mathcal{S}}{\partial x'} \right)_{\substack{x_t \\ x_0}} + \frac{(x - x_t)^2}{2} \left(\frac{\partial^2 \mathcal{S}}{\partial x^2} \right)_{\substack{x_t \\ x_0}} \\
& + \frac{(x' - x_0)^2}{2} \left(\frac{\partial^2 \mathcal{S}}{\partial x'^2} \right)_{\substack{x_t \\ x_0}} + (x - x_t)(x' - x_0) \left(\frac{\partial^2 \mathcal{S}}{\partial x \partial x'} \right)_{\substack{x_t \\ x_0}}
\end{aligned}$$

The Wigner transform

$$\mathcal{P}_\alpha(\mathbf{x},\mathbf{p}) = \left(\frac{1}{2\pi\hbar}\right)^N \int_{-\infty}^{\infty} \mathrm{d}\mathbf{q}\langle\alpha|\mathbf{x}+\mathbf{q}/2\rangle\langle\mathbf{x}-\mathbf{q}/2|\alpha\rangle \mathrm{e}^{i\mathbf{p}\cdot\mathbf{q}/\hbar}$$

The $(\mathbf{x},\mathbf{p})$ behavior in the resulting exponential argument for $\mathcal{P}_\alpha(\mathbf{x},\mathbf{p})$ is

$$\begin{aligned}\mathrm{Arg}_{\substack{x\\p}}\left[\mathcal{P}_\alpha\right] \quad = \quad & \frac{i}{\hbar}\Big\{(\mathbf{x}-\mathbf{x}_0)^T\cdot(\mathbf{A}_0-\mathbf{A}_0^*)\cdot(\mathbf{x}-\mathbf{x}_0)+[\mathbf{p}-\mathbf{p}_0-(\mathbf{A}_0+\mathbf{A}_0^*)\cdot(\mathbf{x}-\mathbf{x}_0)]^T \\ & \cdot(\mathbf{A}_0-\mathbf{A}_0^*)^{-1}\cdot[\mathbf{p}-\mathbf{p}_0-(\mathbf{A}_0+\mathbf{A}_0^*)\cdot(\mathbf{x}-\mathbf{x}_0)]\Big\}\end{aligned}$$

Returning to the quadratic expansion derivatives

$$\begin{aligned}\mathbf{p}_t \quad &= \quad \nabla_{\mathbf{x}}\mathcal{S}(\mathbf{x},\mathbf{x}';t)\;, \qquad\qquad -\mathbf{p}_0 = \nabla_{\mathbf{x}'}\mathcal{S}(\mathbf{x},\mathbf{x}';t) \\ \nabla_{\mathbf{x}}\mathbf{p}_t \quad &= \quad \mathbf{m}_{11}\mathbf{m}_{21}^{-1}\;, \qquad -\nabla_{\mathbf{x}'}\mathbf{p}_0 = \mathbf{m}_{11}^{-1}\mathbf{m}_{22} \\ \nabla^2_{\mathbf{x},\mathbf{x}'}\mathcal{S}(\mathbf{x},\mathbf{x}';t) \quad &= \quad \mathbf{m}_{21}-\mathbf{m}_{11}\mathbf{m}_{21}^{-1}\mathbf{m}_{22}\end{aligned}$$

The stability matrix

$$\begin{pmatrix} \delta\mathbf{p}_t \\ \delta\mathbf{x}_t \end{pmatrix} = \mathbf{M}_t \begin{pmatrix} \delta\mathbf{p}_0 \\ \delta\mathbf{x}_0 \end{pmatrix} = \begin{pmatrix} \mathbf{m}_{11} & \mathbf{m}_{12} \\ \mathbf{m}_{21} & \mathbf{m}_{22} \end{pmatrix}_t \begin{pmatrix} \delta\mathbf{p}_0 \\ \delta\mathbf{x}_0 \end{pmatrix}$$

Its evolution

$$\frac{\mathrm{d}\mathbf{M}_t}{\mathrm{d}t} = \begin{pmatrix} -\left.\frac{\partial^2\mathcal{H}(\mathbf{x},\mathbf{p};t)}{\partial\mathbf{x}\partial\mathbf{p}}\right|_{\mathbf{x}_t,\mathbf{p}_t} & -\left.\frac{\partial^2\mathcal{H}(\mathbf{x},\mathbf{p};t)}{\partial\mathbf{x}^2}\right|_{\mathbf{x}_t,\mathbf{p}_t} \\ \left.\frac{\partial^2\mathcal{H}(\mathbf{x},\mathbf{p};t)}{\partial\mathbf{p}^2}\right|_{\mathbf{x}_t,\mathbf{p}_t} & \left.\frac{\partial^2\mathcal{H}(\mathbf{x},\mathbf{p};t)}{\partial\mathbf{x}\partial\mathbf{p}}\right|_{\mathbf{x}_t,\mathbf{p}_t} \end{pmatrix} \mathbf{M}_t$$

Its initial condition

$$\mathbf{M}_0 = \mathbf{1}$$

Linearized Gaussian wave packet dynamics [3]

$$
\begin{aligned}
\langle \mathbf{x} | \alpha(t) \rangle_{lwpd} &= \exp\left(\frac{i}{\hbar} \left[(\mathbf{x} - \mathbf{x}_t)^T \cdot \mathbf{A}_t \cdot (\mathbf{x} - \mathbf{x}_t) + \mathbf{p}_t^T \cdot (\mathbf{x} - \mathbf{x}_t) + s_t \right] \right) \\
\dot{\mathbf{x}} &= \nabla_{\mathbf{p}} \mathcal{H}(\mathbf{x}, \mathbf{p}; t) \qquad \dot{\mathbf{p}} = -\nabla_{\mathbf{x}} \mathcal{H}(\mathbf{x}, \mathbf{p}; t) \\
\mathbf{A}_t &= \frac{1}{2} \mathbf{B}_t \cdot \mathbf{C}_t^{-1} \quad \text{where} \quad \begin{pmatrix} \mathbf{B}_t \\ \mathbf{C}_t \end{pmatrix} = \mathbf{M}_t \begin{pmatrix} 2\mathbf{A}_0 \\ \mathbf{1} \end{pmatrix} \\
s_t &= s_0 + \mathcal{S}(\mathbf{x}_t, \mathbf{x}_0; t) + \frac{i\hbar}{2} \mathrm{Tr}\left[\ln \mathbf{C}_t \right]
\end{aligned}
$$

Quadratic expansion of the Schrödinger equation [4]

$$
\begin{aligned}
i\hbar \frac{\partial}{\partial t} \langle \mathbf{x} | \alpha(t) \rangle_{lwpd} &= \left[-\frac{\hbar^2}{2m} \nabla_{\mathbf{x}}^2 + V(\mathbf{x}) \right] \langle \mathbf{x} | \alpha(t) \rangle_{lwpd} \\
V(\mathbf{x}) &= V(\mathbf{x}_t) + (\mathbf{x} - \mathbf{x}_t)^T \cdot \nabla_{\mathbf{x}} V(\mathbf{x})|_{\mathbf{x}_t} + \\
&\quad \frac{1}{2} (\mathbf{x} - \mathbf{x}_t)^T \cdot \nabla_{\mathbf{x}} \left(\nabla_{\mathbf{x}} V(\mathbf{x}) \right)|_{\mathbf{x}_t} \cdot (\mathbf{x} - \mathbf{x}_t)
\end{aligned}
$$

Time scales of validity or breakdown

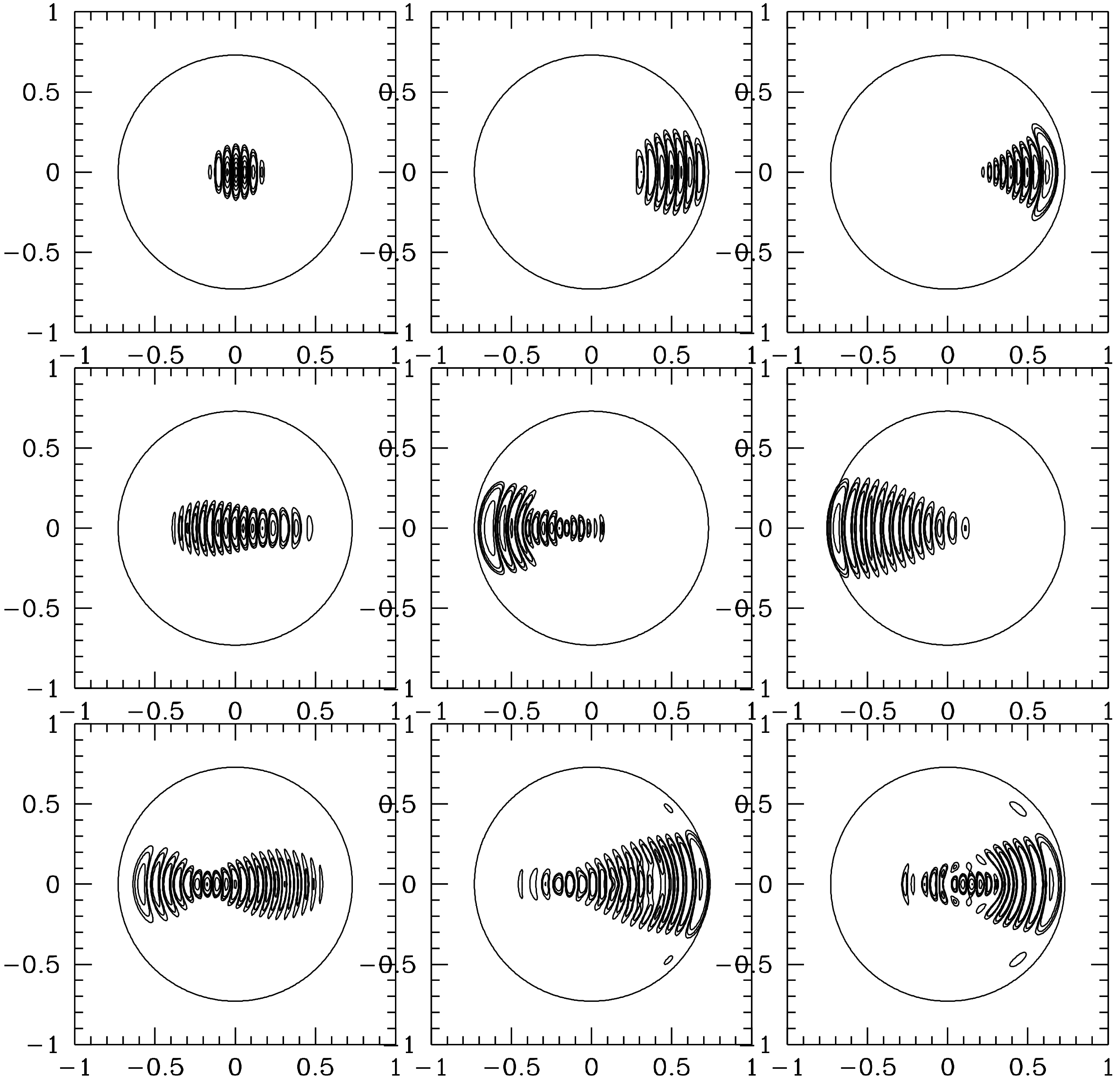
Integrable systems:

$$\tau_b = \sqrt{\frac{\Delta \mathbf{x}^T \cdot \Delta \mathbf{x}}{\Delta \mathbf{v}^T \cdot \Delta \mathbf{v}}} = \begin{cases} \frac{c_I}{\hbar \sqrt{\mathrm{Tr}(\vec{\omega}' \cdot \vec{\omega}')}} & \text{optimal} \\ \frac{c_I}{\sqrt{\hbar \mathrm{Tr}(\vec{\omega}' \cdot \vec{\omega}')}} & \text{not paying attention} \end{cases}$$

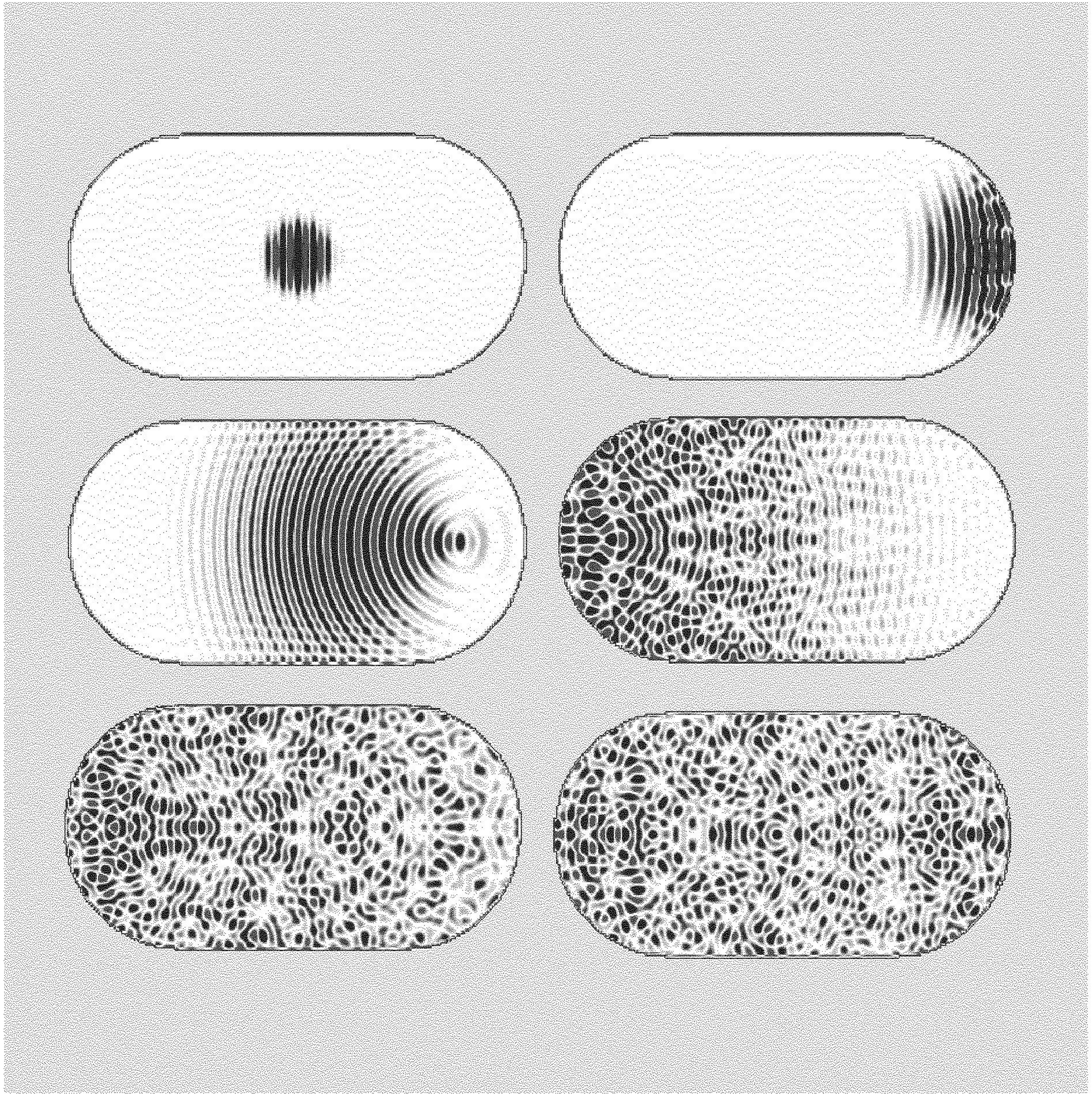
Chaotic systems:

$$\tau_b = \frac{1}{\sum_n \lambda_n} \ln \frac{c_c}{\hbar}$$

Propagating wave packets - Circle



Propagating wave packets - Stadium



Generalized Gaussian wave packet dynamics [5]

Recall the basic Gaussian form

$$\langle \mathbf{x}|\alpha\rangle = \exp\left(\frac{i}{\hbar}\mathcal{S}_0(\mathbf{x};\mathbf{x}_0,\mathbf{p}_0)\right) = \exp\left(\frac{i}{\hbar}\left[(\mathbf{x}-\mathbf{x}_0)^T\cdot\mathbf{A}_0\cdot(\mathbf{x}-\mathbf{x}_0)+\mathbf{p}_0^T\cdot(\mathbf{x}-\mathbf{x}_0)+s_0\right]\right)$$

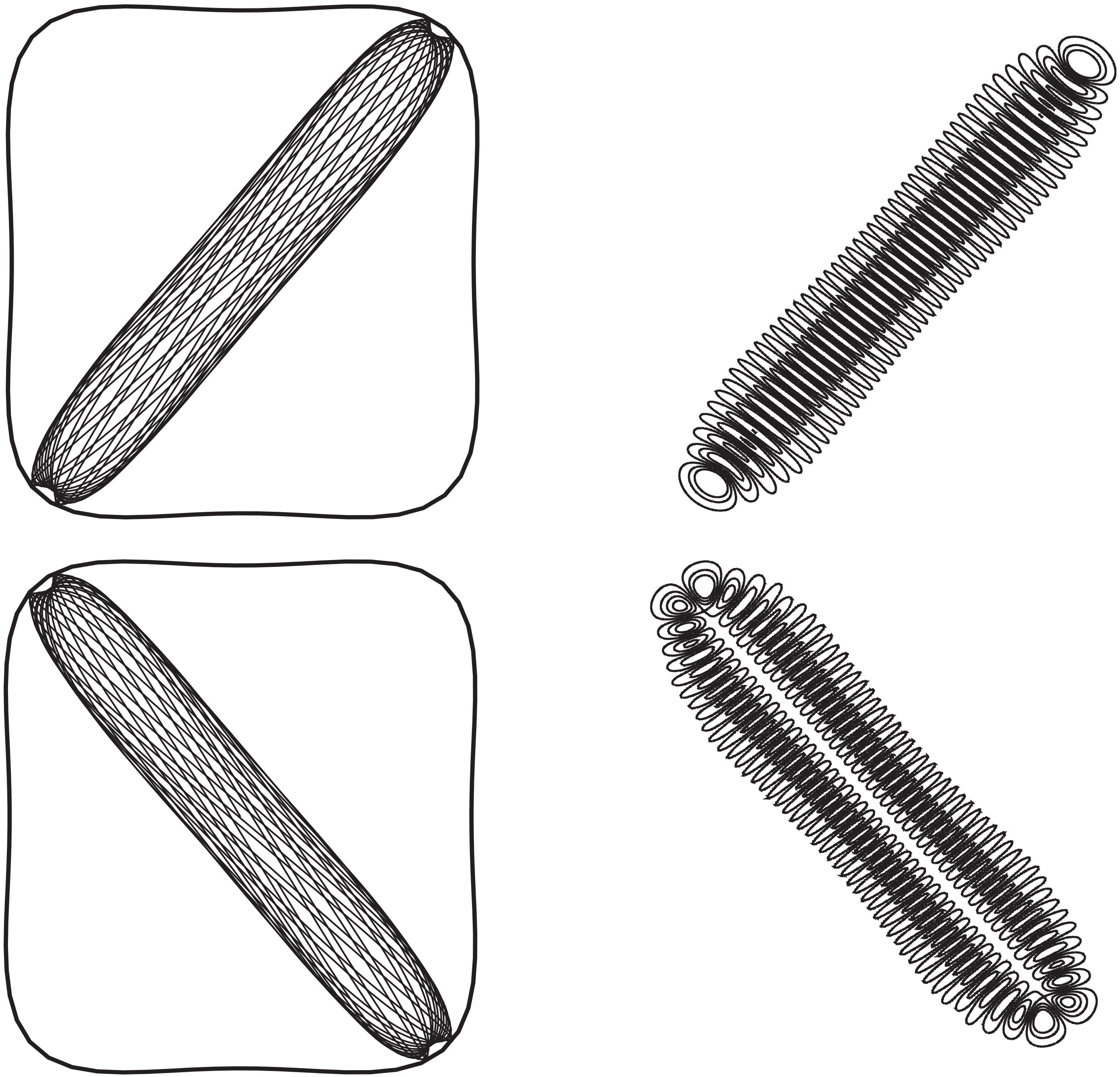
Note that it is invariant if you choose any new $(\mathbf{x}_0', \mathbf{p}_0')$ and s_0' such that

$$\begin{aligned} \mathbf{p}_0' - \mathbf{p}_0 &= 2\mathbf{A}_0\cdot(\mathbf{x}_0' - \mathbf{x}_0) \quad \text{and let} \\ s_0' - s_0 &= \mathbf{x}_0^T\cdot\mathbf{A_0}\cdot\mathbf{x}_0 - {\mathbf{x}_0'}^T\cdot\mathbf{A_0}\cdot\mathbf{x}_0' + {\mathbf{p}_0'}^T\cdot\mathbf{x}_0' - \mathbf{p}_0^T\cdot\mathbf{x}_0 \end{aligned}$$

Complex Lagrangian manifold:

$$\mathbf{p}(\mathbf{x}) = \frac{\partial\mathcal{S}_0(\mathbf{x};\mathbf{x}_0,\mathbf{p}_0)}{\partial\mathbf{x}} = \mathbf{p}_0 + 2\mathbf{A}_0\cdot(\mathbf{x}-\mathbf{x}_0) \qquad [\mathbf{x},\mathbf{p}(\mathbf{x})]$$

Example quantized tori of 2-D coupled quartic oscillators [7]



Linearized Gaussian wave packet dynamics [3]

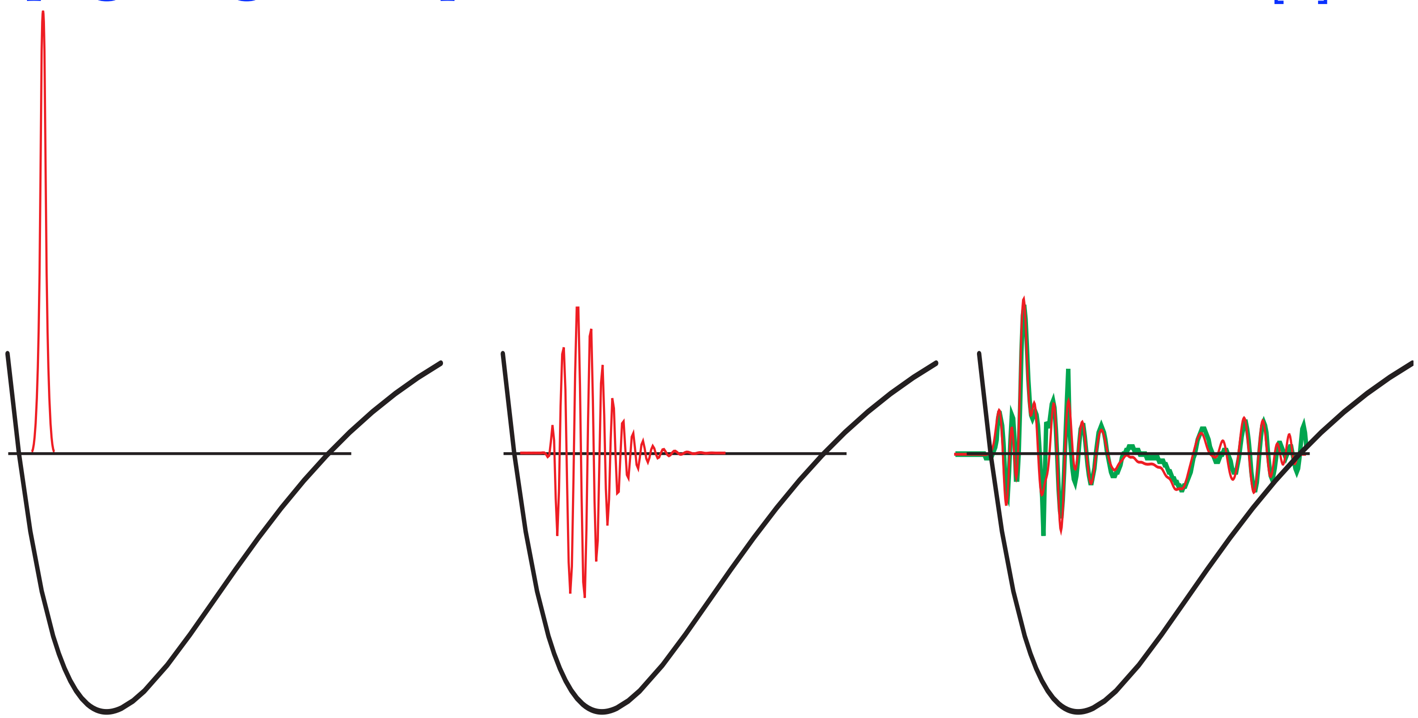
$$\langle \mathbf{x}|\alpha(t)\rangle_{lwpd} = \exp\left(\frac{i}{\hbar}\left[(\mathbf{x}-\mathbf{x}_t)^T\cdot\mathbf{A}_t\cdot(\mathbf{x}-\mathbf{x}_t)+\mathbf{p}_t^T\cdot(\mathbf{x}-\mathbf{x}_t)+s_t\right]\right)$$

$$\dot{\mathbf{x}} = \nabla_{\mathbf{p}}\mathcal{H}(\mathbf{x},\mathbf{p};t) \qquad \dot{\mathbf{p}} = -\nabla_{\mathbf{x}}\mathcal{H}(\mathbf{x},\mathbf{p};t)$$

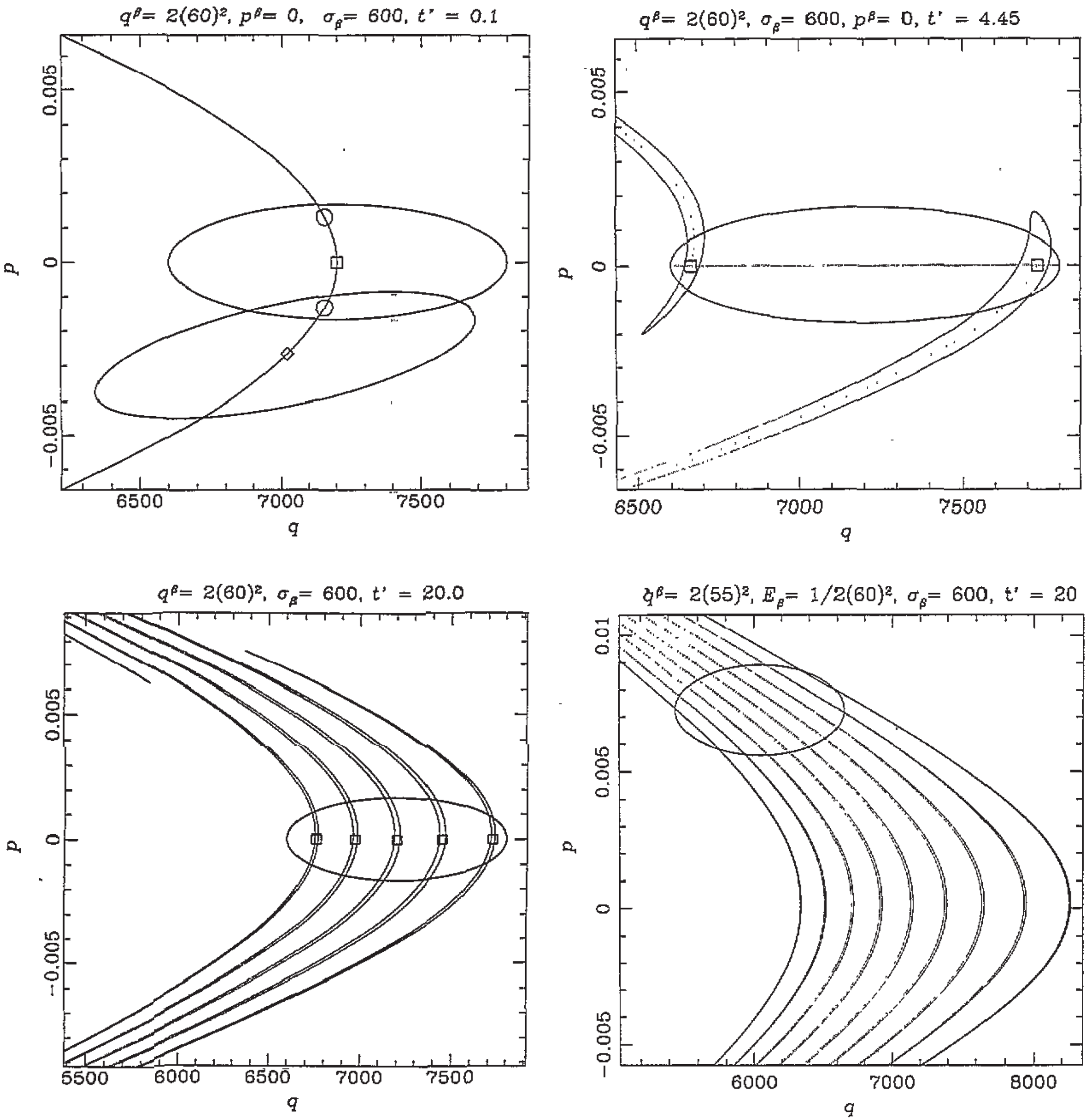
$$\mathbf{A}_t = \frac{1}{2}\mathbf{B}_t\cdot\mathbf{C}_t^{-1} \quad \text{where} \quad \begin{pmatrix}\mathbf{B}_t\\ \mathbf{C}_t\end{pmatrix} = \mathbf{M}_t\begin{pmatrix}2\mathbf{A}_0\\ \mathbf{1}\end{pmatrix}$$

$$s_t = s_0 + \mathcal{S}(\mathbf{x}_t,\mathbf{x}_0;t) + \frac{i\hbar}{2}\mathrm{Tr}\left[\ln\mathbf{C}_t\right]$$

Propagating wave packet - 1-D Morse oscillator [5]



Propagating classical hydrogen orbits [1]



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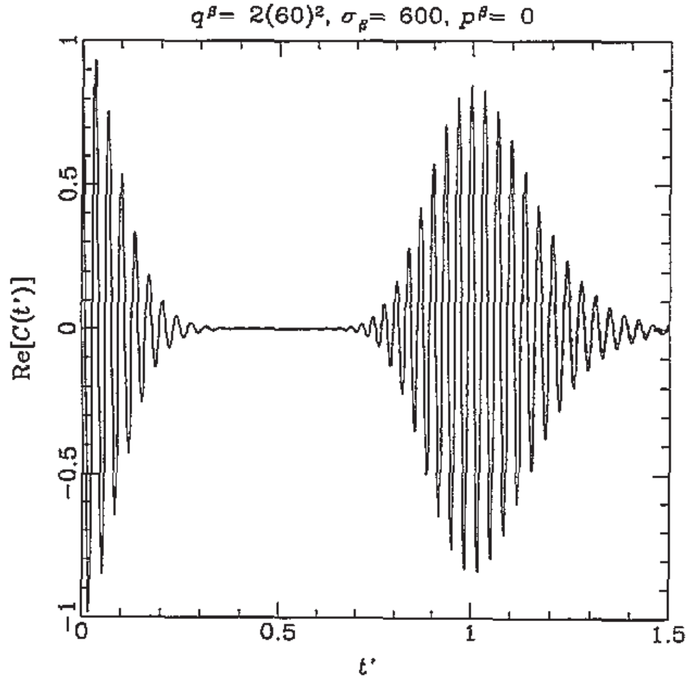
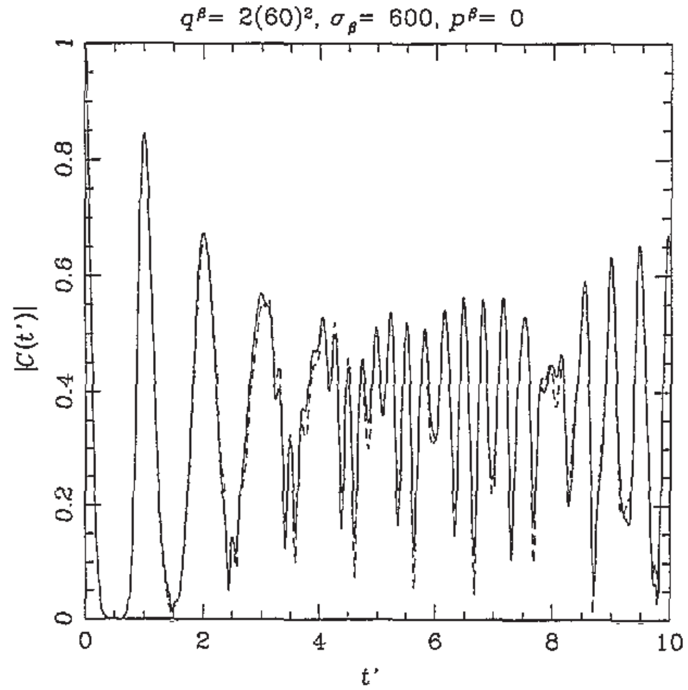
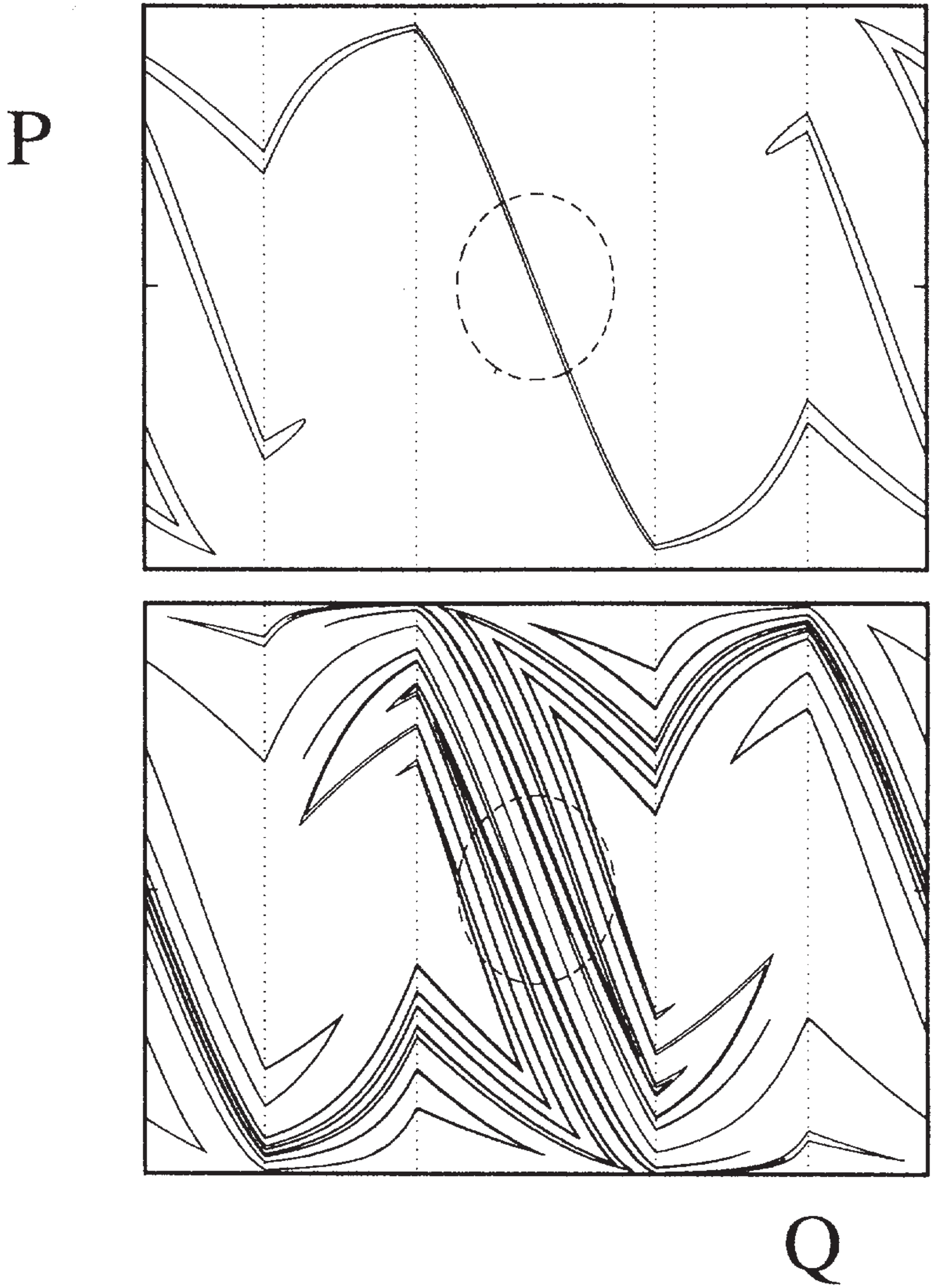


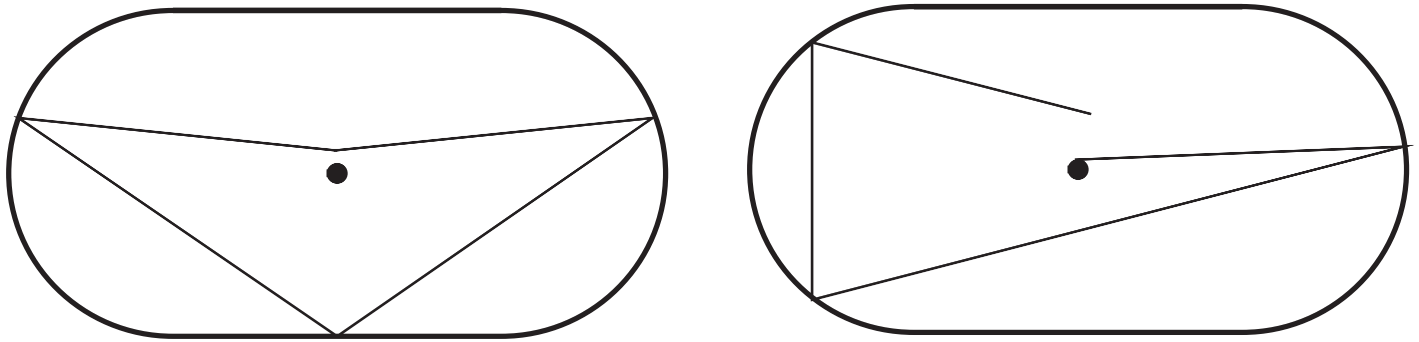


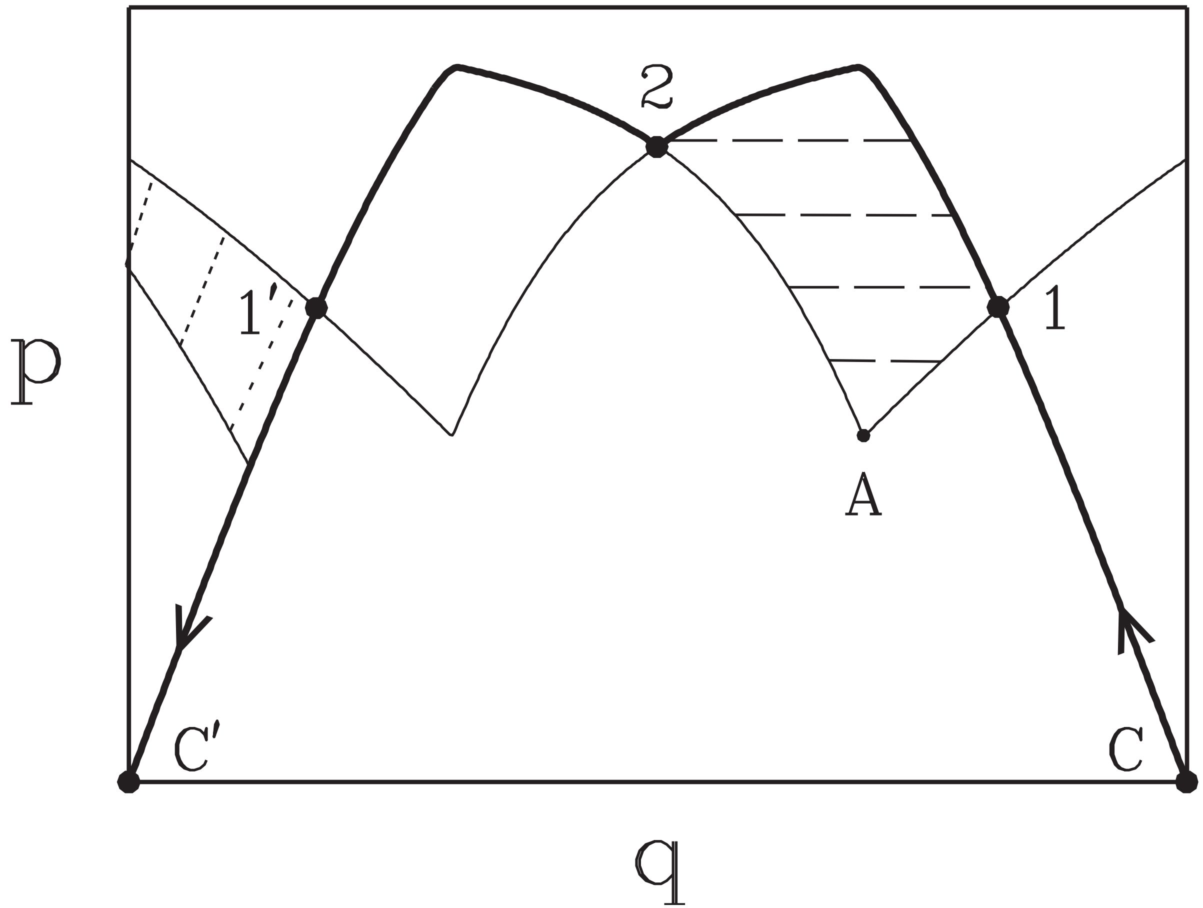
Propagating classically chaotic orbits [8]

Propagating classically chaotic orbits in the stadium [8]

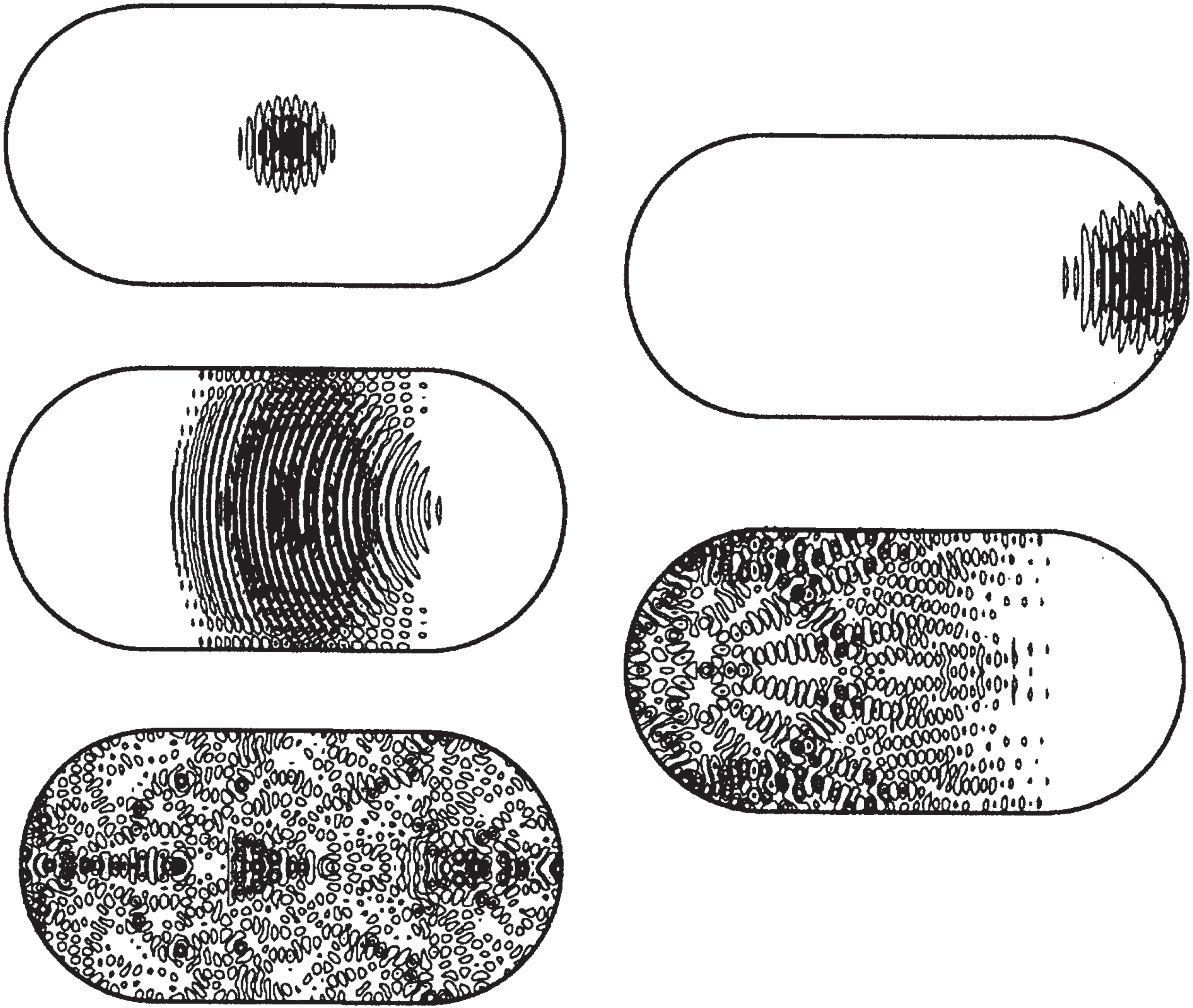


Heteroclinic (homoclinic) orbits in the stadium [8]





Propagating wave packets in the stadium [8]



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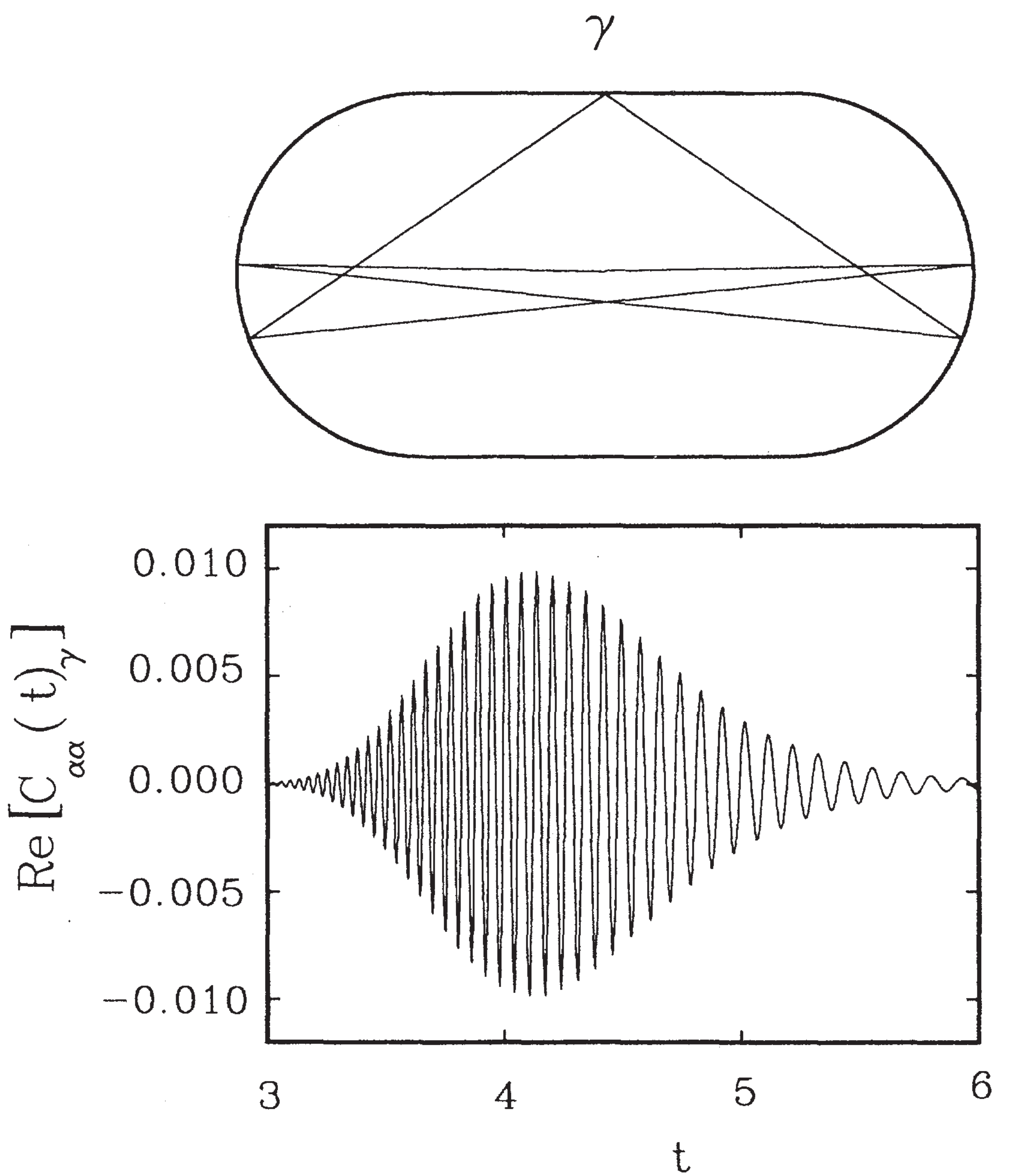

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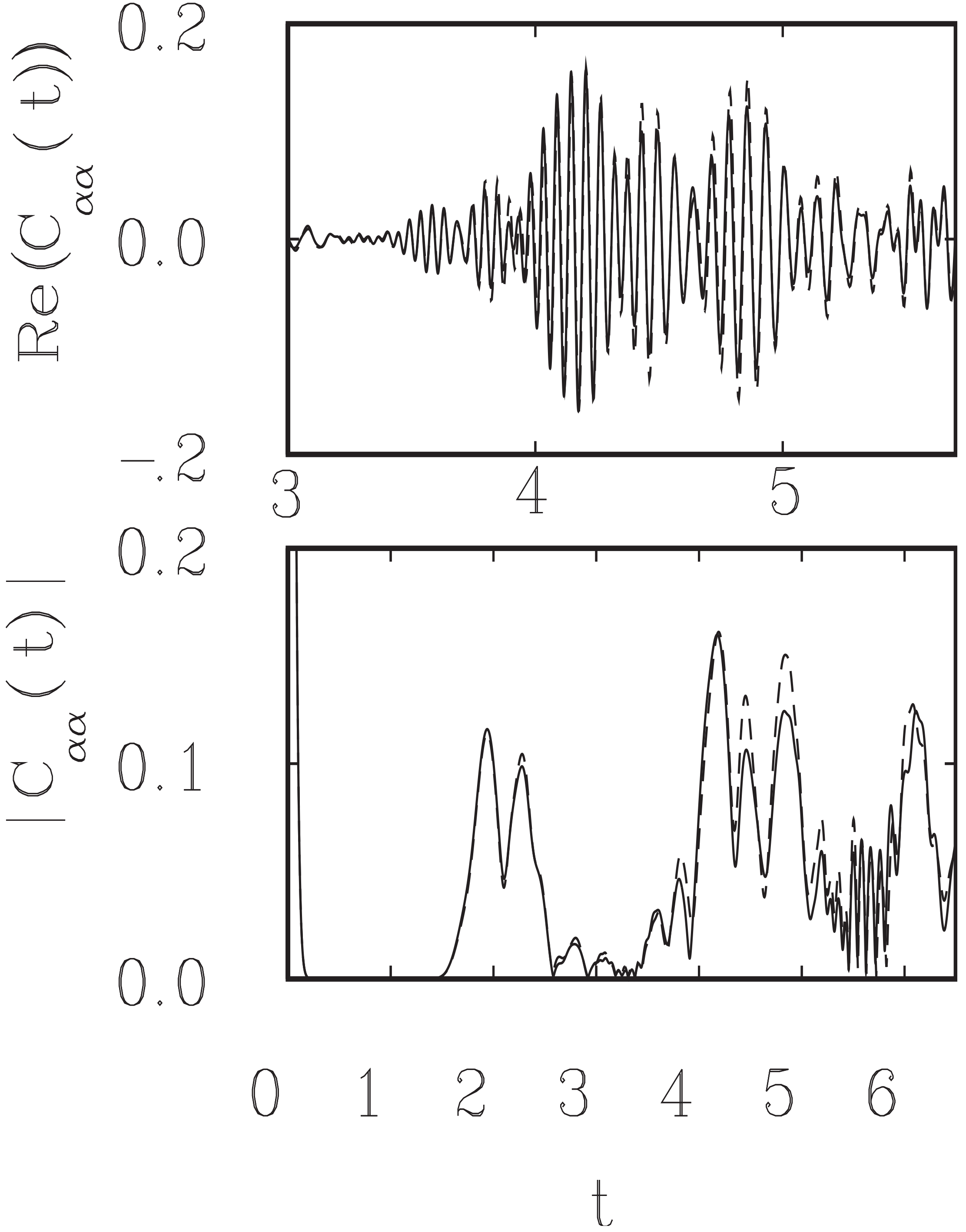
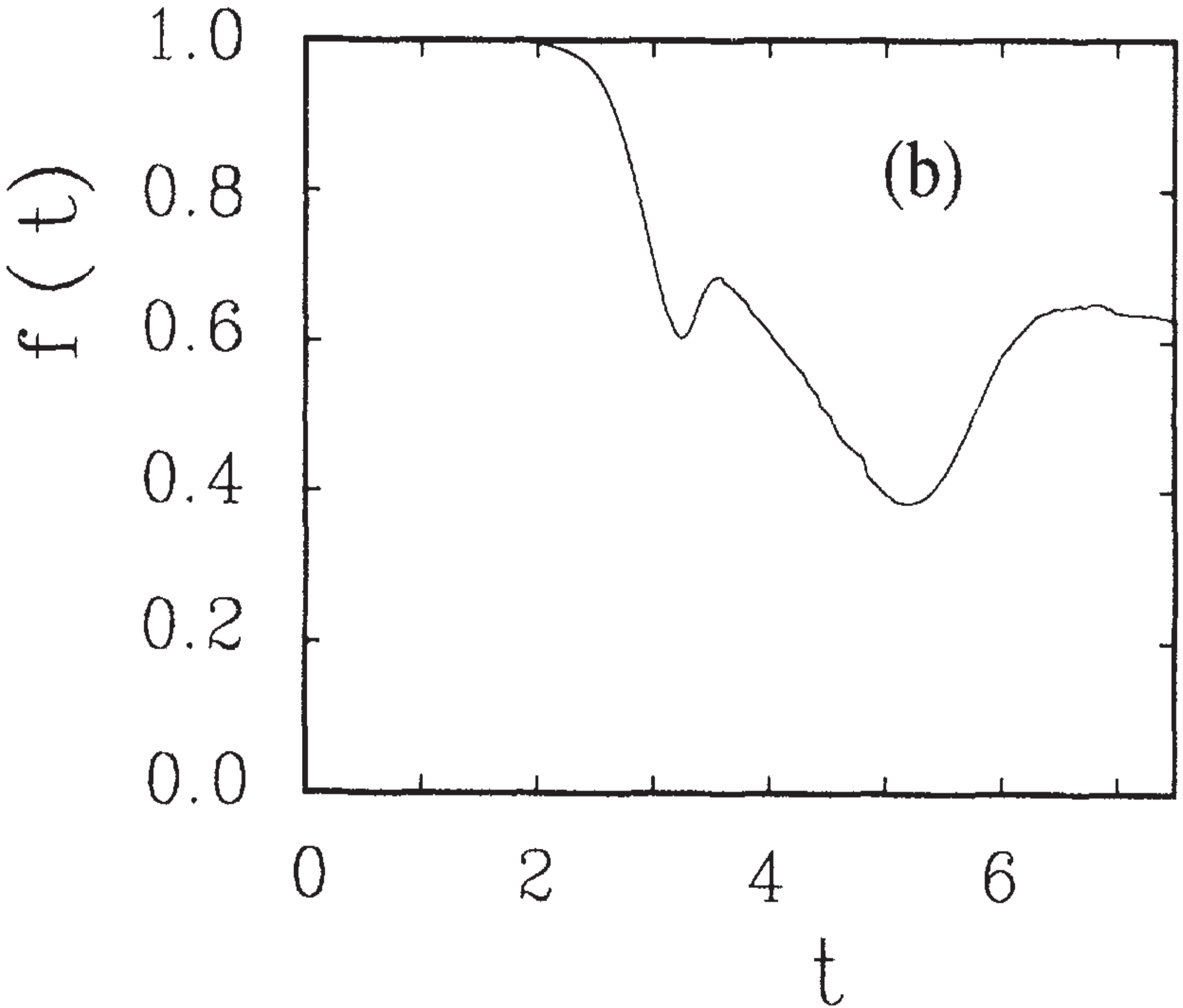
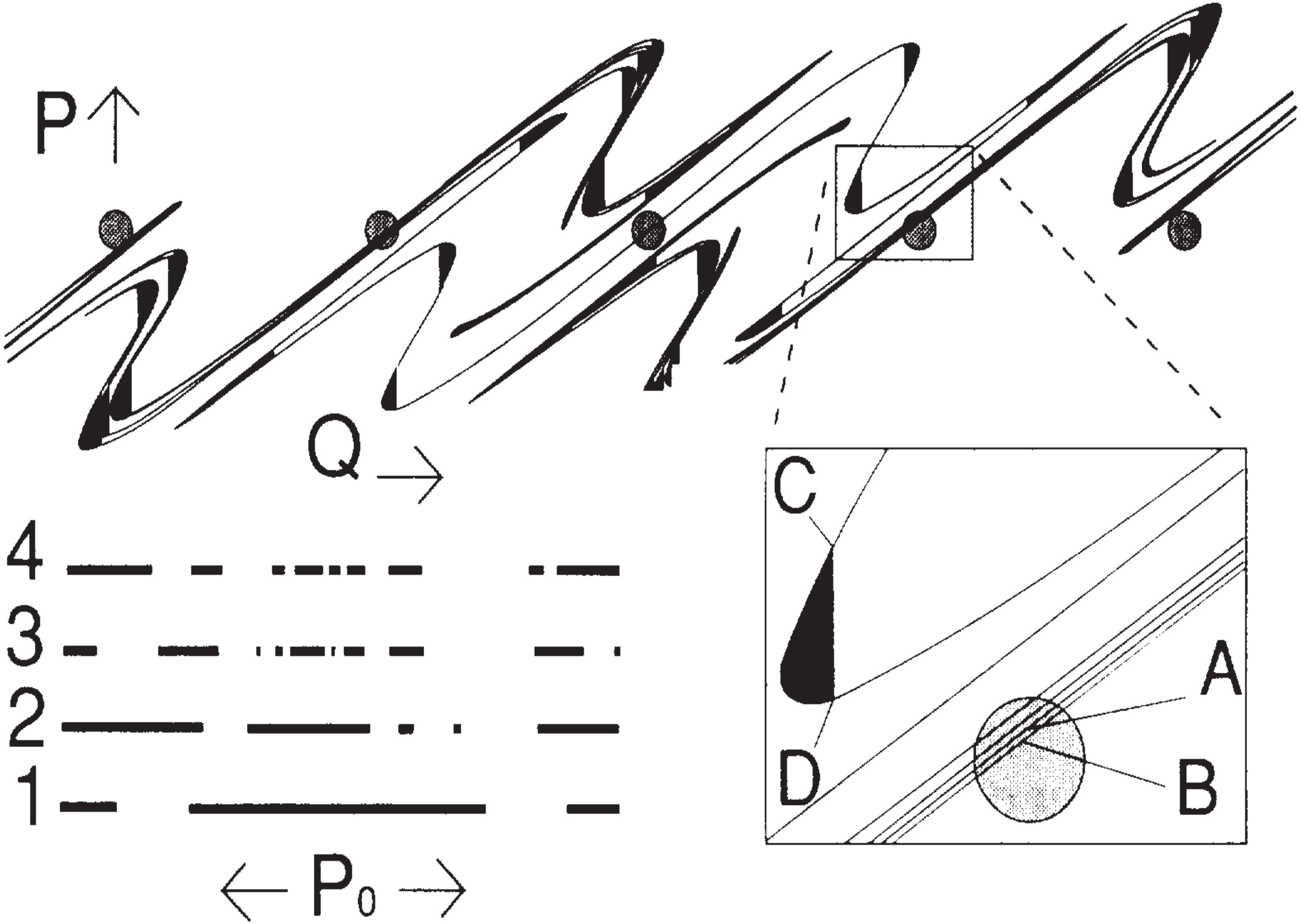


Validity time scales [8]



Validity time scales [6]



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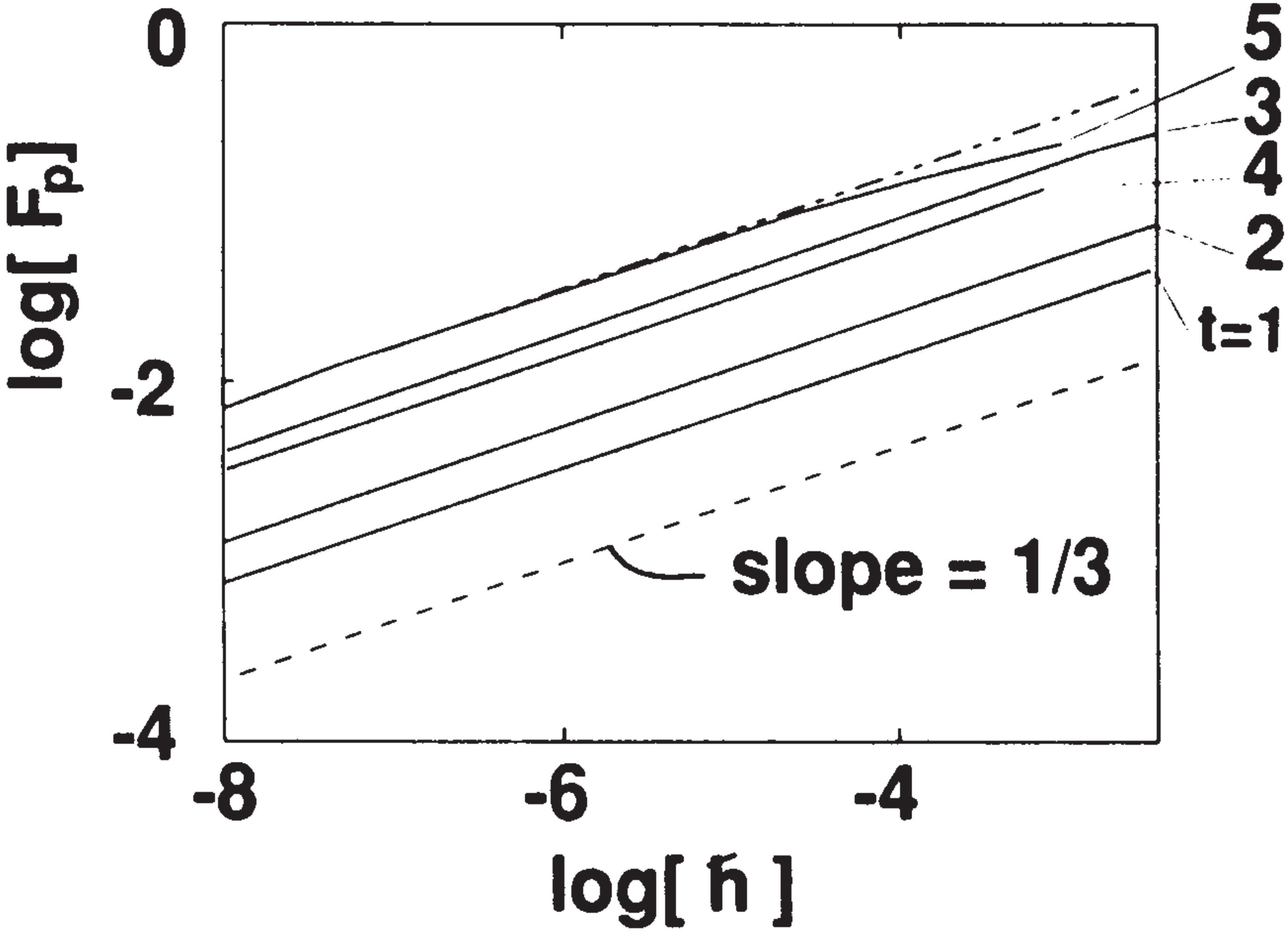
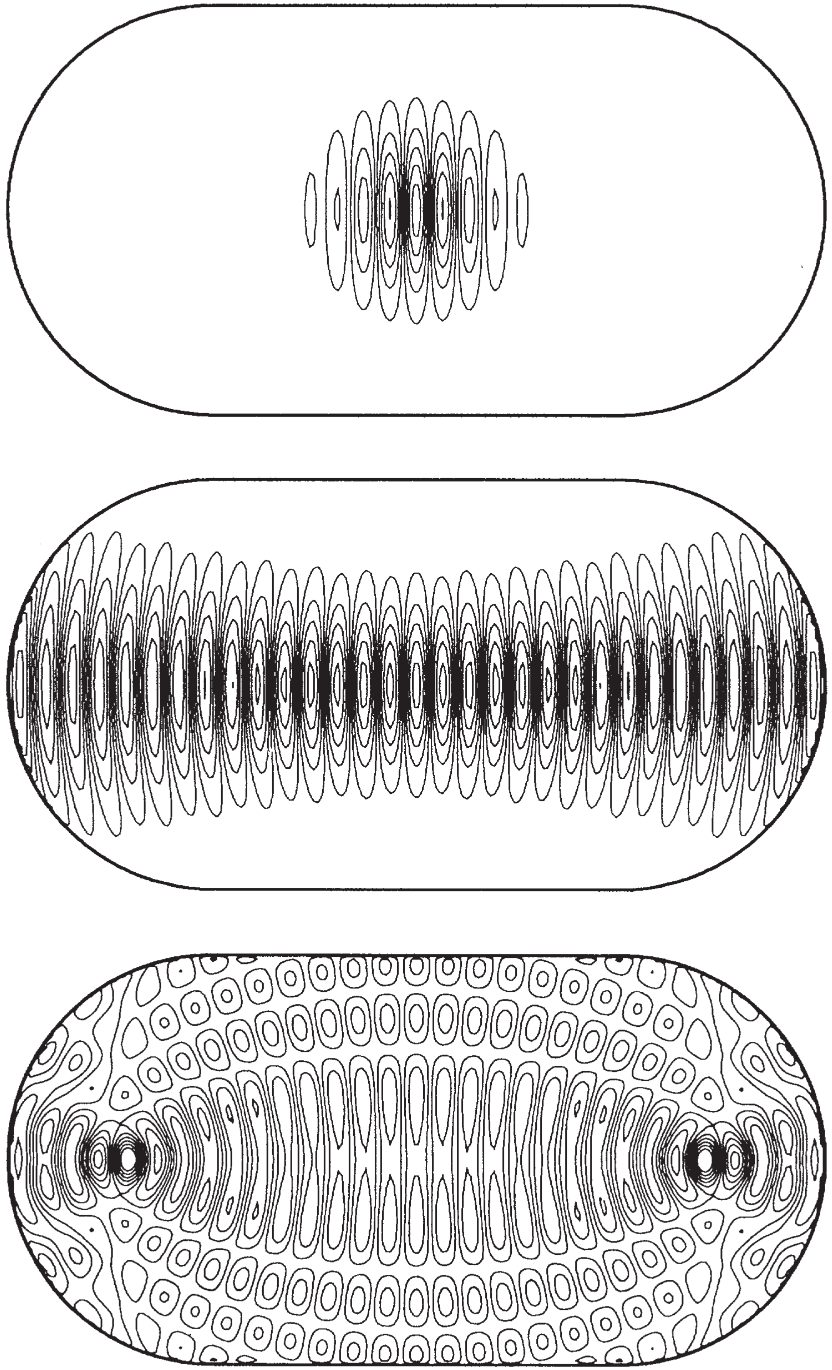


Constructing chaotic eigenstates in the stadium [9]



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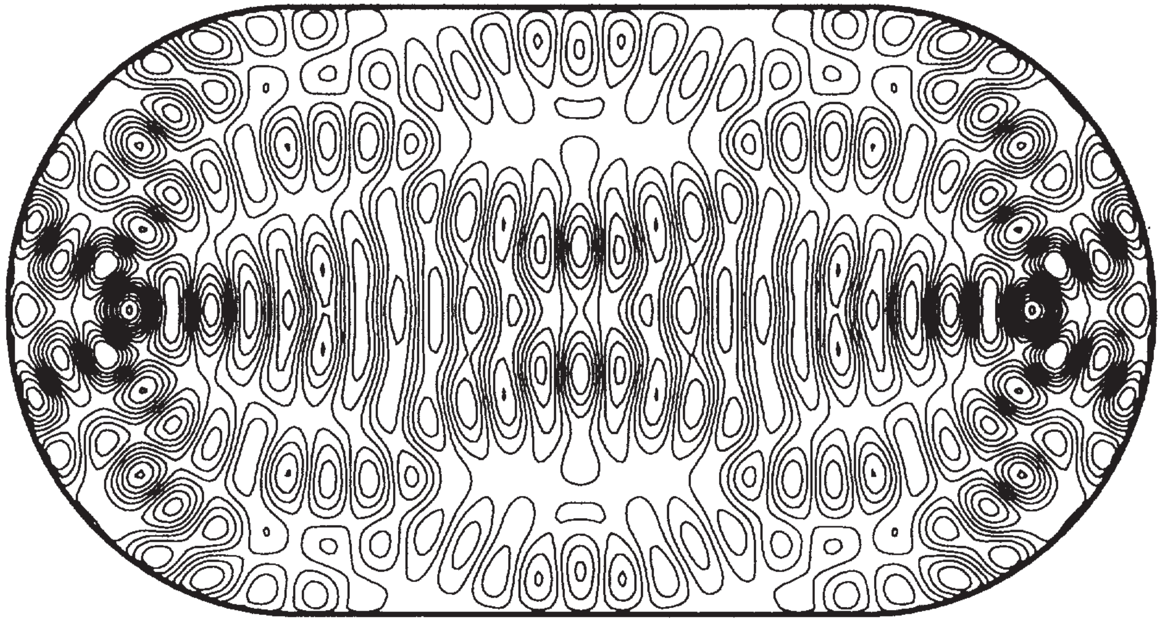

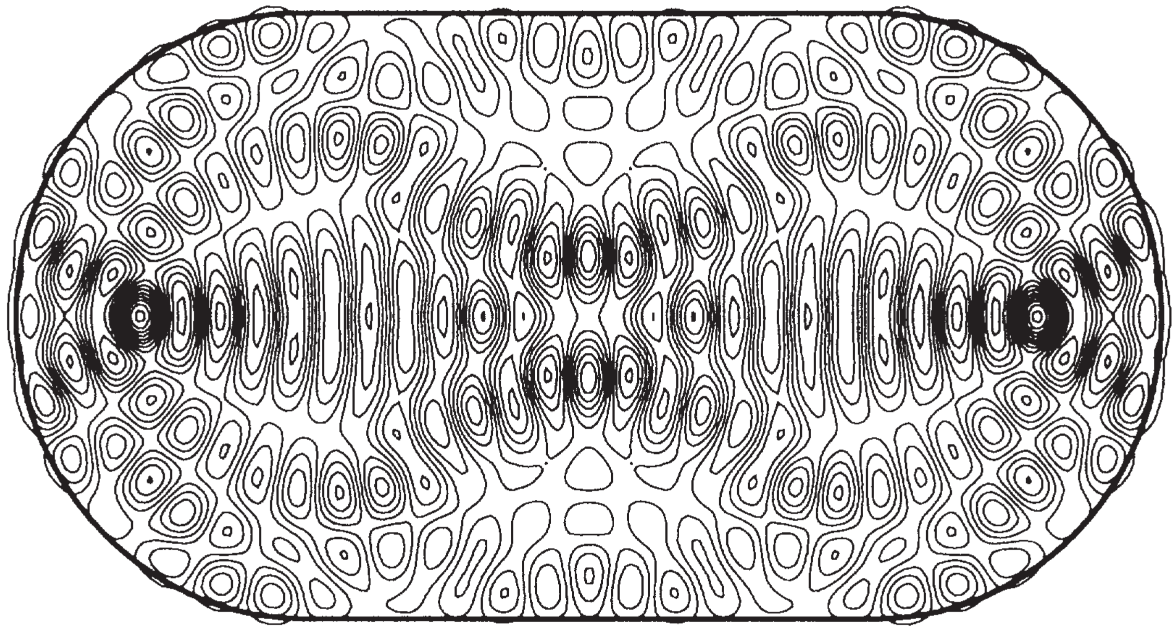

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[1] I. Marianna Suarez Barnes, Michael Nauenberg, Mark Nockleby, and Steven Tomsovic. Classical orbits and semiclassical wave packet propagation in the coulomb potential. J. Phys. A: Math. Gen., 27:3299–3321, 1994.

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