From Hamiltonian to dissipative chaos and back: A primer of active particles

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Publications: Igor S. Aranson and Arkady Pikovsky, “Confinement and collective escape of active particles,” Phys. Rev. Lett. *128*, 108001 (2022); arXiv:2308.08412

Hamiltonian vs dissipative chaos

- Hamiltonian dynamics: phase volume is conserved, Poincaré recurrence theorem
- Dissipative dynamics: phase volume shrinks, attractors are observed

Hamiltonian chaos: long history starting from Poincaré treatise on the three-body problem, with seminal contributions of Hadamard, Birkhoff, KAM, Chirikov and others

In dissipative systems first examples of transient chaos appeared (van der Pol and van der Mark, Cartright and Levinson, and others) and only later examples of strange attractors (Lorenz, Smale and Williams, Roessler, Hénon, and others)

Hamiltonian dynamics with two degrees of freedom

The simplest Hamiltonian autonomous system where chaos can occur is a particle in a two-dimensional potential

$$H = \frac{p_x^2 + p_y^2}{2} + U(x, y)$$

One of the first examples: Hénon-Heiles potential

$$U(x, y) = \frac{x^2 + y^2 + 2x^2 y - \frac{2}{3} y^3}{2}$$

Hénon-Heiles example of Hamiltonian chaos

Michel Hénon
(1931-2013)

THE ASTRONOMICAL JOURNAL VOLUME 69, NUMBER 1 FEBRUARY 1964

The Applicability of the Third Integral Of Motion: Some Numerical Experiments

MICHEL HÉNON* AND CARL HEILES
Princeton University Observatory, Princeton, New Jersey

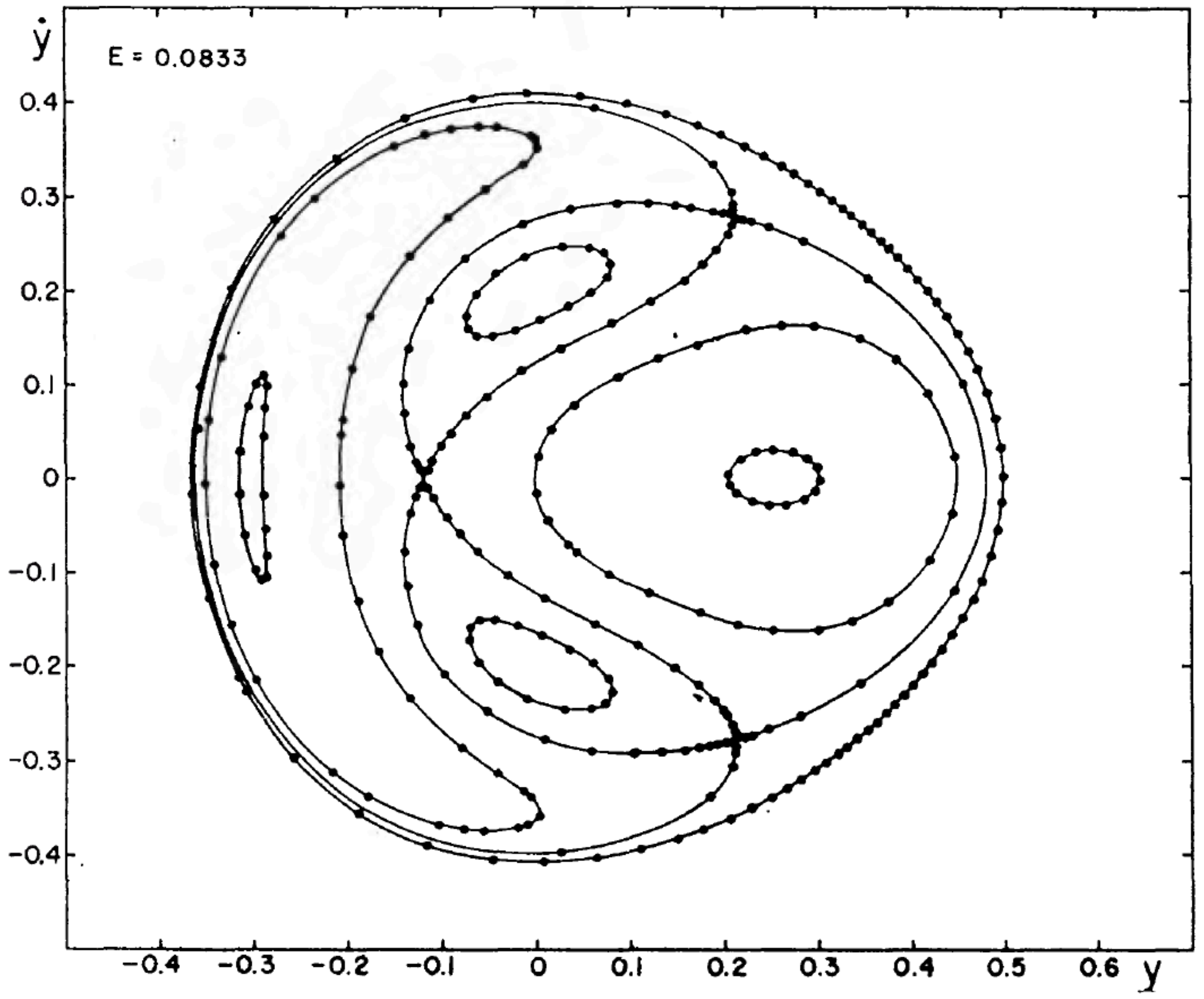


FIG. 4. Results for $E=0.08333$.

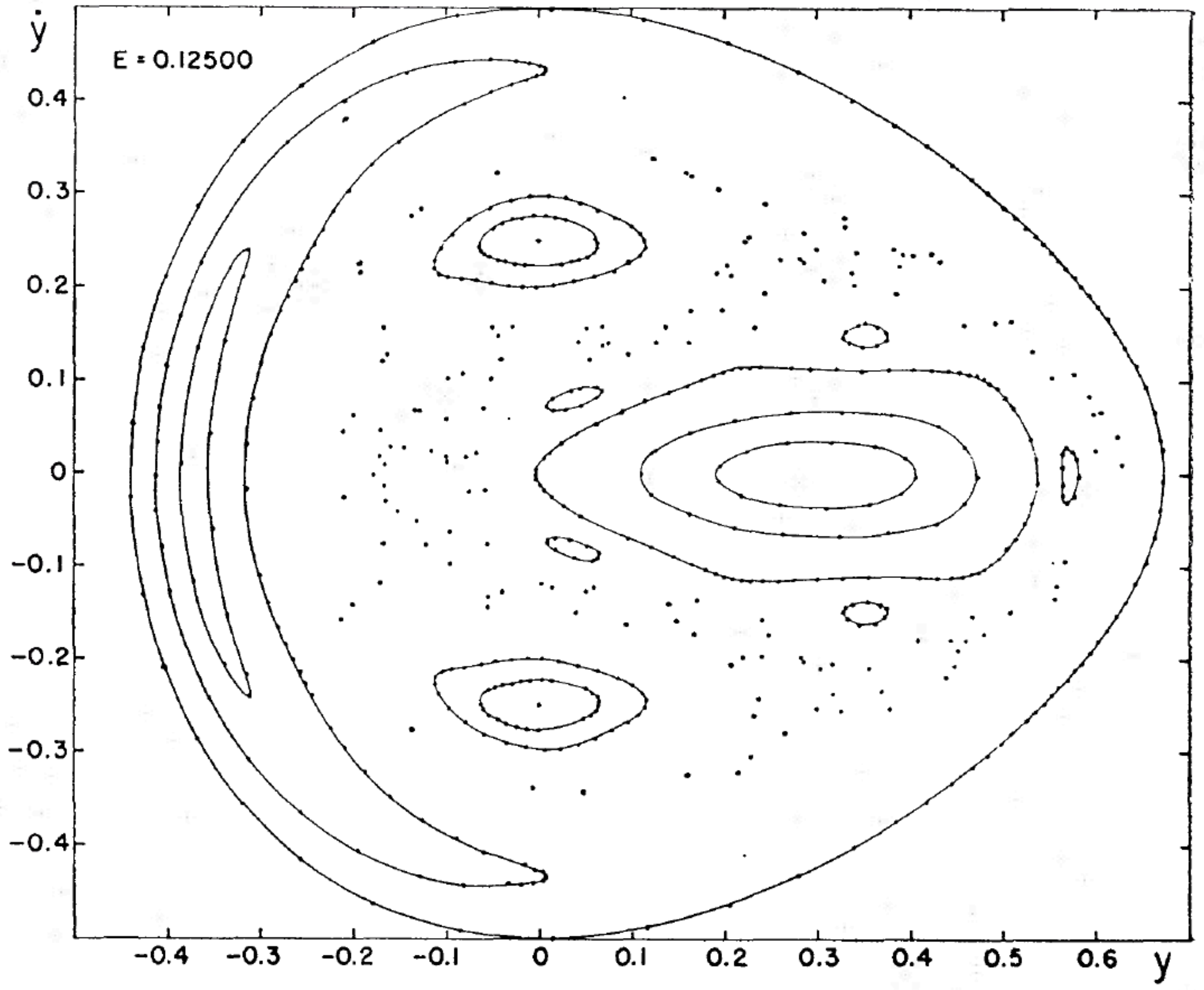


FIG. 5. Results for $E=0.12500$.

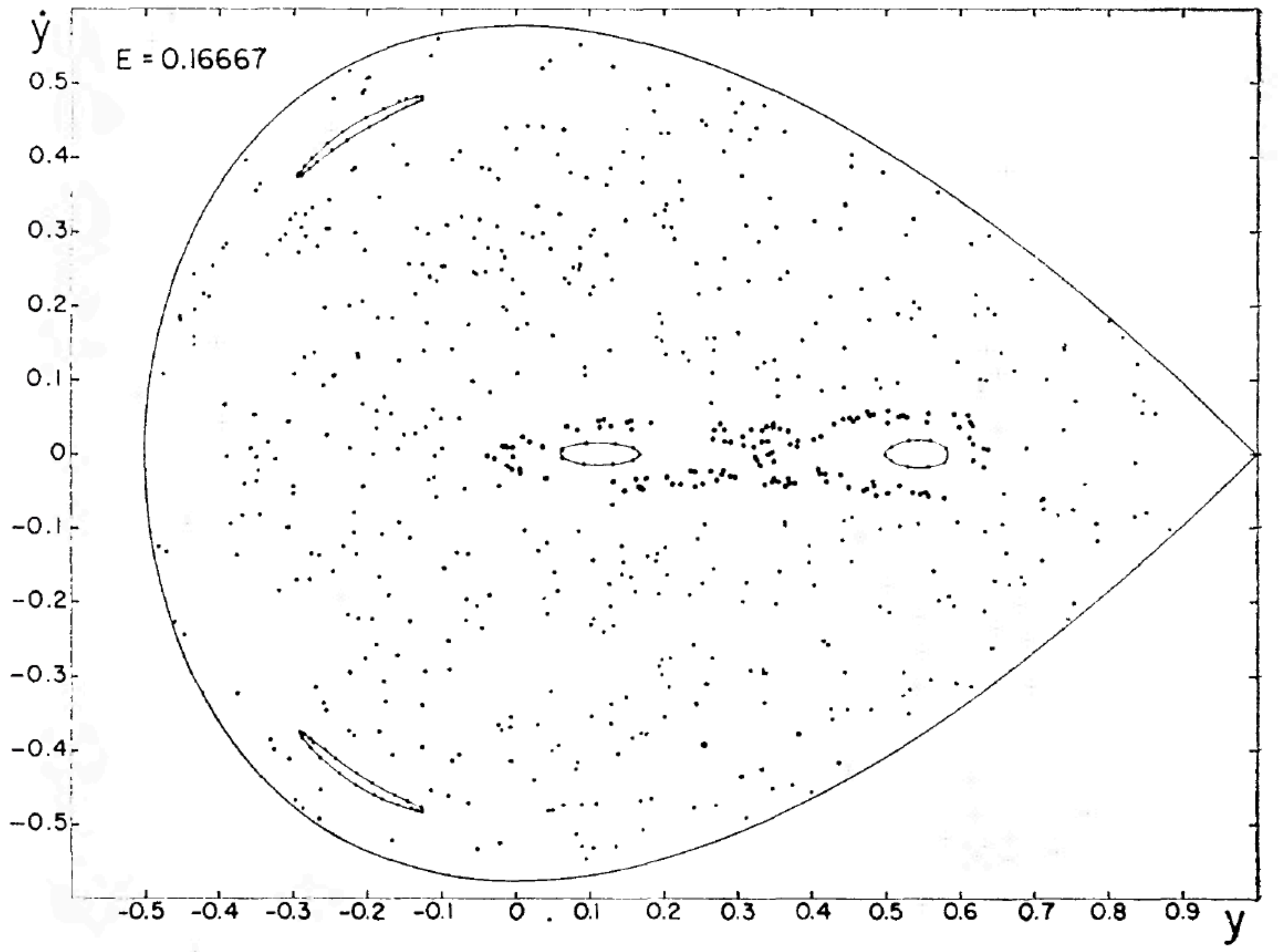


FIG. 6. Results for $E=0.16667$.

Making Hamiltonian system dissipative

Adding pure dissipation: Energy decreases, attractors are steady states at local minima of potential energy

Adding activity:

$$\dot{\vec{r}} = \vec{v} \,, \qquad \dot{\vec{v}} = -\nabla U + \frac{1}{\mu}(V^2 - v^2)\vec{v}$$

An active velocity-dependent force describes convergence (with rate μ^{-1}) of the speed to the preferred speed V ("cruise control") [e.g., Romanczuk et al., Eur. Phys. J. Spec. Topics, 2012, 202:1-62]

There are also other models of active particles, in many of them (e.g., in the famous Vicsek model) noise is included

Here I consider deterministic dynamics only

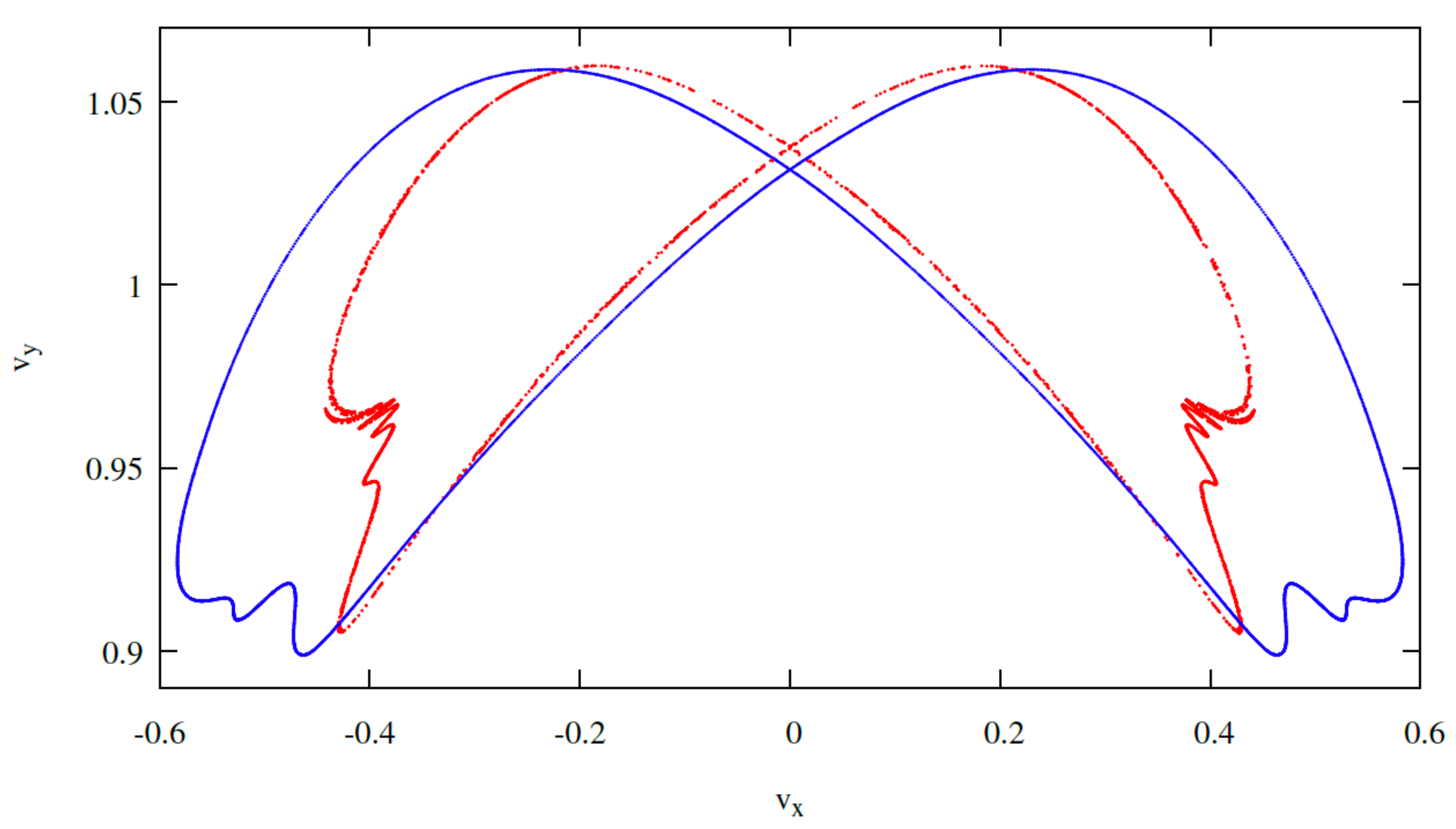
Quasiperiodic and chaotic attractors in a harmonic potential

Numerical solution of the equations:

$$\dot{\vec{r}} = \vec{v}\,, \qquad \dot{\vec{v}} = -\nabla U + \frac{1}{\mu}(V^2 - v^2)\vec{v}\,, \qquad U(x,y) = \frac{x^2 + by^2}{2}$$

yields quasiperiodic and chaotic attractors, but the latter are rare

Poincaré maps for $b = 2$ and different values of activity parameter μ show quasiperiodic (blue) and chaotic (red) attractors



Overactive limit

It is convenient to introduce speed v and direction of motion $\vec{n}$ via $\vec{v} = v\vec{n}$:

$$\dot{\vec{r}} = \vec{v}\,, \quad \dot{\vec{v}} = -\nabla U + \frac{1}{\mu}(V^2 - v^2)\vec{v} \qquad \Rightarrow$$

$$\dot{\vec{r}} = v\vec{n}, \quad \dot{v} = \frac{1}{\mu}(V^2 - v^2)v - \nabla U\vec{n}, \quad \dot{\vec{n}} = \frac{-\nabla U + \vec{n}(\nabla U \cdot \vec{n})}{v}$$

Take the overactive limit (very strong cruise control) $\mu \to 0$, then $v = V$ and the resulting equations are

$$\dot{\vec{r}} = V\vec{n} \qquad V\dot{\vec{n}} = -\nabla U + \vec{n}(\nabla U \cdot \vec{n})$$

In "natural coordinates" $\vec{n} = (\cos\theta, \sin\theta)$ we obtain

$$\frac{dx}{dt} = V\cos\theta \qquad \frac{dy}{dt} = V\sin\theta$$

$$\frac{d\theta}{dt} = \frac{1}{V}\left(-\partial_y U\cos\theta + \partial_x U\sin\theta\right)$$

Hamiltonian formulation

Remarkably, the equations of motion can be formulated as a Hamiltonian system with Hamilton function

$$H(x, y, p_x, p_y) = V\sqrt{p_x^2 + p_y^2} - V^2 \exp\left[-\frac{U(x, y)}{V^2}\right] = 0$$

Because the energy is conserved, $\sqrt{p_x^2 + p_y^2} = V^{-1}\exp[-U(x, y)V^{-2}]$ and a substitution

$p_x = V^{-1}\exp[-U(x, y)V^{-2}]\cos\theta,\ p_y = V^{-1}\exp[-U(x, y)V^{-2}]\sin\theta$

leads to the equations in the standard form

The same Hamiltonian describes the ray dynamics in geometrical optics

$$H(x, y, p_x, p_y) = \sqrt{p_x^2 + p_y^2} - n(x, y) = 0$$

Small velocities: time-scales separation

$$\dot{x} = V\cos\theta, \quad \dot{y} = V\sin\theta, \qquad V\dot{\theta} = -\cos\theta\partial_y U + \sin\theta\partial_x U$$

For small V we have a fast adjustment of the angle θ to the gradient of the potential U according to

$$\dot{\theta} = V^{-1}|\nabla U|\sin(\alpha-\theta), \quad \sin\alpha = -\frac{\partial_y U}{|\nabla U|}, \cos\alpha = -\frac{\partial_x U}{|\nabla U|}$$

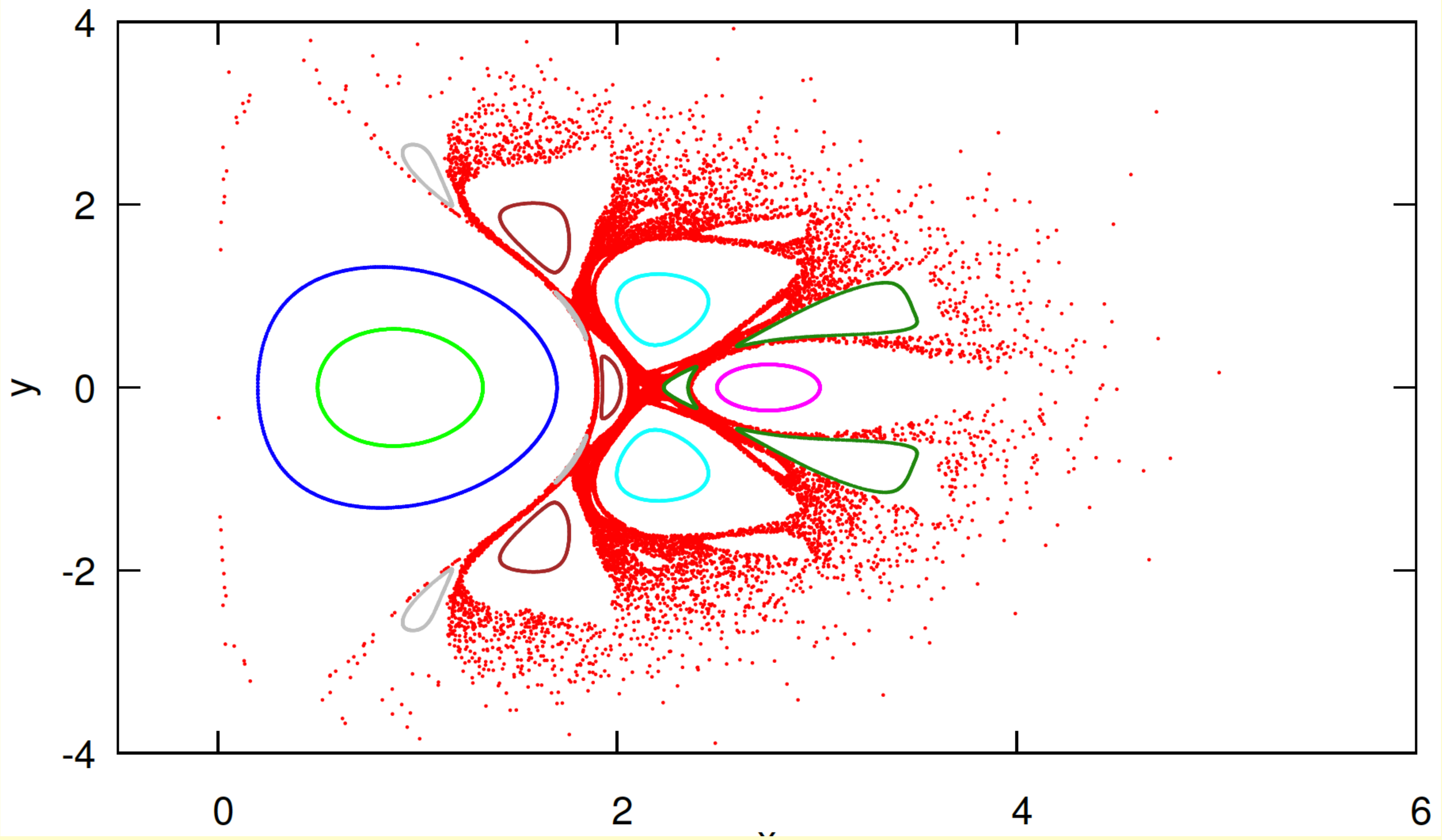
and then slow drift along the gradient toward the minimum of the potential [the dynamics $\dot{\theta} = \sin(\alpha-\theta)$ was used by Chepizhko & Peruani (PRL, 2013) and Peruani & Aranson (PRL, 2018)]

Near the minimum of the potential, the time-scale separation fails

Close to a potential minimum we can consider the potential as a harmonic one

Motion in a harmonic potential

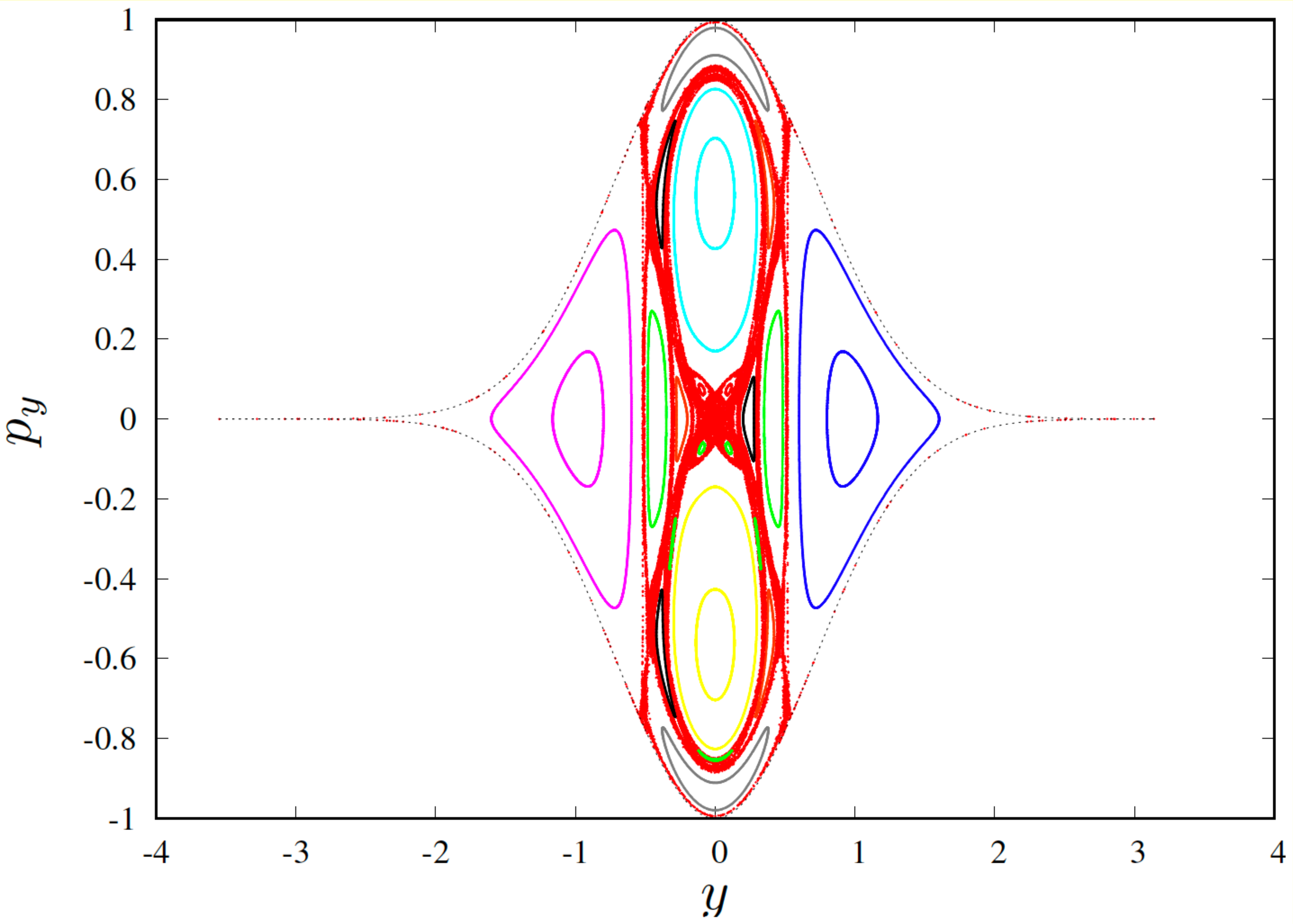
In a harmonic potential $U_h = \dfrac{x^2 + b^2 y^2}{2}$ the velocity parameter can be renormalized to one, and remains only an irrelevant parameter b



- chaotic motion of particles coming from large values of potential
- quasiperiodic motion of particles starting close to the minimum

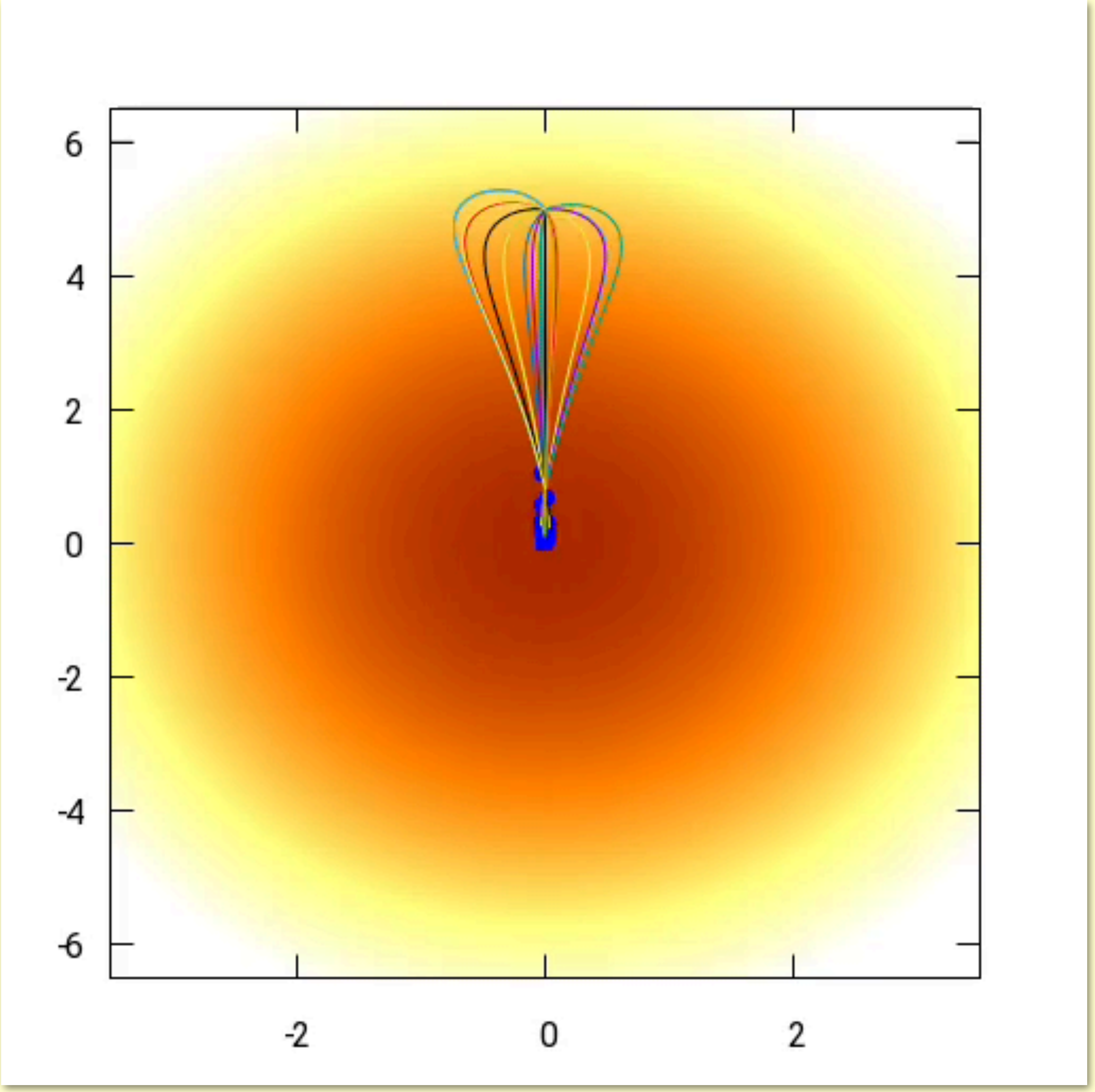
Nonuniform distribution on the Poincare map because we work with non-canonical variables: Density $\sim \exp\left[-\dfrac{U(x,y)}{V^2}\right]$

Motion in a harmonic potential

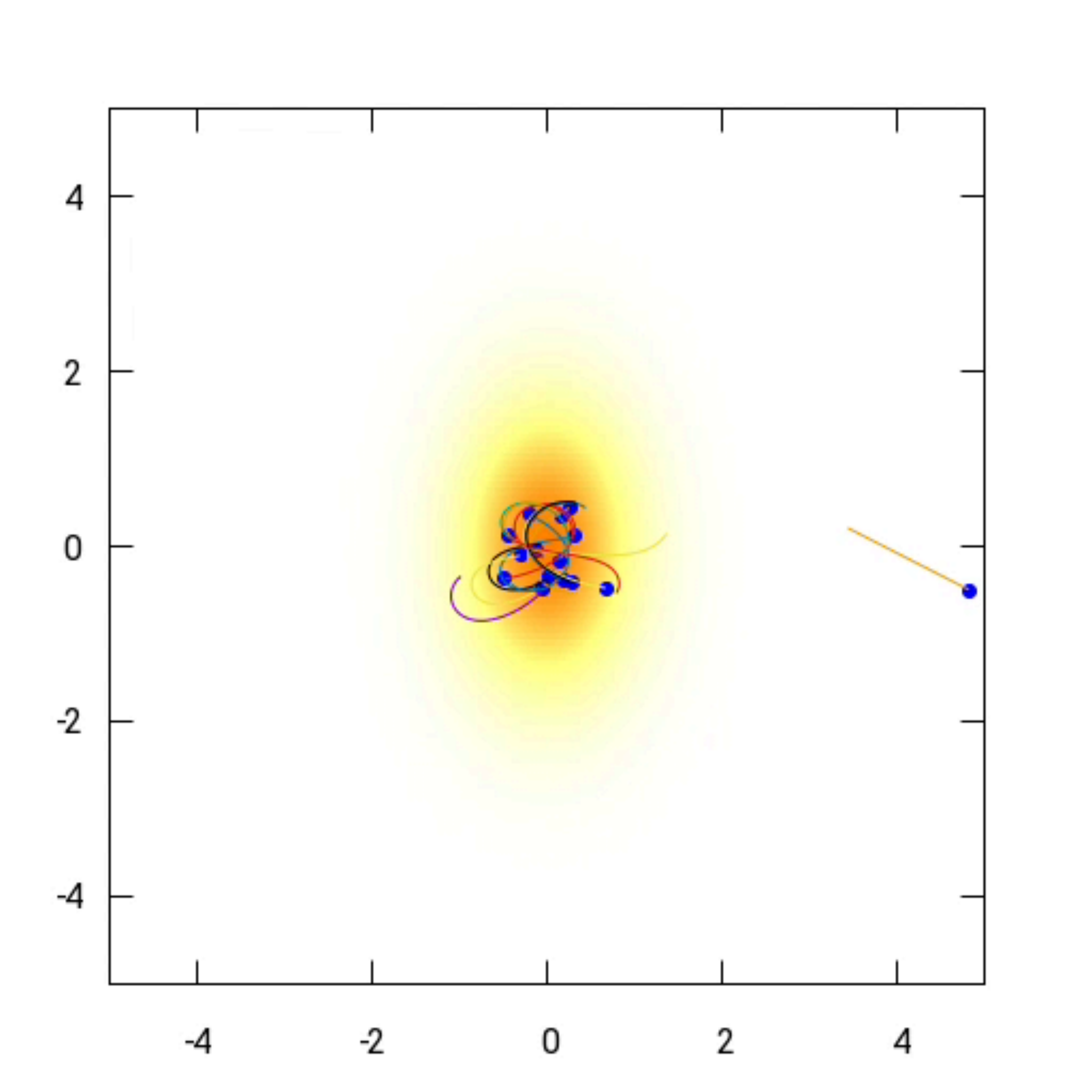


The same dynamics, but the Poincaré map is plotted in canonical variables

Motion in a harmonic potential: movie



Chaotic scattering on a potential well



Alignment: dissipative interaction of particles

Aligning coupling of Kuramoto/Viscek type (global)

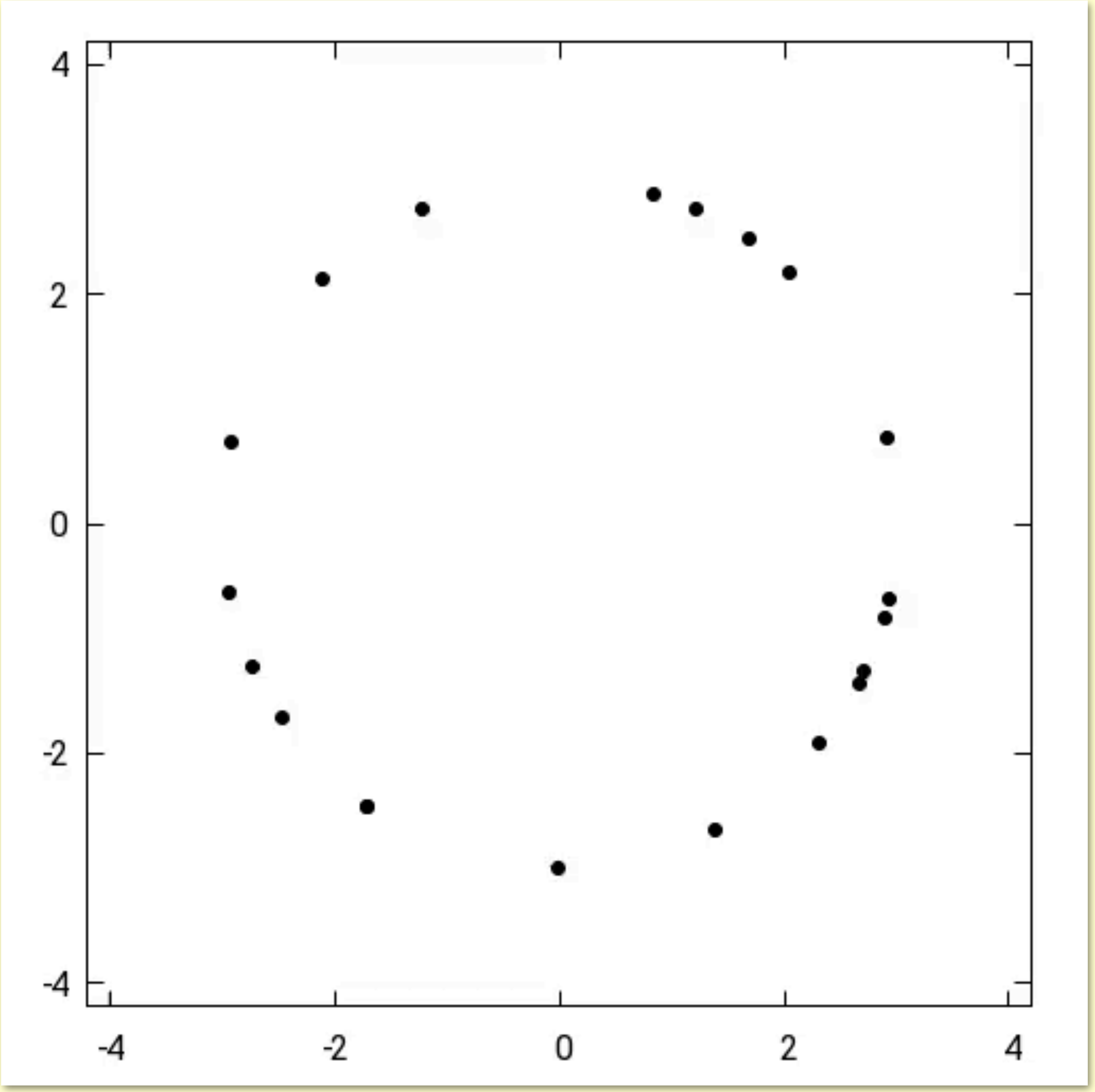
$$\dot{x}_k = V\cos\theta_k \quad \dot{y}_k = V\sin\theta_k$$

$$\dot{\theta}_k = (\epsilon F_y - \partial_y U(\vec{r}_k))\cos\theta_k - (\epsilon F_x - \partial_x U(\vec{r}_k))\sin\theta_k \qquad F_x = \sum_1^N \cos\theta_k, \quad F_y = \sum_1^N \sin\theta_k$$

Synchronization: in a harmonic potential particles build a synchronous cluster
$x_1 = \ldots = x_N,\ y_1 = \ldots = y_N,\ \theta_1 = \ldots = \theta_N,$ in this cluster the aligning force vanishes

Regularization: the dynamics of the final cluster is Hamiltonian quasiperiodic

Alignment: movie



Time-dependent potential and phase volume conservation

I cannot extend the Hamilton function $H(x, y, p_x, p_y) = V\sqrt{p_x^2 + p_y^2} - \exp\left[-\frac{U(x, y)}{V^2}\right] = 0$ to a time-dependent potential $U(x, y, t)$. Thus, another approach is used - calculation of the phase volume evolution in the full equations

$$\frac{dx}{dt} = V\cos\theta \qquad \frac{dy}{dt} = V\sin\theta$$

$$\frac{d\theta}{dt} = \frac{1}{V}\left(-\partial_y U\cos\theta + \partial_x U\sin\theta\right)$$

The divergence rate α is

$$\alpha(t) = W^{-1}\frac{dW}{dt} = \partial_x\dot{x} + \partial_y\dot{y} + \partial_\theta\dot{\theta} = V^{-2}(U_y\dot{y} + U_x\dot{x}) = V^{-2}\left(\frac{dU}{dt} - \frac{\partial U}{\partial t}\right)$$

For a time-independent potential the average divergence rate vanishes

$$\langle\alpha(t)\rangle_T = \frac{1}{T}\int_0^T \alpha(t')dt' = \frac{U_T - U_0}{V^2 T} \underset{T\to\infty}{\to} 0$$

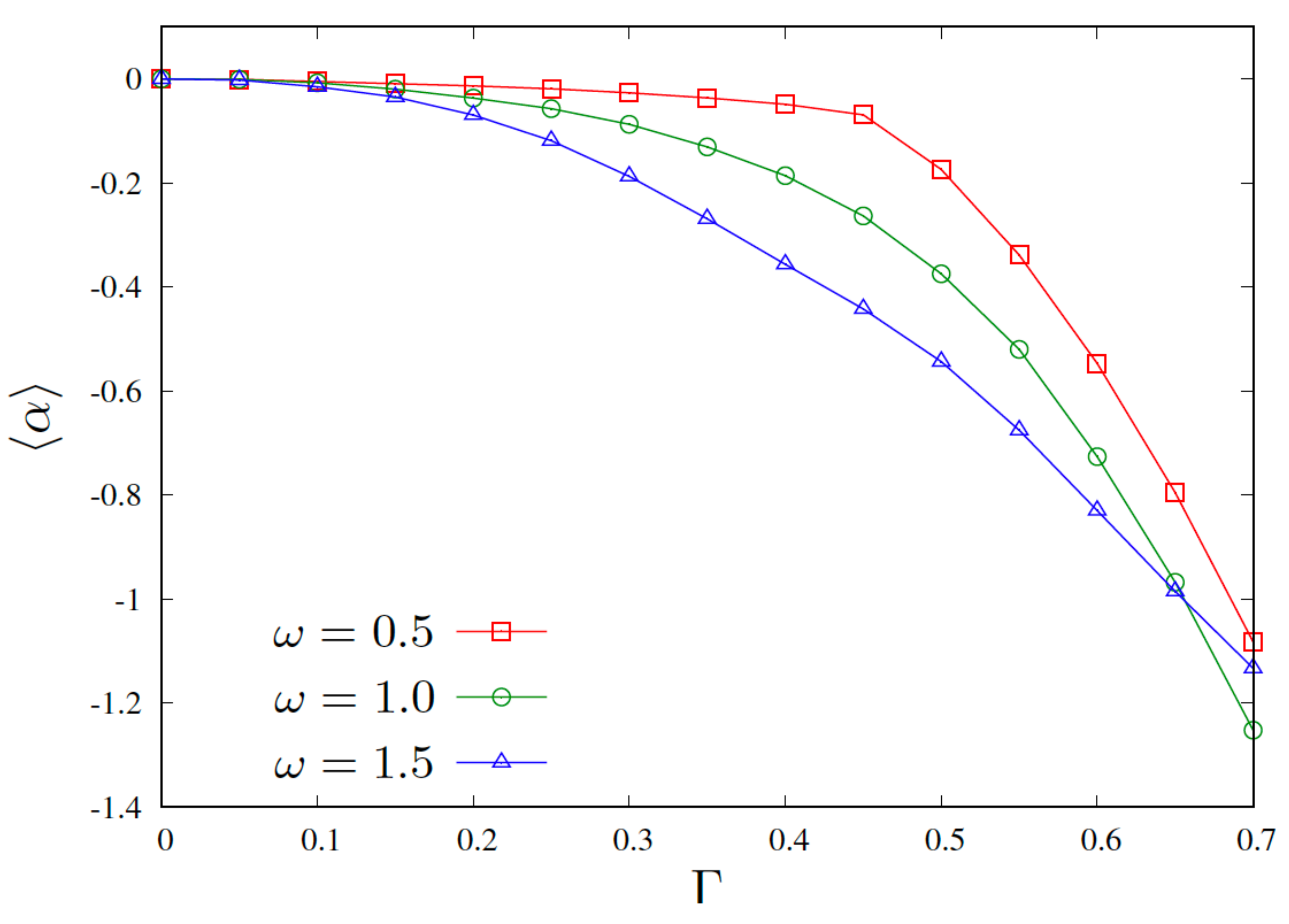
Time-dependent potential and phase volume conservation

The divergence rate α is $\alpha(t) = V^{-2}\left(\frac{dU}{dt} - \frac{\partial U}{\partial t}\right)$

For a time-dependent potential the average divergence rate not necesseraly vanishes

Example: breathing potential

$$U(x,y,t) = \frac{a(1+\Gamma\cos(\omega t))x^2 + b(1+\Gamma\sin(\omega t))y^2}{2}$$



Interacting particles

I cannot write a Hamiltonian formulation for particles interacting with some potential $U(\vec{r}_1, \vec{r}_2)$, but one can check the phase volume conservation

$$\dot{x}_{1,2} = V_{1,2} \cos\theta_{1,2} \,,$$
$$\dot{y}_{1,2} = V_{1,2} \sin\theta_{1,2} \,,$$
$$\dot{\theta}_{1,2} = \frac{1}{M_{1,2}V_{1,2}} \left(-\frac{\partial U}{\partial y_{1,2}} \cos\theta_{1,2} + \frac{\partial U}{\partial x_{1,2}} \sin\theta_{1,2} \right) \,.$$

In general, masses M and velocities V for two particles are different and the phase volume divergence is

$$\alpha(t) = \sum_{m=1,2} \left(\frac{\partial \dot{x}_m}{\partial x_m} + \frac{\partial \dot{y}_m}{\partial y_m} + \frac{\partial \dot{\theta}_m}{\partial \theta_m} \right) = \sum_{m=1,2} (M_m V_m^2)^{-1} \left(\dot{x}_m \frac{\partial U}{\partial x_m} + \dot{y}_m \frac{\partial U}{\partial y_m} \right)$$

Identical and non-identical interacting particles

$$\alpha(t) = \sum_{m=1,2} \left(\frac{\partial \dot{x}_m}{\partial x_m} + \frac{\partial \dot{y}_m}{\partial y_m} + \frac{\partial \dot{\theta}_m}{\partial \theta_m} \right) = \sum_{m=1,2} (M_m V_m^2)^{-1} \left(\dot{x}_m \frac{\partial U}{\partial x_m} + \dot{y}_m \frac{\partial U}{\partial y_m} \right)$$

If particles are identical, then the divergence rate is the total derivative of the potential

$\alpha(t) = (MV^2)^{-1} \dfrac{dU}{dt}$ and on a long term, the phase volume is conserved on average

If the particles are different $M_1 V_1^2 \neq M_2 V_2^2$, the phase volume is not conserved

Many non-identical interacting particles are dissipative

We simulated several particles interacting via a smooth repulsing potential

$$U_{ij}(R) = \begin{cases} D\,|\,(R/\sigma)^2 - 1\,|^7 & R < \sigma\,, \\ 0 & R \geq \sigma\,, \end{cases}$$

in a harmonic confining potential

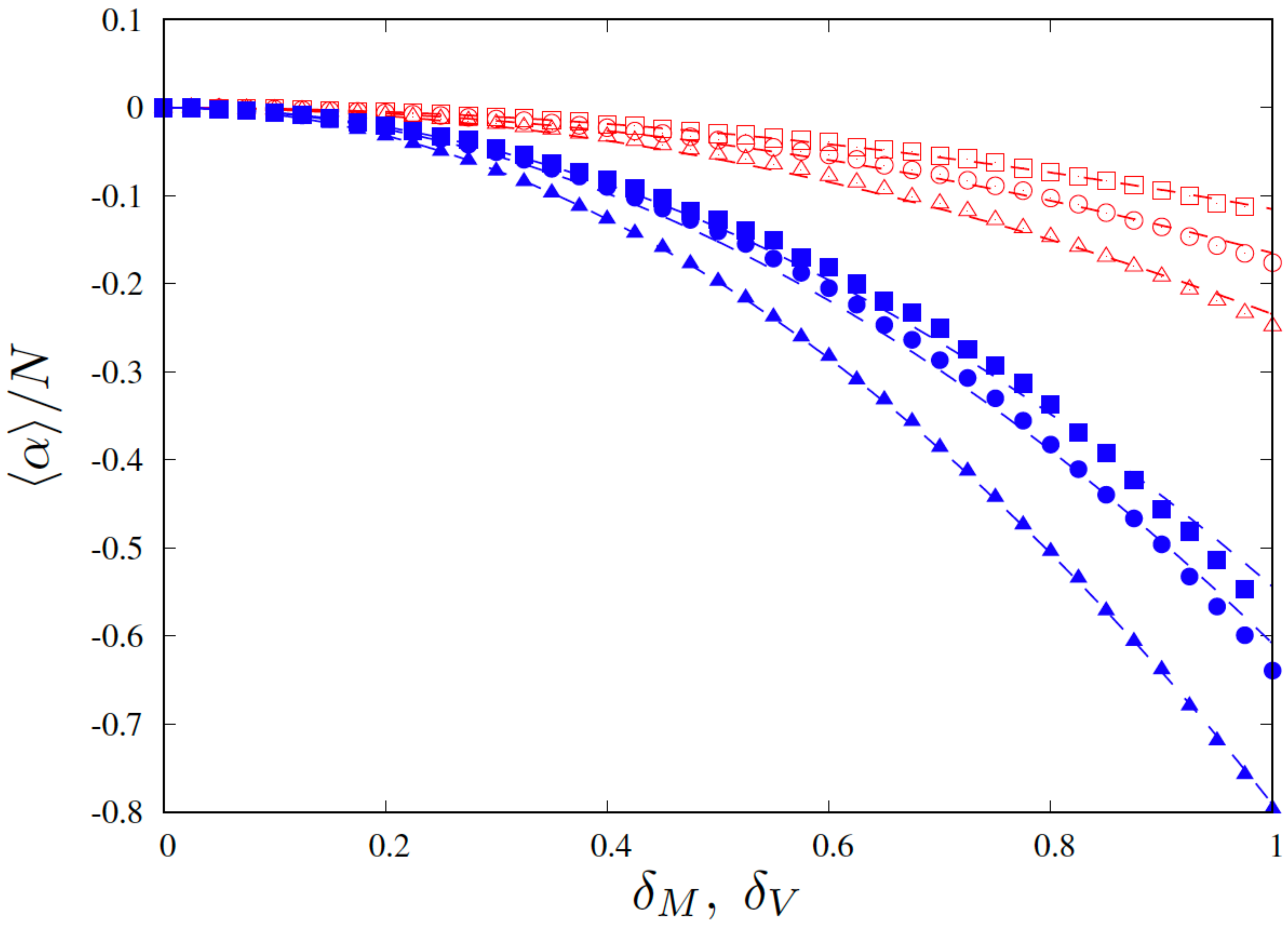


FIG. 5. Particles with potential interaction (parameters $\sigma = 1$, $D = 10^4$, time of averaging 10^5.) Red: rate vs δ_M for $\delta_V = 0$ (the masses of particles are $1 \pm \delta_M/2$); blue: rate vs δ_V (the velocities of particles are $V = 1 \pm \delta_V/2$) for $\delta_M = 0$. Squares: two particles, circles: five particles; triangles: 10 particles. Lines: fits according to the square rate $\sim \delta^2$. All the rates are scaled by the particle number (i.e., convergence rate per particle).

Conservative vs dissipative dynamics

Classical particles

Active particles

Overactive particle ina time-independent potential

Alignment of many overactive particles

Synchronized cluster of aligned particles

Particle in a time-dependent potential

Interacting identical overactive particles

Interacting non-identical overactive particles