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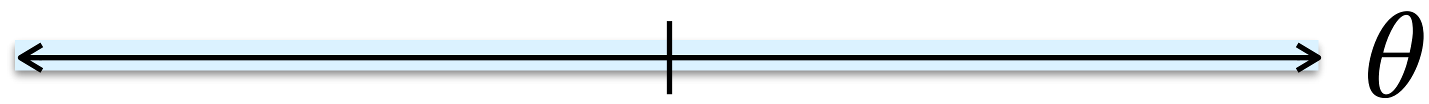
- **Hamiltonian Monte Carlo**

Parameter space



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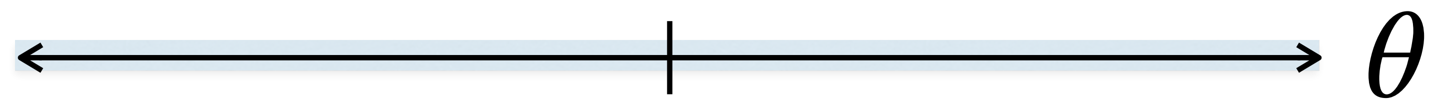

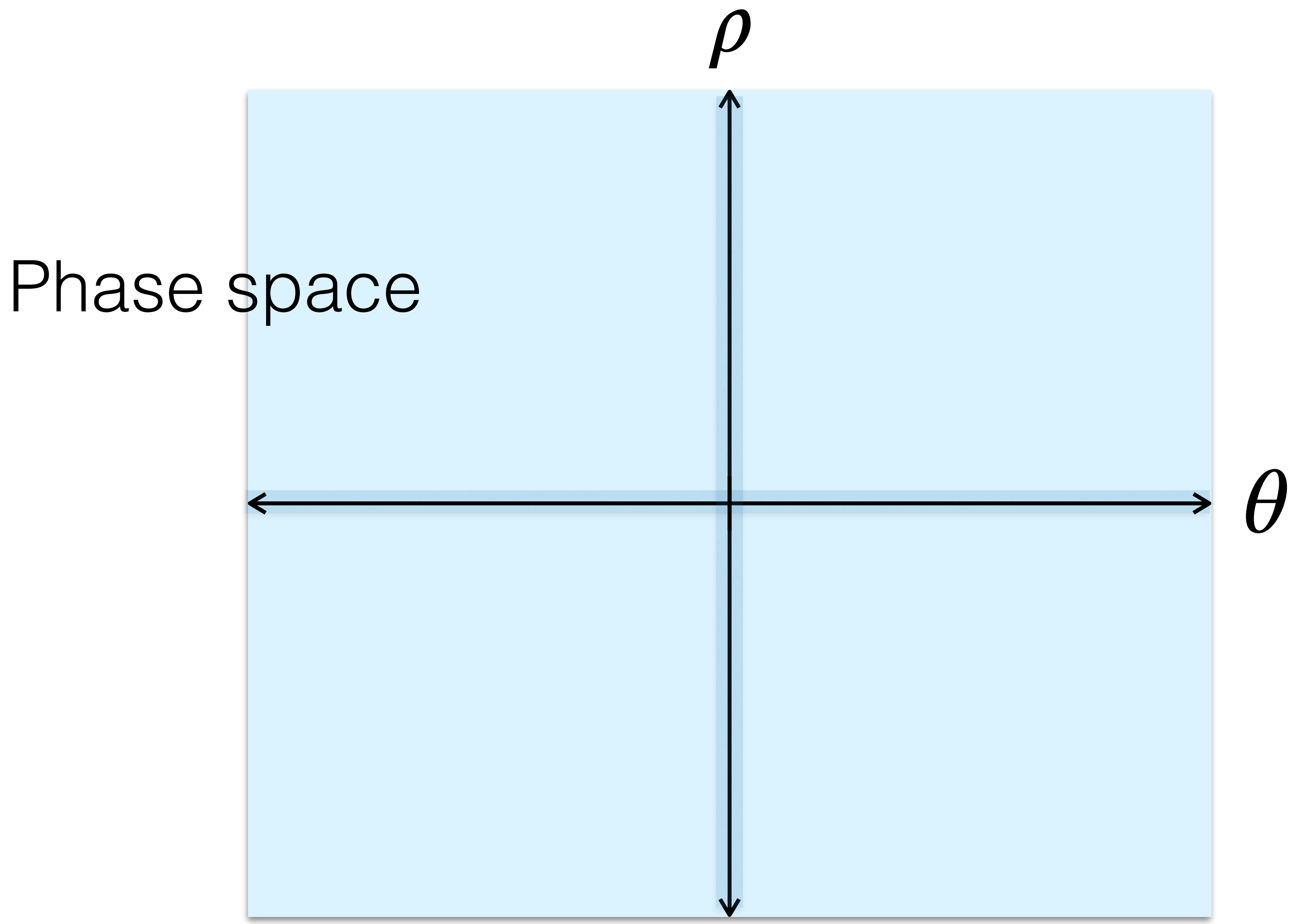
Phase space
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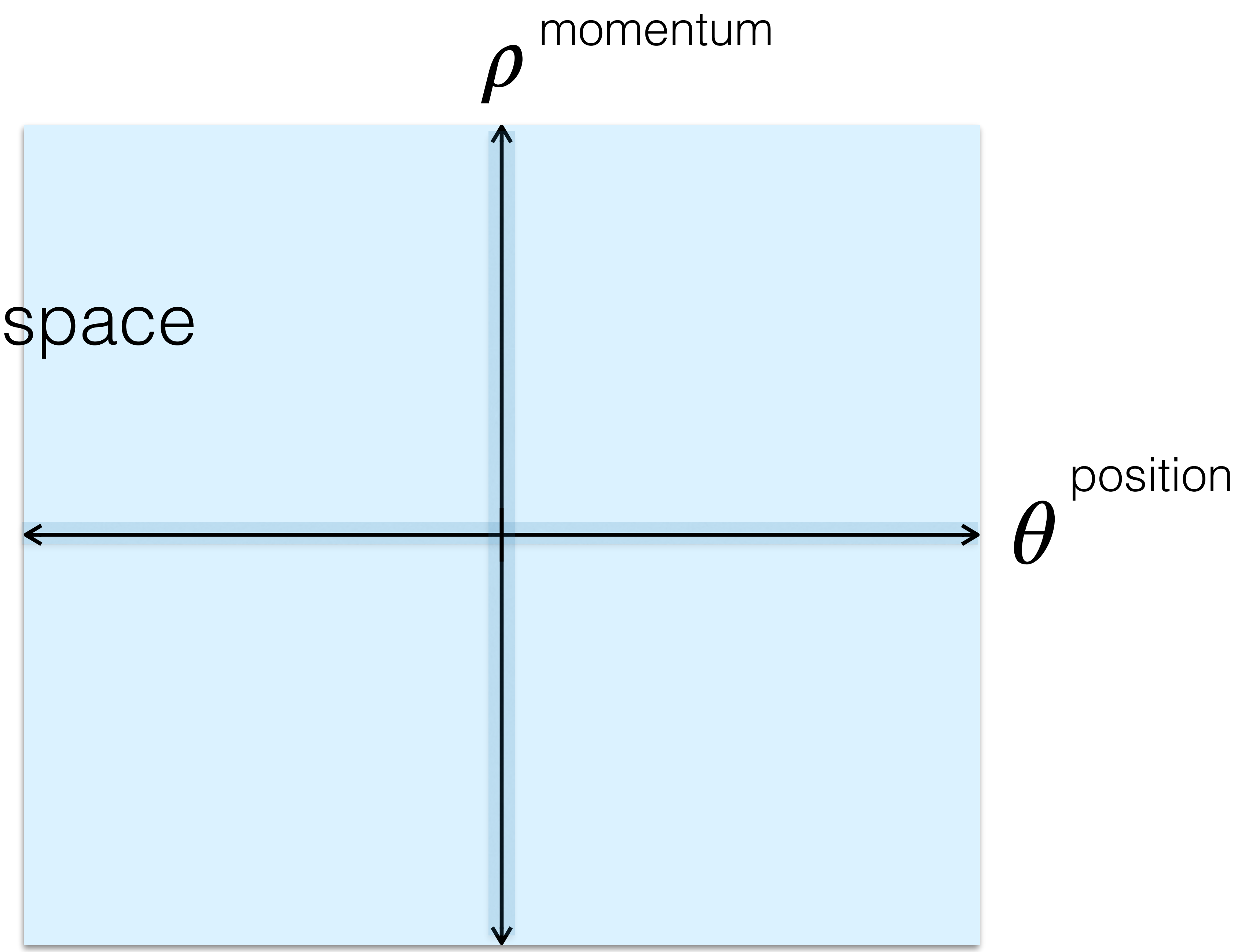

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$$\pi(\theta, \rho)$$

refer to the joint distribution of the parameters and momenta in phase space.

We can explore the the typical set of the target distribution by simulating **Hamiltonian dynamics** in phase space

Hamiltonian Function

$$
\begin{aligned}
\pi(\theta, \rho) &= \exp\{-H(\theta, \rho)\} \\
H(\theta, \rho) &= -\log \pi(\theta, \rho) \\
&= -\log \pi(\rho|\theta) - \log \pi(\theta) \\
&= \underbrace{K(\rho, \theta)}_{\text{kinetic}} + \underbrace{V(\theta)}_{\text{potential}}
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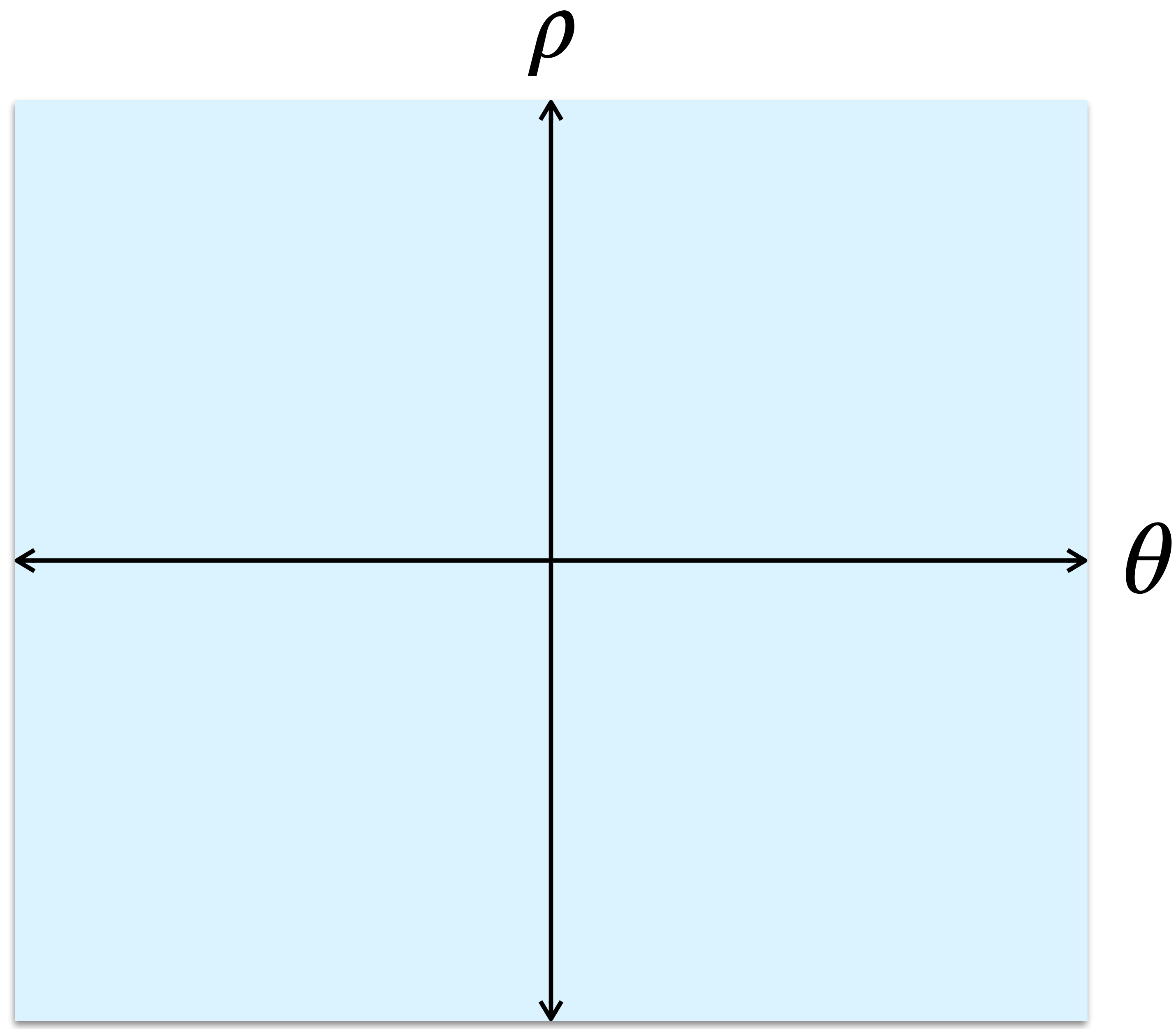
gradient of (log) target dist.

Phase space decomposes into concentric **energy** level sets



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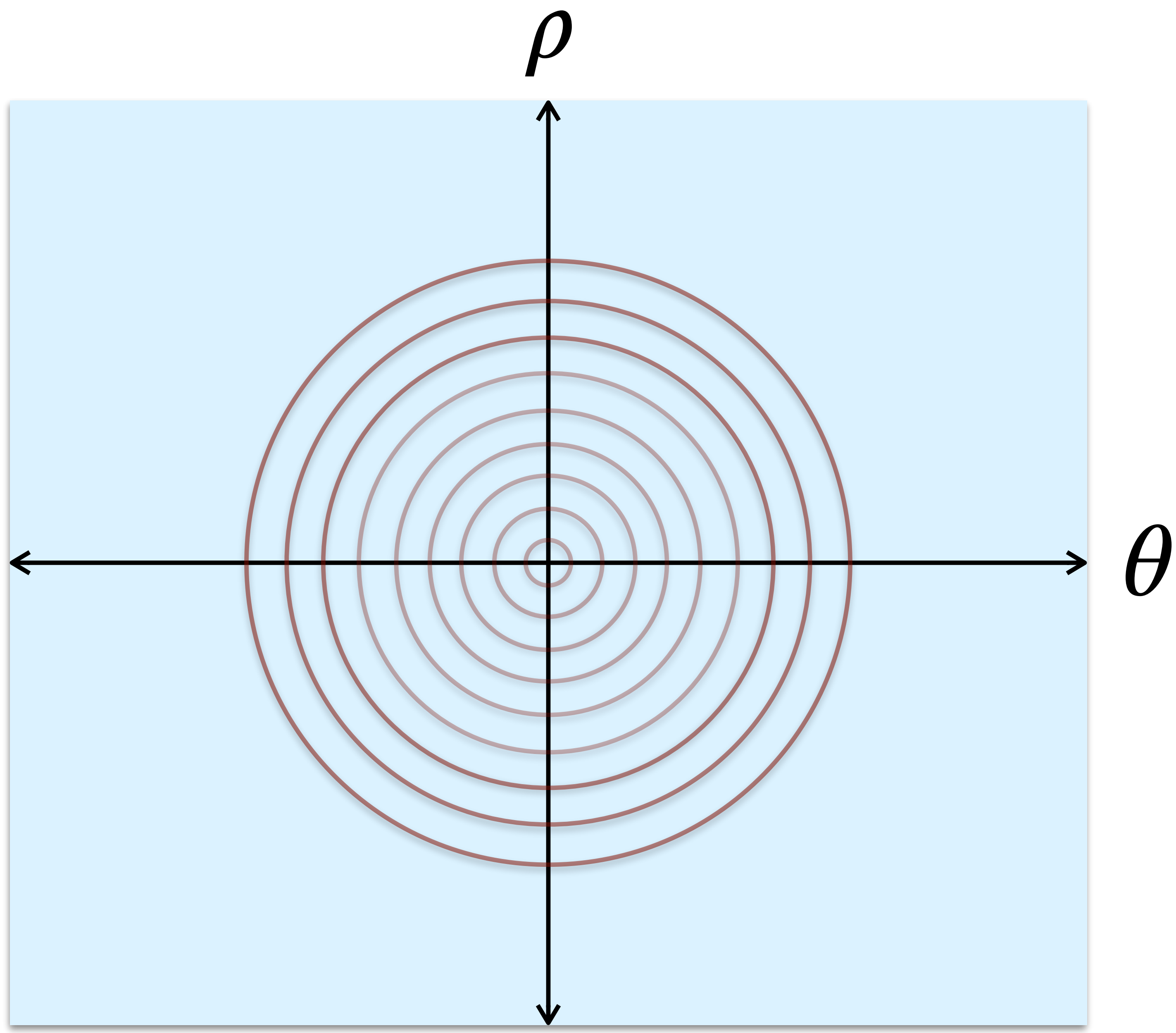

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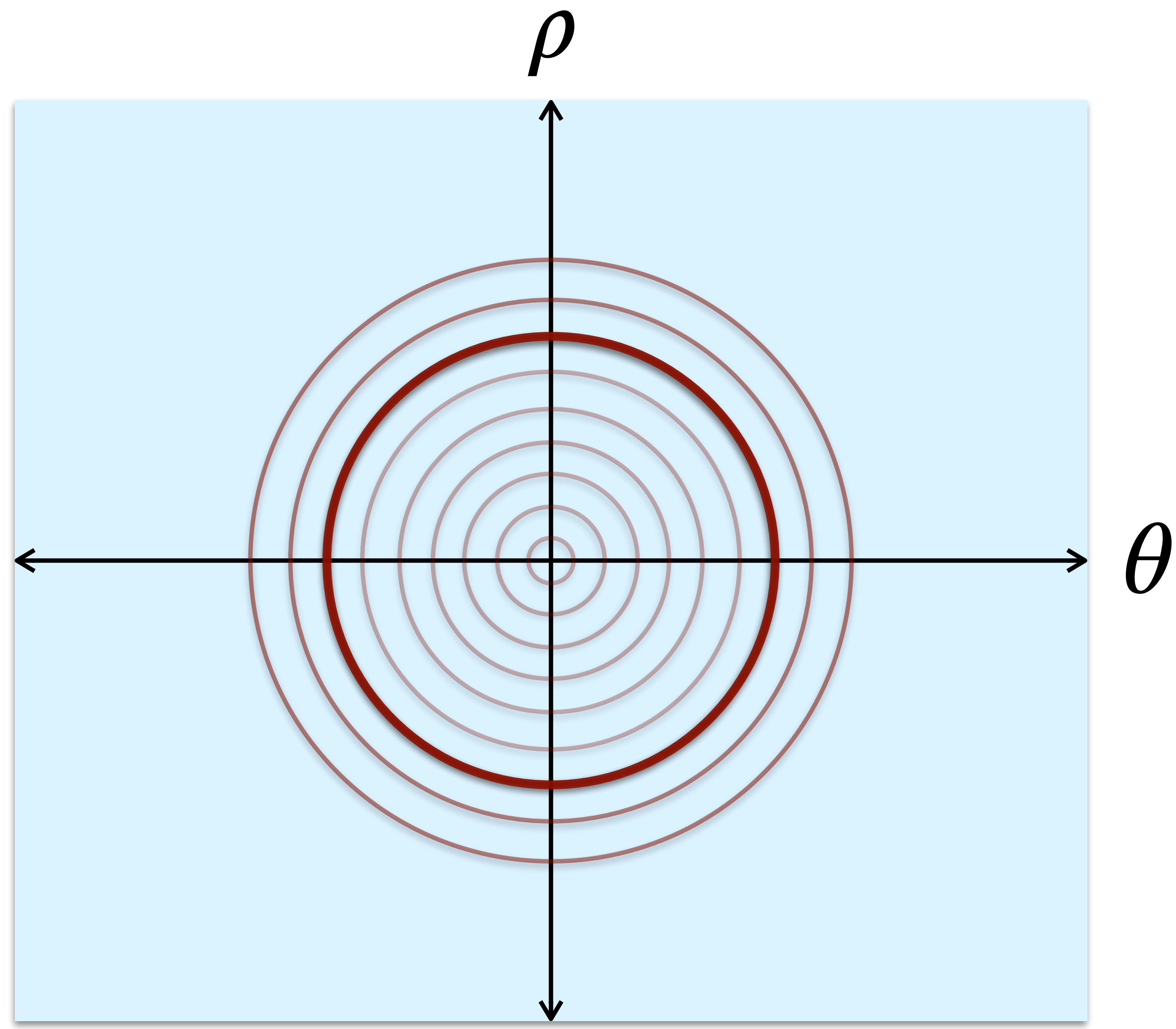
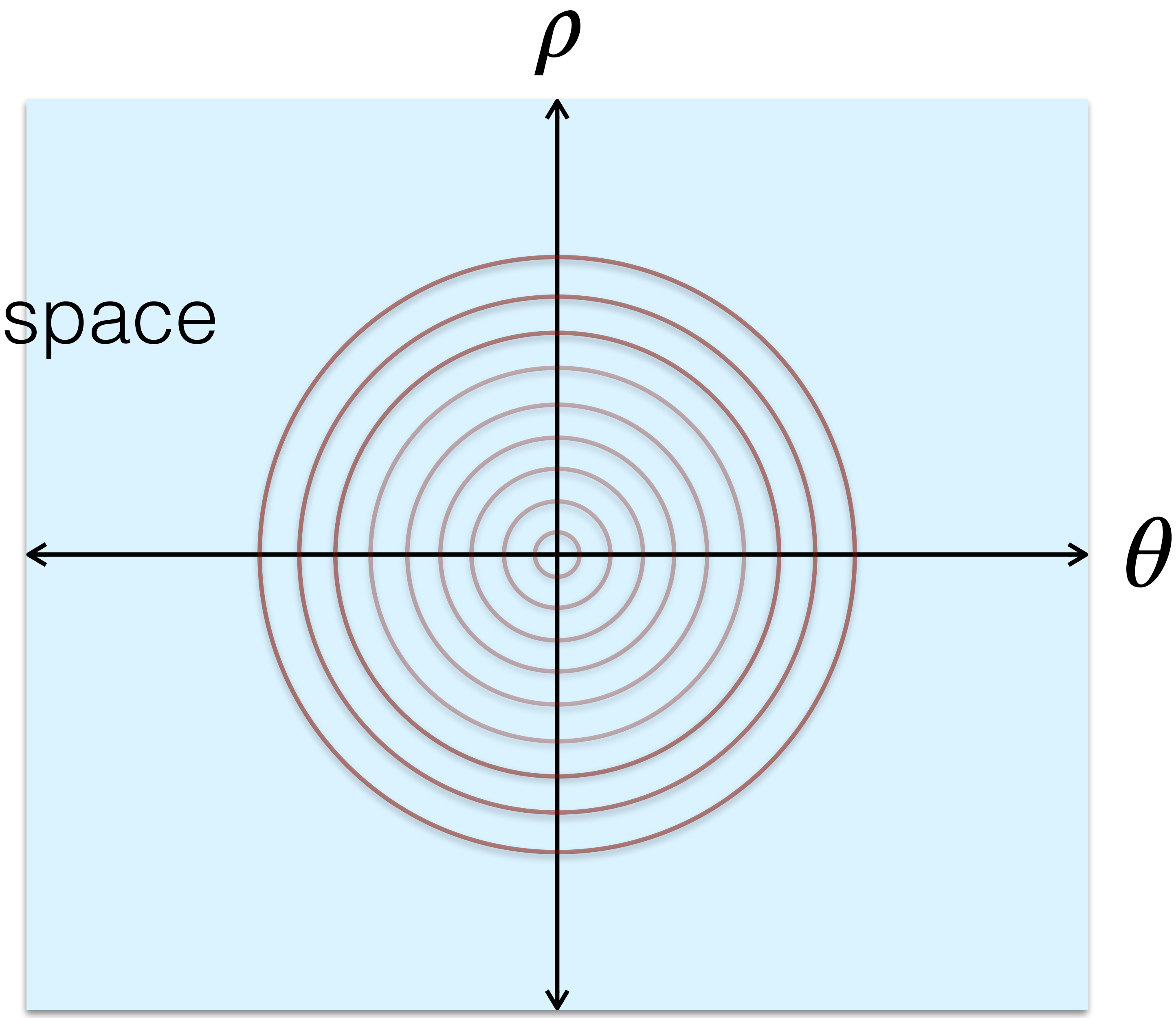


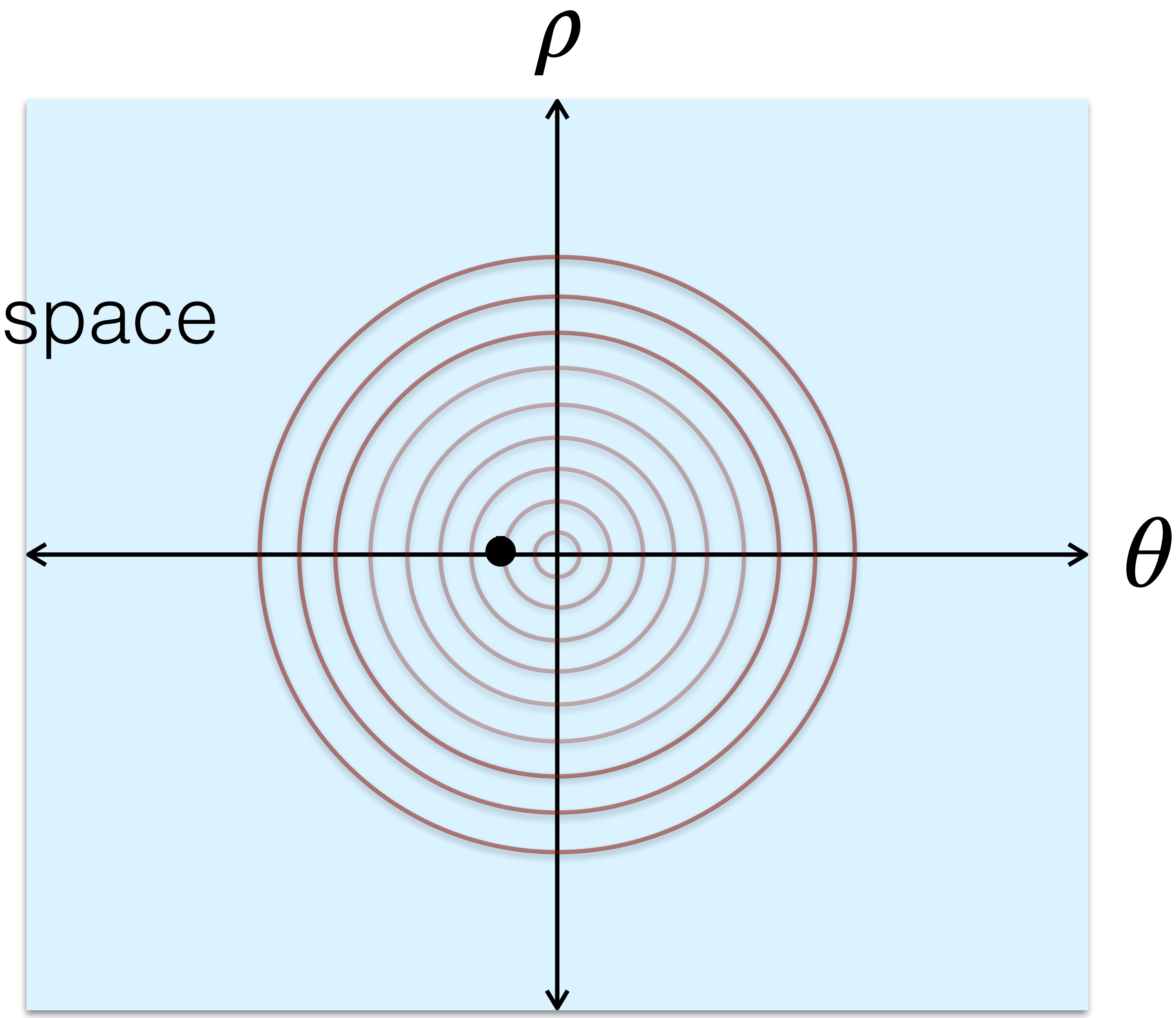
$$H^{-1}(E) = \{\theta, \rho \mid H(\theta, \rho) = E\}$$

Pick an initialization point

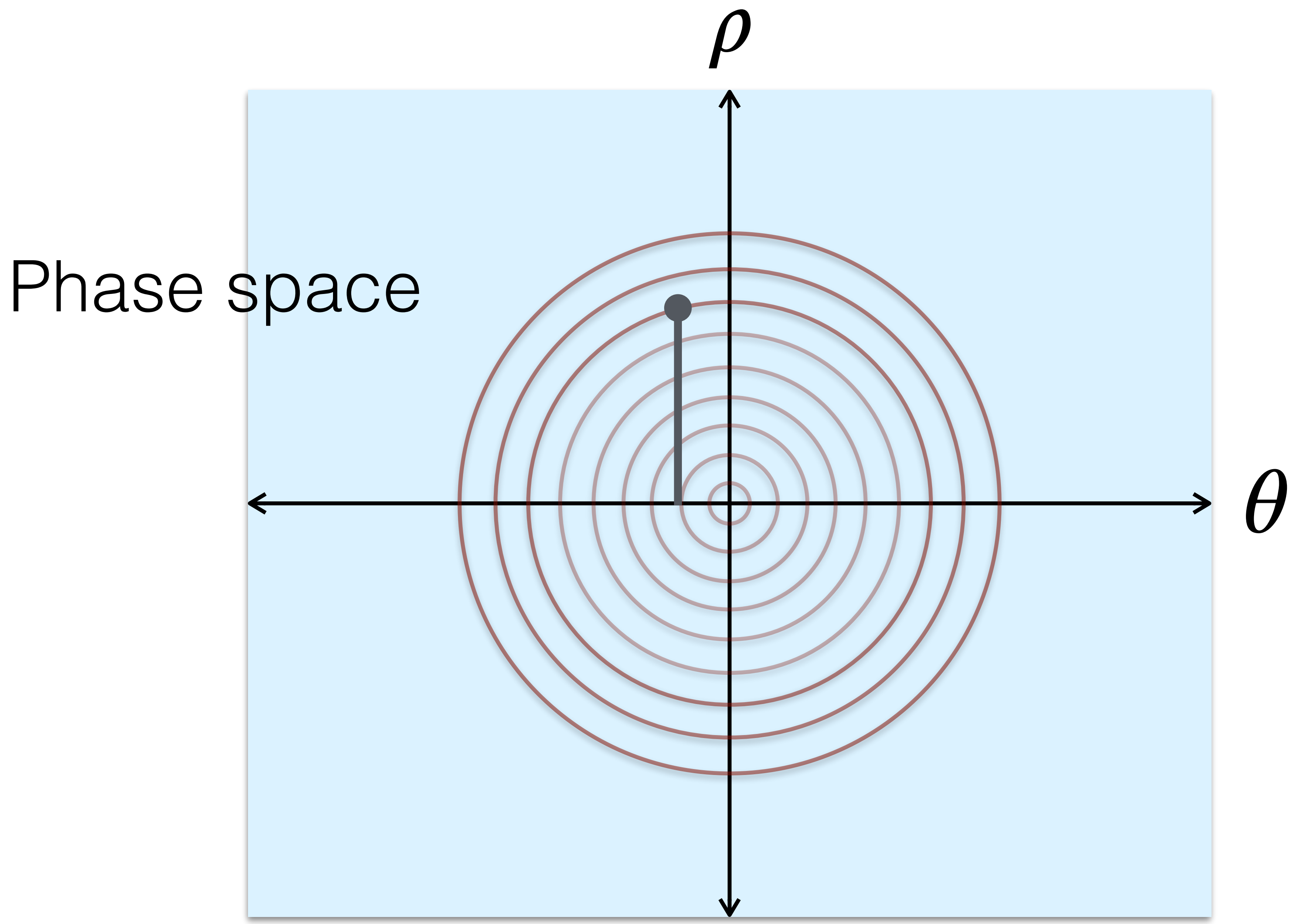


Pick an initialization point

Phase space



Sample momenta to lift into phase space



Deterministic exploration within energy levels sets

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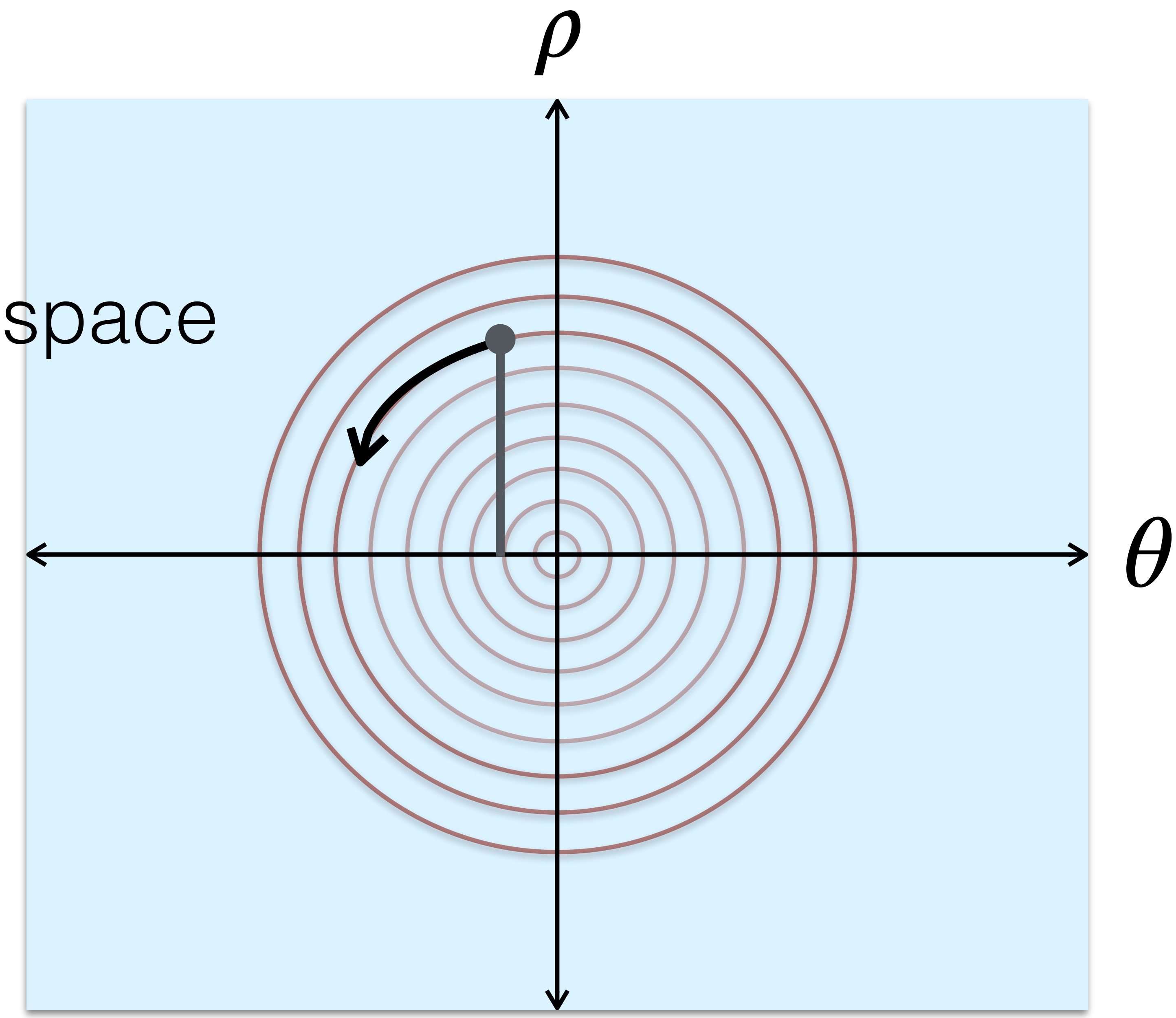

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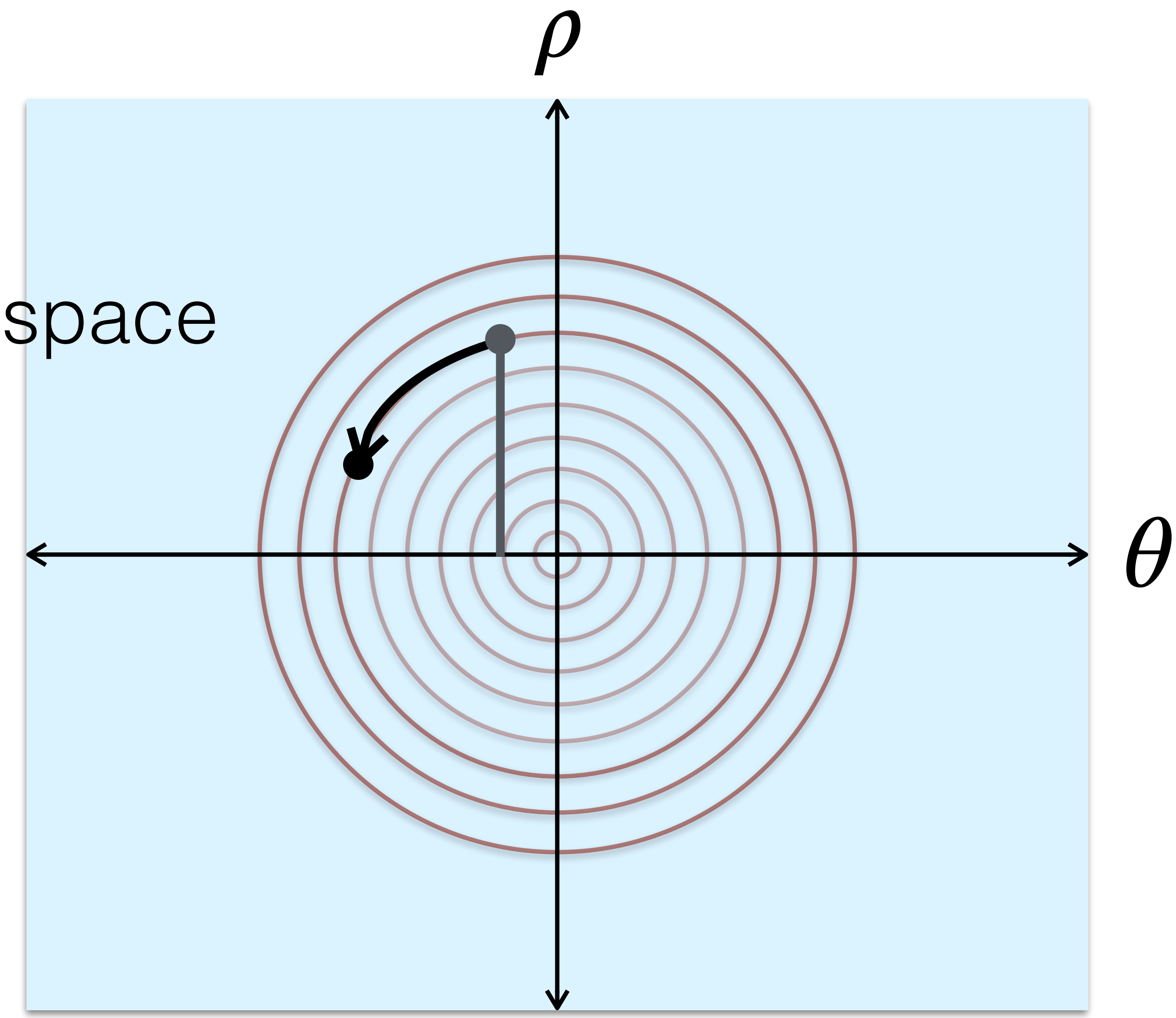
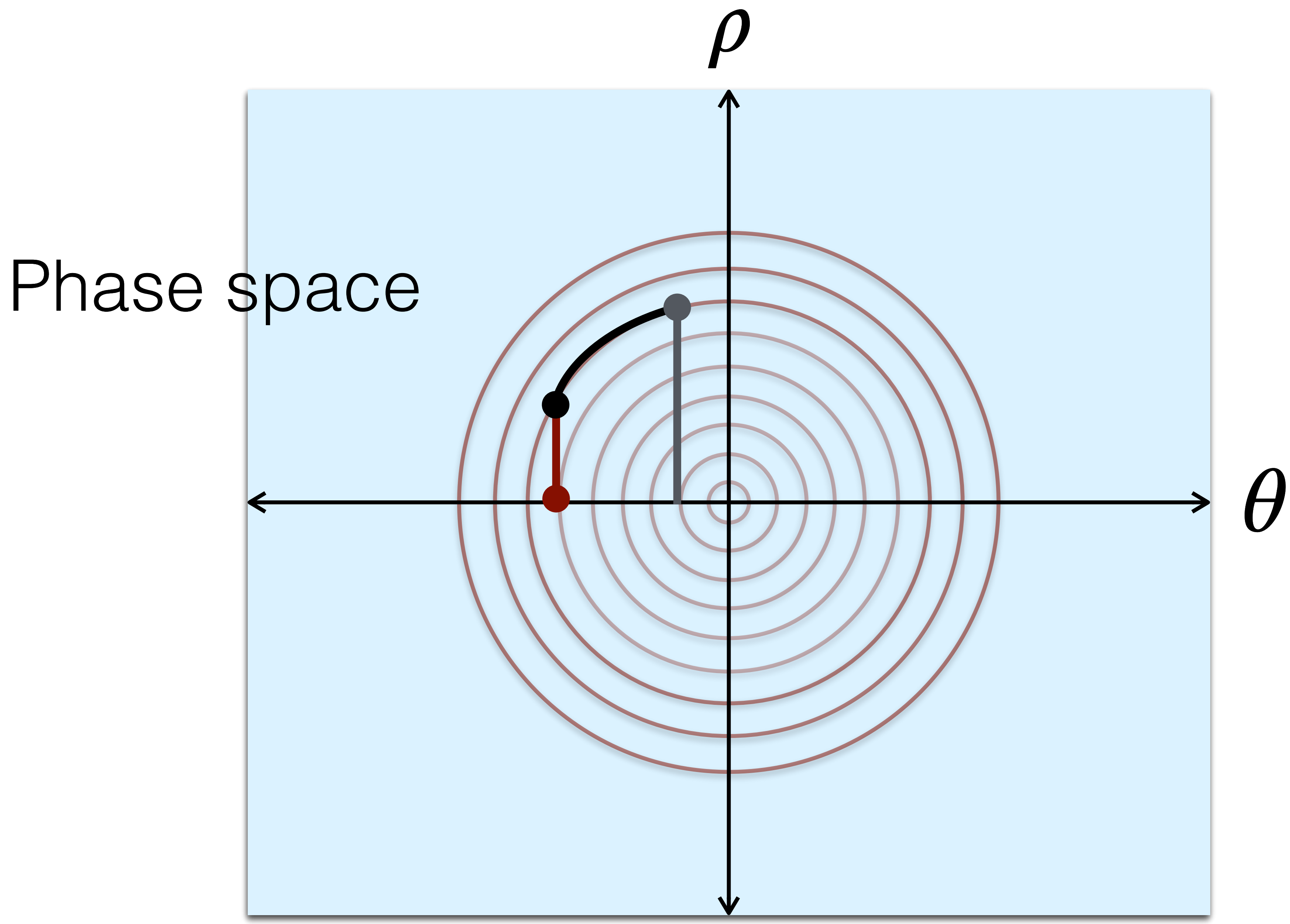
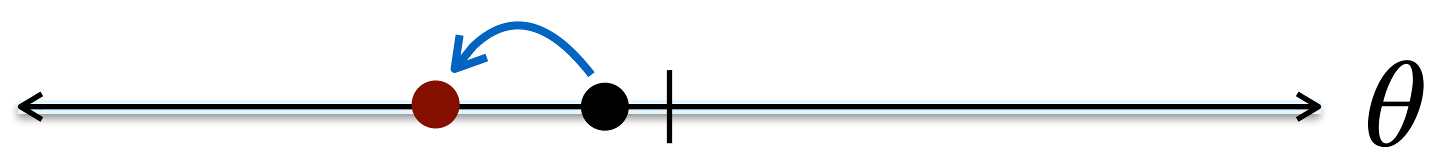


Project back down to parameter space

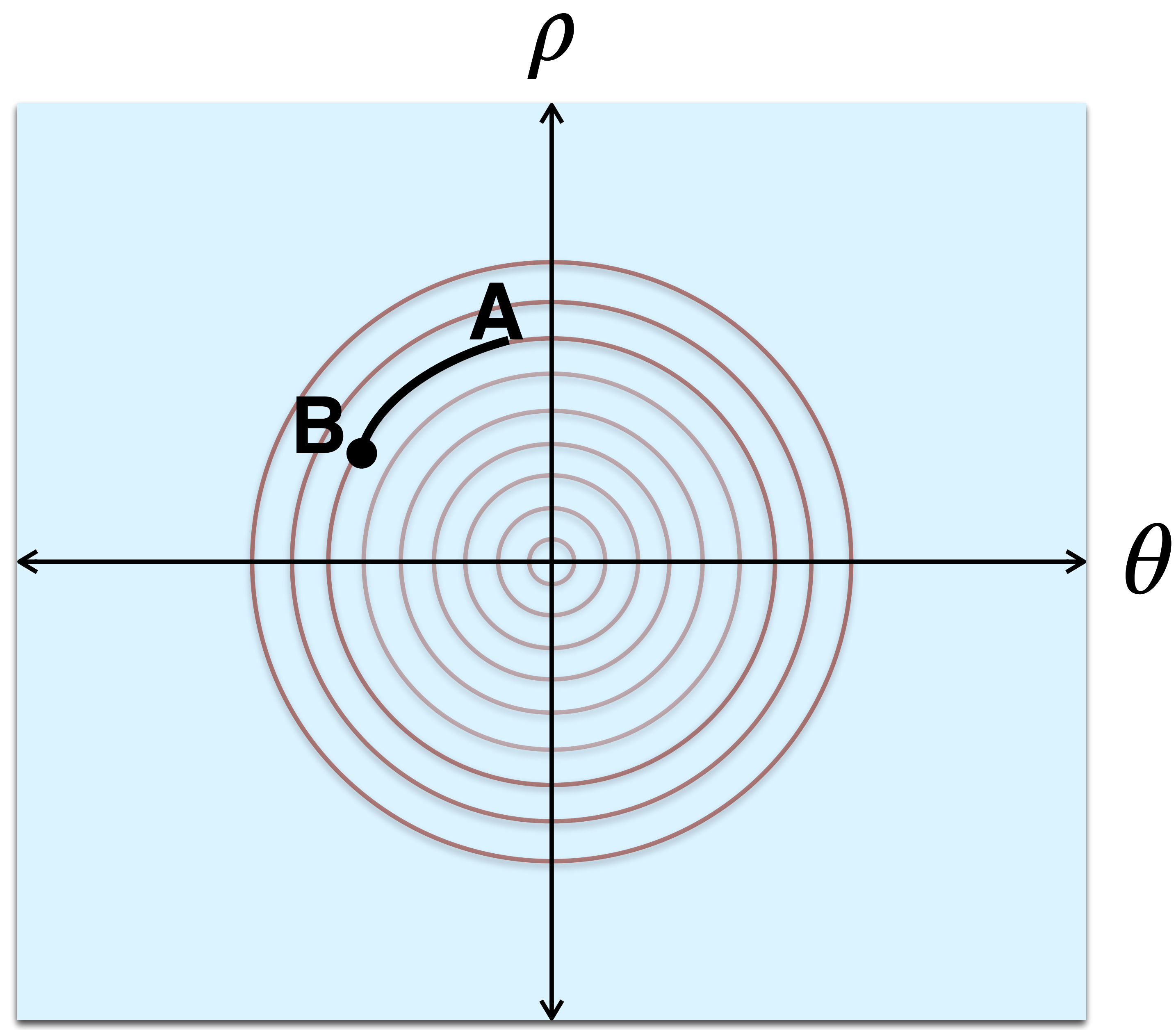


The auxiliary momenta are discarded and we are left with a point in the typical set of the target distribution

Parameter space



In that middle step, how did we actually get from point **A** to point **B**?



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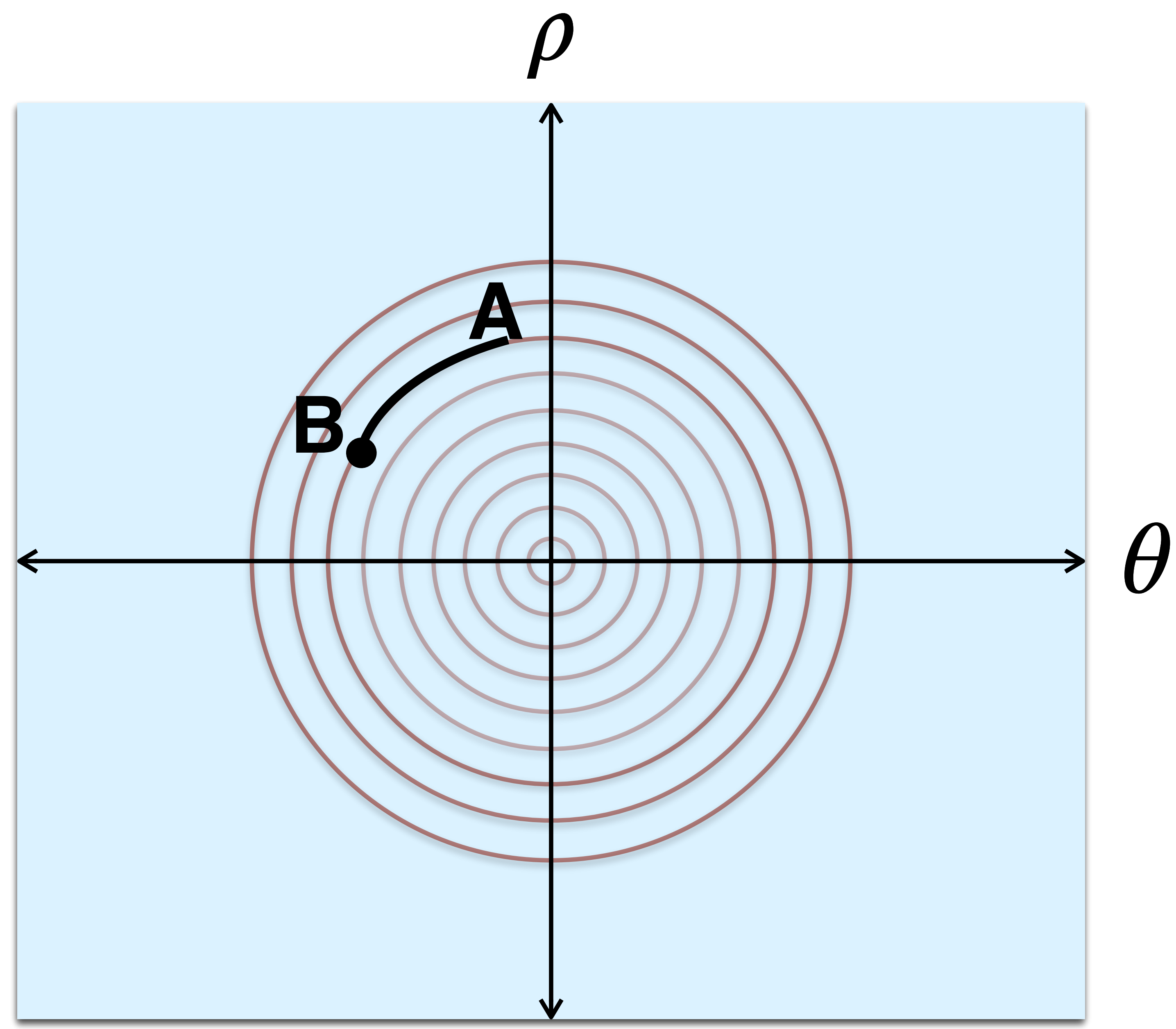

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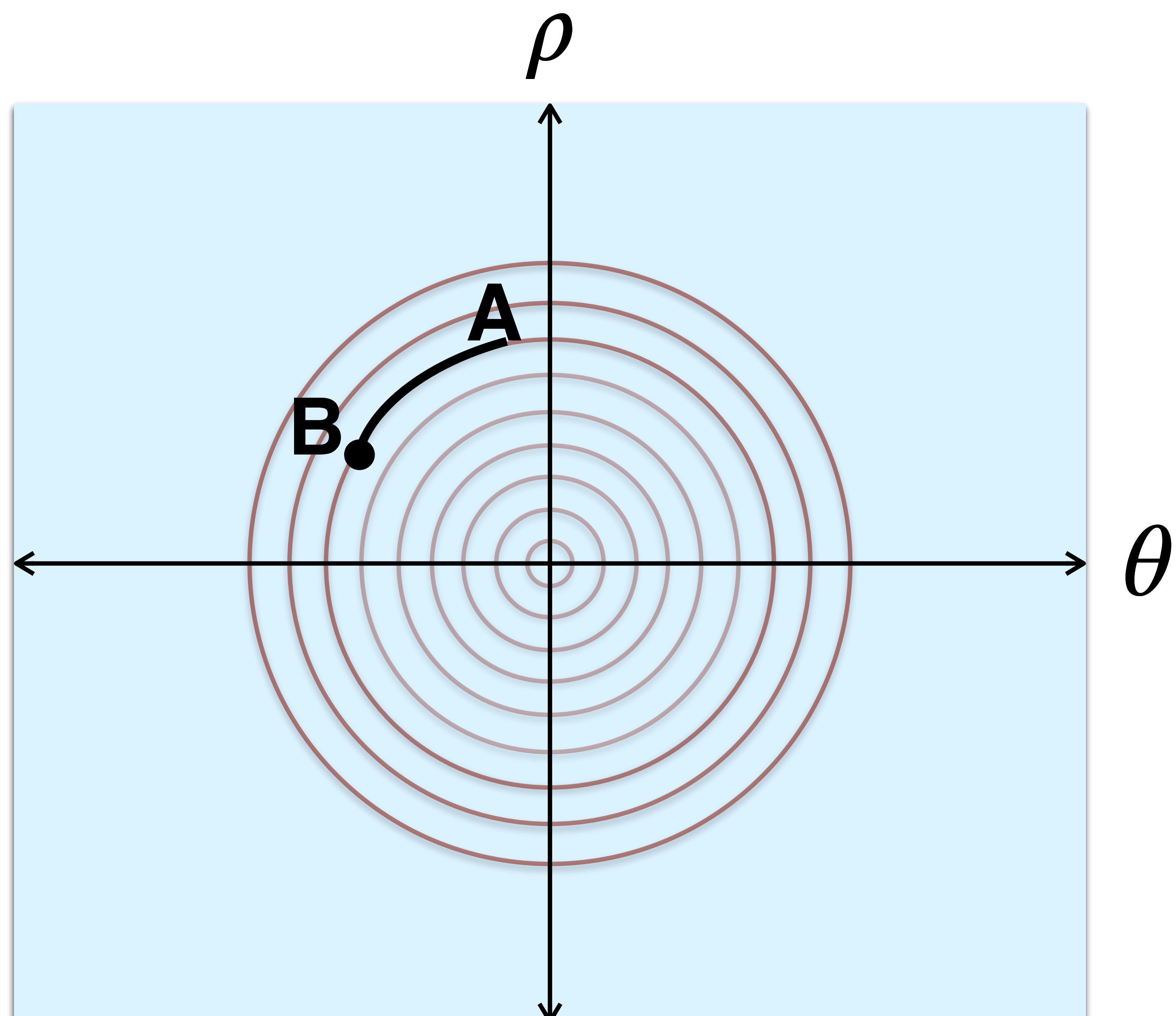
  - Informed by geometry of the system



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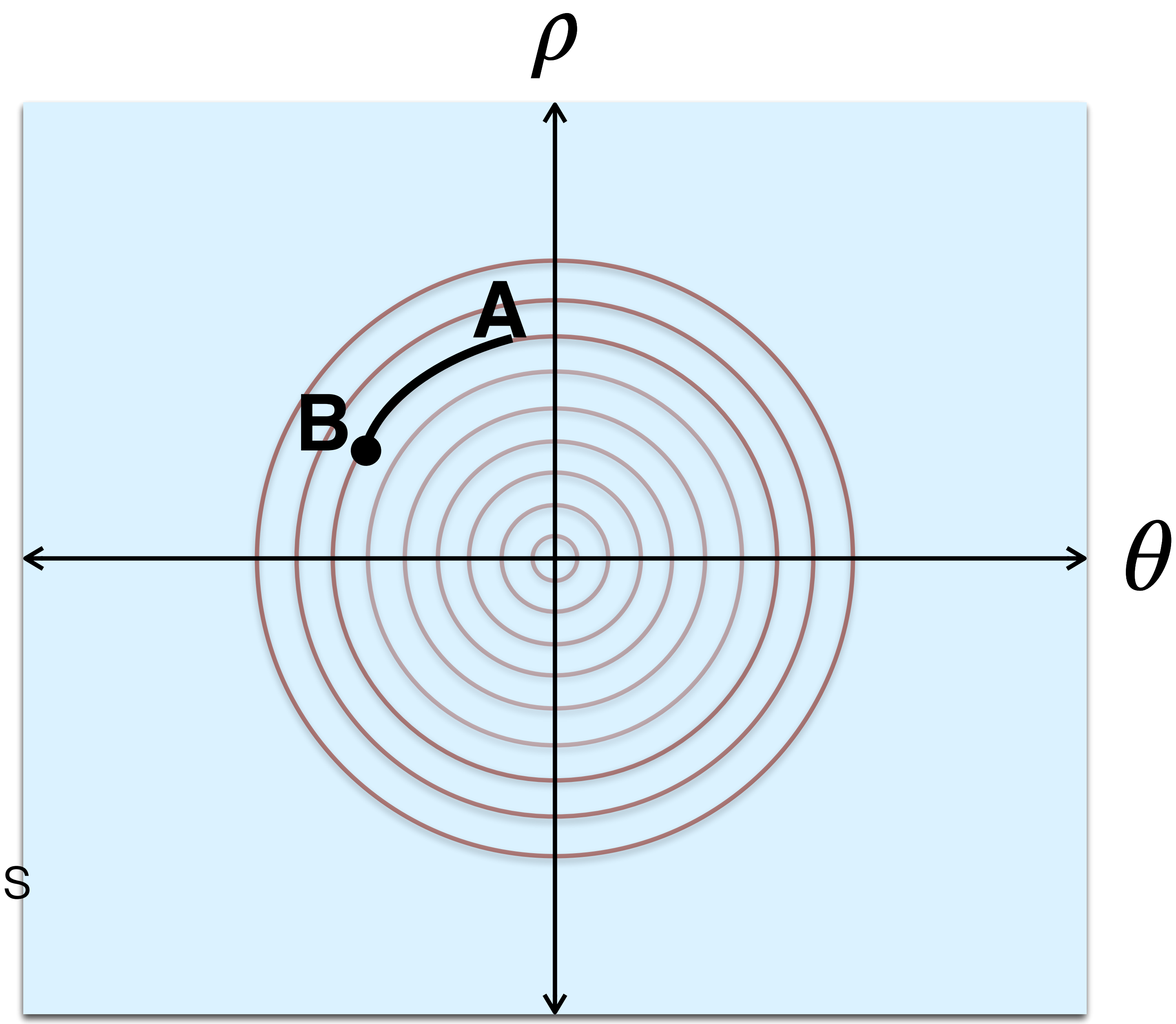
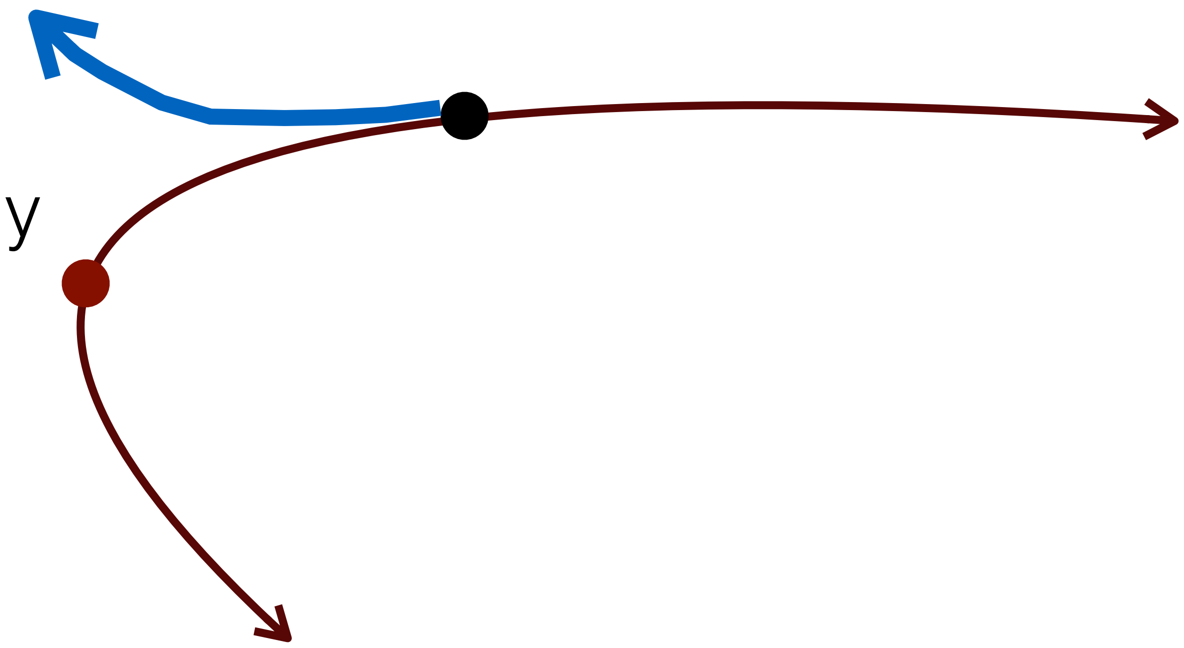
- Motivates new MCMC diagnostics
  - Divergent transitions
  - Comparison of marginal & conditional energy distributions



Most numerical integrators suffer from drift

- Trajectories deviate from typical set
- The size of the error increases rapidly with dimension



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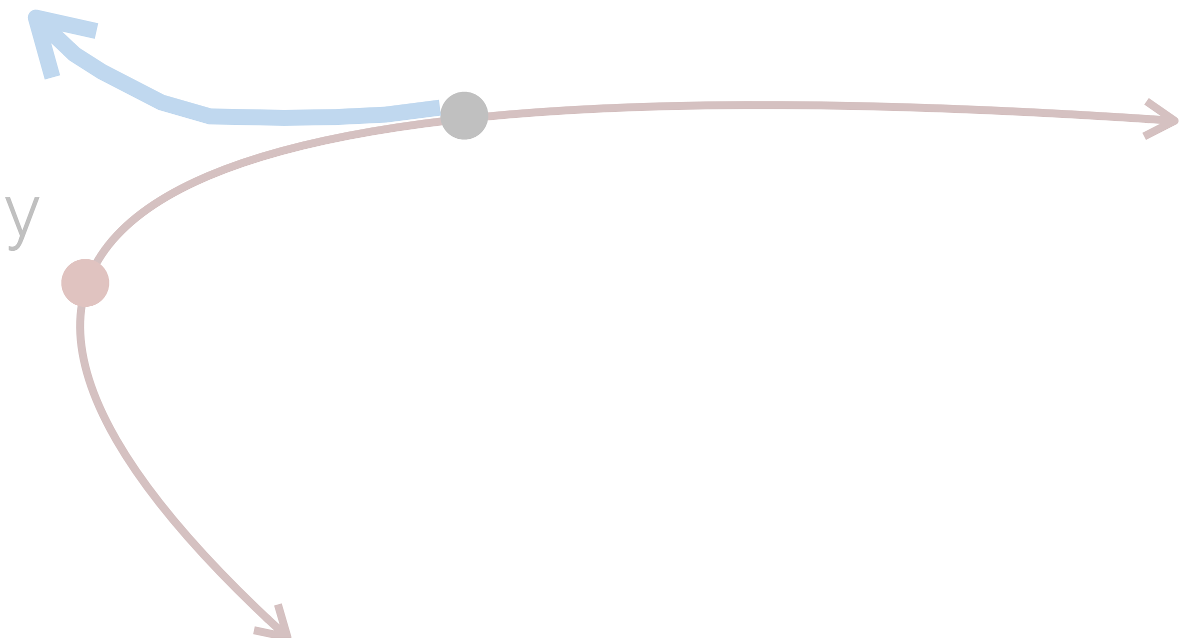
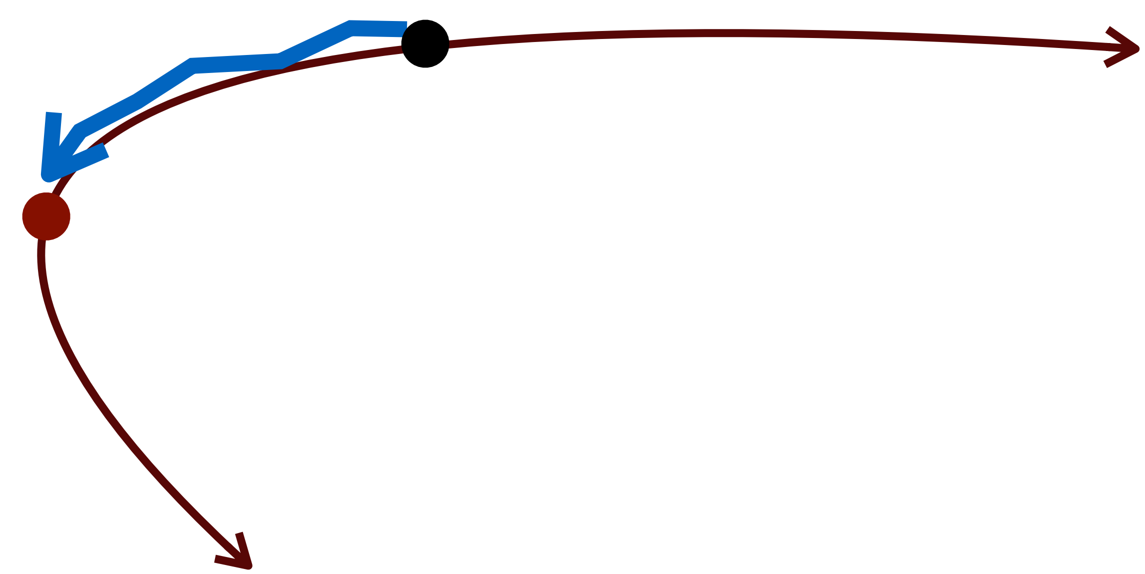


Symplectic integrators preserve volume in phase space

- Trajectories oscillate around exact energy level set, even for long integration times
- Scale well to higher dimensions
- Pathologies easy to diagnose (divergence)



Comparison of algorithms on **highly correlated** 250-dimensional Gaussian distribution

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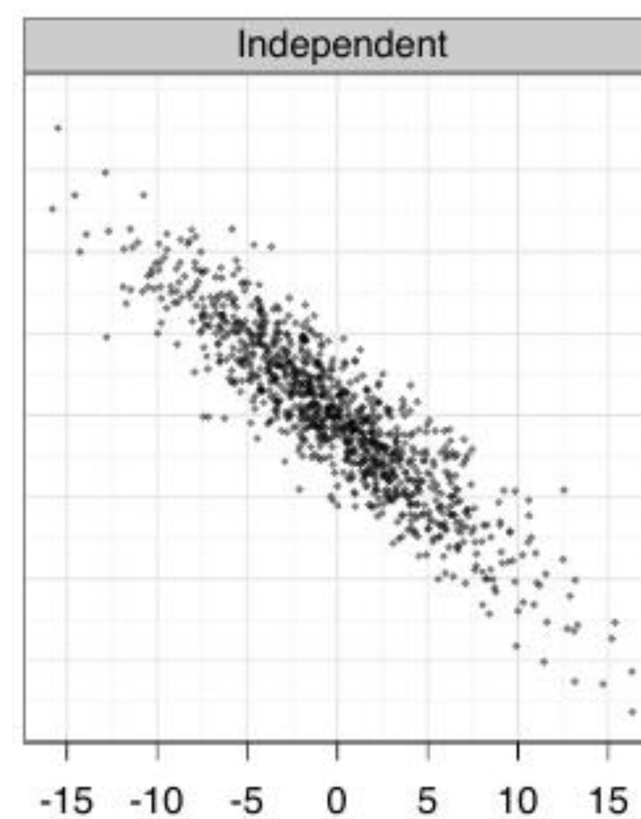

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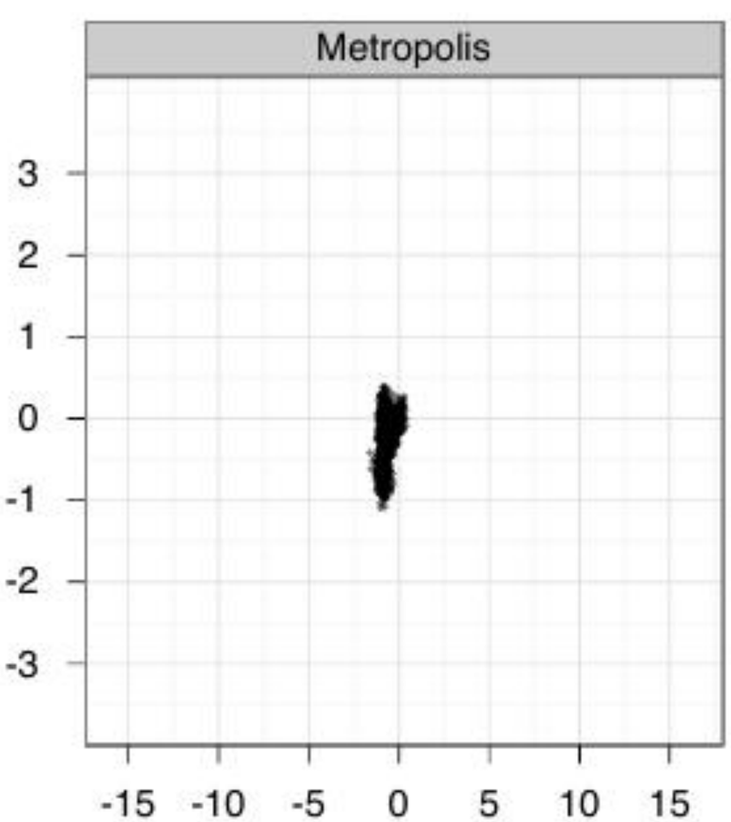

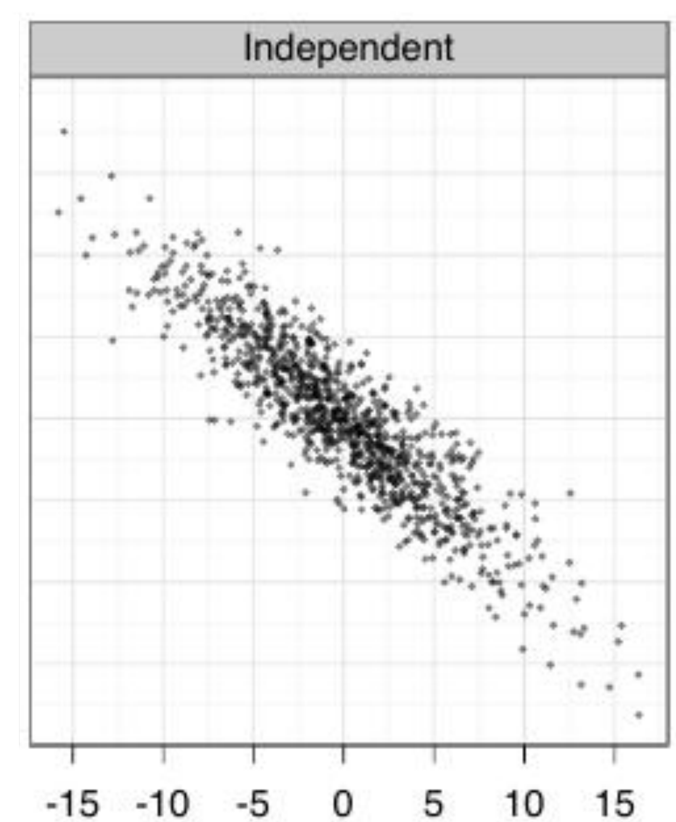

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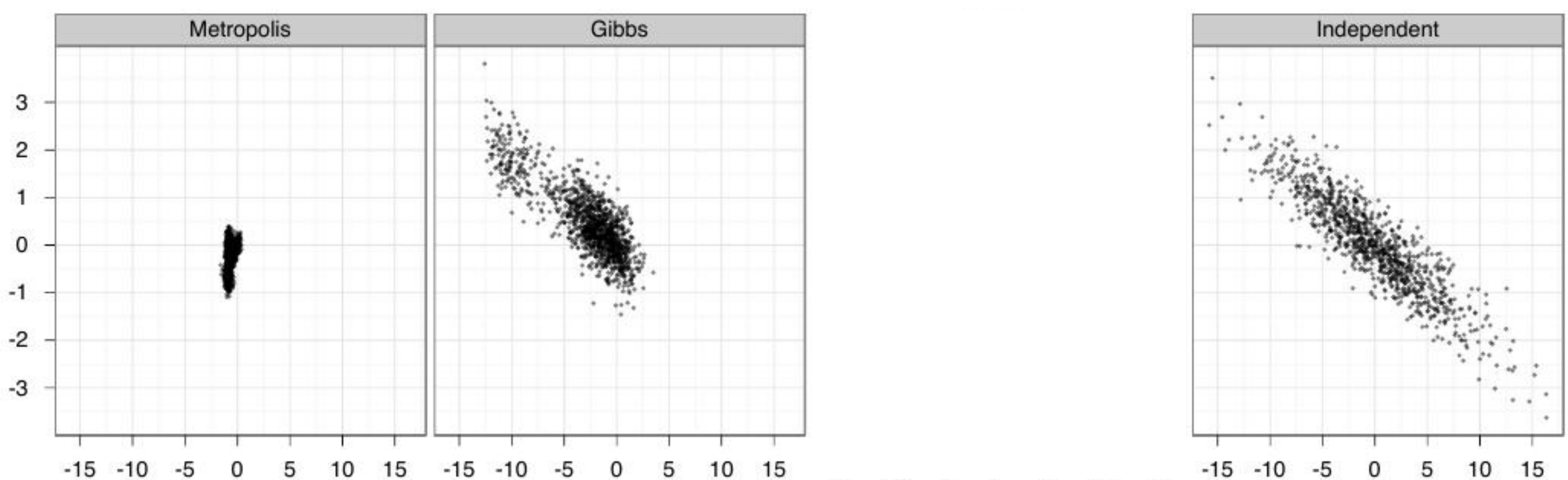

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