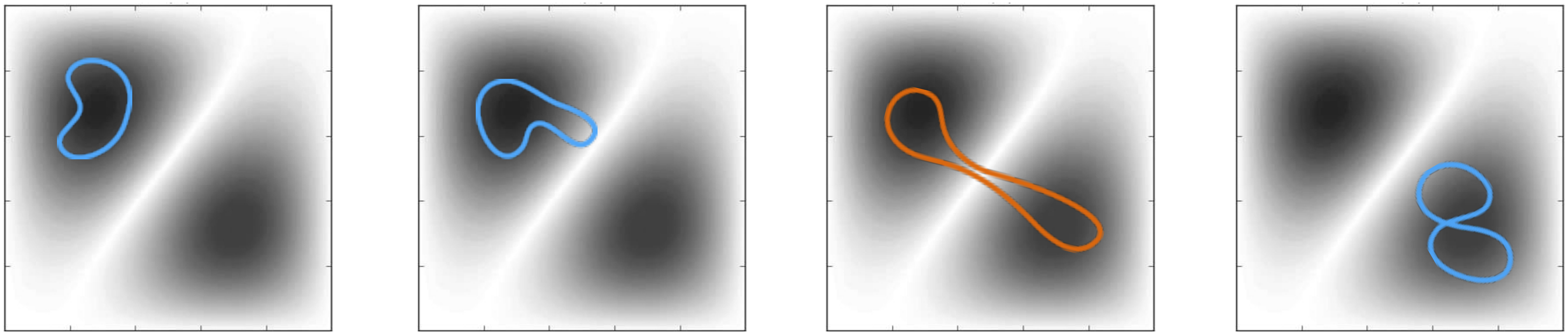


Quantum Monte Carlo Tunneling from Quantum Chemistry to Quantum Annealing

Guglielmo Mazzola (Institute Theoretical Physics, ETH, Zurich)

M. Troyer (Microsoft ← ETH)
S. Isakov, V. Smelyanskiy (Google)

1. Motivation: Quantum Annealing
2. Tunneling with Quantum Monte Carlo
3. "Is a simulated Quantum Computer (QC) faster than a real QC?"
4. Implication for realistic systems: quantum reaction rates from PIMC?

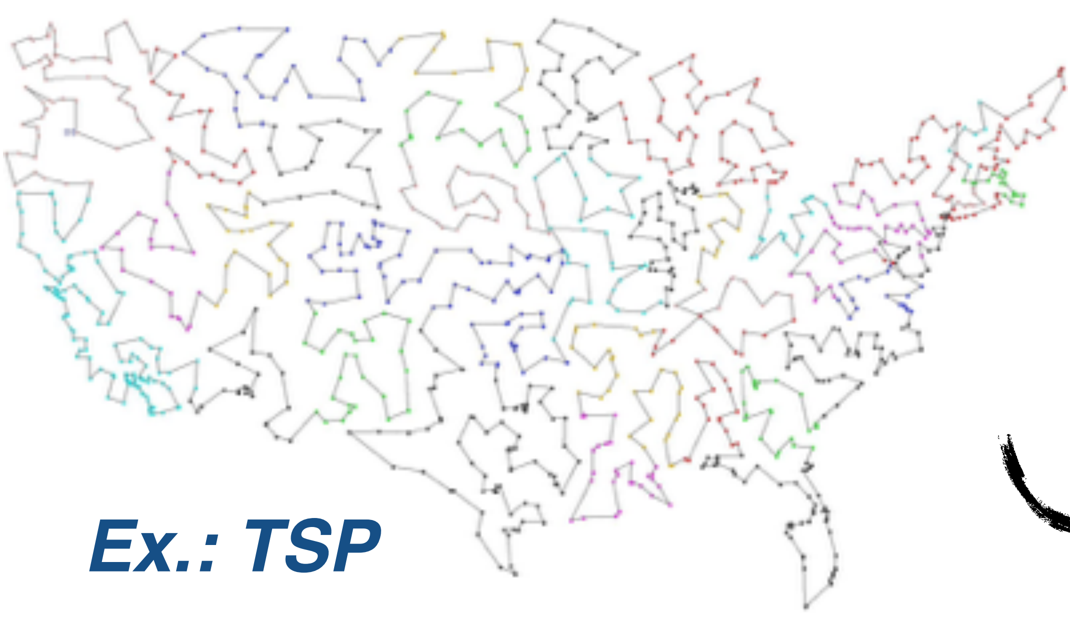
5. Many body quantum state tomography with Neural Networks

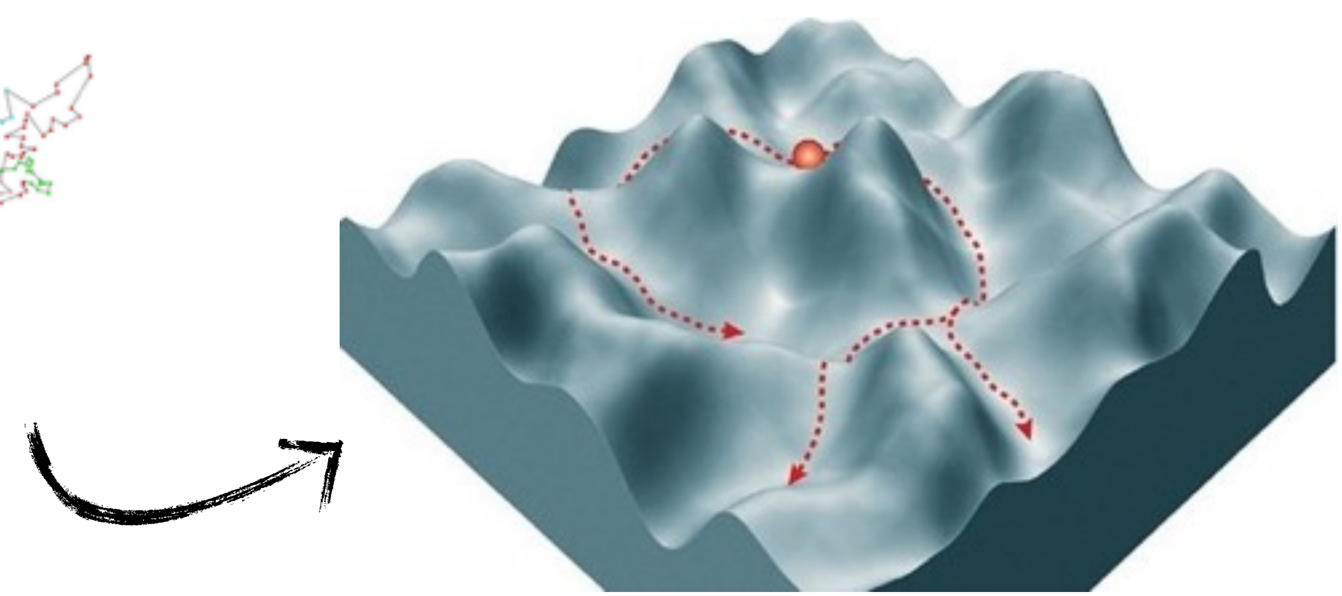
Outline

Hard optimization problems

Find an optimal solution among several possibilities.

Encode the problem into a **cost function**, s.t. the solution is optimal when we find the **global minimum** of this function.



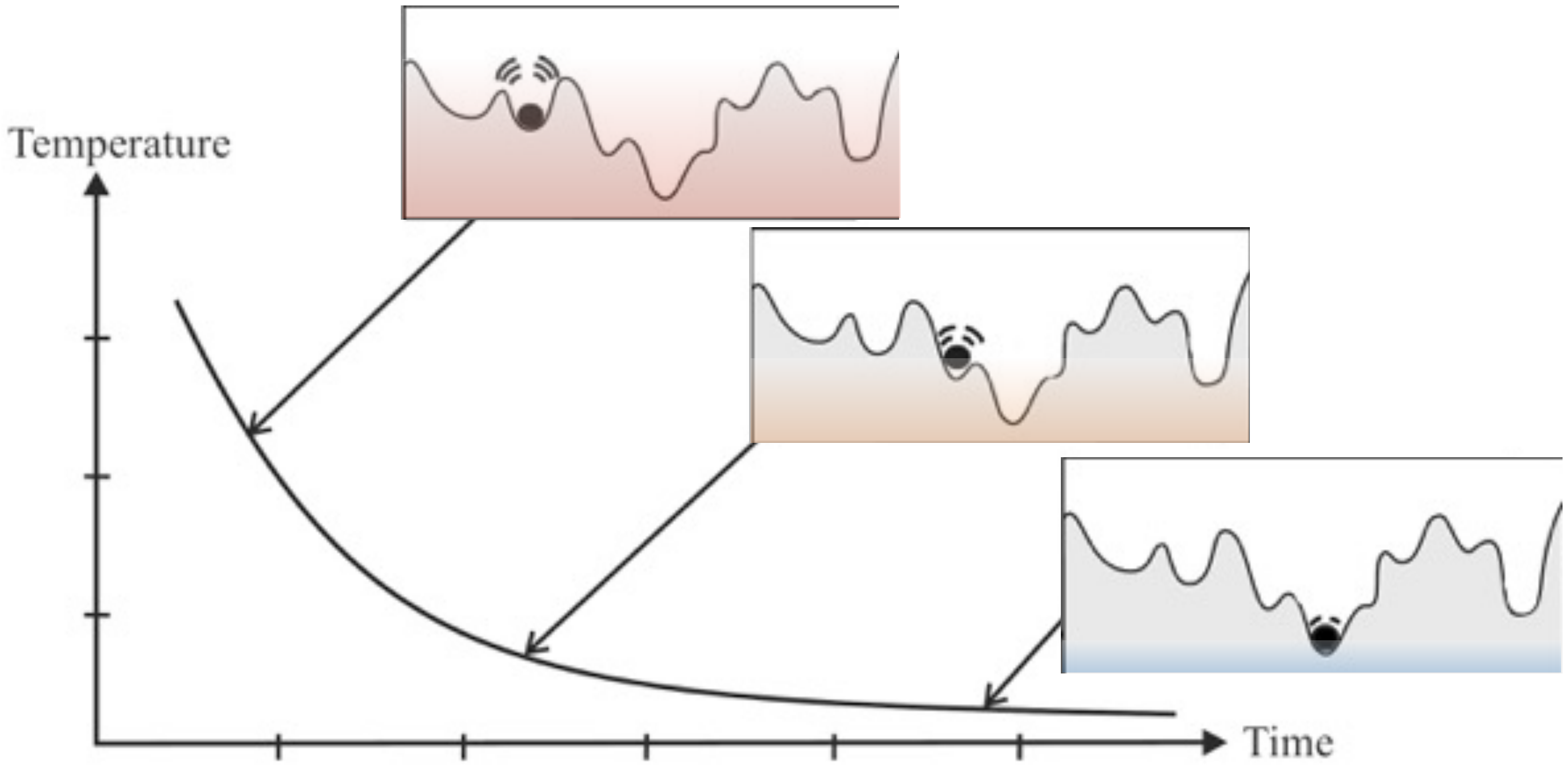


The (exponentially) large number of **local minima** makes the problem hard.

The Classical approach (benchmark)

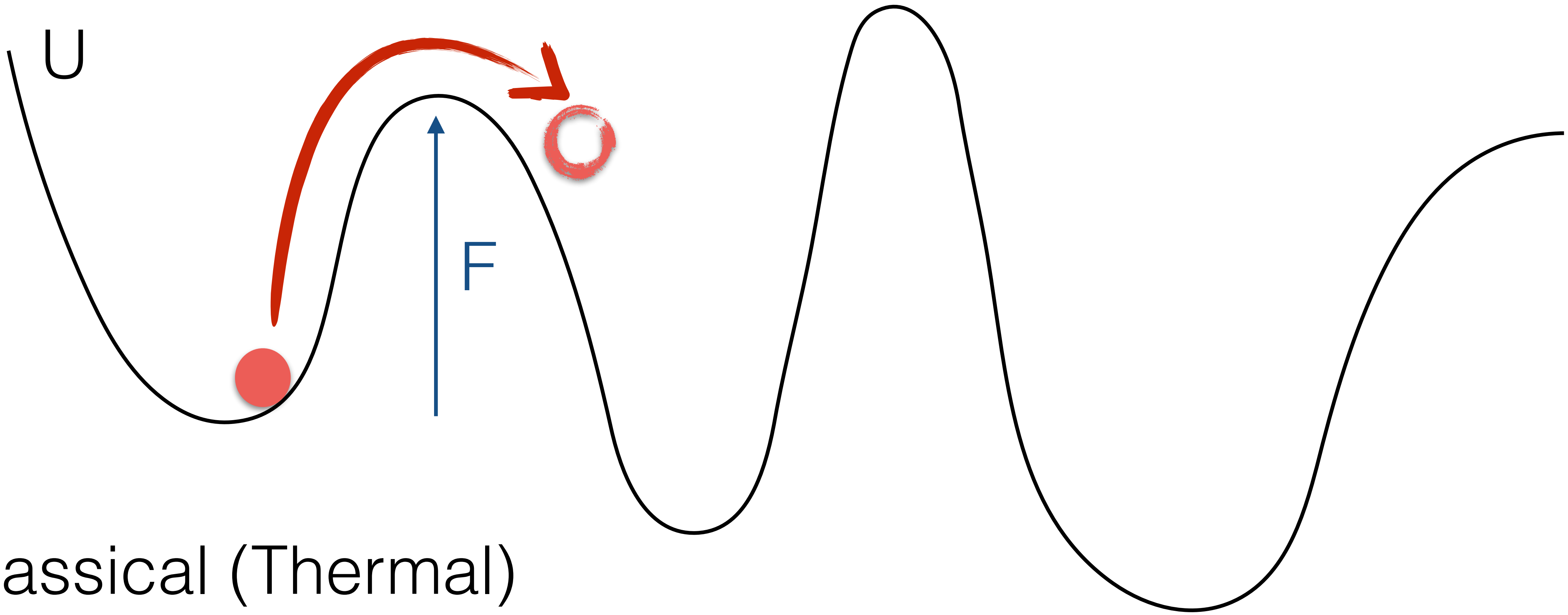
Annealing: *slowly* cooling a material to eliminate defects, i.e. reach the stable crystal configuration.

Simulated Annealing: *emulates this process with MC*



Classical vs Quantum

Efficiency = overcoming energy barriers.

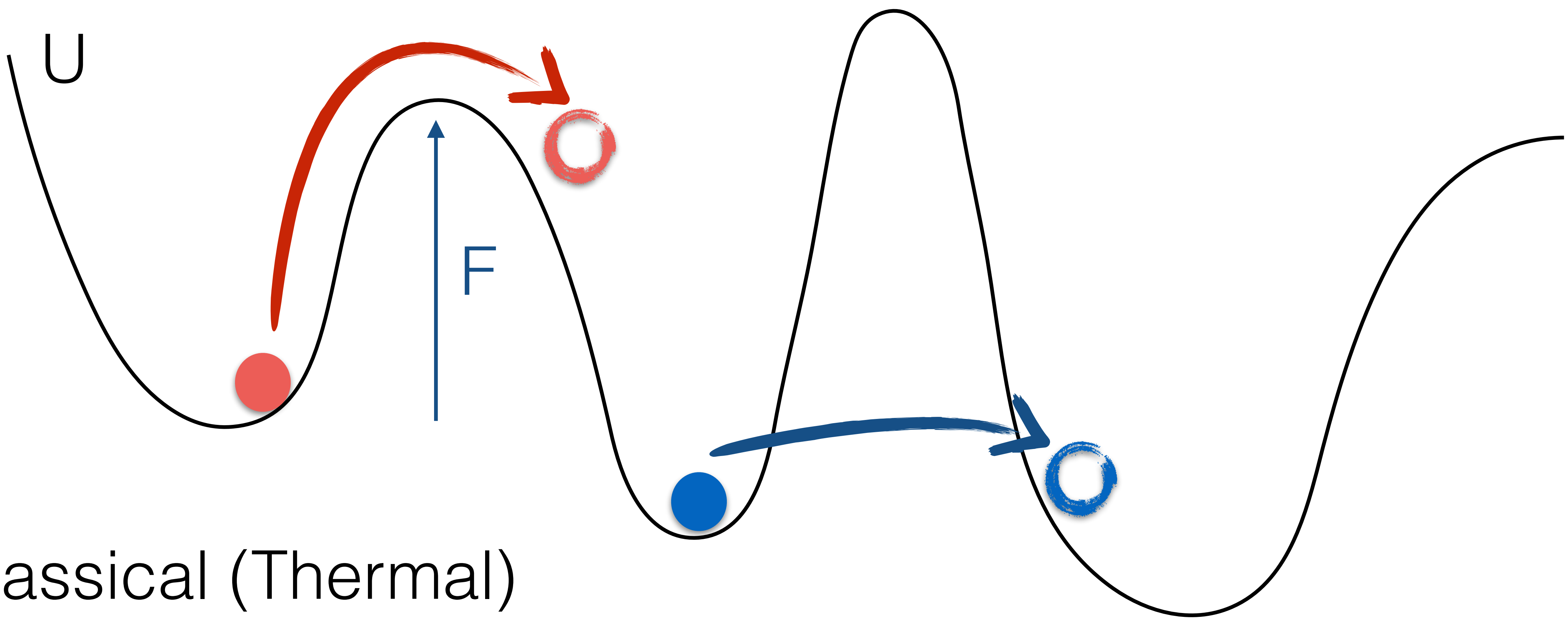


Classical (Thermal)

Prob.  = $\exp(-F/kT)$

Classical vs Quantum

Efficiency = overcoming energy barriers.



Classical (Thermal)

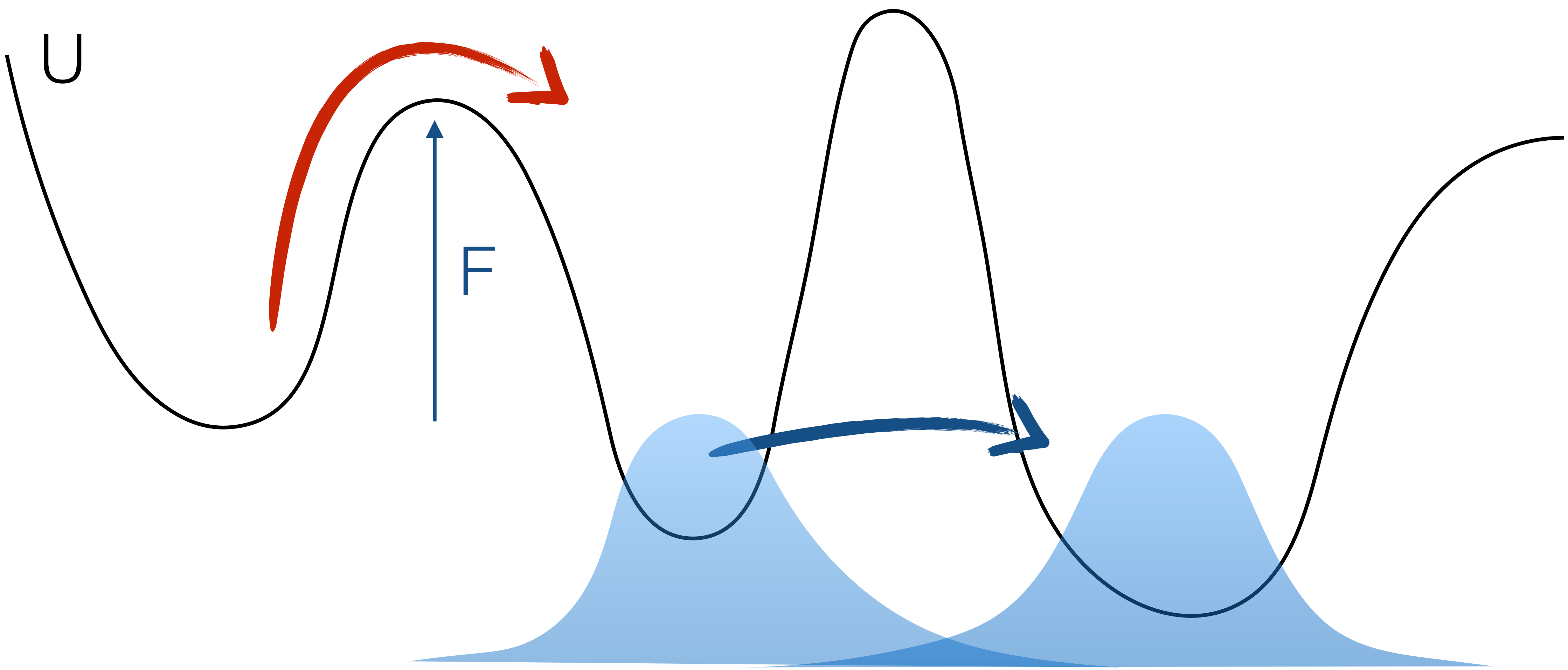
Prob. → = exp(- F/kT)

Quantum (Tunneling)

Prob. → $= \Delta^2$

Classical vs Quantum

Efficiency = overcoming energy barriers.



overlap

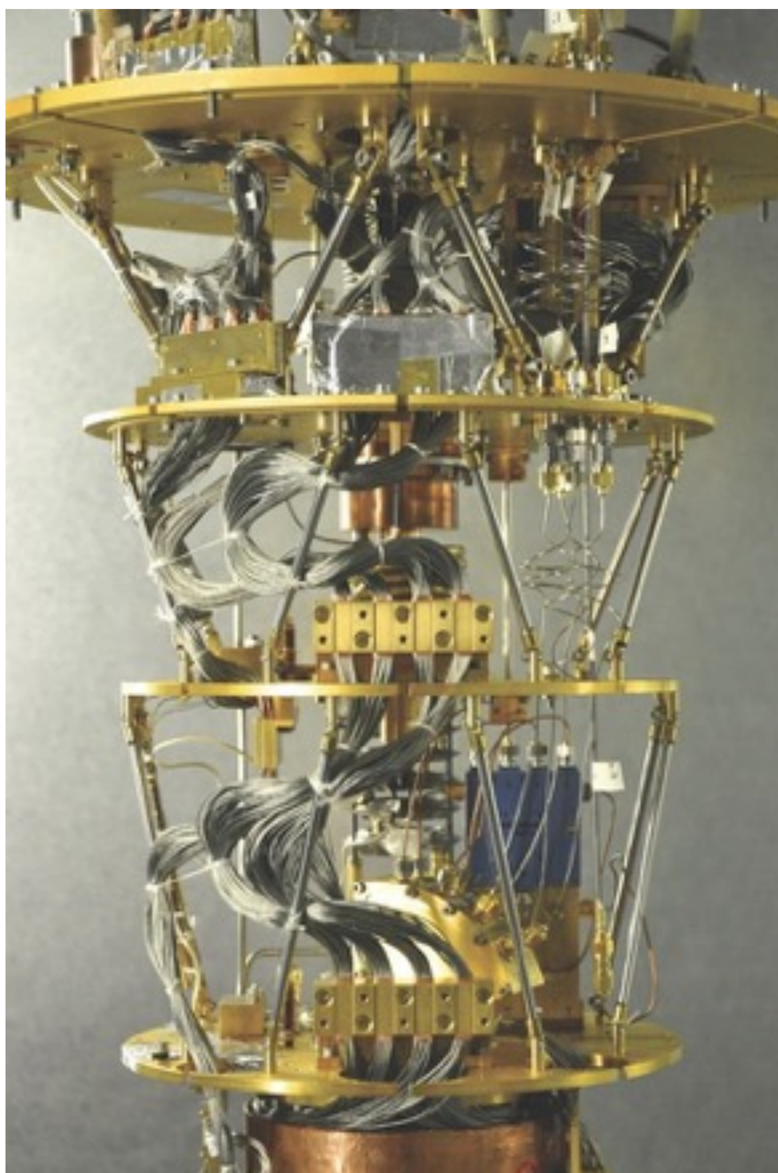
Quantum (Tunneling)

Prob. ● → ○ $= \Delta^2$

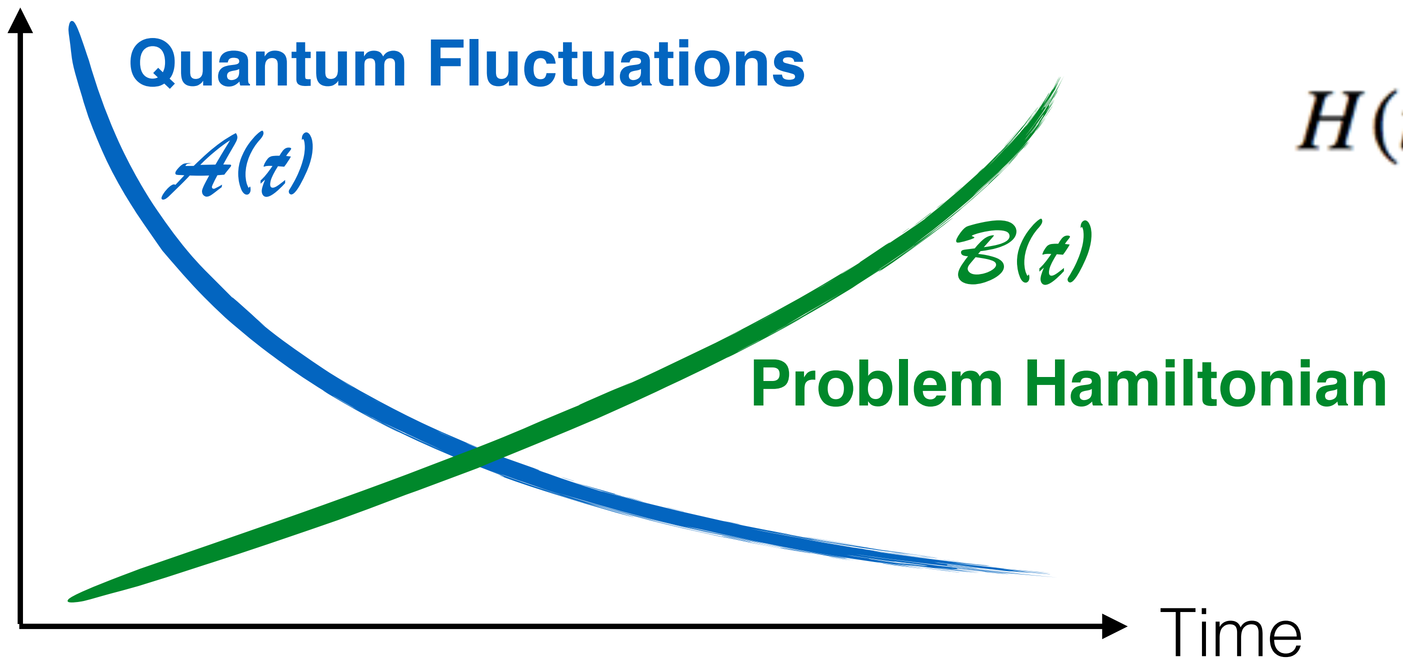
for tall but thin barriers, quantum wins!

D-Wave Device

Can a Quantum Device solve this problem faster than a Classical one?



Quantum Annealing



$$H(t) = B(t)\sum_{i<j} J_{ij}\sigma_i^z\sigma_j^z - A(t)\sum_i \sigma_i^x$$

Ising problem

Transverse magnet field

Quantum adiabatic theorem: if the Hamiltonian changes slowly, we stay in the ground state. $T_{QA} \propto \Delta^{-2}$

The ground state at t=0 is easy to prepare, the final ground state $t=t_{fin}$, is the classical solution to the problem.

QA vs SQA

Numerical simulations of QM on classical computers.

Comparison within the same quantum approach (tunneling).

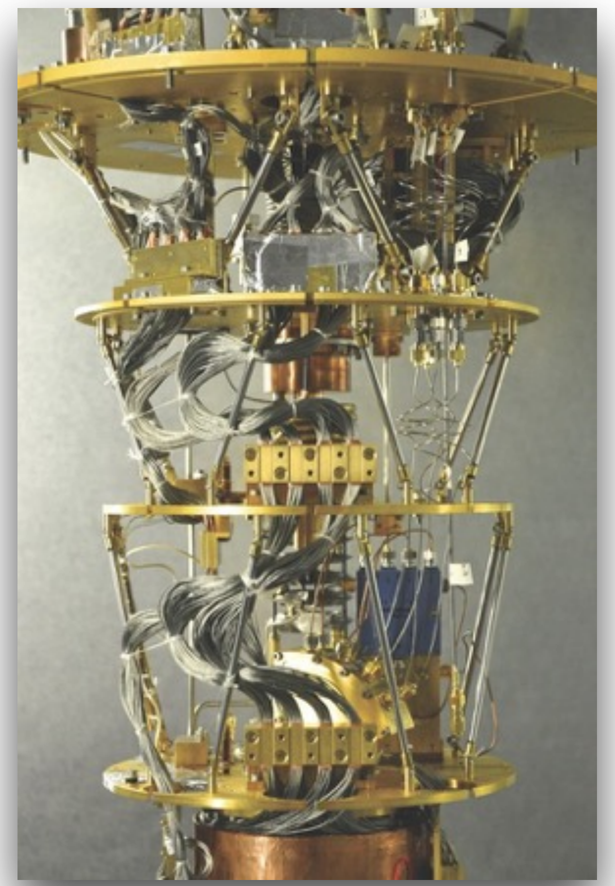
Direct integration of time-dependent Schroedinger eq. is **impossible** for more than 50 spins..

$$\frac{d}{dt}|\psi(t)\rangle = -iH(t)|\psi(t)\rangle$$

Early works on SQA are done using **Quantum Monte Carlo (QMC)**. Which is an equilibrium technique!

SQA as a sequence of equilibrium QMC simulations. How does this compare to the real QA performance?

Experiment: compare runtimes of QA device vs QMC



The runtime of the (ideal) Quantum device is dictated by the Quantum Adiabatic theorem:

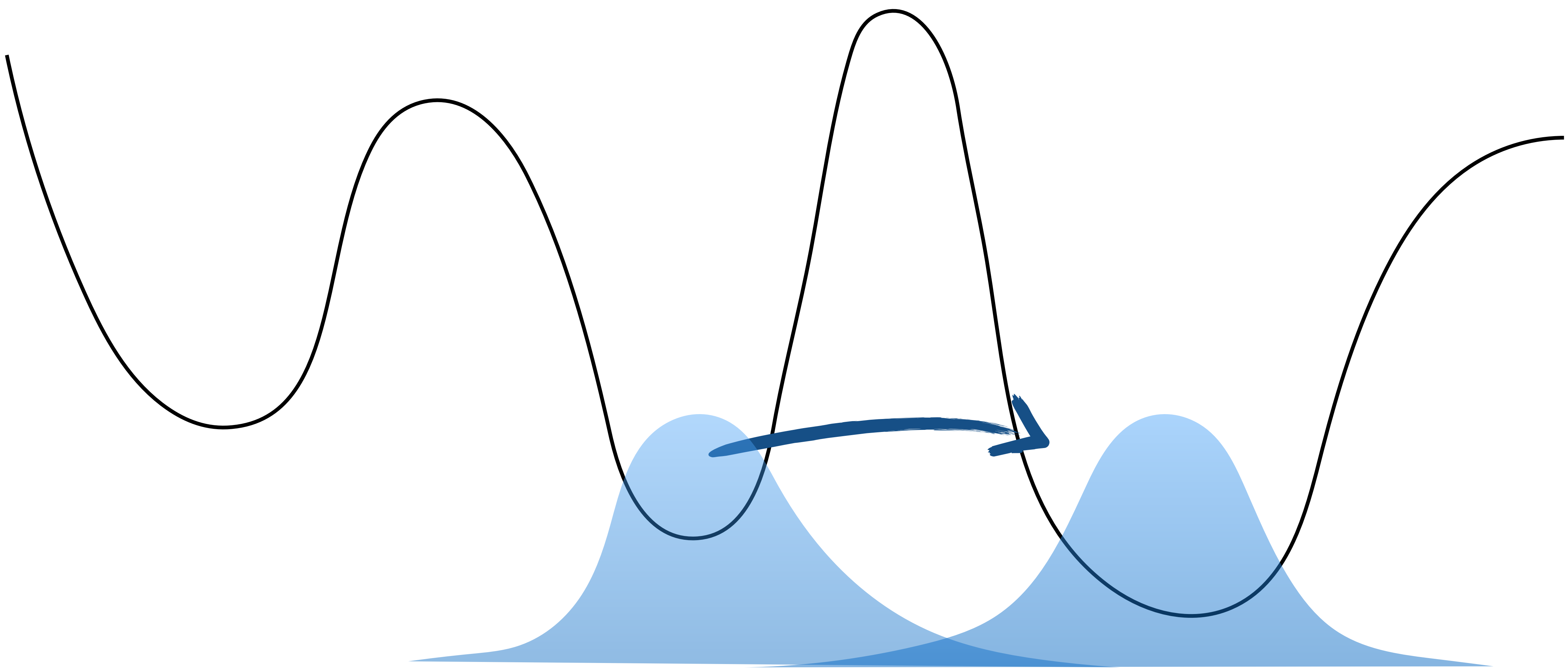
$$T_{QA} \propto \Delta^{-2}$$

How does the runtime of a QMC simulated annealing algorithm scale?

$$T_{QMC} \propto T_{QA} \ ?$$

A simpler problem: Quantum Tunneling rate

What is the tunnelling rate of QMC compared to QM?



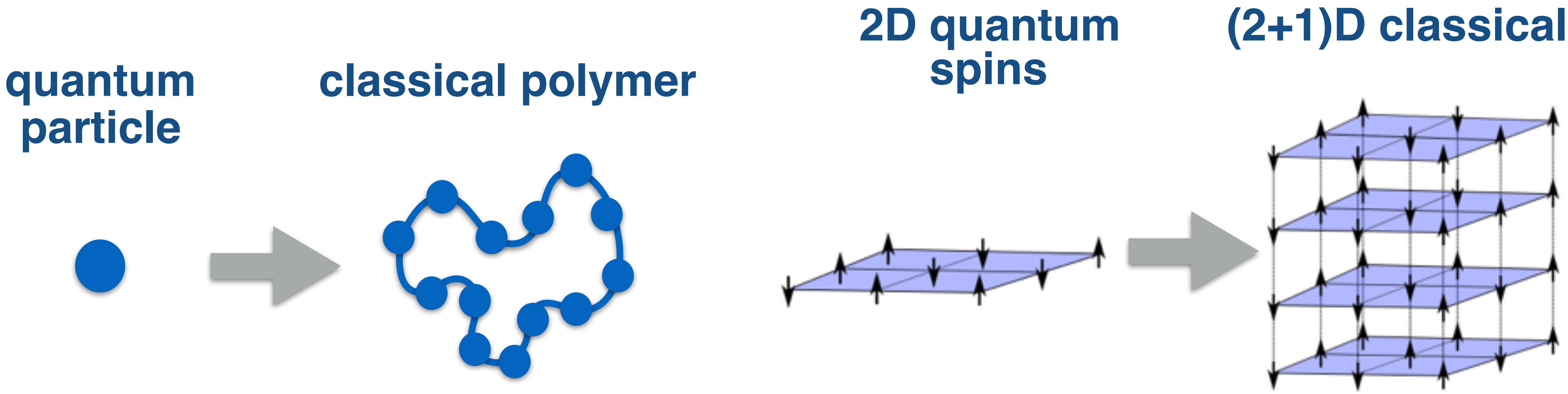
overlap

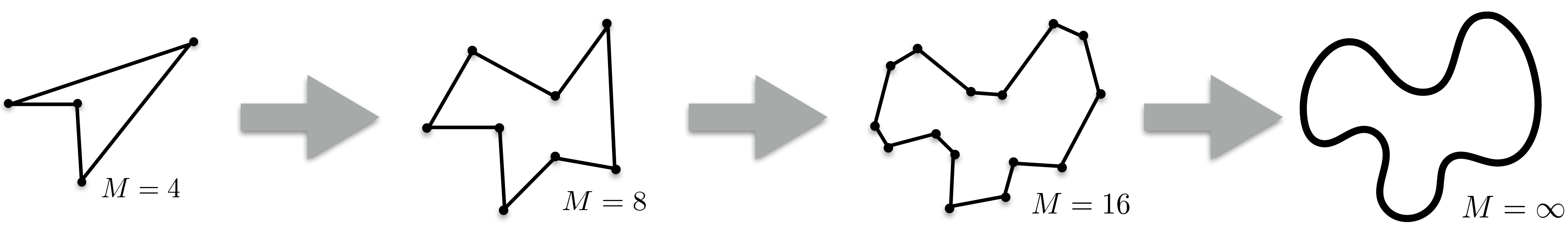
Quantum (Tunneling)

Prob. ● → ○ $=\Delta^2$

Path Integral Monte Carlo… in one slide

QMC mimics quantum fluctuations, using an extended classical systems. It follows from the path integral formulation of quantum mechanics.





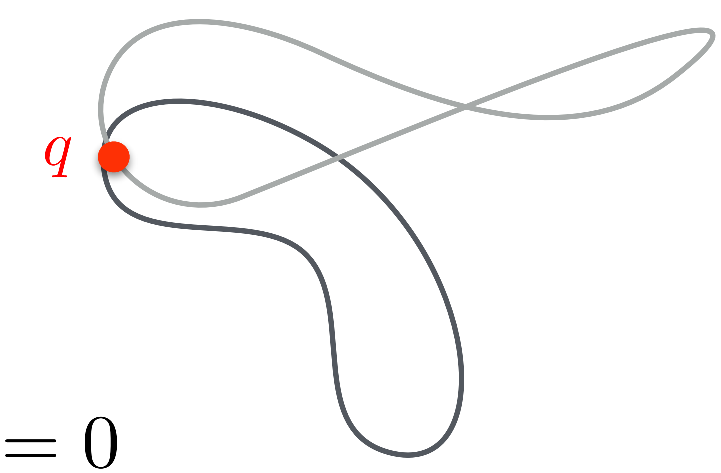
Simulations are exact in the infinite beads limit.

Path Integral Monte Carlo

$$Z = \int dq \, \langle q | e^{-\beta H} | q \rangle = \int dq \; dq_1 \; dq_2 \cdots dq_M \; \langle q | e^{-\tau H} | q_1 \rangle \langle q_1 | e^{-\tau H} | q_2 \rangle \cdots \langle q_M | e^{-\tau H} | q \rangle$$

$$Z = \sum_{\text{paths}} e^{-\mathcal{S}[\text{path}]}$$

Sum of all possible paths or trajectories in imaginary time $q(\tau)$



Each path contributes with $e^{-\mathcal{S}[q(\tau)]}$

Dominant contributions come from paths $\frac{\partial \mathcal{S}[q(\tau)]}{\partial q(\tau)} = 0$

Form of $\mathcal{S}[q(\tau)]$ is system dependent.

Path Integral Monte Carlo pseudodynamics

Doing the integral with Monte Carlo by sampling ring-polymer configurations (paths) with Metropolis weight $e^{-\mathcal{S}[q(\tau)]}$

Evolution of the classical path as a function of the simulation time t

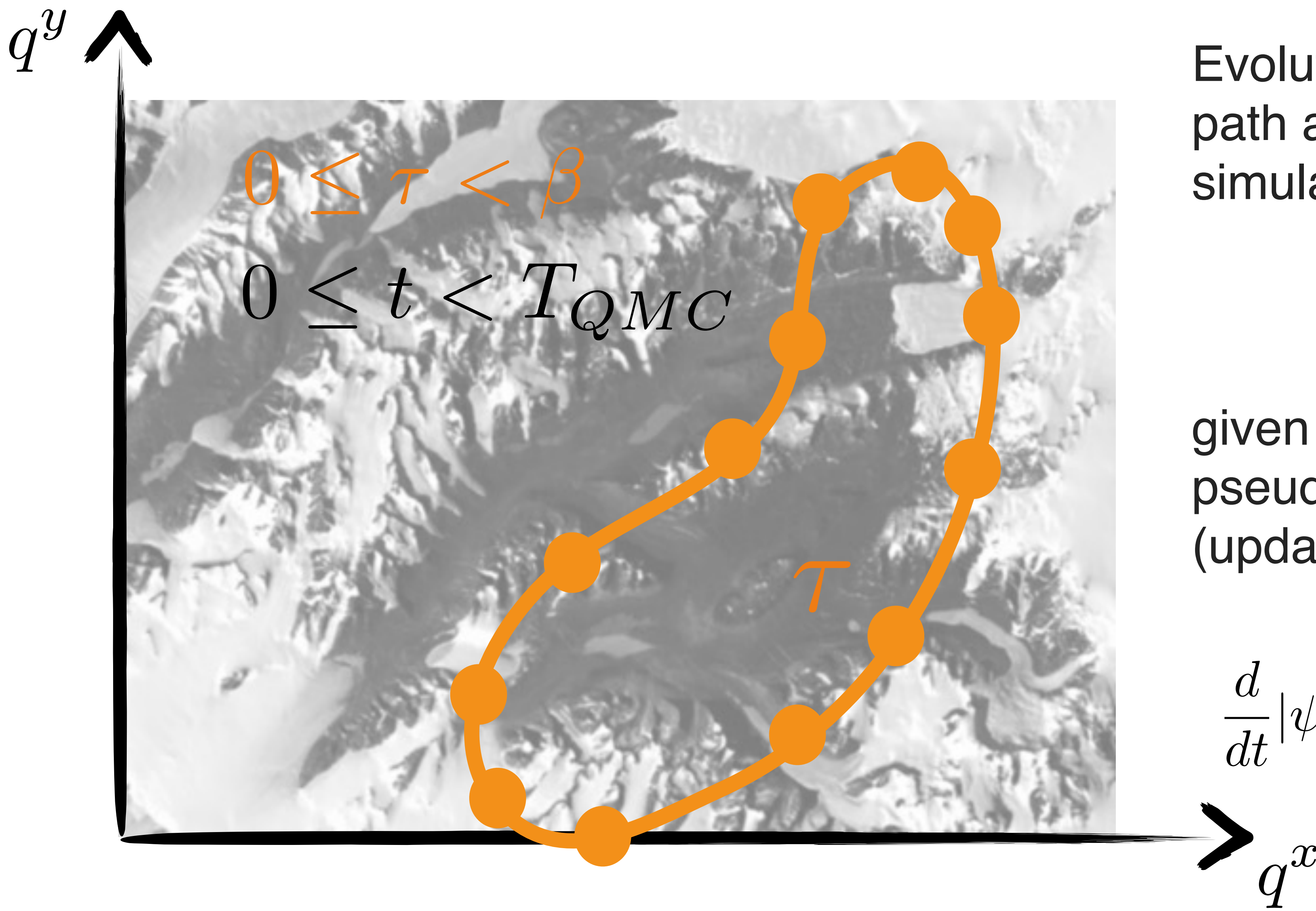
$$q(\tau, t)$$

given by the Metropolis pseudo-dynamics (updates).

$$\frac{\partial q(\tau,t)}{\partial t} = -\frac{\delta \mathcal{S}[q(\tau,t)]}{\delta q(\tau,t)} + \eta(\tau,t)$$

Path Integral Monte Carlo pseudodynamics

Doing the integral with Monte Carlo by sampling ring-polymer configurations (paths) with Metropolis weight $e^{-\mathcal{S}[q(\tau)]}$



Evolution of the classical path as a function of the simulation time t

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$$\frac{d}{dt}|\psi(t)\rangle = -iH(t)|\psi(t)\rangle$$

Path Integral Monte Carlo pseudodynamics

Stochastic quantization (Parisi, 81') $q(\tau) \to q(\tau, t)$

If the classical field evolves through a Langevin equation

$$\frac{\partial q(\tau,t)}{\partial t} = -\frac{\delta \mathcal{S}[q(\tau,t)]}{\delta q(\tau,t)} + \eta(\tau,t)$$

then $\lim_{t\to\infty} P[q(\tau,t)] = e^{-\mathcal{S}[q(\tau)]}$

Path Integral Monte Carlo pseudodynamics

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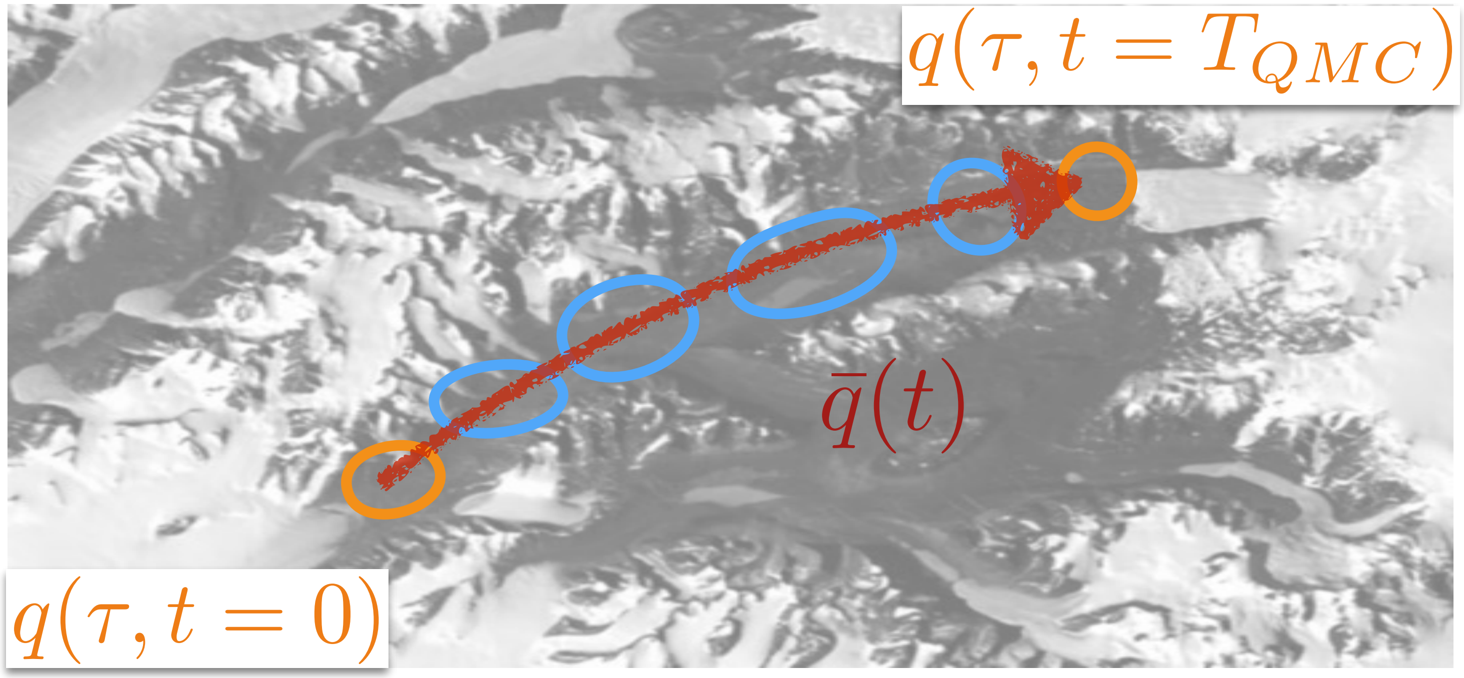
Diffusion of a classical object!



Most probable pathway for this diffusion over a time T_{QMC} is:

$$\frac{d^2\bar{q}}{dt^2} = -\frac{\delta}{\delta q}\left[\left(\frac{\delta \mathcal{S}}{\delta q}\right)^2 - 2\frac{\delta^2 \mathcal{S}}{\delta q^2}\right]$$

Transition states of the dynamics: instantons

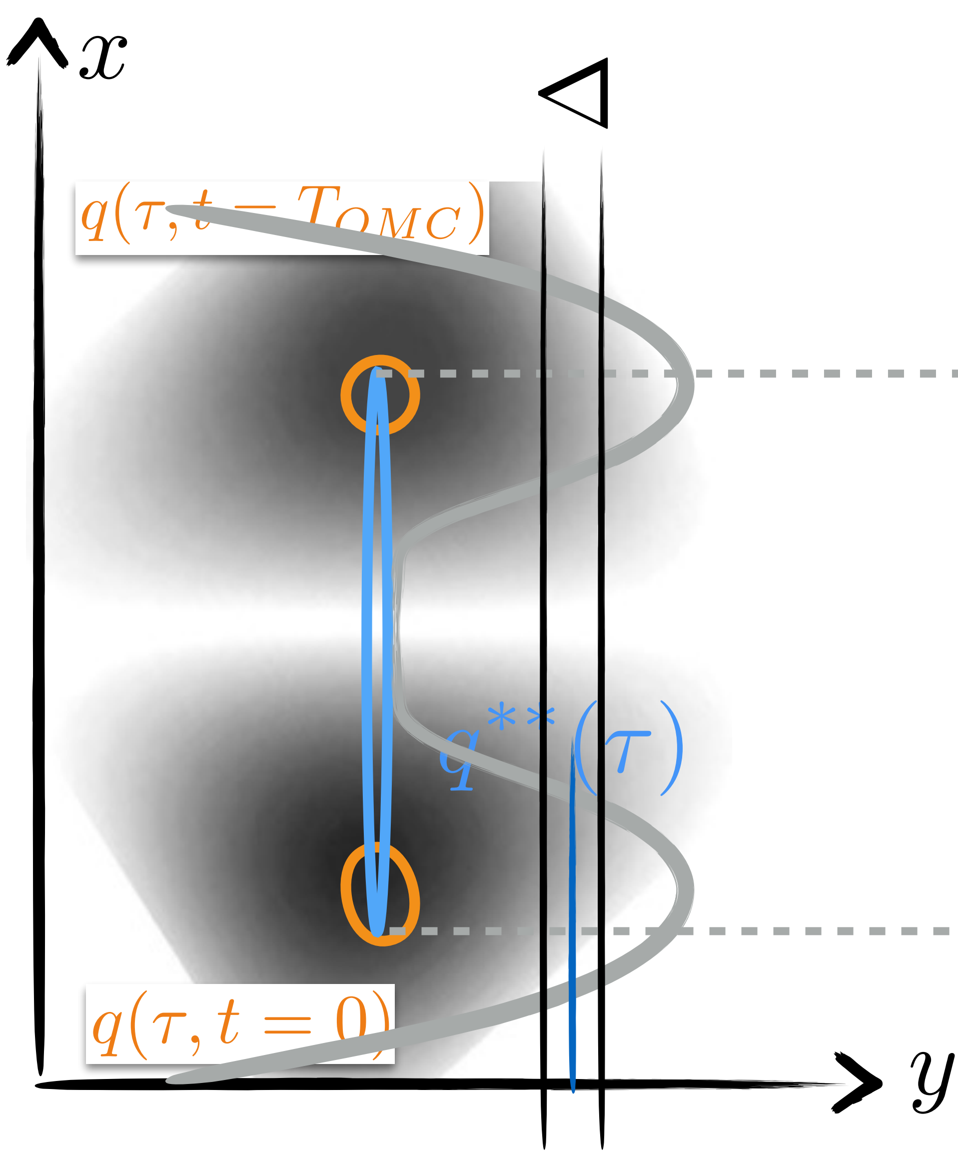
Consider double well problems

$$\frac{\partial q(\tau,t)}{\partial t} = -\frac{\delta \mathcal{S}[q(\tau,t)]}{\delta q(\tau,t)} + \eta(\tau,t)$$

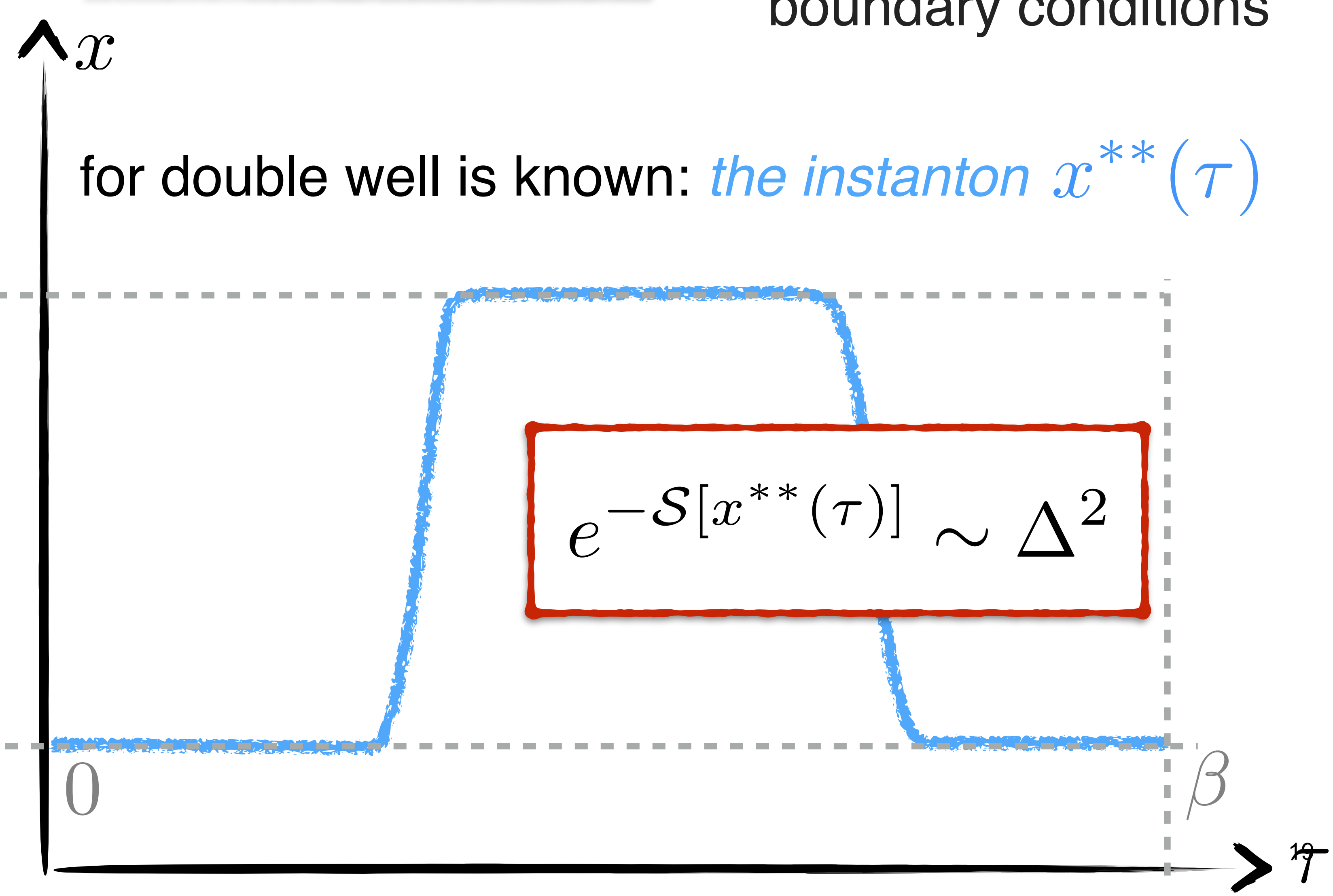
Transition states defined by:

$$\frac{\delta \mathcal{S}[q(\tau,t)]}{\delta q(\tau,t)} = 0$$

Transition state (TS) is the saddle point with non-trivial boundary conditions



for double well is known: *the instanton* $x^{**}(\tau)$

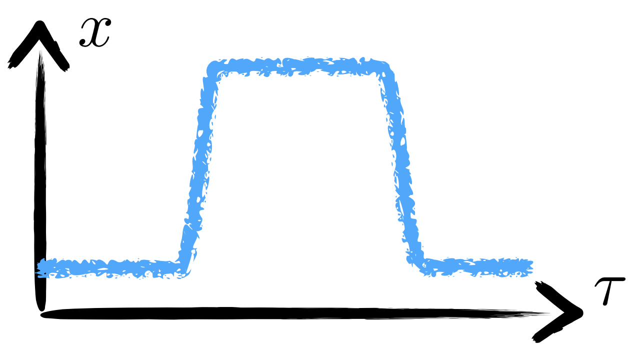


Transition states of the dynamics: instantons

The classical field, in a PIMC simulation, evolves through a Langevin equation,

$$\frac{\partial q(\tau,t)}{\partial t} = -\frac{\delta \mathcal{S}[q(\tau,t)]}{\delta q(\tau,t)} + \eta(\tau,t)$$

In a double well model, we know the transition state (transition path or trajectory in imaginary time) $q^{**}(\tau)$



The escape rate of this classical thermally activated event is given by Kramers theory (Boltzmann weight at the TS)

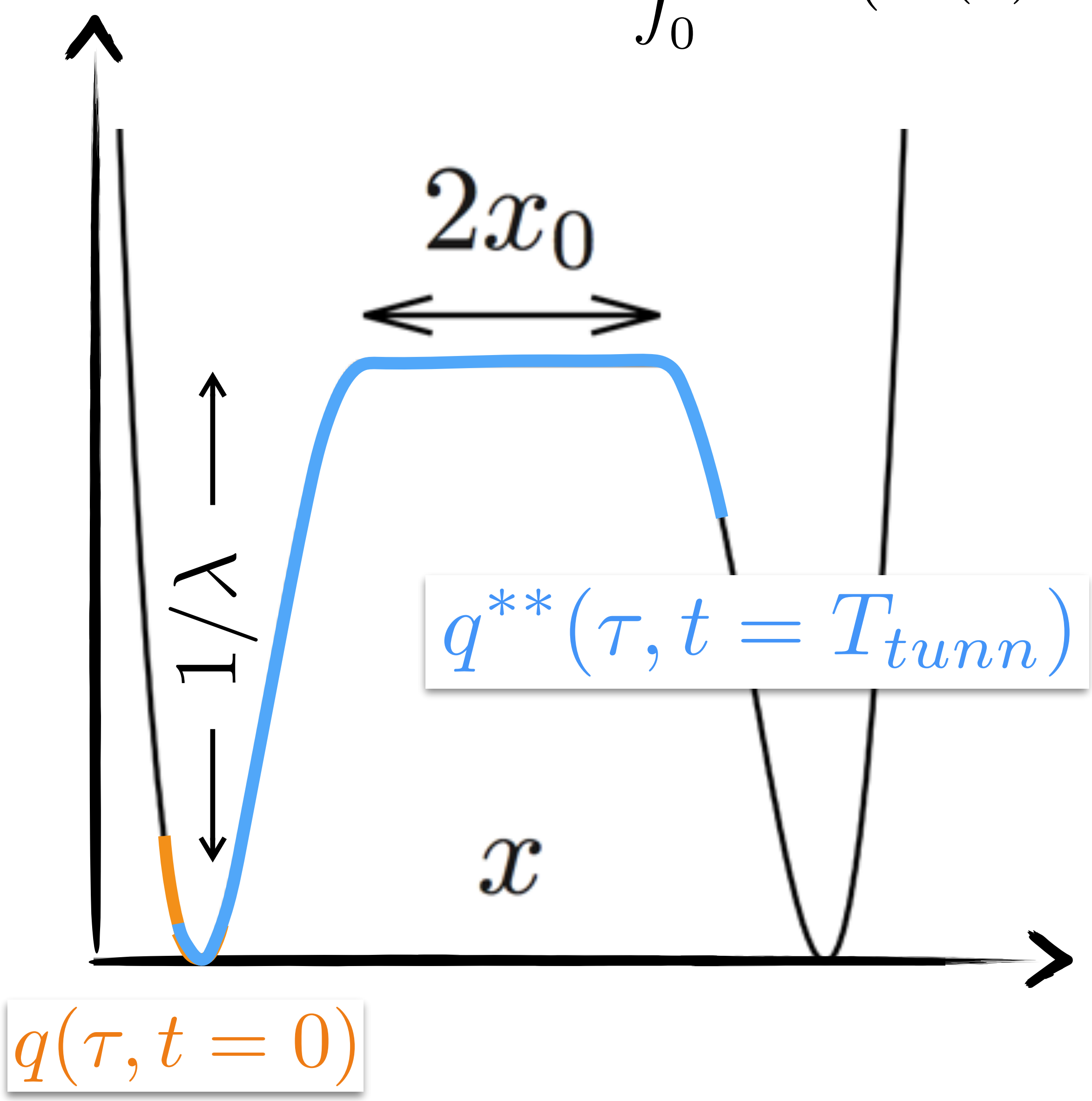
$$k \propto e^{-\mathcal{S}[q^{**}(\tau)]} \sim \Delta^2$$

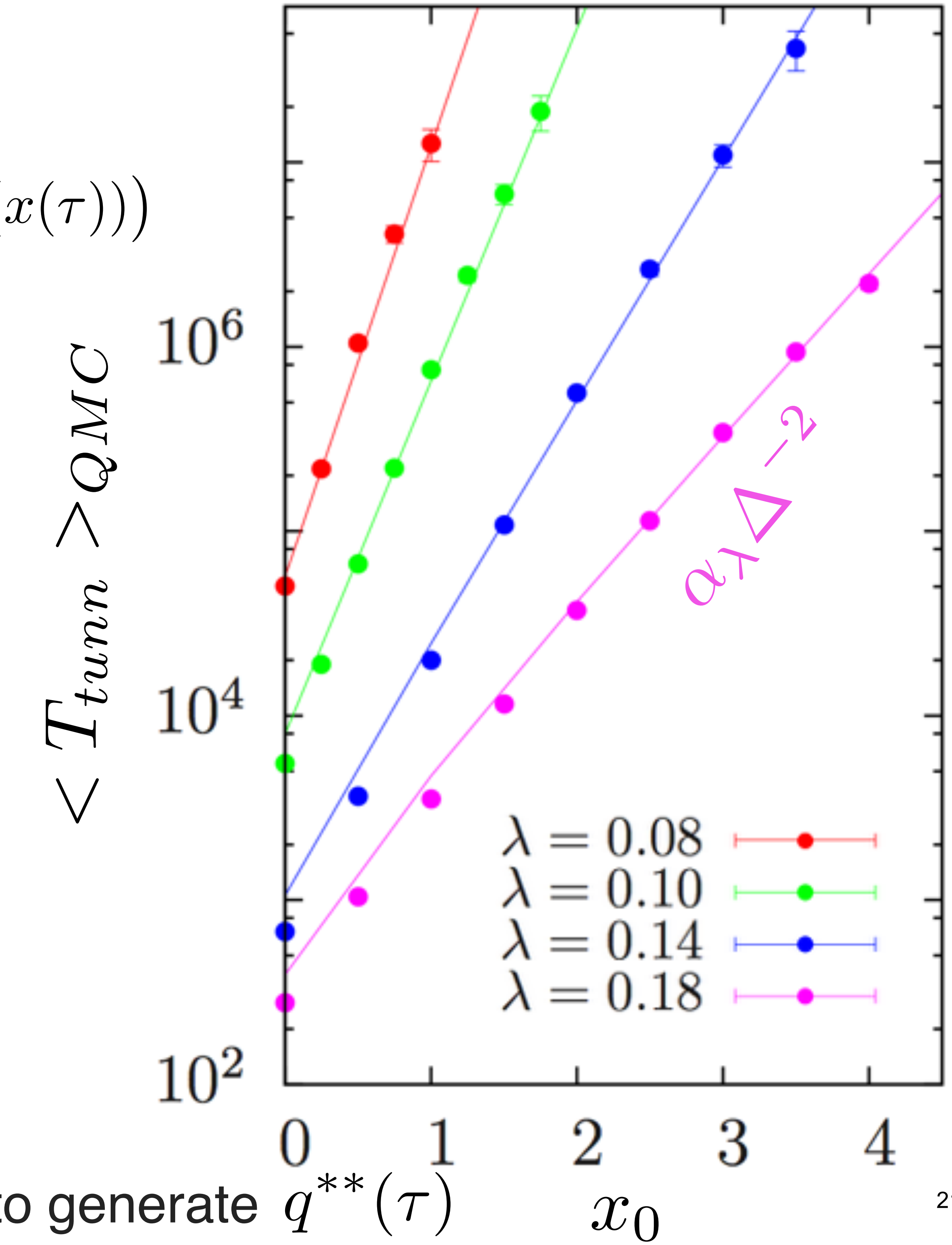
Therefore we expect that the QMC tunneling rate must scale as $\sim \Delta^2$

Continous space model: 1D double well

$$H = -\frac{\partial^2}{\partial x^2} + V(x)$$

$$\mathcal{S} = \int_0^\beta d\tau \ \left(\dot{x}^2(\tau) + V(x(\tau))\right)$$





T_{tunn} : Number of QMC updates required to generate $q^{**}(\tau)$

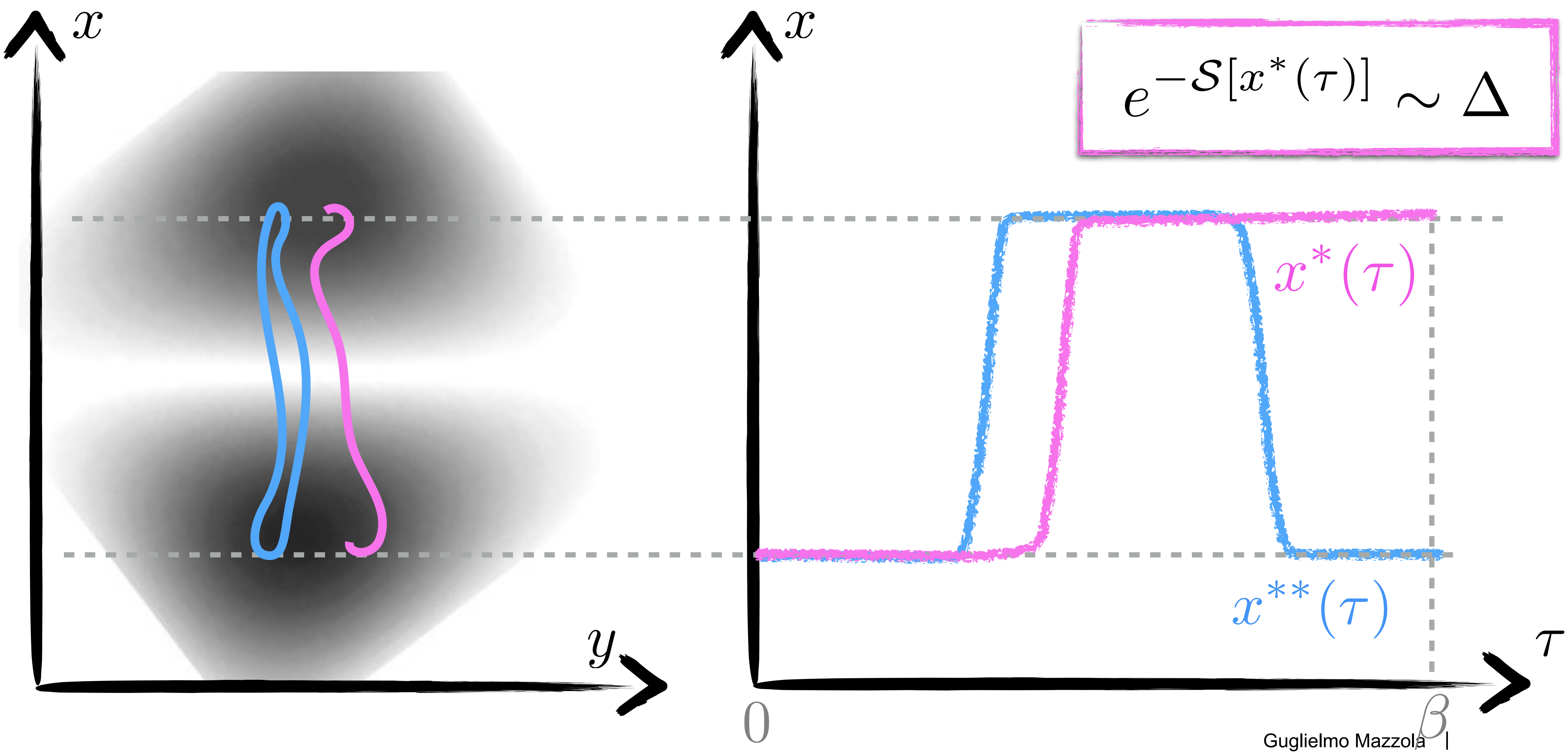
Transition states of the dynamics: instantons

Computing the thermal density matrix requires closed paths in imag. time

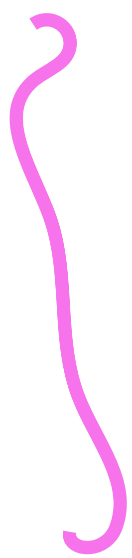
$$Z = \int dq \, \langle q | e^{-\beta H} | q \rangle$$

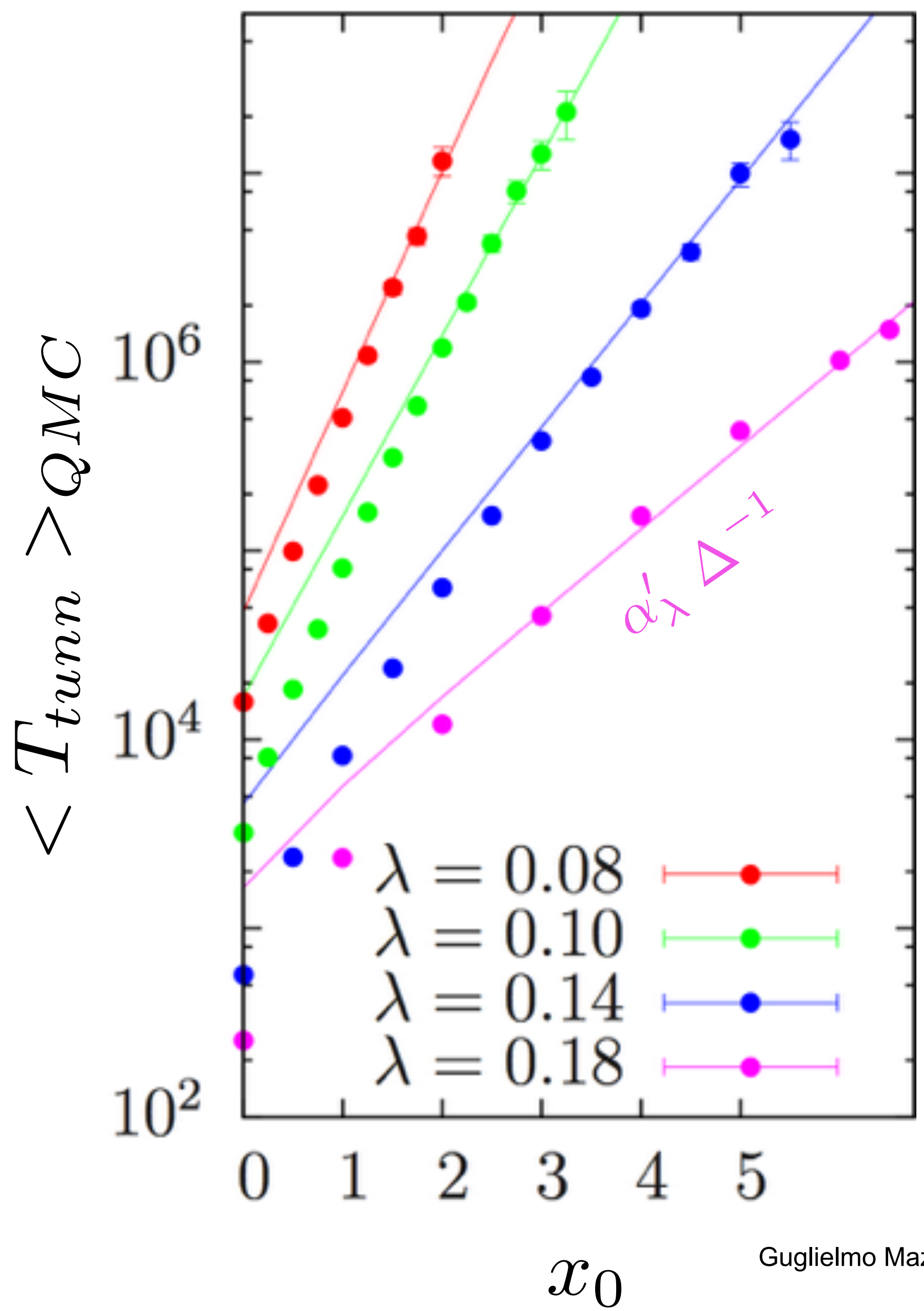
$$e^{-\mathcal{S}[x^{**}(\tau)]} \sim \Delta^2$$

$$e^{-\mathcal{S}[x^{*}(\tau)]} \sim \Delta$$



PIMC with Open Boundary Conditions

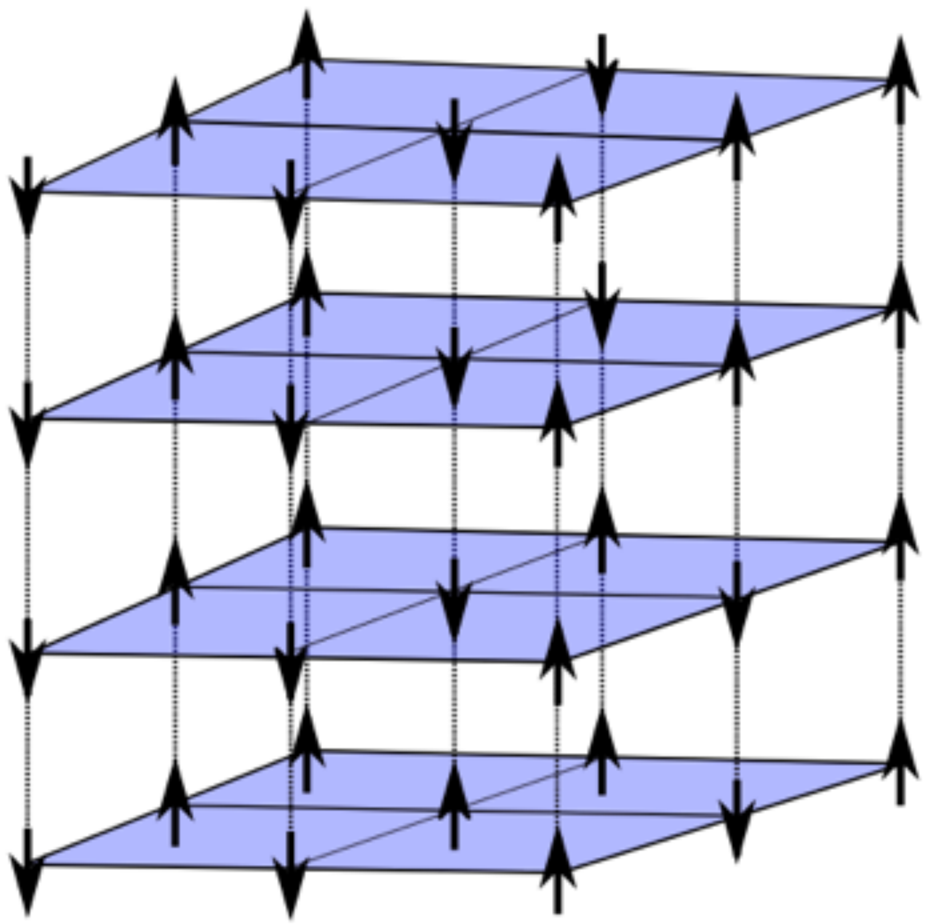


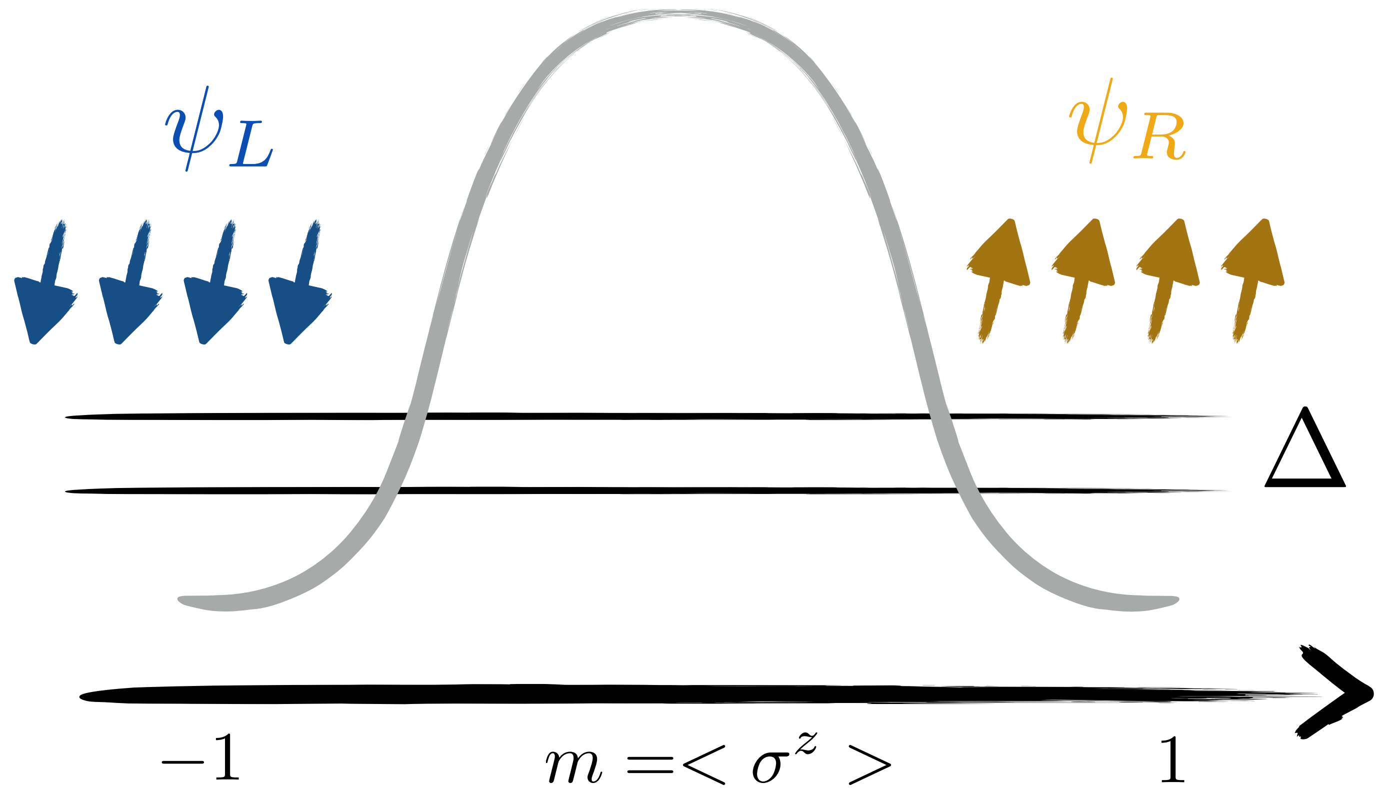


Ferromagnetic Ising system

Consider now a spin system.

$$H = J \sum_{i,j} \sigma_i^z \sigma_j^z + \Gamma \sum_i \sigma_i^x$$





Path integral construction lead to an extended lattice (formally similar to the previous ring polymer)

$$\psi_0 = \frac{1}{\sqrt{2}} (\psi_L + \psi_R)$$

Ferromagnetic Ising system

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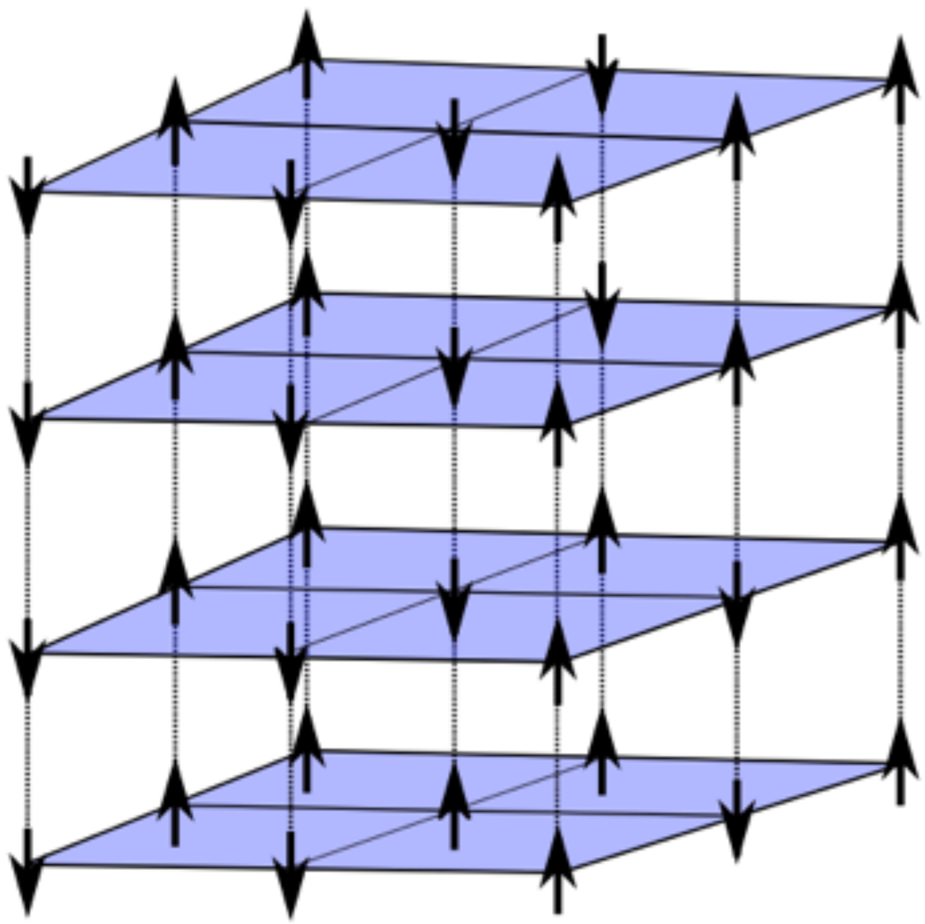
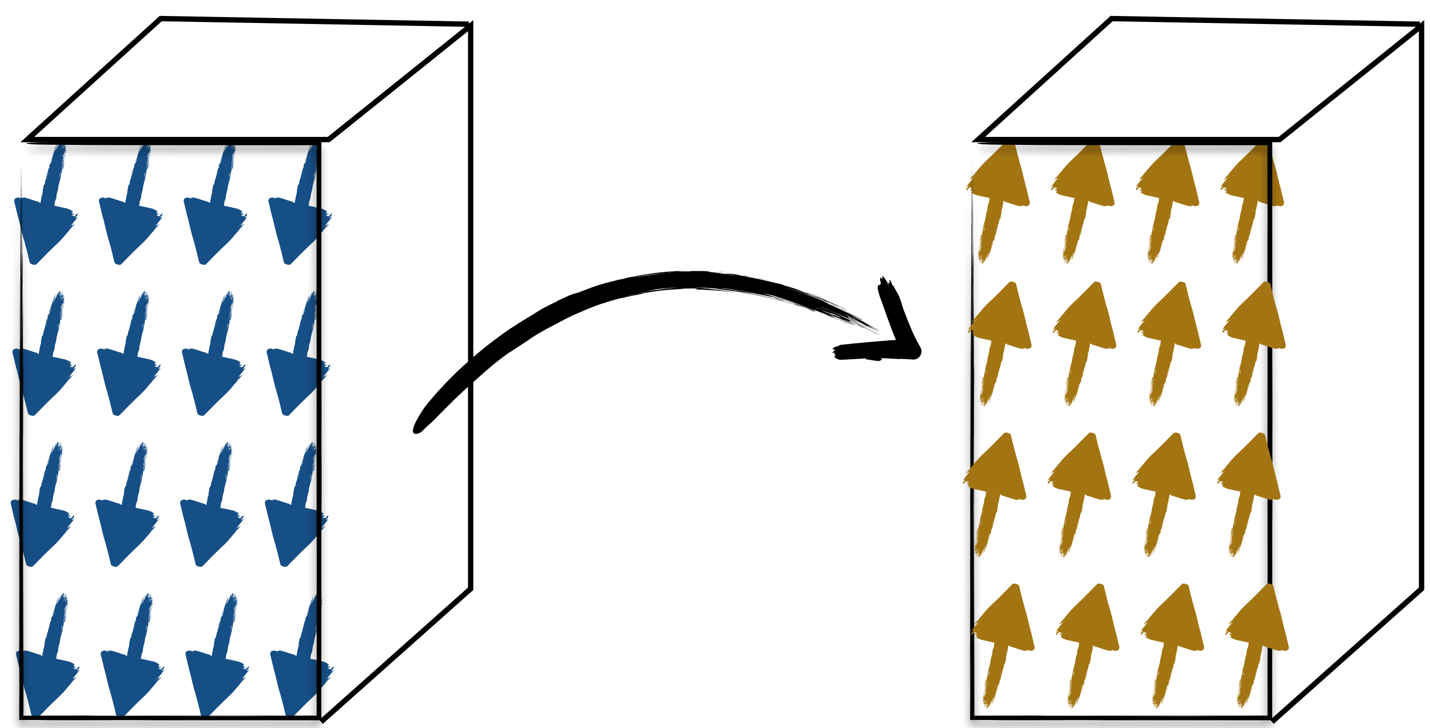
$$H = J\sum_{i,j}\sigma_i^z\sigma_j^z + \Gamma\sum_i\sigma_i^x$$

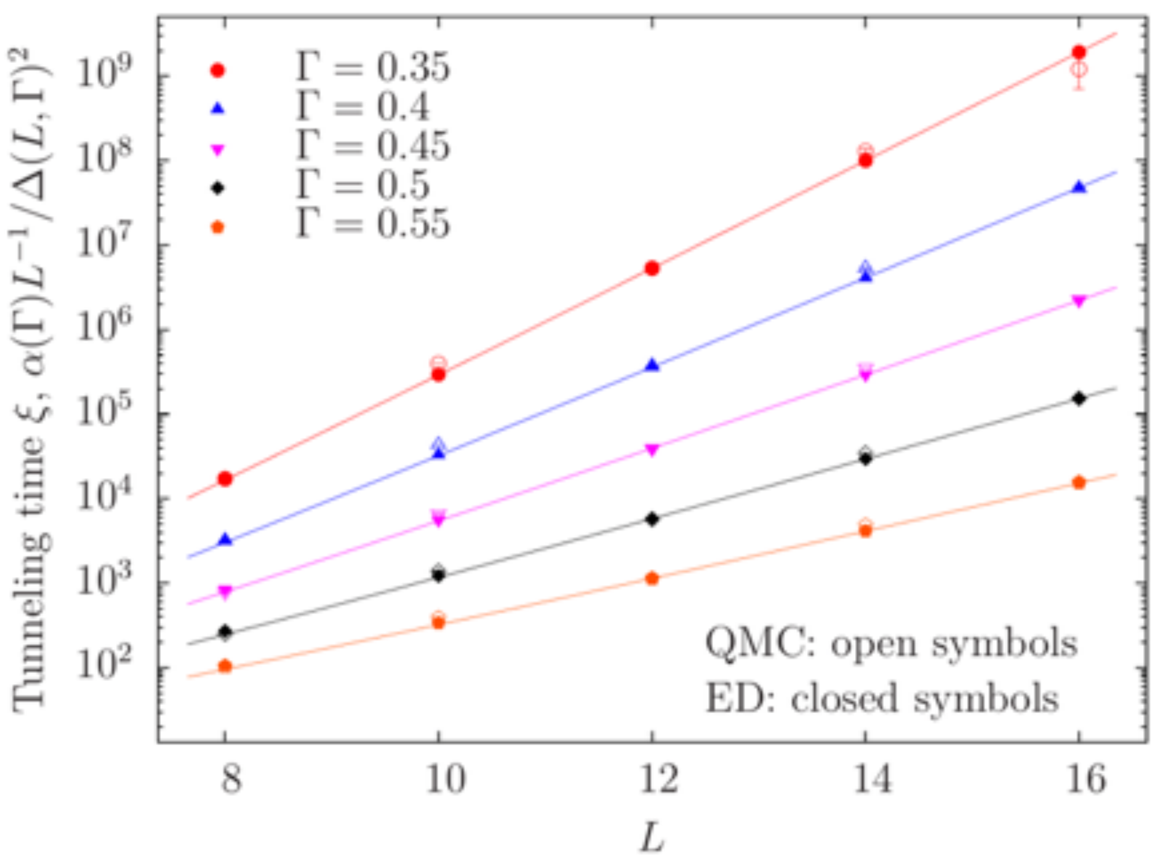




Path integral construction lead to an extended lattice (formally similar to the previous ring polymer)

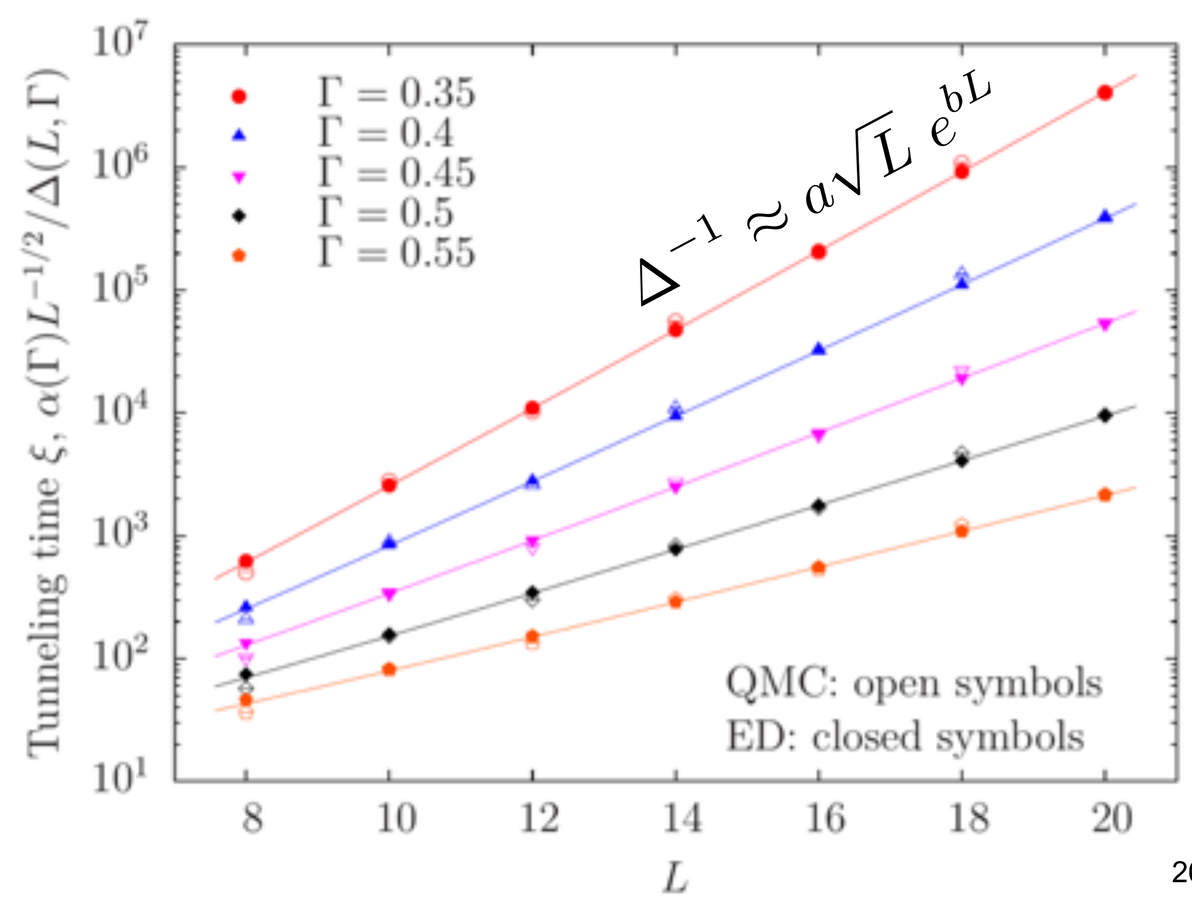
QMC tunneling rate in ferromagnetic Ising system

Let's measure QMC tunneling time as a function of the system size L.



$$< T_{PBC} >\sim 1/\Delta^2$$

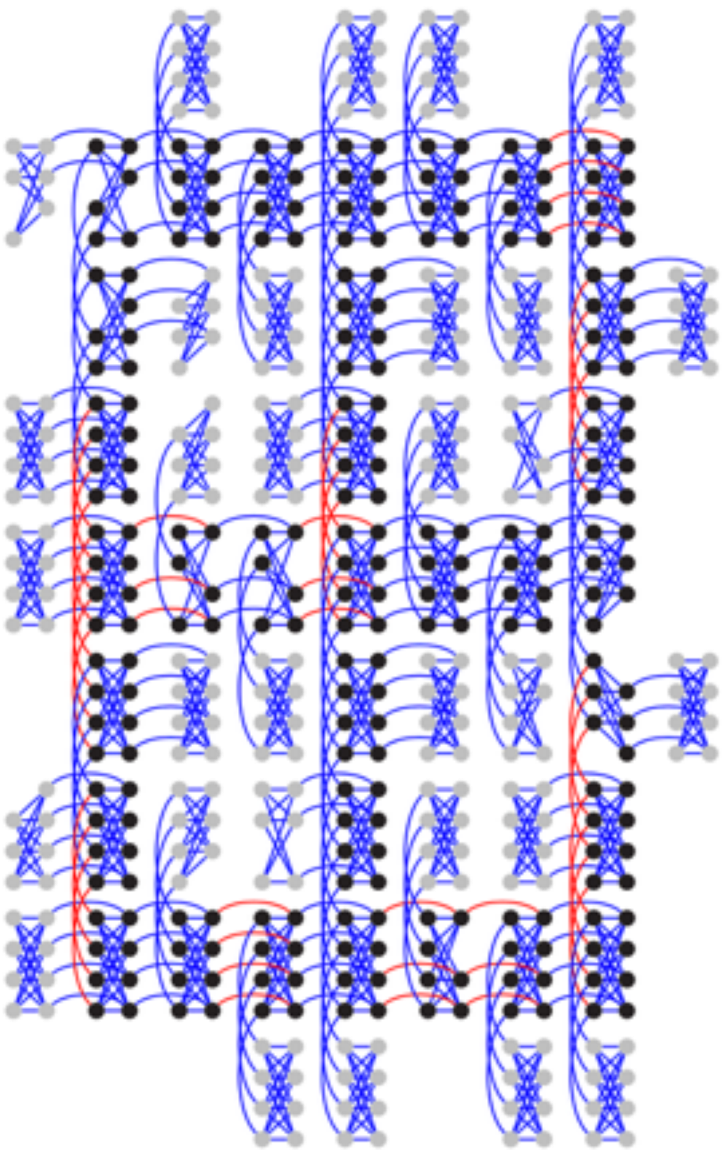
$$< T_{OBC} >\sim 1/\Delta$$

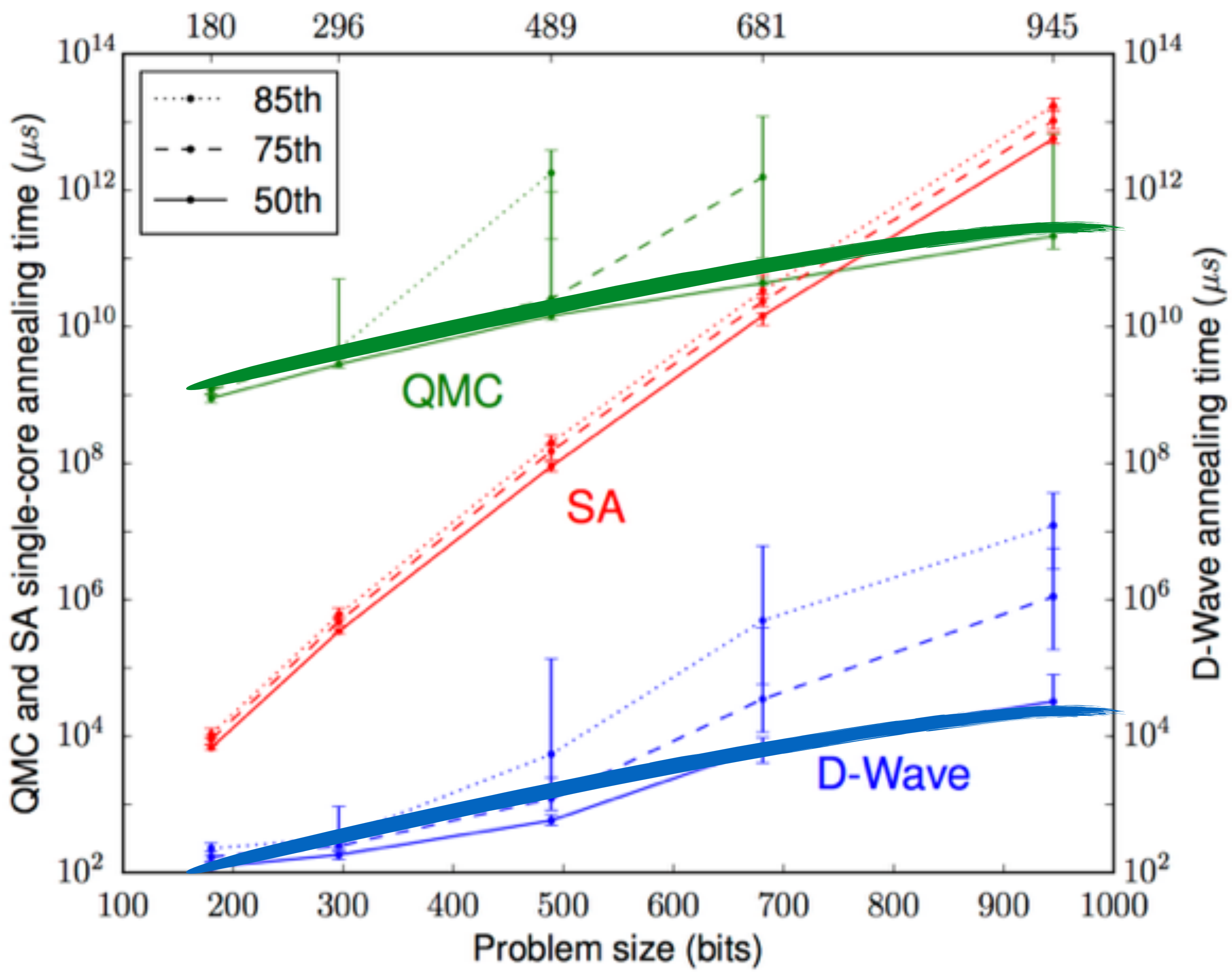


S.V. Isakov, G. Mazzola, V.N. Smelyanskiy, Z. Jiang, S. Boixo, H. Neven, and M. Troyer
Phys. Rev. Lett. 117, 180402 (2016)

QMC annealing performance

"Google" instances



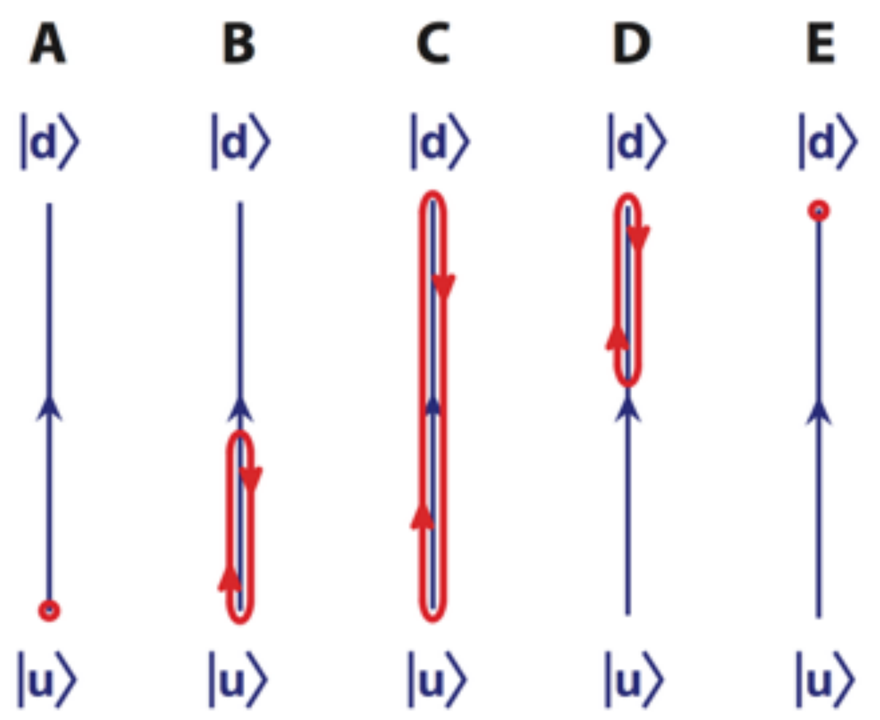


Denchev et. al. 2016

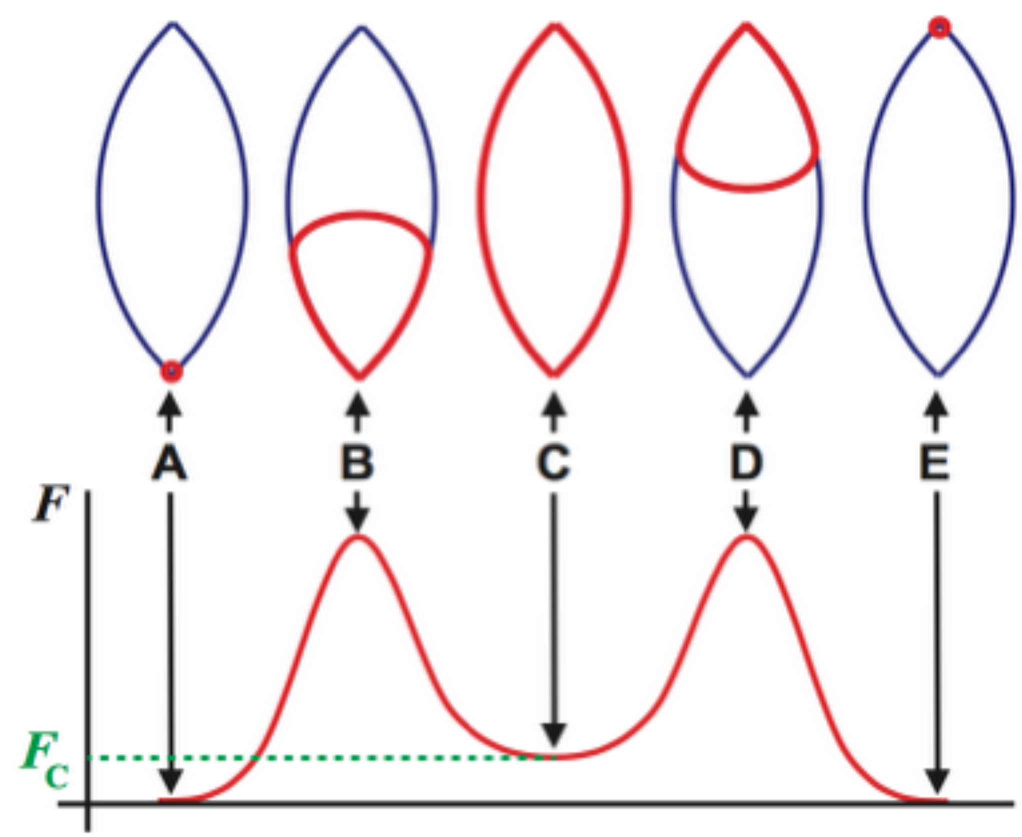
Is this property general?

A. “Topological obstructions”

single path



two degenerate paths

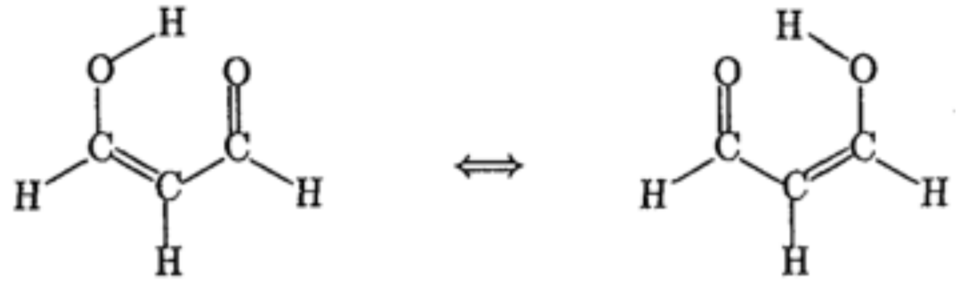


activation energy to reach paths **c,d** is not degenerate with **a,b**

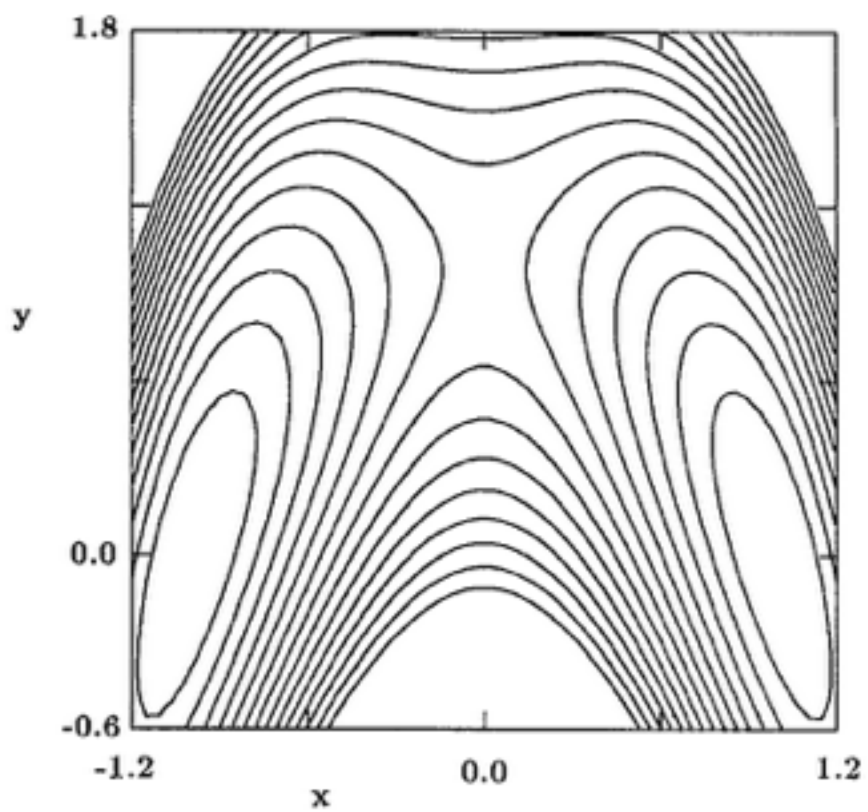
from Andriash and Amin, arXiv:1703.09277 (2017)

Is this property general?

B. Explore physical system to explore possible **counterexamples**: multidimensional tunnelling in **quantum chemistry** reactions.



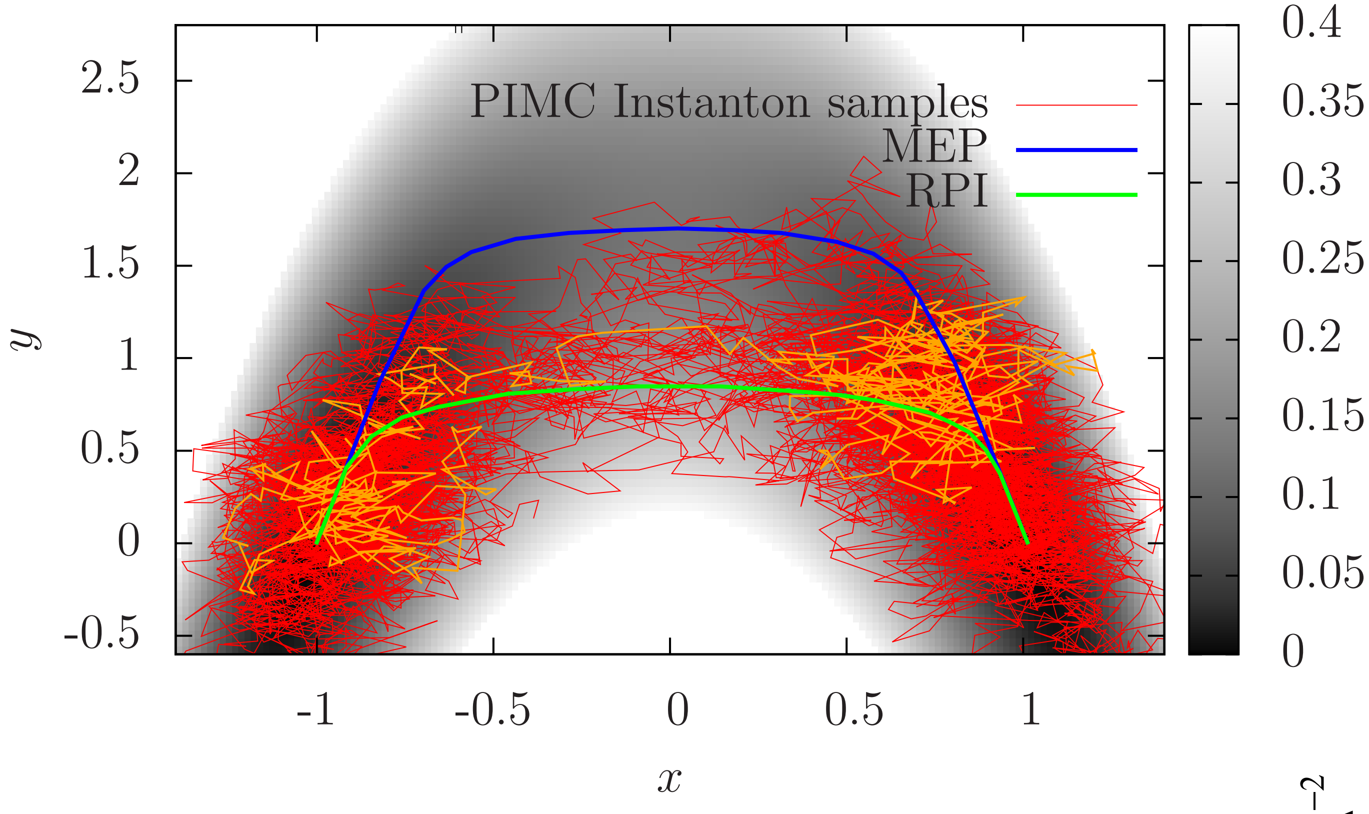
e.g.: proton transfer in malonaldehyde



1. Intrinsic multidimensionality
2. Multiple equivalent tunneling paths.

Tanaka et. al. J. Chem. Phys. 100 (I), 98 (1994)

Is this property general?

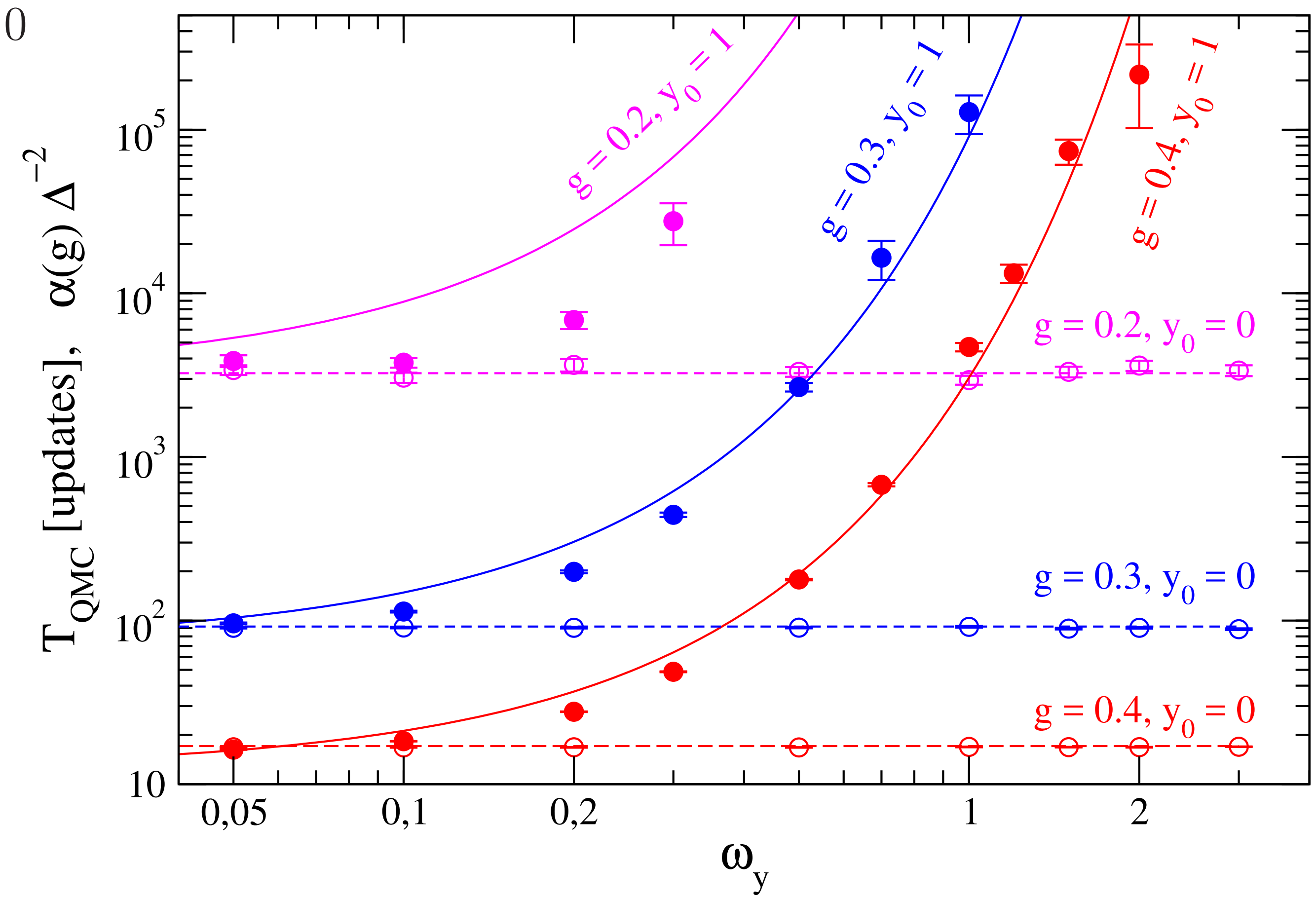


$$H = \Theta + V_A \ ,$$

$$\Theta = -\frac{g^2}{2}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right) \ ,$$

Yes.

QMC **ground state** tunnelling is always mediated by instantons.



G. Mazzola, V.N. Smelyanskiy, and M. Troyer

arXiv: 1703.08189 (2017)

PIMC/PIMD tunneling rate scales as incoherent quantum tunneling rate for tunneling in double well-like models.

Since incoherent tunneling is the driving process occurring in a AQC, PIMC is as efficient as a QC to solve optimisation process.

PIGS tunnels faster than PIMC (quadratic speed-up): more efficient of present AQC!

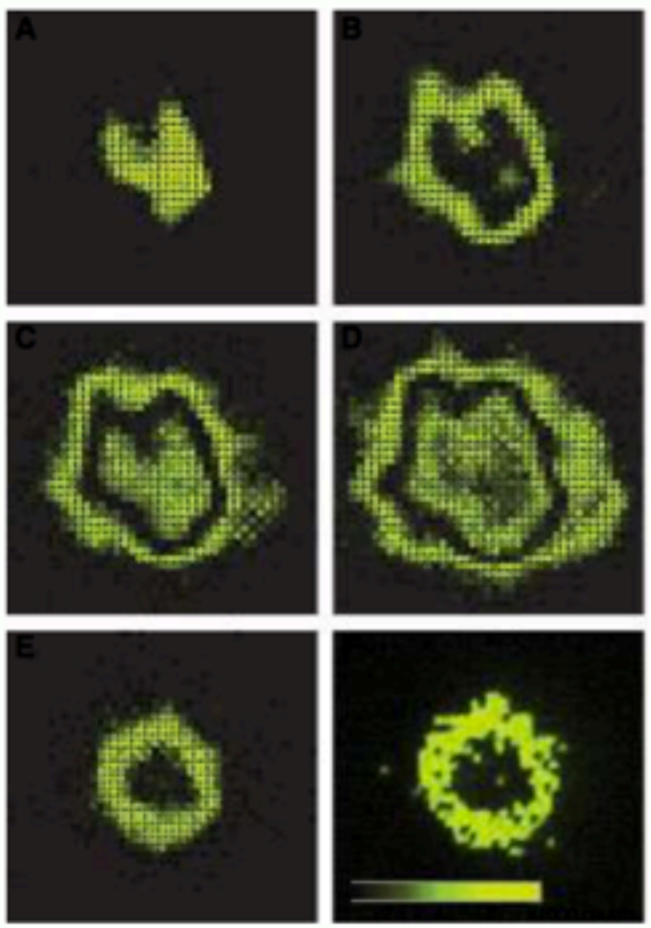
Of course this holds only for sign-problem free quantum driving hamiltonians!

Conclusions/1

Quantum State Tomography

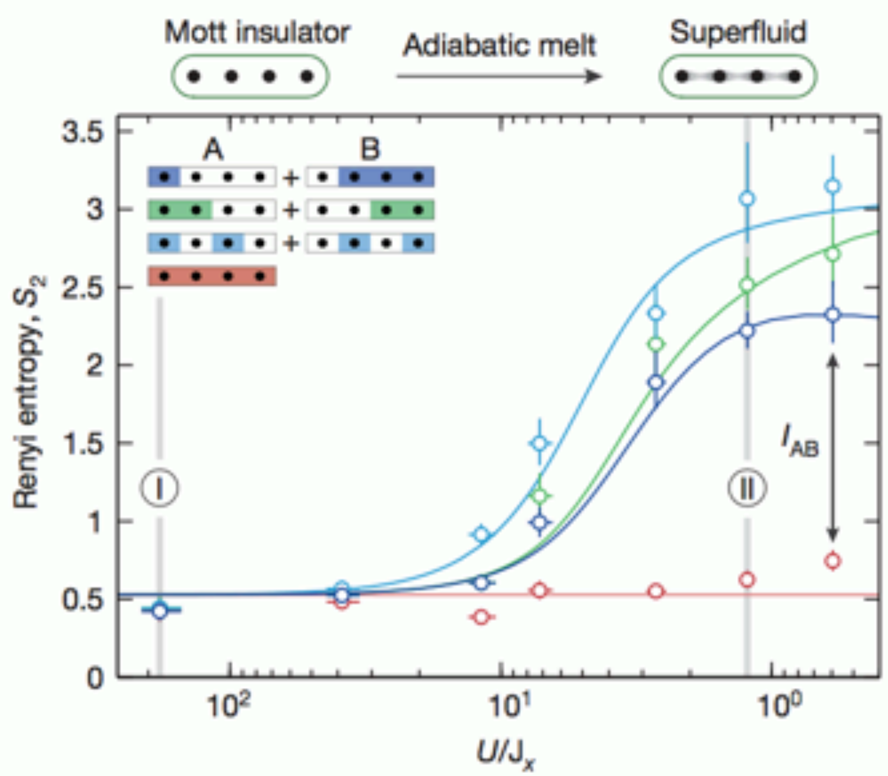
Can we "learn" a quantum state from a limited set of measurements?

Cold atomic gases



W. Bakr et al, Science (2010)

Entanglement



R. Islam et al, Nature (2015)

Quantum devices

Image: D-Wave 2000Q

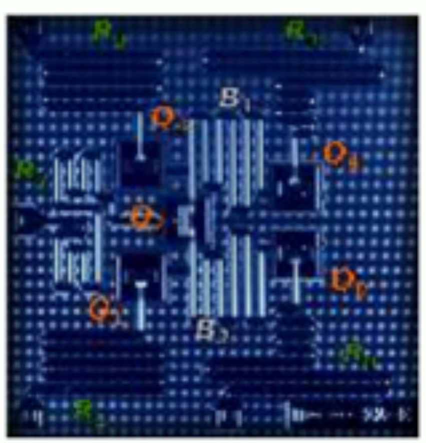


Image: ibmqx2

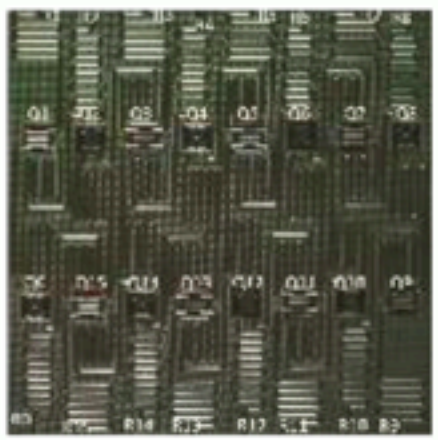


Image: ibmqx3

Quantum State Tomography

From a limited set of simple measurements, reconstruct the full many-particle quantum state.

Example: W state

$$|\Psi_W\rangle = \frac{1}{\sqrt{N}}\left(|100\ldots\rangle + ... + |\ldots 001\rangle\right).$$

Standard QST for an 8 site system requires 656.000 measurement for 99% fidelity! Hilbert space scales exponentially with N.

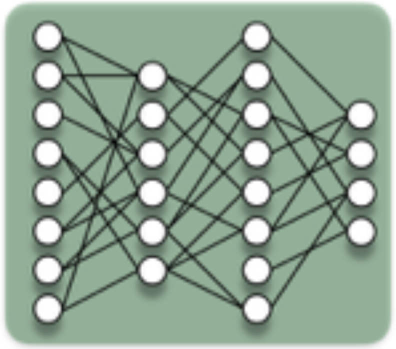
It's *clear* that for structured problem a more "compact" representation should exist.

Quantum State Tomography

Neural networks (NN) are very good variational wavefunctions!

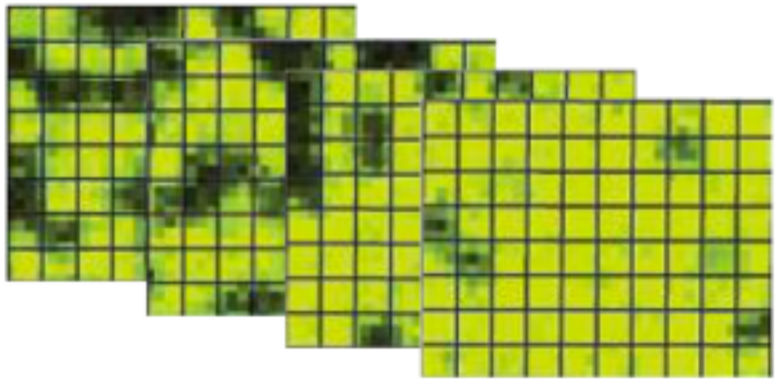
Solving the quantum many-body problem with artificial neural networks,
G. Carleo and M. Troyer. Science 355, pp. 602-60 (2017)

$(\boldsymbol{\lambda}, \boldsymbol{\mu})$

$\psi_{\boldsymbol{\lambda},\boldsymbol{\mu}}(\boldsymbol{\sigma}) =$ 

Here, we train a NN using configurations extracted from the ground state. So that NN can learn quantum mechanics.

Many-body quantum state tomography with neural networks,
G Torlai, G Mazzola, J Carrasquilla, M Troyer, R Melko, G Carleo, arXiv:1703.05334 (2017)

In a given basis $\boldsymbol{\sigma}^{[b]}$:  $\longrightarrow$ $P_b(\boldsymbol{\sigma}^{[b]}) \propto |\Psi(\boldsymbol{\sigma}^{[b]})|^2$

Quantum State Tomography

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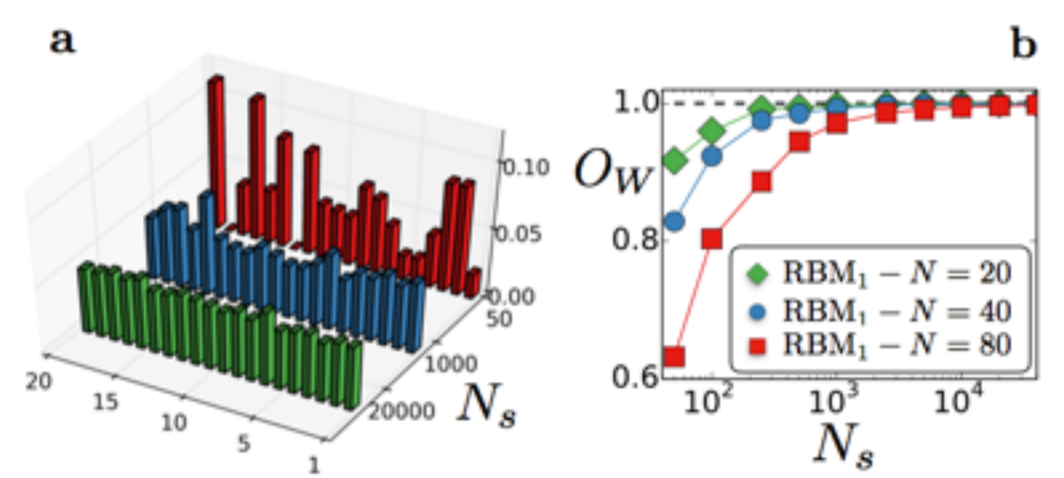
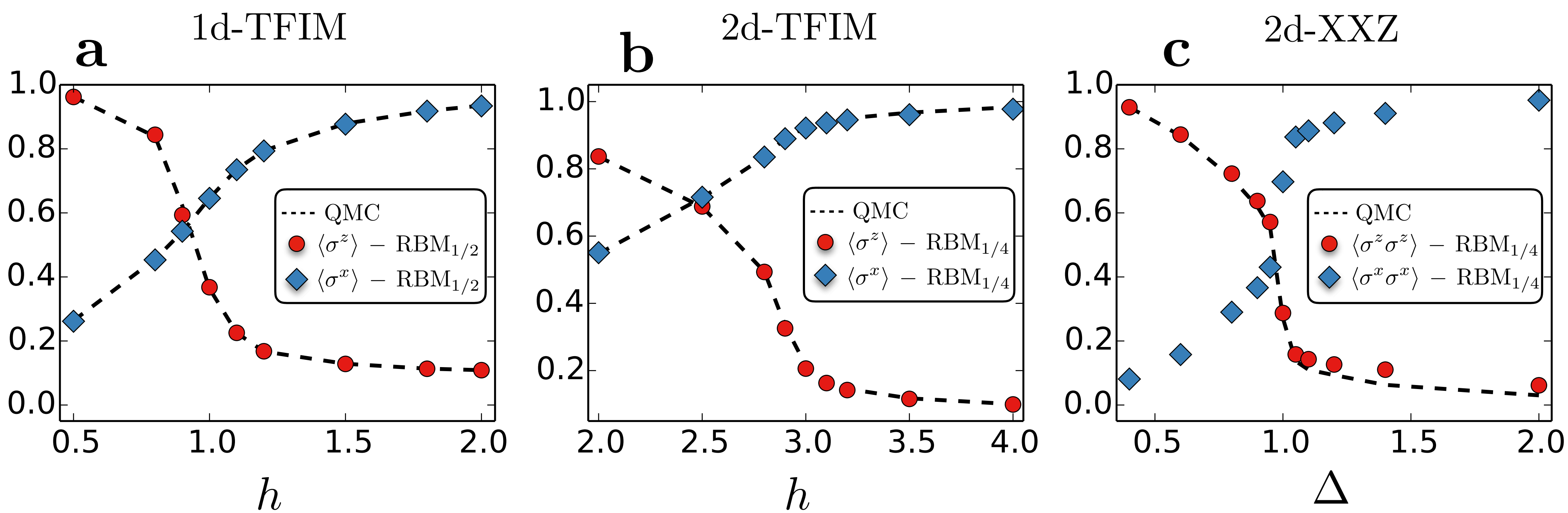
Our NN only requires about ~100 measurements



Tomography of PIMC

We generate syntetic measurements for several models and train the NN.



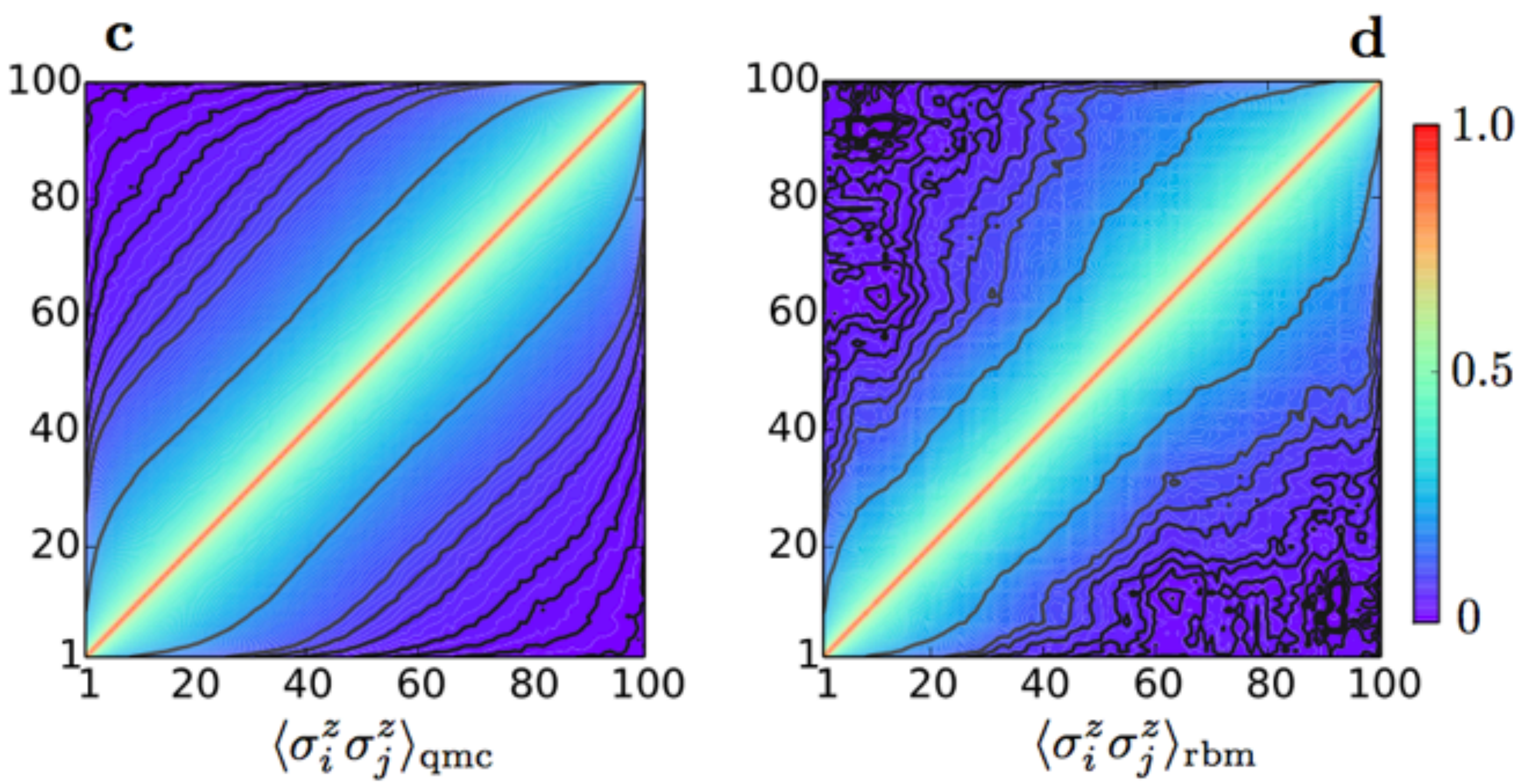
$$\mathcal{H} = -\sum_{\langle ij\rangle} \sigma_i^z \sigma_j^z - h \sum_i \sigma_i^x$$

$$\mathcal{H} = \sum_{\langle ij\rangle} \left[\Delta \left(\sigma_i^x \sigma_j^x + \sigma_i^y \sigma_j^y \right) + \sigma_i^z \sigma_j^z \right]$$

Tomography of PIMC

Once we have a NN representation of the ground state, trained with PIMC samples, we can reconstruct all possible quantities.

Example: n-spin correlation functions, but also entanglement entropy…

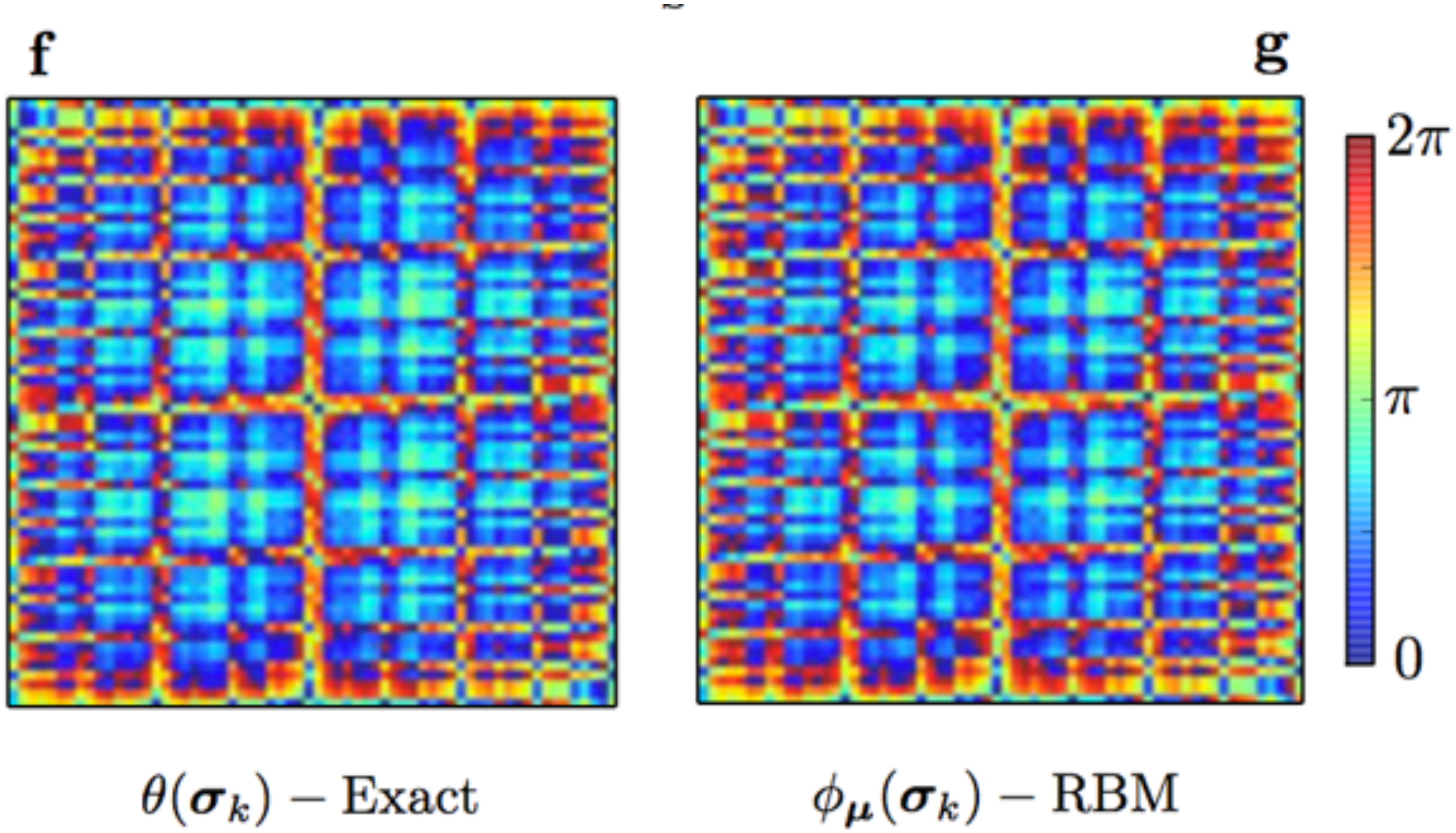


$$\mathcal{H} = -\sum_{\langle ij \rangle} \sigma_i^z \sigma_j^z - h \sum_i \sigma_i^x$$

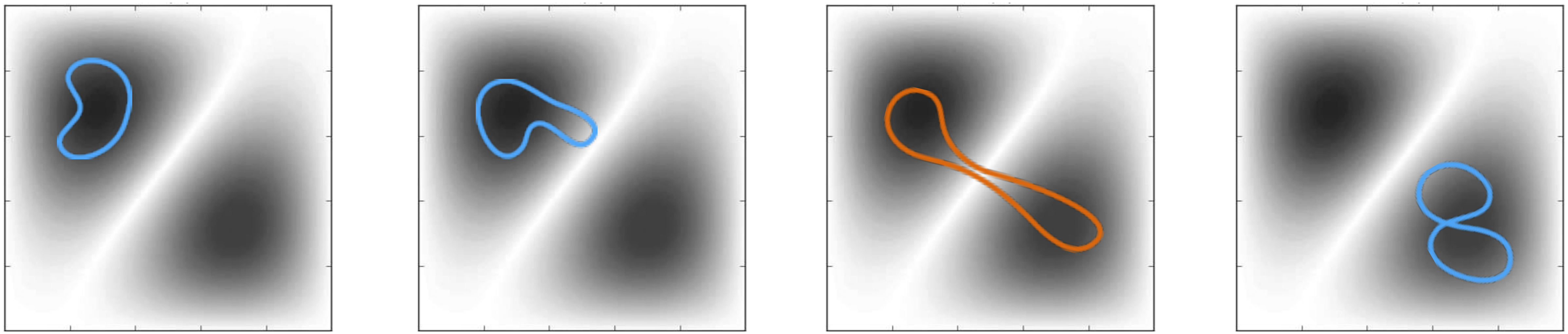
Tomography of Quantum Systems

Generalization to states with complex phase is also possible!

Example: unitary evolution of transverse field Ising.



N=12 spin system, i.e. reconstruction of 2^12=4096 phases, here re-arranged as a 2d array.



Thank you!