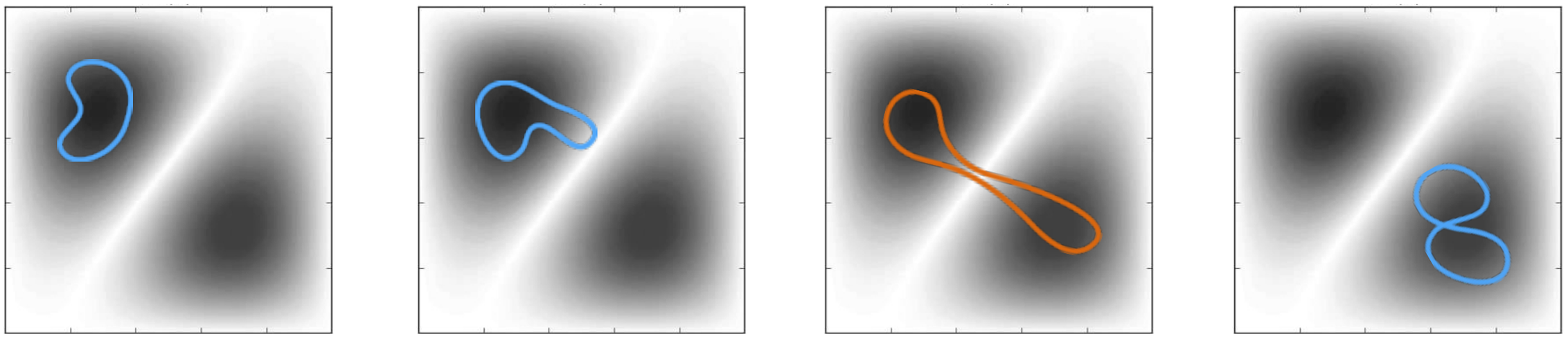


Simulating Quantum Annealing with Quantum Monte Carlo

Guglielmo Mazzola (ETH)

M. Troyer (ETH)
S. Isakov, V. Smelyanskiy, S. Boixo, H. Neven (Google)
Z. Jiang (NASA)

1. ***Introduction*: QA vs SQA (the story so far)**
2. *Introduction*: Quantum Monte Carlo (QMC) for SQA
3. Tunneling with QMC and with QA
4. Conclusions

Outline

SQA

~2000

Simulations

QA

2011

SA

1983

Hardwares

CA

~10.000 b.C.

Implement “Quantum Mechanics”

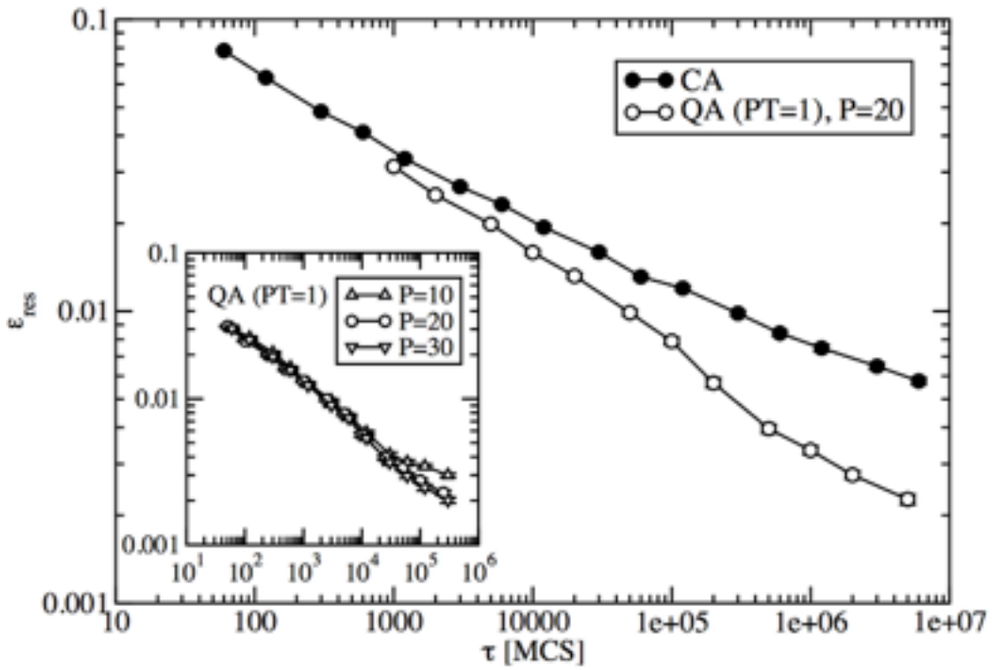
Implement classical optimization

Run on Classical Hardwares

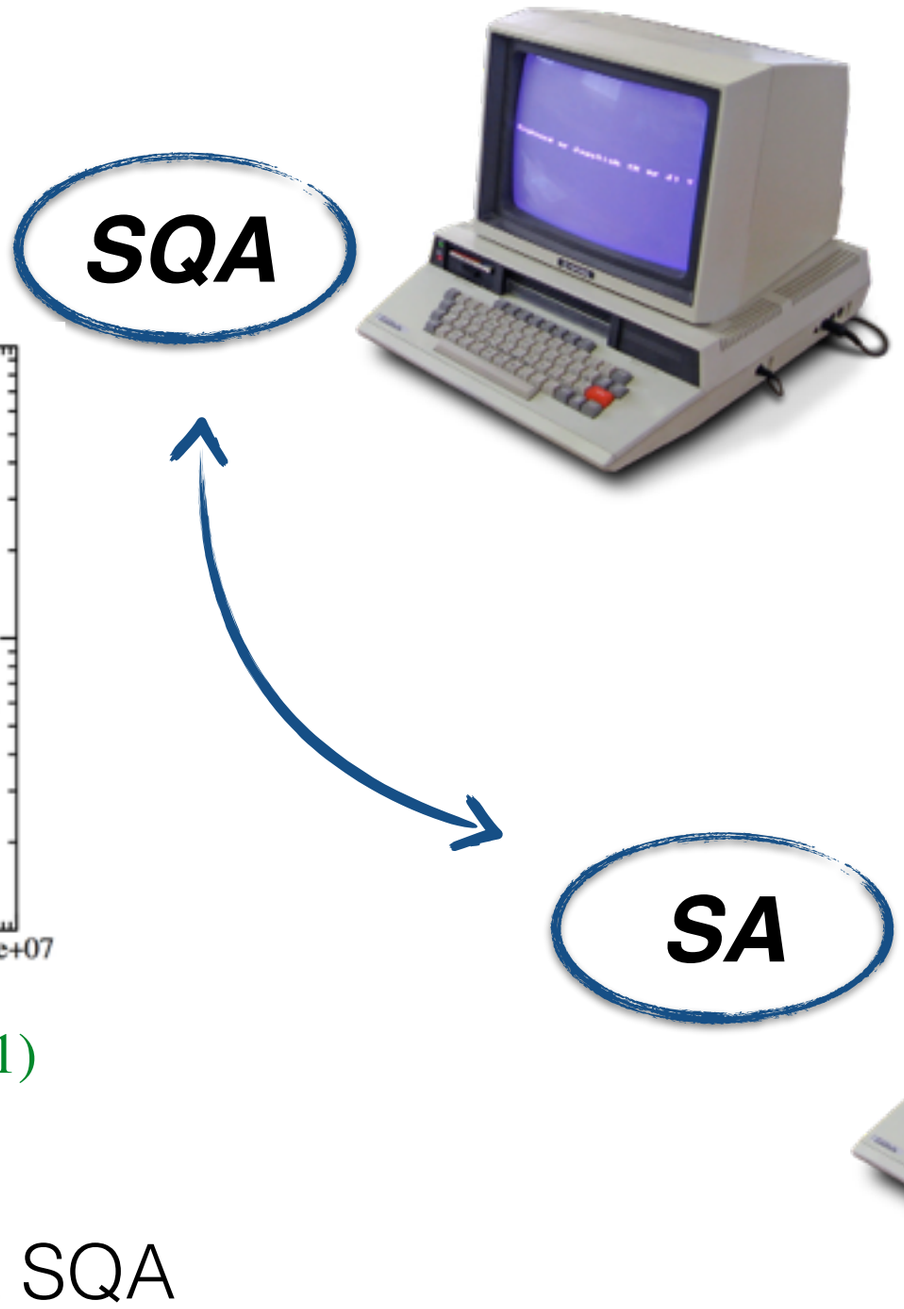
QA

Quantum Hardware

SA

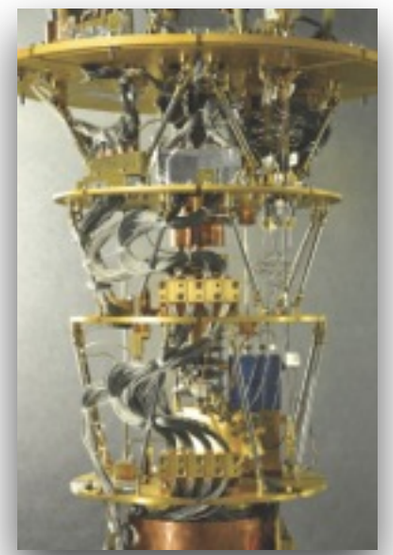


Santoro et. al. ***Science* 295,** 2427 (2001)

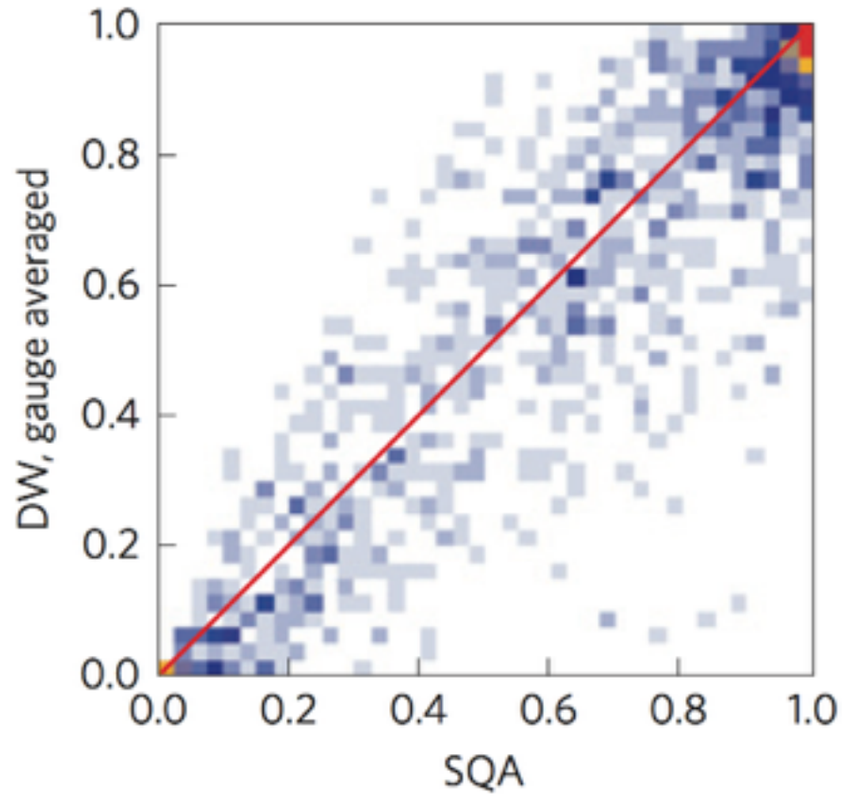


2001: early evidence that SQA outperform SA for 2D random Ising glasses

2014: D-Wave correlates with SQA

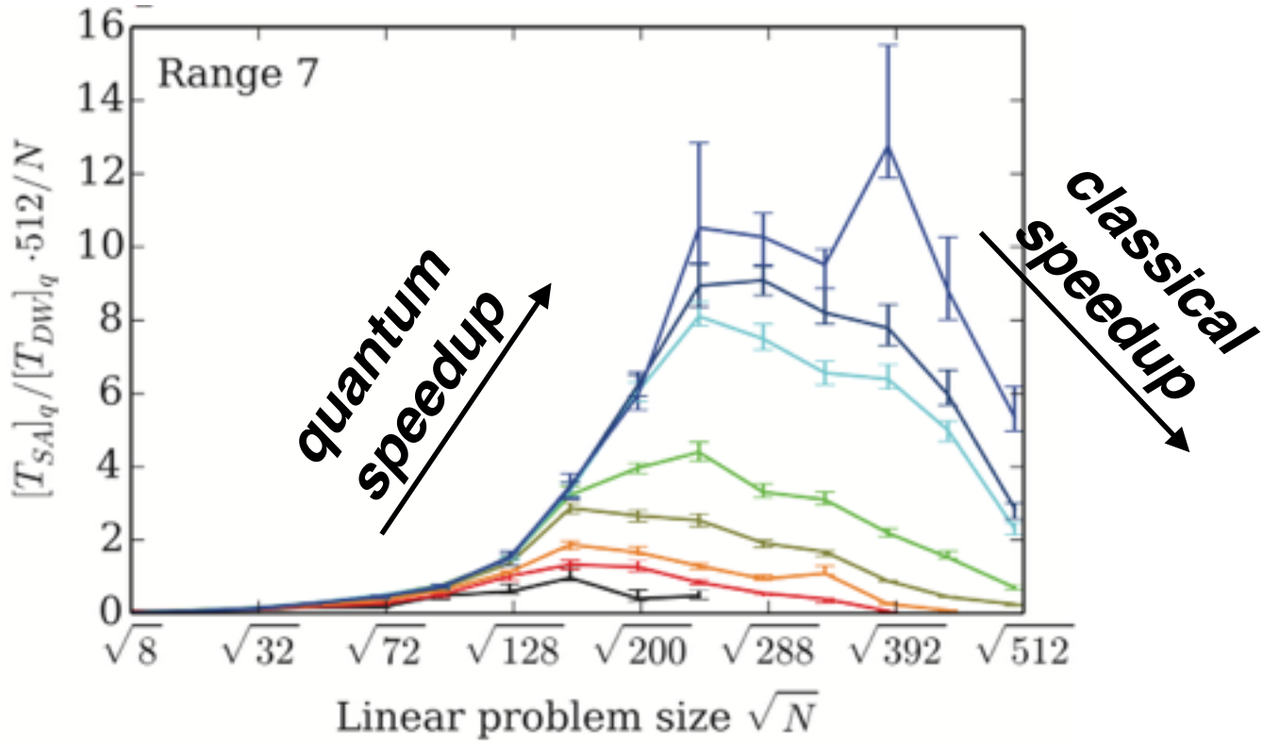


QA



Boixo et. al. ***Nat. Phys.*** **10,** 218 (2014)

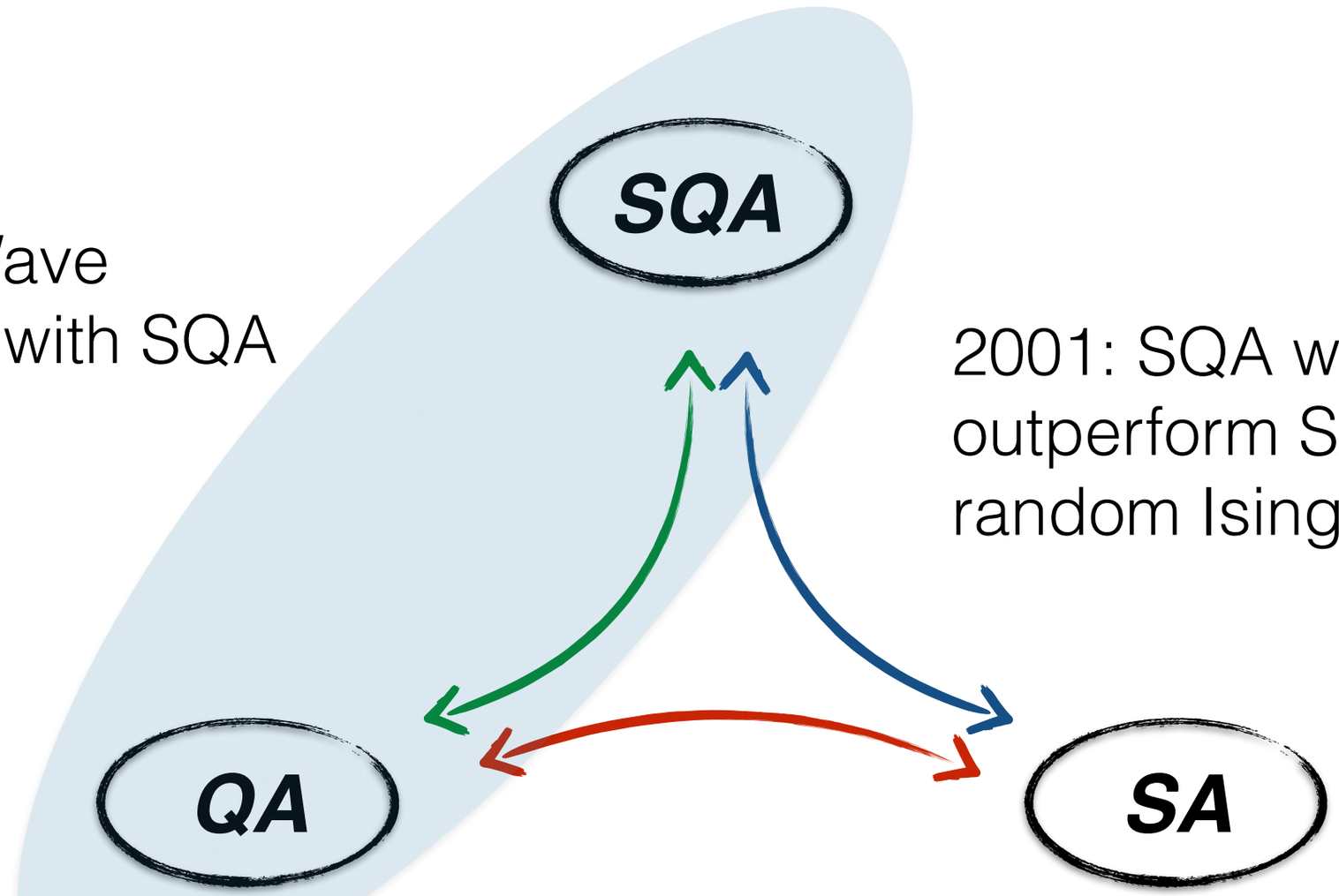
2014: D-Wave does not display quantum speed-up compared to SA.



Ronnow et. al. ***Science*, 345,** 420 (2014)

QA ⟷ **SA**

2014: D-Wave correlates with SQA



2001: SQA with QMC outperform SA for 2D random Ising glasses

N.B. stoquastic drivers such as transverse field hamiltonians always assumed

2014: D-Wave does not display quantum speed-up compared to SA.

V. Denchev et. al. arXiv:1510.08057

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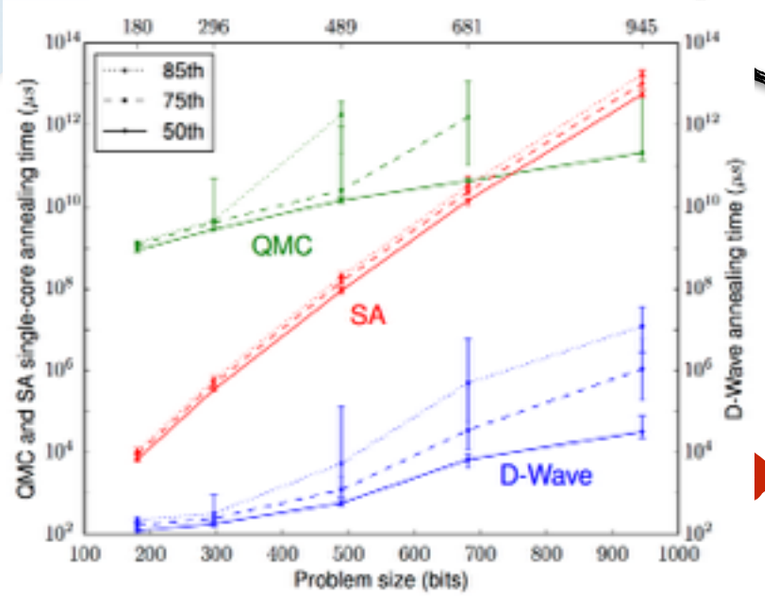
2001: SQA with QMC outperform SA for 2D random Ising glasses

SQA

QA

SA



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V. Denchev et. al. arXiv:1510.08057

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Outline

Simulating Quantum Annealing

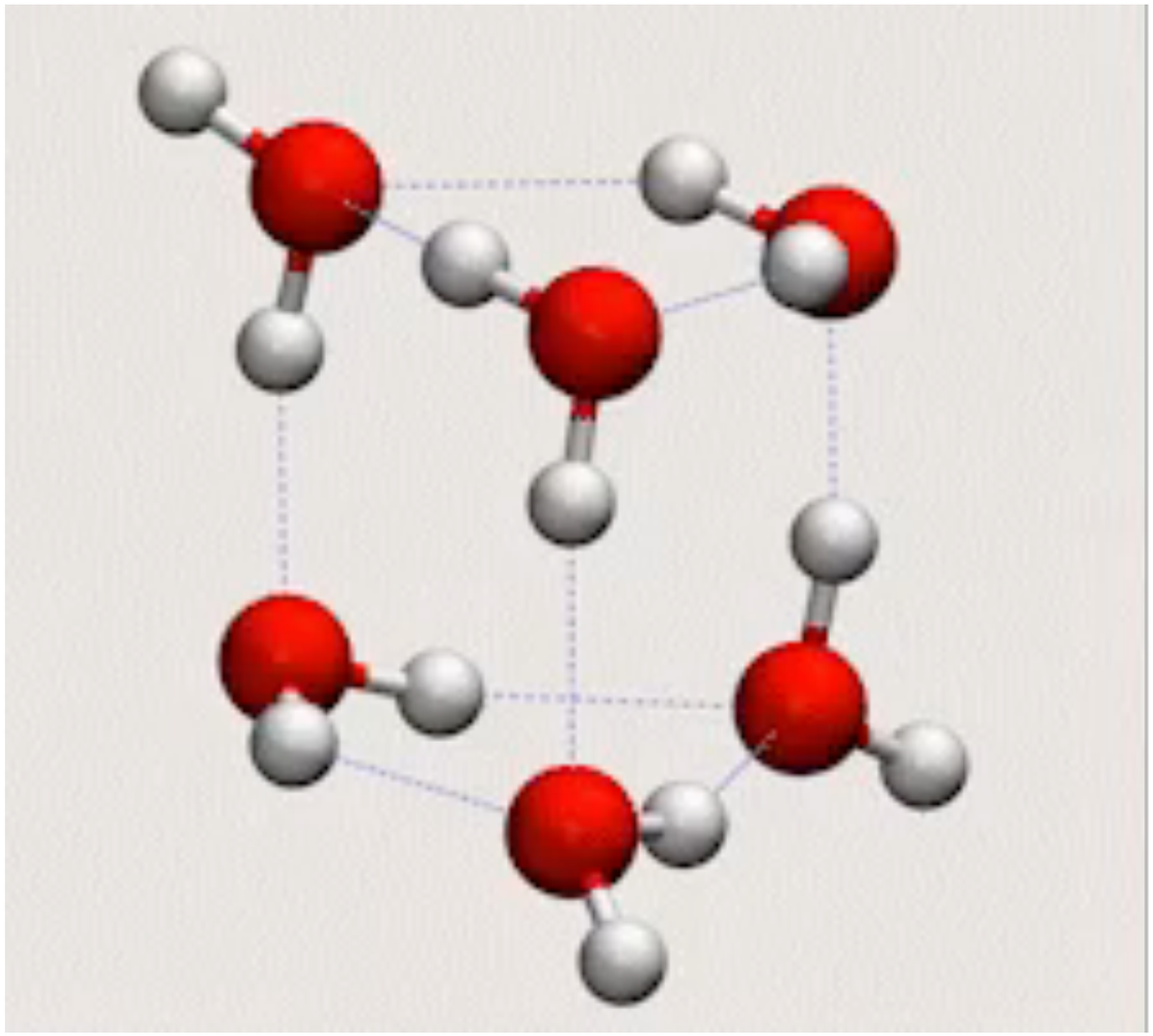
Ideally we would like to solve time-dependent Schroedinger equation:

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

Hilbert space scales exponentially with the size!

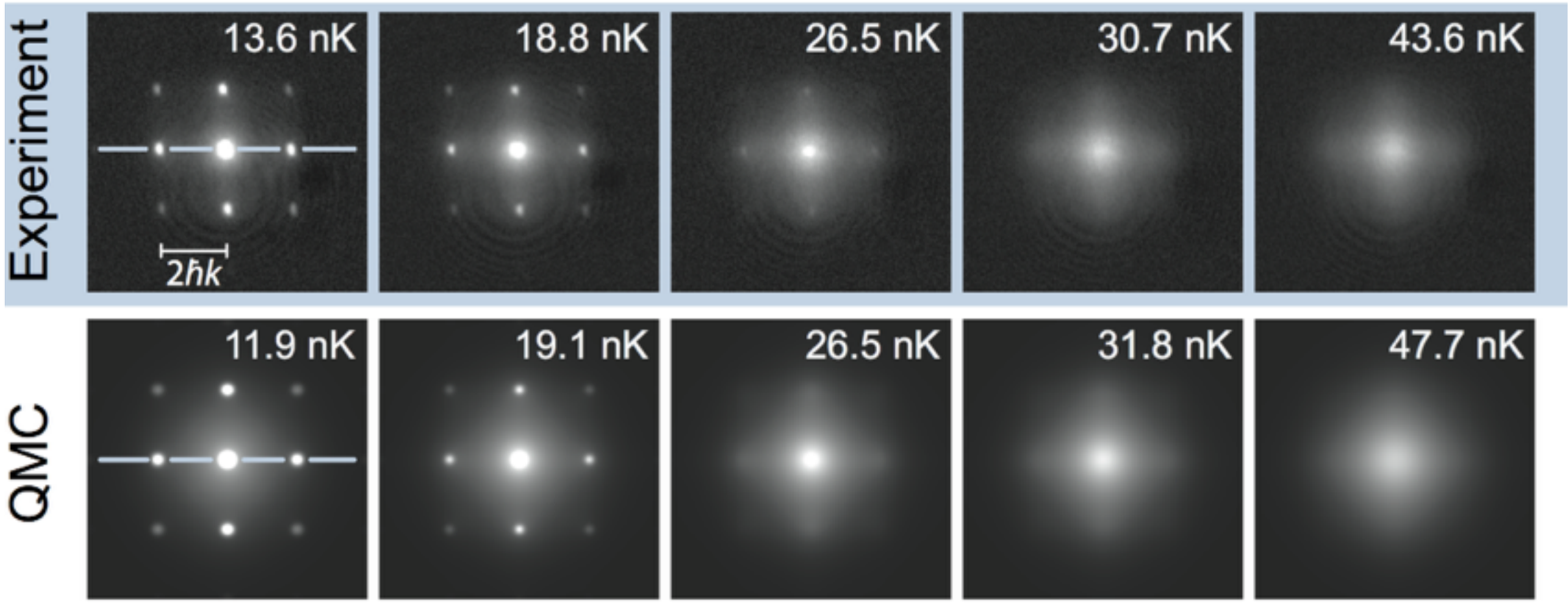
System size: ~40 spins

Quantum tunneling in the smallest droplet of water



Richardson et al. "**Concerted** hydrogen-bond breaking by **quantum tunneling** in the water hexamer prism."
***Science* 351, 1310 (2016)**

Quantum Monte Carlo simulations



Ultracold bose gas

S. Trotzky, L. Pollet, F. Gerbier, U. Schnorrberger, I. Bloch, N. V. Prokof'ev, B. Svistunov & M. Troyer

***Nature Physics* 6,** 998–1004 (2010)

Simulating Quantum Annealing

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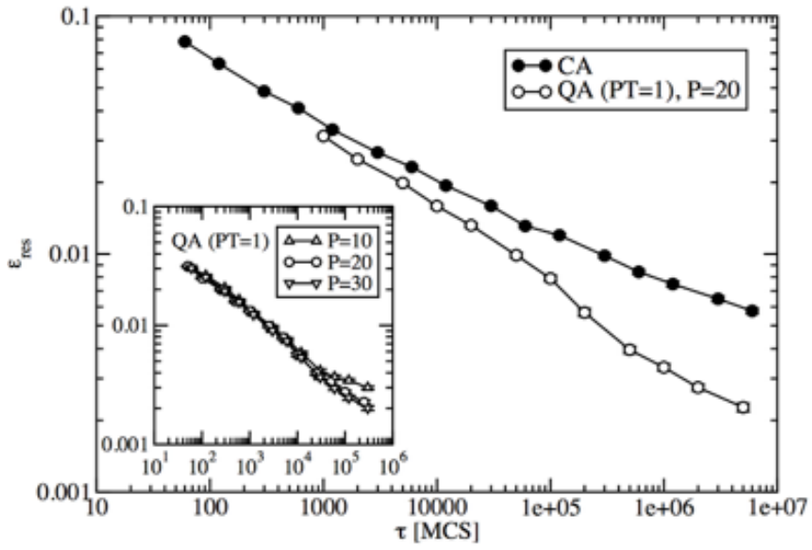
$$\frac{d}{dt}|\psi(t)\rangle = -iH(t)|\psi(t)\rangle$$

Hilbert space scales exponentially with the size!

System size: ~40 spins

Quantum Monte Carlo (PIMC)

Computational effort scales linearly with size!



Santoro et. al. ***Science* 295,** 2427 (2001)

System size: ~10.000 spins

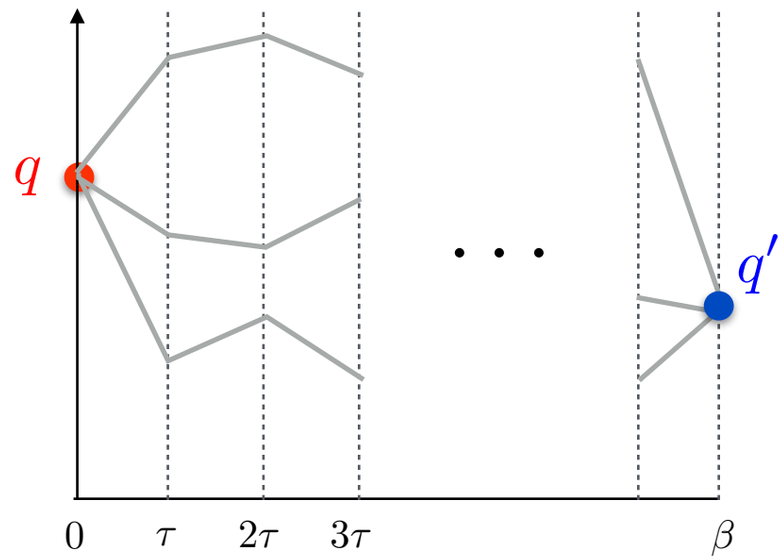
Path Integral Monte Carlo

Density matrix is an operator: $\rho = e^{-\beta H}$ $\qquad Z = \mathrm{Tr}\ e^{-\beta H}$

Matrix elements are difficult to compute: $\langle q|e^{-\beta H}|q'\rangle$ because $H = H_1 + H_2$, $[H_1, H_2] \neq 0$

instead $e^{-\tau H} \approx e^{-\tau H_1} e^{-\tau H_2}$ $\qquad e^{-\beta H} = \lim_{M\to\infty} \left[e^{-\frac{\beta}{M} H_1} e^{-\frac{\beta}{M} H_2} \right]^M$

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



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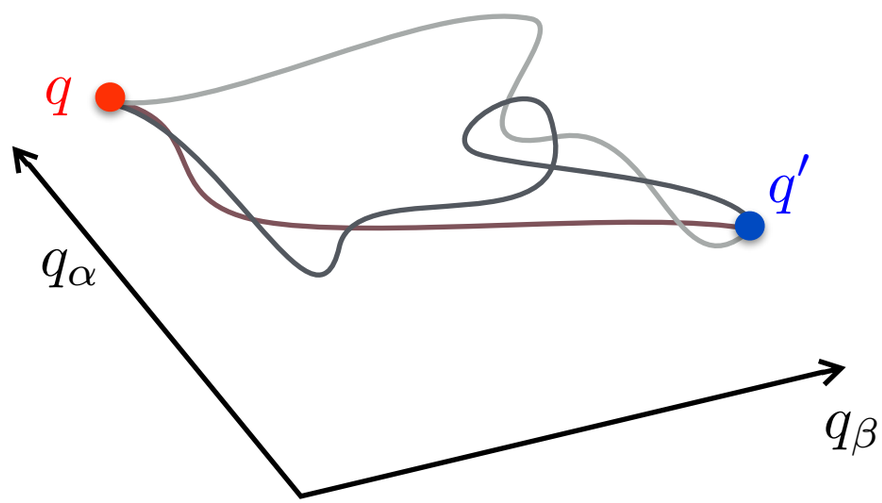

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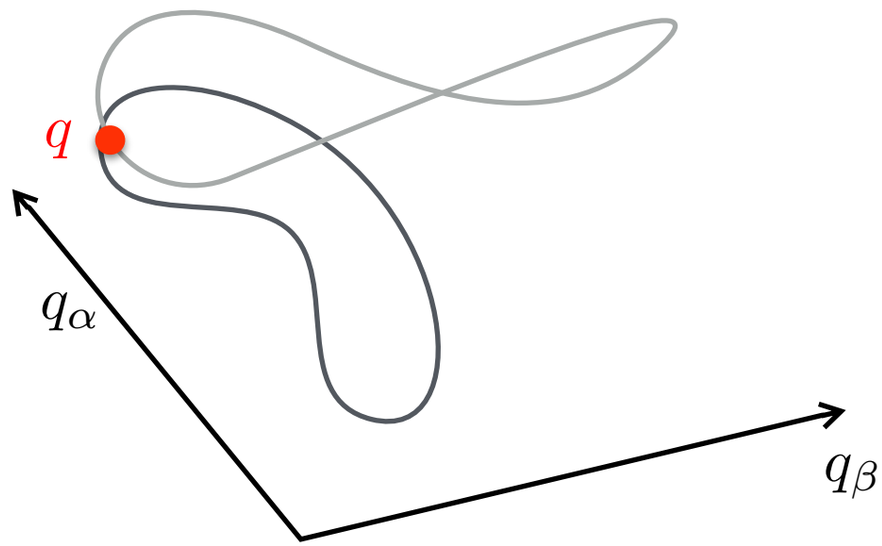

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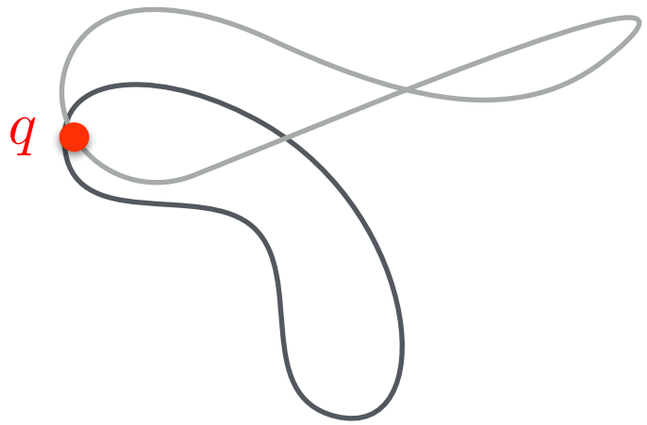


Path Integral Monte Carlo

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

$$\langle q_1|e^{-\tau H}|q_2\rangle \cdots \langle q_M|e^{-\tau H}|q\rangle$$

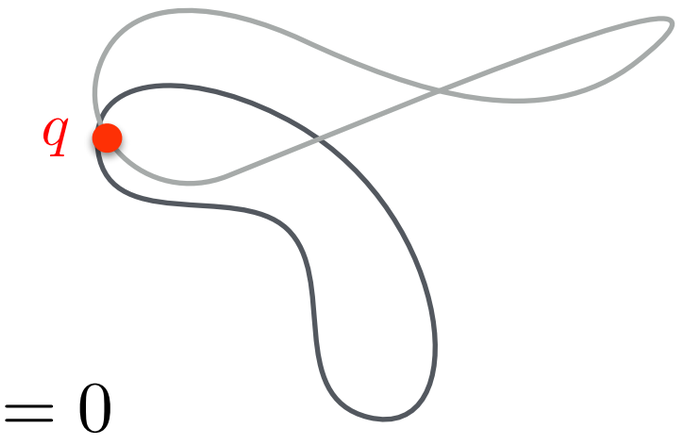
$$Z = \sum_{\text{paths}} e^{-\mathcal{S}[\text{path}]}$$

NB: only possible for stoquastic H

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

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

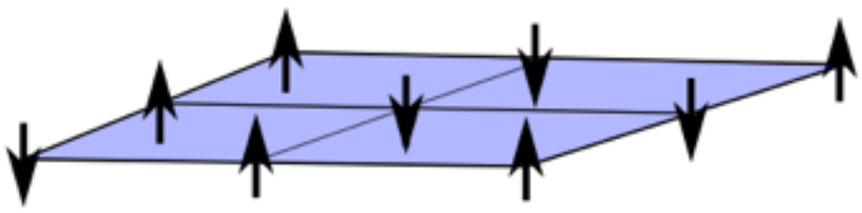
Dominant contributions come from paths $\dfrac{\partial \mathcal{S}[q(\tau)]}{\partial q(\tau)} = 0$

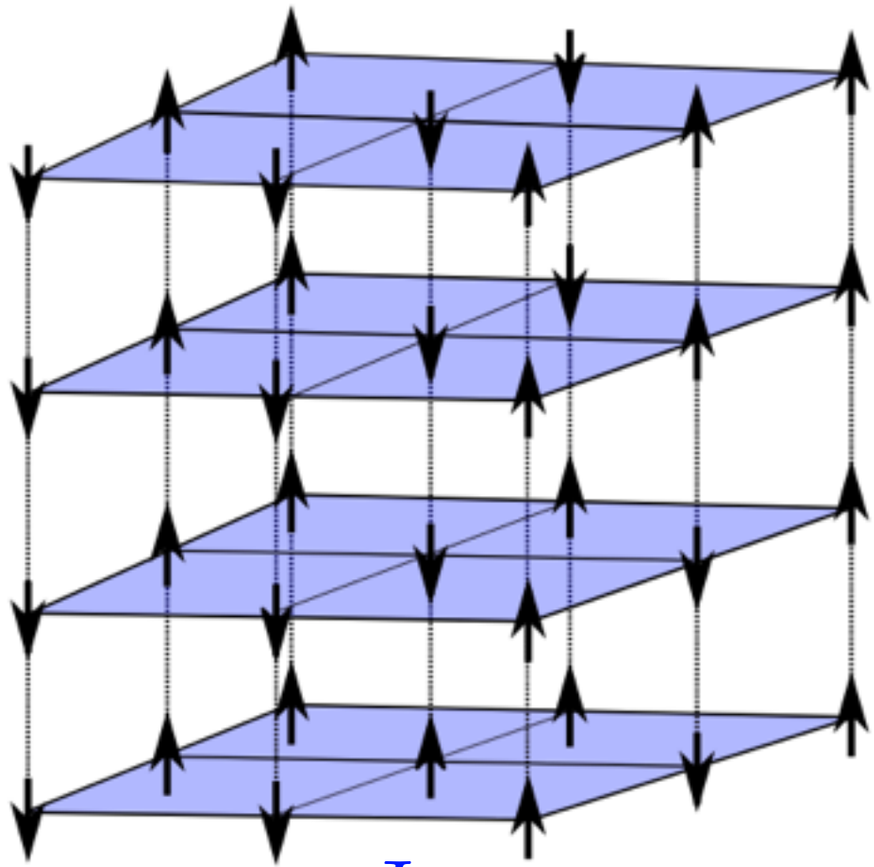


Form of $\mathcal{S}[q(\tau)]$ is system dependent.

Path Integral Monte Carlo: spin systems

$$H = \sum_{ij} J_{ij}\sigma_i^z\sigma_j^z + \Gamma\sum_i \sigma_i^x$$





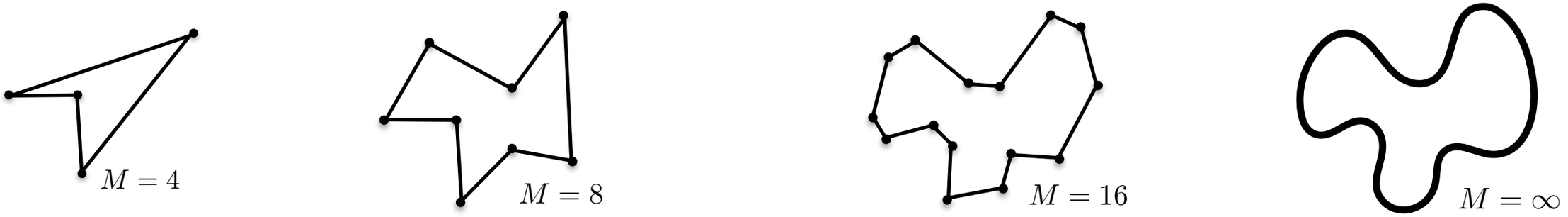
$$e^{-\mathcal{S}[q(\tau)]} = e^{-\beta\mathcal{H}/M}$$

$$\mathcal{H} = \sum_{k=1}^{M}\left(\sum_{ij} J_{ij}s_i^k s_j^k + J^\perp \sum_i \quad s_i^k s_i^{k+1}\right)$$

Path Integral Monte Carlo: physical limit

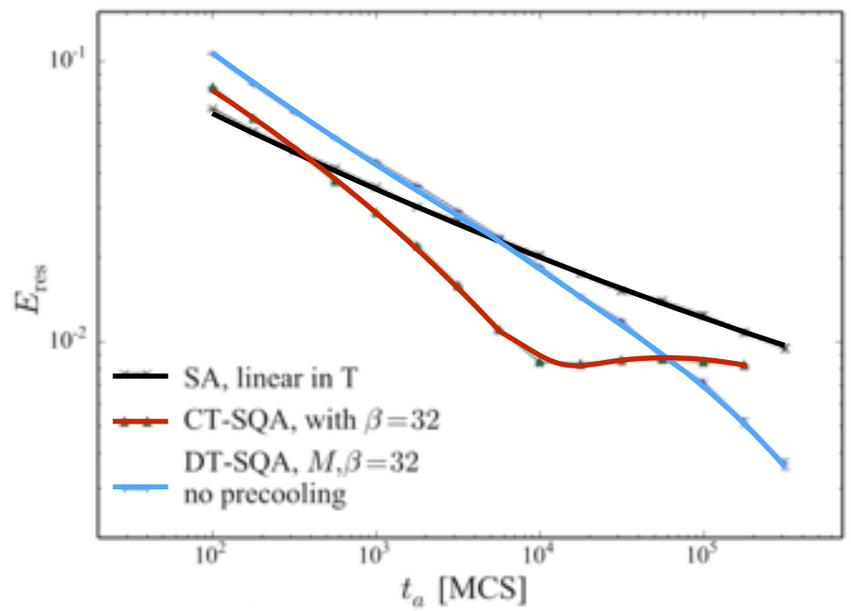
$$e^{-\beta H} = \lim_{M\to\infty} \left[e^{-\frac{\beta}{M} H_1} e^{-\frac{\beta}{M} H_2} \right]^M$$

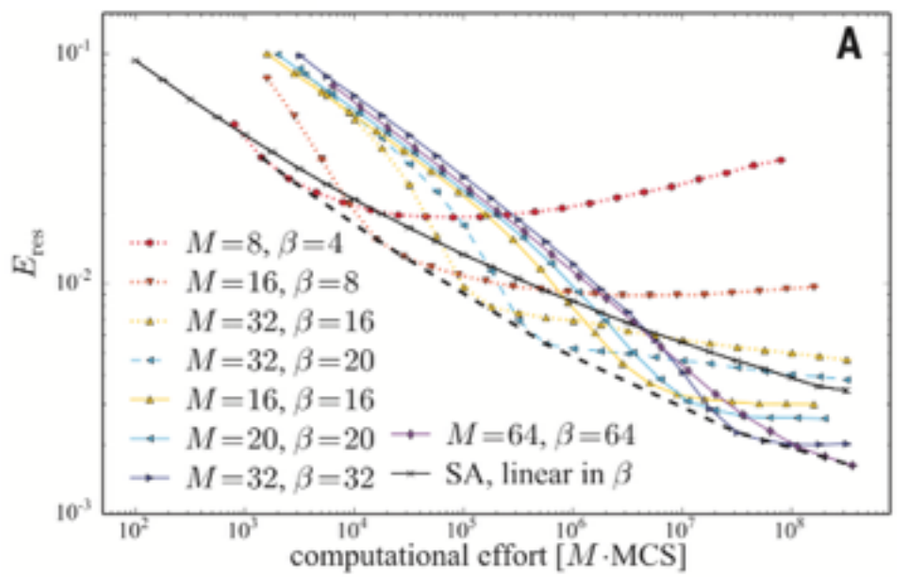
PIMC samples the correct partition function in the *physical* limit $M \to \infty$



One could also optimise M at given β

Continuous time limit (CT)





Heim et. al. ***Science* 348,** 215 (2015)

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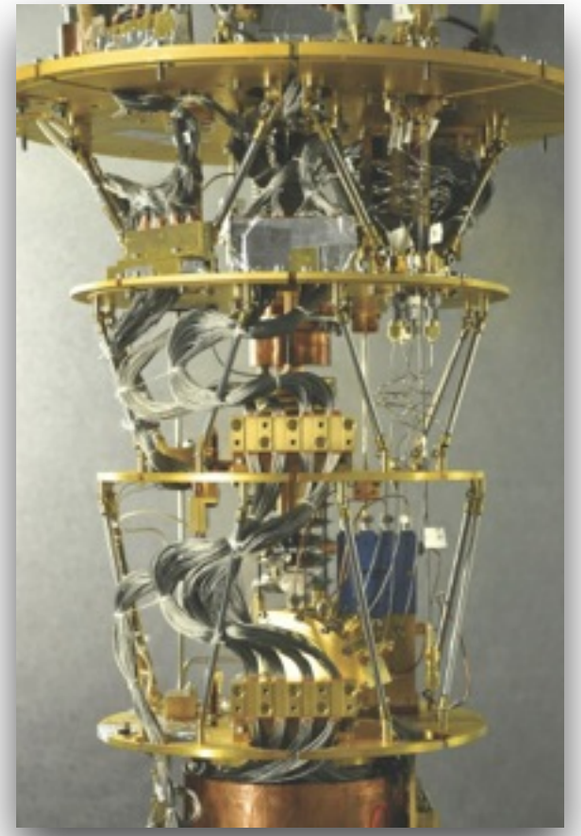
Outline

Experiment: compare runtimes of QA device vs QMC



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

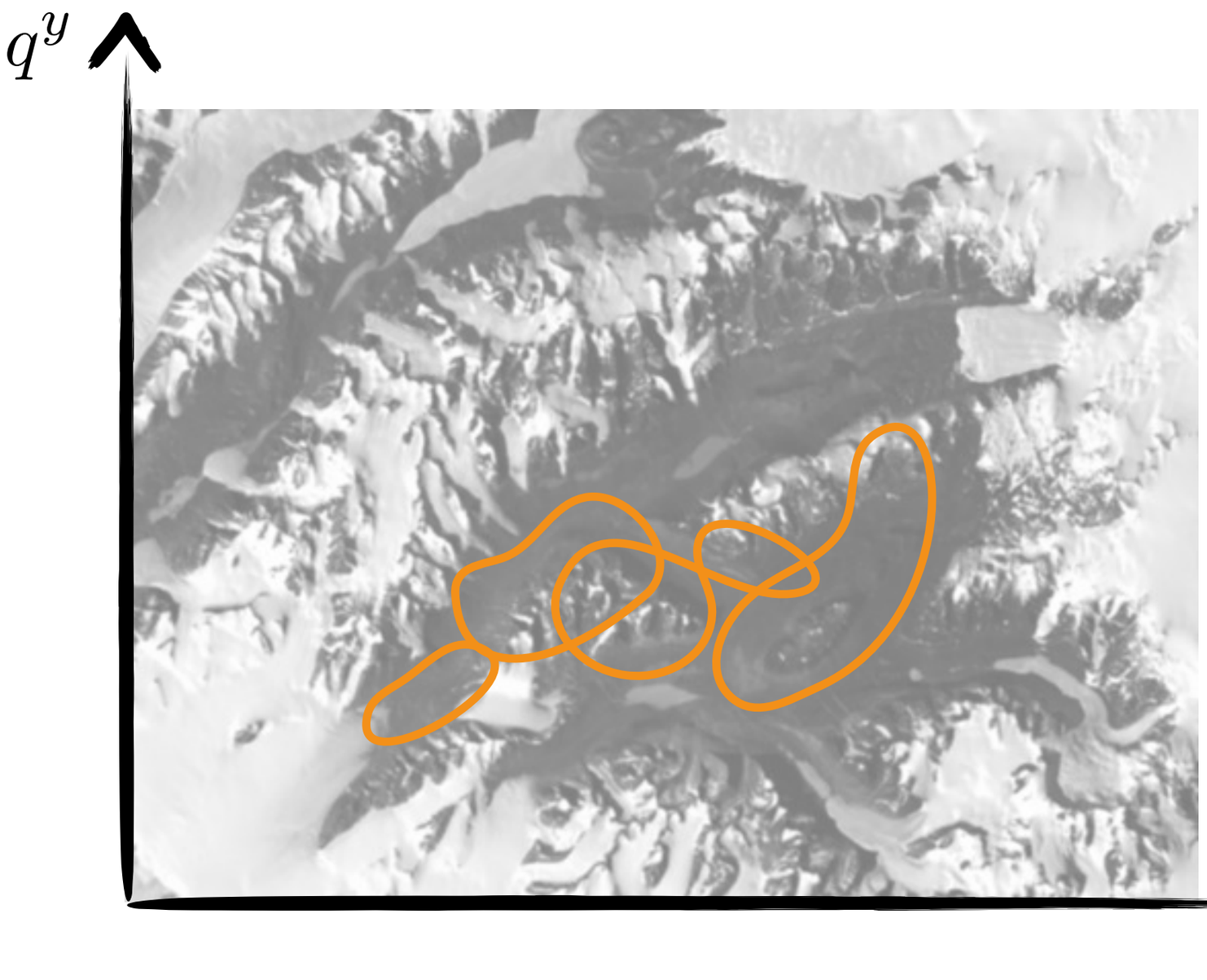
$$T_{QA} \propto \Delta^{-2}$$

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

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

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).

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

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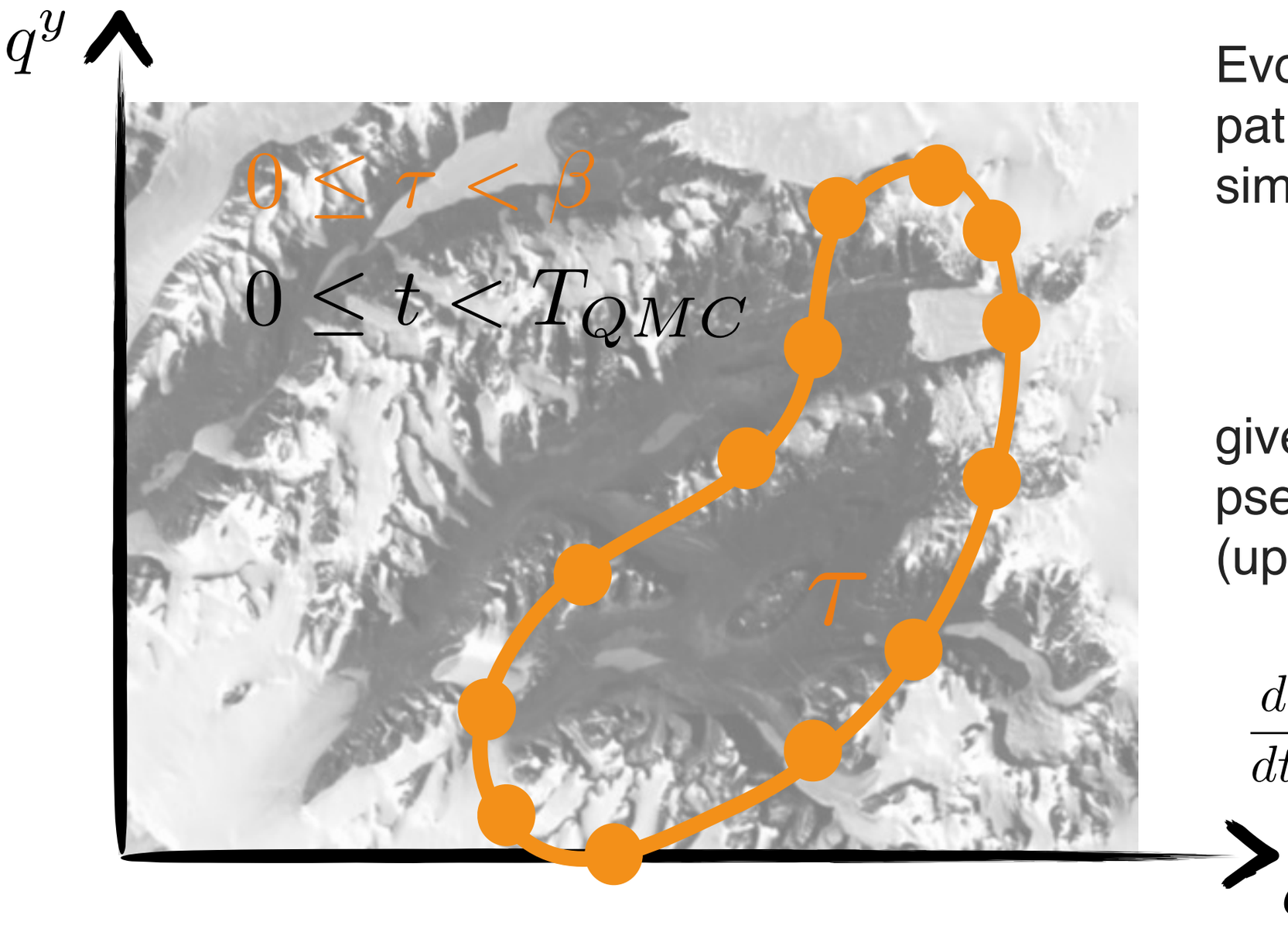

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$$\frac{d}{dt}|\psi(t)\rangle = -iH(t)|\psi(t)\rangle$$

Transition states of the dynamics: instantons

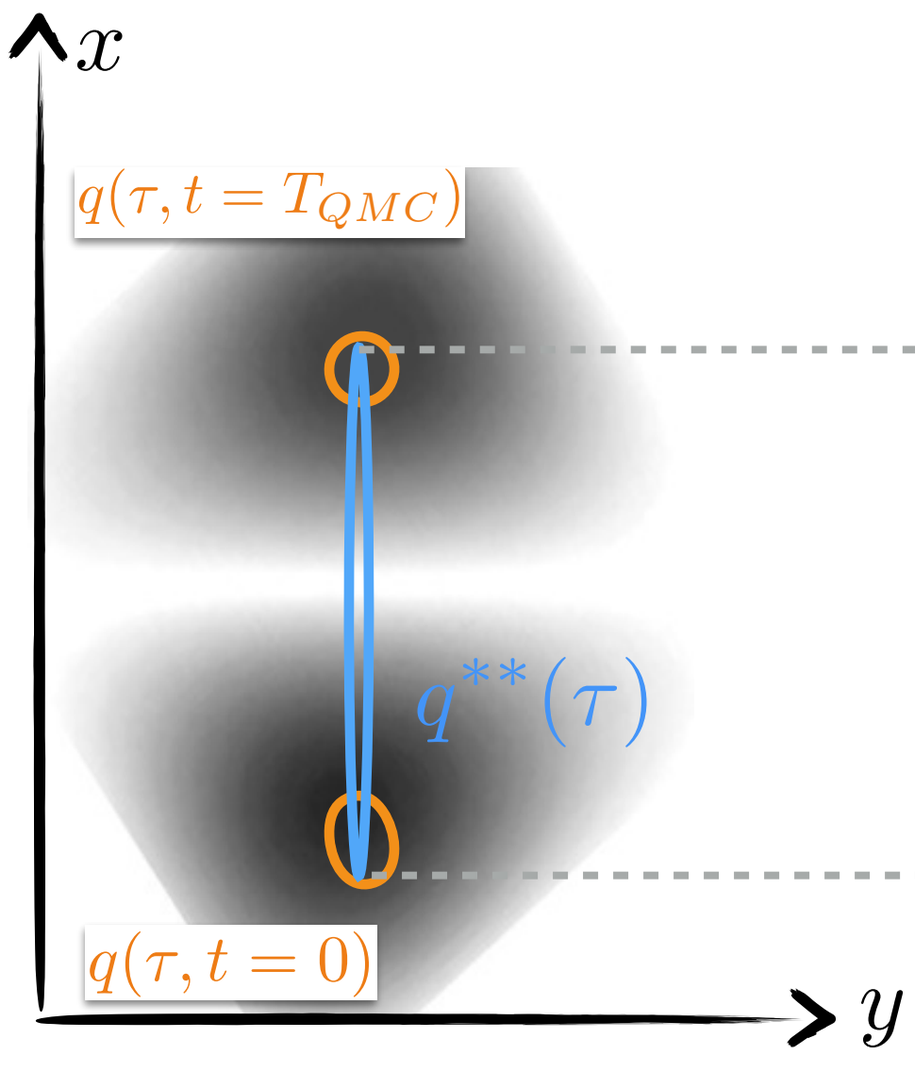
Consider double well problems

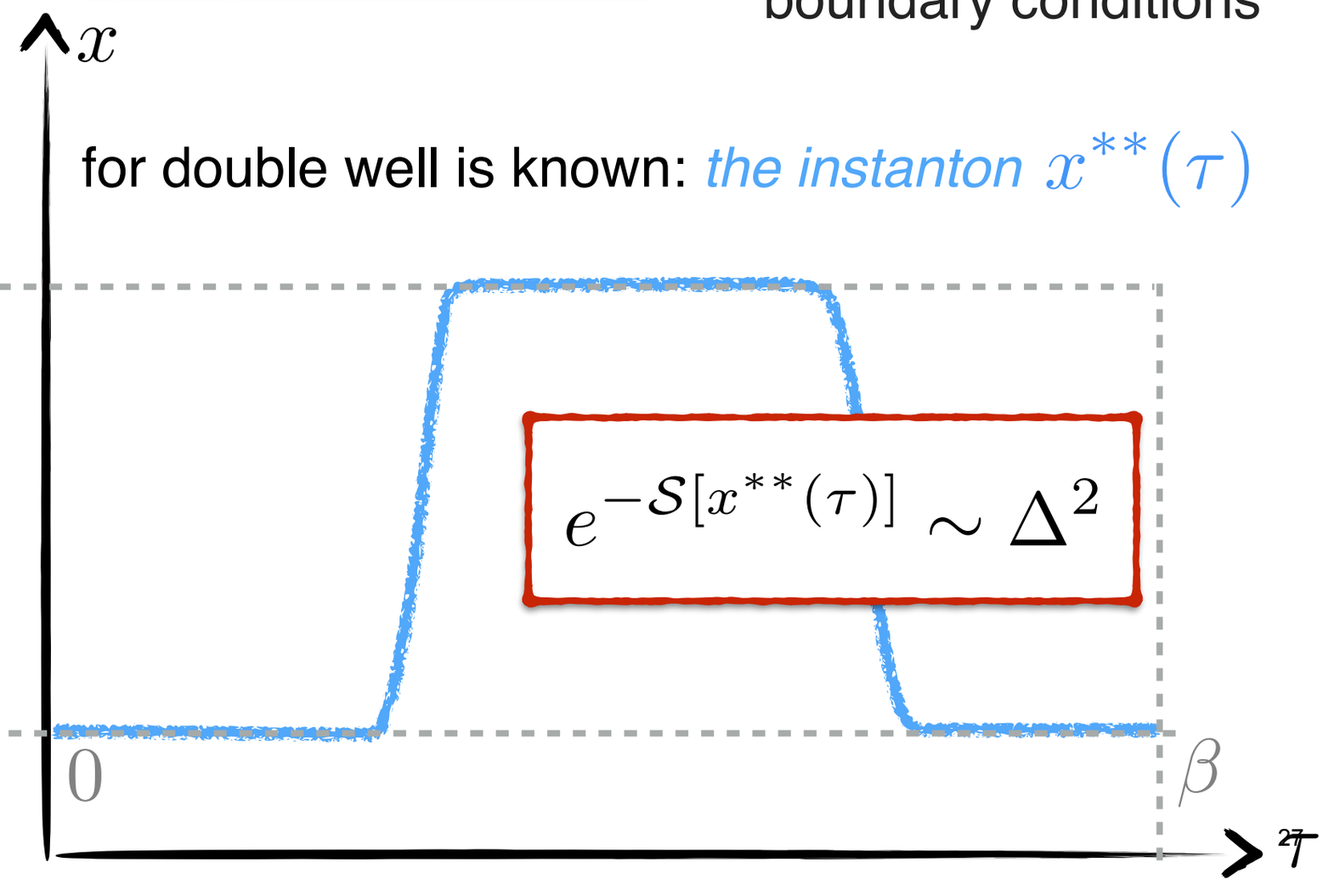
$$\frac{\partial q(\tau,t)}{\partial t} = -\frac{\delta \mathcal{S}[q(\tau,t)]}{\delta q(\tau,t)} + \eta(\tau,t)$$

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





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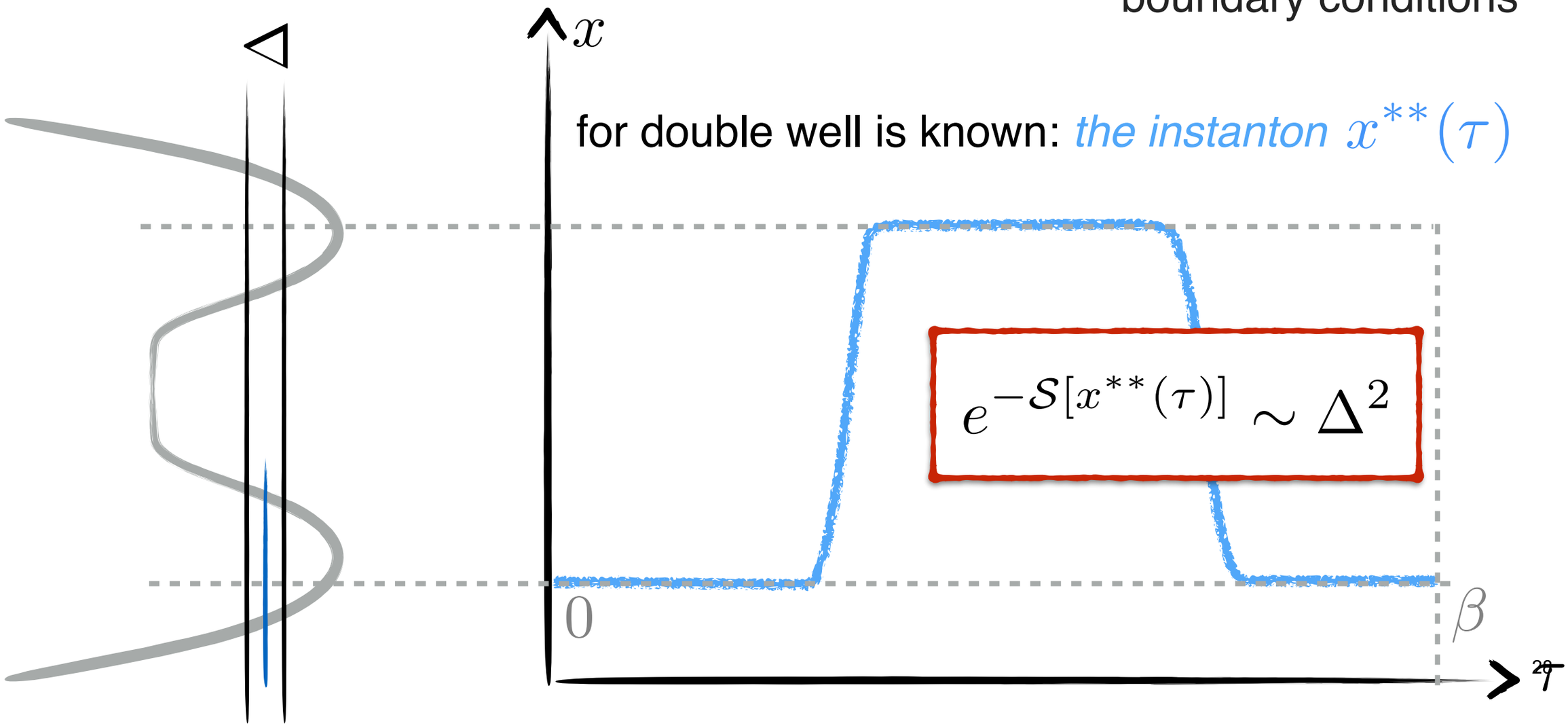
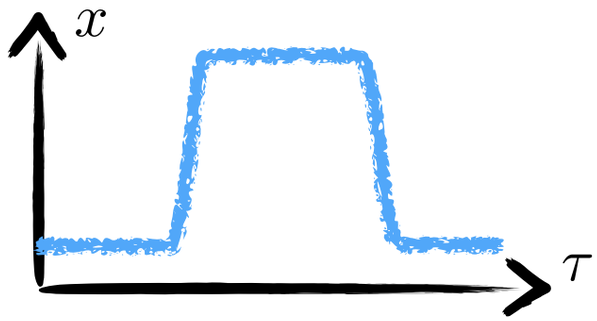


Transition states of the dynamics: instantons

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)

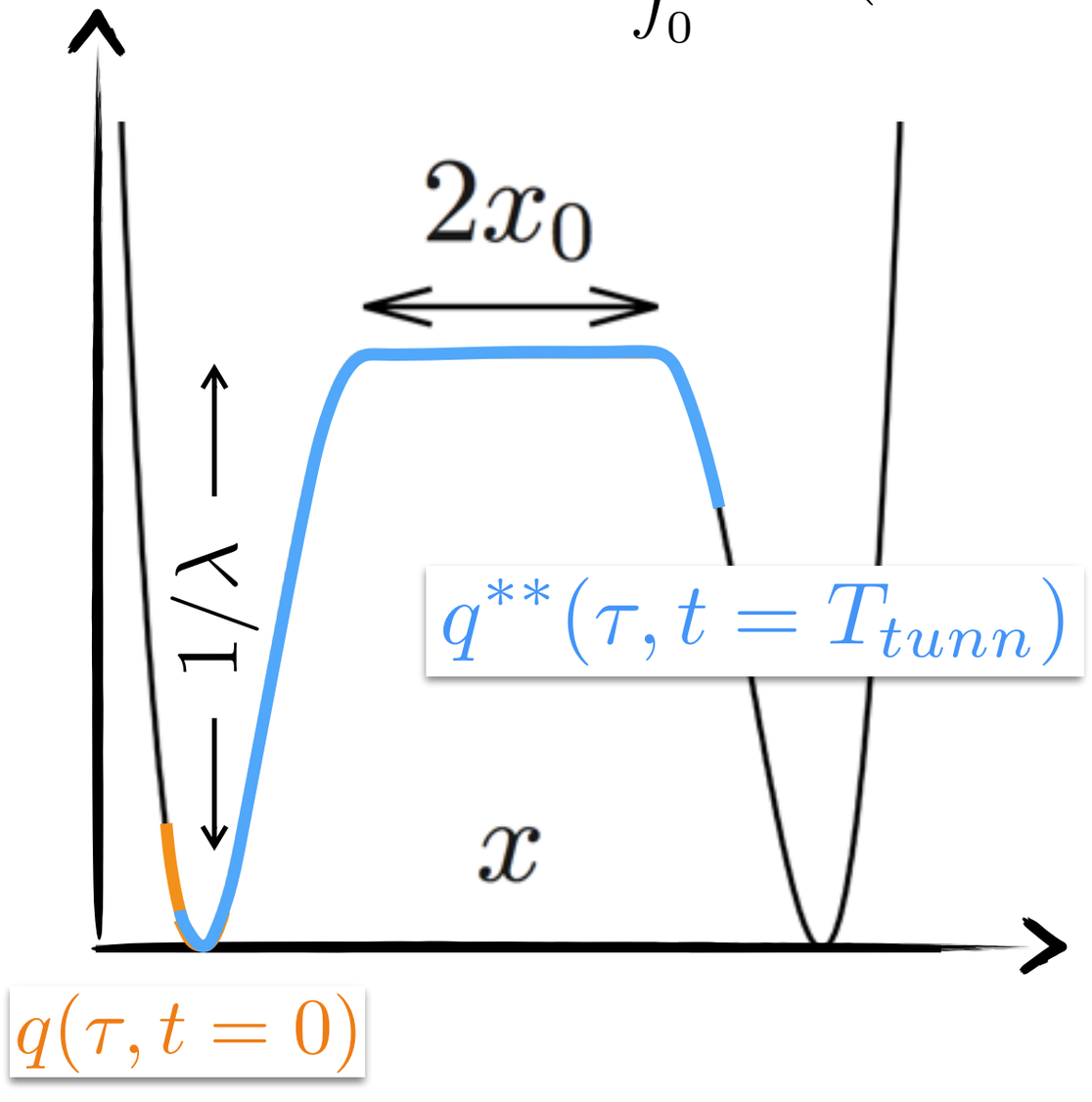
$$k \propto e^{-\mathcal{S}[q^{**}(\tau)]} \sim \Delta^2$$

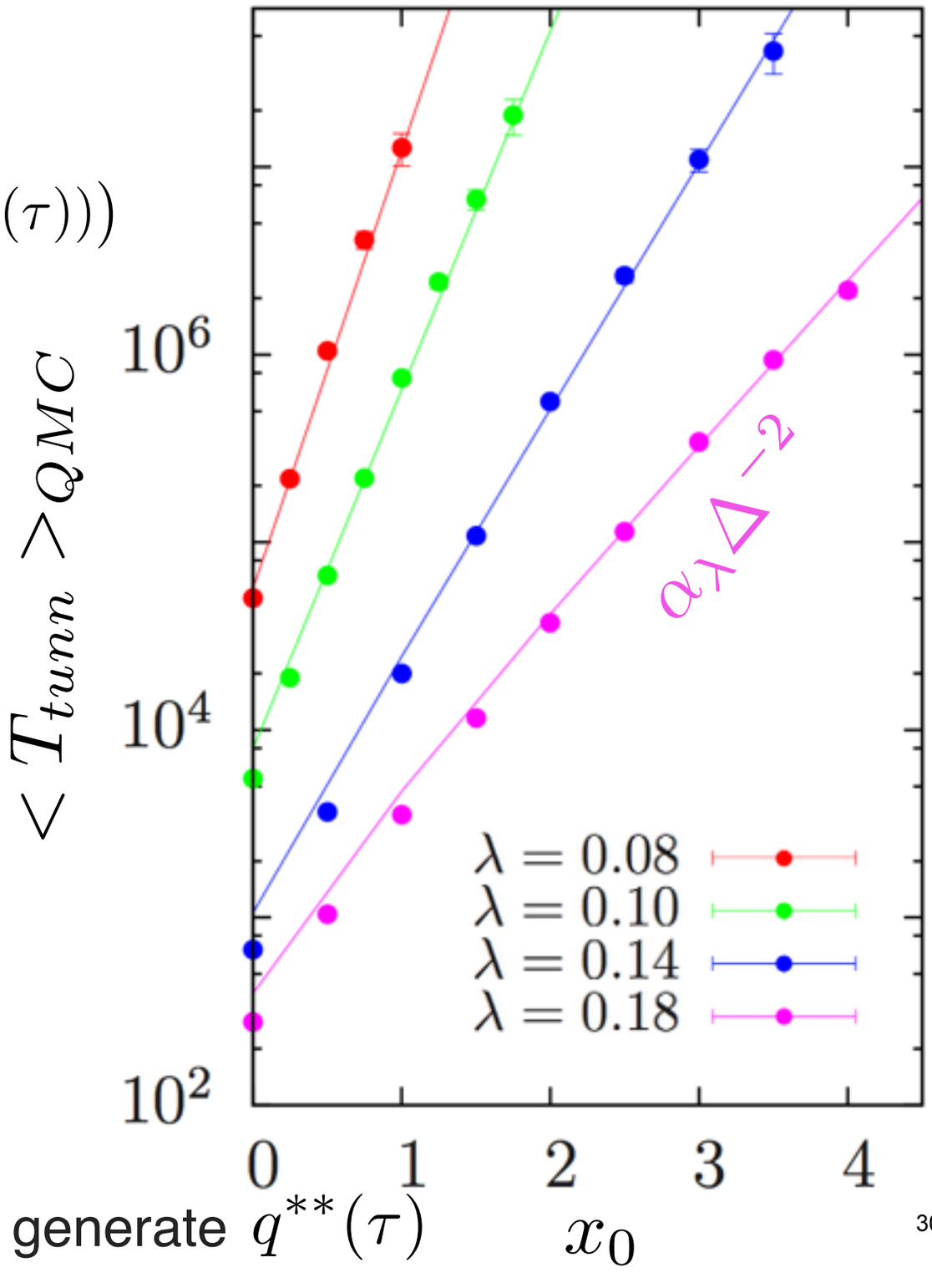
Therefore we expect that the QMC tunneling rate must scale as $\sim \Delta^2$

Continous space model: 1D double well

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

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



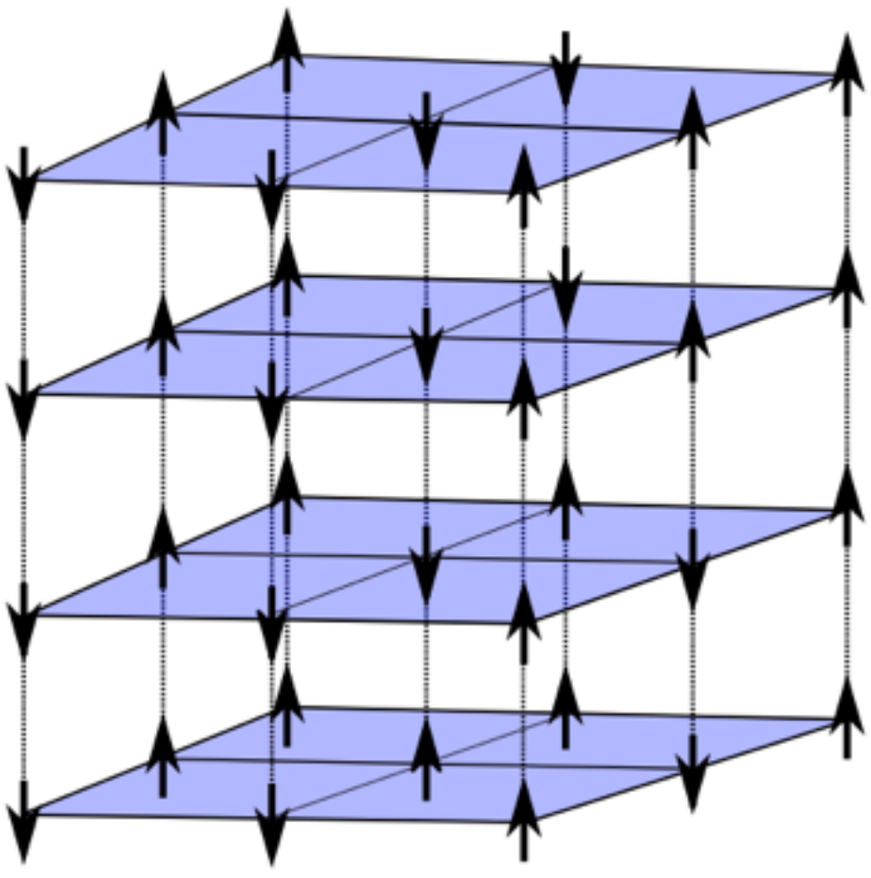


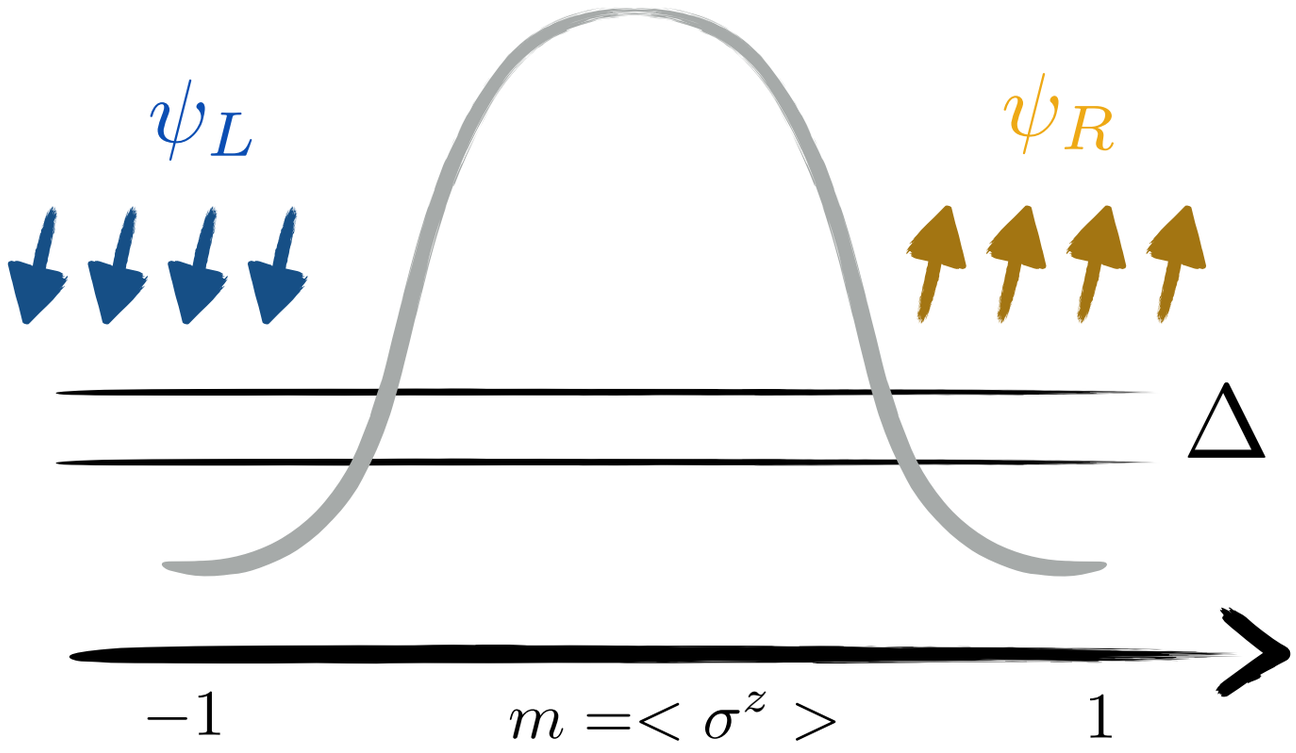
T_{tunn} : Number of QMC updates required to generate $q^{**}(\tau)$

Ferromagnetic Ising system

Consider now a spin system.

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

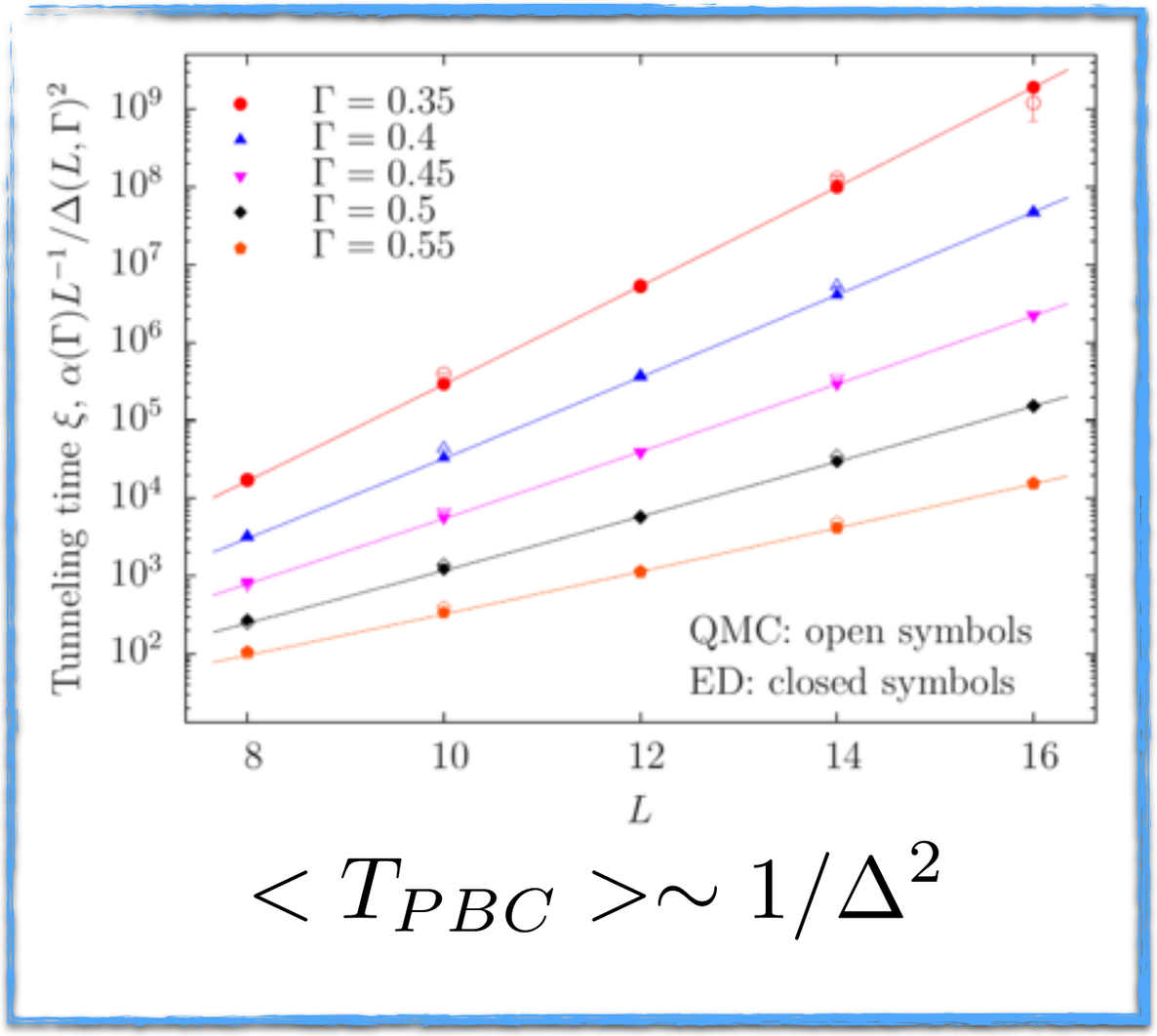




Path integral construction lead to an extended lattice (formally similar to the previous ring polymer)

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

QMC tunneling rate in ferromagnetic Ising system



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

"Understanding Quantum Tunneling through Quantum Monte Carlo Simulations"

S.V. Isakov, G. Mazzola, V.N. Smelyanskiy, Z. Jiang, S. Boixo, H. Neven, and M. Troyer

arXiv:1510.08057

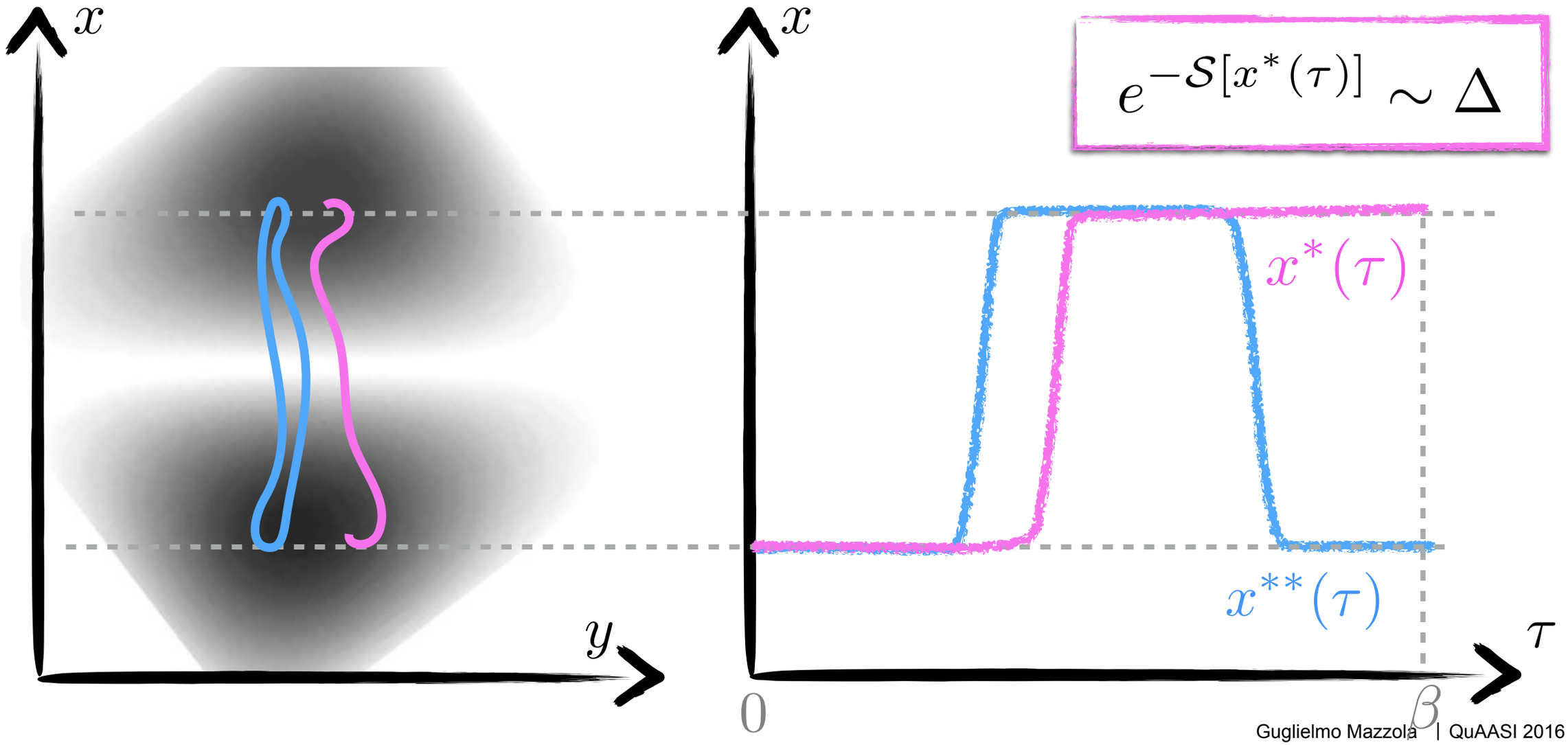
Transition states of the dynamics: instantons

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

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

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

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



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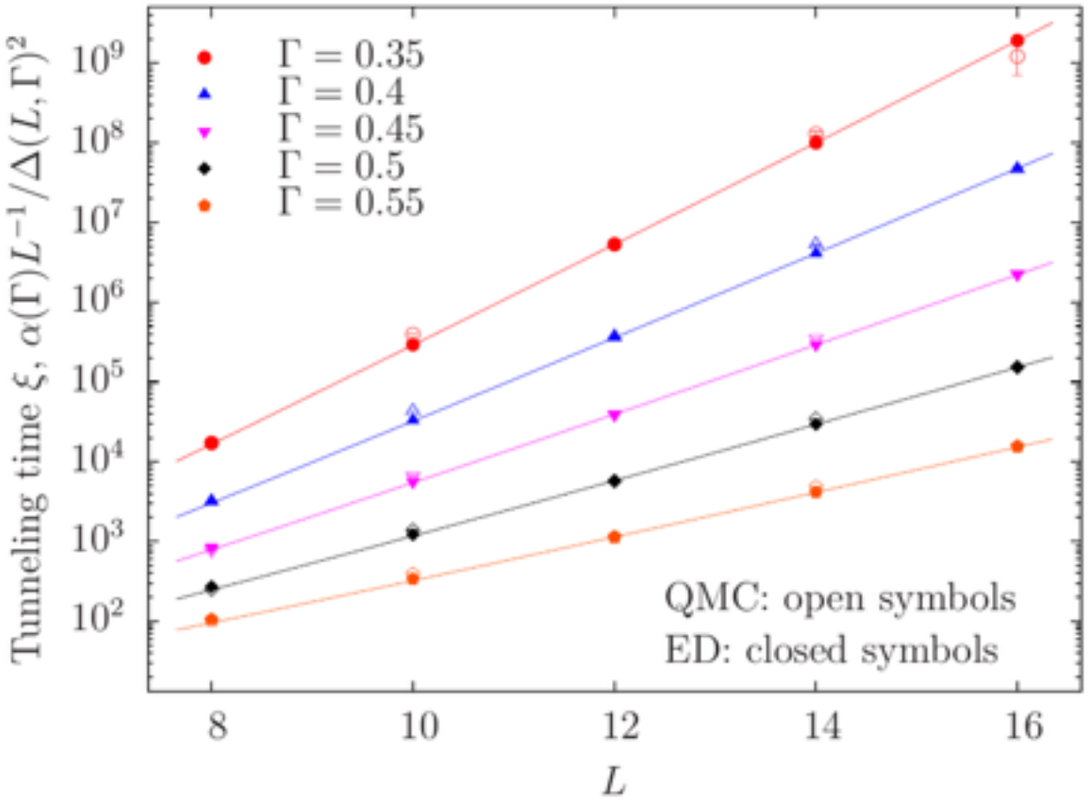
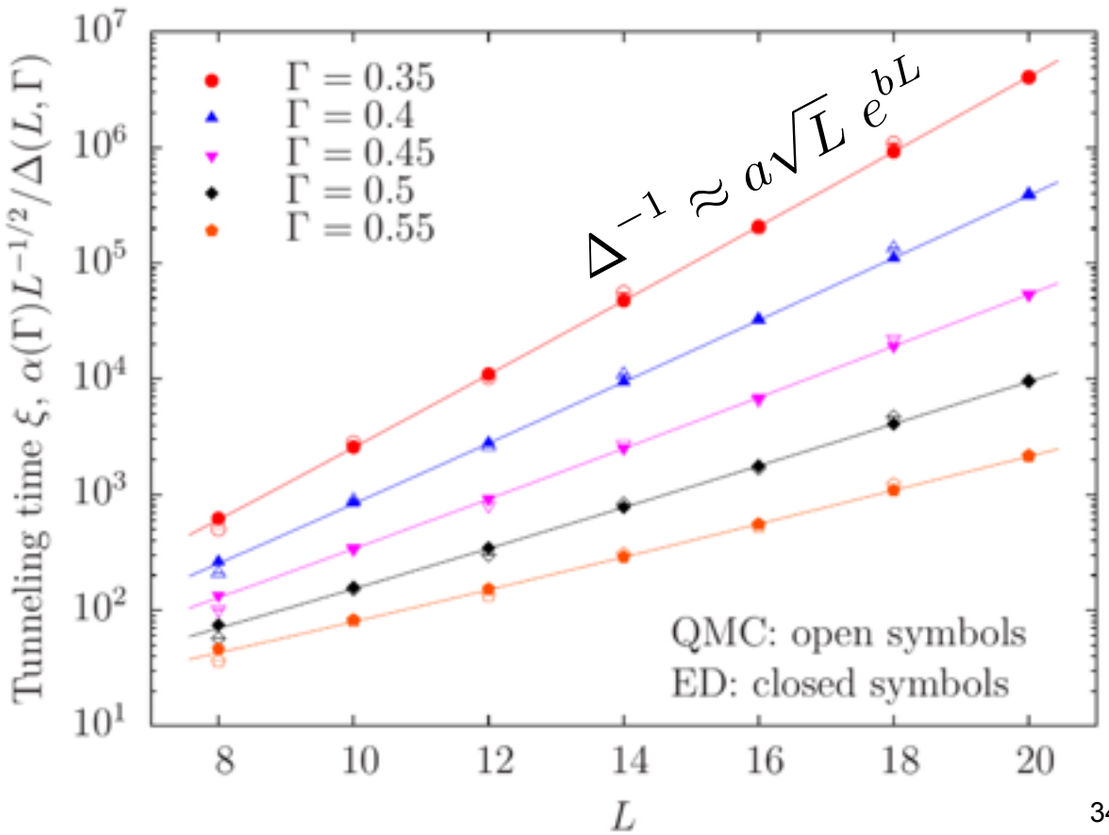


$$< T_{PBC} > \sim 1/\Delta^2$$

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

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



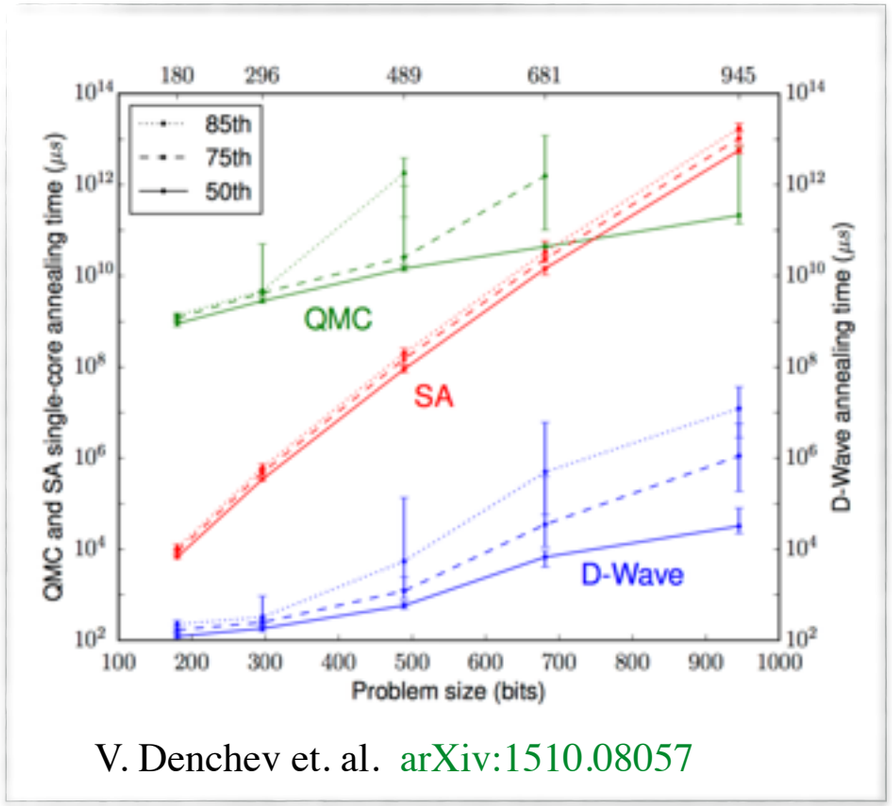
"Understanding Quantum Tunneling through Quantum Monte Carlo Simulations"

S.V. Isakov, G. Mazzola, V.N. Smelyanskiy, Z. Jiang, S. Boixo, H. Neven, and M. Troyer

arXiv:1510.08057

Conclusions /1

We show that, for a double well model, we can identify the transition state of the PIMC pseudodynamics, *the instanton* $q^{**}(\tau)$, and the autocorrelation time scales as Δ^{-2}

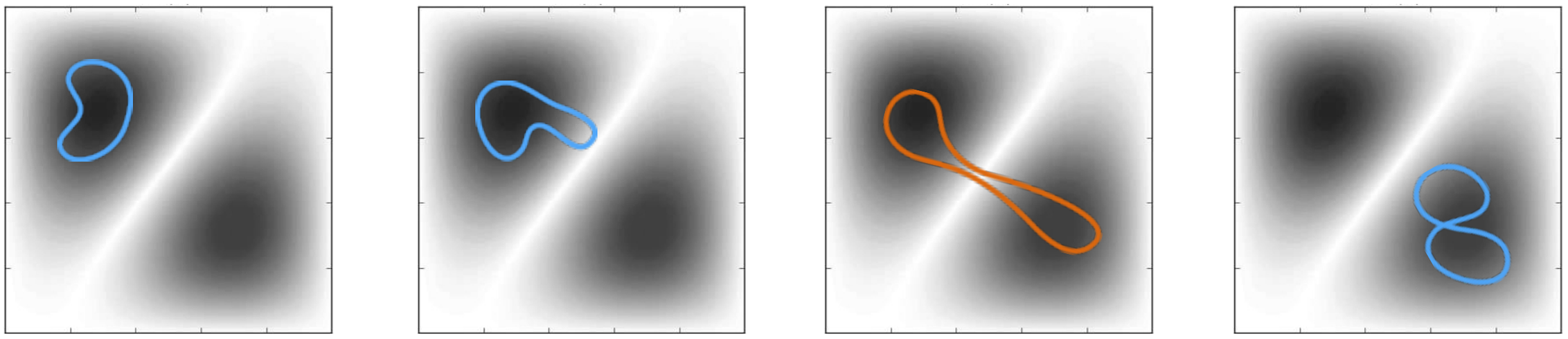


V. Denchev et. al. arXiv:1510.08057

We propose a simple modification of the PIMC algorithm, with open boundary conditions in imaginary time, which implies a quadratic speedup (quantum inspired classical algorithm).

We are currently working on finding possible exceptions to this matching, exploring models (borrowed from chemistry) which feature multidimensional tunnelling.

Clearly, also Hamiltonians with sign-problem (***non stoquastic***), beyond the Transverse field, may show scaling advantage compared to QMC.



Thank you!