Understanding Quantum Annealing using projective Monte Carlo algorithms

Inack Estelle Maeva
ICTP/SISSA

Workshop on Understanding Quantum Phenomena with Path Integrals: From Chemical Systems to Quantum fluids and Solids

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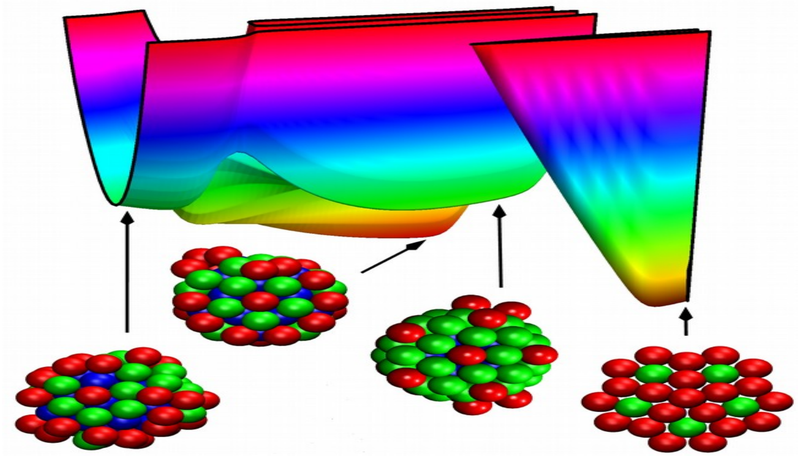
The Abdus Salam International Centre for Theoretical Physics

SISSA

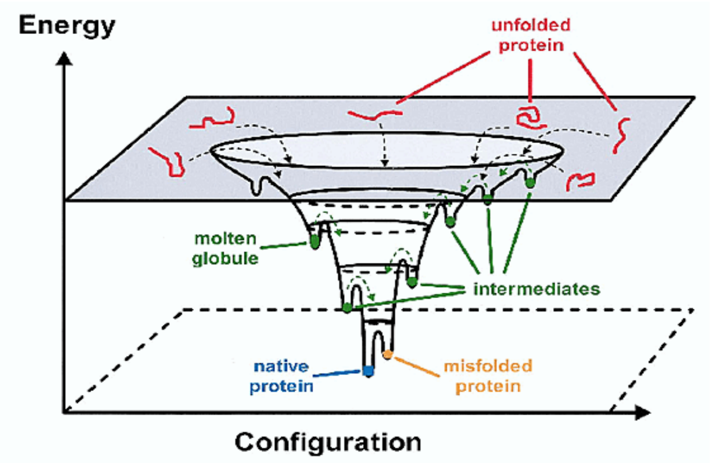
INFN

Optimization Problems

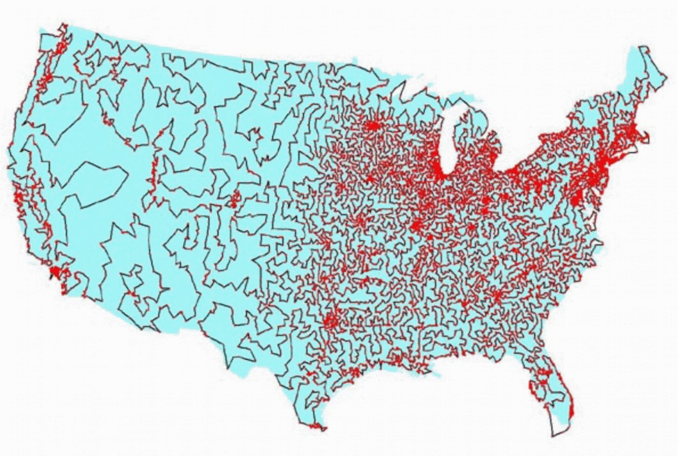
Lennard-Jones Clusters



Protein Folding

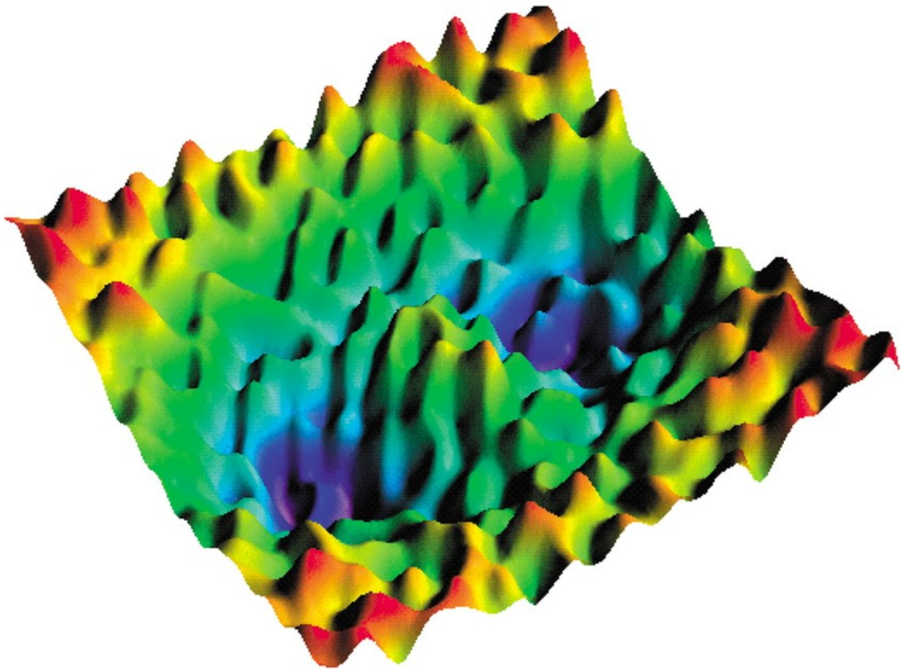


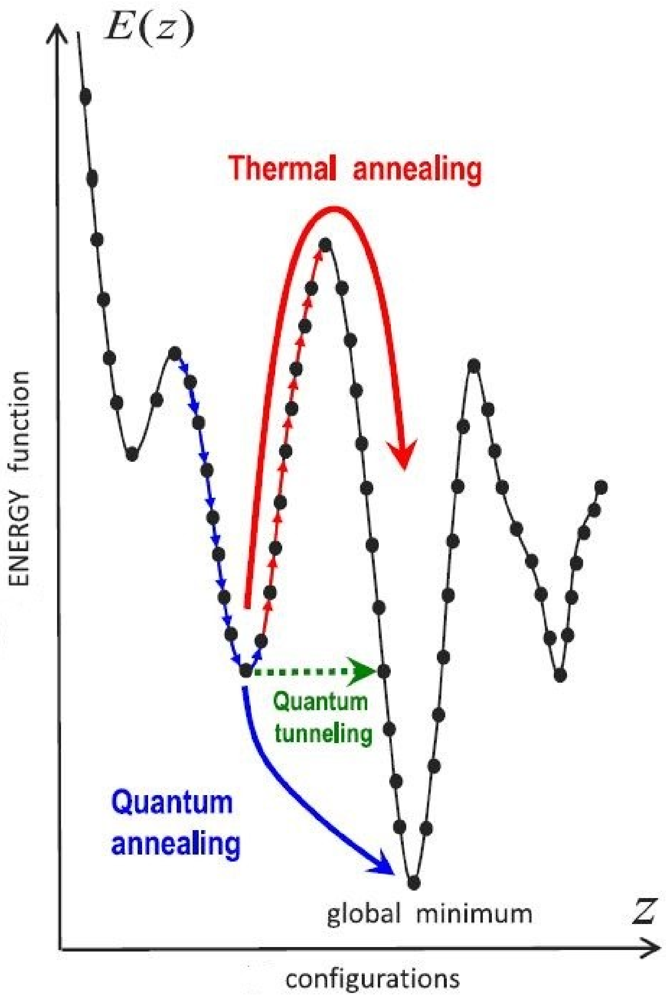
Traveling salesman



Etc ...

Simulated Classical Annealing Vs Quantum Annealing





- S. Kirkpatrick, C. D. Gelatt, and M. P. Vecchi, Science 220, 671 (1983).
- A. Finnila, M. Gomez, C. Sebenik, C. Stenson, and J. Doll, Chem. Phys. Lett. 219, 343 (1994).
- G. E. Santoro, R. Martonak, E. Tosatti, and R. Car, Science 295, 2427 (2002).
- B. Heim, T. F. Rønnow, S. V. Isakov, and M. Troyer, Science 348, 215 (2015).

Quadratic unconstrained binary optimization (QUBO) problems

$$H_{cl} = -\sum J_{ij}\sigma_i^z \sigma_j^z - \sum h_i \sigma_i^z$$

Finding the ground state of H_{cl} is a very hard problem

Trick:

- Introduce $H_{kin} = -\Gamma(t)\sum_i \sigma_i^x$
- At t=0, $\Gamma \gg J_{ij}, h_i$
- At $t=t_f$, $\Gamma = 0$

How slow? Adiabatic theorem

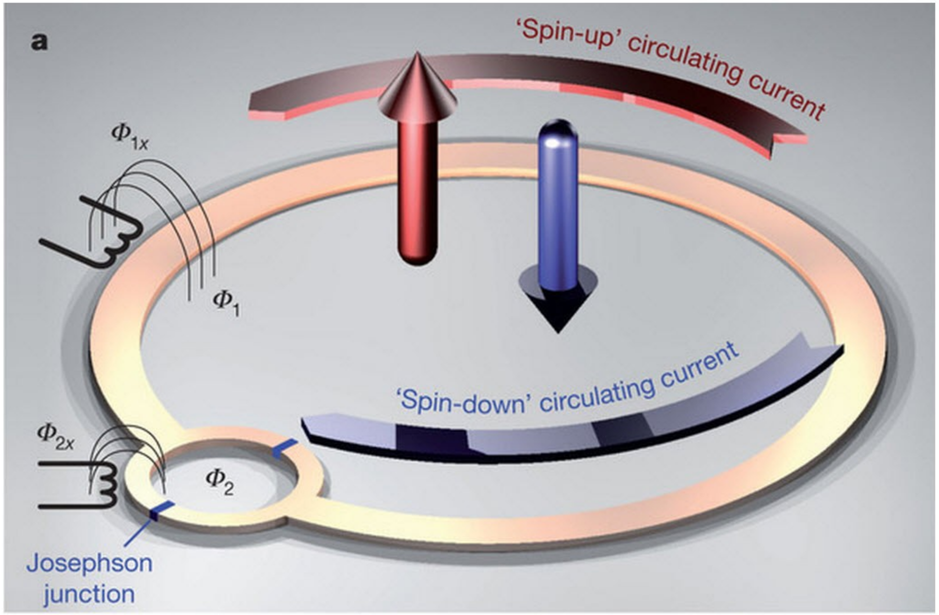
$$t_f \gg \frac{\alpha}{\Delta_m^2}$$

QA with an annealer

$$H_{cl} = -\sum J_{ij}\sigma_i^z \sigma_j^z$$

$$H_{kin} = -\Gamma(t)\sum_i \sigma_i^x$$

$$\Gamma(t) = \Gamma_o\left(1 - \frac{t}{t_f}\right)$$



Simulated QA with QMC

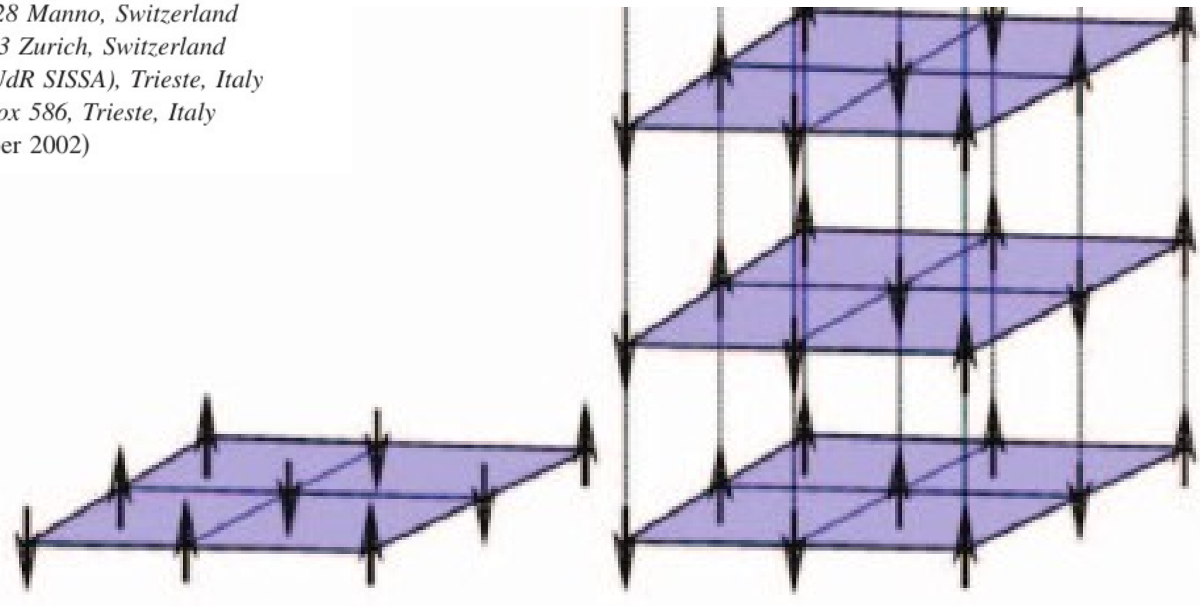
PHYSICAL REVIEW B **66**, 094203 (2002)

Quantum annealing by the path-integral Monte Carlo method: The two-dimensional random Ising model

Roman Martoňák,[1,*] Giuseppe E. Santoro,[2] and Erio Tosatti[2,3]
[1]*Swiss Center for Scientific Computing, Via Cantonale, CH-6928 Manno, Switzerland and ETH Zurich, Physical Chemistry, Hoenggerberg, CH-8093 Zurich, Switzerland*
[2]*International School for Advanced Studies (SISSA) and INFM (UdR SISSA), Trieste, Italy*
[3]*International Center for Theoretical Physics (ICTP), P.O. Box 586, Trieste, Italy*
(Received 22 March 2002; published 13 September 2002)

Theory of Quantum Annealing of an Ising Spin Glass

Giuseppe E. Santoro,[1] Roman Martoňák,[2,3] Erio Tosatti,[1,4*] Roberto Car[5]



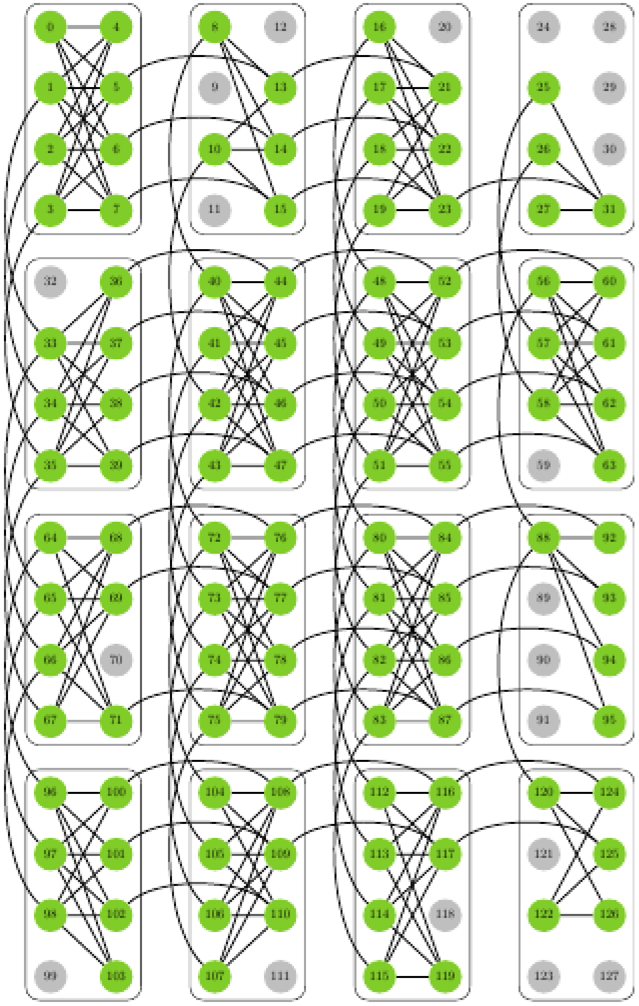
Path Integral Monte Carlo (PIMC)

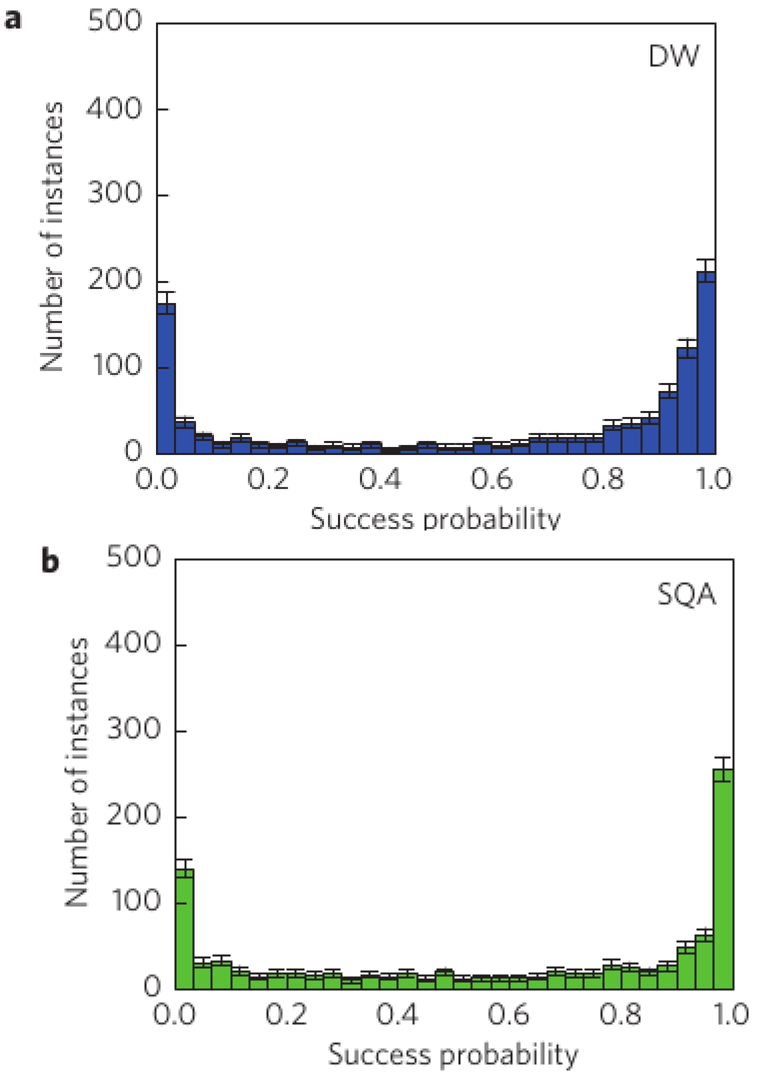
- G. E. Santoro, R. Martonak, E. Tosatti, and R. Car, Science 295, 2427 (2002).
- B. Heim, T. F. Rønnow, S. V. Isakov, and M. Troyer, Science 348, 215 (2015)

Comparison between SQA and Dwave 1

Ising glass on Chimera graphs

$$H_{cl} = -\sum_{i<j} J_{ij}\, \sigma_i^z \sigma_j^z$$

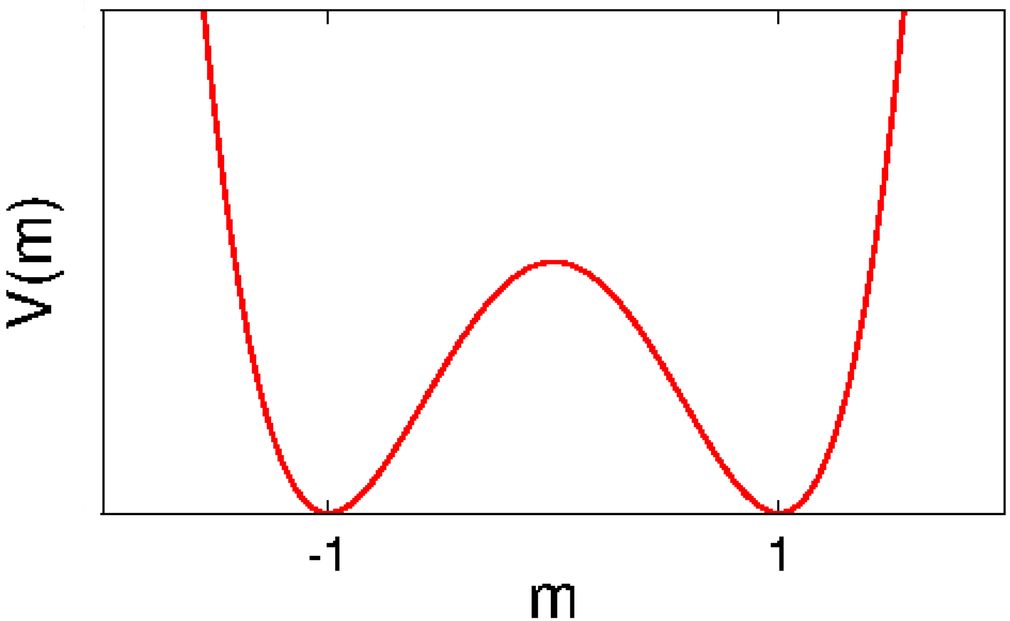




S. Boixo et al., Nat. Phys. 10, 218–224 (2014).

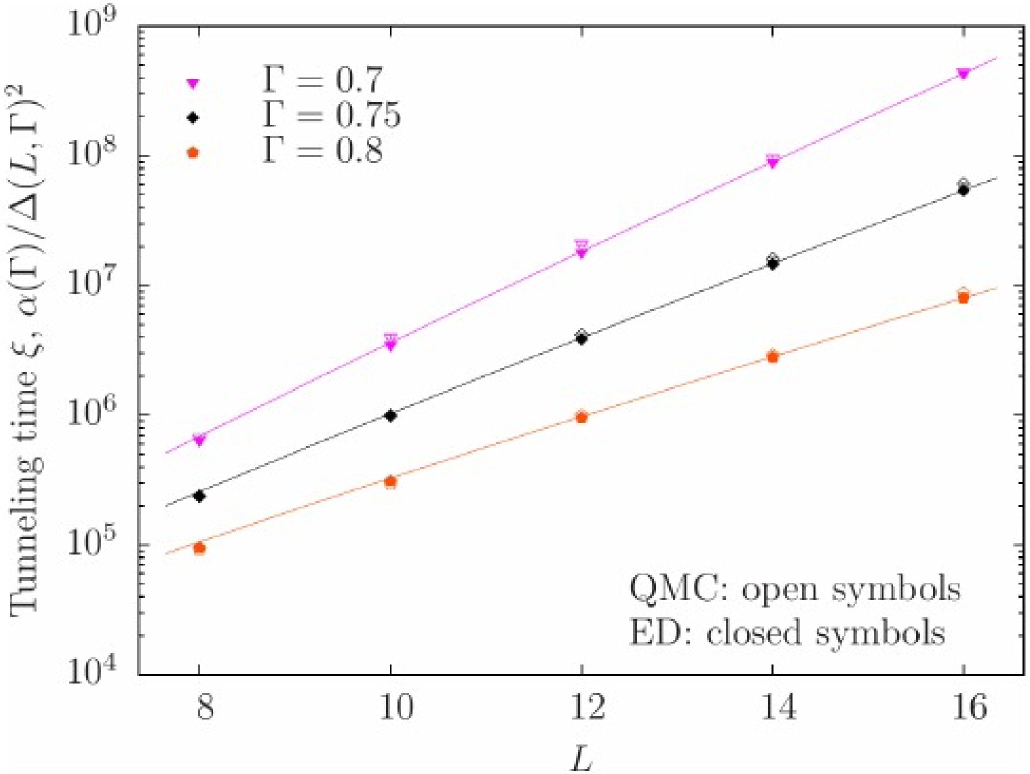
- **SQA done with PIMC is consistent with DWave**

Tunneling time studies



The quantum Ising chain

$$\hat{H} = -J \sum_{\langle i,j \rangle} \sigma_i^z \sigma_j^z - \Gamma \sum_i \sigma_i^x$$



$$\xi \propto \alpha(\Gamma)/\Delta^2$$

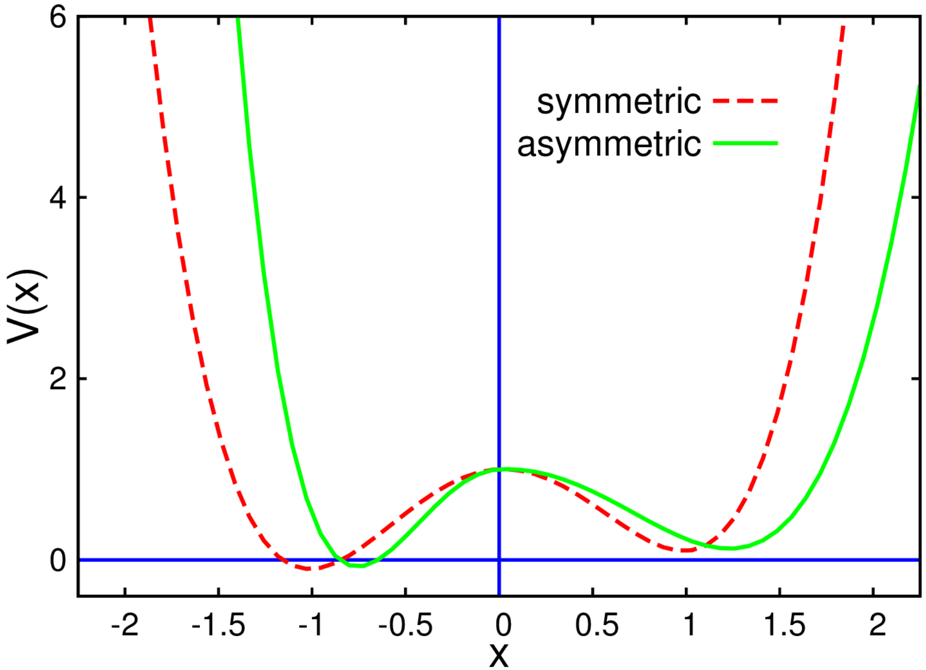
$$\Delta = E_1 - E_0$$

- **PIMC tunneling time scaling is like the one of a quantum annealer**

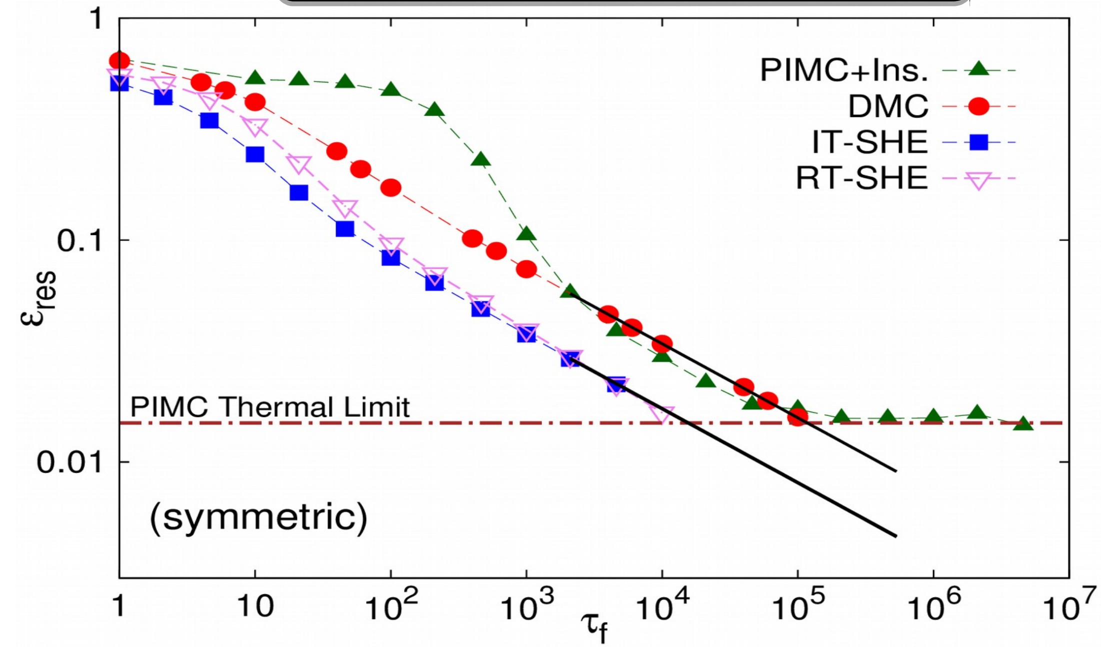
Isakov et al, Phys. Rev. Lett. 117, 180402 (2016)

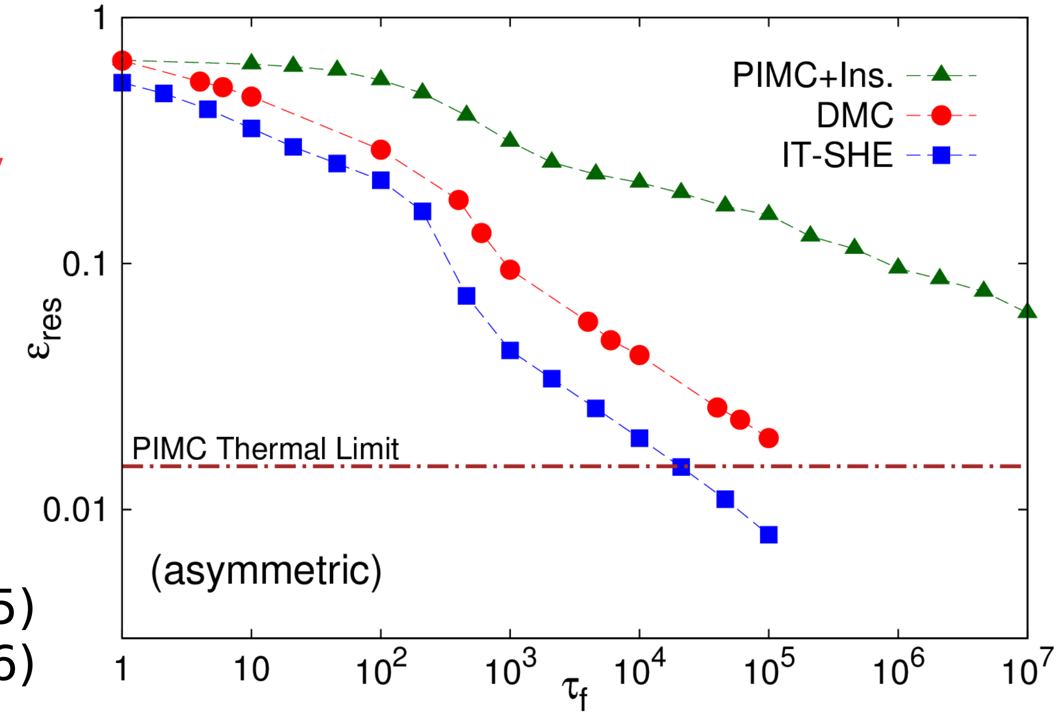
SQA comparison of PIMC and DMC

$$H(\tau) = -D(\tau)\nabla^2 + V(x) \qquad D = \frac{1}{2m_\tau}$$



Conjecture: $\varepsilon_{res}^{imaginary}(\tau_f) \ll \varepsilon_{res}^{real}(\tau_f)$





- **DMC performs asymptotically like deterministic IT-SHE**
- **PIMC cannot simulate QA, whereas DMC can**

E. M. I., S. Pilati, Phys. Rev. E. 92, 053304 (2015)

Stella et al, Phys. Rev. B 72, 014303 (2005)
Stella et al, Phys. Rev. B 73, 144302 (2006)

DMC on Quantum Ising models

$$\hat{H} = \underbrace{-\sum_{\langle ij \rangle} J_{ij}\, \sigma_i^z \sigma_j^z}_{\textit{Potential Energy}} - \underbrace{\Gamma(\tau) \sum_i \sigma_i^x}_{\textit{Fictitious Kinetic Energy}}$$

Evolve the Schrödinge
equation in
imaginary time

$$\Psi(\boldsymbol{X}, \tau_f) = e^{-\hat{H}\tau_f}\, \Psi(\boldsymbol{X}, 0)$$

$$\Psi(\boldsymbol{X}, \tau + \Delta\tau) = \sum_{X'} G(\boldsymbol{X}', \boldsymbol{X}, \Delta\tau)\, \Psi(\boldsymbol{X}', \tau)$$

$$G(\boldsymbol{X}', \boldsymbol{X}, \Delta\tau) \approx G_d(\boldsymbol{X}', \boldsymbol{X}, \Delta\tau)\, G_b(\boldsymbol{X}', \boldsymbol{X}, \Delta\tau)$$

$$\textit{where} \quad G_d(\boldsymbol{X}', \boldsymbol{X}, \Delta\tau) = P_F^{\delta} (1 - P_F)^{N-\delta}$$

$$P_F = \frac{\sinh(\Delta\tau\, \Gamma(\tau))}{\exp(\Delta\tau\, \Gamma(\tau))}$$

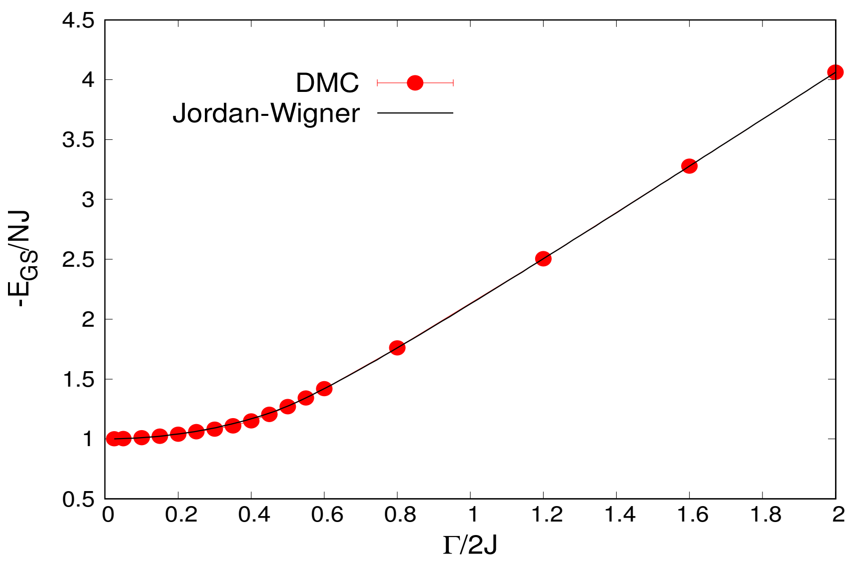
$$G_b(\boldsymbol{X}', \boldsymbol{X}, \Delta\tau) = \exp(-\Delta\tau [E_o(\boldsymbol{X}') - N\,\Gamma(\tau) - E_{ref}])$$

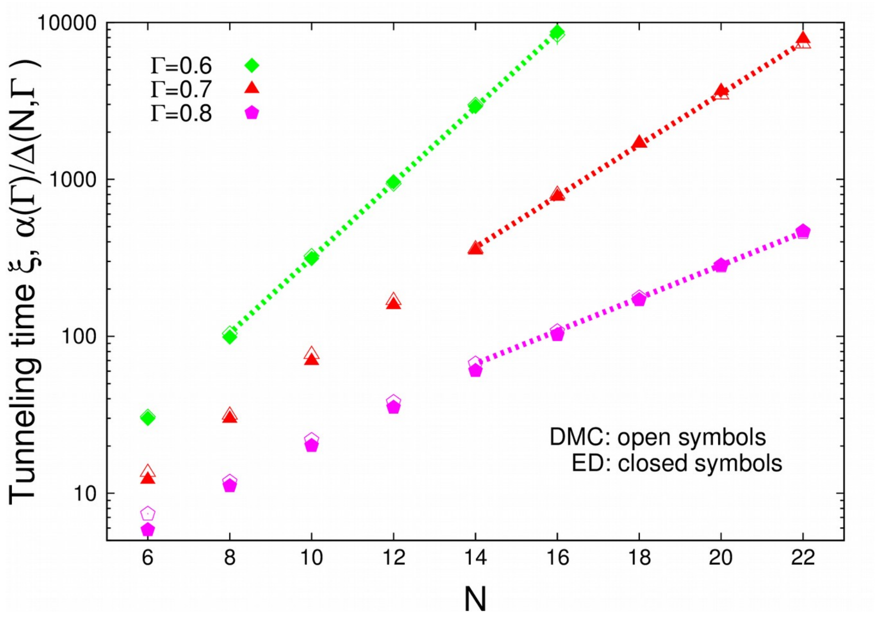
Tunneling time results

The quantum Ising chain (QIC)

$$\hat{H} = -J \sum_{\langle i,j \rangle} \sigma_i^z \sigma_j^z - \Gamma \sum_i \sigma_i^x$$

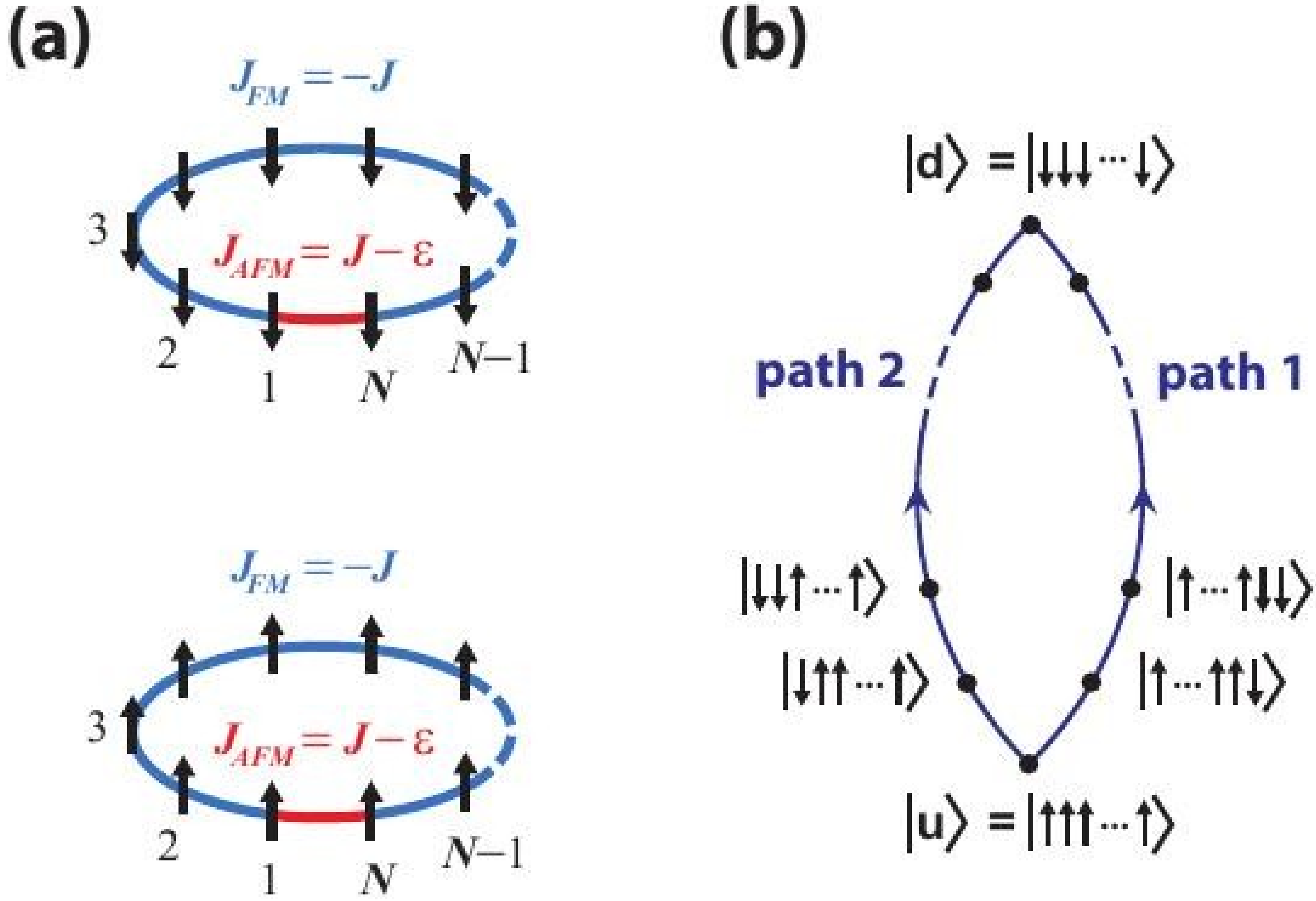
$$\xi \propto \alpha(\Gamma)/\Delta$$





- **As a benchmarch DMC simulates ground state properties**
- **DMC tunneling time is identical to PIMC with open boundary conditions.** Isakov et al, Phys. Rev. Lett. 117, 180402 (2016)

A simple model with frustration



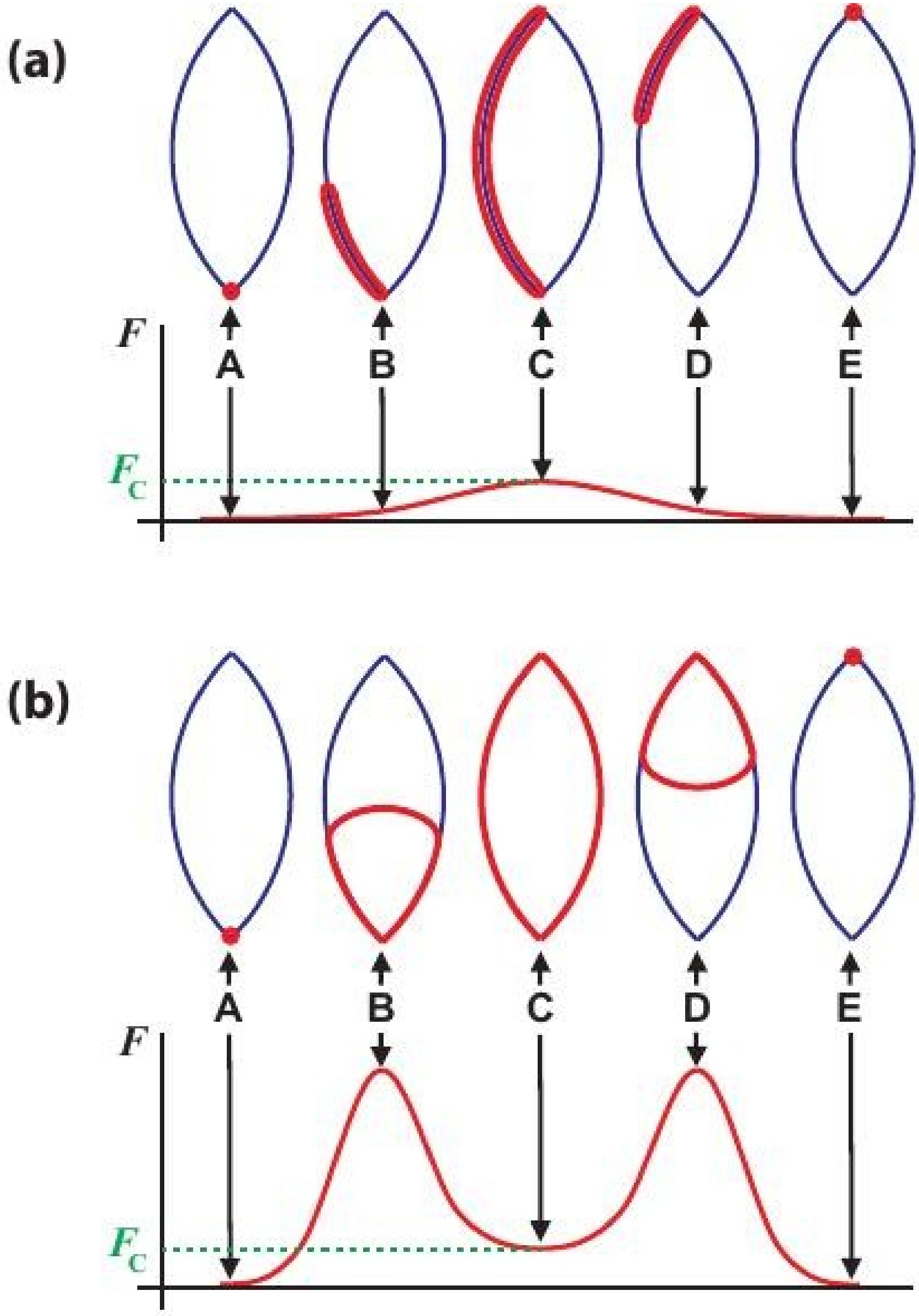
- **PIMC tunneling time is twice that of incoherent quantum tunneling**

$$\xi_{PBC}^{PIMC} \propto 2/\Delta^2$$

E. Andriyash and M. H. Amin. arXiv:1703.09277, 2017

E. Andriyash and M. H. Amin.

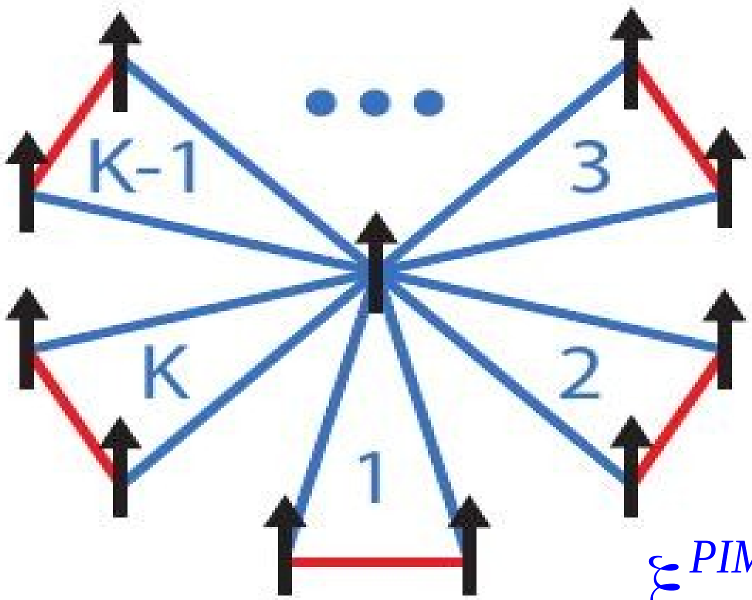
arXiv:1703.09277, 2017

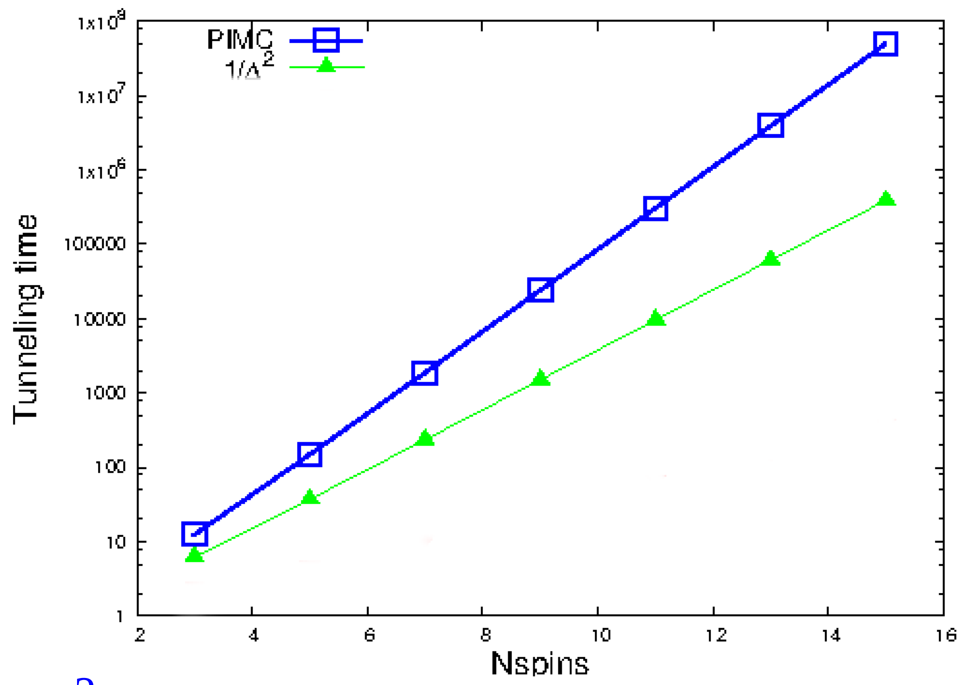


Tunneling time studies

$$H_{cl} = -J \sum_{i=1}^{K} \sum_{j=2i}^{2i+1} \sigma_1^z \sigma_j^z + (J - \varepsilon) \sum_{i=1}^{K} \sigma_{2i}^z \sigma_{2i+1}^z$$

Shamrock: A model of frustrated rings



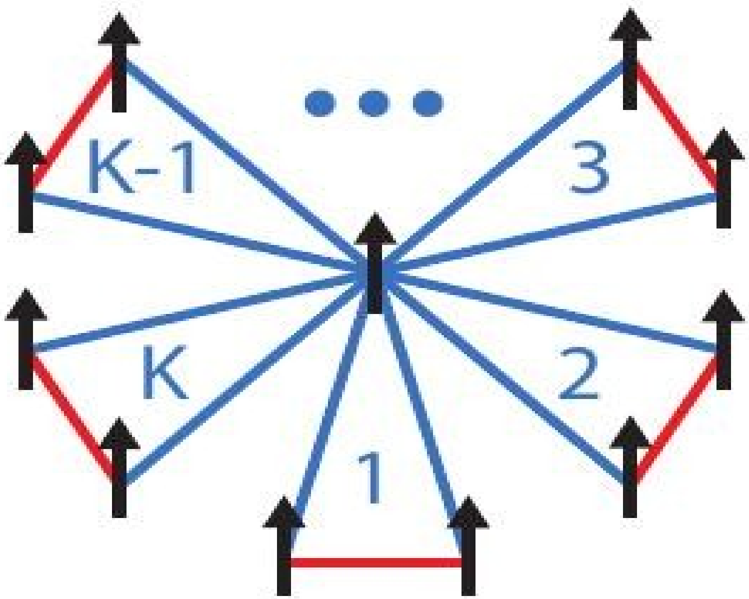


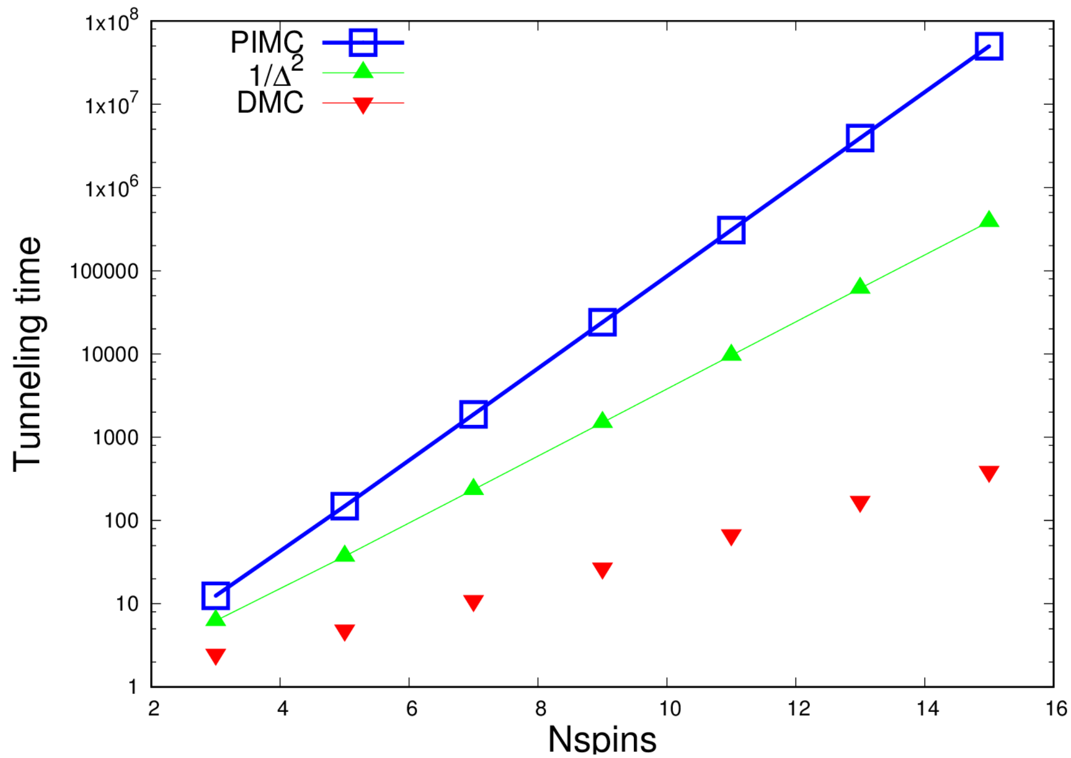
$$\xi_{PBC}^{PIMC} \propto 2^K / \Delta^2$$

- **PIMC scaling is worse than incoherent quantum tunneling**
- **It suggests than in some cases it cannot simulate QA**

E. Andriyash and M. H. Amin. arXiv:1703.09277, 2017

Tunneling time results





- **DMC scaling is the same as in the QIC**
- **It has better scaling than PIMC and incoherent quantum tunneling.**

$$\xi^{PIMC}_{PBC} \propto 2^K / \Delta^2$$

$$\xi^{DMC} \propto \alpha / \Delta$$

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