Title: Simulating quantum annealing via projective quantum Monte Carlo algorithms

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URL: http://pirsa.org/18100093

Abstract: <p>We implement projective quantum Monte Carlo (PQMC) methods to simulate quantum annealing on classical computers. We show that in the regime where the systematic errors are well controlled, PQMC algorithms are capable of simulating the imaginary-time dynamics of the Schroedinger equation both on continuous space models and discrete basis systems. We also demonstrate that the tunneling time of the PQMC method is quadratically faster than the one of incoherent quantum annealing. It shows remarkable stability when applied to frustrated systems compared to finite-temperature path integral Monte Carlo algorithm, the method mostly chosen to do comparisons with quantum annealers. However, a major drawback of the PQMC method comes from the finite number of random walkers needed
to implement the simulations. It grows exponentially with the system size when no or poor guiding wave-functions are utilized. Nevertheless, we demonstrate that when good enough guiding wave-functions are used â€“ in our case we choose artificial neural networks â€“ the computational complexity seems to go from exponential to polynomial in the system size. We advocate for a search of more efficient guiding wave functions since they could determine when PQMC simulations are feasible on classical computers, a question closely related to a provable need or speed-up of a quantum computer.</p>

<p>References:
- E. M. Inack and S. Pilati, Phys. Rev. E 92, 053304 (2015)
- E. M. Inack, G. Giudici, T. Parolini, G. Santoro and S. Pilati, Phys. Rev. A 97, 032307 (2018)
- E. M. Inack, G. Santoro, L. Dellâ€™Anna, and S. Pilati, arXiv:1809.03562v1</p>

Simulating quantum annealing via projective quantum Monte Carlo algorithms

Inack Estelle Maéva
ICTP/SISSA

Perimeter institute seminar
26th October 2018

Collaborators: T. Parolini (SISSA), G. Giudici (SISSA), L. Dell'Anna (UniPD), G. Santoro (SISSA), S. Pilati (University of Camerino)

The Abdus Salam International Centre for Theoretical Physics

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SISSA 40!

Outline:

- Introduction to quantum annealing

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- Simulating quantum annealing on continuous space models

PHYSICAL REVIEW E **92**, 053304 (2015)

Simulated quantum annealing of double-well and multiwell potentials

E. M. Inack[1,2] and S. Pilati[1]

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[2] *SISSA, International School for Advanced Studies and INFN, Sezione di Trieste, I-34136 Trieste, Italy*

(Received 28 August 2015; revised manuscript received 15 October 2015; published 19 November 2015)

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- Tunneling dynamics in DMC simulations

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Understanding quantum tunneling using diffusion Monte Carlo simulations

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[5]*Dipartimento di Fisica e Astronomia "Galileo Galilei," Università di Padova, 35131 Padova, Italy*
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- Boosting projective QMC simulations via artificial neural networks

Projective quantum Monte Carlo simulations guided by unrestricted neural network states

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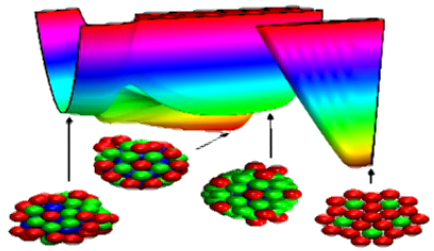
- SQA using projective QMC on the quantum Ising chain
  Inack, Santoro, Pilati, work in progress

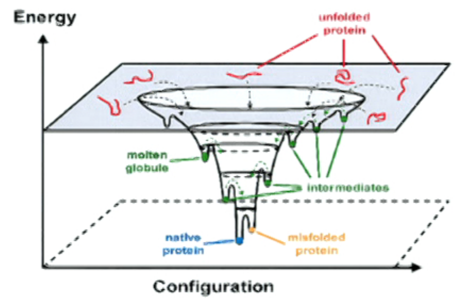
Optimization Problems are ubiquitous in different fields

Traveling salesman

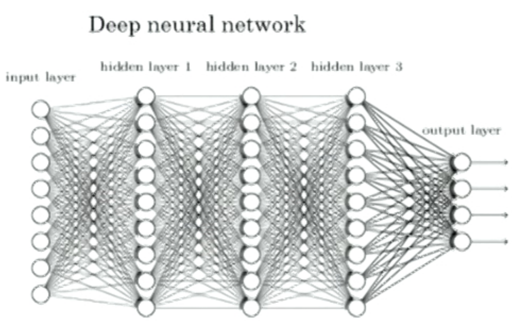
Clusters of atoms



Protein Folding



Machine Learning

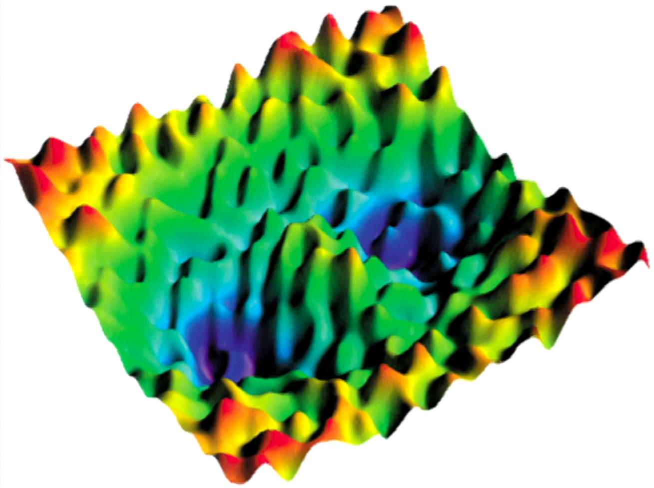


Luggage handling

Etc ...

Classical Annealing (CA) Vs Quantum Annealing (QA)

Rugged and exponentially large



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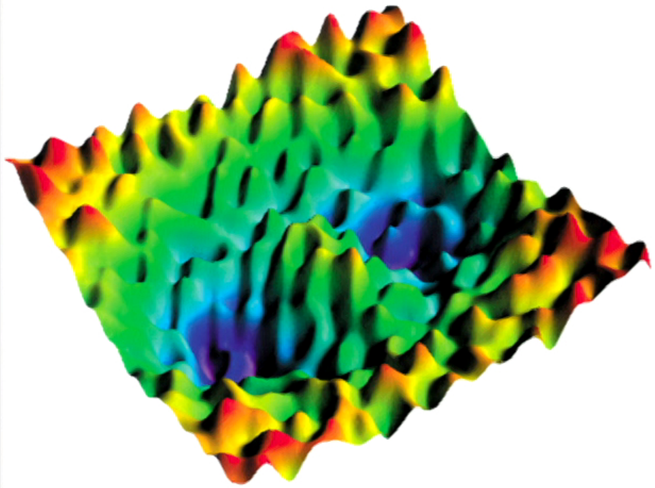

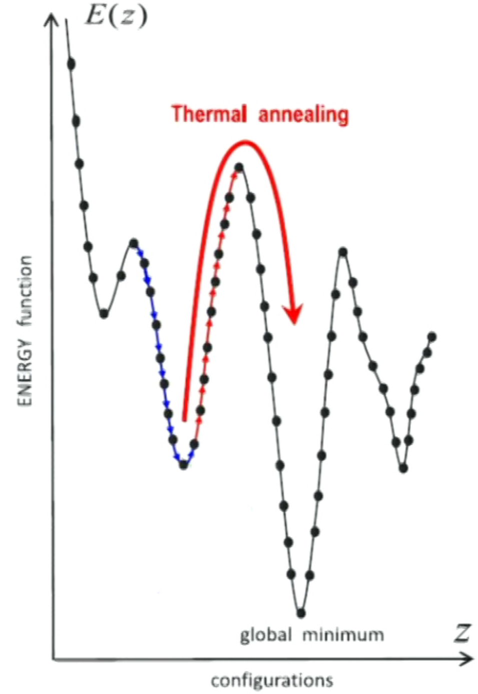

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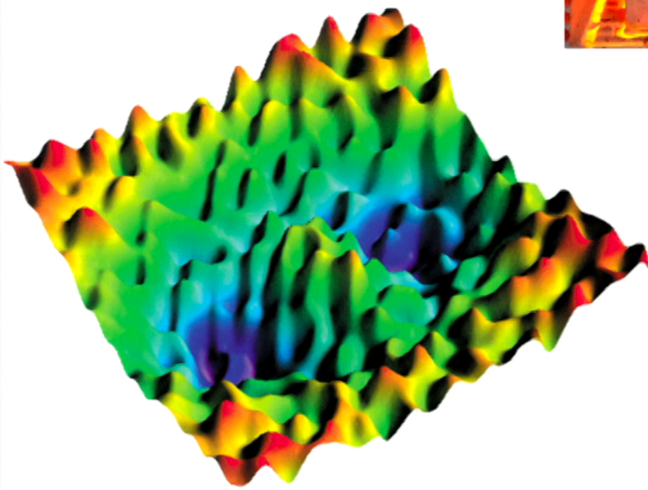

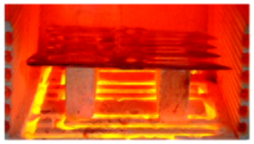

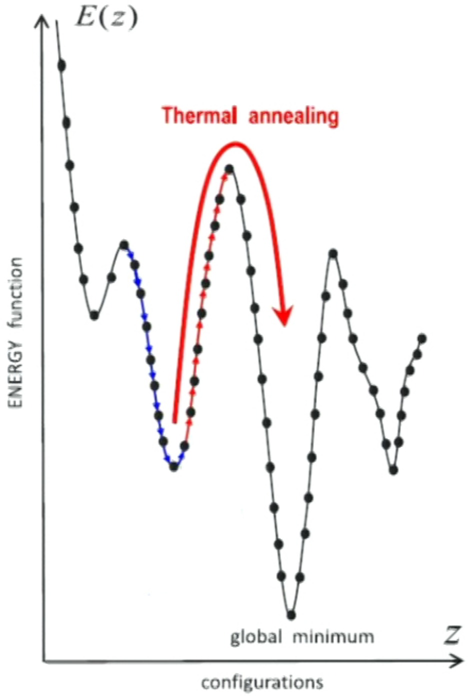

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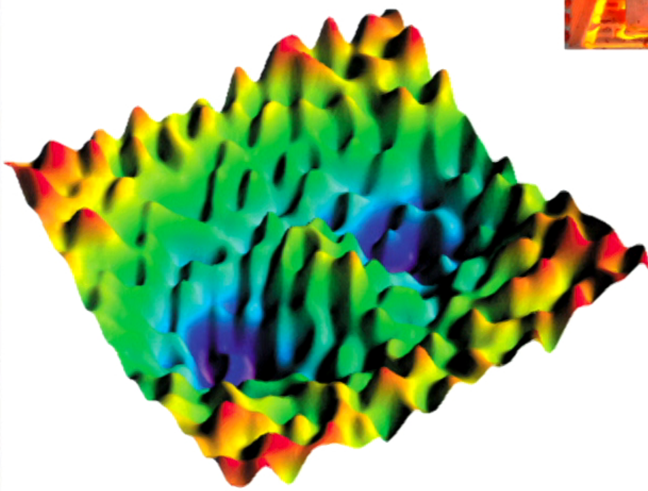

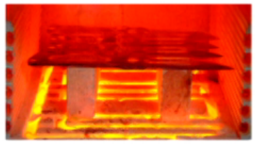

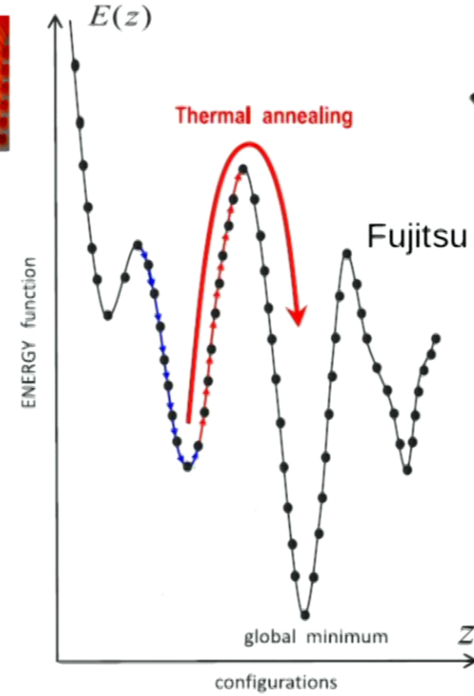

Fujitsu digital annealer

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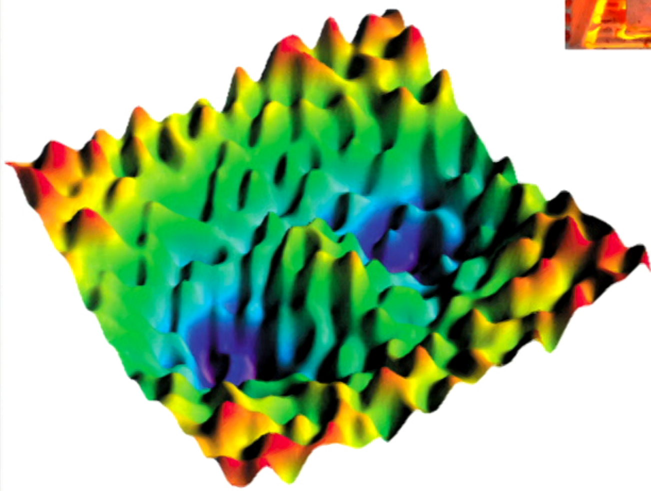

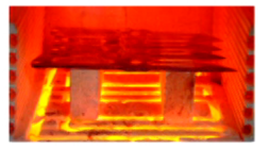

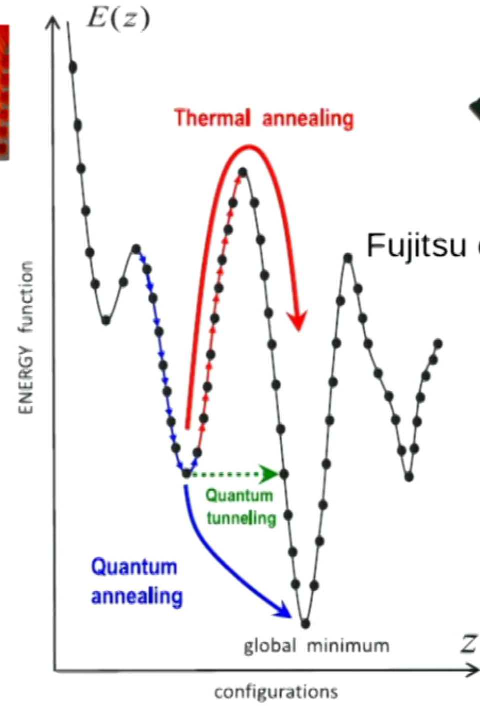

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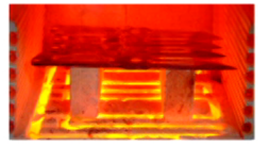
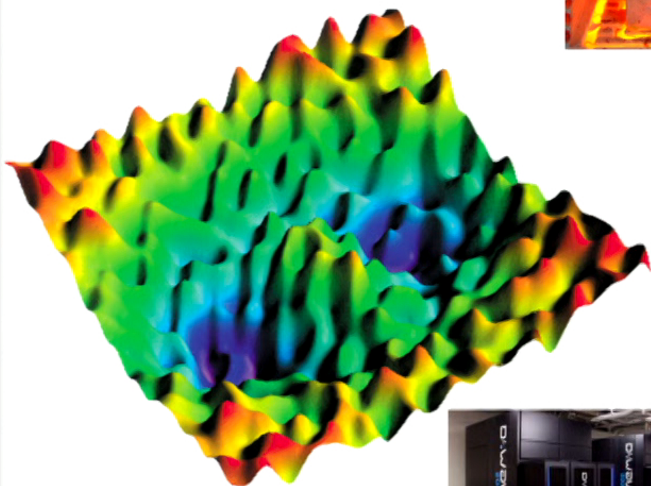
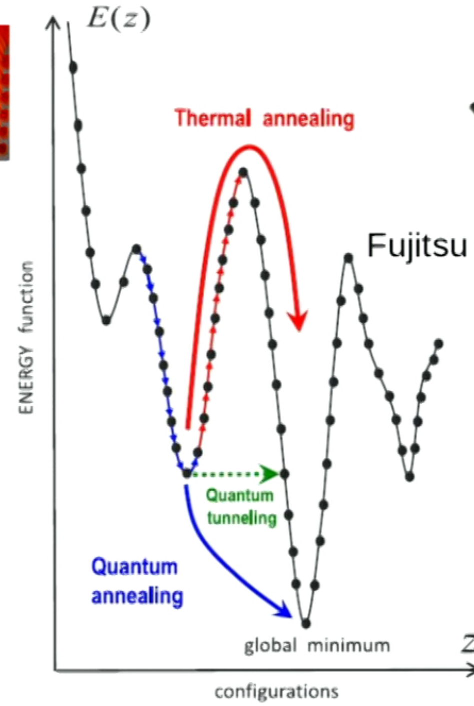




DWave quantum annealer



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Most Optimization problems

[Lucas, Front. Phys. (2014)]

$$H_{cl} = \sum_{p} \sum_{j_{1,\ldots}, j_p} J_{j_{1,\ldots}, j_p} \sigma^z_{j_1} \ldots \sigma^z_{j_p}$$

Most Optimization problems

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$$H_{cl}=\sum_p \sum_{j_{1,\ldots},j_p} J_{j_{1,\ldots},j_p} \sigma^z_{j_1} \ldots \sigma^z_{j_p}$$

E.g: Disordered Ising glass in a random longitudinal field

$$H_{cl}=-\sum_{i,j} J_{ij} \sigma^z_i \sigma^z_j - \sum_i h_i \sigma^z_i$$

Finding the ground state among 2^N classical states: **a very hard problem**

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QA idea:

- Introduce $H_{kin}(t) = -\Gamma(t) \sum_i \sigma^x_i + \ldots$

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$$H_{cl}=\sum_p \sum_{j_{1,\dots},j_p} J_{j_{1,\dots},j_p}\,\sigma^z_{j_1}\dots\sigma^z_{j_p}$$

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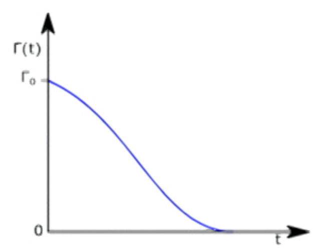

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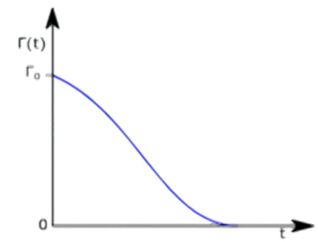

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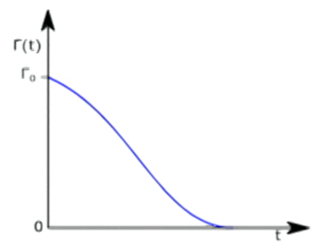
- At t=0, $H_{kin} \gg H_{cl}$



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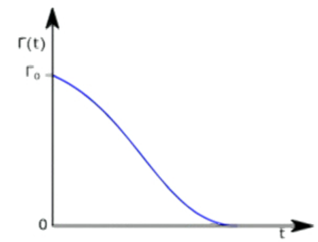
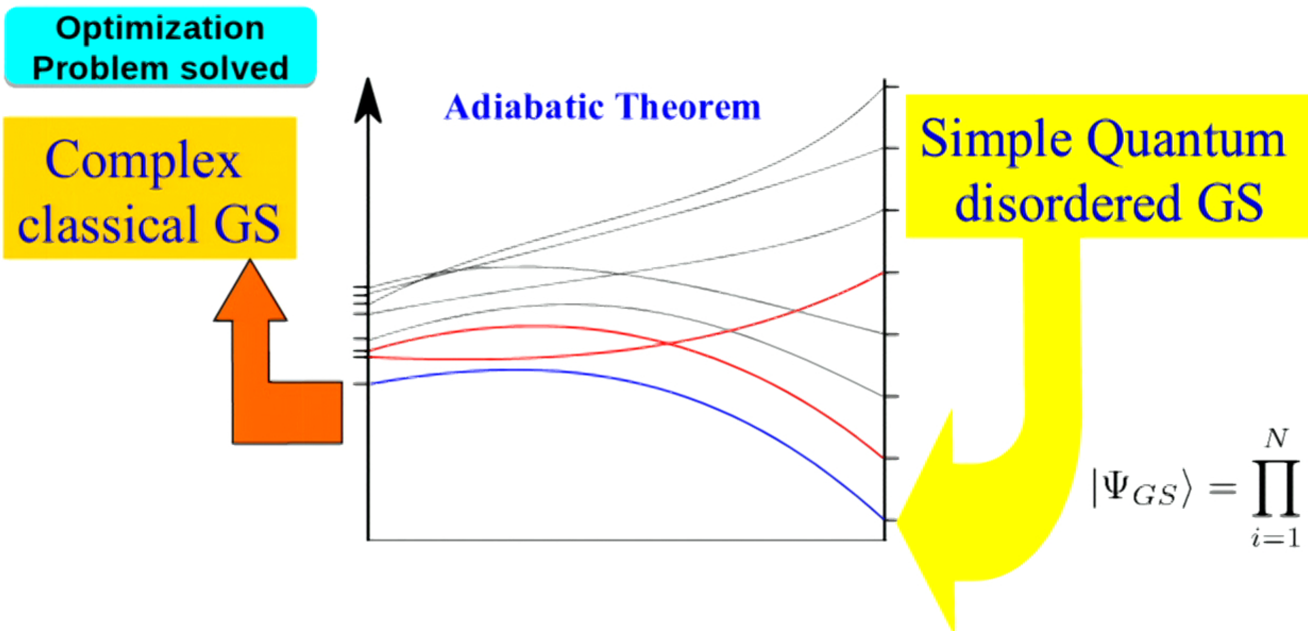
- At t=0, $H_{kin} >> H_{cl}$
- At $t=t_f$, $H_{kin} = 0$



QA: there is no free lunch

$$\hat{H}(t) = H_{cl} + H_{kin}(t)$$

$$i\hbar \frac{\partial}{\partial \tau}|\Psi\rangle = \hat{H}(t)|\Psi\rangle$$



$$|\Psi_{GS}\rangle = \prod_{i=1}^{N} \frac{|\uparrow\rangle_i + |\downarrow\rangle_i}{\sqrt{2}}$$

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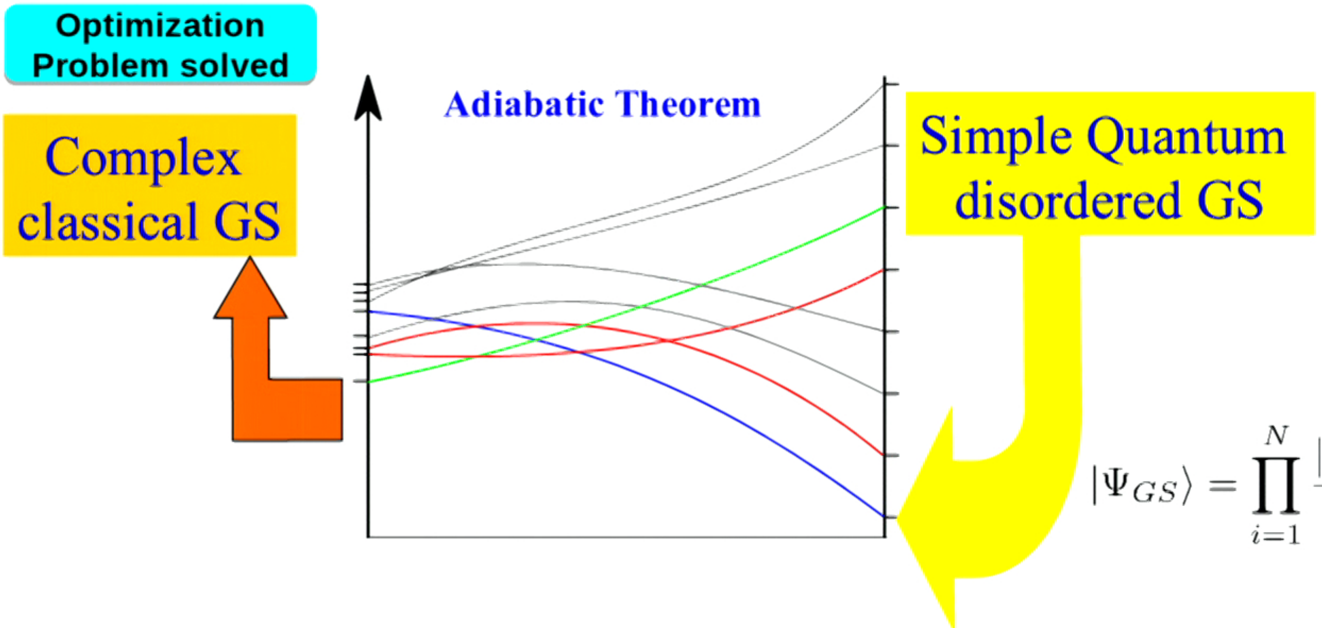

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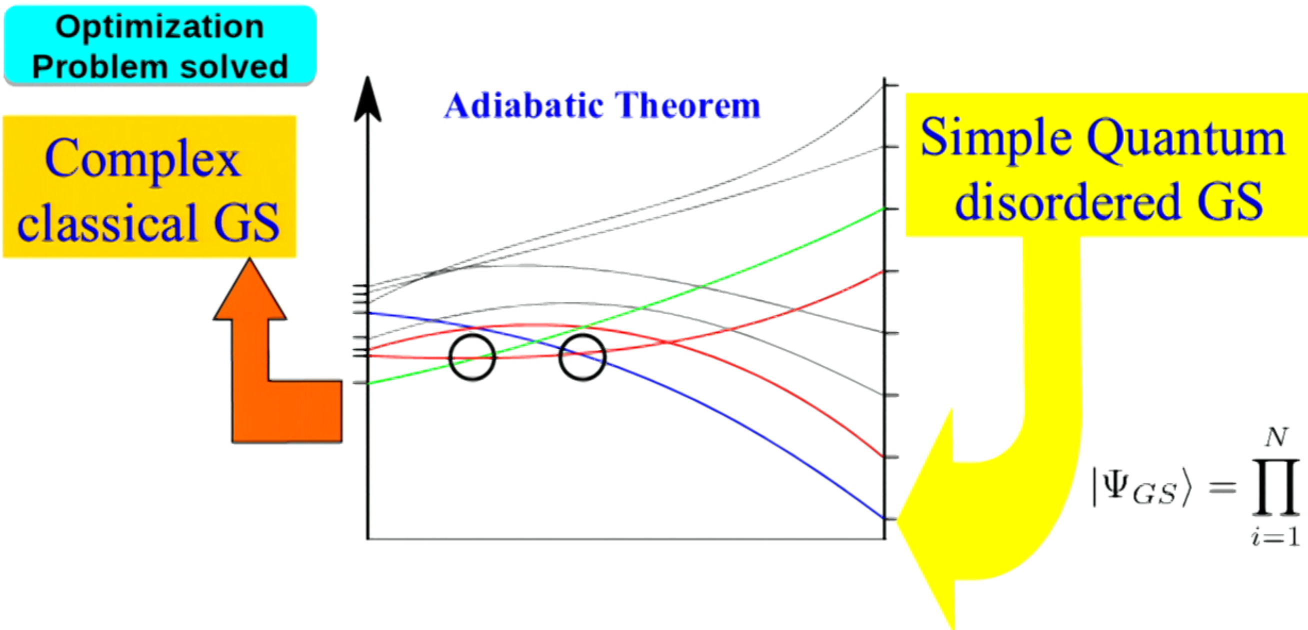

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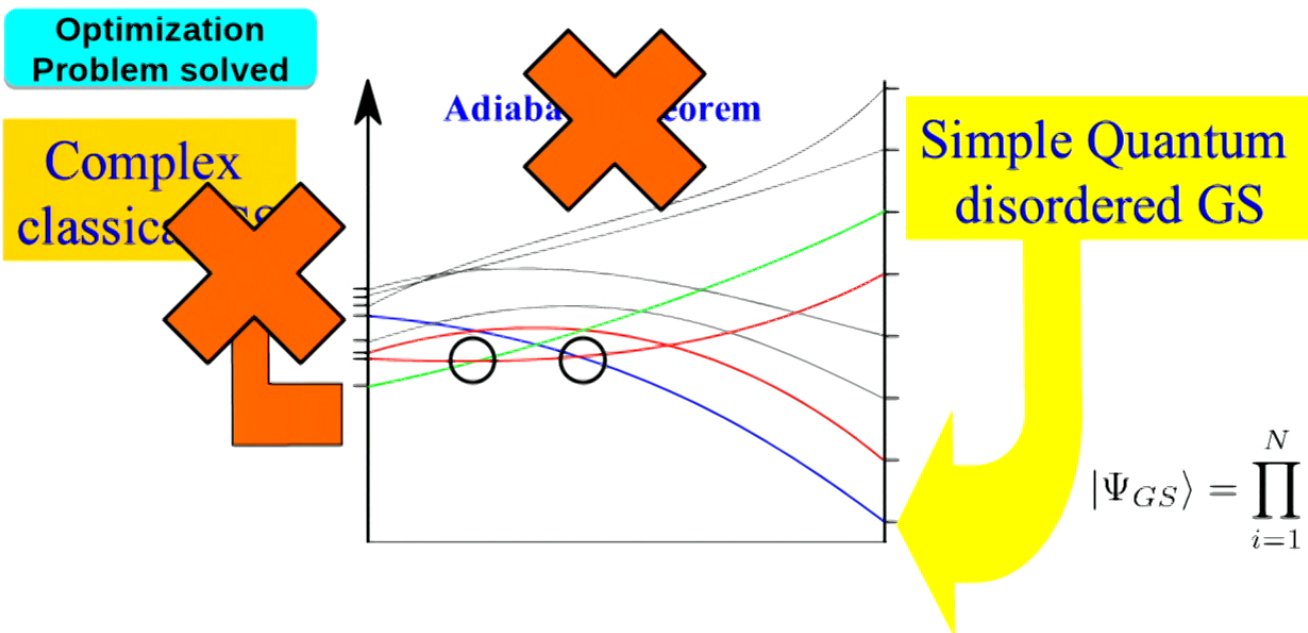

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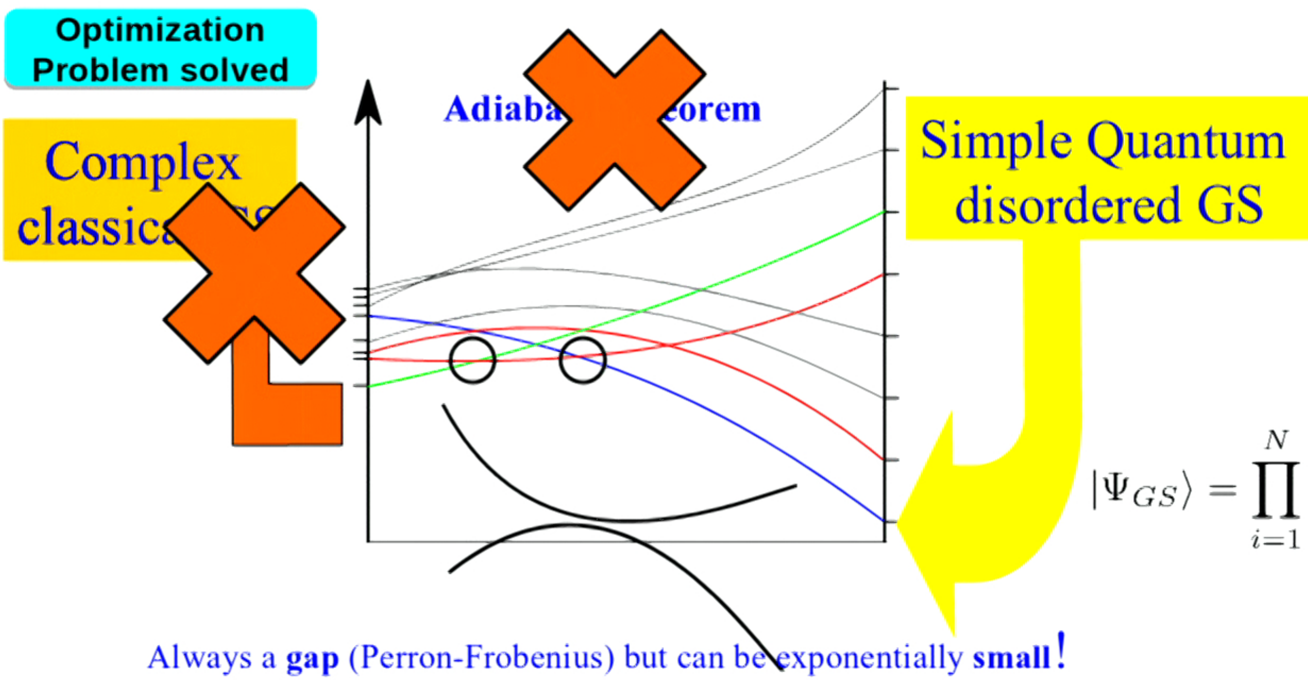

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Always a **gap** (Perron-Frobenius) but can be exponentially **small**!

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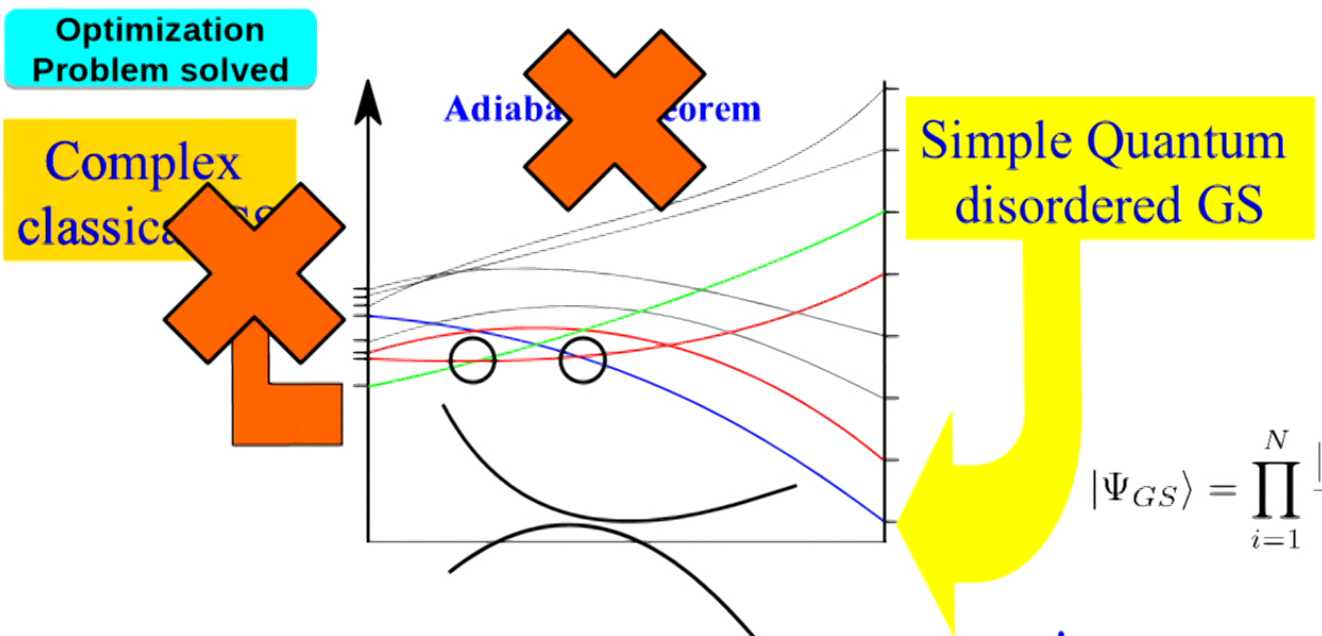

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$$t_{ad} \gg \frac{\alpha}{\Delta_m^2}$$

Simulated QA with Quantum Monte Carlo (QMC)

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

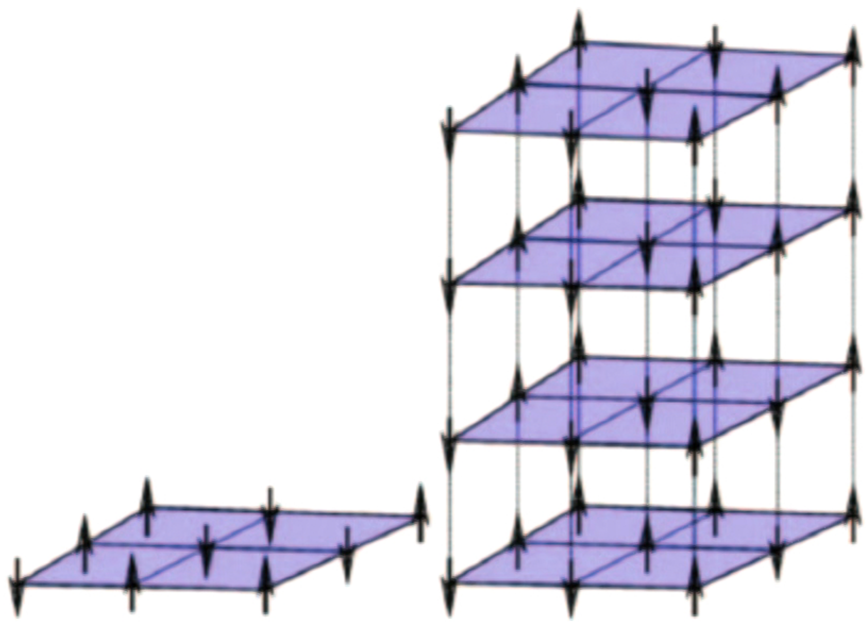
**Quantum annealing by the path-integral Monte Carlo metl
The two-dimensional random Ising model**

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]

Simulated QA with Quantum Monte Carlo (QMC)



Path Integral Monte Carlo (PIMC)

- Santoro, Martonak, Tosatti, and Car, Science 295, 2427 (2002)
- Heim, Rønnow, Isakov, and Troyer, Science 348, 215 (2015)

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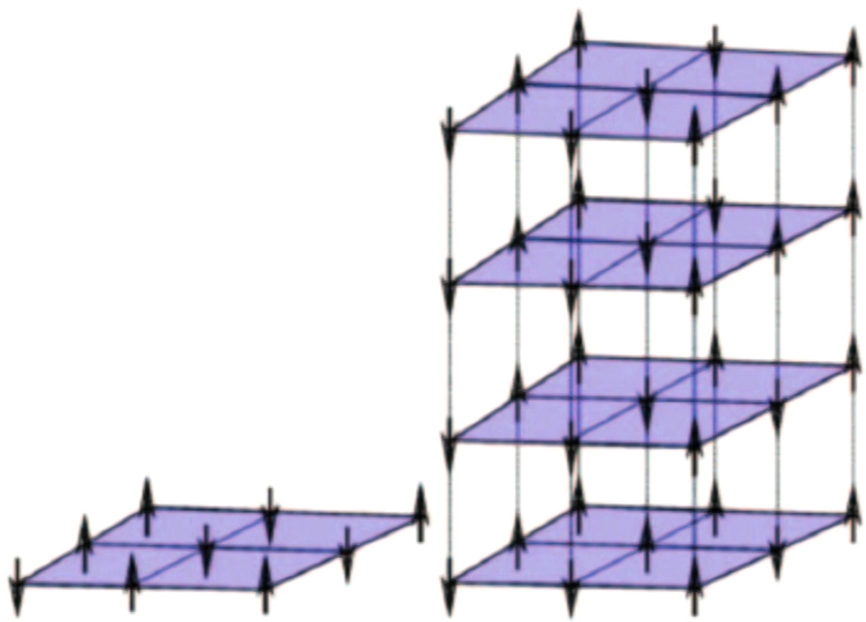

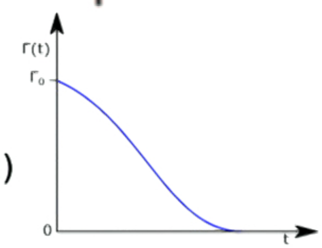

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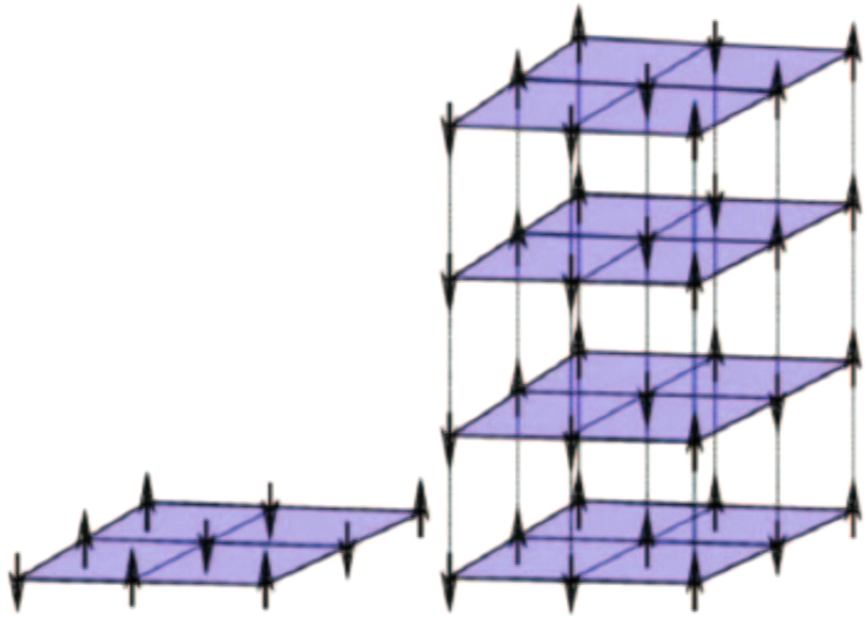
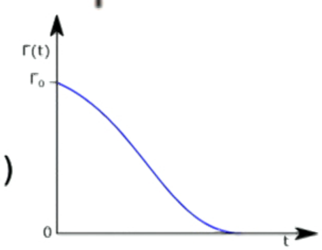
Monte Carlo dynamics not clearly related to a quantum dynamics





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Our Motivation: Real Vs imaginary time QA of the ***deterministic*** Schroedinger equation (SHE)

$$\varepsilon_{res} = \frac{\langle \Psi_0(\tau_f) | H_{cl} | \Psi_0(\tau_f) \rangle}{\langle \Psi_0(\tau_f) | \Psi_0(\tau_f) \rangle} - E_{GS}$$

$$\varepsilon_{res}^{imaginary}(\tau_f) \leqslant \varepsilon_{res}^{real}(\tau_f)$$

Stella, Santoro, Tosatti, Phys. Rev. B 72, 014303 (2005)
S. Morita and H. Nishimori, J. Math. Phys. 49, 125210 (2008)

Assumption:
Adiabatic perturbation theory holds

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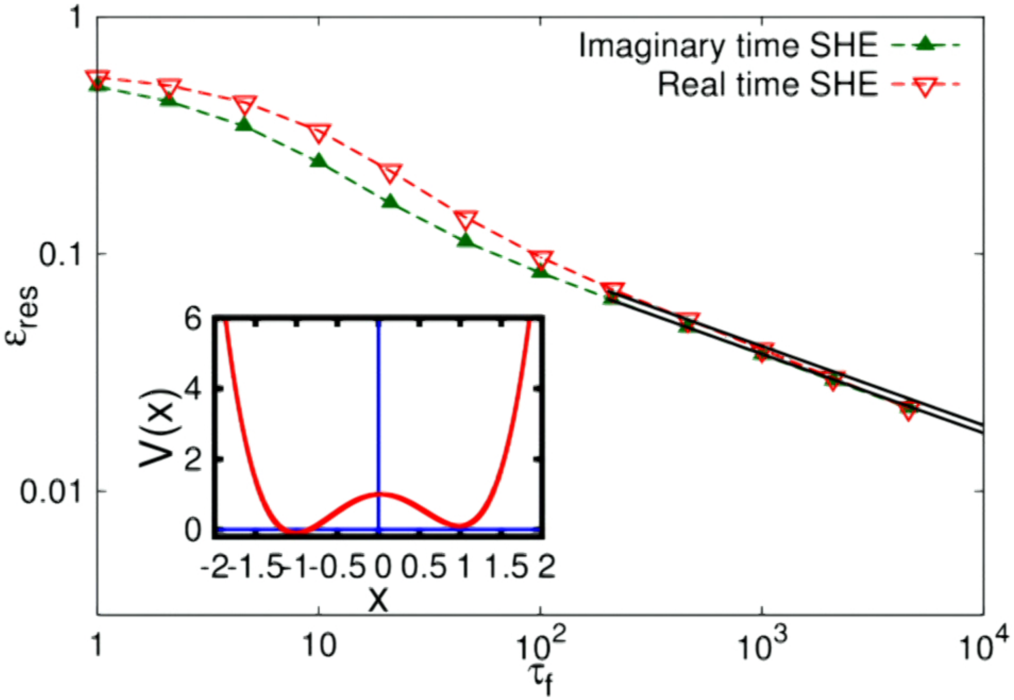
Symmetric double-well potential



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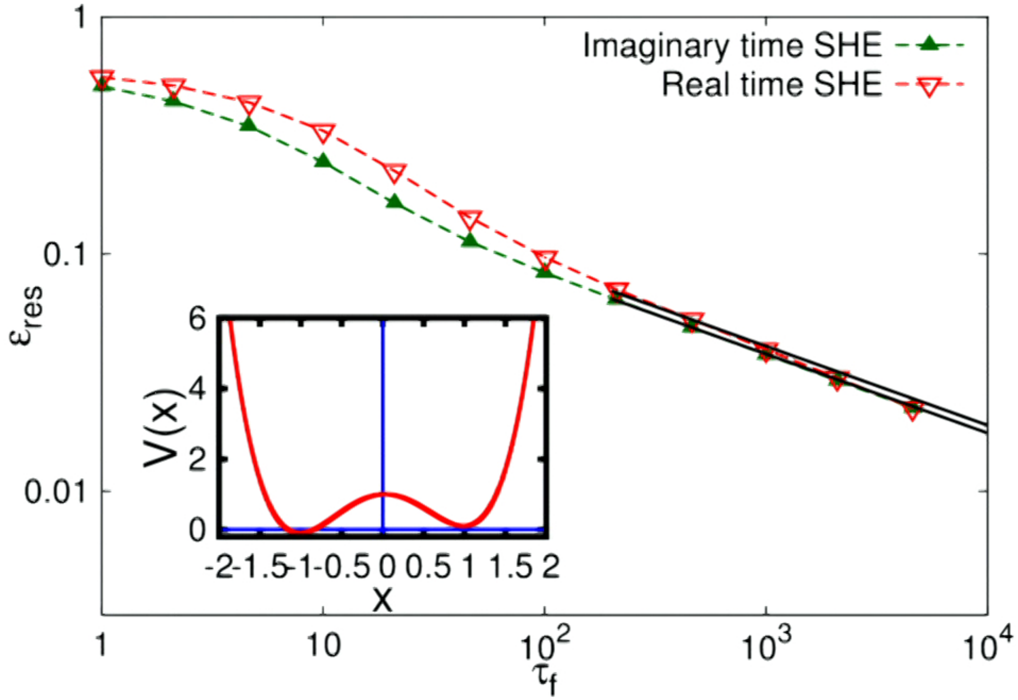

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Can we simulate stochastically the imaginary-time dynamics of the SHE?

<u>Method</u>: projective QMC (PQMC) in a nutshell

Kalos, Levesque, Verlet 1974

Let's consider the Schroedinger equation (SHE) at $\tau = \frac{it}{\hbar}$

$$-\frac{\partial}{\partial\tau}|\Psi(\tau)\rangle = (\hat{H} - E_{ref})|\Psi(\tau)\rangle$$

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$$\xrightarrow{\tau_f \to \infty} c_0 e^{-(\mathbf{E_0} - E_{ref})\tau_f}|\mathbf{\Psi_0}\rangle$$

- PQMC finds the ground state properties of ***quantum*** systems.

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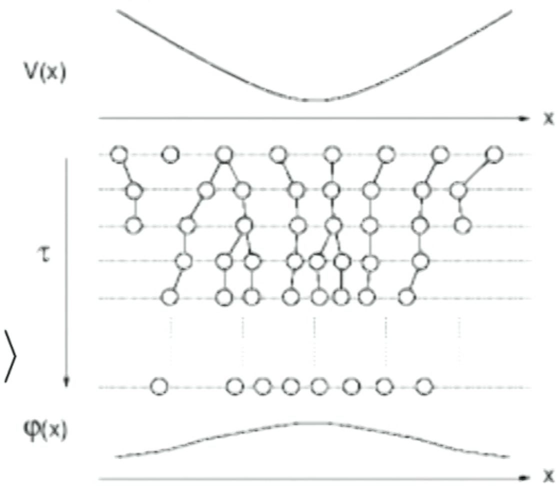

Image from: J. Thijssen, Computational Physics, Cambridge University Press

- PQMC finds the ground state properties of ***quantum*** systems.
- A large population of random walkers N_w is evolved through: ***diffusion*** + ***branching (****death/birth process****)***

Outline:

- Introduction to quantum annealing
- Simulating quantum annealing on continuous space models
  Inack, Pilati, PRE 92, 053304 (2015)
- Tunneling dynamics in QMC simulations
  Inack, Giudici, Parolini, Santoro, Pilati, PRA 97, 032307 (2018)
- Boosting projective QMC simulations via artificial neural networks
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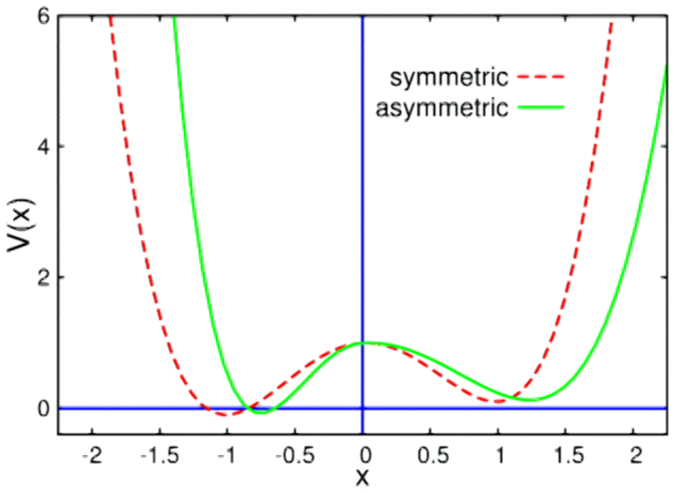
  Inack, Santoro, Pilati, work in progress
- Conclusions and perspectives

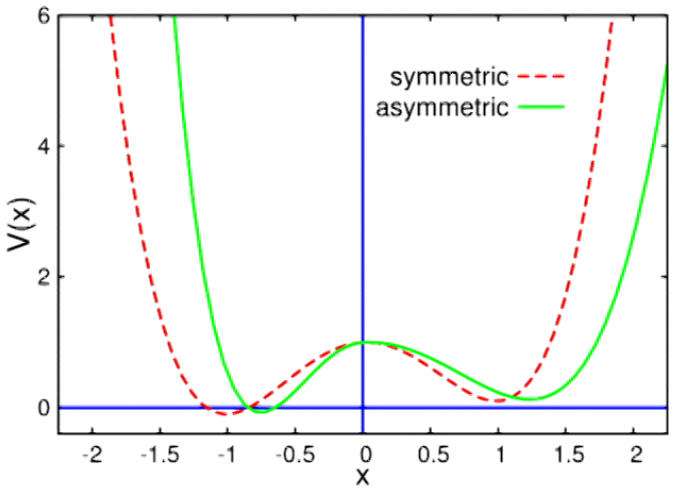
Simulated QA on double-well potentials

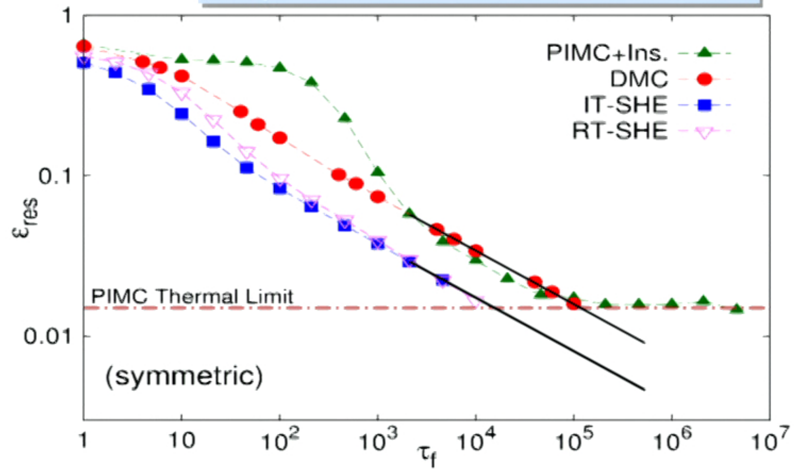


Stella et al, PRB 72, 014303 (2005)
Stella et al, PRB 73, 144302 (2006)

Simulated QA on double-well potentials

NOTE: “time” scales are different, only asymptotic slopes matter





- **DMC performs asymptotically like deterministic IT-SHE**

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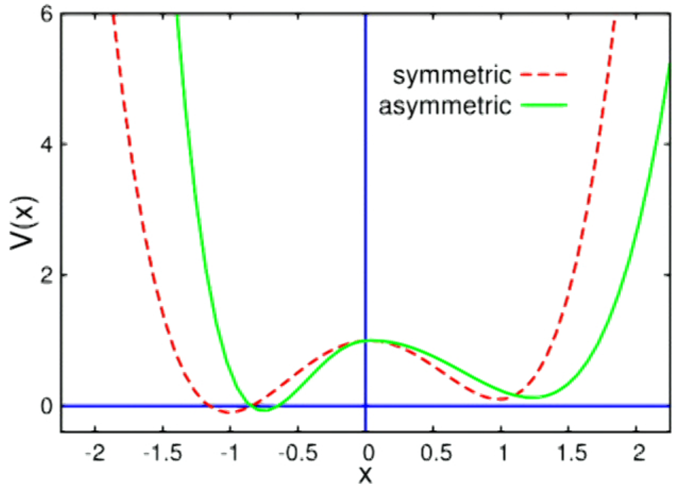
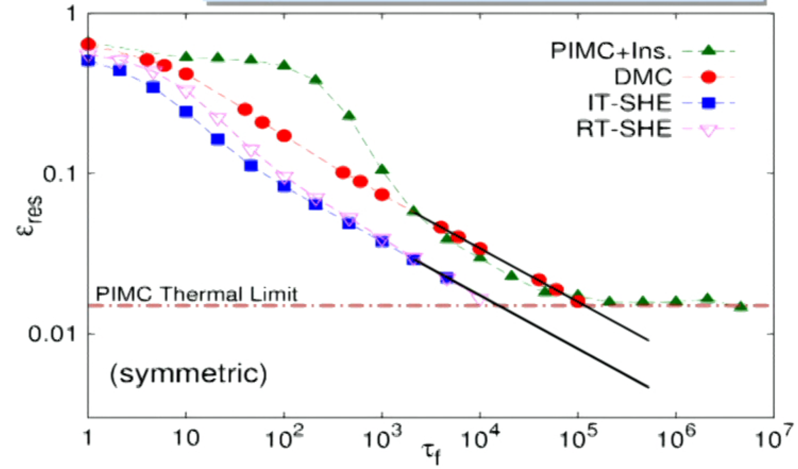
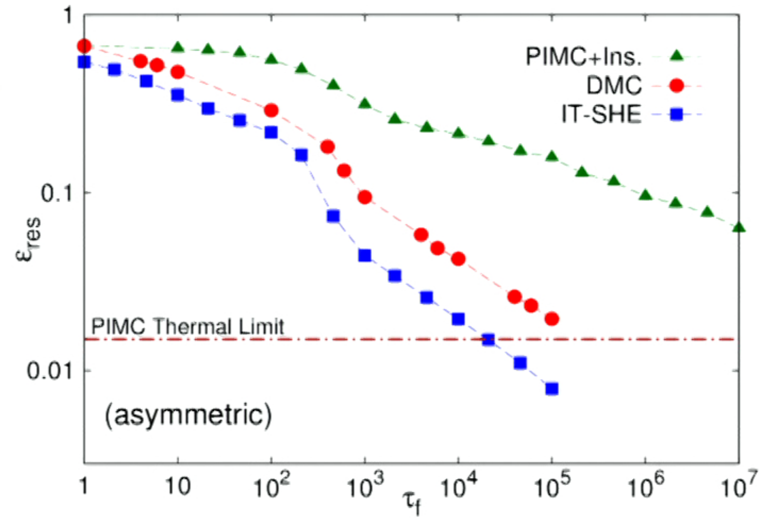






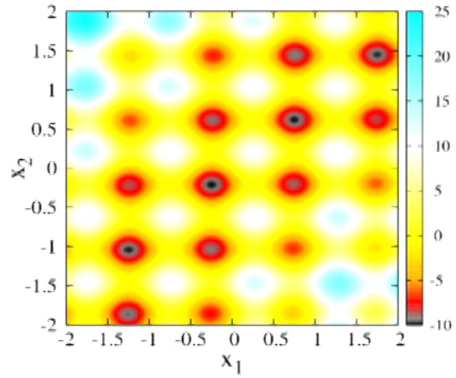
- DMC performs asymptotically like deterministic IT-SHE
- DMC outperforms PIMC even with instanton move

Inack, Pilati, PRE 92, 053304 (2015)

Stella et al, PRB 72, 014303 (2005)
Stella et al, PRB 73, 144302 (2006)

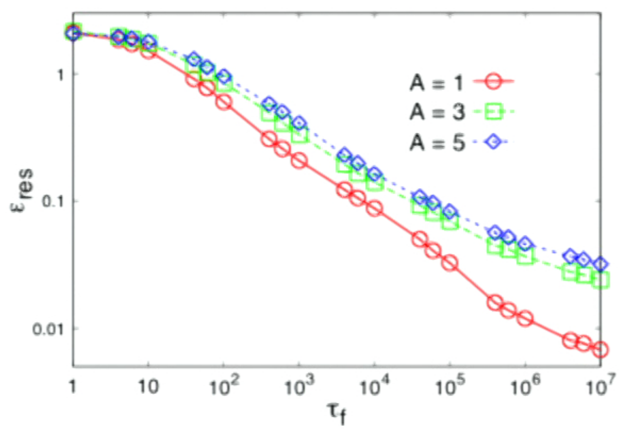
Simulated QA on multiwell potentials

$$V(x_1,x_2) = A[\sin(b_1\pi x_1) + \sin(b_2\pi x_2)] + \frac{1}{2}k_{\text{trap}}(x_1^2 + x_2^2) + \frac{1}{2}k_{\text{rel}}(x_1 - x_2)^2$$

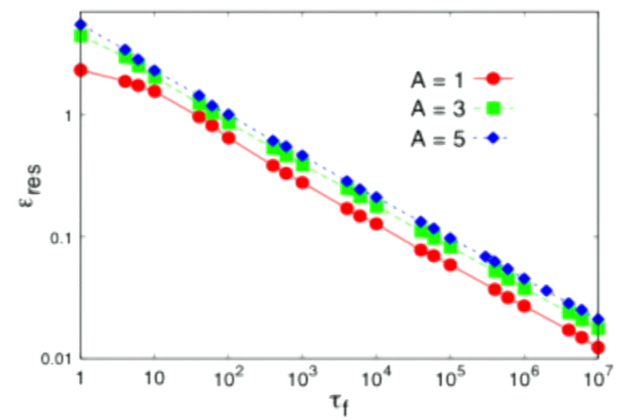


...increasing the barriers height

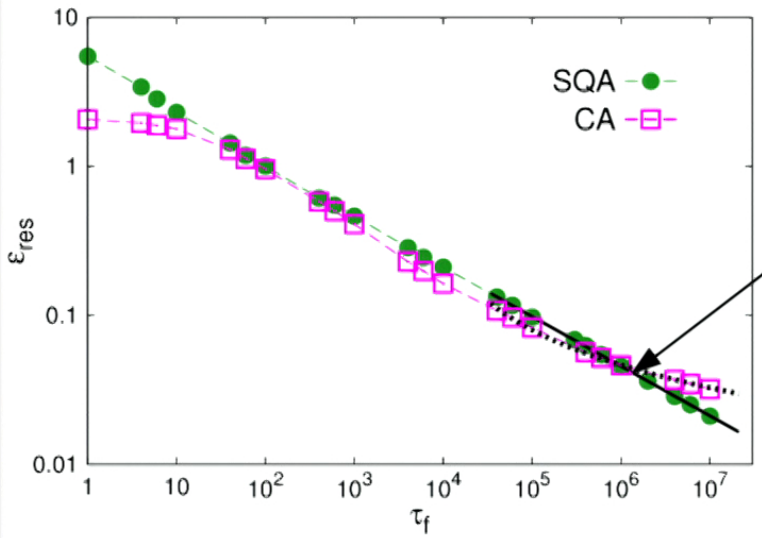
the efficiency of CA degrades



the efficiency of DMC remains constant

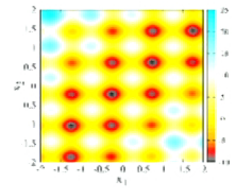


SQA vs CA on multiwell potentials



$$\varepsilon_{res}^{SQA} \sim \tau_f^{-1/3}$$

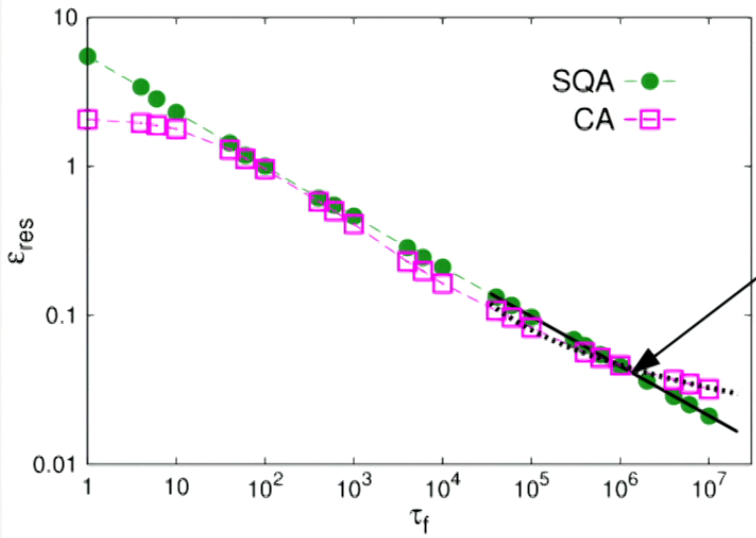
$$\varepsilon_{res}^{CA} \sim \ln^{-1}(c\,\tau_f)$$



Inack, Pilati,
PRE 92, 053304 (2015)

Simulated quantum annealing outperforms CA

SQA vs CA on multiwell potentials



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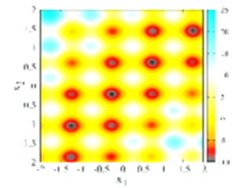

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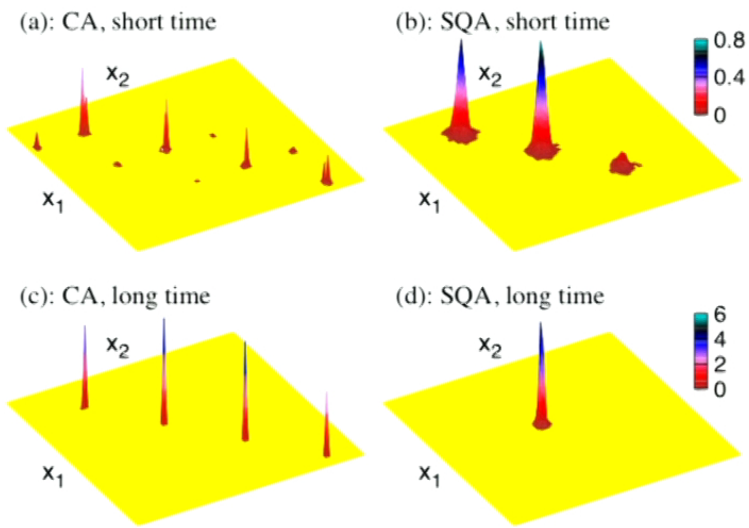

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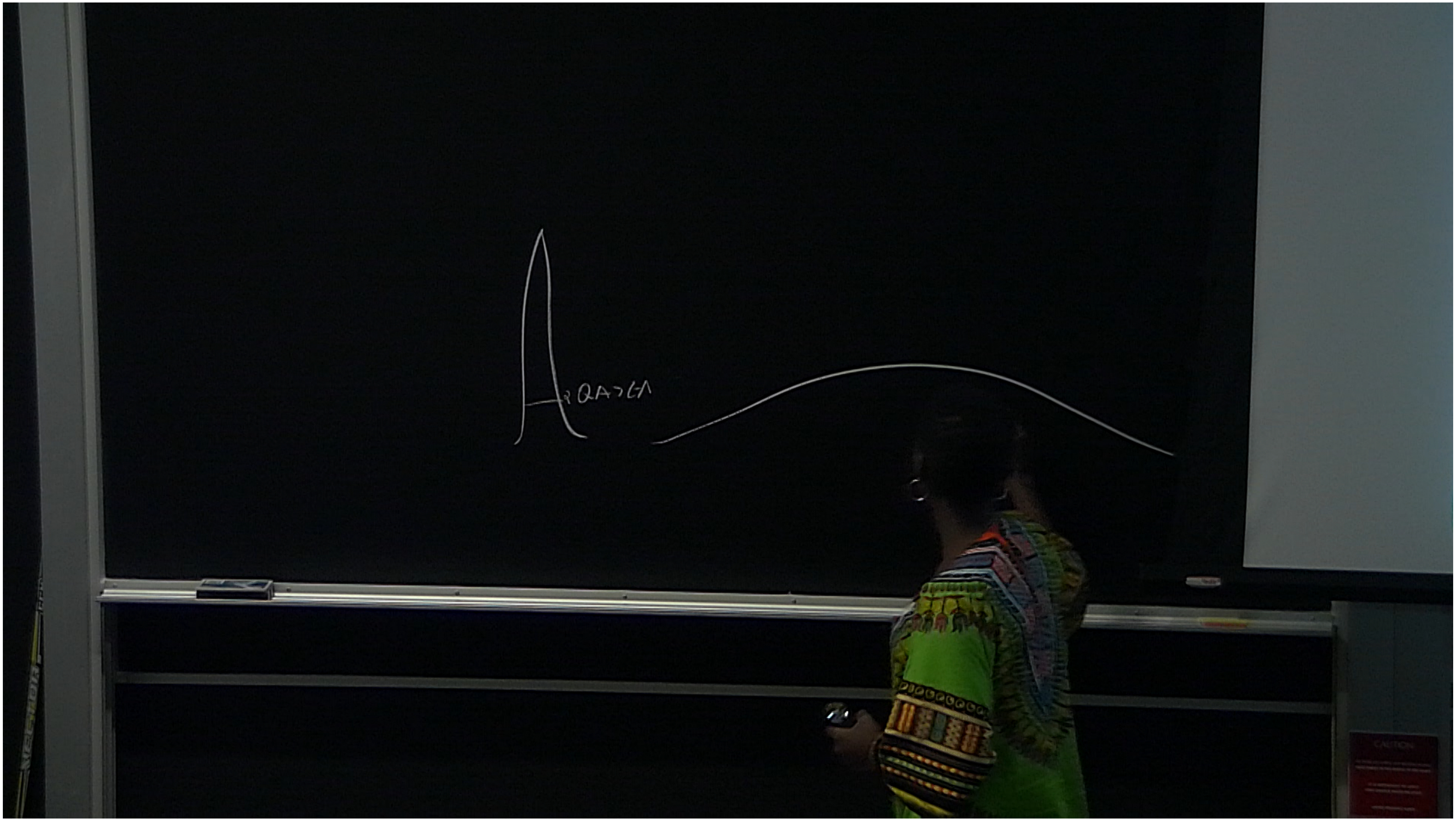

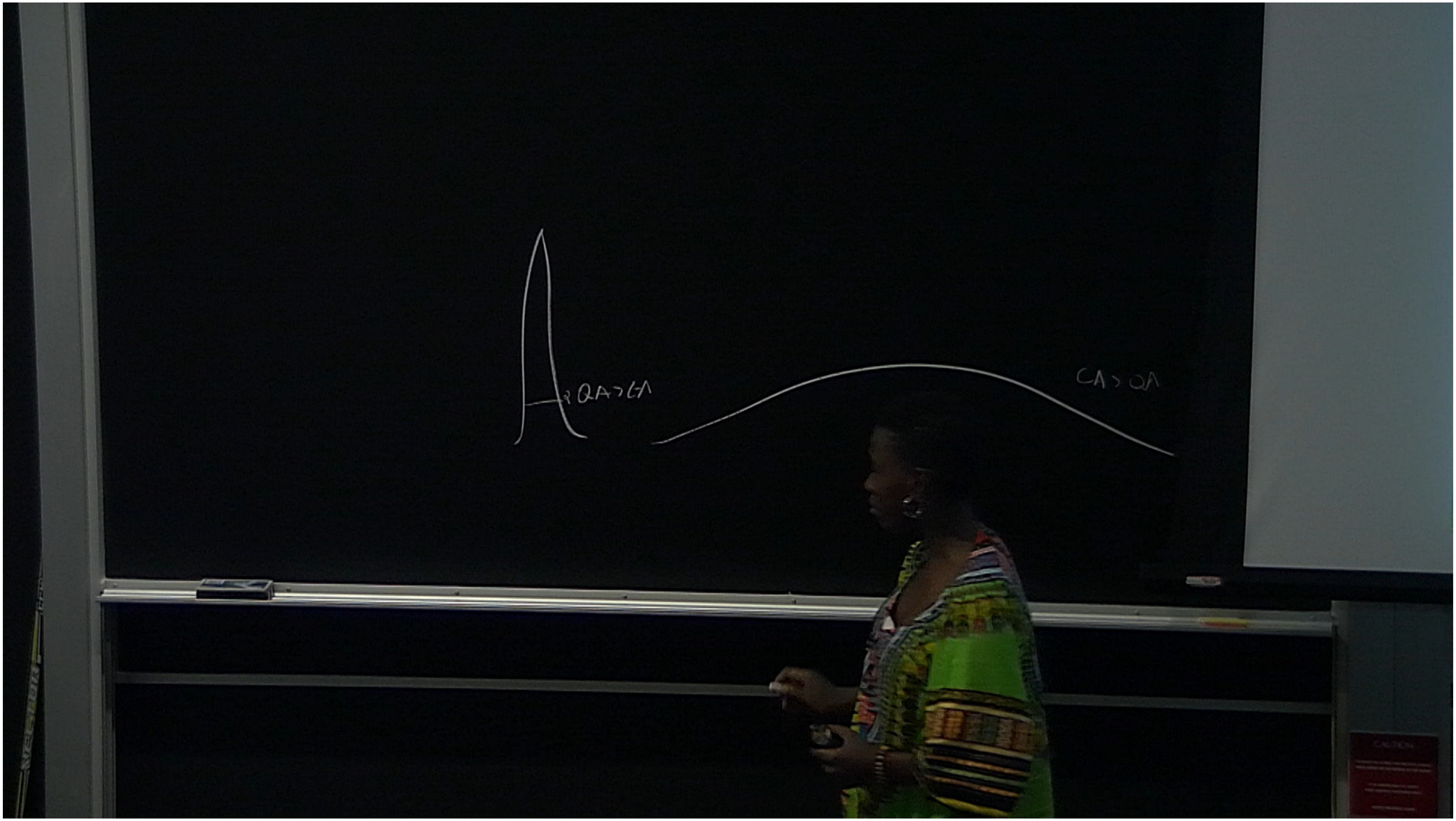
QA > CA
CA > QA

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Tunneling in the double-well potential

PRL 117, 180402 (2016) PHYSICAL REVIEW LETTERS week ending 28 OCTOBER 2016

Understanding Quantum Tunneling through Quantum Monte Carlo Simulations

Sergei V. Isakov,[1] Guglielmo Mazzola,[2] Vadim N. Smelyanskiy,[3] Zhang Jiang,[4,5] Sergio Boixo,[3] Hartmut Neven,[3] and Matthias Troyer[2]

[1]*Google, 8002 Zurich, Switzerland*
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[3]*Google, Venice, California 90291, USA*
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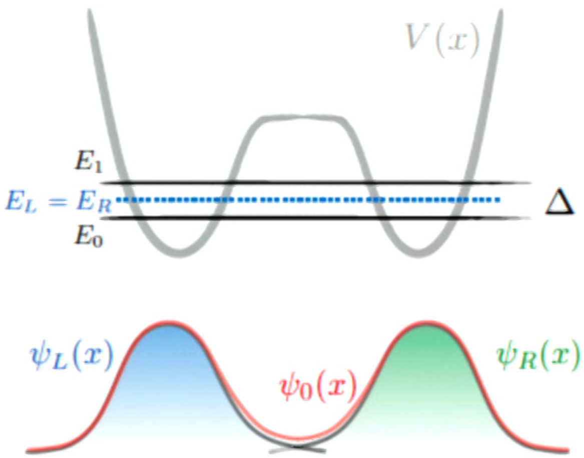

$\psi_{\mathbf{0}}$ Ground state wave-function

$\psi_{\mathbf{1}}$ First excited state

$$\psi_{\mathbf{L}} \equiv \frac{\psi_{\mathbf{0}} - \psi_{\mathbf{1}}}{\sqrt{2}}$$

$$\psi_{\mathbf{R}} \equiv \frac{\psi_{\mathbf{0}} + \psi_{\mathbf{1}}}{\sqrt{2}}$$

$$\Delta = E_1 - E_0$$

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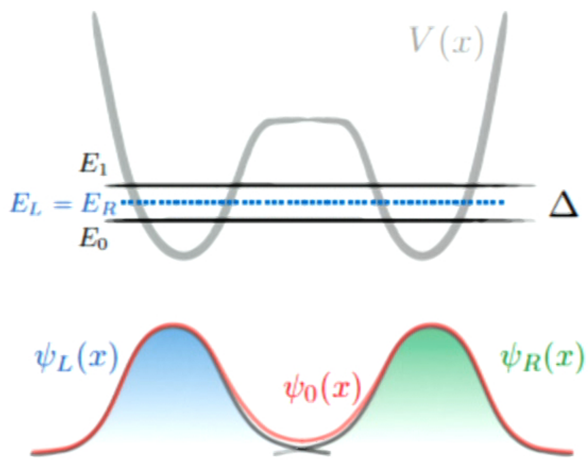

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$$\Delta = E_1 - E_0$$

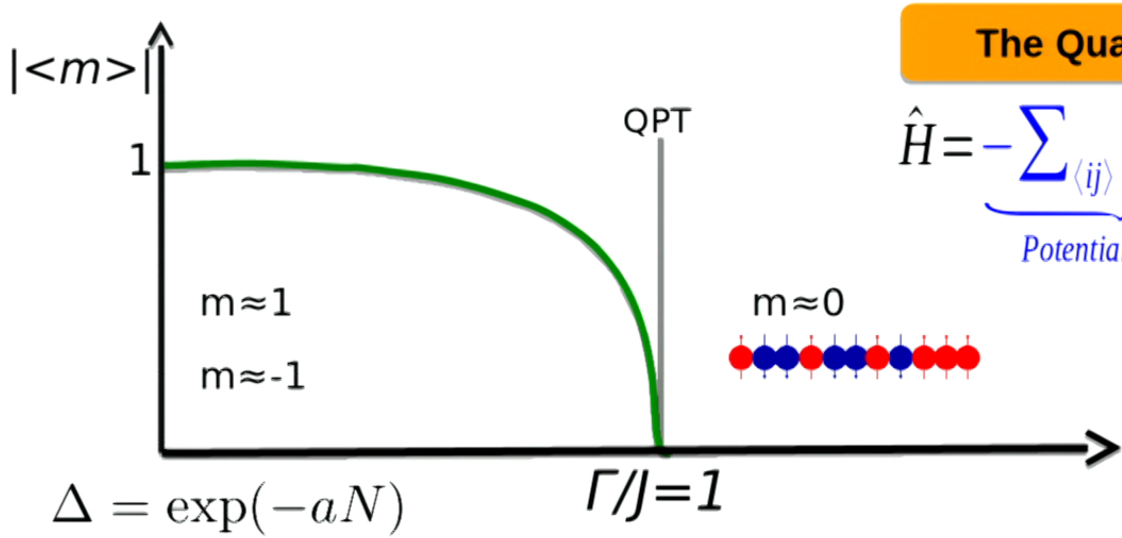
Quantum annealing tunneling time

$$\xi_{anneal} \propto \frac{\alpha}{\Delta^2}$$

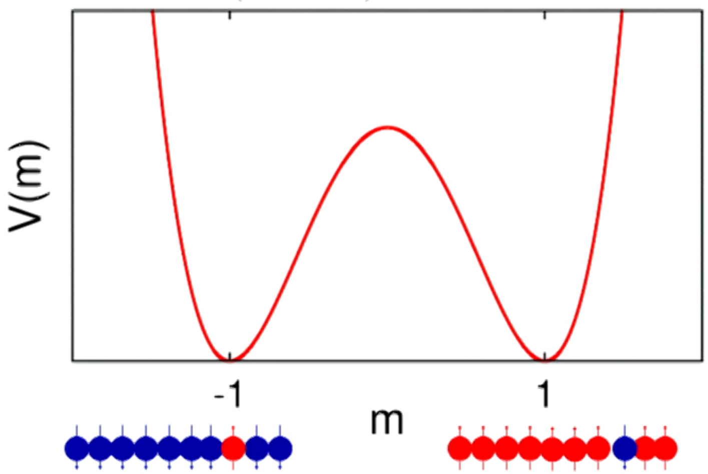
What is the tunneling time of QMC simulations?

The Quantum Ising chain

$$\hat{H} = \underbrace{-\sum_{\langle ij \rangle} J \sigma_i^z \sigma_j^z}_{\text{Potential Energy}} - \underbrace{\Gamma \sum_i \sigma_i^x}_{\text{Kinetic Energy}}$$



$$\Delta = \exp(-aN)$$



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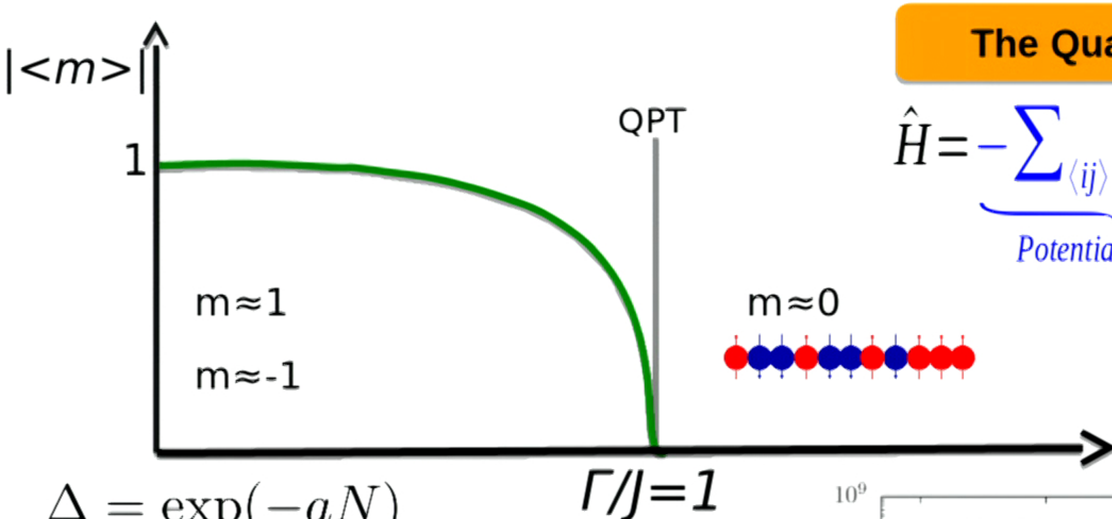

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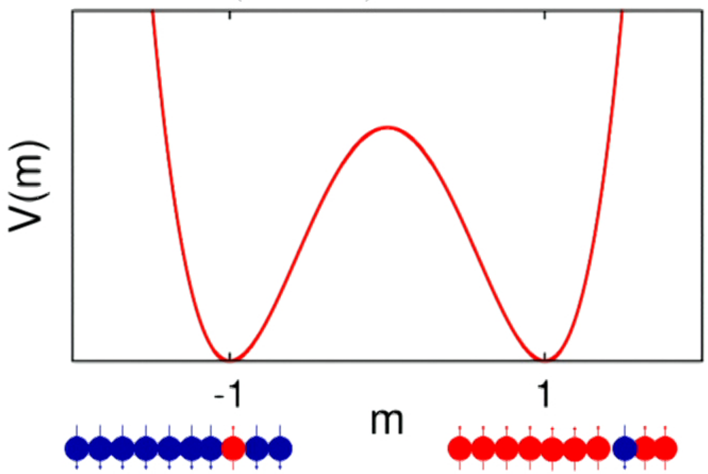
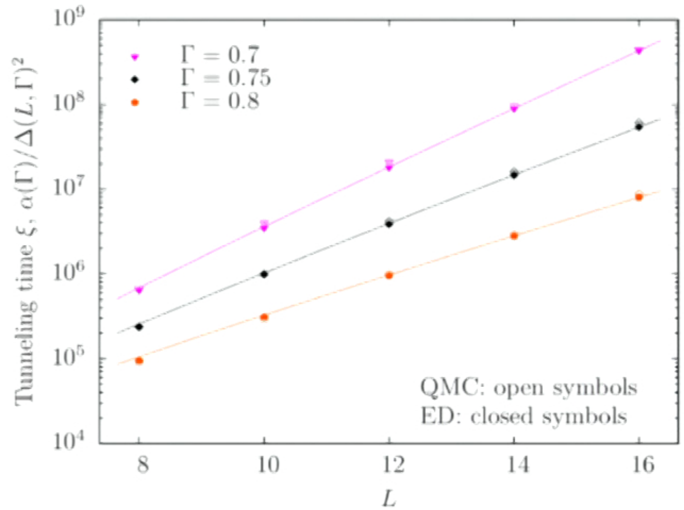
$$\xi_{PIMC} \propto \frac{\alpha}{\Delta^2}$$

PIMC scales like QA

$$\Delta = \exp(-aN)$$





Isakov, Mazzola, Smelyanskiy, Jiang, Boixo, Neven, Troyer, PRL (2016)
Mazzola, Smelyanskiy, Troyer, PRB (2017)

Shamrock: A model of frustrated rings

Can quantum Monte Carlo simulate quantum annealing?

Evgeny Andriyash[1] and Mohammad H. Amin[1,2]

[1] *D-Wave Systems Inc., 3033 Beta Avenue, Burnaby BC Canada V5G 4M9*

[2] *Department of Physics, Simon Fraser University, Burnaby, BC, Canada V5A 1S6*

Shamrock: A model of frustrated rings

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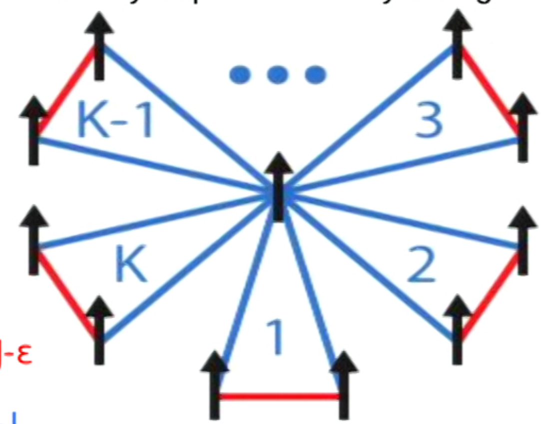
Currently implemented by Google



$J_{AFM} = J - \varepsilon$

$J_{FM} = -J$

Shamrock: A model of frustrated rings

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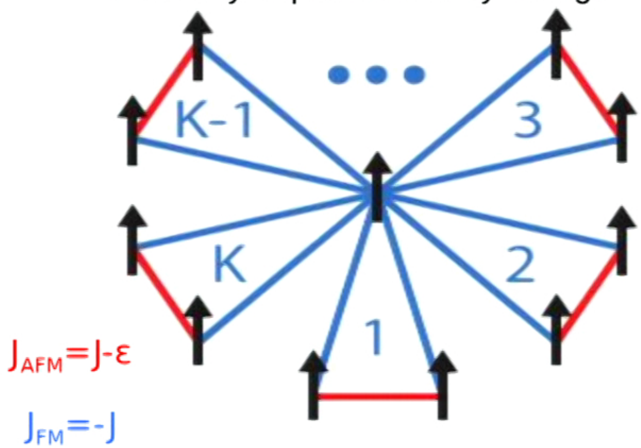
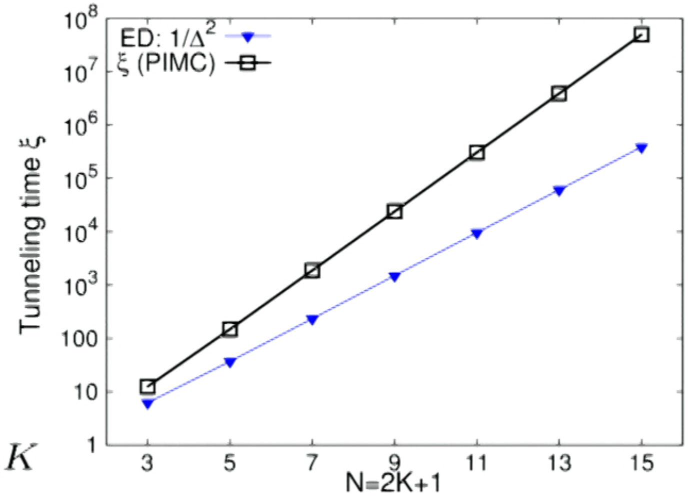


$$\xi_{PIMC} \propto \frac{2^K}{\Delta^2}$$



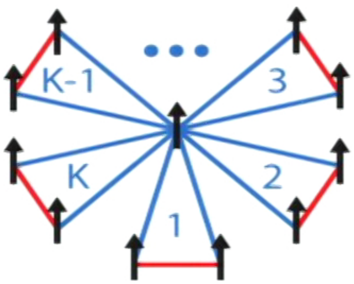
Number of spins

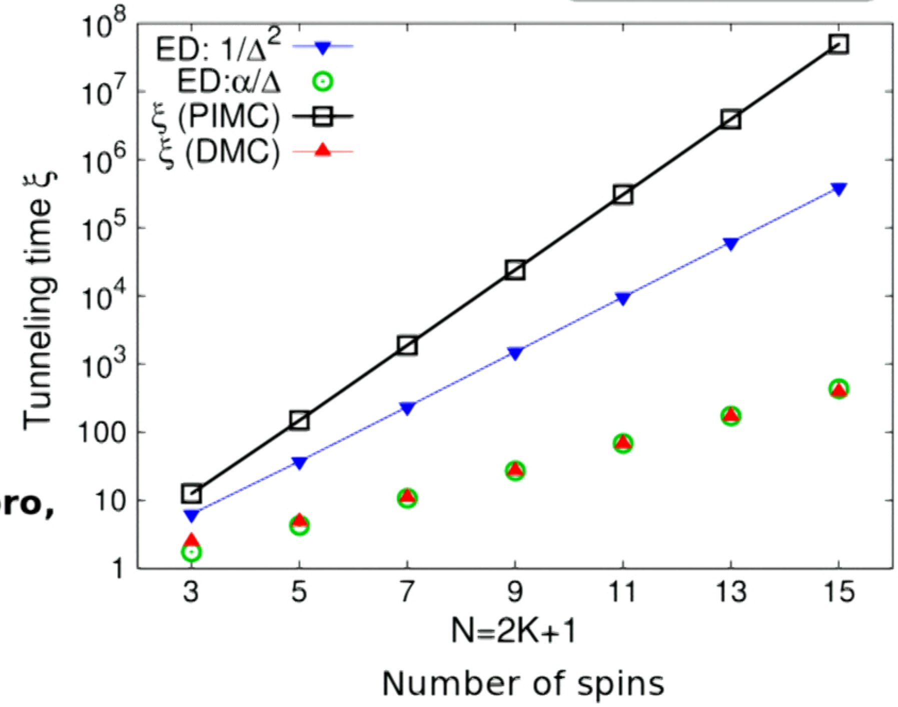
PIMC dynamics slows down due to "topological" obstructions,
It is slower than QA!

M. B. Hastings, Quantum Inf. Comput. 13, 1038 (2013)

Shamrock: A model of frustrated rings

PQMC results





Inack, Giudici, Parolini, Santoro, Pilati, PRA (2018)

- ➢ PIMC dynamics slows down due to "topological" obstructions, **It is slower than QA!**
- ➢DMC dynamics scales like $1/\Delta$ (i.e., **"faster" than QA**)

Projective quantum Monte Carlo method

$$-\frac{\partial}{\partial \tau}|\Psi(\tau)\rangle = (\hat{H} - E_{ref})|\Psi(\tau)\rangle$$

Projective quantum Monte Carlo method

$$-\frac{\partial}{\partial \tau}|\Psi(\tau)\rangle = (\hat{H} - E_{ref})|\Psi(\tau)\rangle$$

Evolve the Schrödinger equation in imaginary time

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

$$w(\boldsymbol{X}') = \sum_{X} G(\boldsymbol{X}, \boldsymbol{X}', \Delta\tau) \neq 1$$

G is not a stochastic matrix

This is not a classical Markov chain

Projective quantum Monte Carlo method

$$-\frac{\partial}{\partial \tau}|\Psi(\tau)\rangle = (\hat{H} - E_{ref})|\Psi(\tau)\rangle$$

Evolve the Schrödinger equation in imaginary time

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

$$w(\mathbf{X}') = \sum_{X} G(\mathbf{X}, \mathbf{X}', \Delta\tau) \neq 1$$

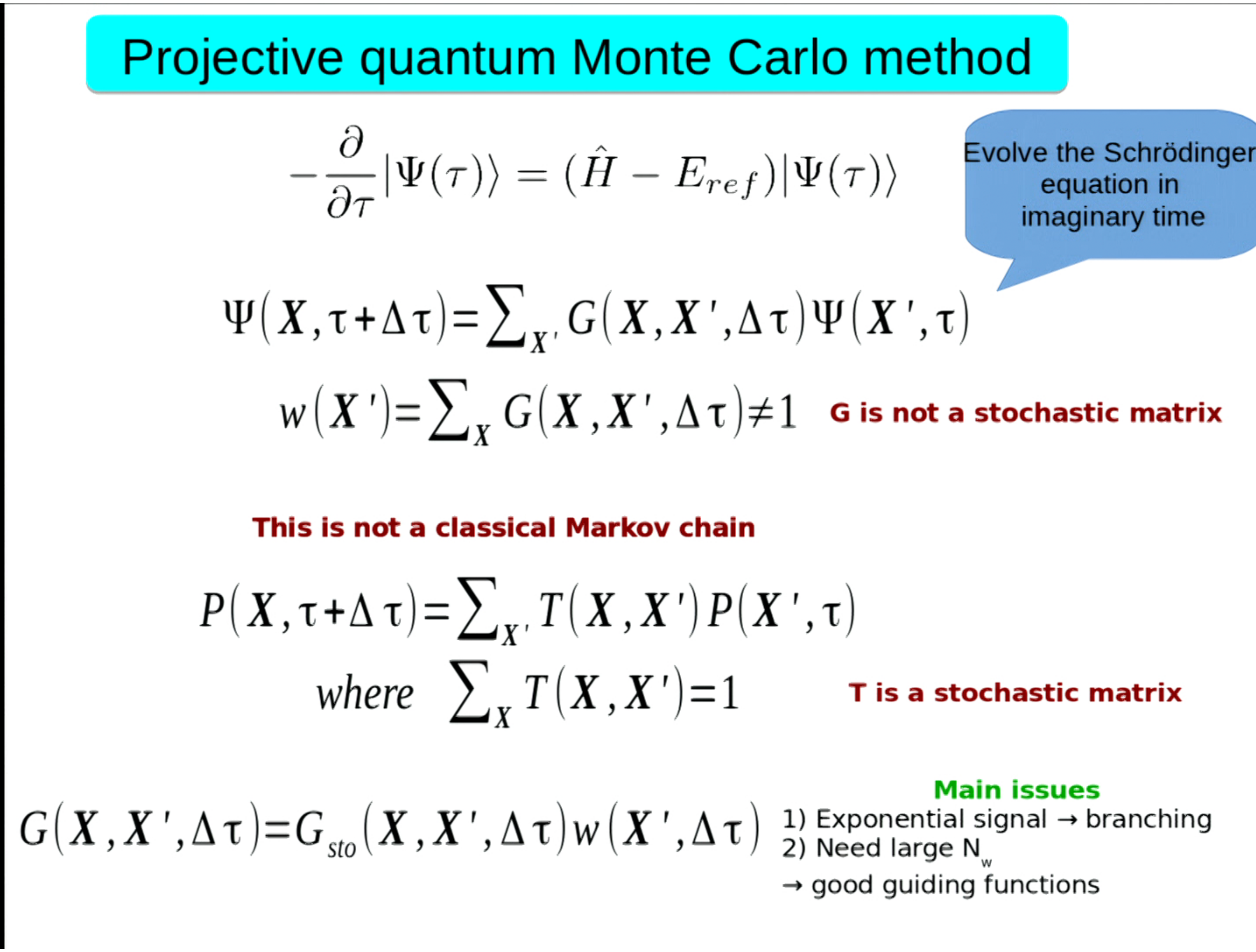
G is not a stochastic matrix

This is not a classical Markov chain

$$P(\mathbf{X}, \tau+\Delta\tau) = \sum_{X'} T(\mathbf{X}, \mathbf{X}') P(\mathbf{X}', \tau)$$

$$\text{where} \quad \sum_{X} T(\mathbf{X}, \mathbf{X}') = 1$$

T is a stochastic matrix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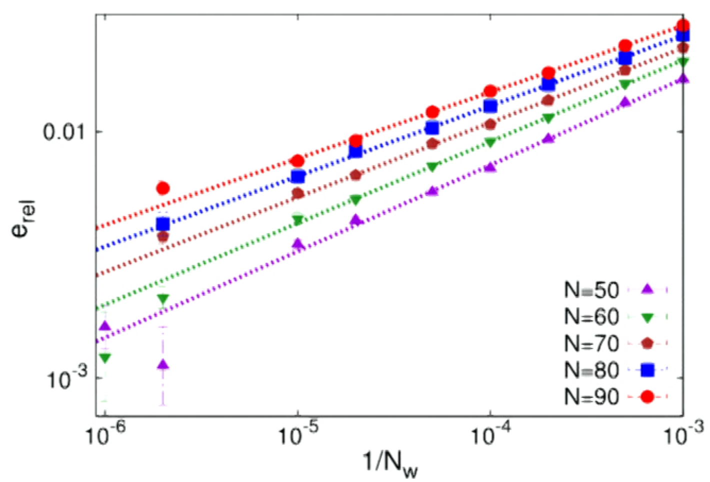
Main issues
1) Exponential signal → branching
2) Need large N_w
→ good guiding functions

Systematic errors in PQMC algorithms

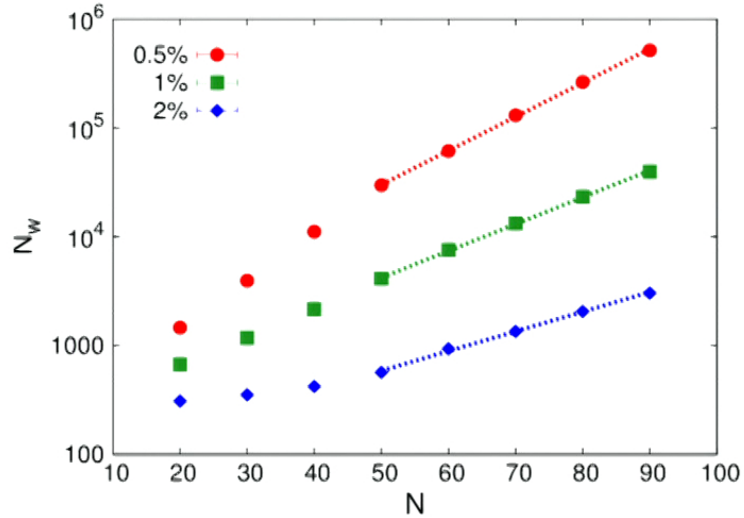
Model: Quantum Ising chain

Relative error w.r.t. exact ground state energy



Inverse number of random walkers

# of walkers required to keep relative err. fixed



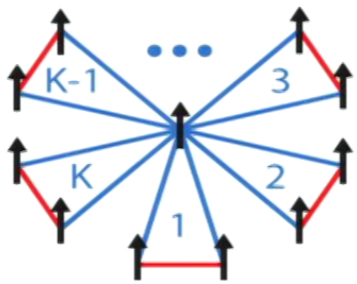
System size

Inack, Giudici, Parolini, Santoro, Pilati, PRA (2018)

Exponentially growing computational cost

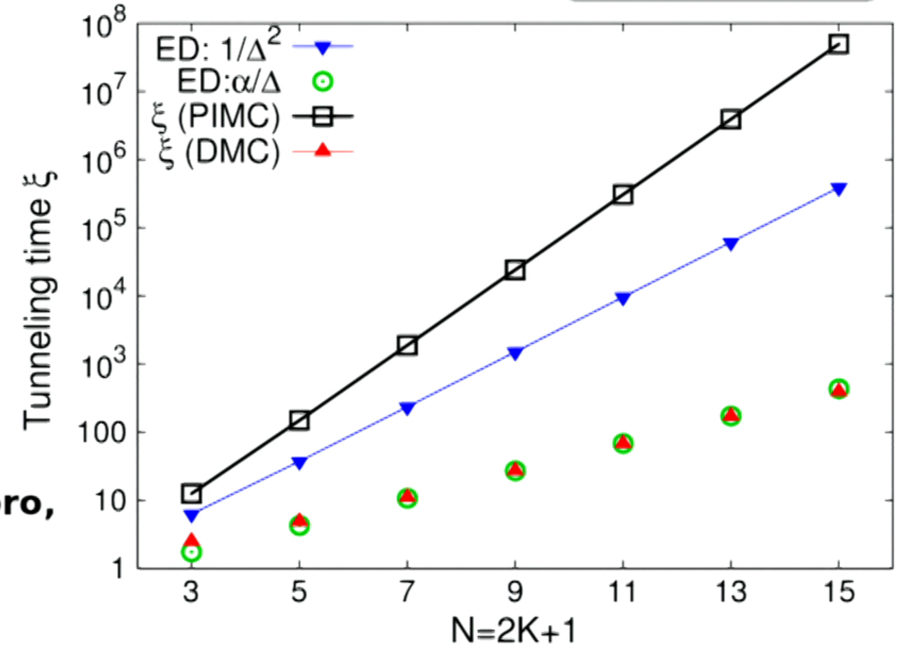
Note: here we use "simple" PQMC algorithm: no guiding wave function.

Shamrock: A model of frustrated rings



Inack, Giudici, Parolini, Santoro, Pilati, PRA (2018)

PQMC results



Number of spins

- ➢ PIMC dynamics slows down due to "topological" obstructions, **It is slower than QA!**
- ➢DMC dynamics scales like $1/\Delta$ (i.e., **"faster" than QA**)

Systematic errors in PQMC algorithms

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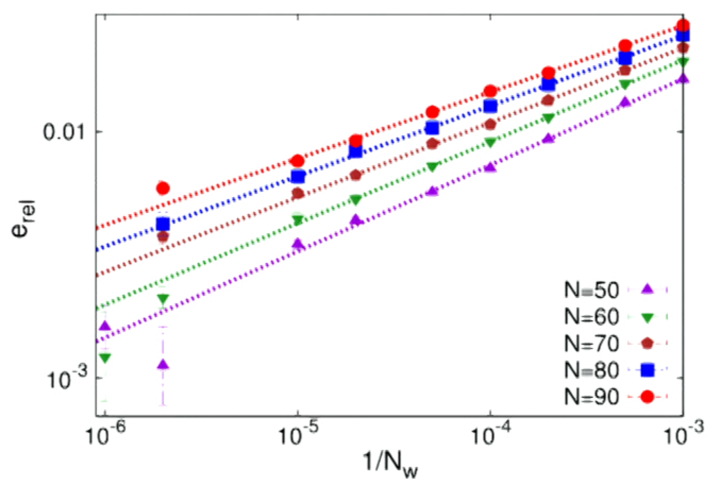

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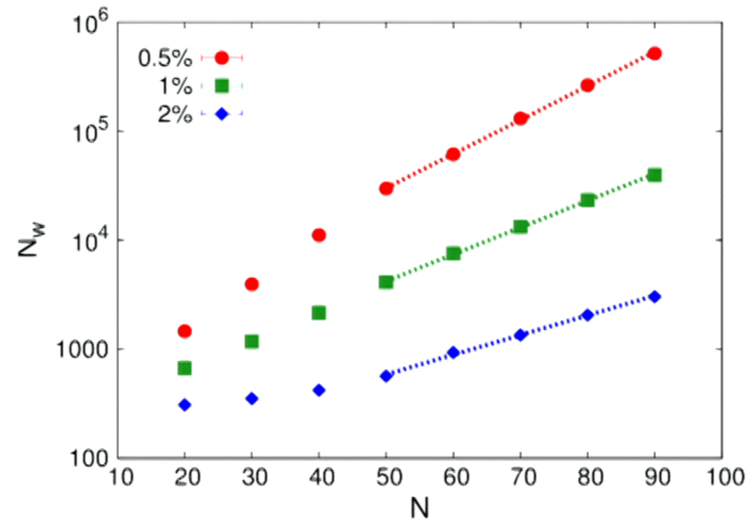

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Projective QMC with importance sampling

$$f(\mathbf{x},\tau) = \Psi(\mathbf{x},\tau)\psi_\kappa(\mathbf{x})$$

The modified Schroedinger equation in imaginary-time leads to:

continuous space

Drift-diffusion Langevin equation

$$\mathbf{x} = \mathbf{x}' + \frac{\Delta\tau}{m}F_\kappa(\mathbf{x}') + \eta\sqrt{\frac{\Delta\tau}{m}}$$

Branching

$$w(\mathbf{x}',\Delta\tau) = e^{-\Delta\tau\left(E_{loc}(\mathbf{x}')-E_{ref}\right)}$$

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Idea: use artificial neural networks as guiding wave functions

RESEARCH ARTICLE

MANY-BODY PHYSICS

Solving the quantum many-body problem with artificial neural networks

Giuseppe Carleo[1*] and Matthias Troyer[1,2]

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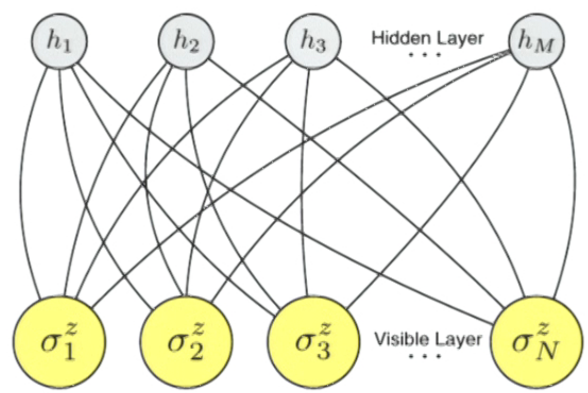
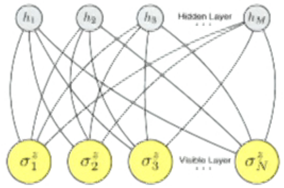


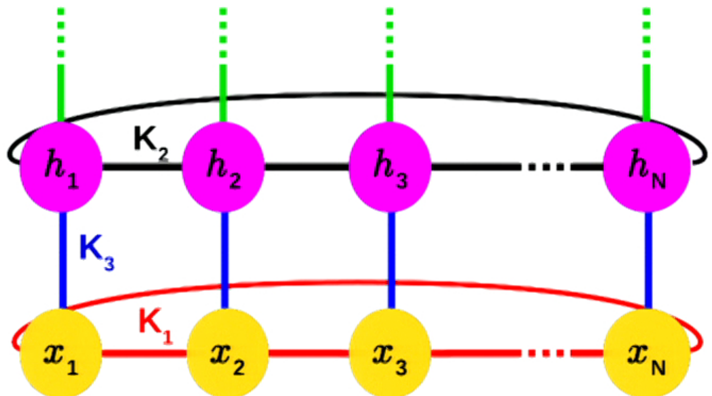
Unrestricted Boltzmann machines as variational wave functions

Idea: use Boltzmann machine (BM) as guiding wave function

- Carleo, Troyer, Science (2017): restricted Boltzmann machines
- This work: unrestricted Boltzmann machine



$$\psi_K(\mathbf{x}) = \sum_{\mathbf{h}} e^{-\mathbf{K_1}\sum_{<\mathbf{i},\mathbf{j}>}\mathbf{x_i x_j} - \mathbf{K_2}\sum_{<\mathbf{i},\mathbf{j}>}\mathbf{h_i h_j} - \mathbf{K_3}\sum_{\mathbf{i}}\mathbf{x_i h_i}}$$



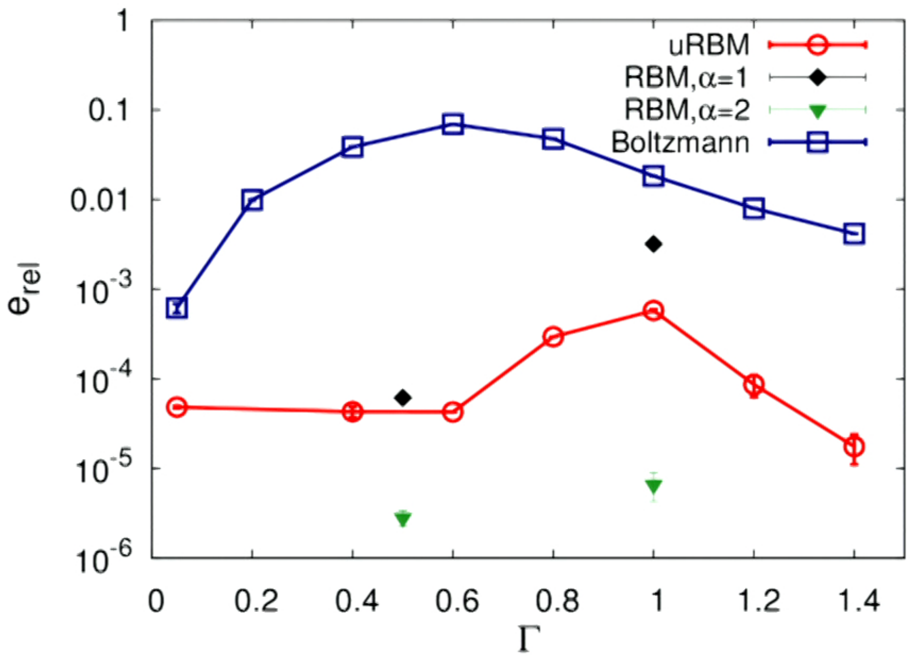
Variational parameters: K_1, K_2, K_3

Hidden variables: h_1, $h_{2,\ldots,}$ h_N

Visible variables: x_1, $x_{2,\ldots,}$ x_N

Comparison between variational wave-functions

Quantum Ising chain



α is the hidden-density layer

$$e_{rel} = \left| \frac{E_v - E_{GS}}{E_{GS}} \right|$$

- **uRBM is more efficient compared with the RBM at α=1**
- **The efficiency of the RBM increases with α**

Inack, Dell'Anna, Santoro, Pilati, arXiv:1809.03562v1

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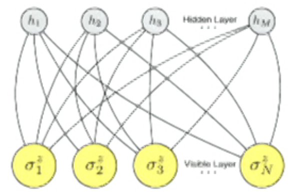

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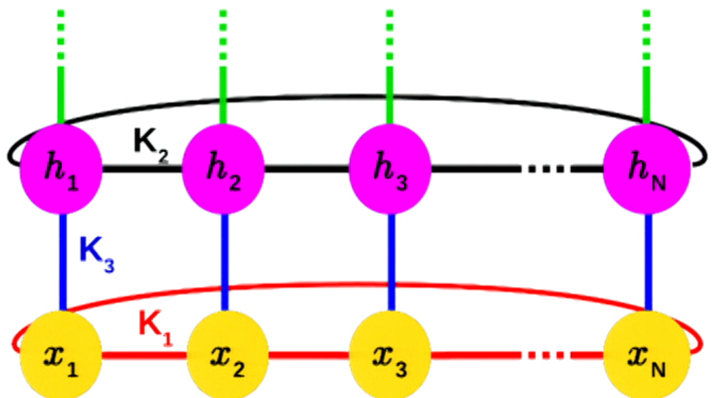

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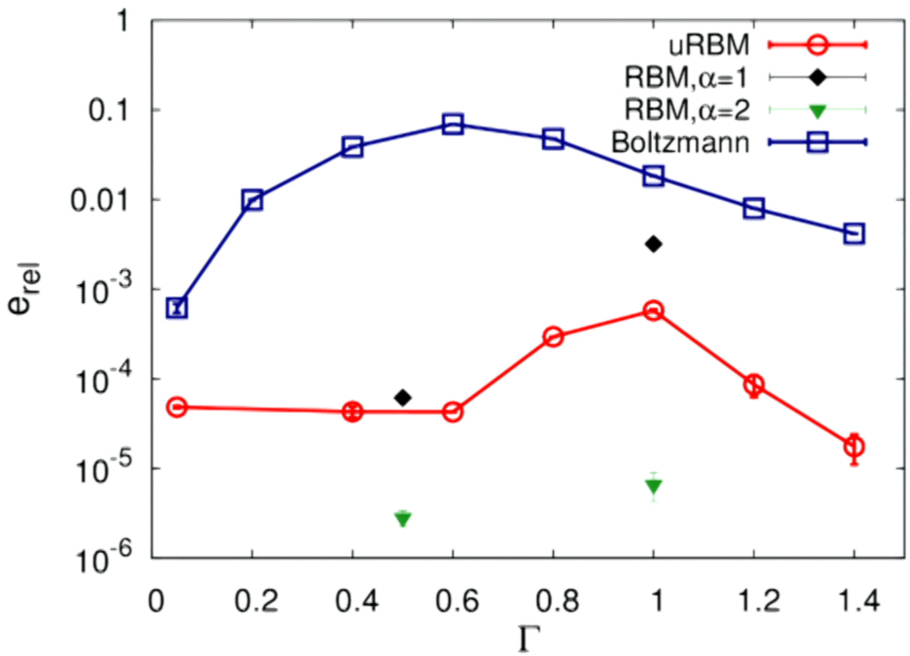

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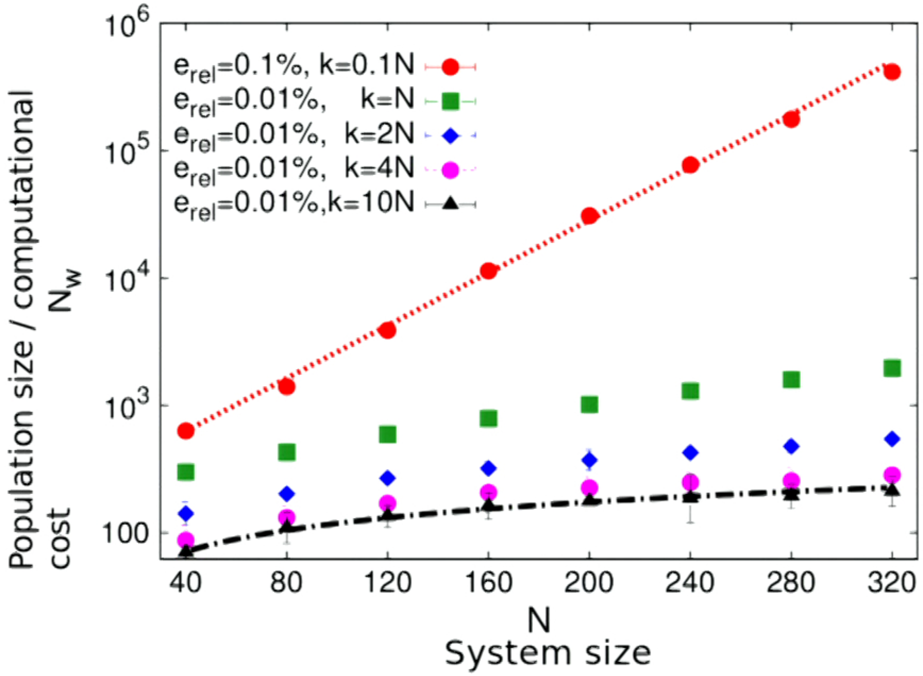
Computational complexity of PQMC guided by unrestricted BM

- Needs combined sampling of both visible and hidden spins
- Correlations among hidden-spin configurations affect systematic errors
- Needs efficient sampling of hidden-spins, especially at the critical point

k = # of updates of hidden spins variables every visible spin

Quantum Ising chain: Γ = 1



$N_w \propto e^{aN}$ a=0.023(3)

Inack, Dell'Anna, Santoro, Pilati, arXiv:1809.03562v1

$N_w \propto N^b$ b=0.55(1)

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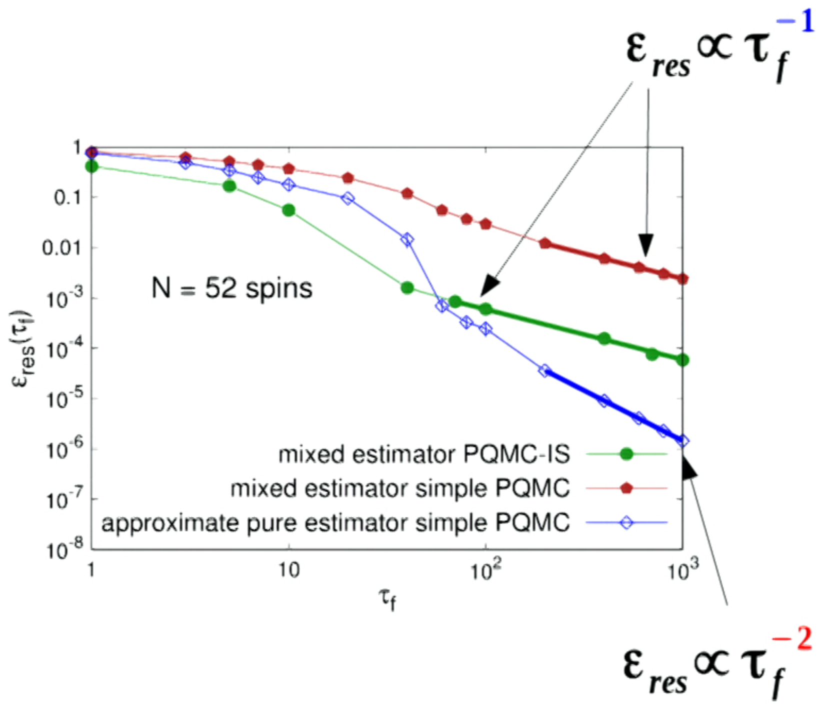
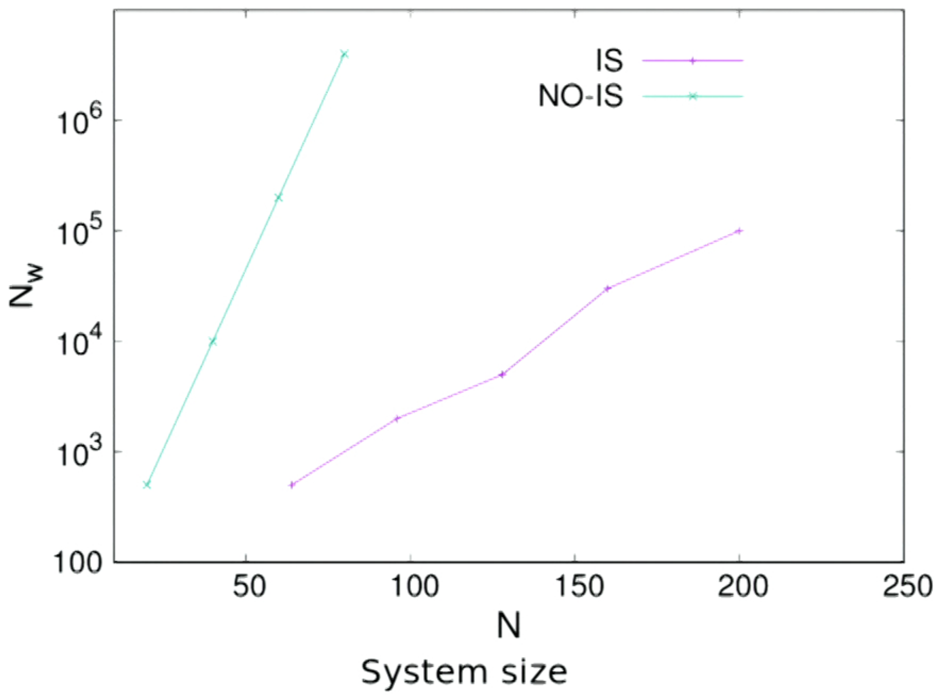
SQA with results on the Ising chain (work in progress)



PQMC results for different estimators

➢**PQMC performs asymptotically like deterministic IT-SHE (Zanca, Santoro, PRB 2016)**

SQA computational complexity on the Ising chain (work in progress)



Quasiadiabatic limit

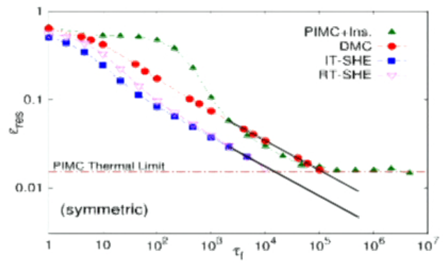
$$\tau_f = 500$$

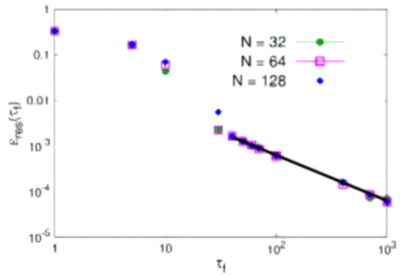
$$\varepsilon_{res} \sim 10^{-4}$$

- Importance sampling betters the scaling but it's still exponential
- Better guiding wave-functions may improve the scaling

Summary and perspectives

- Projective QMC methods can simulate quantum annealing





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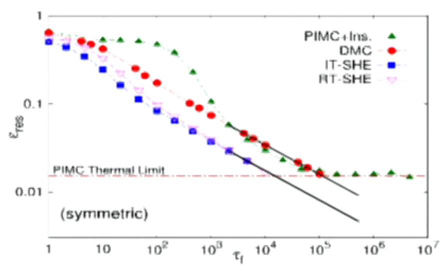

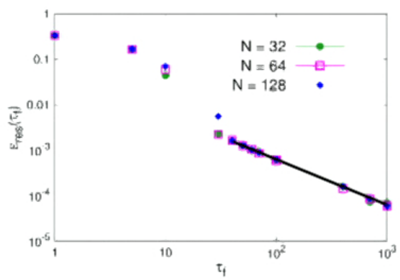

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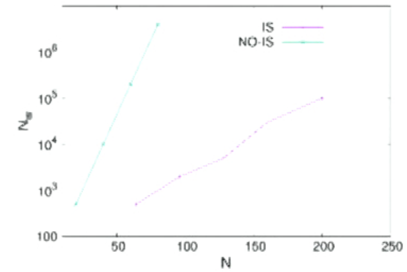

Good guiding functions needed

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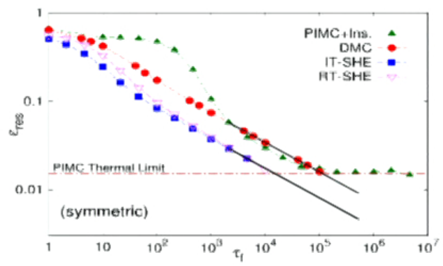

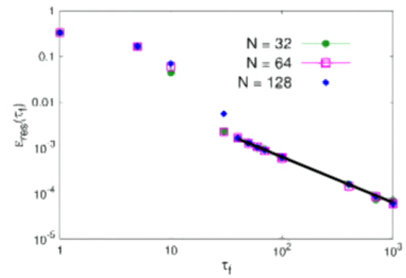

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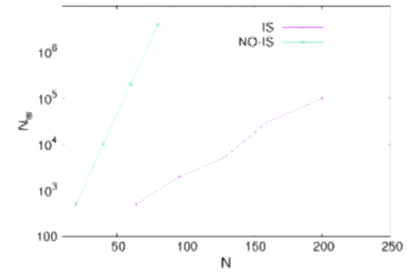
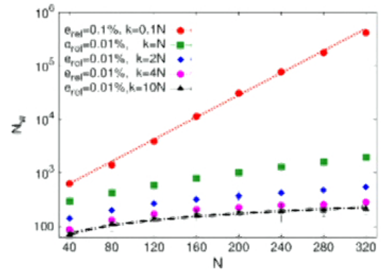


Good guiding functions needed

- Major improvements of computational scaling with unrestricted Boltzmann machines



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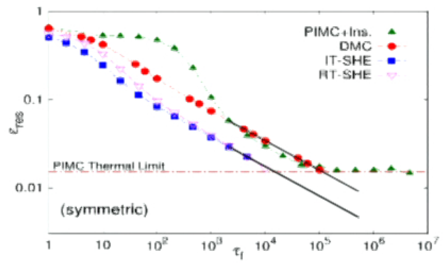

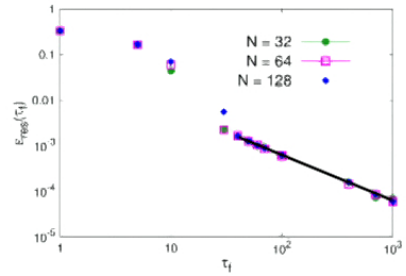

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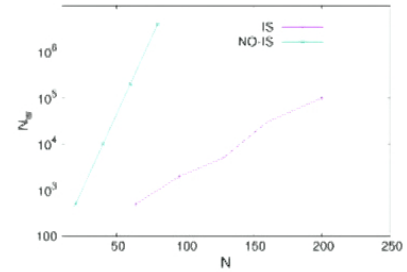

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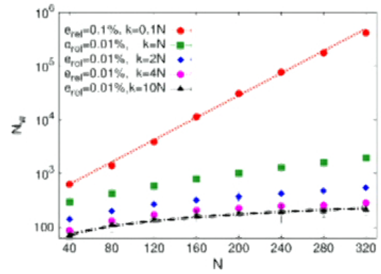
In future works: Combine uRBMs with SQA



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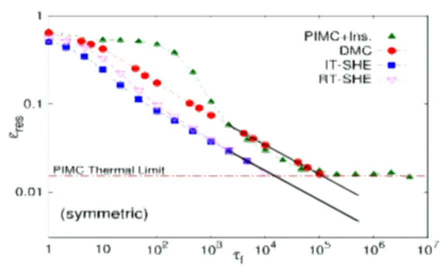

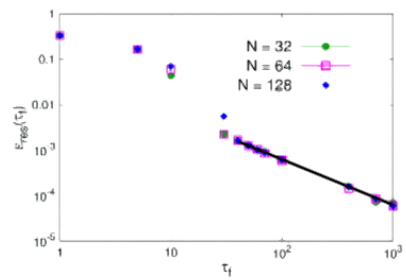

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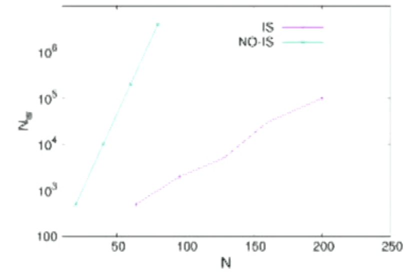

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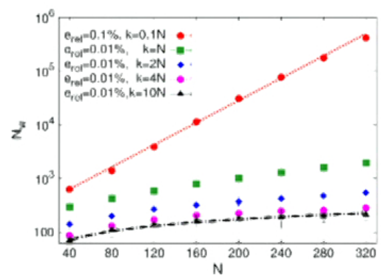

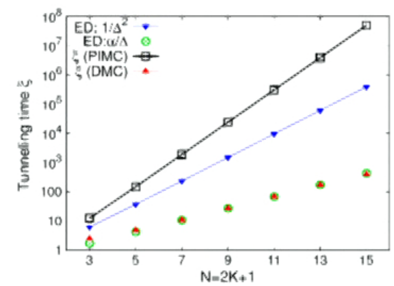

- Tunneling time in Projective QMC simulations scales much faster than quantum annealing and PIMC

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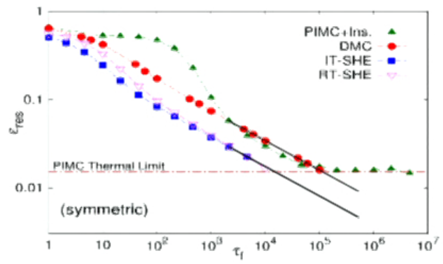

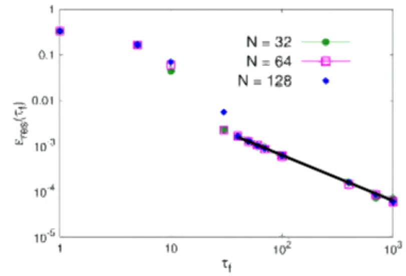

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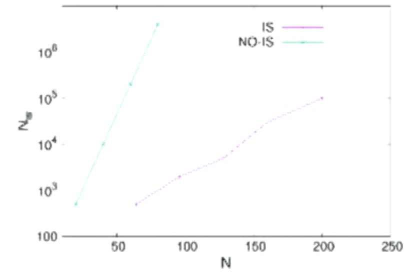

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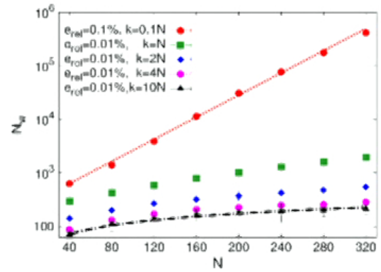

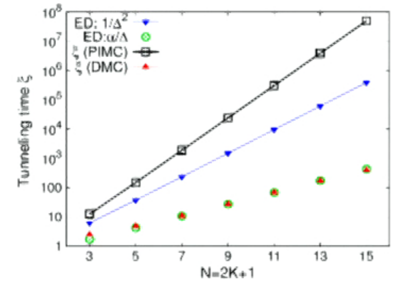

- Tunneling time in Projective QMC simulations scales much faster than quantum annealing and PIMC

- **This suggests that imaginary-time based methods could be more efficient for solving optimization problems**

Thank you for your kind attention!