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Optimization with Quantum Mechanics

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Optimization with Quantum Mechanics

Quantum annealing via adiabatic evolution

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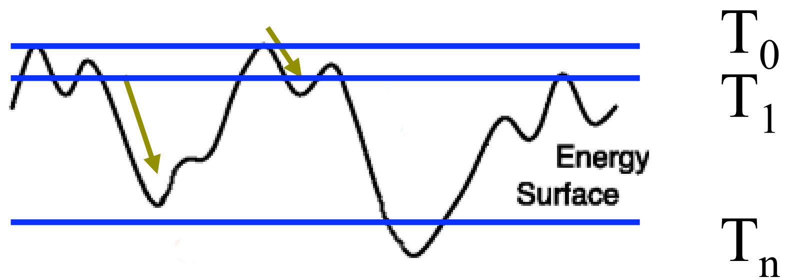
Outline

- Introduction: Complex systems
- Basic idea of Quantum Annealing
- Path-Integral MC results: Ising glass, TSP, 3-SAT
- Lessons from a simple case: Double-well potential
- 1D Random Ising Chain, an ideal playground.
- Thoughts and Perspectives

Optimization of a complex system

Problem: Searching the optimal state (absolute minimum) of a complex energy (cost) function with many *local minima* separated by *barriers*

Simulated annealing



Gradient-based minimization fails
(trapping into local minima)

Ex: NP-complete problems

- Spin glass. N Ising spins on a lattice interacting with random exchange constants: find the ground state.
- Traveling Salesman. Given N towns, find the shortest route to visit them all.
- k-SAT (satisfiability). Search for a binary N-bit string which satisfies M constraints, each involving k given bits.
- Lennard-Jones clusters. Find minimal energy configuration of a cluster of N LJ particles

Ising spin glass

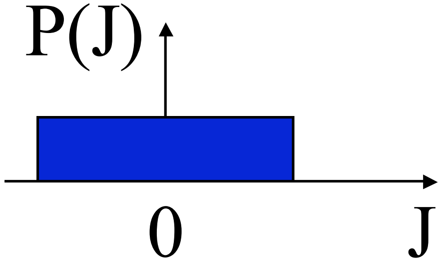
- N Ising spins $\sigma_i^z = \pm 1 \longleftarrow 2^N$ configurations

$$H = -\sum_{ij} J_{ij}\sigma_i^z\sigma_j^z$$

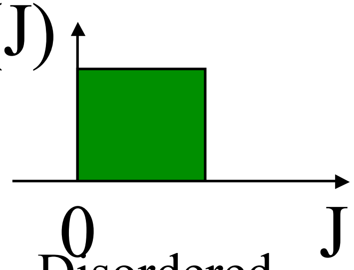
$J_{ij} > 0$ Ferro

$J_{ij} < 0$ Antiferro

Random J_{ij}

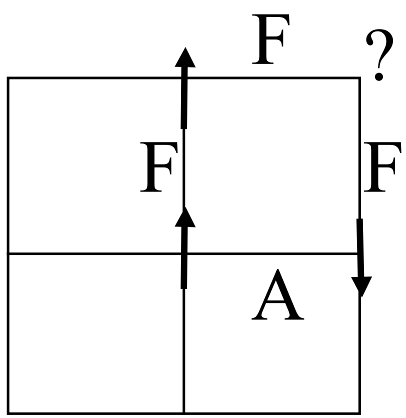


Spin Glass



Disordered Ferromagnet

Disorder $\Rightarrow$ Frustration



An Ising ferro-glass: $LiHo_{1-x}Y_xF_4$

See T.Rosenbaum, J.Phys.:Cond. Mat. 8, 9759 (96)

$LiHoF_4$ An insulating S=1/2 (due to Ho) Ising dipolar-coupled ferromagnet with Tc=1.53K

- Doping with Y (non magnetic) introduces disorder in the couplings J_{ij}
- One can apply a magnetic field $H_\perp$ perpendicular to the Ising easy axis (z)
- ⇨ experimental realization of Ising glass in transverse field

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

can be changed by changing $H_\perp$

tunable quantum disordering term

Basic Idea of Quantum Annealing

(Quantum Adiabatic Evolution)

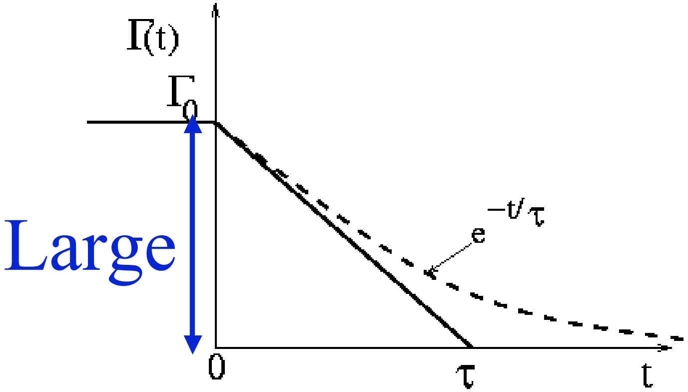
- Schrödinger evolution

$$i\hbar\frac{d}{dt}\Psi(t) = [H_{class} + \Gamma(t) H_{kin}]\Psi(t)$$

$$H_{class} = -\sum_{ij} J_{ij}\sigma_i^z\sigma_j^z \qquad H_{kin} = -\sum_i \sigma_i^x$$

$$\begin{cases} \sigma_i^x \equiv \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \\ \sigma_i^x \left|\uparrow\right\rangle_i \equiv \left|\downarrow\right\rangle_i \end{cases}$$

$$GS \equiv \prod_i^N \left(\left|\uparrow\right\rangle_i + \left|\downarrow\right\rangle_i \right)$$



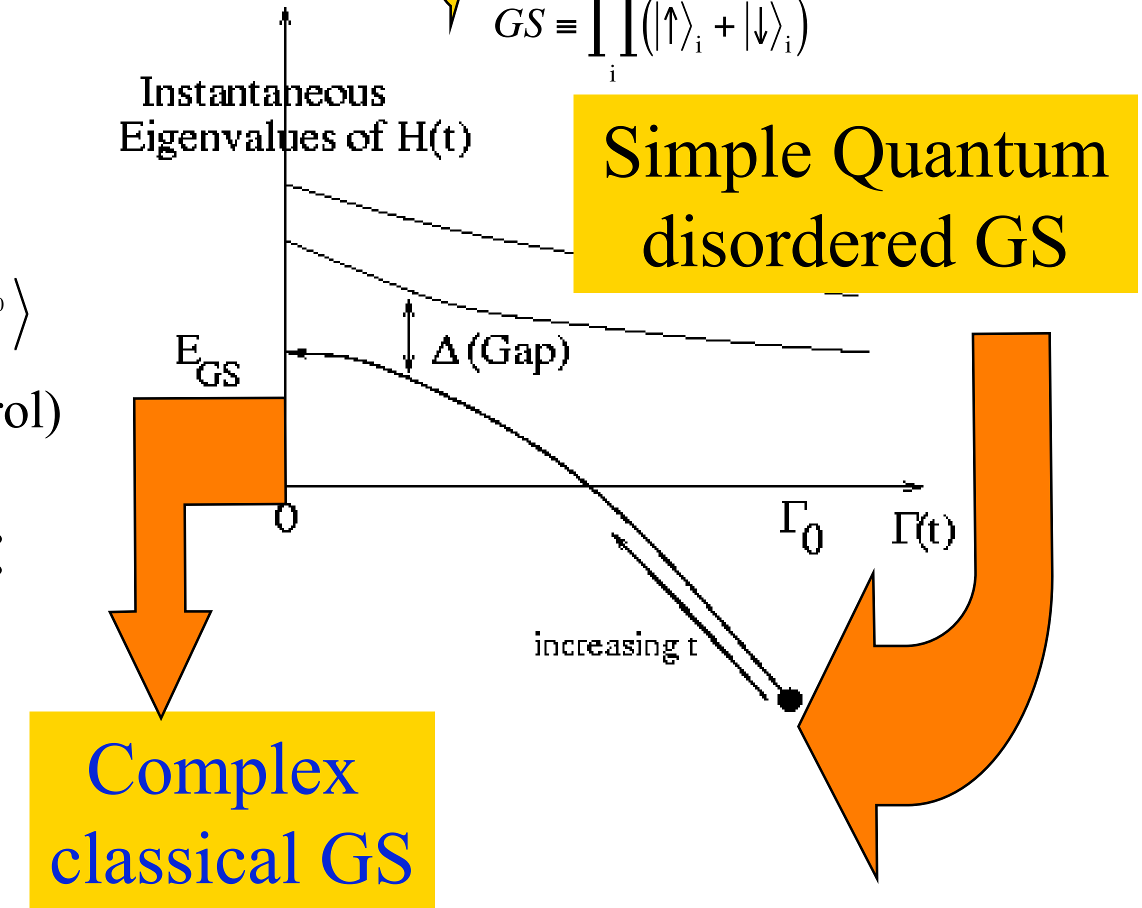
- Start from $\Psi(t=0) = \left|\Psi_{GS}^{\Gamma=\Gamma_0}\right\rangle$

(Assumed known or under control)

IF *adiabaticity* holds:

$$\Psi(t) \approx \left|\Psi_{GS}^{\Gamma=\Gamma(t)}\right\rangle$$

Very fast convergence!



Quantum Computing?

Adiabatic Quantum Computation is Equivalent to Standard Quantum Computation

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December 21, 2005

No recipe to construct, *in general*

H_{in} and H_{fin}

Schor's algorithm for **integer factorization** can be in principle expressed as an **AQC**:

$$H(t) = \left(1 - \frac{t}{\tau}\right) H_{in} + \left(\frac{t}{\tau}\right) H_{fin}$$

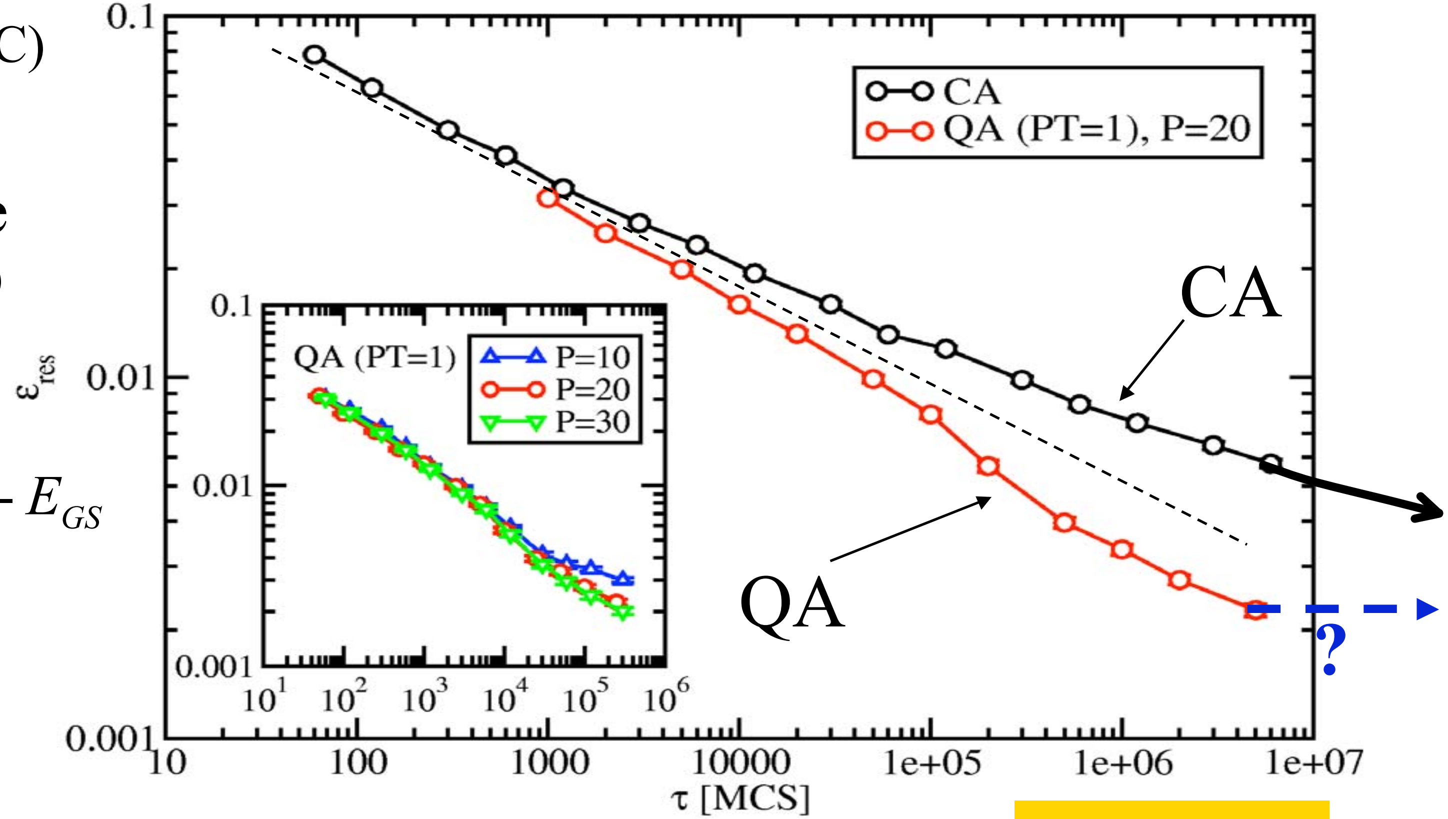
PIMC simulations (2D Ising)

SCIENCE 295, 2427 (2002).

(Path-Integral MC)

80x80 sample
(fixed couplings)

$$\varepsilon_{res}(\tau) \equiv \overline{E_{fin}(\tau)} - E_{GS}$$



Large τ behaviour ? Power-law or log ?

LOG !

12 hours against 14 years

PIMC on 3-SAT

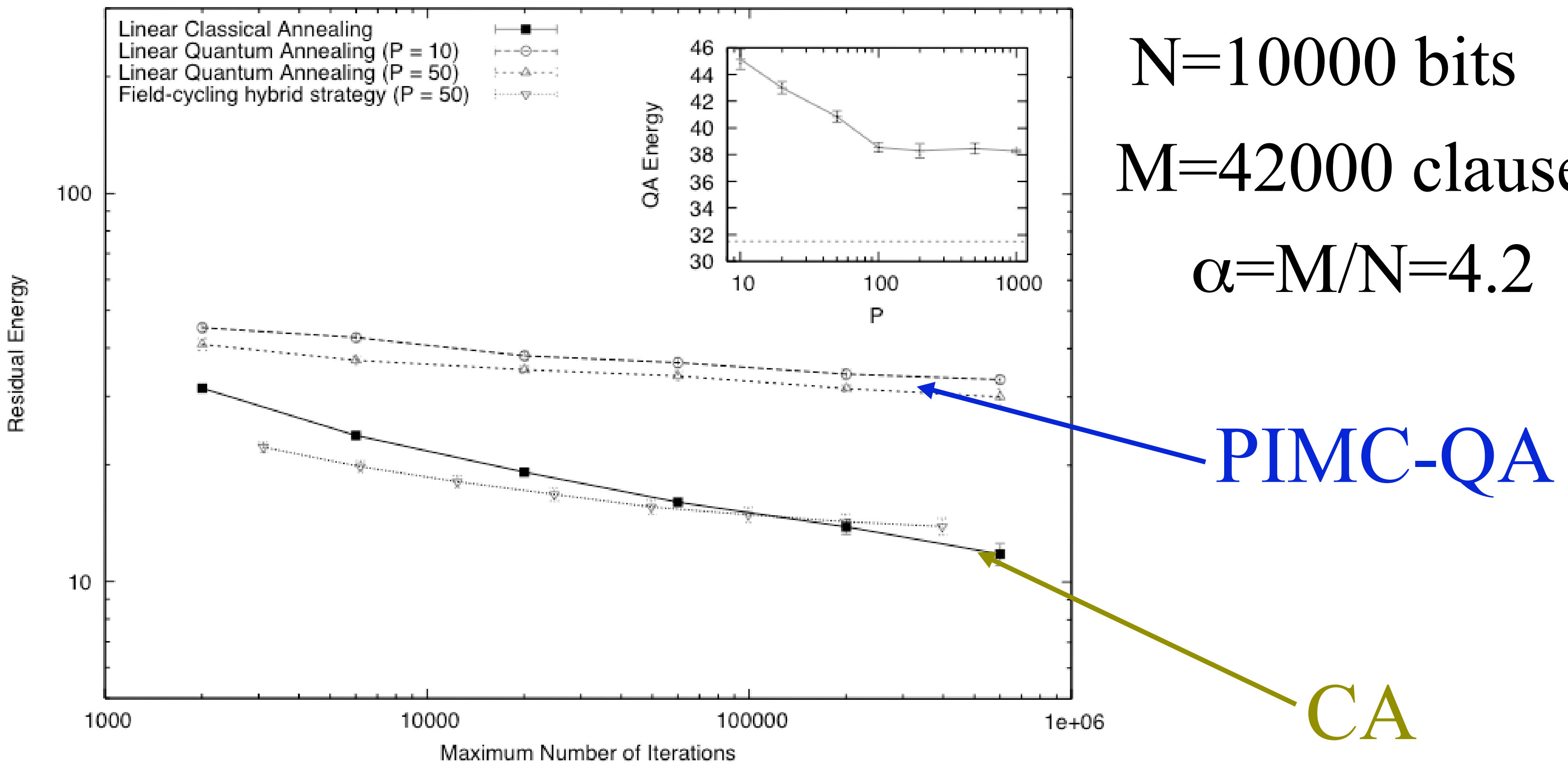
PRE **71**, 066707 (2005); cond-mat/0502468

Very Hard instance

N=10000 bits

M=42000 clauses

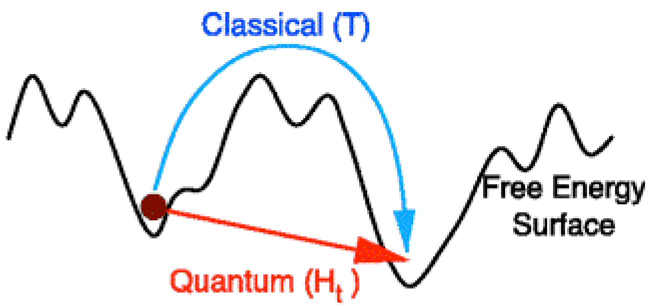
α=M/N=4.2



QA has a worse "slope"!

Questions

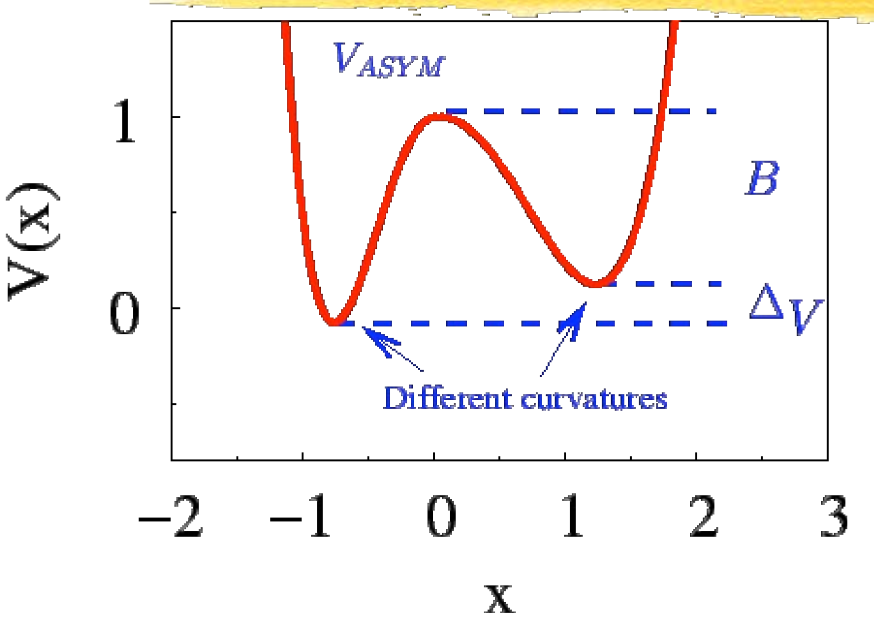
- When is Quantum Mechanics (QM) more effective than Simulated Annealing?



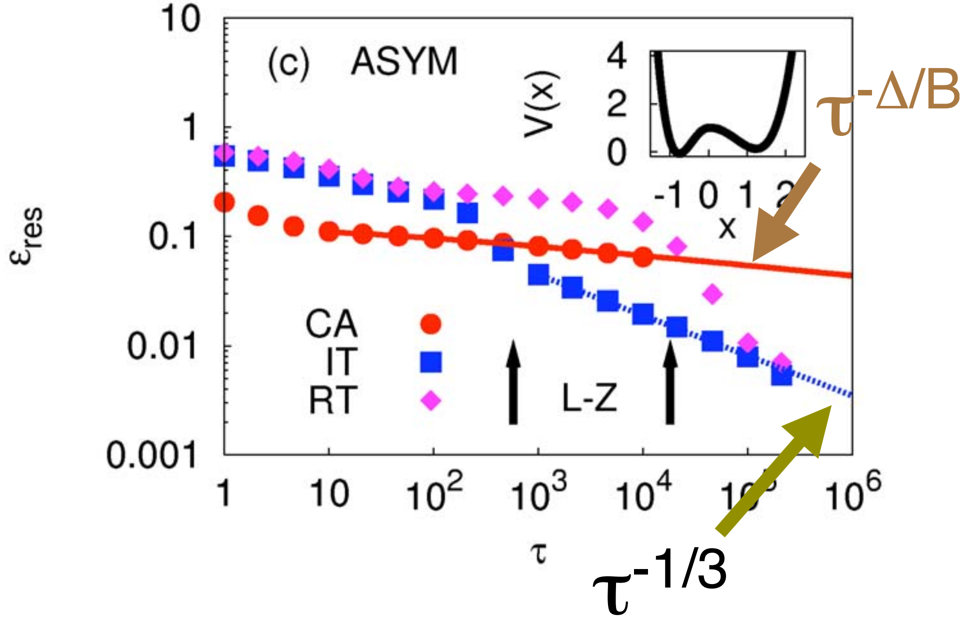
- Can QM generally solve NP-complete problems?

Double Well Potential

PRB **72**, 014303 (2005); cond-mat/0502129



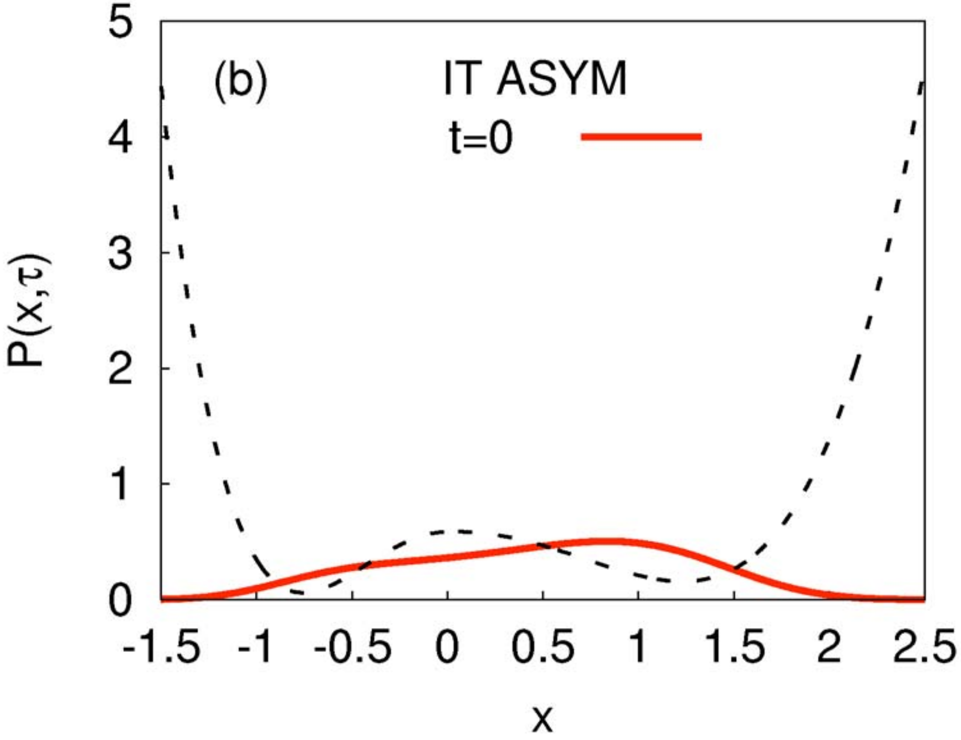
$$\epsilon_{res}(\tau) = \langle V(\tau)\rangle - V_{min}$$

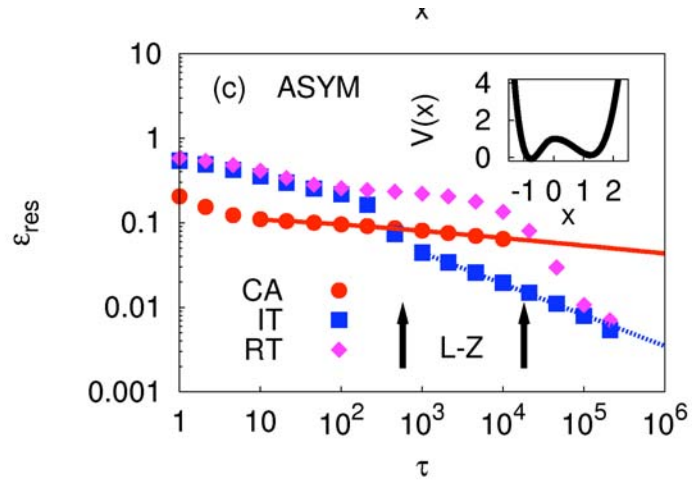


$$V(x) = \begin{cases} V_0 \frac{(x^2 - a_+^2)^2}{a_+^4} + \delta\, x & \text{for } x \geq 0 \\ V_0 \frac{(x^2 - a_-^2)^2}{a_-^4} + \delta\, x & \text{for } x < 0 \end{cases}$$

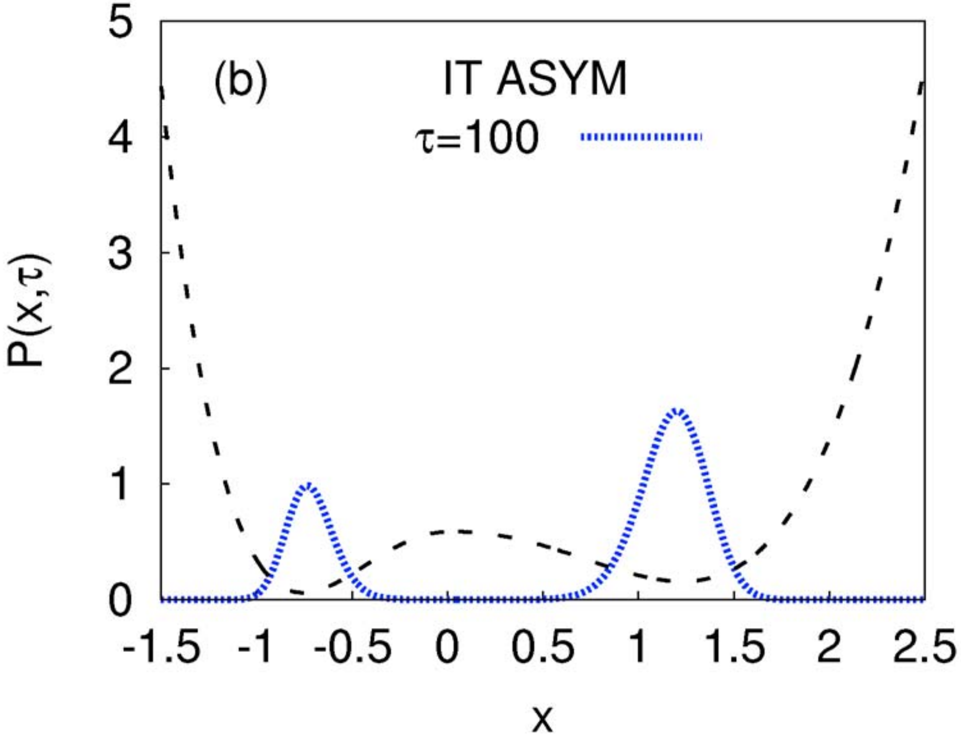
Huse & Fusher PRL **57**, 2203

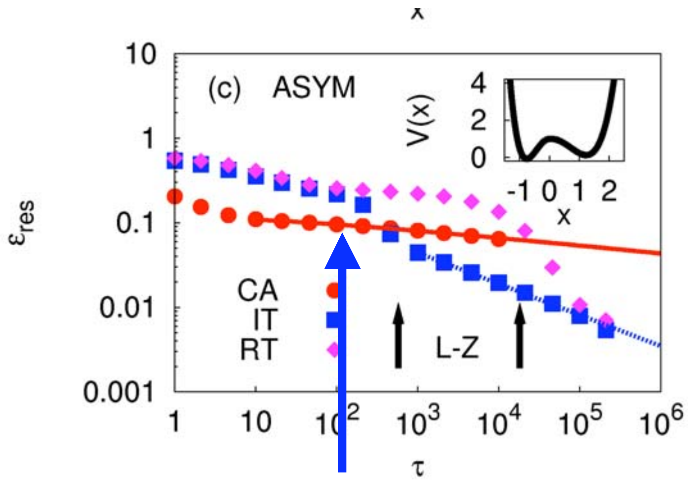
Schrödinger QA



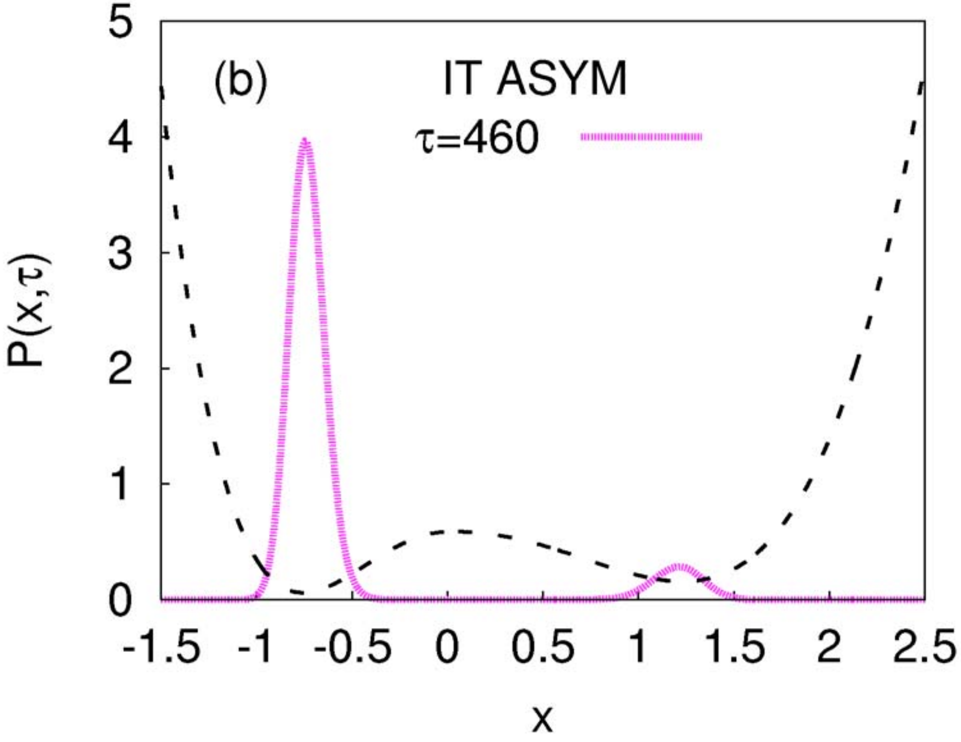


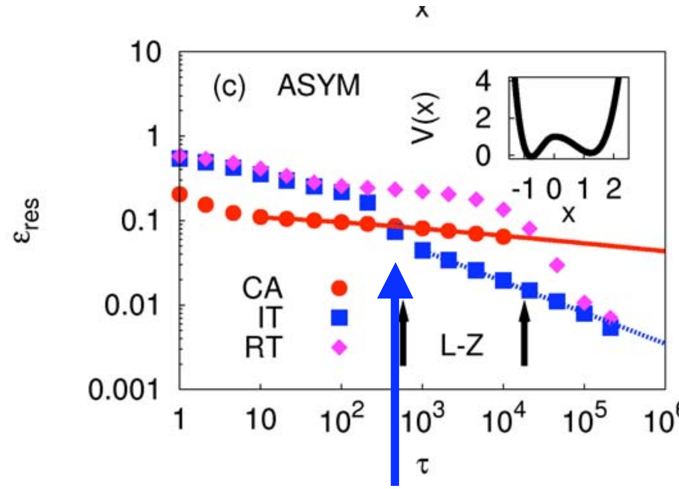
Schrödinger QA



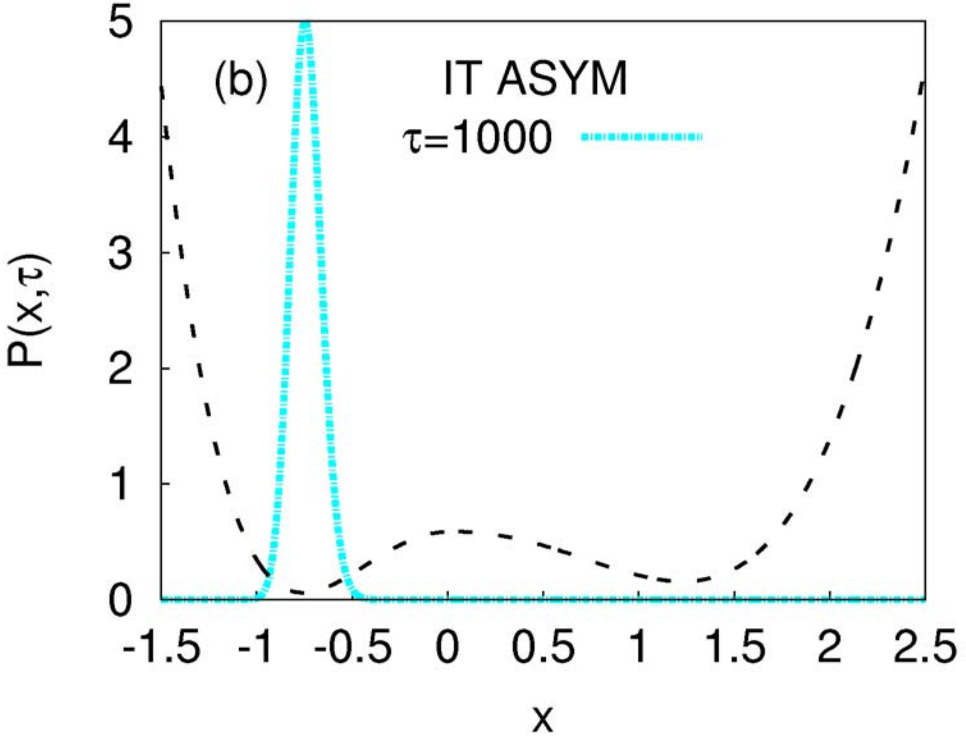


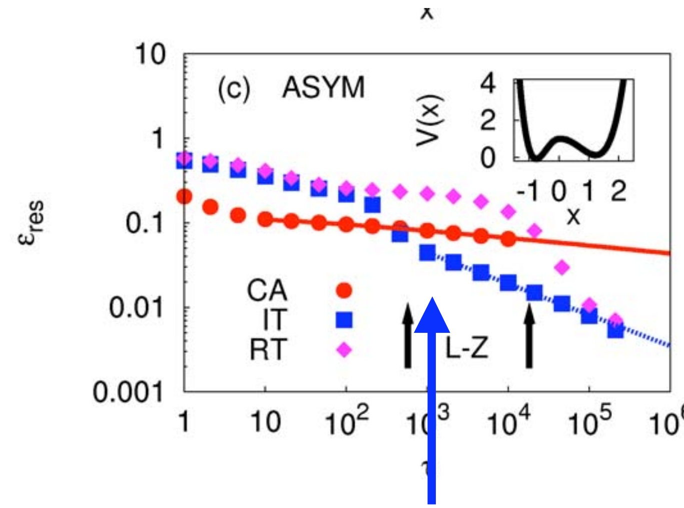
Schrödinger QA



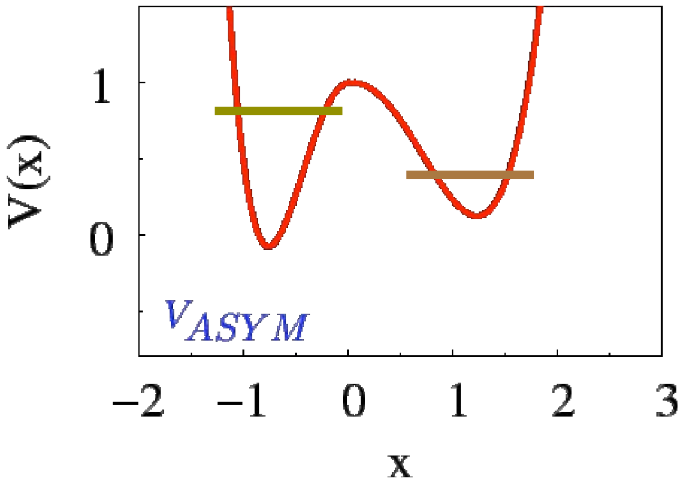


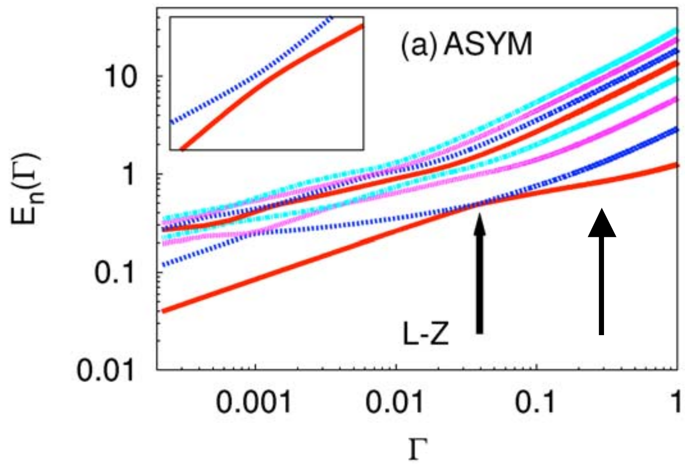
Schrödinger QA



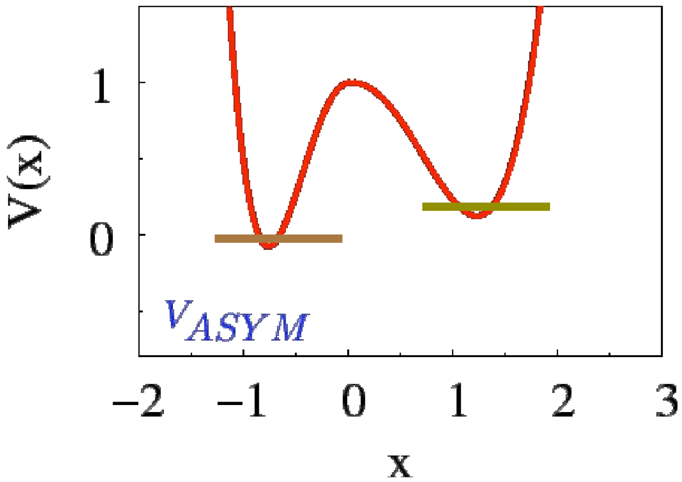


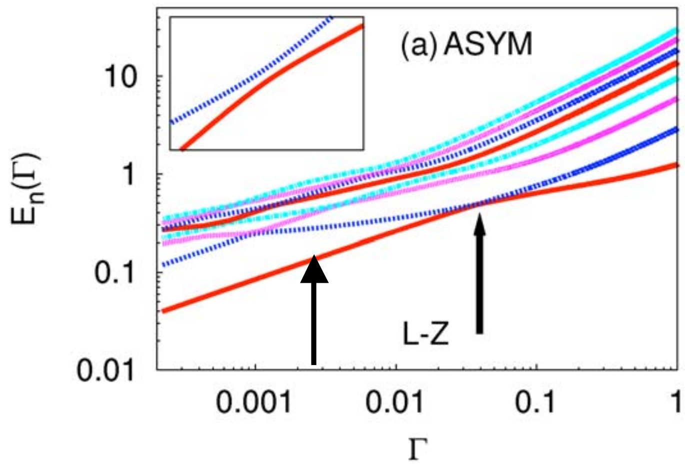
Instantaneous Spectrum



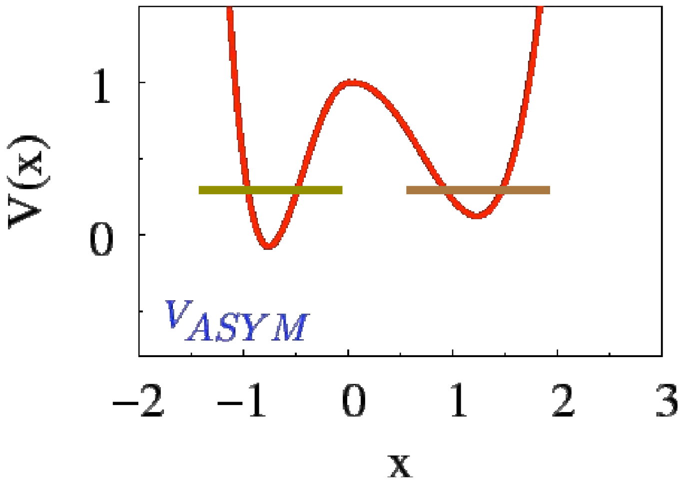


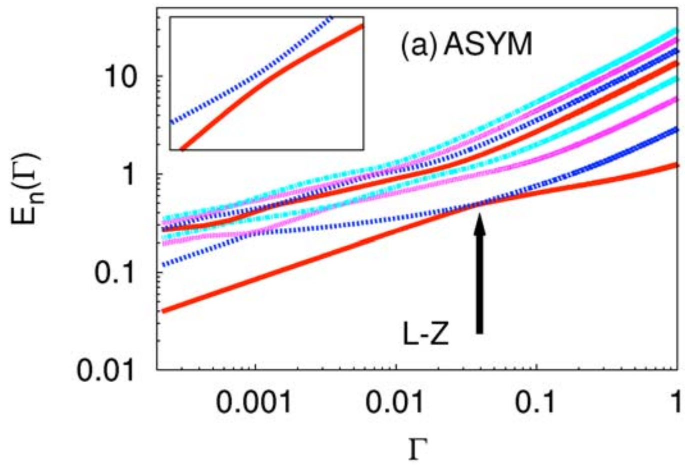
Instantaneous Spectrum



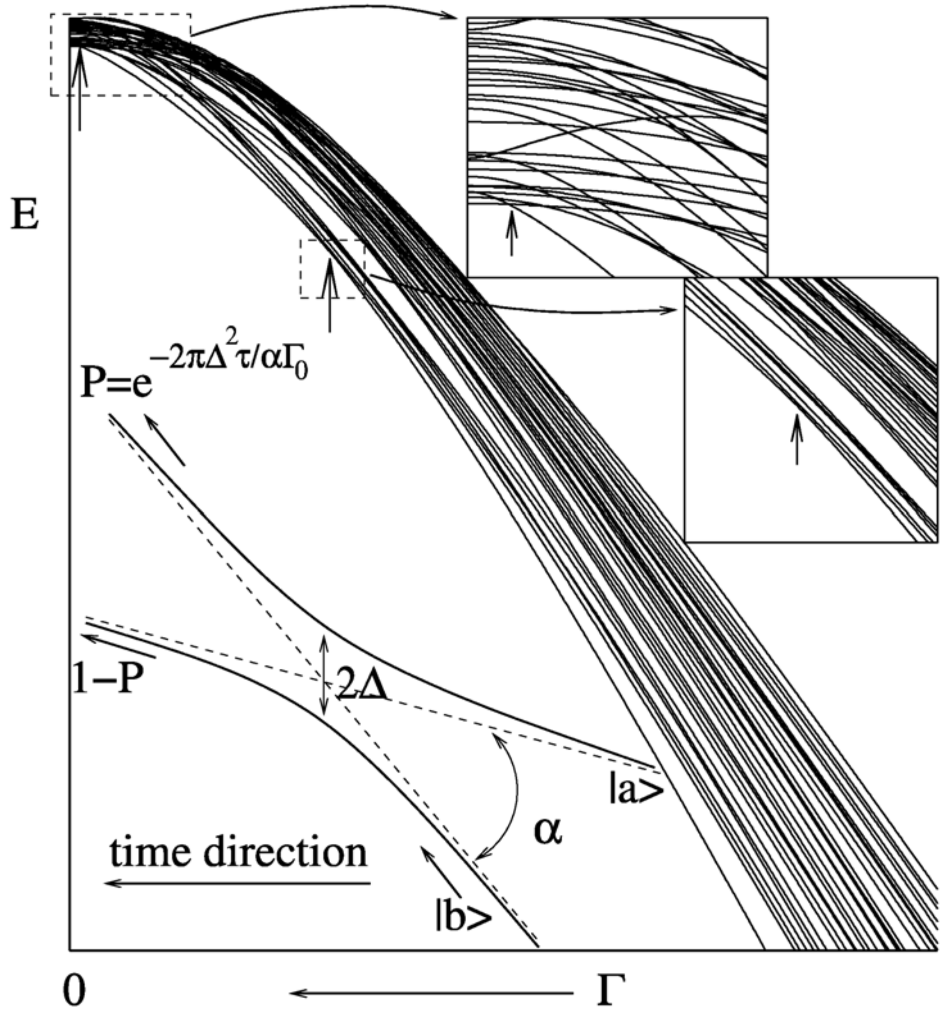


Instantaneous Spectrum





Landau-Zener tunneling



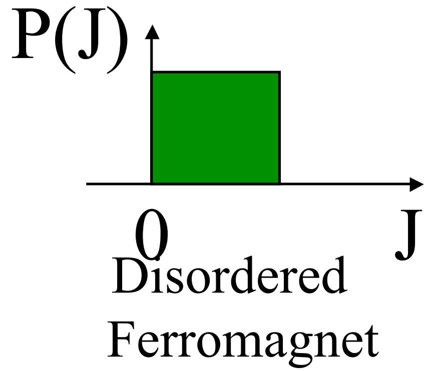
$$P_{ex} = e^{-\frac{\tau}{\tau_{LZ}}}$$

$$\tau_{LZ} \propto \frac{\Gamma_0}{4\Delta^2}$$

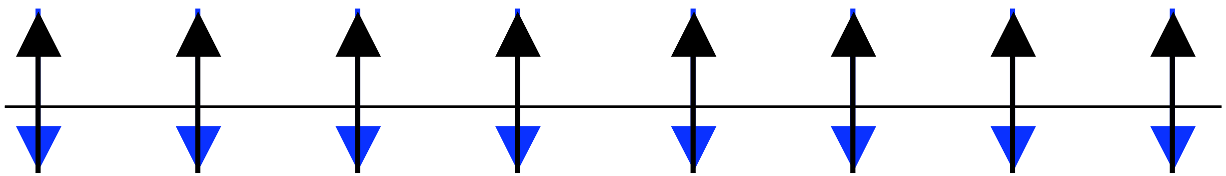
Science **295,** 2427 (2002)

Random Ising Chain (1D)

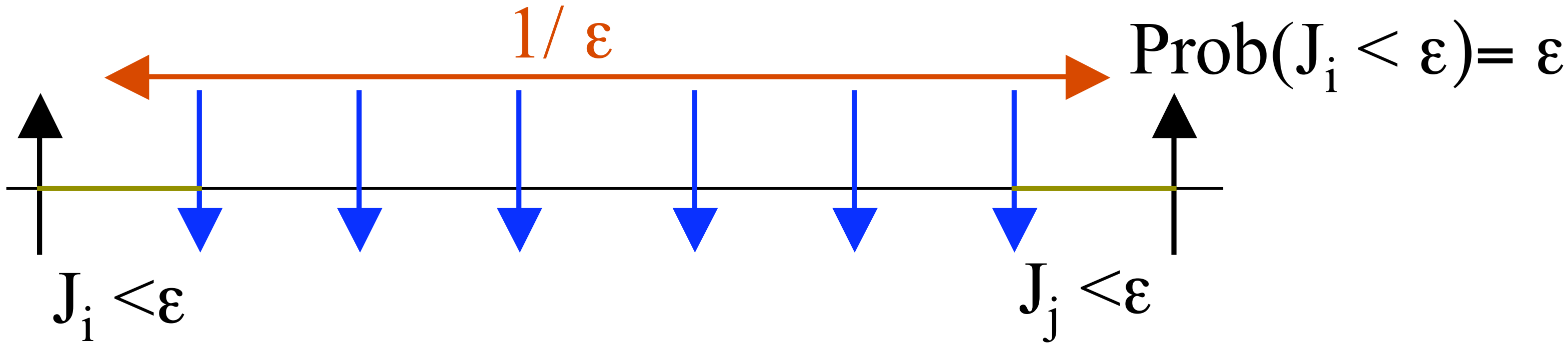
$$H = -\sum_i J_i \sigma_i^z \sigma_{i+1}^z$$



- GS is trivial: ferromagnetic state with all spin up (down)

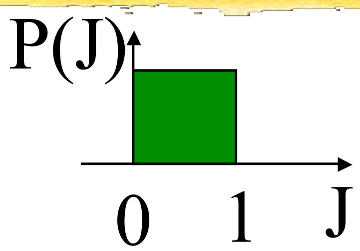


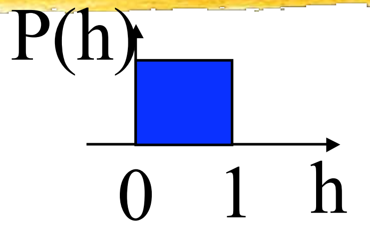
- Low energy defects (**domain walls** pinned at smallest J_i)



Random Ising Chain in Transverse Field

(Work in progress with T. Caneva and R. Fazio)

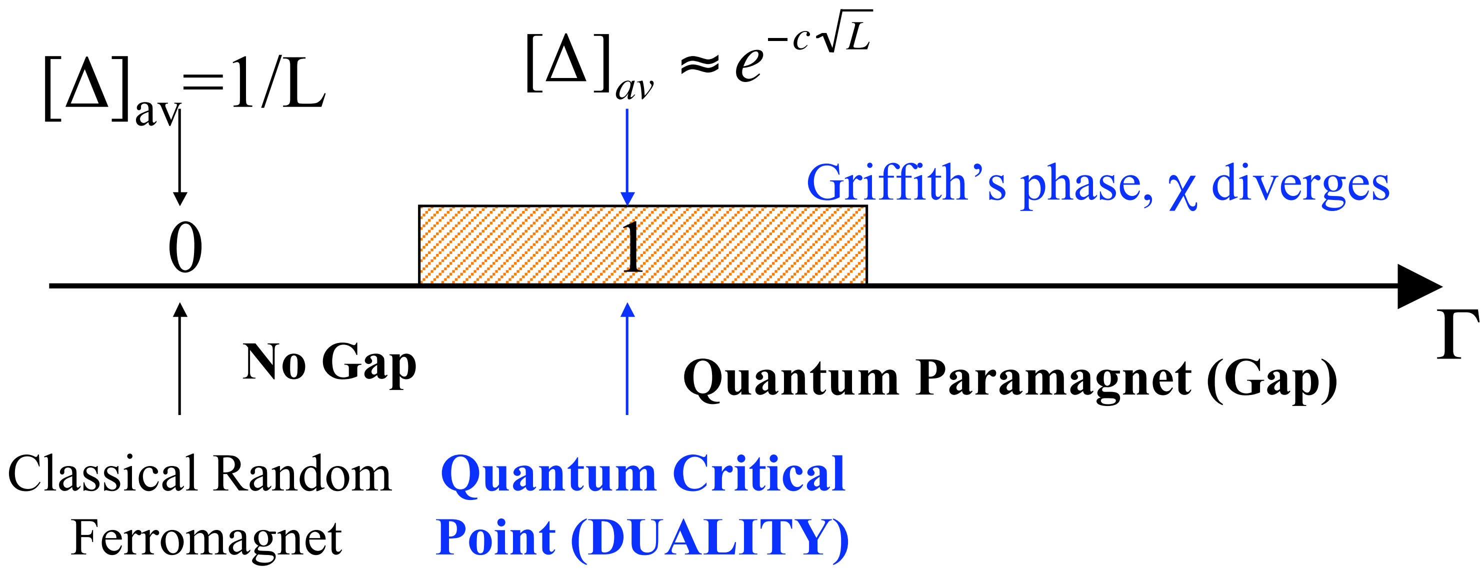




$$H = -\sum_i J_i \sigma_i^z \sigma_{i+1}^z - \Gamma \sum_i h_i \sigma_i^x$$

Statics: Phase diagram

D. Fisher, PRB 51, 6411 (95)

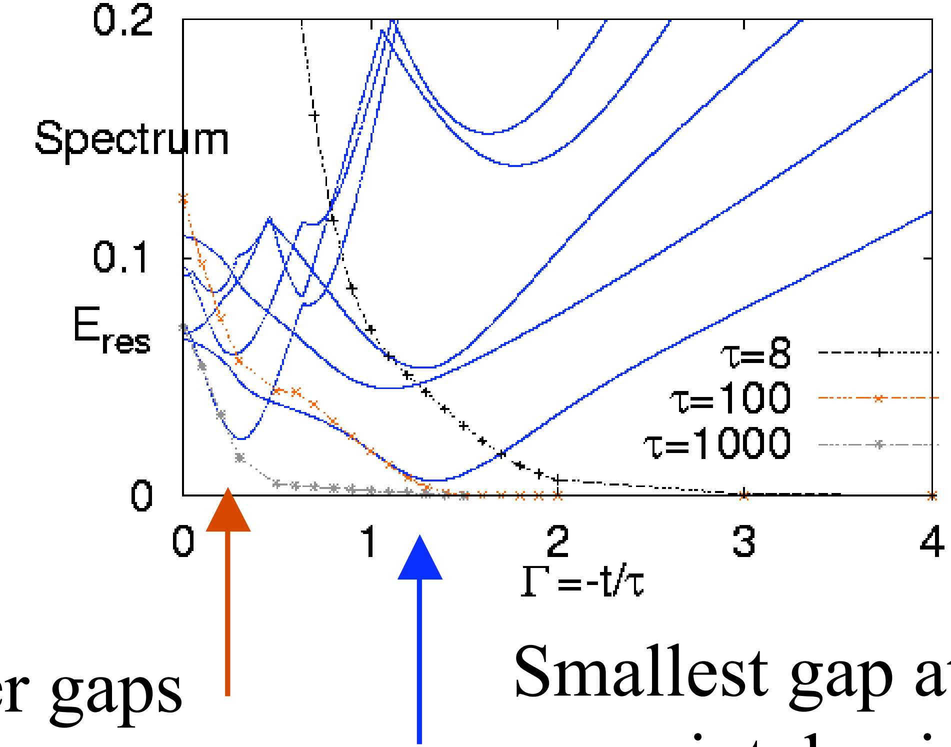


Gaps and QA Schroedinger evolution

Random Ising Chain: Instance with L=32

$$H(t) = -\sum_i J_i \sigma_i^z \sigma_{i+1}^z - \Gamma(t) \sum_i h_i \sigma_i^x$$

(Time-dependent Bogoliubov-de Gennes)



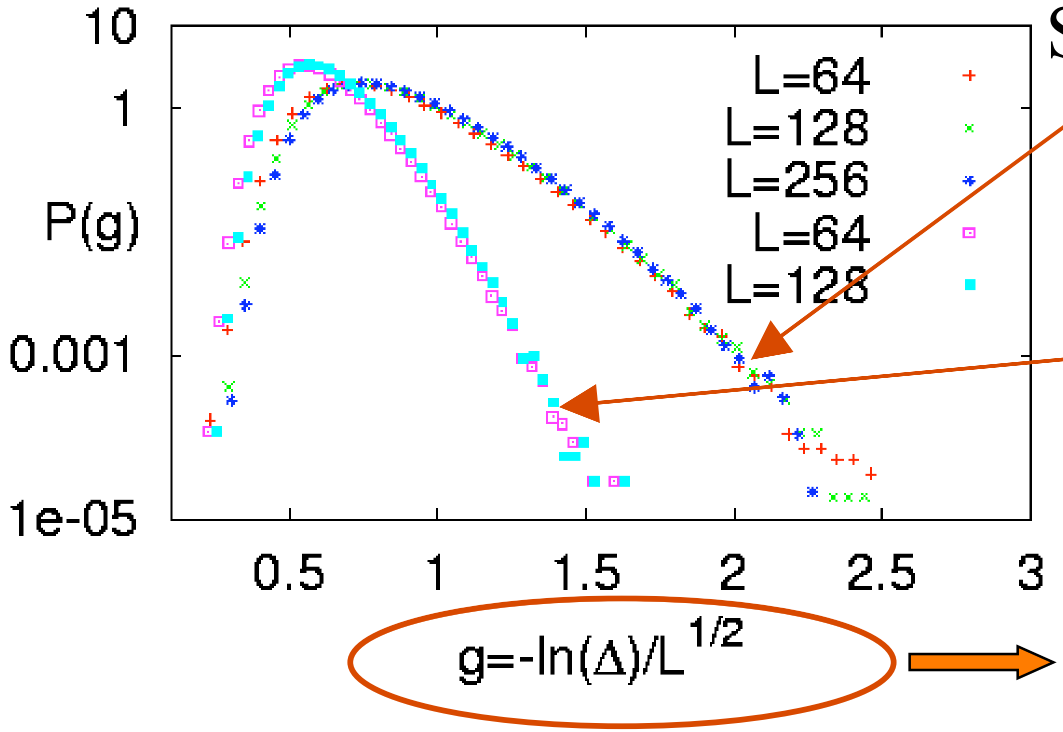
…but higher gaps not irrelevant

Smallest gap at critical point dominates

Gaps distributions

(Bogoliubov diagonalizations)

At critical point Γ=1, universal scaling of gaps



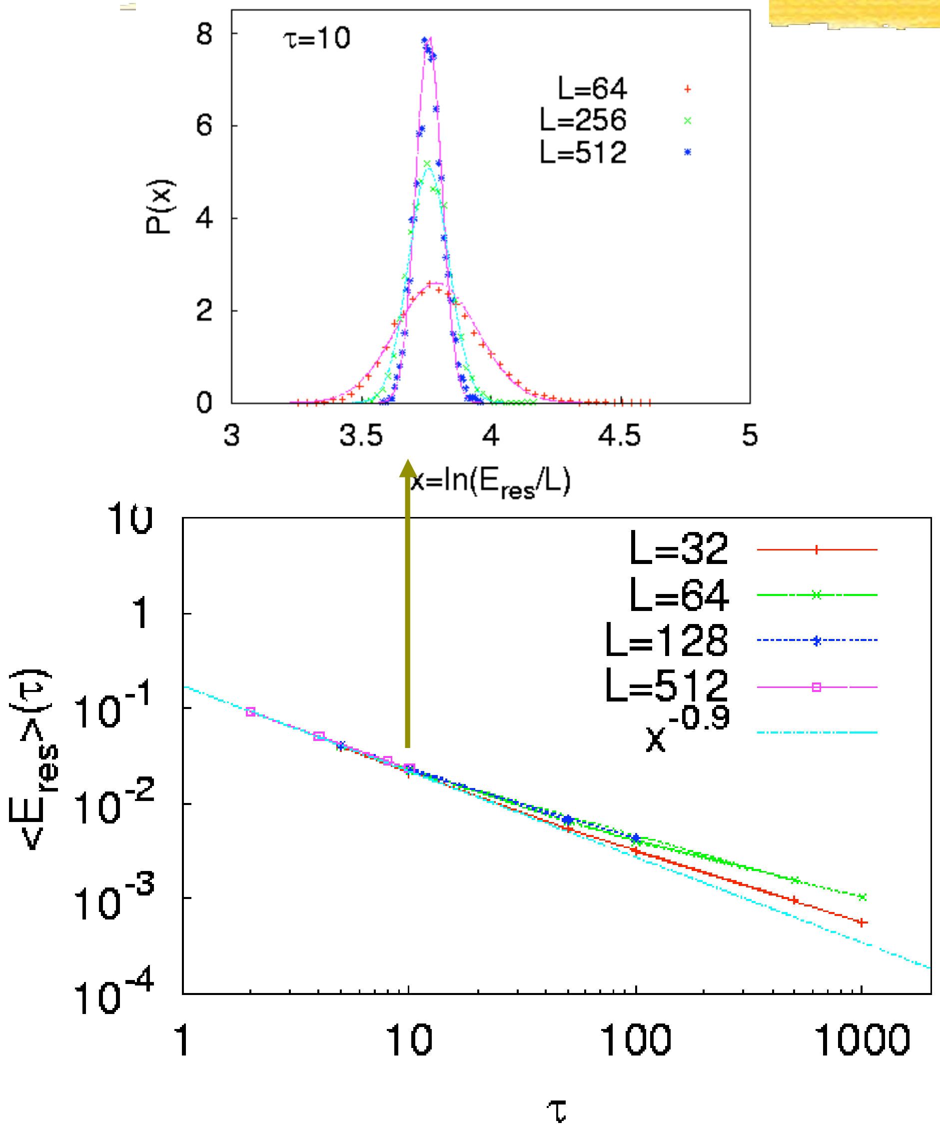
Smallest gap seen by the dynamics

Next eigenvalue

$$\Delta \approx e^{-g\sqrt{L}}$$

The two sets of gap distributions tend to overlap!

Residual energy



$$\tau_{LZ} \propto \frac{\Gamma_0}{4\Delta^2}$$

$$\Delta \approx e^{-g\sqrt{L}}$$

$$\tau_{LZ} \propto e^{C\sqrt{L}}$$

$$\left[E_{res}\right]_{av} \propto [\log(\tau)]^{-\zeta}$$

Quantum Computing?

- Schor's factorization: an NP problem (**not NP-complete**!) becomes Quantum-Polynomial. But it is a problem **without disorder**, equivalent to finding the **period of a function** where QM excels…

- Probably the question of P/NP has nothing to do with the physics of annealing (quantum adiabatic evolution): even polynomial problems can be **hard** for QA-AQC if **disorder is present**!

- Good candidate: 1D Random Ising Chain

Coworkers and References

Roman Martonák (ETH Zürich, and FEI-Bratislava)
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References:

SCIENCE 295, 2427 (2002).
PRB **66**, 094203 (2002).
PRE **70**, 057701 (2004).
PRB **72**, 014303 (2005); cond-mat/0502129.
PRE **71**, 066707 (2005); cond-mat/0502468.
PRB **73**, 144302 (2006); cond-mat/0512064.
Review: J Phys A (in press).