Imaginary time quantum annealing using quantum Monte Carlo

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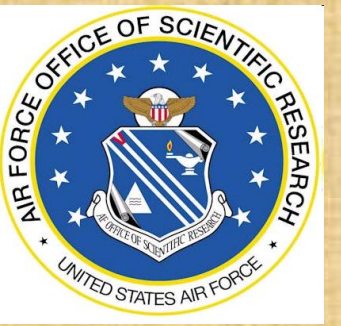


Outline

1. *Non-adiabatic response in real and imaginary times.*
2. *Kibble-Zurek mechanism and universal dynamics near continuous phase transitions.*
3. *Application to spin glass transitions: Quantum annealing vs. Simulated annealing.*
4. *Dynamical localization transition near critical points.*

Non-adiabatic response in real and imaginary time dynamics

Consider an arbitrary unitary transformation of the wave function

$$|\psi(\vec{\lambda})\rangle = U^{\dagger}(\vec{\lambda})|\Psi\rangle$$

Infinitesimal transformations are like the Schrödinger equation

$$i\hbar\partial_{\lambda_\alpha}|\psi(\vec{\lambda})\rangle = -\mathcal{A}_\alpha|\psi\rangle,\ \mathcal{A}_\alpha = i\hbar U^{\dagger}\partial_{\lambda_\alpha}U,\ \mathcal{A}_\alpha^{\dagger} = \mathcal{A}_\alpha$$

Hamiltonian equations of motion in a moving frame

$$i\partial_t|\psi\rangle = (U^{\dagger}HU - \dot{\lambda}_a\mathcal{A}_a)|\psi\rangle$$

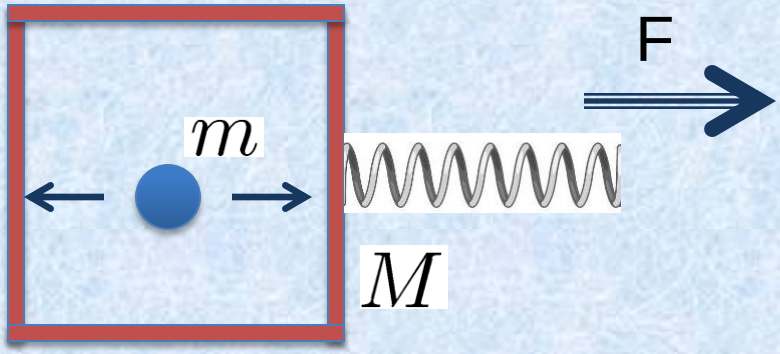
Special instantaneous frame, where U diagonalizes the instantaneous Hamiltonian. Convenient near the adiabatic limit

$$|\psi\rangle = |\psi_0(\vec{\lambda})\rangle \ \Rightarrow\ A_\alpha = \langle\mathcal{A}_\alpha\rangle$$

Berry connection is the expectation value of the gauge potential

First order perturbation theory

$$a_n \approx -\dot{\lambda}\frac{\langle n|\mathcal{A}_\lambda|0\rangle}{\mathcal{E}_n-\mathcal{E}_0} = -i\dot{\lambda}\frac{\langle n|\partial_\lambda H|0\rangle}{(\mathcal{E}_n-\mathcal{E}_0)^2}$$



$$H = \frac{p^2}{2m} + V(x - X_0(t))$$

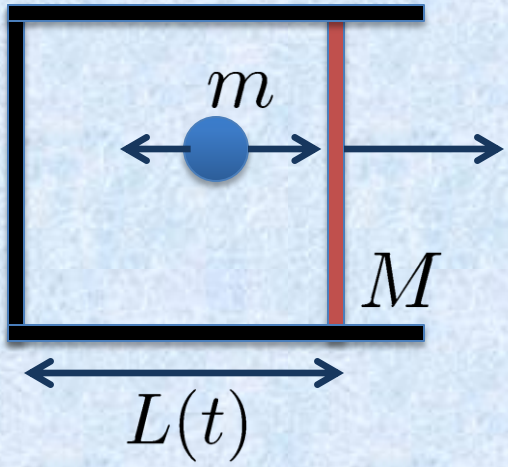
$$U = \exp\left[-\frac{i}{\hbar}pX_0(t)\right]$$

$$\tilde{H} = U^\dagger H U - \dot{X}_0\mathcal{A}_{X_0} = H - \dot{X}_0 p$$

Compute leading correction to the energy due to the Galilean term

$$\Delta E_1 = \langle 0| - \dot{X}_0 p|0\rangle = 0$$

$$\Delta E_2 = \sum_n (E_n - E_0)|a_n|^2 = \dot{X}_0^2 \sum_{n\neq 0} \frac{\langle 0|p|n\rangle\langle n|p|0\rangle}{E_n - E_0} = m\dot{X}_0^2 \frac{8}{\pi^2}\sum_{n=1}^{\infty}\frac{16n^2}{(4n^2-1)^3} = \frac{m\dot{X}_0^2}{2}$$



$$\phi_n(x) = \sqrt{\frac{2}{L}} \sin \frac{\pi n x}{L}$$

$$\partial_L \phi_n(x) = -\frac{1}{2L}\phi_n(x) - \sqrt{\frac{2}{L}} \frac{\pi n x}{L^2} \cos \frac{\pi n x}{L} = \mathcal{D}\phi_n(x)$$

$$\mathcal{D} = \frac{px + xp}{2L}$$

Dilation operator

Moving frame

$$\tilde{H} = U^\dagger H U - \dot{X}_0 \mathcal{A}_{X_0} = \frac{p^2}{2mL^2(t)} - \dot{L}\mathcal{D}$$

Can absorb L^2 into time dilatation:

$$dt = L^2 d\tau, \quad H \to L^2 H$$

Leading non-adiabatic correction.

$$\Delta E_2 = \dot{L}^2 \sum_{m \neq n} \frac{\langle n|\mathcal{D}|m\rangle\langle m|\mathcal{D}|n\rangle}{E_m - E_n} = m\dot{L}^2 \frac{16}{\pi^2} \sum_{m \neq m} \frac{n^2 m^2}{(m^2 - n^2)^3} = \frac{m\dot{X}_0^2}{2}\left(\frac{1}{3} - \frac{1}{2\pi^2 n^2}\right)$$

Recover “quantum” dilatation mass: the classical result plus an additional quantum correction.

Leading corrections to generalize forces (beyond Born-Oppenheimer approximation)

$$M_\mu \approx -\langle 0|\partial_\mu H|0\rangle - \sum_n{}' \left(a_n^* \langle n|\partial_\mu H|0\rangle + a_n \langle 0|\partial_\mu H|n\rangle\right)$$

$$M_\mu = M_\mu^0 + i\dot{\lambda}(\chi_{\mu\lambda} - \chi_{\lambda\mu}) = M_\mu^0 + F_{\mu\lambda}\dot{\lambda}$$

$$\chi_{\lambda\mu} = \sum_{n\neq 0} \frac{\langle 0|\partial_\lambda \mathcal{H}|n\rangle\langle n|\partial_\mu \mathcal{H}|0\rangle}{(\mathcal{E}_n - \mathcal{E}_0)^2} = \langle 0|\mathcal{A}_\lambda \mathcal{A}_\mu|0\rangle_c$$

$$i(\chi_{\mu\lambda} - \chi_{\lambda\mu}) = i\langle 0|[\mathcal{A}_\mu, \mathcal{A}_\lambda]|0\rangle = \partial_\mu A_\lambda - \partial_\lambda A_\mu = F_{\mu\lambda}$$

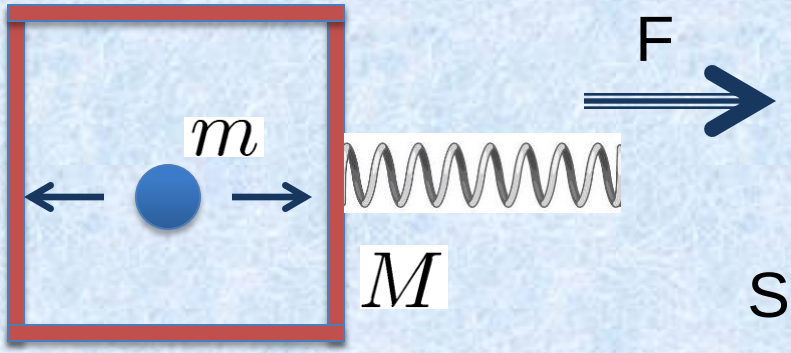
Leading non-adiabatic corrections give the Berry curvature for generalized forces and mass tensor for the energy (metric tensor for energy fluctuations).

Repeat similar analysis for imaginary time dynamics

Imaginary time Schrödinger equation in a moving frame

$$\tilde{\partial}_\tau |\psi\rangle = -\left(\mathcal{H}(\tau) - i\dot{\lambda}\mathcal{A}_\lambda\right)|\psi\rangle,$$

$$a_n \approx i\dot{\lambda}\frac{\langle n|\mathcal{A}_\lambda|0\rangle}{\mathcal{E}_n - \mathcal{E}_0} = -\dot{\lambda}\frac{\langle n|\partial_\lambda H|0\rangle}{(\mathcal{E}_n - \mathcal{E}_0)^2}$$



$$\Delta E_2 = \sum_n (E_n - E_0)|a_n|^2 = \frac{m\dot{X}_0^2}{2}$$

Same expression as in the real time

$$M_\mu = M_\mu^0 + v_\lambda(\chi_{\mu\lambda} + \chi_{\lambda\mu}) = M_\mu^0 + 2g_{\mu\nu}v_\nu$$

Similar analysis applies to classical Markov systems

$$\partial_t P = M(z(t))P$$

L. D'Alessio, Y. Kafri, A.P. 2015

Generalized Kubo response (imaginary time) and the metric tensor.

$$M_\mu \approx 2 g_{\mu\lambda} v_\lambda$$

Real time $\delta E^2 \approx v_\mu g_{\mu\lambda} v_\lambda$

Hamiltonian: $\mathcal{H} = \mathcal{H}(\vec{\lambda})$. Ground state wave-function: $\psi_0 = \psi_0(\vec{\lambda})$.

Consider the following change $\vec{\lambda} \to \vec{\lambda} + \delta\vec{\lambda}$

$$||\psi_0(\vec{\lambda}) - \psi_0(\vec{\lambda} + \delta\vec{\lambda})||^2 \approx 1 - |\langle \psi_0(\vec{\lambda}) | \psi_0(\vec{\lambda} + \delta\vec{\lambda}) \rangle|^2 = g_{\alpha\beta} d\lambda_\alpha d\lambda_\beta$$

$\chi_{\alpha\beta}$ - geometric tensor (Provost, Vallee, 1980; Venuti Zanardi, 2007)

$$\chi_{\alpha\beta} = \langle 0 | \overleftarrow{\partial_\alpha} \partial_\beta | 0 \rangle_c = \langle \mathcal{A}_\alpha \mathcal{A}_\beta \rangle_c, \; g_{\alpha\beta} = \Re[\chi_{\alpha\beta}]$$

g is the metric tensor, characterizes the Riemann manifold of ground statates (density matrices).

Metric tensor can be extracted from response of physical observables in the imaginary time dynamics.

Analytic structure of the non-adiabatic response

$$i\frac{da_n}{d\lambda}\dot{\lambda}+i\dot{\lambda}\sum_m a_m\langle n|d_\lambda|m\rangle=\mathcal{E}_n a_n \;\Rightarrow\; \frac{da_n}{d\lambda}=i\sum_m a_m\mathcal{A}_{nm}+\frac{i\mathcal{E}_n}{v_\lambda}a_n$$

$$\frac{d\alpha_n}{d\lambda}\dot{\lambda}+\dot{\lambda}\sum_m \alpha_m\langle n|d_\lambda|m\rangle=-\mathcal{E}_n\alpha_n \;\Rightarrow\; \frac{d\alpha_n}{d\lambda}=i\sum_m \alpha_m\mathcal{A}_{nm}-\frac{\mathcal{E}_n}{v_\lambda}\alpha_n$$

Asymptotically (excluding LZ type nonanalytic corrections)

$$a_n(v_\lambda)=\alpha_n(iv_\lambda),\; a_n^*(v_\lambda)=\alpha_n^*(-iv_\lambda)$$

We can get real time result by analytic continuation in the complex velocity plane.

For observables need something else

$$\langle\mathcal{O}\rangle=\langle\psi(v)|\mathcal{O}|\psi(v)\rangle=\langle\psi(-iv)|\mathcal{O}|\psi(iv)\rangle$$

Use left and right expectation values in imaginary time.

$$\tilde{O}(v) = \langle \psi(-v) | \mathcal{O} | \psi(v) \rangle$$

Analytic continuation $v \to iv$ gives
the real time expectation value in all orders in v

$$O(v) = \tilde{O}(iv)$$

In particular, can extract the Berry curvature from the imaginary time dynamics (M. Kolodrubetz, 2013)

$$M_\mu \approx 2 v_\lambda g_{\lambda\mu}$$

$$M_\mu \approx v_\lambda F_{\lambda\mu}$$

$$\tilde{M}_\mu \approx -i v_\lambda F_{\lambda\mu}$$

Critical points: diverging susceptibilities. Scaling theory.

(Pokrovsky, Patashinski, 1963-1965, Kadanoff 1966)

Diverging correlation length

$$\xi = \frac{1}{|\lambda|^{\nu}},\ \lambda = (T - T_c), h - h_c, \ldots \text{ is the tuning parameter.}$$

Power law correlations (scale invariance) at the critical point

$$\langle m(x) m(x') \rangle \sim \frac{1}{|x - x'|^{2\alpha}}, \quad \dim[m(x)] = \alpha$$

Finite size scaling hypothesis close to the critical point

$$\langle m(x) \rangle = L^{-\alpha} f(L/\xi) = L^{-\alpha} f(L|\lambda|^{\nu}), \quad f \text{ is the scaling function}$$

$$\langle m(x) m(x') \rangle \sim \frac{1}{|x - x'|^{2\alpha}} \tilde{f}(|x - x'|/\xi)$$

Extend scaling theory to nonequilibrium – universal dynamics (both in real and imaginary time)

(C. De Grandi, A.P., A. Sandvik, 2011, Chandran et al. 2012, Kolodrubetz et. al. 2012)

$$\xi = |\lambda|^{-\nu} \Rightarrow \xi = \frac{1}{|\lambda|^{\frac{1}{\nu}}} \Rightarrow \dim[\lambda] = 1/\nu$$

$$t \sim \frac{1}{\xi^{-z}} \Rightarrow \dim[t] = -z$$

$$v = \frac{d\lambda}{dt} \Rightarrow \dim[v] = \frac{1}{\nu} + z = \frac{1+z\nu}{\nu} \Rightarrow \xi_v \sim \frac{1}{v^{\frac{\nu}{z\nu+1}}}$$

We can now use normal scaling theory using this new length scale

$$\boxed{M_\mu(\lambda) = L^{-\Delta_\mu} f(L/\xi_\lambda, L/\xi_v),\ \Delta_\mu = \dim[M_\mu]}$$

The shortest scale dominates. At the critical point

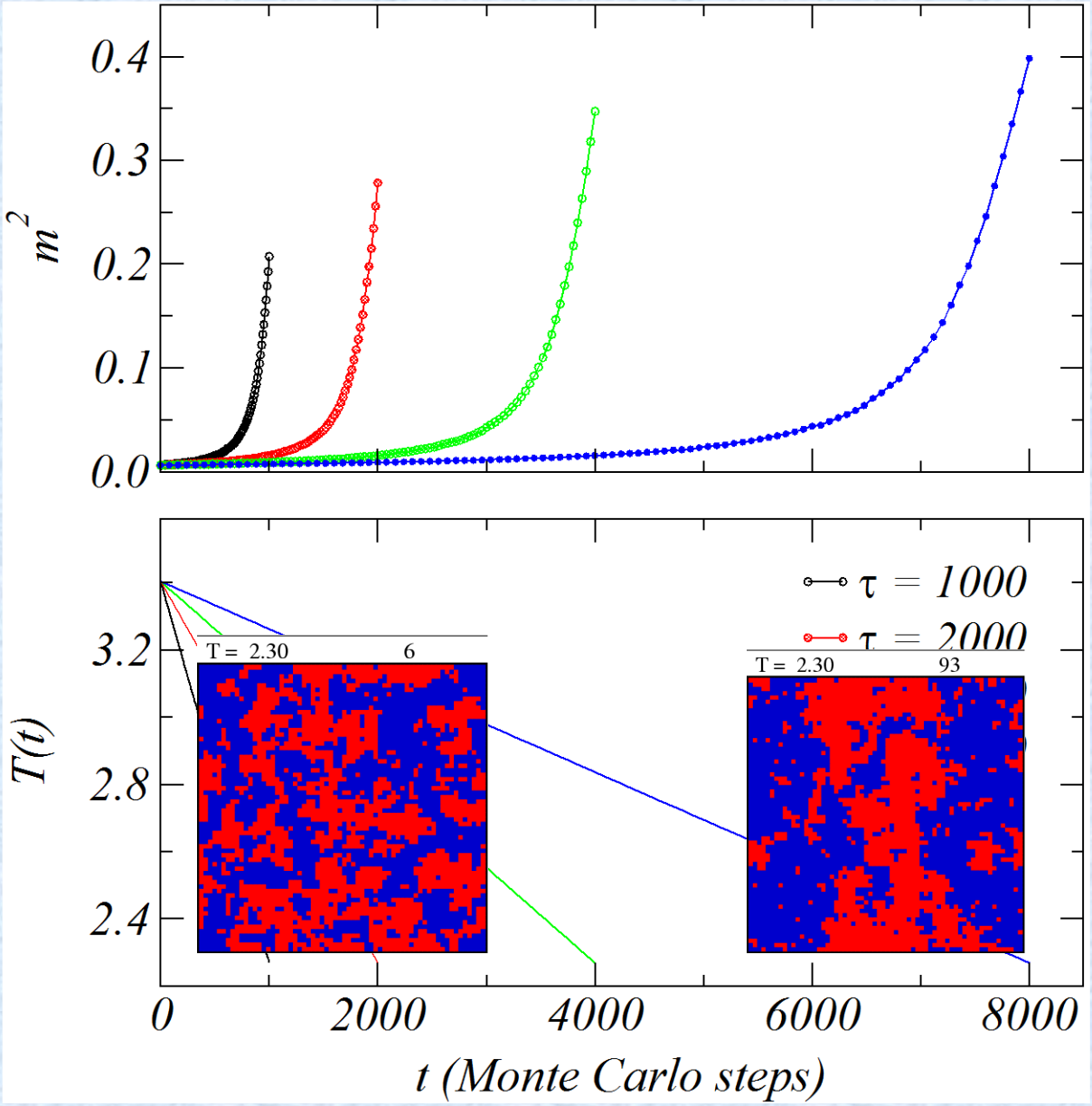
$$\xi_\lambda = \infty \Rightarrow M_\mu = L^{-\Delta_\mu} f(L/\xi_v)$$

If $M \sim L^d$ is extensive then

$$f(x) \sim x^{d+\Delta_\mu} \Rightarrow M_\mu \sim L^d v^{\frac{(d+\Delta_\mu)\nu}{z\nu+1}}$$

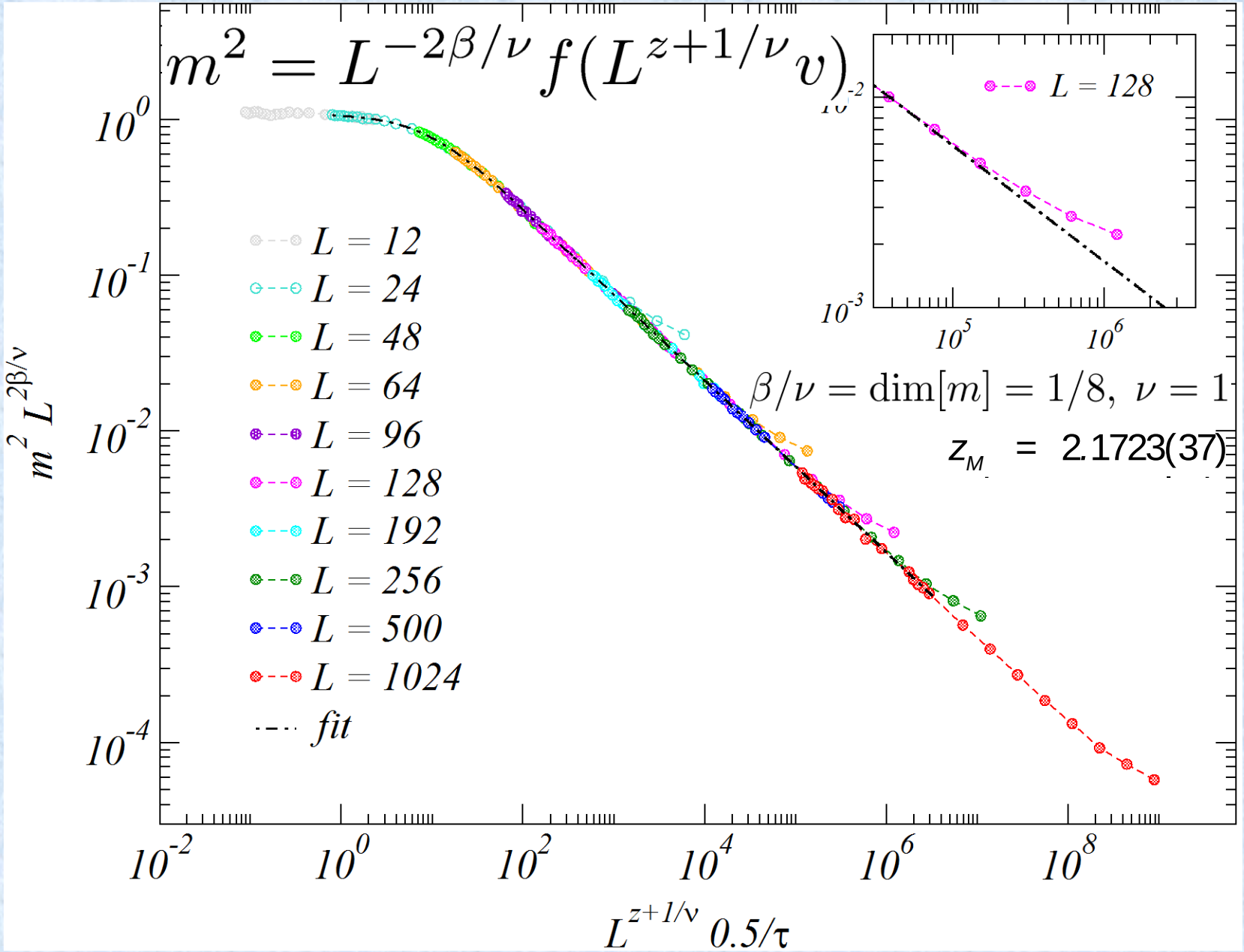
Instead slowly quench T to the critical point. Metropolis dynamics

(C.-W. Liu, A. P., A. Sandvik 2013)



Magnetization

Temperature



Very accurate determination of the dynamical exponent.

Quantum Ising model in 2D (imaginary time QMC)

$$\mathcal{H} = -s \sum_{\langle i,j \rangle} \sigma_i^z \sigma_j^z - (1-s) \sum_i \sigma_i^x \ , \ s : 0 \to 1$$

$$\frac{\partial \psi}{\partial \tau} = -\mathcal{H}(s)\psi, \quad s(\tau) = v\tau$$

Scan through QCP, look for Binder cumulant:

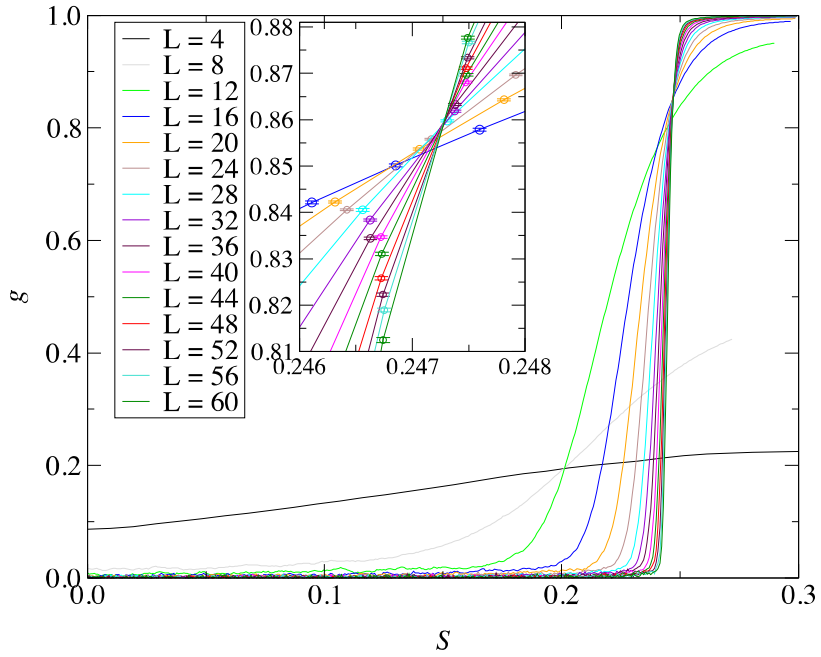
$$g_L = \frac{1}{2}\left(3 - \frac{\langle m_L^4 \rangle}{\langle m_L^2 \rangle^2}\right)$$

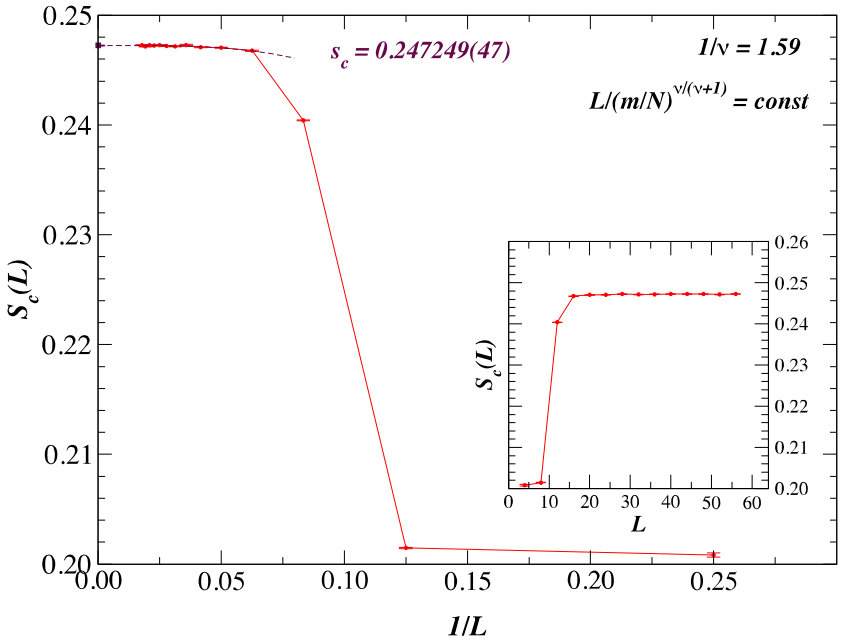
Expect the scaling form

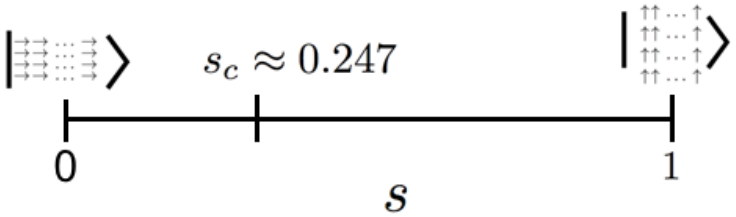
$$g_L = f\left[L(s-s_c)^\nu, Lv^{\frac{\nu}{z\nu+1}}\right]$$

If the second argument is constant (or flows to zero) expect a crossing point at $s = s_c$

Numerical simulations (imaginary time quantum annealing)







extrapolated critical point:

$s_c \approx 0.247249(47)$

Either the best or close to the best accuracy for simulations on a small computer cluster.

Comparison of real and imaginary time ramps for small systems

Example: linear ramp of transverse-field Ising ferromagnet

$$H(s) = -s \sum_{\langle ij \rangle} \sigma_i^z \sigma_j^z - (1-s) \sum_{i=1}^{N} \sigma_i^x \qquad s \in [0,1], \quad s = vt$$

2D square-lattice system; $N=L^2$

Start from eigenstate of H(s=0) at t=0

- Instantaneous ground state $|\Psi_0(t)\rangle = |\Psi_0(s[t])\rangle$

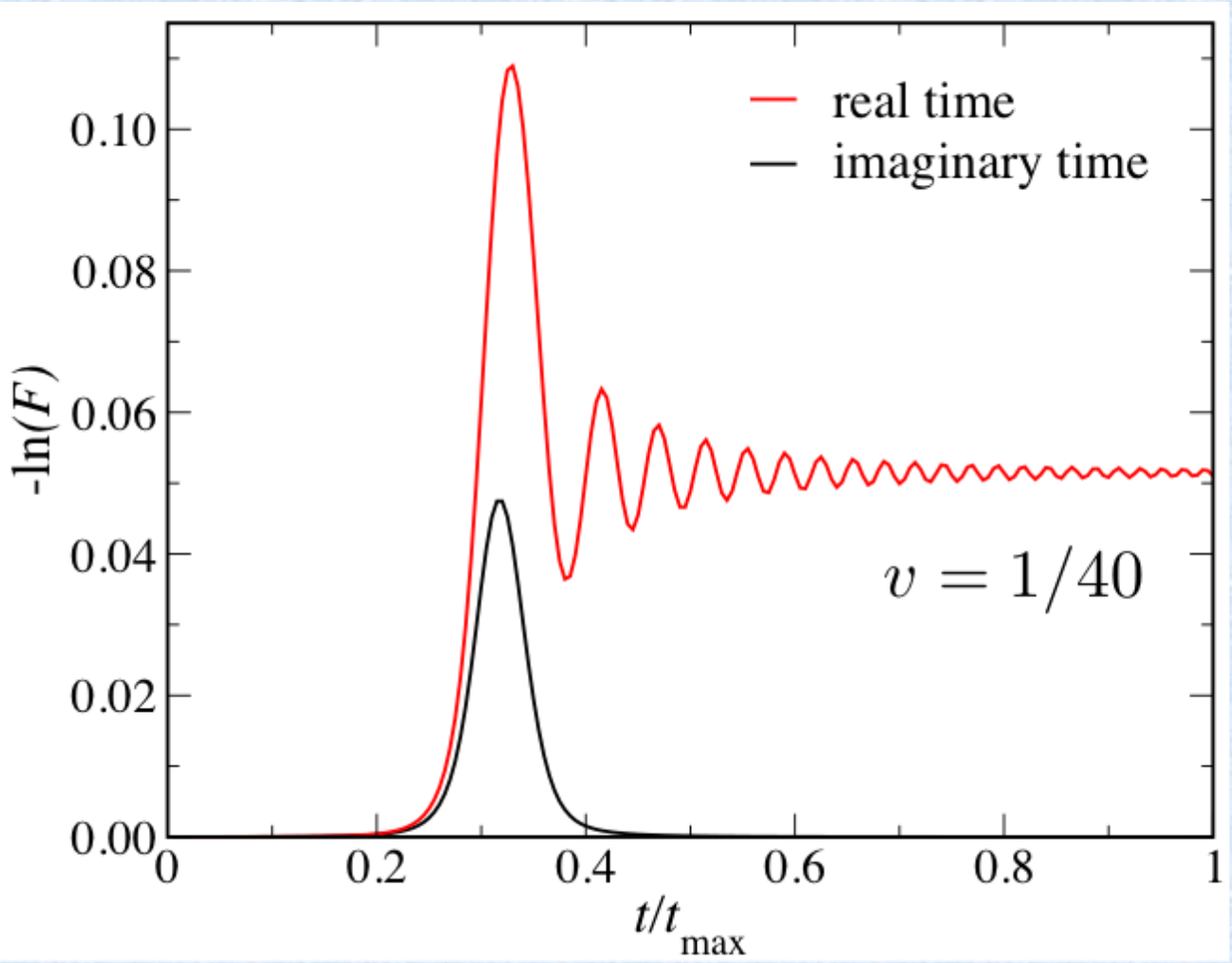
- Actual state during evolution $|\Psi(t)\rangle$

Distance between these states given by log-fidelity

$$-\ln[F(t)] = -\frac{1}{2} \ln\left(|\langle \Psi_0(t) | \Psi(t) \rangle|^2\right)$$

Integrate Schrödinger equation numerically for small L

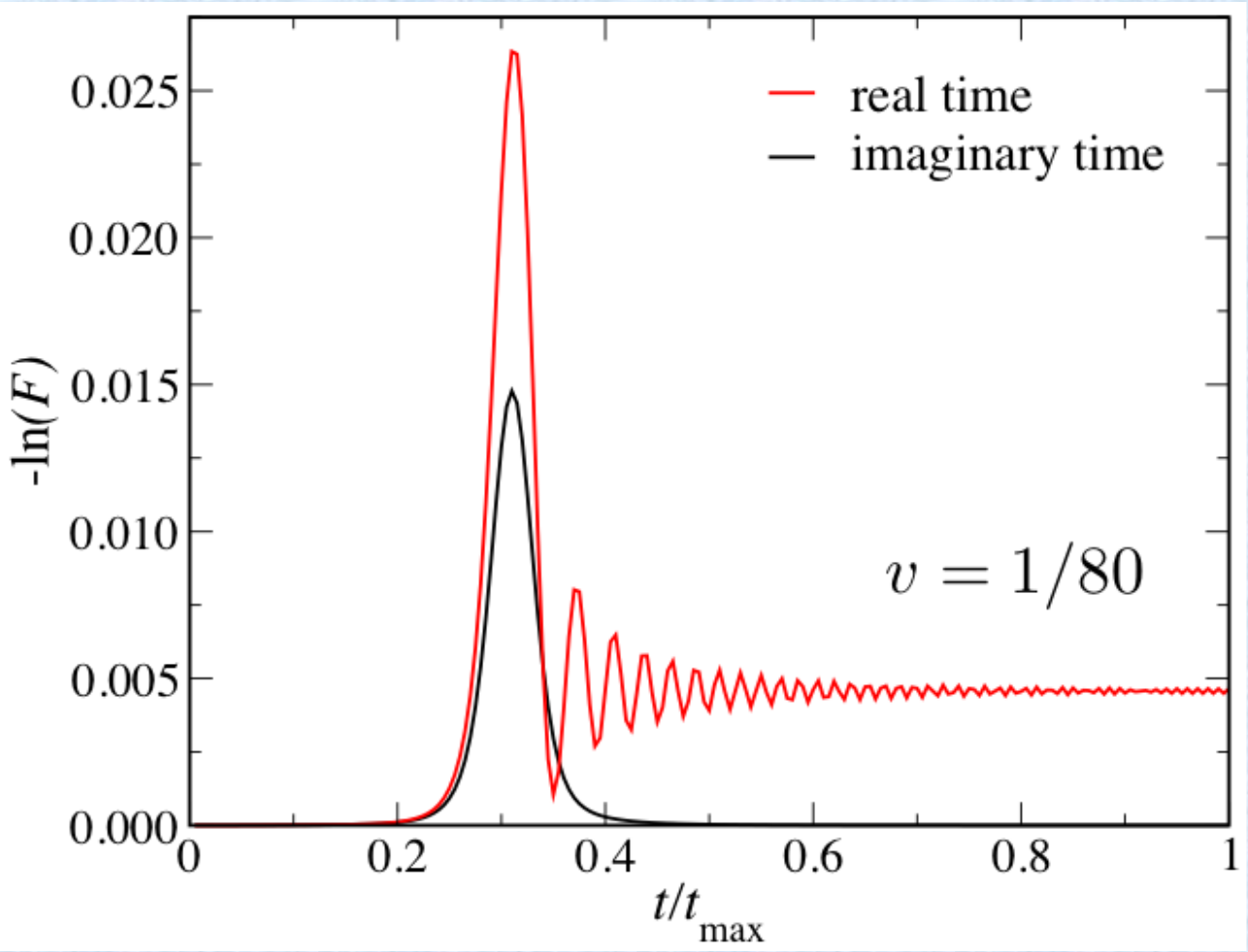
- compare real and imaginary time



Main peak reflects quantum phase transition at $S_c \approx 0.25$

Before QCP perturbation theory works and have good agreement.

Beyond QCP in real time the system remains excited



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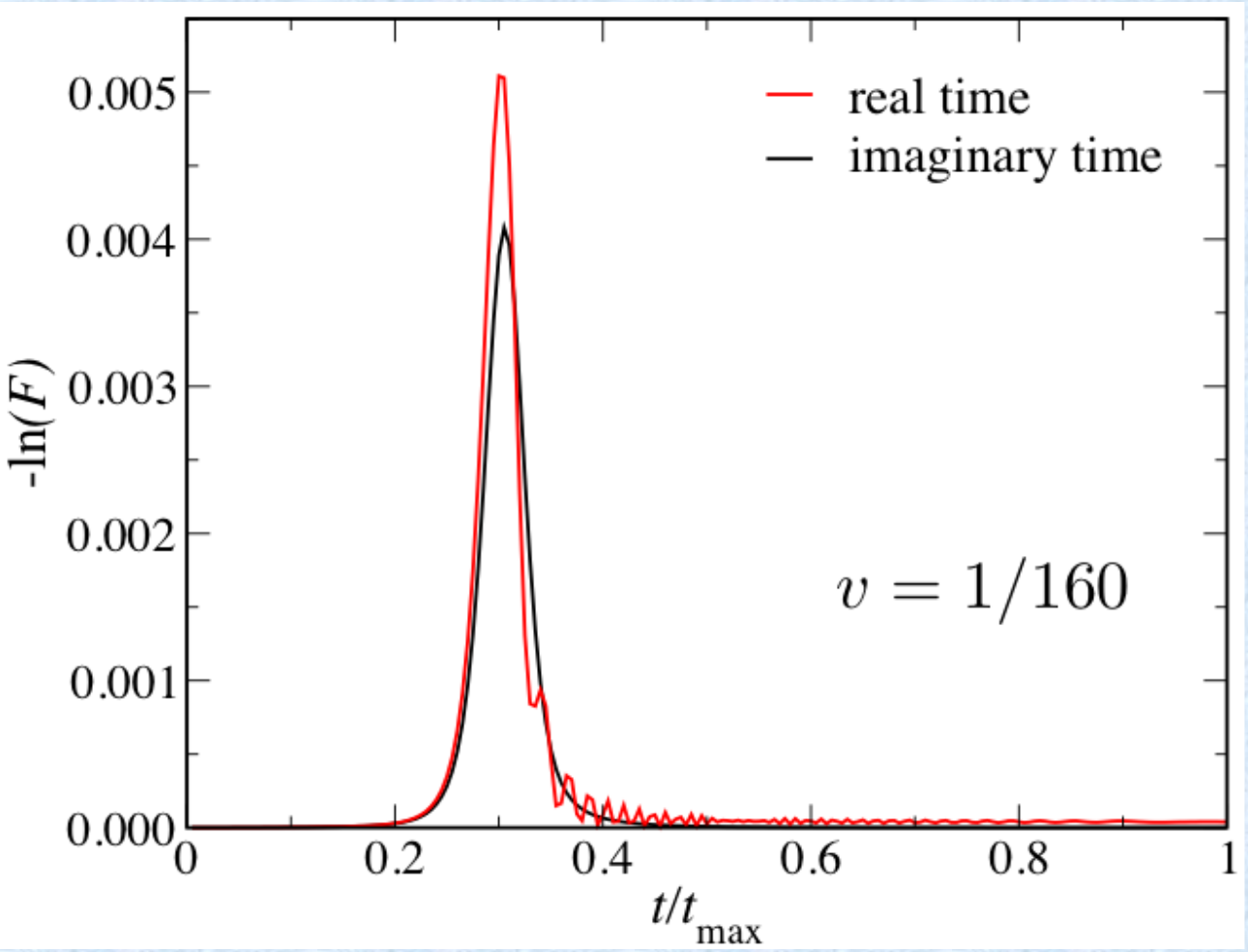
Imaginary time more efficient in reaching ground state for $s \rightarrow 1$



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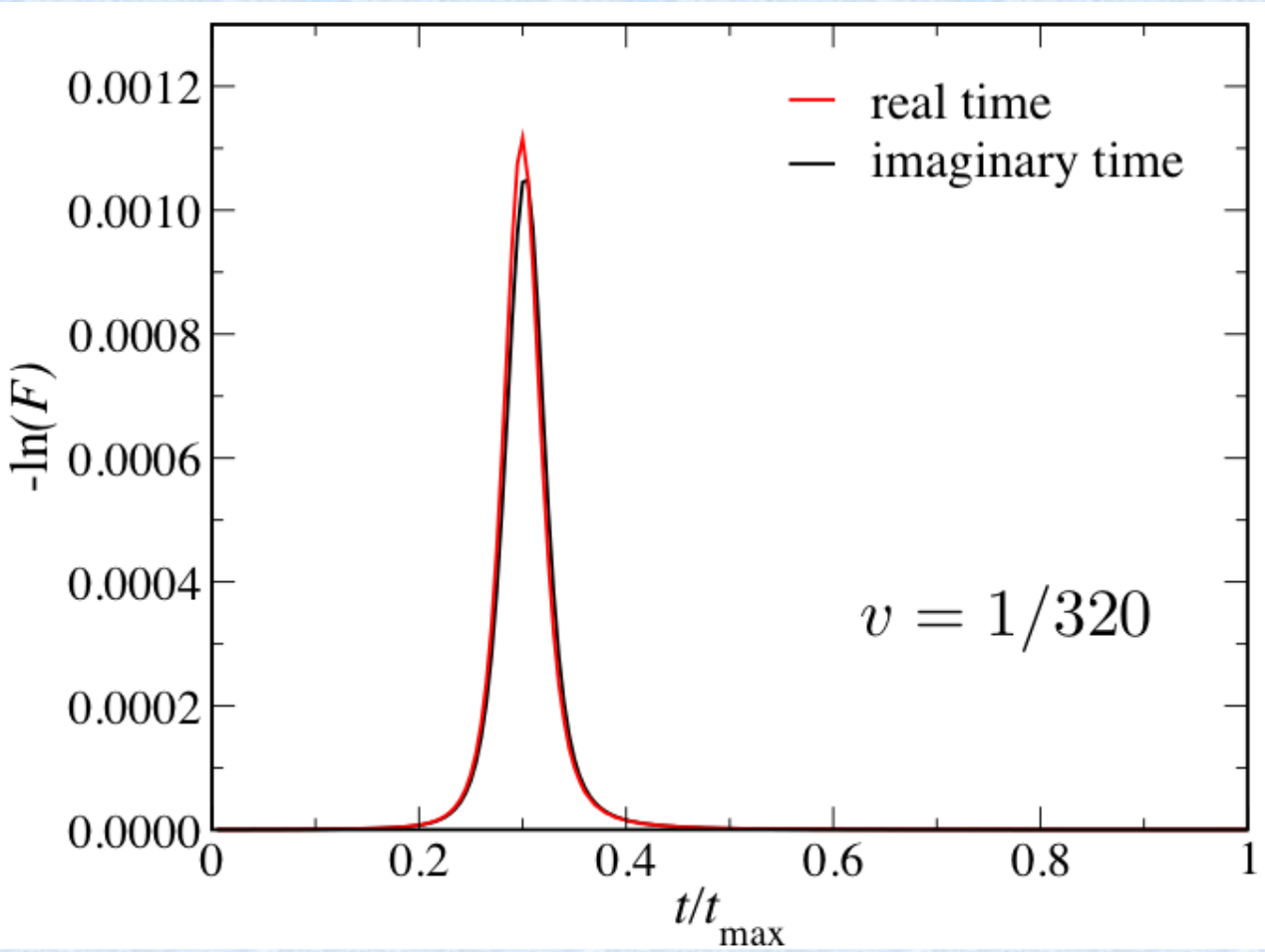


Differences between real and imaginary time come in at order v^2

Same dynamic susceptibility accessed in real and imaginary time

Dynamic exponent z is same in real and imaginary time!

De Grandi, Polkovnikov, Sandvik, PRB 2011

Schrödinger dynamic in imaginary time t=iτ

$$|\Psi(\tau)\rangle = U(\tau,\tau_0)|\Psi(\tau_0)\rangle \qquad U(\tau,\tau_0) = T_\tau \exp\left[-\int_{\tau_0}^{\tau} d\tau' H[s(\tau')]\right]$$

Implemented in quantum Monte Carlo as:

$$|\Psi(\tau)\rangle = \sum_{n=0}^{\infty} \int_{\tau_0}^{\tau} d\tau_n \int_{\tau_0}^{\tau_n} d\tau_{n-1} \cdots \int_{\tau_0}^{\tau_2} d\tau_1 [-H(\tau_n)] \cdots [-H(\tau_1)] |\Psi(0)\rangle$$

Simpler scheme: evolve with just a H-product
(Liu, Polkovnikov, Sandvik, PRB 2013)

$$|\Psi(s_M)\rangle = H(s_M)\cdots H(s_2)H(s_1)|\Psi(0)\rangle, \quad s_i = i\Delta_s, \quad \Delta_s = \frac{s_M}{M}$$

Time unit is ∝ 1/N, velocity is $v \propto N\Delta_s$

Difference in v-dependence between product evolution and imaginary-time Schrödinger dynamics is O(v²)
- same critical scaling behavior, dynamic susceptibilities

Quantum annealing vs. simulated quantum annealing

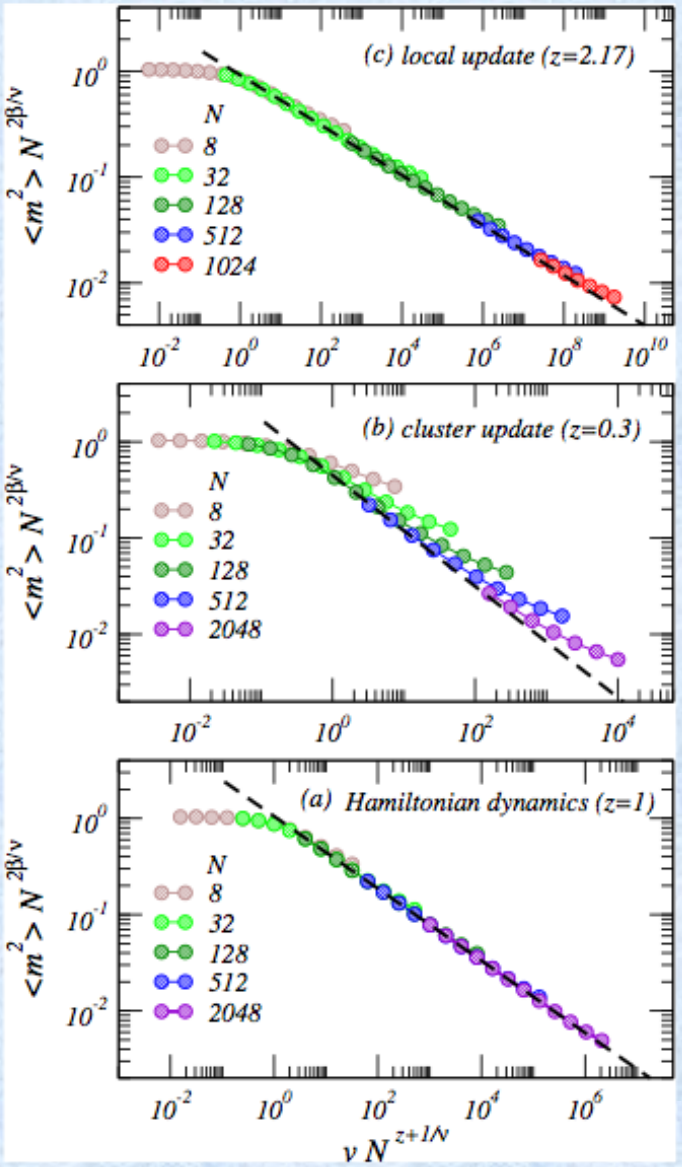
Recent work claimed the D-wave machine shows behavior similar to "simulated quantum annealing"
[S. Boixio, M. Troyer et al., Nat. Phys. 2014]

H(s) evolved in simulation time

Is this the same as Hamiltonian quantum dynamics?

NO! Only accesses the dynamics of the QMC method

Demonstration for 1D Ising model with transverse field shows this
z =1 for true Hamiltonian dynamics
z = 2.17 or z=0.30 for simulation-time dynamics (local or cluster updates)



Application to Quantum Annealing

Goal: find the ground state of a disordered classical model

NP-hard problem. Many applications in many fields.

Thermal annealing. Take this system at finite temperature

$$Z = \sum_{\{\sigma_i\}} \exp[-\beta \sum_{ij} J_{ij}\sigma_i\sigma_j]$$

and slowly decrease it. In the adiabatic limit the system should gradually relax to the ground state.

Quantum Annealing

Introduce an auxiliary quantum term and slowly anneal it to zero

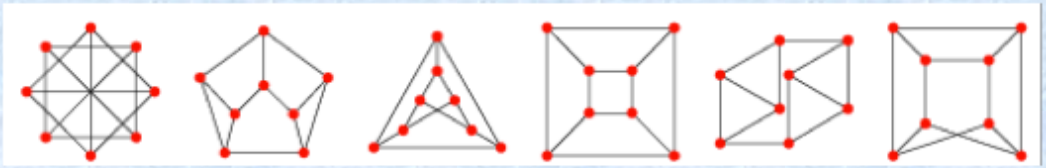
$$s = vt$$

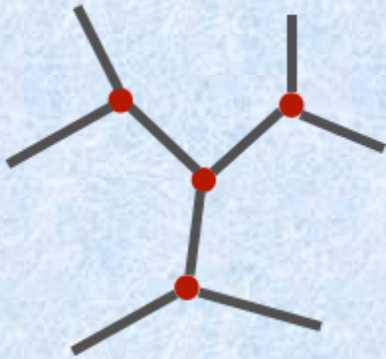
In the adiabatic limit follow the ground state.

Both thermal (simulated) annealing and quantum annealing have problems in glass phases. Hopes are that quantum annealing can be more efficient.

N spins, randomly connected, coordination-number 3

N=8





Classical model has mean-field glass transition
- Tc known exactly (Krazakala et al.)

The quantum model was studied recently:
Farhi, Gosset, Hen, Sandvik, Shor, Young, Zamponi, PRA 2012

- $s_c \approx 0.37$ from quantum cavity approximation
- QMC consistent with this s_c, power-law gaps at s_c

More detailed studies with quantum annealing

Edwards-Anderson spin-glass order parameter

$$q = \frac{1}{N}\sum_{i=1}^{N} \sigma_i^z(1)\sigma_i^z(2)$$

(1) and (2) are independent simulations (replicas)

Extracting Quantum-glass transition

Using Binder cumulant

$$U(s, v, N) = U[(s - s_c)N^{1/\nu'}, vN^{z'+1/\nu'}]$$

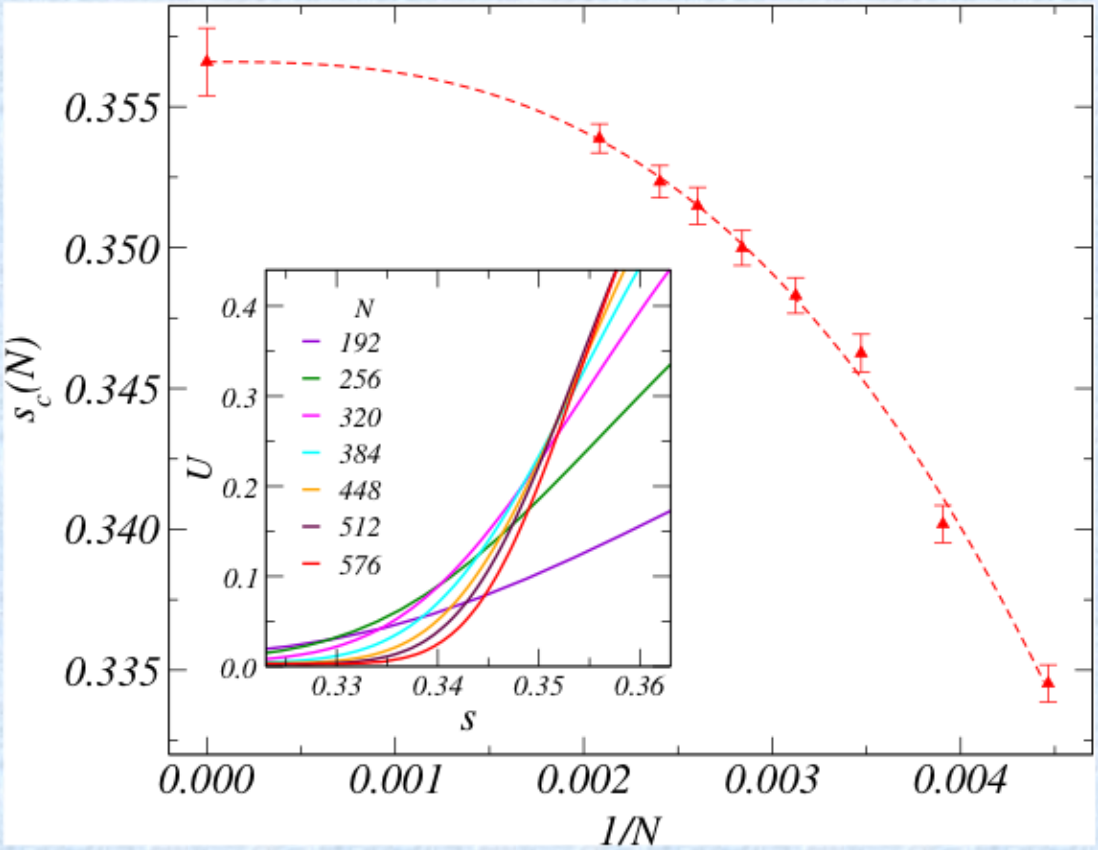
But now we don't know the exponents. Use

$$v \propto N^{-\alpha}, \quad \alpha > z' + 1/\nu'$$

Best result for α=17/12

s_c = 0.3565 +/- 0.0012

$\alpha = 17/12$



Velocity Scaling at the Glass Transition

Study evolution to s_c
- several system sizes N
- several velocities

$\beta/\nu' \approx 0.43(2)$
$z'+1/\nu' \approx 1.3(2)$

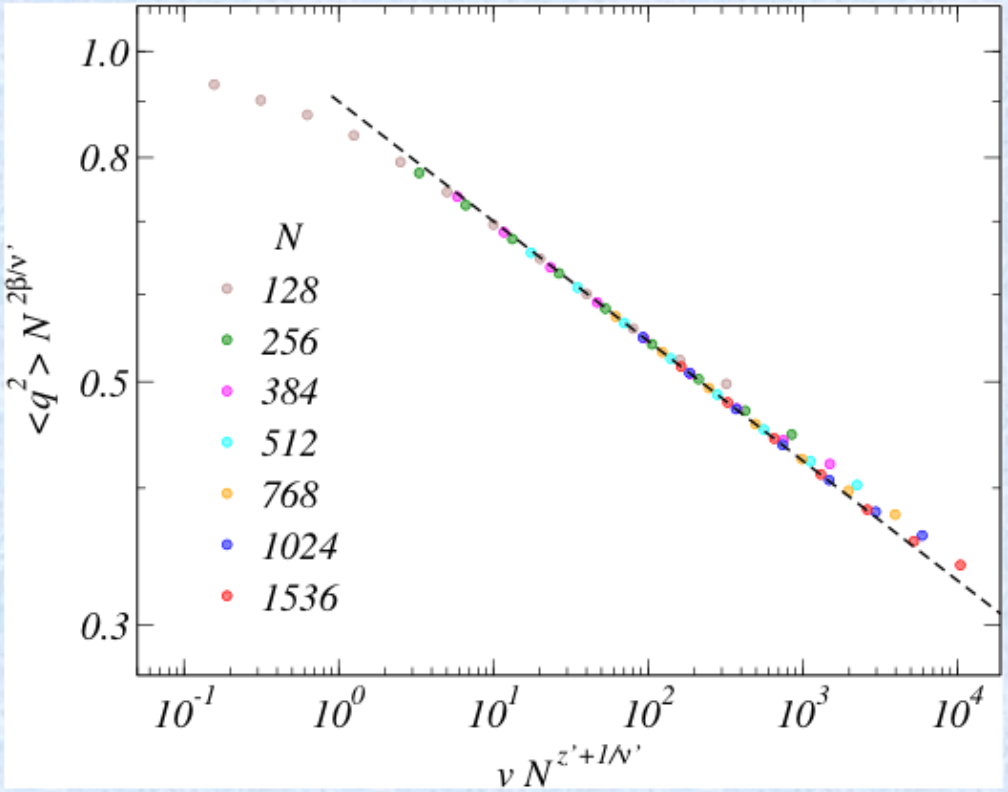
Same as fully connected (Sherrington-Kirkpatrick)?

$\beta/\nu' \approx 0.42(2)$
$z'+1/\nu' \approx 1.4(2)$

Differ from values expected for d=∞: (Read, Sachdev, Ye, 1995)

$\beta/\nu' = 1/2$
$z'+1/\nu' = 3/4$

$$\langle q^2(s_c)\rangle \propto N^{-2\beta/\nu'} f(vN^{z'+1/\nu'})$$



Relevance to Quantum Computing

The time needed to stay adiabatic up to s_c scales as

$$t \sim N^{z'+1/\nu} \qquad z' + 1/\nu' \approx 1.3$$

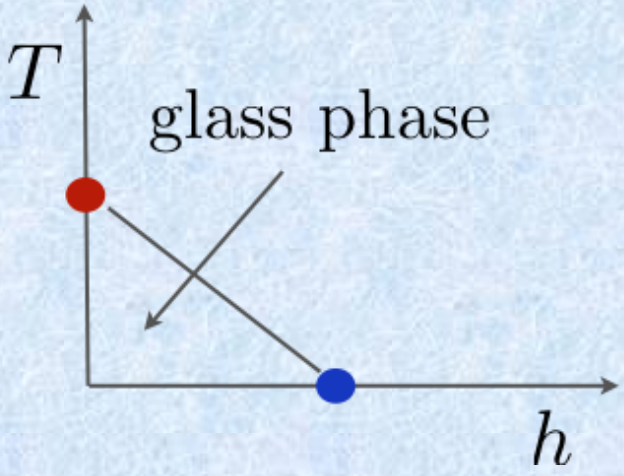
Reaching s_c, the degree of ordering scales as

$$\sqrt{< \langle q^2 \rangle >} \sim N^{-\beta/\nu'} \qquad \beta/\nu' \approx 0.43$$

Let's compare with the know classical exponents (finite-temperature transition of 3-regular random graphs)

Classical	**Quantum**
$\beta/\nu' = 1/3$	**$\beta/\nu' \approx 0.43$**
$z'+1/\nu' = 1$	**$z'+1/\nu' \approx 1.3$**

- **It takes longer for quantum annealing to reach its critical point**

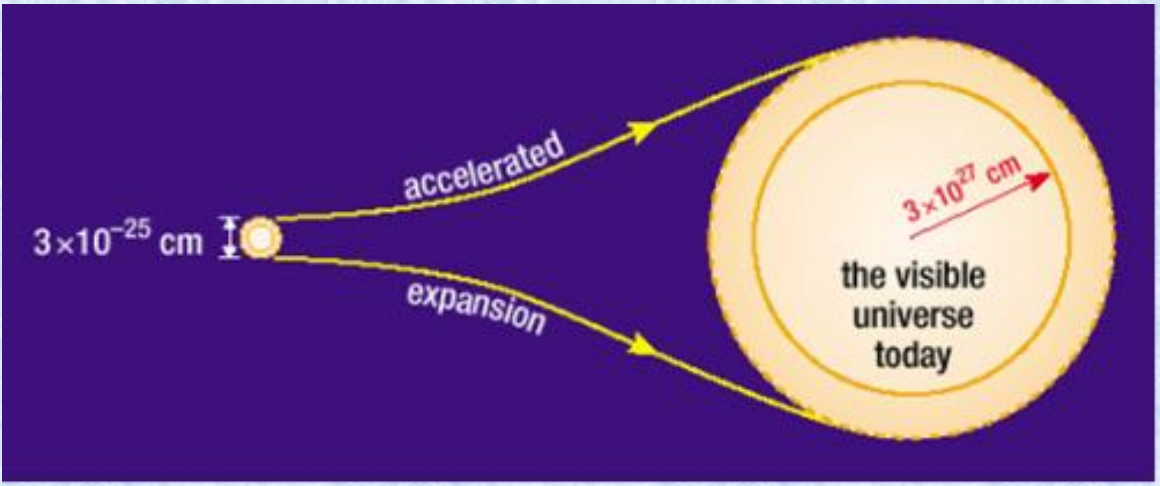


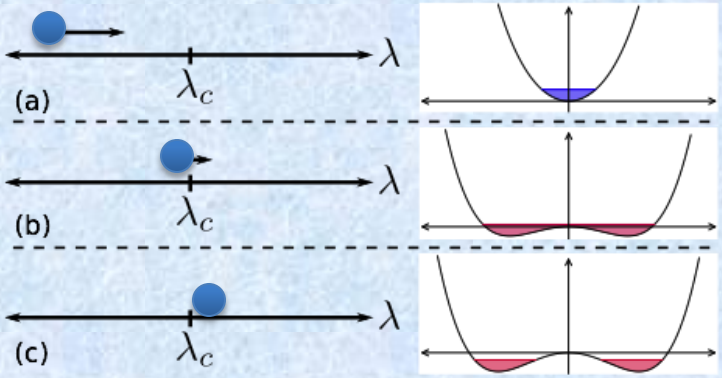
Origin of KZ scaling is that many excitations are created near QCP. Like moving in a swamp: lots of drag and added mass.

Image taken from: http://allthingspoliticaltoday.com

As the ball gets heavier it is harder to move even if there is a slope.
Can get stuck.

From a snowball to inflation in cosmology (hypothetical scenario)





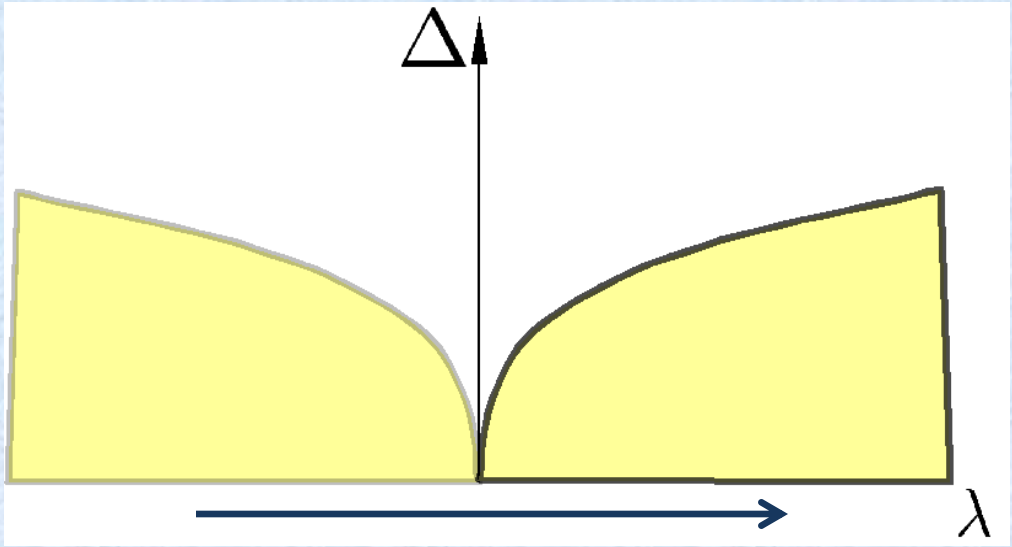
$$H_\phi = \int d^d x \left[|\Pi(x)|^2 + |\nabla\phi(x)|^2 + \lambda|\phi(x)|^2 + u|\phi(x)|^4 \right] + H_0(\lambda)$$

Scalar field rolls affecting the Higgs mass. Near QCP (zero Higgs mass) it gets very heavy and dynamically localizes.

Related ideas: L. Kofman et. al. (2004)

The Kibble-Zurek type scaling argument one more time

$$H_\phi = \int d^d x \left[|\Pi(x)|^2 + |\nabla\phi(x)|^2 + \lambda|\phi(x)|^2 + u|\phi(x)|^4 \right] + H_0(\lambda)$$



Scaling dimension of velocity

$$[d\lambda/dt] = [\lambda] - [t] = z + 1/\nu$$

Divergent KZ correlation length

$$\xi_{KZ} = \frac{1}{|\dot{\lambda}|^{\frac{\nu}{z\nu+1}}}$$

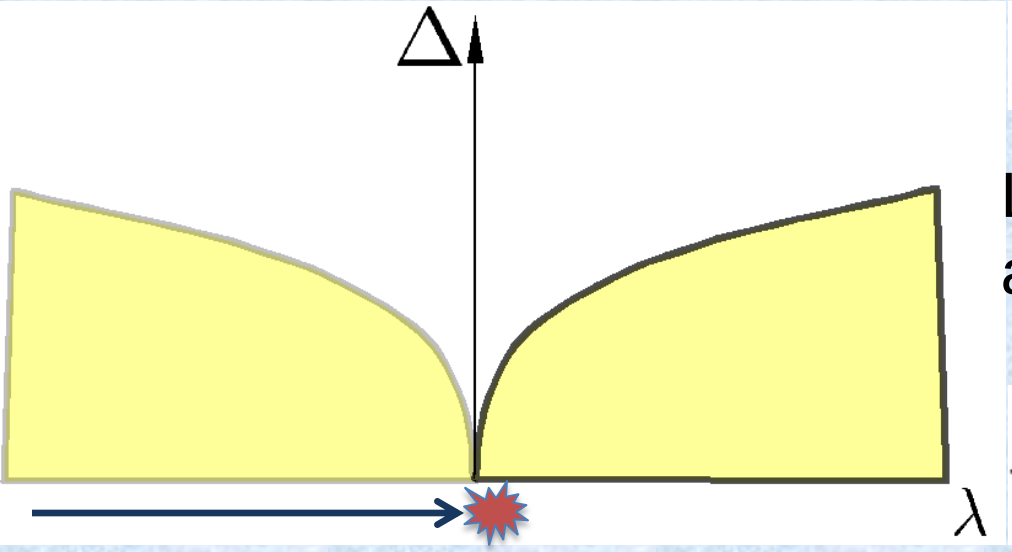
Characteristic gap $\Delta \sim 1/\xi_{KZ}^z$

Energy (heat) density $Q/L^d \sim \Delta\xi_{KZ}^d \sim |\dot{\lambda}|^{\frac{(d+z)\nu}{z\nu+1}}$

Initial kinetic energy $K/L^d \sim \mu\dot{\lambda}^2$

Can expect localization if $Q > K$

Localization from the Kibble-Zurek



$$K < Q \Leftrightarrow \mu\dot{\lambda}^2 < |\dot{\lambda}|^{\frac{(d+z)\nu}{z\nu+1}}$$

Localization is expected if we absorb more energy than it has

$$\frac{(d+z)\nu}{z\nu+1} < 2 \Leftrightarrow d < z + \frac{2}{\nu}$$

The slower the system goes the more likely it is localized

Alternative way to understand this result. Mass renormalization near QCP

$$E \to E + \frac{\kappa}{2} L^d \dot{\lambda}^2$$

$$[\kappa] = [E] + d - 2[\dot{\lambda}] = z + d - \frac{2}{\nu} - 2z = d - z - \frac{2}{\nu}$$

Negative scaling dimension = divergence. Small dimensionality implies divergent mass.

Check numerically. Transverse field Ising model with magnetic field as a dynamical degree of freedom

$$H = \frac{p_\lambda^2}{2\mu L} + H_{\rm TFI}(\lambda) - E_{\rm gs}(\lambda)$$

$$H_{\rm TFI}(\lambda) = -\sum_j (1-\lambda) s_j^z + s_j^x s_{j+1}^x, \quad E_{\rm gs}(\lambda) = \langle 0 | H_{\rm TFI} | 0 \rangle$$

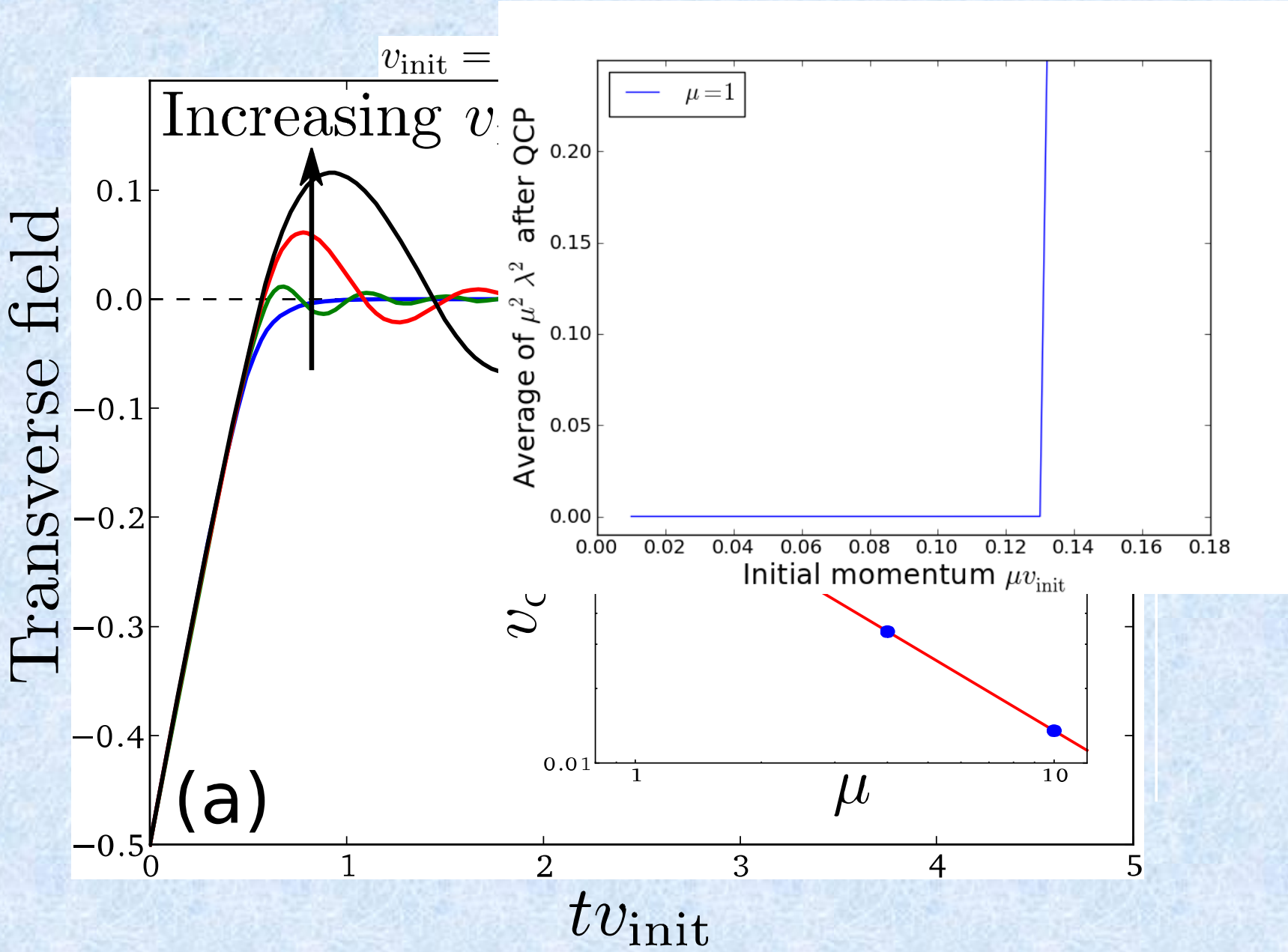
First subtract the GS energy so that the field moves in a flat potential (later revise this assumption).

Trapping condition

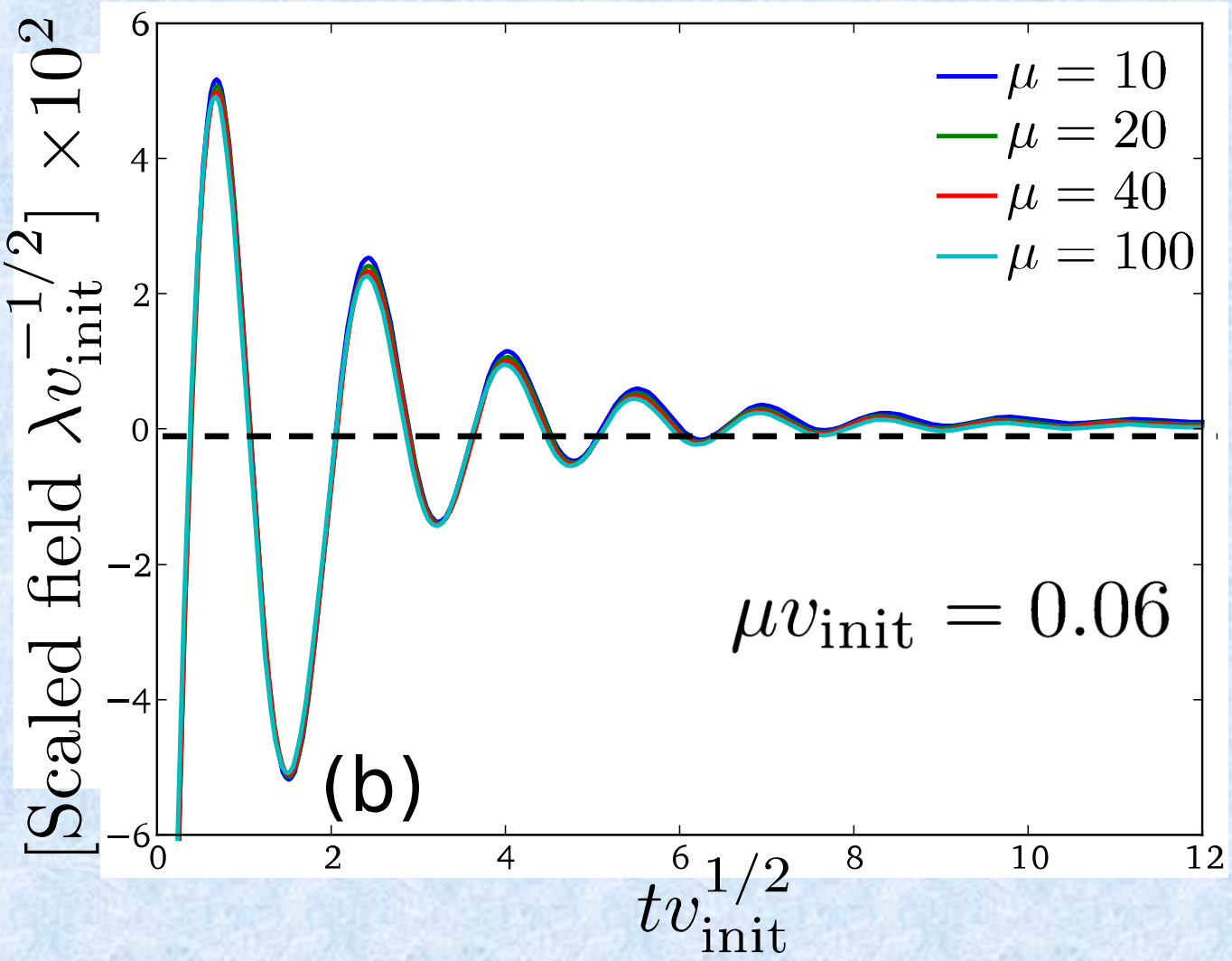
$$K < Q \;\Leftrightarrow\; \mu\dot{\lambda}^2 < |\dot{\lambda}|^{\frac{(d+z)\nu}{z\nu+1}} = |\dot{\lambda}|, \quad d = z = \nu = 1$$

Expect trapping when $\mu|\dot{\lambda}| < \text{const} \sim 1$

Observe sharp transition to the trapping regime at $\mu v_{\text{init}} \approx 0.13$



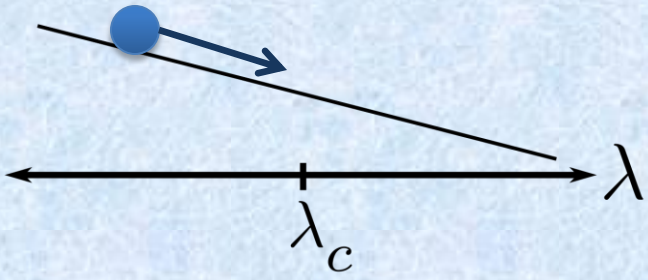
Scaling collapse of the dynamics in the trapping regime



Trapping slightly off QCP due to irrelevant terms in the Hamiltonian.

Finite slope

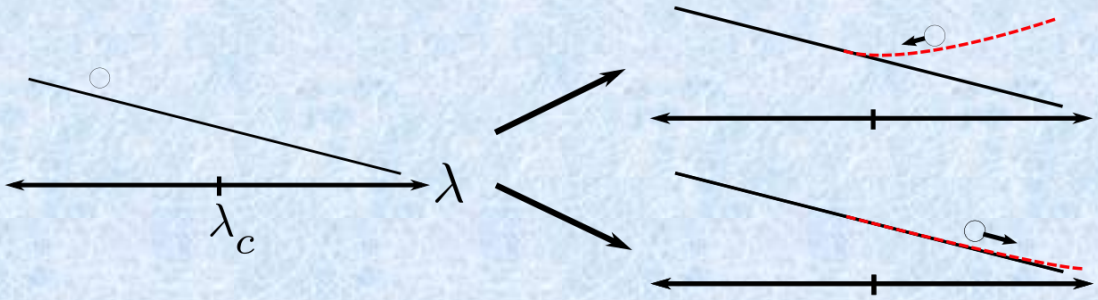
$$H = \frac{p_\lambda^2}{2\mu L} + H_{\rm TFI}(\lambda) - E_{\rm gs}(\lambda) - \alpha\lambda$$



Start from the rest at some $\lambda_{\rm ini}$ and release the system. What will happen?

Naïve answer: will roll down, perhaps stumble a bit near QCP and move on. Wrong!

The system can be truly self-trapped due to heating



Expect two scenarios:
Untrapped (adiabatic)
Trapped (enough heating)

Start far from QCP: not too fast

$$K \sim \mu\dot{\lambda}^2 \sim \alpha\lambda_{\rm init} \lesssim Q \sim |\dot{\lambda}|, \Rightarrow \alpha\lambda_{\rm init} \lesssim \sqrt{\frac{\alpha\lambda_{\rm init}}{\mu}}$$

$$\lambda_{\rm init} \lesssim \frac{1}{\mu\alpha}$$

Start near QCP : not too slow

$$\mu \to \kappa \sim \frac{1}{\lambda_{\rm init}^2} \Rightarrow \lambda_{\rm init} \lesssim \frac{1}{\mu\alpha} \to \lambda_{\rm init} \lesssim \frac{\lambda_{\rm init}^2}{\alpha} \quad \Rightarrow \quad \lambda_{\rm init} > \alpha$$

$$[\kappa] = z - d - 2/\nu = -2, \; [\lambda] = 1/\nu = 1 \Rightarrow [\kappa] \sim \lambda^{-2}$$

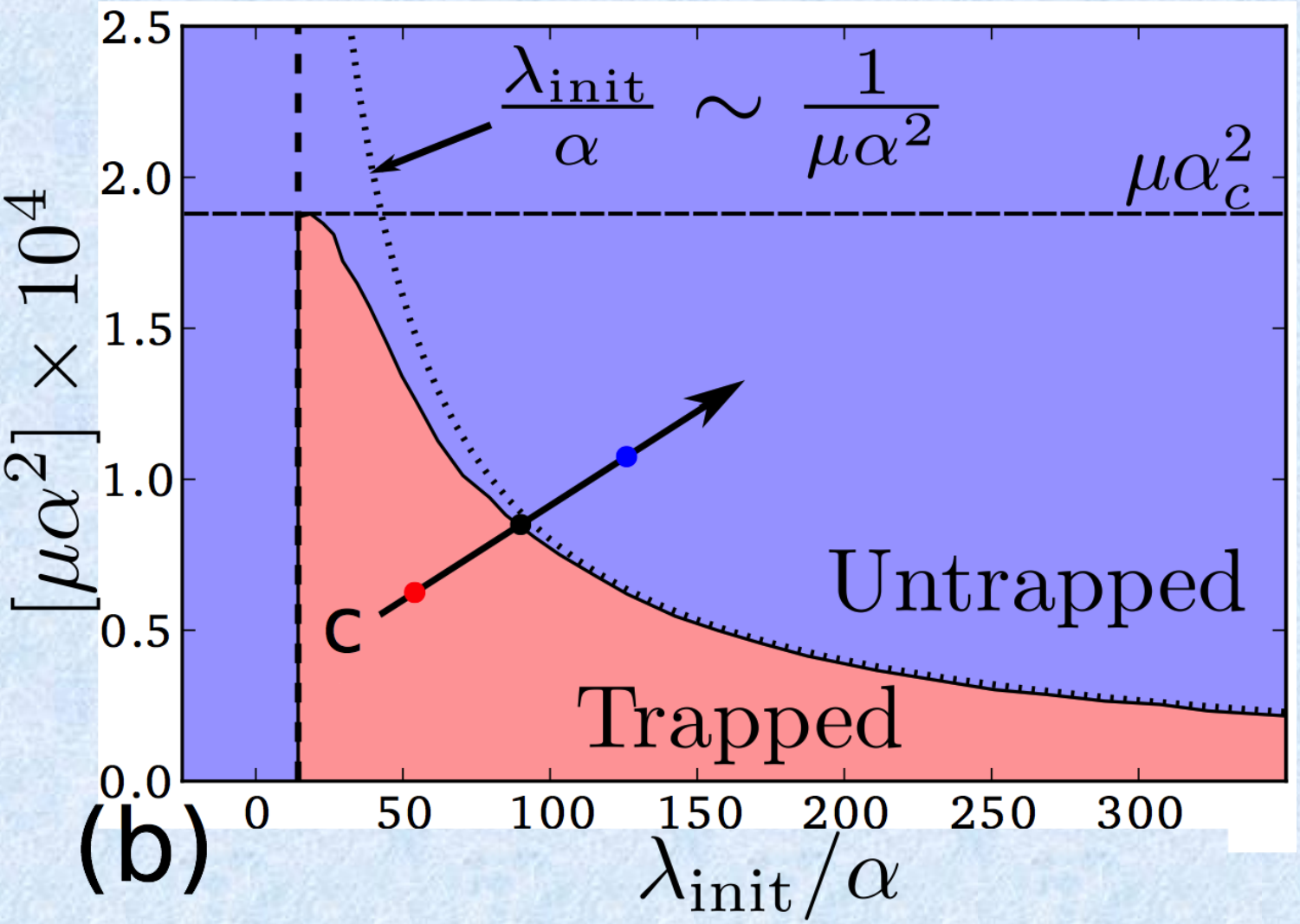
Expect trapping when

$$1 \lesssim \frac{\lambda_{\rm init}}{\alpha} \lesssim \frac{1}{\mu\alpha^2}$$

Trapping is possible only if

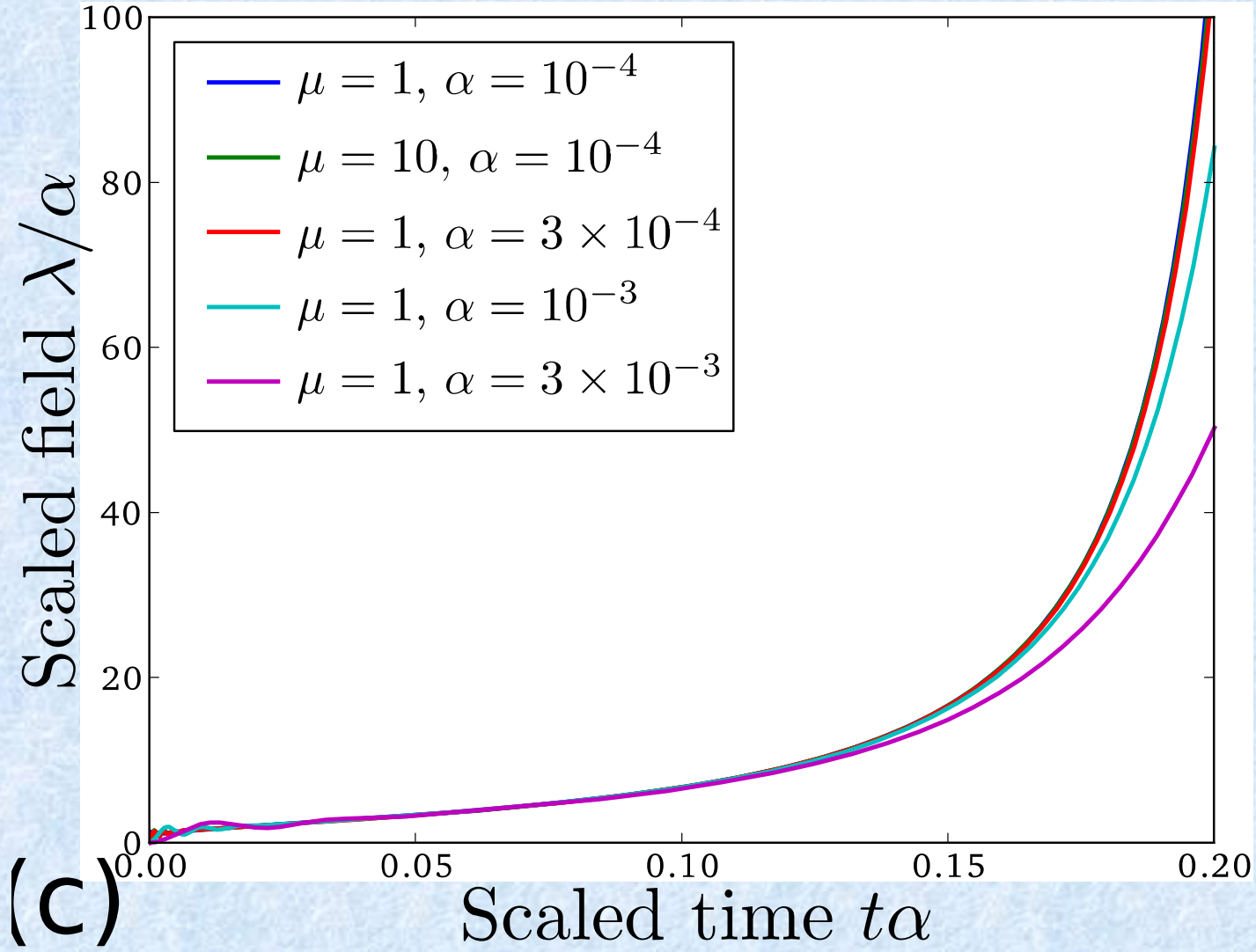
$$\mu\alpha^2 \ll 1$$

Numerical phase diagram



Numerical constants are not very small, but this is quite typical.

Interesting non-equilibrium dynamics if start near QCP.
Bare mass is irrelevant and can be set to zero.



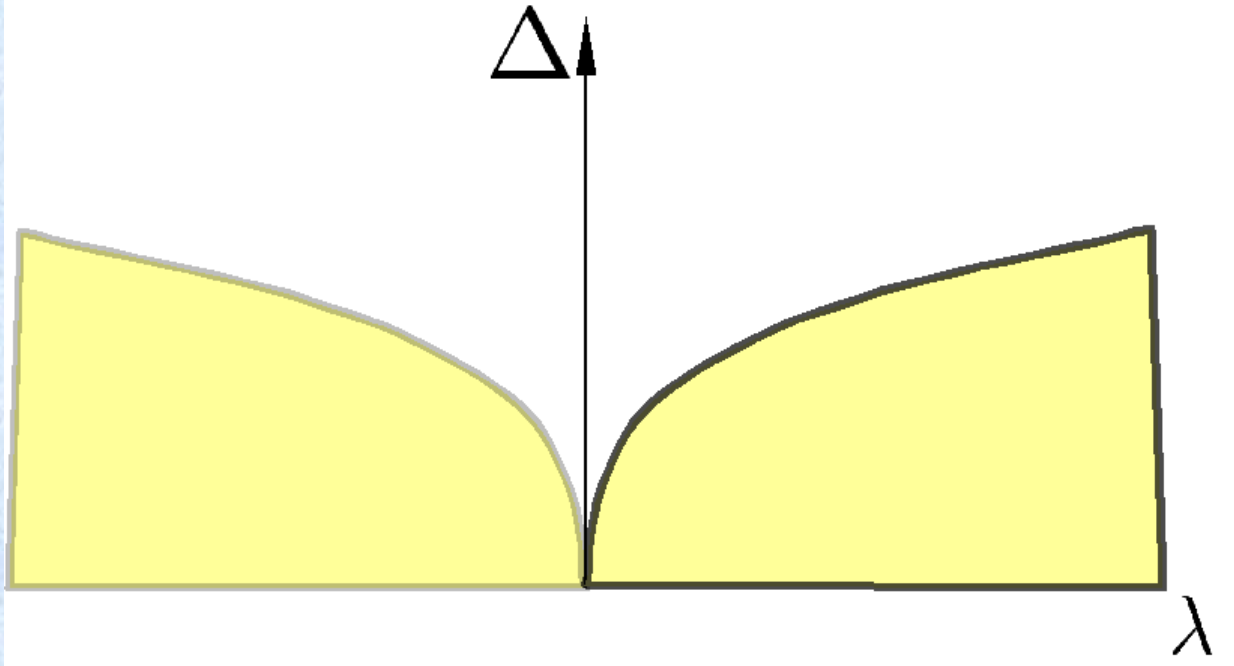
(c)

Except for transients and long times have a full scaling collapse

Outlook: dynamic trapping is consistent with thermodynamic trapping

$$H_{tot}(\lambda) = H_0(\lambda, p_\lambda) + H(\lambda, \{\hat{s}_j\})$$

Consider a fixed energy state. Equilibrium: maximize entropy



The entropy is maximized near QCP where excitations are cheapest.

From scaling expect entropy maximum near QCP.

Can the same happen with MBL/glass type transitions with heavy/light atoms?

Summary

- Can use non-adiabatic response in real and imaginary times to get non-trivial susceptibilities: Berry curvature, Fubini-Study metric and Fidelity susceptibility, added mass, …
- Can use this scaling theory to accurately determine both equilibrium and dynamical critical exponents in classical and quantum systems. Applications to quantum annealing.
- Can use simulate quantum annealing in imaginary time and likely get upper bounds to real time annealing protocols.
- Dynamical localization of macroscopic slow fields near critical points. Potential applications to Higgs mass.

Berry phase and geometry. Aharonov-Bohm effect.

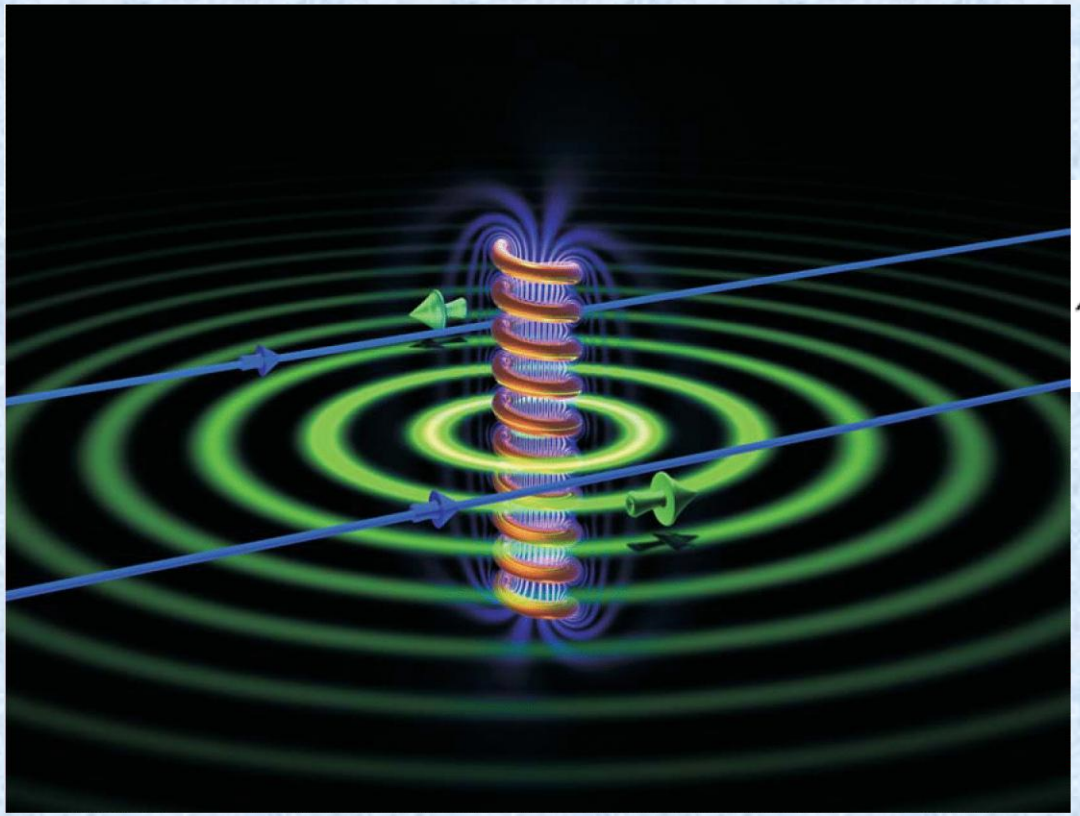


Image: H. Batelaan and A. Tonomura, Physics Today, Sep. 2009

A charged particle outside of a solenoid

$$\mathcal{H} = \frac{\left(\vec{p} - \frac{e}{c}\vec{A}\right)^2}{2m} + V(\vec{r} - \vec{R}_0)$$

No magnetic field

$$\vec{\nabla} \times \vec{A} = 0 \Rightarrow \vec{A} = \vec{\nabla}\Phi \Rightarrow \Phi(\vec{r}) = \int \vec{A} d\vec{l}$$

Gauge transformation

$$\psi = \tilde{\psi} e^{i\frac{e}{c\hbar}\Phi(\vec{r})}$$

$$\tilde{\mathcal{H}} = \frac{\vec{p}^2}{2m} + V(\vec{r} - \vec{R}_0)$$ does not depend on $\vec{A}$

Total accumulated (Aharonov-Bohm) phase for a closed path $\gamma_0 = \frac{e}{c\hbar} \oint \vec{A} d\vec{l}$

Geometric phase: S. Pancharatnam (1956), M. V. Berry (1984)

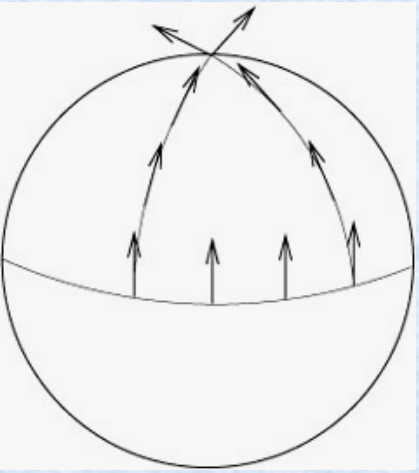
$$\psi = \tilde{\psi} e^{i\frac{e}{c\hbar}\Phi(\vec{r},\vec{R}_0)},\ \Phi(\vec{r},\vec{R}_0) = \int_{\vec{R}_0}^{\vec{r}} \vec{A}(\vec{r}\,')d\vec{r}\,'$$

Berry: imagine that we adiabatically move $\mathbf{R}_0$ around the solenoid

$$\gamma_0 = \frac{e}{c\hbar}\oint \vec{A}d\vec{l} = \frac{e}{c\hbar}\oint d\vec{r}\,\vec{\nabla}_r\Phi(\vec{r},\vec{R}_0) =$$

$$= -\frac{e}{c\hbar}\oint d\vec{R}_0\vec{\nabla}_{\vec{R}_0}\Phi(\vec{r},\vec{R}_0) = i\oint d\vec{R}_0\langle\psi|\vec{\nabla}_{\vec{R}_0}|\psi\rangle$$

The integral is taken over an arbitrary path outside the solenoid.



Geometric interpretation: the Berry phase is the phase obtained by a parallel transport of the ground state $|\psi_0(\vec{R}_0)\rangle$ around a closed loop.

These ideas can be extended to an arbitrary parameter manifold $\vec{\lambda}$

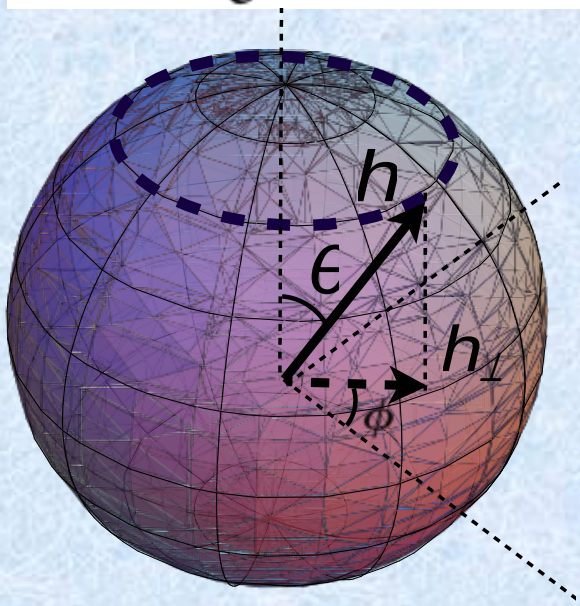
The Hamiltonian and the ground state are functions of the parameter

$$\mathcal{H} = \mathcal{H}(\vec{\lambda}), \quad |\psi_0\rangle = |\psi_0(\vec{\lambda})\rangle$$

$$A_\alpha = i\langle 0|\partial_{\lambda_\alpha}|0\rangle$$ Berry connection (vector potential)

$$F_{\alpha\beta} = \partial_\alpha A_\beta - \partial_\beta A_\alpha$$ Berry curvature (Magnetic field).

$$\gamma_0 = \oint_{\mathcal{C}} \vec{A}\cdot d\vec{\lambda} = \int_{\mathcal{A}} F_{\alpha\beta} d\lambda_\alpha \wedge d\lambda_\beta$$ Berry phase (flux)



Example: spin in a magnetic field

$$|\psi_0\rangle = \begin{pmatrix} \cos(\theta/2)\mathrm{e}^{i\phi/2} \\ \sin(\theta/2)\mathrm{e}^{-i\phi/2} \end{pmatrix}. \quad A_\phi = \frac{1}{2}(1-\cos(\theta))$$

$$\gamma_0 = \pi(1-\cos(\theta))$$

General gauge transformations in quantum systems

Consider an arbitrary unitary transformation of the basis.

$$|\psi(\vec{\lambda})\rangle = U^{\dagger}(\vec{\lambda})|\Psi\rangle$$

Infinitesimal transformations are like the Schrödinger equation

$$i\partial_{\lambda_\alpha}|\psi(\vec{\lambda})\rangle = -\mathcal{A}_\alpha|\psi\rangle,\ \mathcal{A}_\alpha = iU^{\dagger}\partial_{\lambda_\alpha}U,\ \mathcal{A}_\alpha^{\dagger} = \mathcal{A}_\alpha$$

Hamiltonian equations of motion in a moving frame

$$i\partial_t|\psi\rangle = (U^{\dagger}HU - \dot{\lambda}_a\mathcal{A}_a)|\psi\rangle$$

Special instantaneous frame, where U diagonalizes the instantaneous Hamiltonian. Convenient near the adiabatic limit

$$|\psi\rangle = |\psi_0(\vec{\lambda})\rangle \ \Rightarrow\ A_\alpha = \langle\mathcal{A}_\alpha\rangle$$

Berry connection is the expectation value of the gauge potential