Quantum Dissipative Systems

Takeo Kato (ISSP, University of Tokyo)

Collaborators

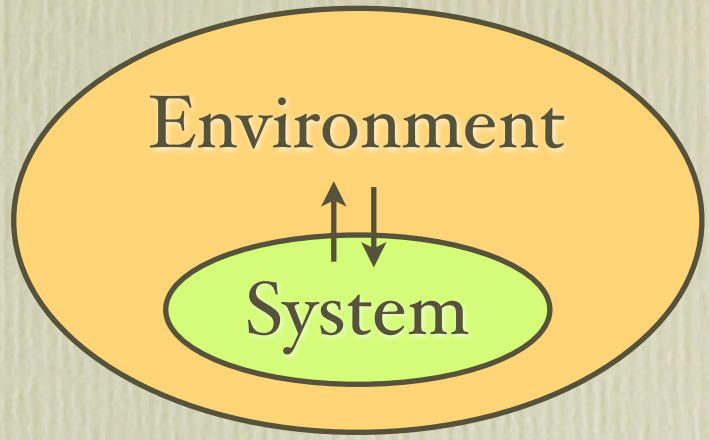
Takeshi Matsuo (Chiba University)

Naoki Kimura (Osaka City University)

Open Quantum Systems

Langevin Equation

$$M\ddot{q} + \eta\dot{q} + \frac{\partial V}{\partial q} = \xi(t)$$



Caldeira Leggett model

$$H = \frac{p^2}{2M} + V(q) + \sum_j \left\{ \frac{p_j^2}{2m_j} + \frac{1}{2} m\omega_j^2 \left(x_j - \frac{C_j q}{m\omega_j^2} \right)^2 \right\}$$

$$J(\omega) = \frac{\pi}{2} \sum_j \frac{C_j^2}{m_j \omega_j} \delta(\omega - \omega_j) = \eta\omega$$ Ohmic damping

General form

$$J(\omega) = A\omega^s$$

$s > 1$ Superohmic

$s < 1$ Subrohmic

Relevant Systems/Phenomena

- ✓ Macroscopic Quantum Phenomena (MQP)
  - Josephson devices, quasi-particle tunneling
- ✓ Fabrication of quantum bits (qubits)
  - Various systems, various decoherence sources
- ✓ Polaron problem, heavy particle motion in metals
- ✓ Impurity problem in Tomonaga-Luttinger Liquids
- ✓ Dynamical mean-field study of phonon systems

Outline of the talk

- ✓ Striking features of Ohmic damping (Analytic)
  - Localization transition
  - Relation to the Kondo problem
  - Experiments of Josephson devices
- ✓ Simulation of quantum dissipation (Numerical)
  - Path-integral Monte Carlo (PIMC) method
  - Resistance-shunted Josephson junctions
  - Dissipative double-well potential systems

Path-integral formalism

$$Z = \oint \mathcal{D}q(\tau) \prod_j \oint \mathcal{D}x_j(\tau) \exp(-S)$$

$$= \oint \mathcal{D}q(\tau) \exp(-S_{\rm eff})$$

Retardation effect

Effective action

$$S_{\rm eff} = \int d\tau \left(\frac{1}{2} M \dot{q}^2 + V(q) \right) + \int d\tau \int d\tau' k(\tau - \tau') q(\tau) q(\tau')$$

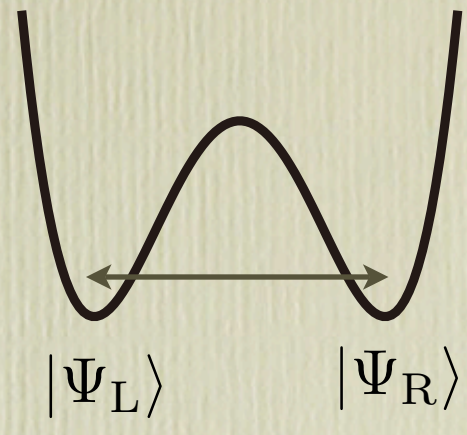
Damping kernel $k(\tau) \sim \dfrac{A}{(\tau - \tau')^{s+1}}$

Long-range interaction along imaginary time

$\longrightarrow$ Significant effects on quantum mechanics of the system

Localization transition

Simple derivation for double-well systems



Adiabatic bases (two-state approx.)

$$|\Psi_{\rm R}\rangle = |\sigma_z = 1\rangle \prod_a |a+\rangle$$

$$|\Psi_{\rm L}\rangle = |\sigma_z = -1\rangle \prod_a |a-\rangle$$

$p\omega_c < \omega < \omega_c$

$(p\omega_c \ll \Delta)$

Renormalized tunneling matrix

$$\Delta' = \Delta \prod_a \langle a+|a-\rangle = \Delta \exp\left(-\int_{p\omega_c}^{\omega_c} \frac{a^2}{2\pi\hbar}\frac{J(\omega)}{\omega^2} d\omega\right)$$

$$= \Delta p^{\alpha}$$

For $\alpha > 1$ $\Delta' \to 0$ $(p \to 0)$

Particle is localized.

$$\alpha = \frac{\eta a^2}{2\pi\hbar}$$ Dimensionless damping strength

Kondo problem

Spin-boson model (two-state approximation)

$$H = -\frac{\Delta}{2}\sigma_x + \sum_i \omega_i \left(a_i^\dagger a_i + \frac{1}{2} \right) + \frac{a}{2}\sigma_z \sum_i \frac{C_i}{\sqrt{2m_i\omega_i}}(a_i + a_i^\dagger)$$

↕ Equivalent! (by bosonization technique)

$$H = \sum_{k,\sigma} \varepsilon_k c_{k,\sigma}^\dagger c_{k,\sigma} + \frac{J_\perp}{2} \sum_{k,k'} (c_{k,\uparrow}^\dagger c_{k',\downarrow} S^- + c_{k,\downarrow}^\dagger c_{k',\uparrow} S^+)$$
$$+ \frac{J_\parallel}{2} \sum_{k,k'} (c_{k,\uparrow}^\dagger c_{k,\uparrow} - c_{k,\downarrow}^\dagger c_{k,\downarrow}) S^z$$

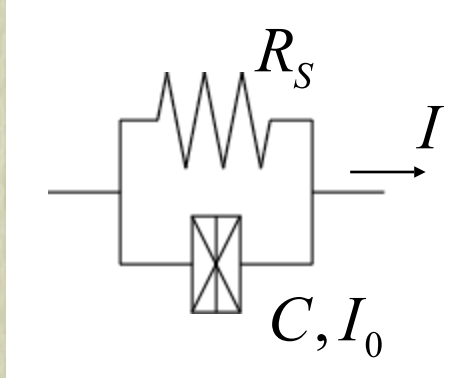
Parameter relations

$$\frac{\Delta}{\omega_c} = \rho J_\perp \qquad \alpha = \left(1 + \frac{2\delta}{\pi} \right)^2$$

$$\delta = -\frac{\pi \rho J_\parallel}{4} + O(J_\parallel^2)$$

Phase shift

Josephson devices



Classical equation of motion

$$C\left(\frac{\Phi_0}{2\pi}\right)^2\ddot{\phi}+\frac{1}{R}\left(\frac{\Phi_0}{2\pi}\right)^2\dot{\phi}+\frac{\partial V}{\partial\phi}=0$$

$$V(\phi)=-I\frac{\Phi_0}{2\pi}\phi-E_{\mathrm{J}}\cos\phi$$

E_{J} : Josephson energy

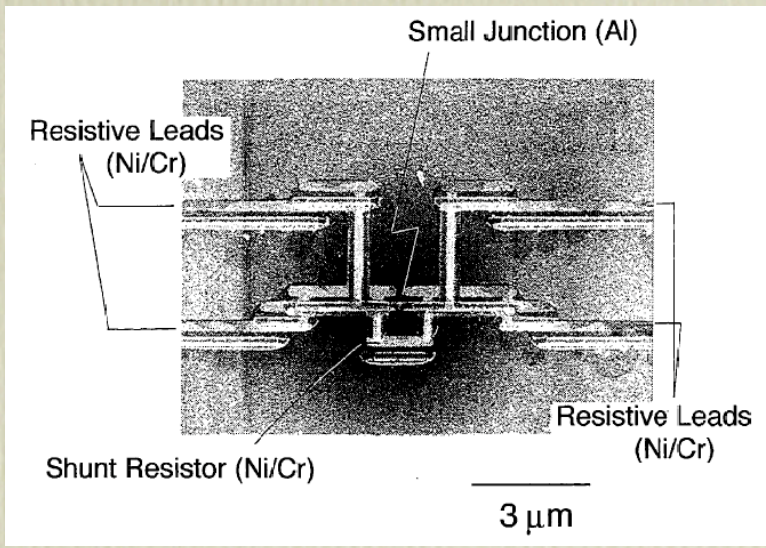
$E_{\mathrm{C}}=\dfrac{(2e)^2}{2C}$: Charging energy

$1/R$: Damping factor

Two control parameters

$$E_{\mathrm{J}}/E_{\mathrm{C}},\ \alpha=R_{\mathrm{Q}}/R$$

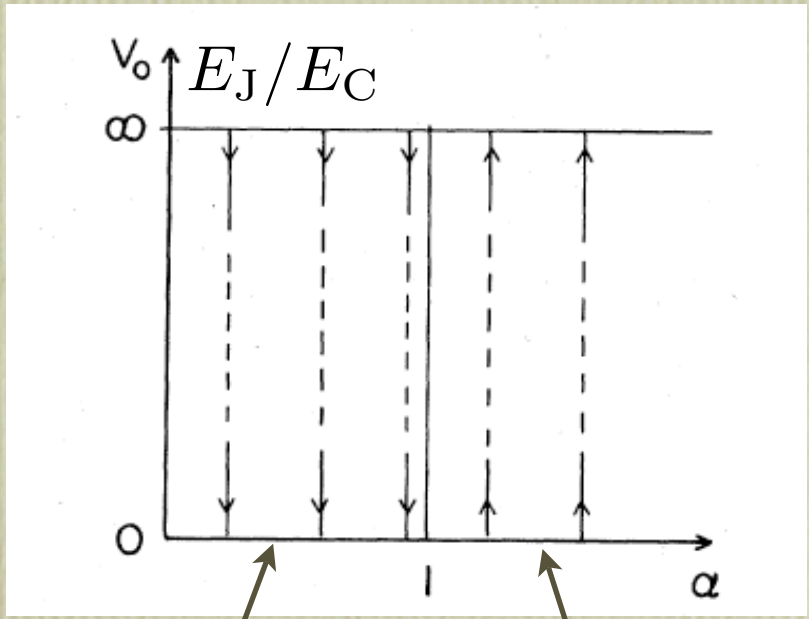
$(R_{\mathrm{Q}}=h/(2e)^2=6.45\ \mathrm{k}\Omega)$



Yagi et.al. 1997

Phase diagram

Renomalization group
(Perturbative approach)



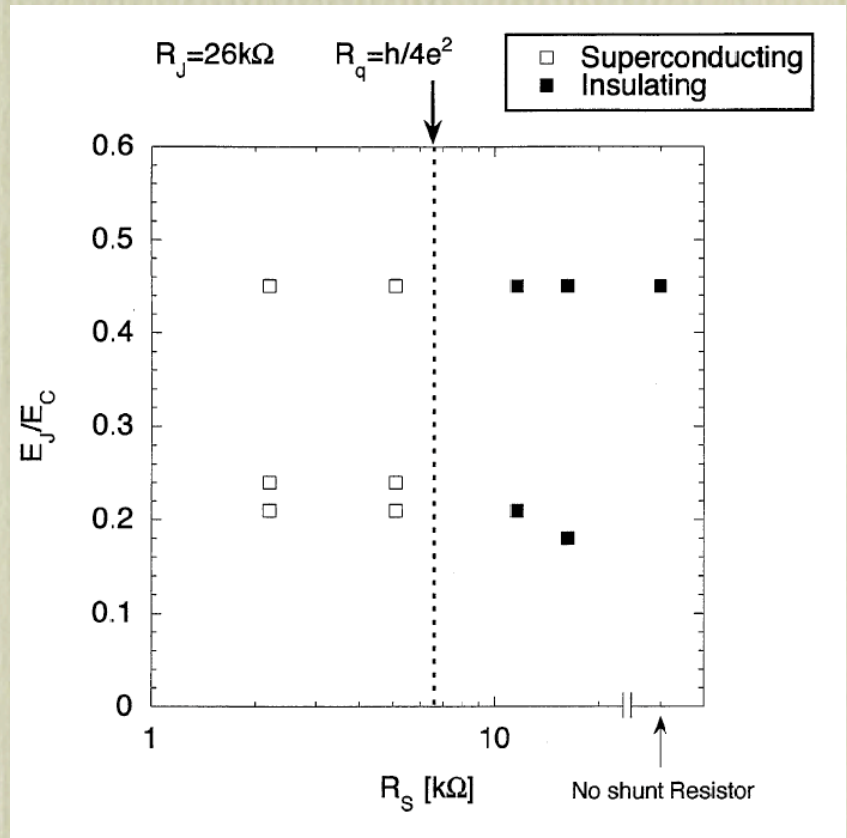
$\alpha = R_Q/R$

delocalized
(insulator)

localized
(superconductor)

Fisher-Zwerger 1985

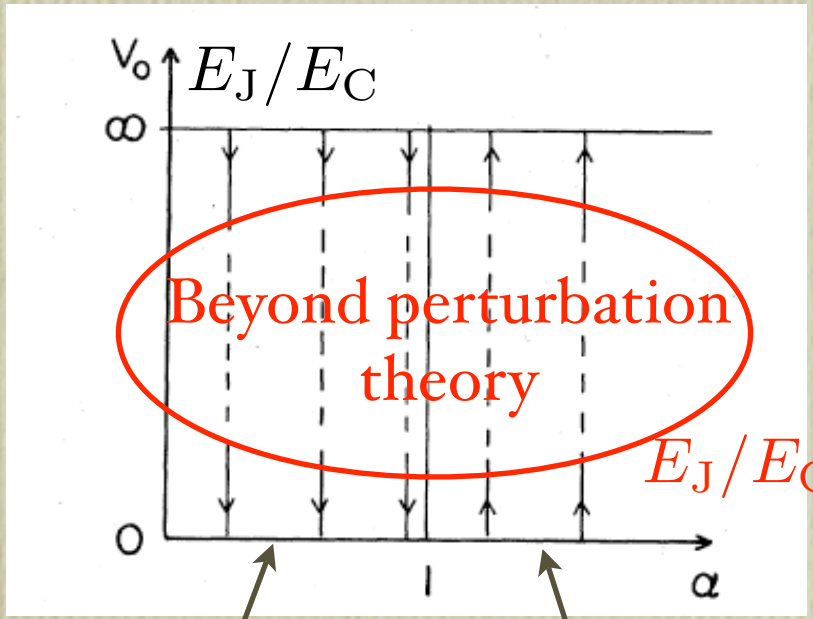
Experiment



Yagi et. al. 1997

Phase diagram

Renomalization group
(Perturbative approach)

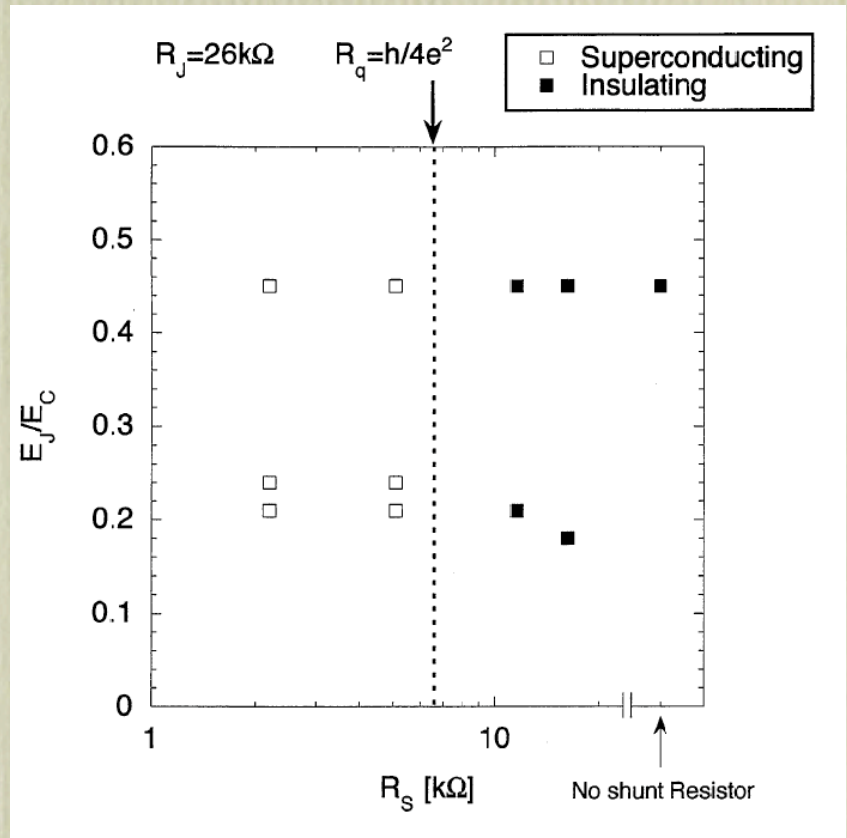


delocalized
(insulator)

localized
(superconductor)

Fisher-Zwerger 1985

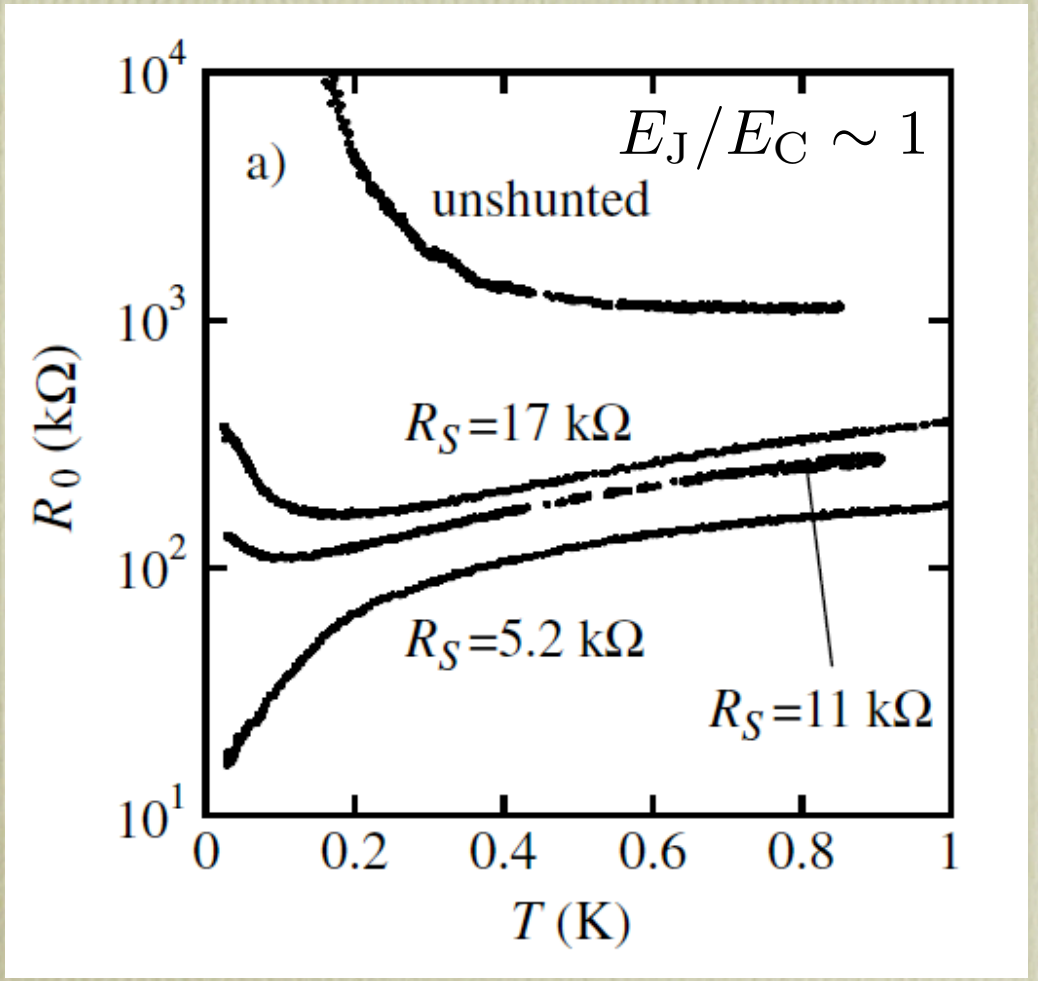
Experiment



Yagi et. al. 1997

Temperature dependence

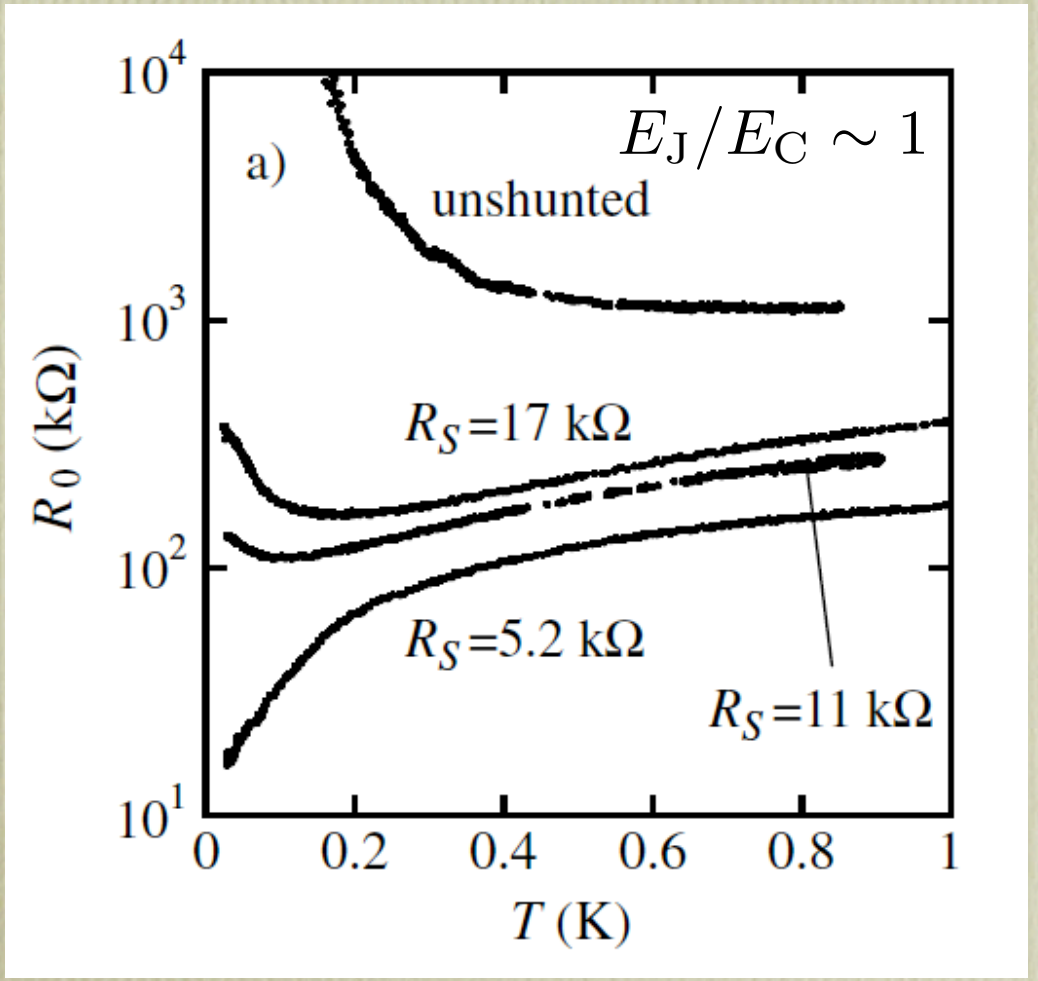
Miyazaki et.al. 2002



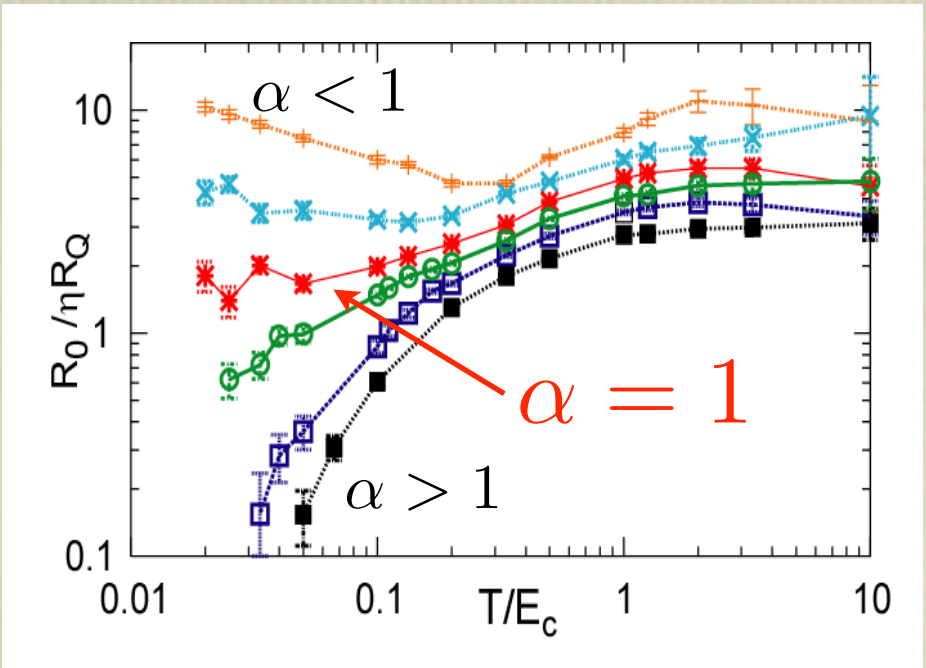
Phase transition at $\alpha = 1$

Temperature dependence

Miyazaki et.al. 2002



Kimura and TK, 2004



Numerical simulation by Path-Integral Monte Carlo

Phase transition at $\alpha = 1$

Path-Integral Monte Carlo

- Imaginary-time path-integral formulation
- Discretization of the particle path
- No approximation except for discretization errors
  - (Exact in the limit of the large Trotter number)
- Application to Helium 4, melting problem, etc.
- Local update, Uniform update, Cluster update
  - (Particle exchange for Bosonic systems)
- Improvement on local updates

Discretization of the path

$$Z = \oint \mathcal{D}q(\tau) \exp(-S_{\text{eff}})$$

$$S_{\text{eff}} = \int d\tau \left(\frac{1}{2} M \dot{q}^2 + V(q) \right) + \int d\tau \int d\tau' k(\tau - \tau') q(\tau) q(\tau')$$

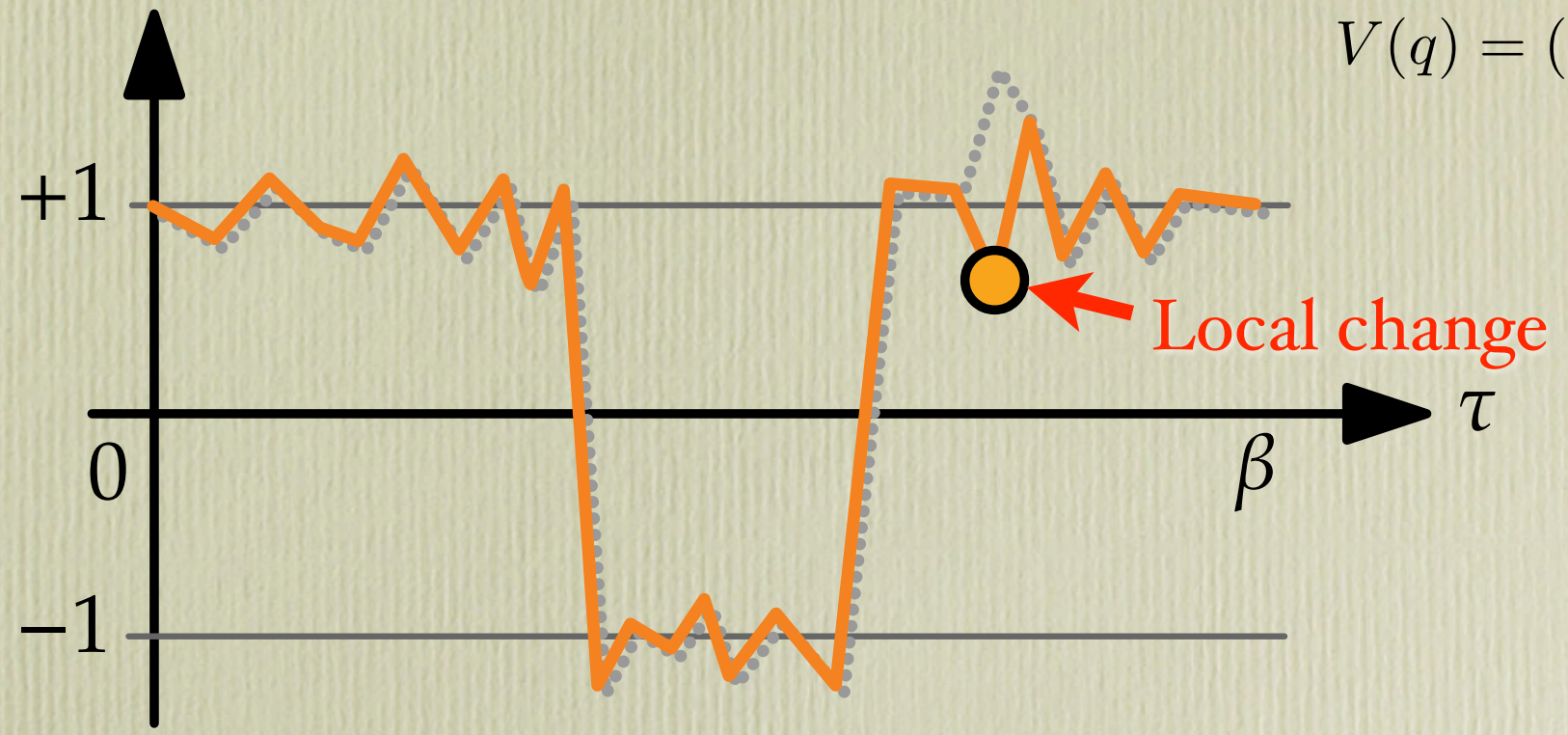
↓ Discretization $\quad q(\tau) \to q_j \quad (0 \le j \le N-1)$

$$Z = \int \prod_j \mathrm{d}q_j \exp(-S_{\text{eff}}(\{q_j\}))$$

$$S_{\text{eff}}(\{q_j\}) = \sum_{i<j} K(i-j) q_i q_j + \Delta\tau \sum_j V(q_j)$$

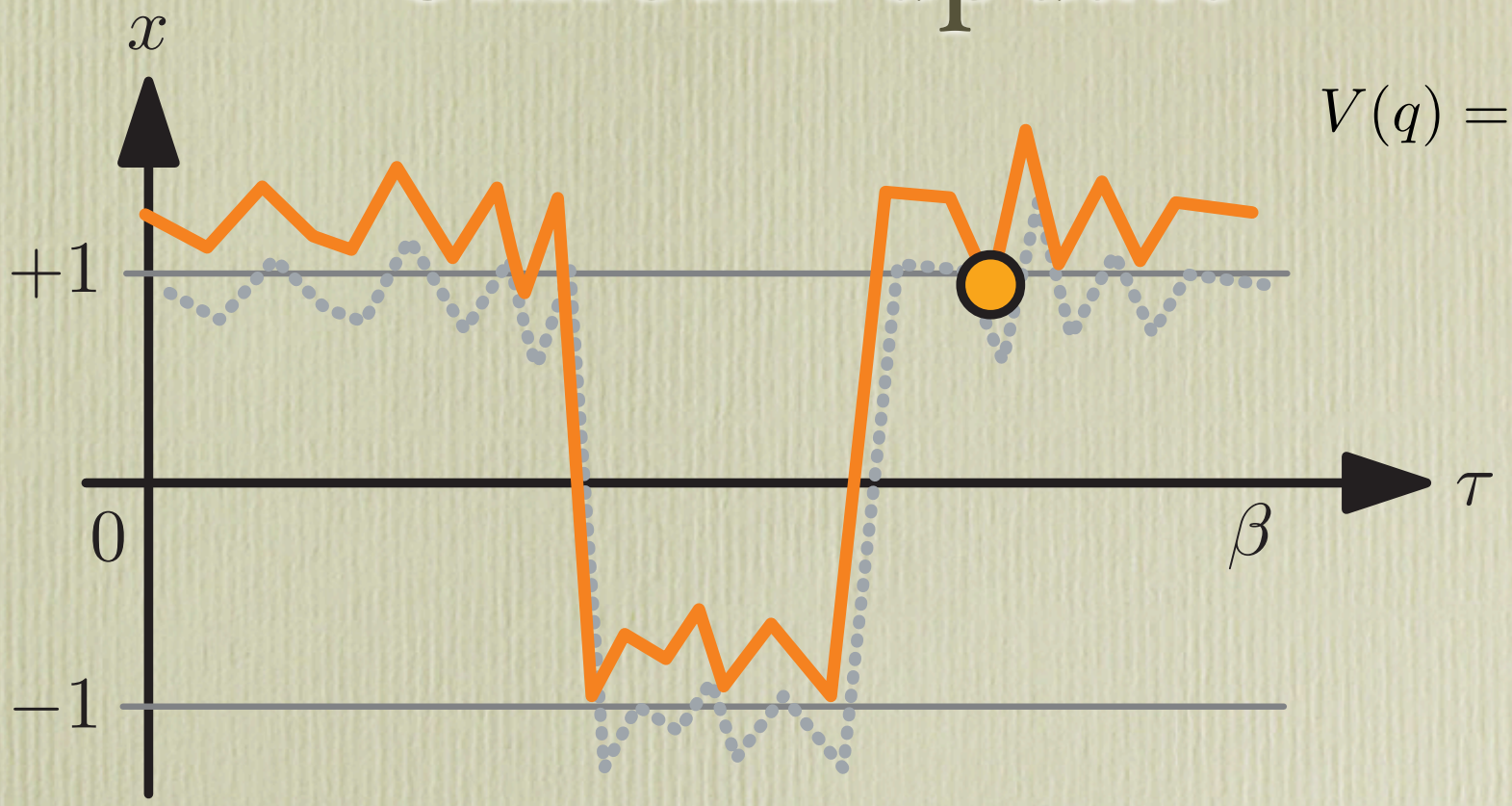
The problem is mapped to a classical statistics of 'polymers'

Local update (traditional)



1. Change the path locally as $q_j^{(\mathrm{new})} = q_j^{(\mathrm{old})} + \epsilon$ $\epsilon \in [-\delta, \delta]$ for fixed j
2. Generate a random number g
3. Accept this change if $g < \min[e^{-(S[\{q_j^{(\mathrm{new})}\}] - S[\{q_j^{(\mathrm{old})}\}])}, 1]$
4. Do this procedure for all path fragments

Uniform update

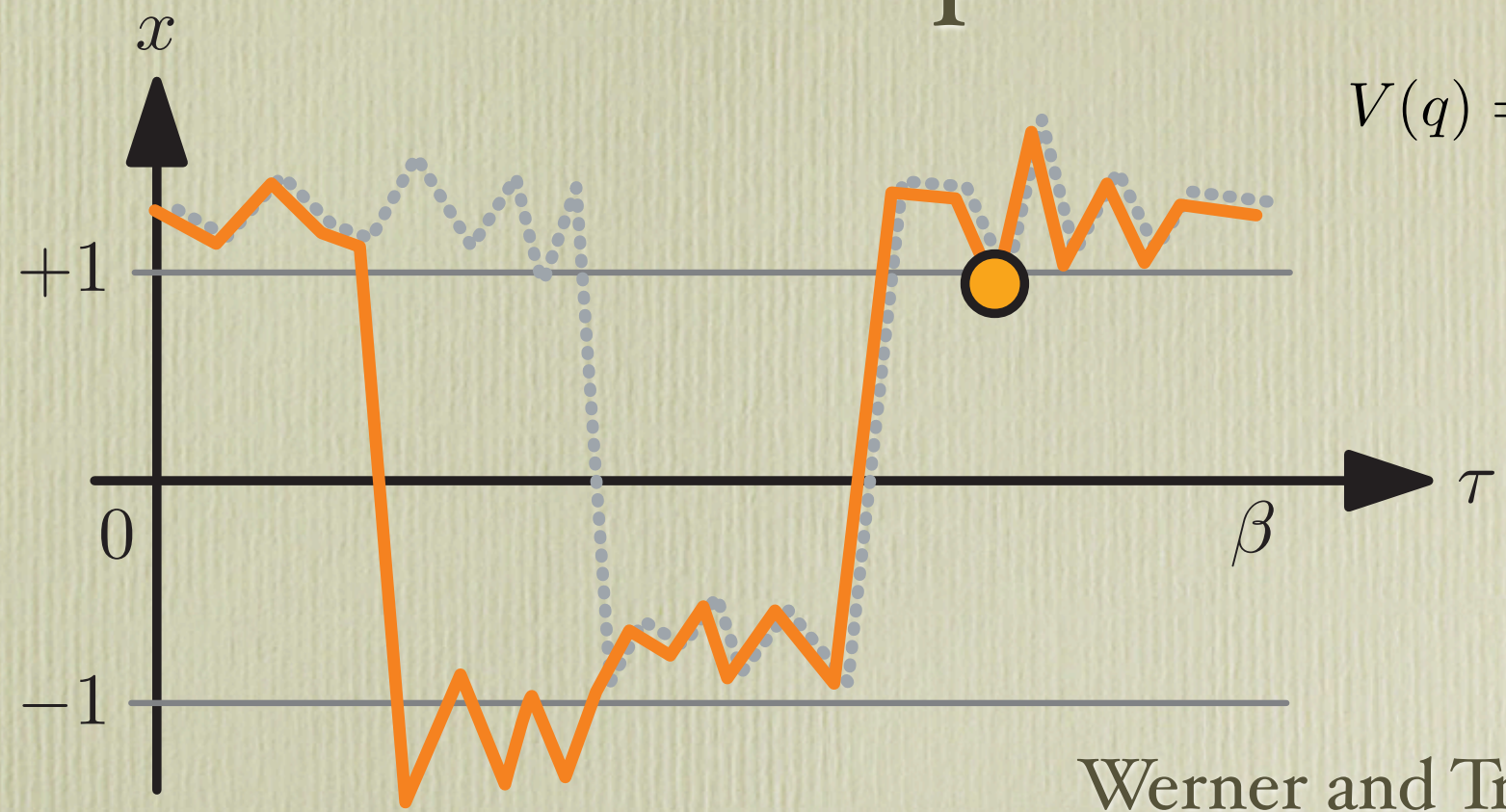


$V(q) = (q^2 - 1)^2$

1. Change the path uniformly as $q_j^{(\mathrm{new})} = q_j^{(\mathrm{old})} + \epsilon$ $\epsilon \in [-\delta, \delta]$ for all j
2. Generate a random number $g \in [0, 1]$
3. Accept this change if $g < \min[e^{-(S_{\mathrm{pot}}[\{q_j^{(\mathrm{new})}\}] - S_{\mathrm{pot}}[\{q_j^{(\mathrm{old})}\}])}, 1]$

(This update becomes important for high temperatures.)

Cluster update



$V(q) = (q^2 - 1)^2$

Werner and Troyer, 2005

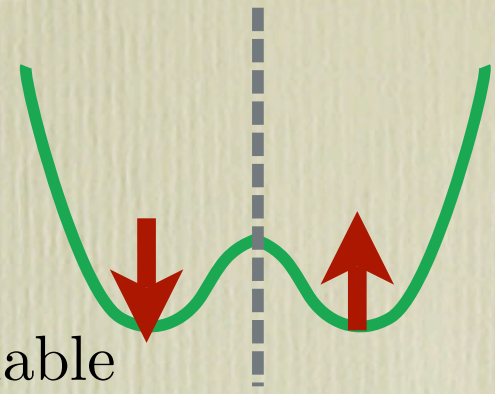
1. Define a cluster by choosing the path fragments.

(Details of cluster construction is described next.)

2. All the path fragments of the cluster is changed as $q_j \to -q_j$

Cluster construction

$$
\begin{aligned}
S &= \sum_{i<j} K(i-j) q_i q_j \\
&= \sum_{i<j} K(i-j) |q_i||q_j| \sigma_i \sigma_j \\
&= \sum_{i<j} J(i-j) \sigma_i \sigma_j
\end{aligned}
$$



$q_i \equiv |q_i| \sigma_i$

σ_i : Ising variable

Potential term is irrelevant for sign change of the path

$$V(-q) = V(q)$$

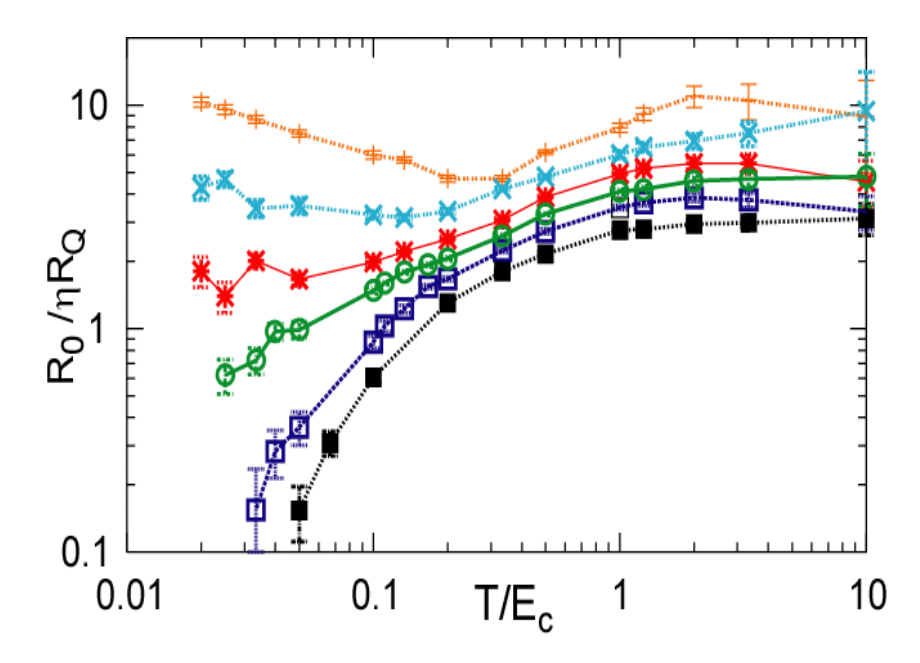
Wolff algorithm (long-range version)

1. Choose j randomly. Current spin = j. Add spin j to a stack.
2. Try to activte the bond between the current spin j and another spin k with the probability $1 - e^{-2J_{j,k}}$
3. Try this for all possible spin k. If successed, add spin k to a stack. Remove the current spin j from the stack.
4. Repeat 2 and 3 until the stack become empty.

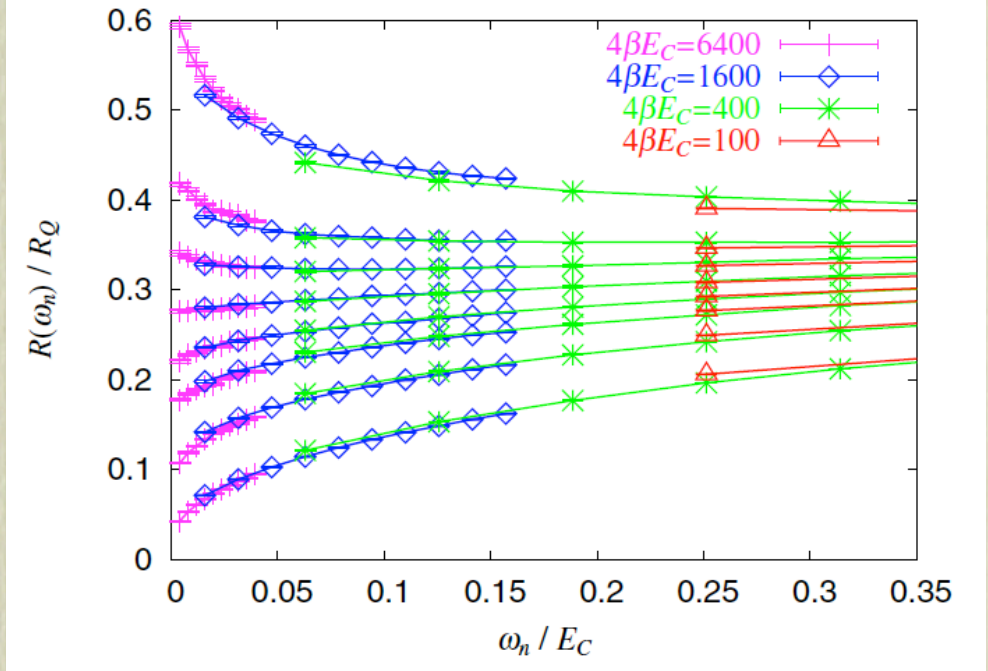
Comparison

Periodic potential $V(q) = \cos q$

Kimura and TK, 2004



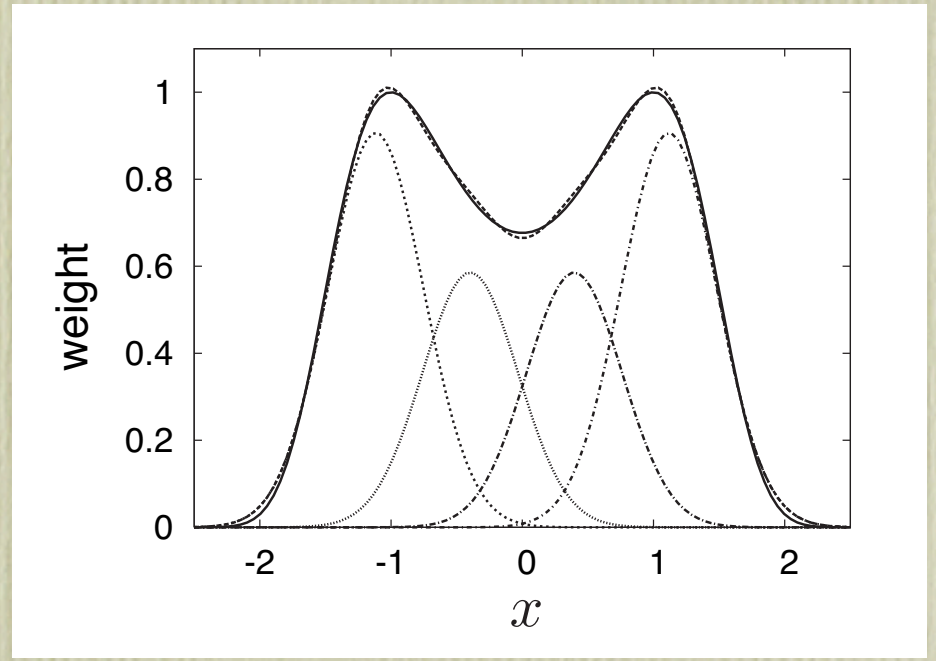
Werner and Troyer, 2005



Without cluster updates

With cluster updates

Improved local update



Double-well potential

$$V(q) = (q^2 - 1)^2$$

Approximate decomposition

$$e^{-\Delta\tau V(q)} \simeq \sum_{m=1}^{M} \mu_m e^{-\lambda(q-\sigma_m)^2}$$

(Matsuo and TK, unpublished)

$$Z = \sum_{\{m_j\}} \int \prod_j \mathrm{d}q_j \exp(-\tilde{S})$$

(Step 1) Path {q_j} is changed for fixed {m_j}

(Setp 2) Auxiliary field {m_j} is changed for fixed {q_j}

Improved local update (Step 1)

Consider the update $\{q_j\} \to \{m_j\}$

Weight

$$\exp(-S[\{q_j\},\{m_j\}]) = f(\{q_j\}) \prod_j w(q_j, m_j)$$

$$w(q_j, m_j) = \mu_{m_j} \exp(-\lambda(x_j - \sigma_{m_j})^2)$$

1. From the configuration q_j, choose m_j with the probability

$$t(m_j|q_j) = \frac{w(q_j, m_j)}{\sum_{m_j} w(q_j, x_j)}$$

2. This update can be done efficiently, because only local information is needed for it.

Improved local update (Step 2)

Consider the update $\{m_j\} \to \{q_j\}$

$$
\begin{aligned}
S &\simeq \sum_n \left(c_n |\tilde{q}_n|^2 + \lambda N |\tilde{q}_n - \tilde{\sigma}_n|^2 \right) \\
&\simeq \sum_n (c_n + \lambda N) \left| \tilde{q}_n - \frac{\lambda N \tilde{\sigma}_n}{c_n + \lambda N} \right|^2
\end{aligned}
$$

$$
c_n = \frac{16N^2}{\beta g^2} \sin^2 \frac{\pi n}{N} + \frac{\pi^2 \alpha}{2} |n|
$$

$$
q_j = \sum_n \tilde{q}_n e^{-2\pi \mathrm{i} jn/N}
$$

$$
\sigma_j = \sum_n \tilde{\sigma}_n e^{-2\pi \mathrm{i} jn/N}
$$

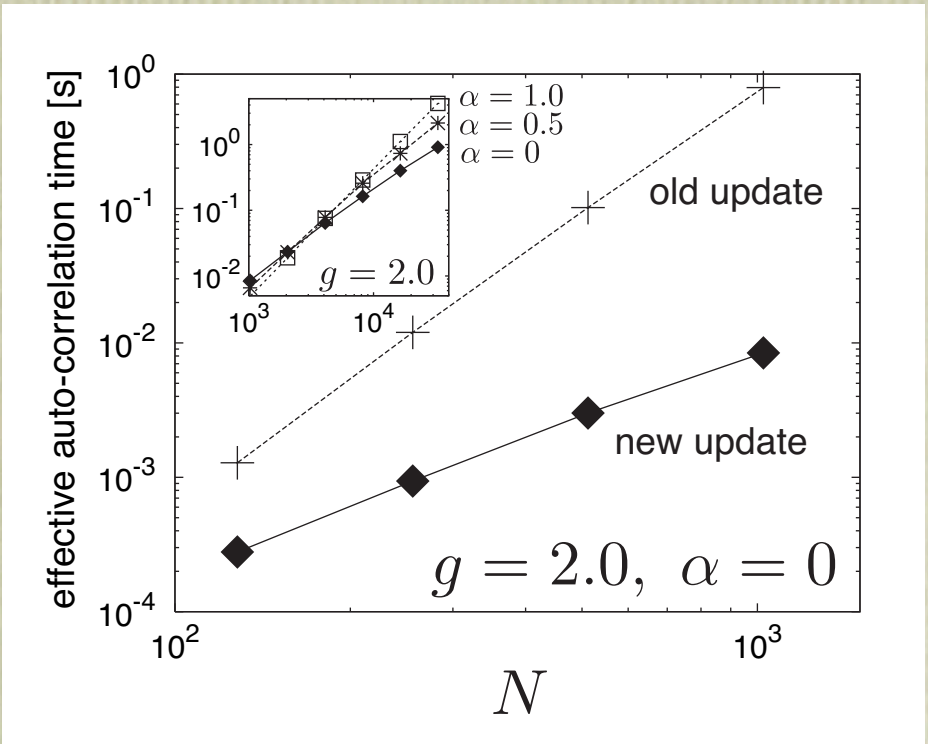
1. Calculate the Fourier components.
2. Generate a random number with the Gaussian distribution with the average $\dfrac{\lambda N \tilde{\sigma}_n}{c_n + \lambda N}$ and width $\dfrac{1}{2\sqrt{c_n + \lambda N}}$
3. All the Fourier components are updated at once.

   (No rejection. Very efficient.)

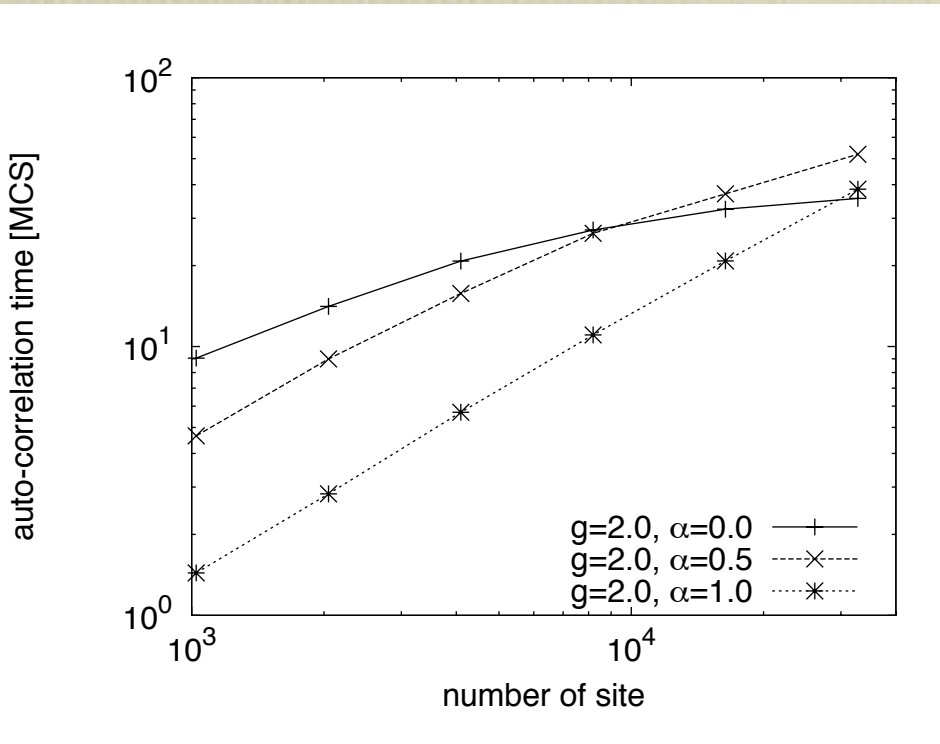
Efficiency

$$V(q) = (q^2 - 1)^2$$

Effective CPU time



Auto-correlation time



Traditional $O(N^2 \log N)$

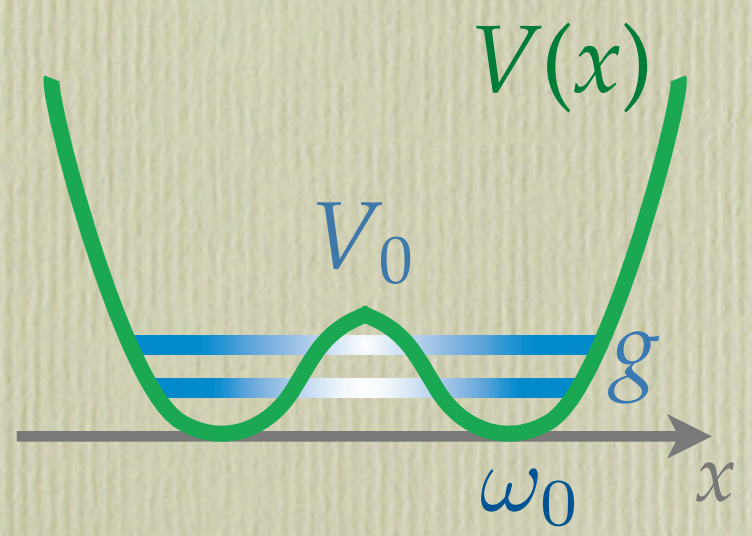
Improved $O(N \log N)$

Local update O(1)

Cluster update O(N)

Localization transition

$$g = \frac{\hbar\omega_0}{V_0}, \quad V_0 = 1$$



$$Z = \int \mathcal{D}q(\tau) \exp(-S[q(\tau)])$$

$$S[q(\tau)] = \int d\tau \left\{ \frac{4}{g} \left(\frac{dq}{d\tau} \right)^2 + (q^2 - 1)^2 \right\} - \int d\tau \int d\tau' k(\tau - \tau') q(\tau) q(\tau')$$

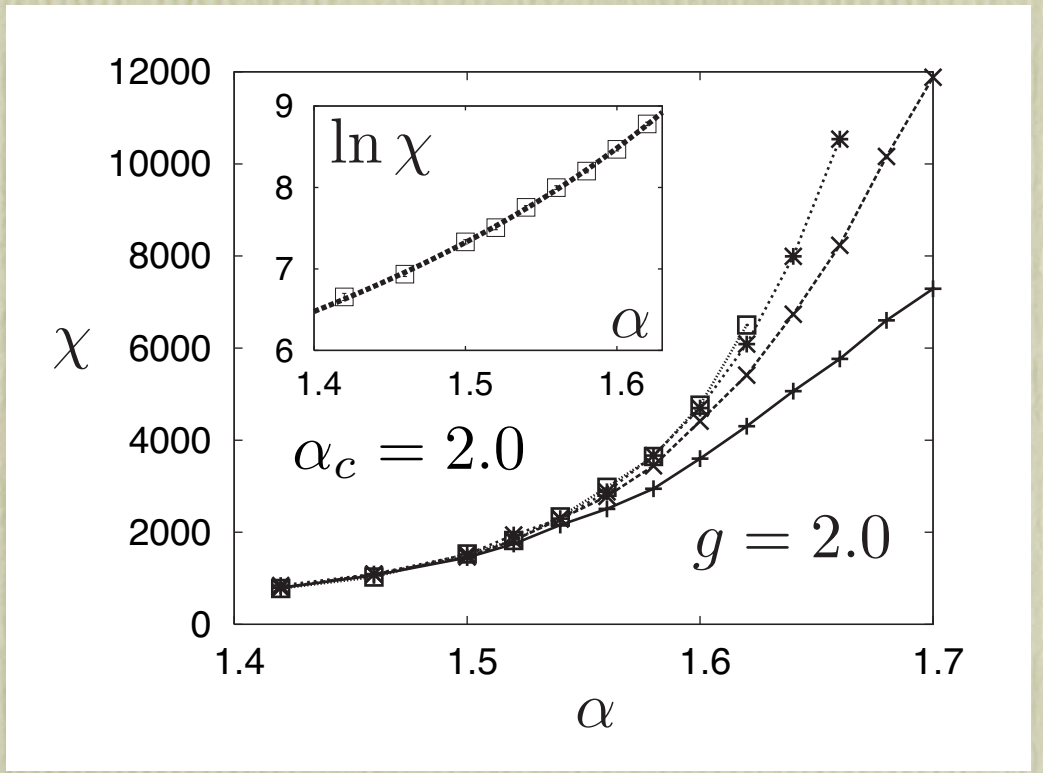
Two-state limit

$$g \to 0 \ : \ \alpha_c = 1$$

Problem : Localization transition for general g

Is there localization transition even when quantum fluctuation dominates the potential barrier?

Determine the critical point



$N = 2^{14}, 2^{15}, 2^{16}, 2^{17} (\simeq 1.2\times) 10^5$

Susceptability

$$\chi \equiv \langle \frac{1}{N^2} \sum_{i,j} q_i q_j \rangle / \langle \frac{1}{N} \sum_j q_j \rangle^2$$

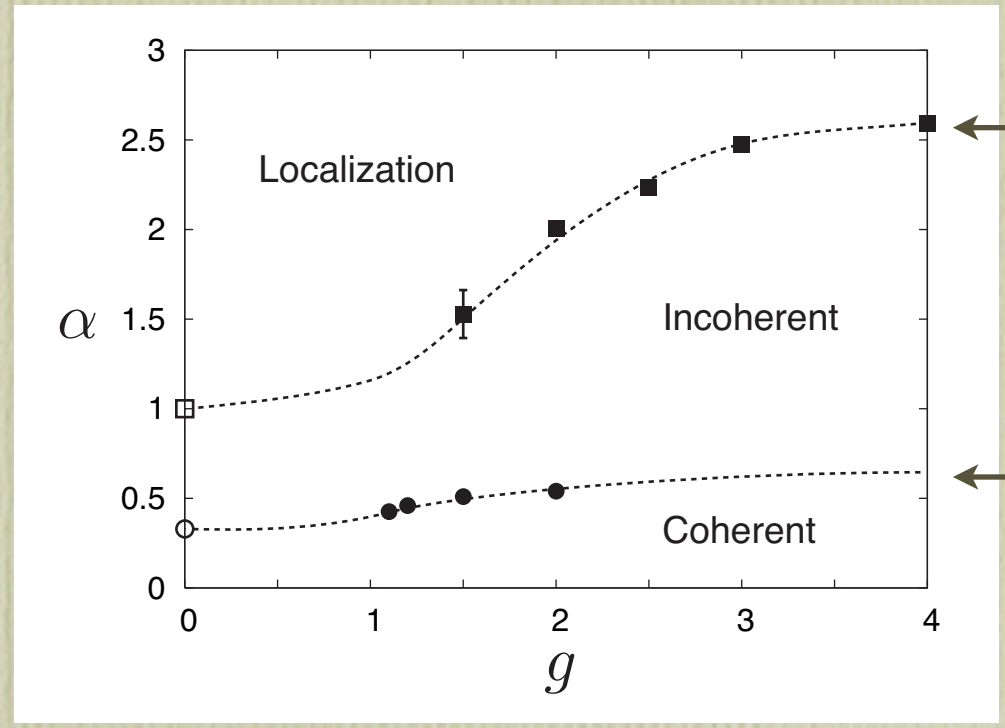
Long-range Ising universality

$$\chi \propto e^{b_1 |\alpha - \alpha_c|^\nu + b_2 |\alpha - \alpha_c|^{-\nu}}$$

$$\nu = 1/2$$

Kosterlitz-Thouless transtion (Luijten 2001)

Phase diagram



← Localization transition

← Coherent-incoherent crossover

1. Localization transition occurs even for a small barrier.

   cf. Renormalization approach by Fisher et.al.

2. Tendency of saturation in critical dissipation strength

Summary

- Brief introduction to ‘dissipative quantum systems’
- Brief review on Path-Integral Monte Carlo (PIMC)
- Recent improvement of local updates
- Future problems: Application to other systems
  - Impurity problem in Tomonaga-Luttinger Liquid
  - Field theoretical model, e.g., phi4 model
  - Phonon: Nonlinearity, electron-phonon