Development and Application of Worm-type Algorithm in Classical and Quantum Lattice Models

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Outline

◆Worm Algorithm

- Markovian-Chain Monte Carlo (MCMC) method
- Worm algorithm for Ising and Bose-Hubbard models
- Worm algorithm for other models

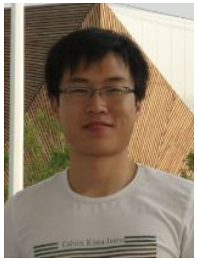
◆ Applications

- Quantum critical dynamics
- N-component loop models

Nikolay Prokof’ev
UMass, Amherst

Boris Svistunov
UMass, Amherst

Timothy Garoni
Monash University



Qingquan Liu
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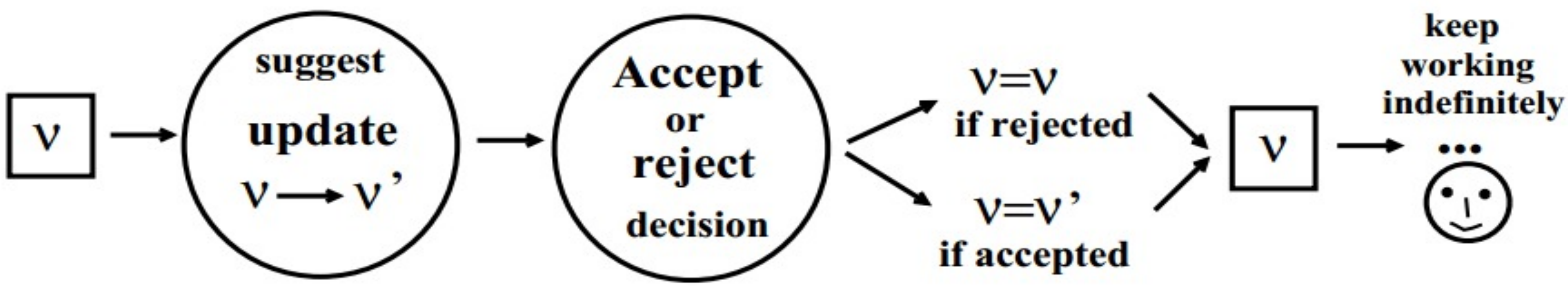
Introduction to MCMC

- **Given a statistical system—e.g, Ising model**

Partition Sum: $Z = \sum_{\nu} W_{\nu}$ (W_{ν} : weight of configuration ν)

To-be-calculated observable: $\langle A \rangle = \sum_{\nu} A(\nu) W_{\nu} / Z$

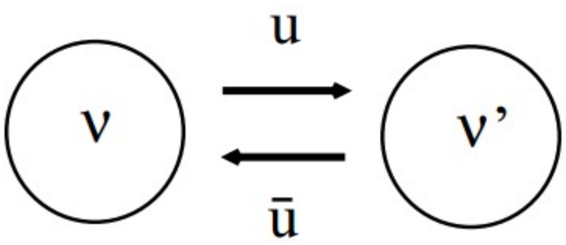
- **Procedure for Markov-Chain Monte Carlo method**



GOAL: Probability of each configuration $\propto W_{\nu}$

Introduction to MCMC

- **Sufficient conditions**



  – Detailed balance (easy to satisfy)

$$W_{\nu} p_u P_u^{acc}(\nu \to \nu') = W_{\nu'} p_{\bar{u}} P_{\bar{u}}^{acc}(\nu' \to \nu)$$

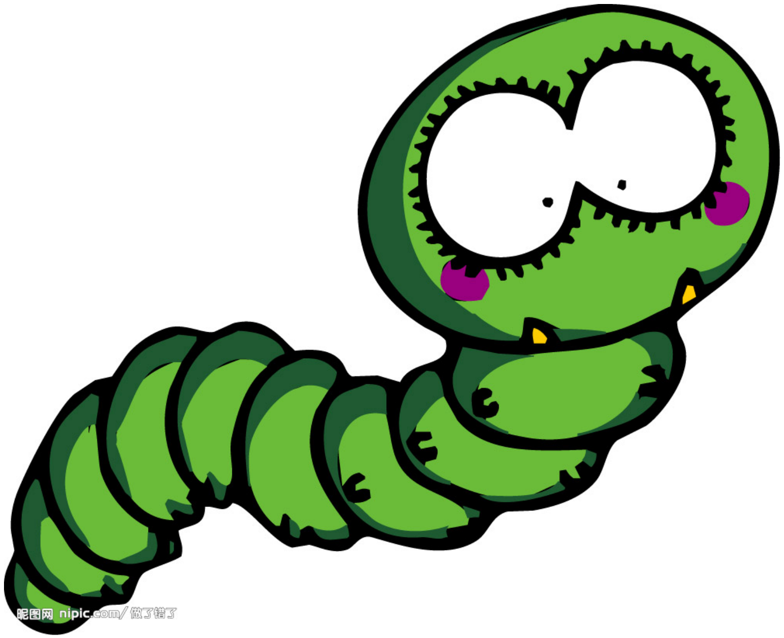
p_u : probability to choose "update u"

$P_u^{acc}(\nu \to \nu')$: acceptance probability

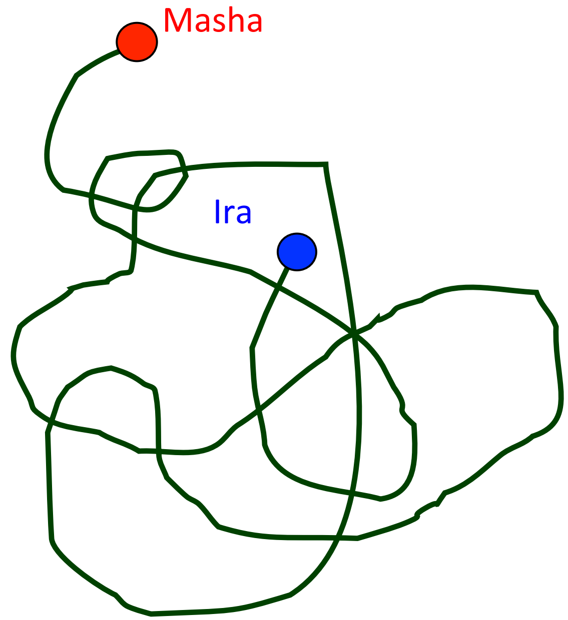
  – Ergodicity (difficult to prove)

➢ Different update schemes ←→ Different algorithms

What is worm?



A cartoon picture of a worm

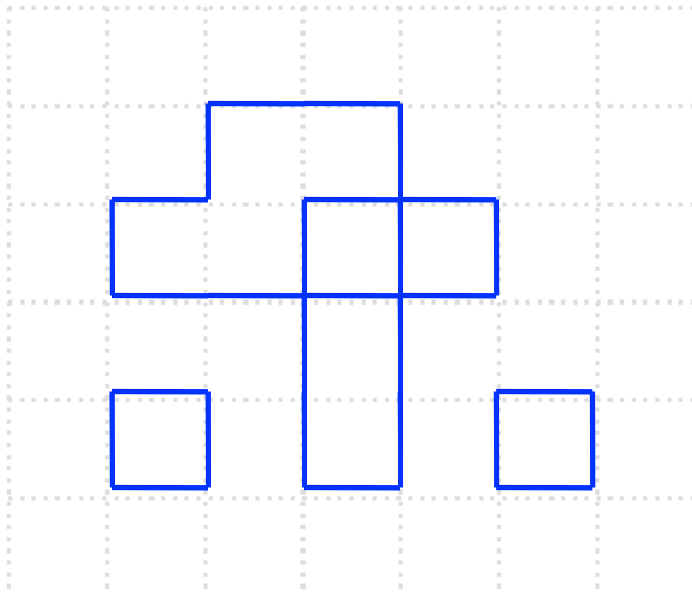


Worm in worm algorithm

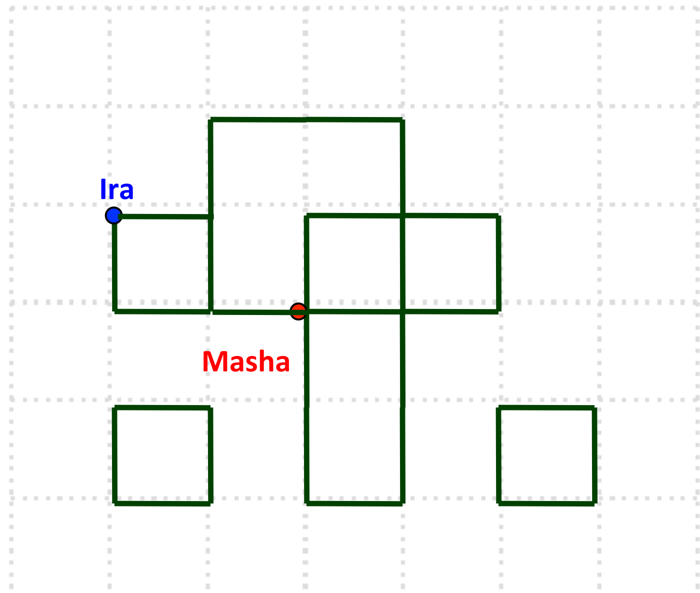
What is worm?

Configuration space $\{v\}$:

close loops



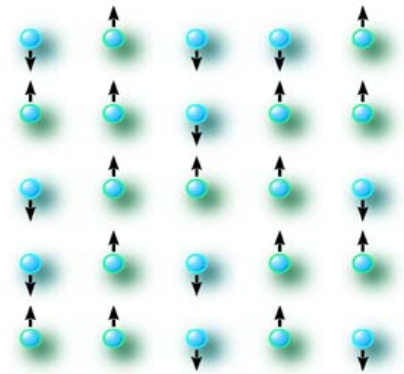
Worm state space (A,I,M)



Simple Idea: Extend configuration space!

Worm algorithm for Ising model

- **Ising model**



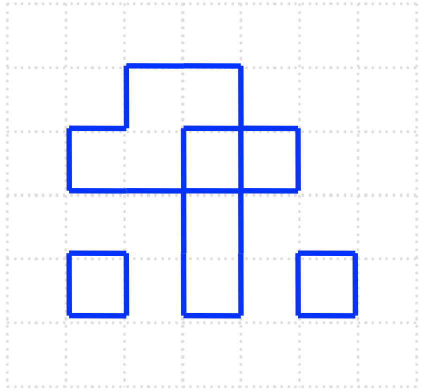
Consider the Ising model on G

$$Z_{\text{Ising}} = \sum_{\sigma \in \{-1,+1\}^V} \prod_{ij \in E} e^{\beta \sigma_i \sigma_j}$$

$\Downarrow$

The high-temperature expansion is

$$Z_{\text{Ising}} = \left(2^{|V|} \cosh^{|E|} \beta\right) \sum_{A \in \mathcal{C}(G)} (\tanh \beta)^{|A|}$$

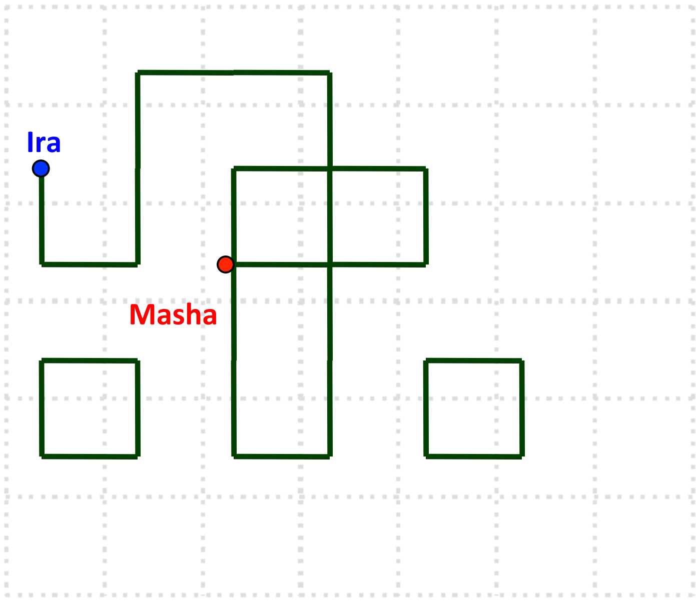


Worm algorithm for Ising model

- **Partition sum in worm sector:**

$$Z_{worm} = \sum_{\{(A,I,M)\}} \tanh \beta^{|A|}$$

Worm state space (A,I,M)



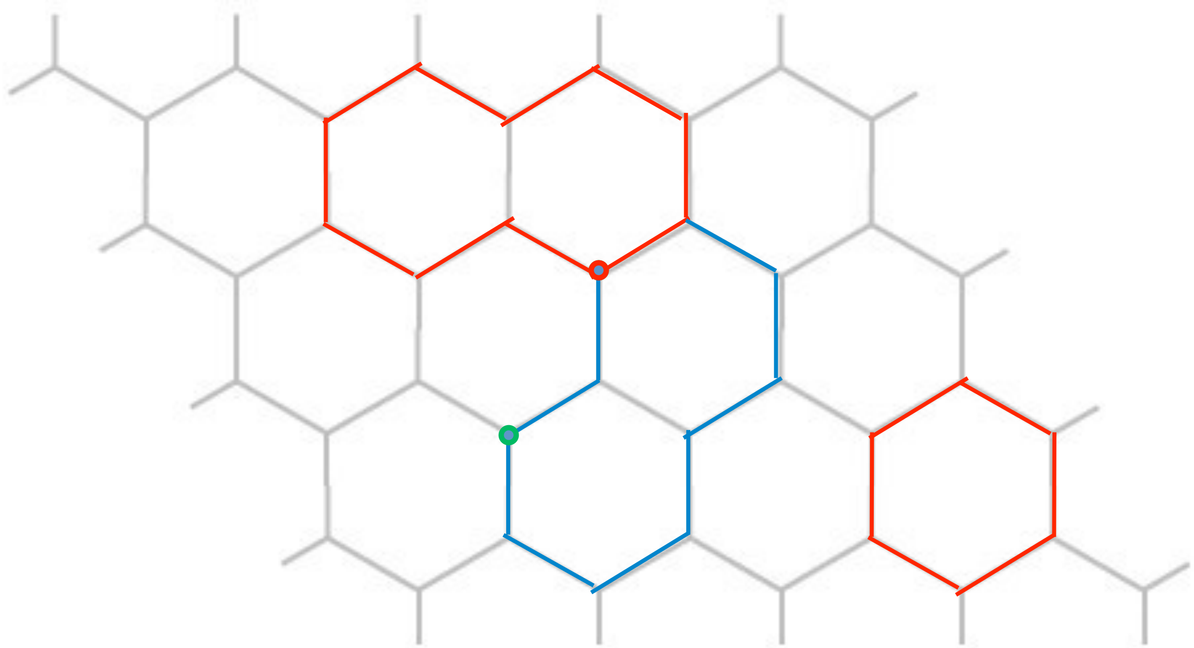
Standard worm update

i) Start in configuration (A, I, M)
ii) Pick I or M, say I
iii) Choose one of I's neighbor, say L
iv) Propose $(A, I, M) \to (A\Delta IL, L, M)$
v) Accept the propose with probability p

! Just a Metropolis method.

Worm algorithm for Ising model

- **Demonstration**



Worm Algorithm for Bose-Hubbard Model

An efficient update scheme for the continuous-time (imaginary) path-integral (world-line) representation of interacting bosonic or spin systems without sign problem.

Interacting Particles on a lattice:

$$H = H_0 + H_1 = \sum_{ij} U_{ij} n_i n_j - \sum_i \mu_i n_i \quad - \sum_{<ij>} t(n_i, n_j)\, b_j^+ b_i$$

diagonal

off-diagonal

$$Z = \mathrm{Tr}\, e^{-\beta H} \equiv \mathrm{Tr}\, e^{-\beta H_0}\, e^{-\int_0^\beta H_1(\tau)\, d\tau}$$

$$H_1(\tau) = e^{\beta H_0} H_1\, e^{-\beta H_0}$$

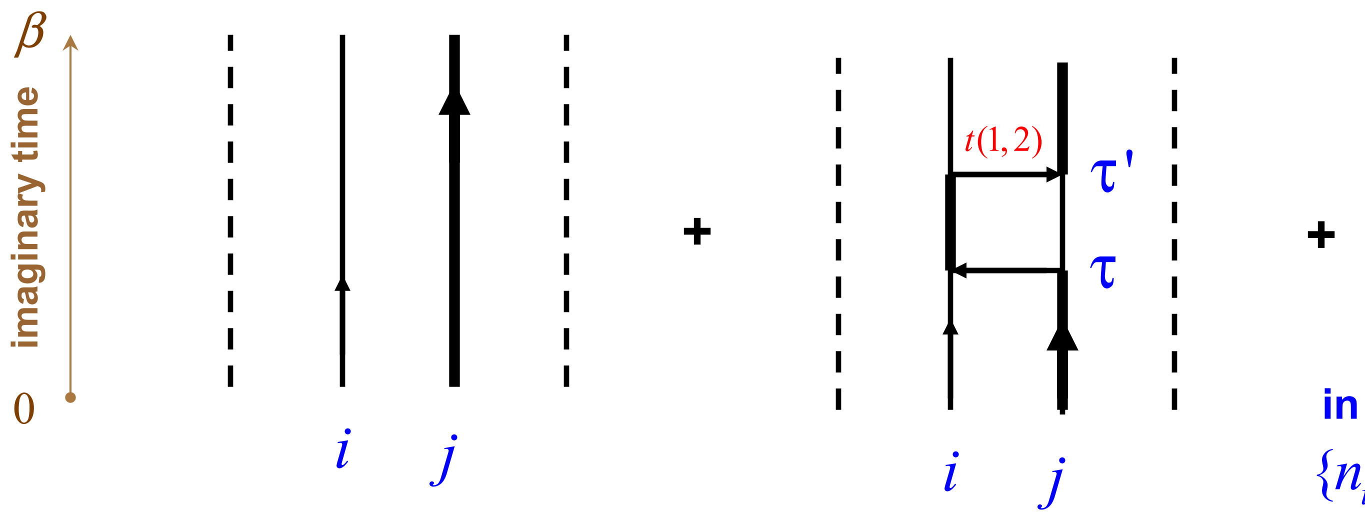
$$= \mathrm{Tr}\, e^{-\beta H_0} \left\{ 1 - \int_0^\beta H_1(\tau)\, d\tau + \int_{\tau'}^\beta \int_0^\beta H_1(\tau)\, H_1(\tau')\; d\tau\, d\tau' + \ldots \right\}$$

In the diagonal basis set (occupation-number representation): $\langle \{n_i\} | = \langle \{n_1, n_2, n_3, \ldots\} |$

$$Z = \sum_{\{n_i\}} \left\langle \{n_i\} \right| \; e^{-\beta H_0} - \int_0^\beta e^{-(\beta-\tau) H_0} H_1 e^{-\tau H_0}\; d\tau + \int_{\tau'}^\beta \int_0^\beta e^{-(\beta-\tau) H_0} H_1\, e^{-(\tau-\tau') H_0} H_1\, e^{-\tau' H_0}\; d\tau\, d\tau' + \ldots \left| \{n_i\} \right\rangle$$

Each term describes a particular evolution of $\{n_i\}$ as imaginary "time" increases

0-order term **one of the 2-order terms**



in this example

$\{n_i\} = 0, 1, 2, 0$

$$Z = \sum_{\{n_i(\tau)\}} e^{-\int_0^\beta U(\{n_i(\tau)\})\, d\tau} \prod_{k=1}^{K} \left\langle \{n_i(\tau_k + 0)\} \,|\, (-H_1 d\tau_k) \,|\, \{n_i(\tau_k - 0)\} \right\rangle$$

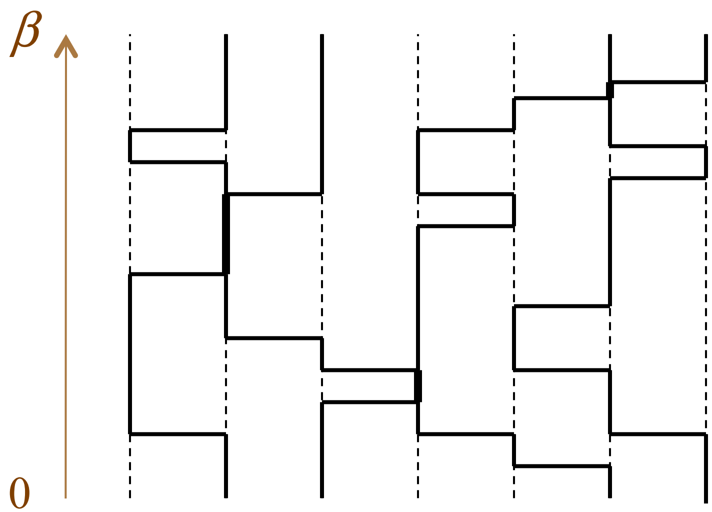
all possible trajectories
for N particles with
K hopping transitions

potential
energy
contribution

off-diagonal matrix elements for the trajectory with K kinks at times
$\beta > \tau_K > \ldots > \tau_2 > \tau_1 > 0$ (ordered sequence on the β -cylinder)

in this example, for K=2, it equals
$t\sqrt{2} \times t\sqrt{2}$ **for bosons**

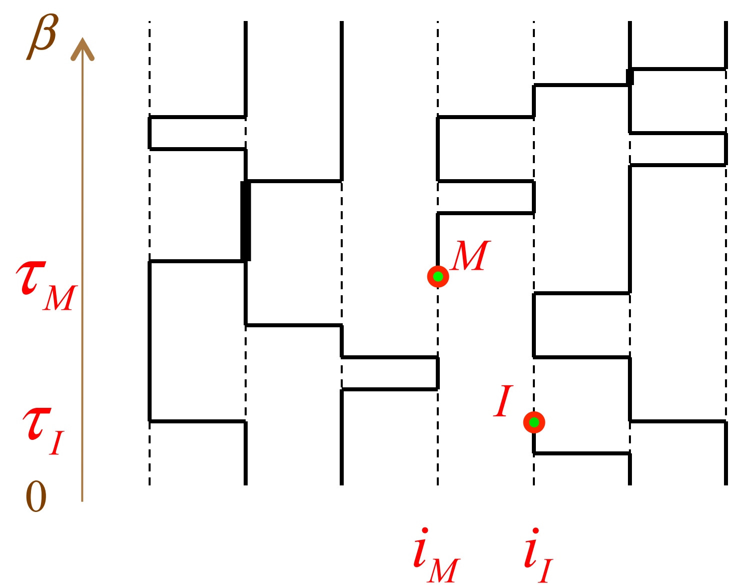
high-order term for $Z = \mathrm{Tr}\, e^{-\beta H}$



Similar expansion in hopping terms for

$$G_{IM} = \mathrm{Tr}\, b_M^+(i_M, \tau_M)\, b_I(i_I, \tau_I)\, e^{-\beta H}$$

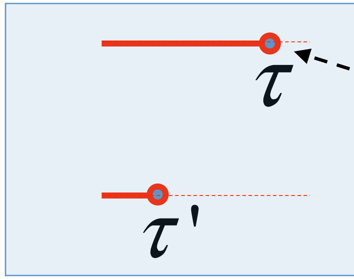
+ two special points for Ira and Masha



The rest is worm algorithm in this $Z \cup G_{IM}$ configuration space:
draw and erase lines using exclusively Ira and Masha

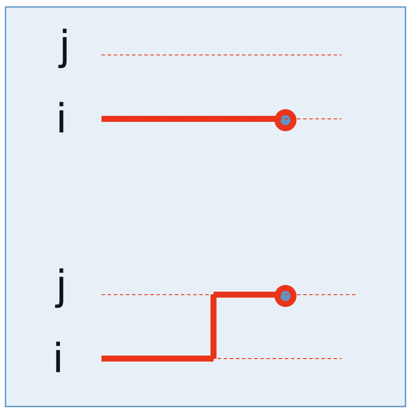
ergodic set of local updates

time shift:

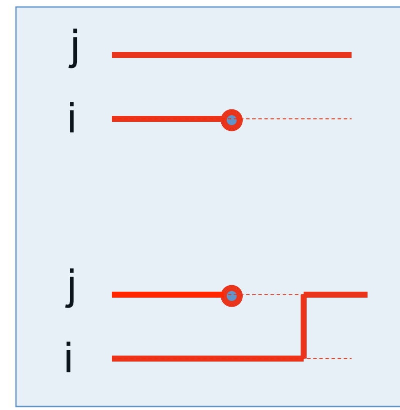


Ira or Masha

space shift ("particle" type):

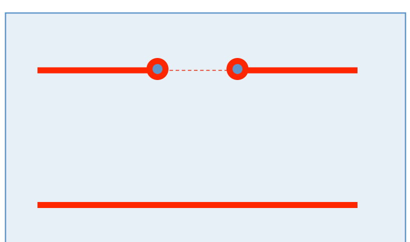


space shift ("hole" type):

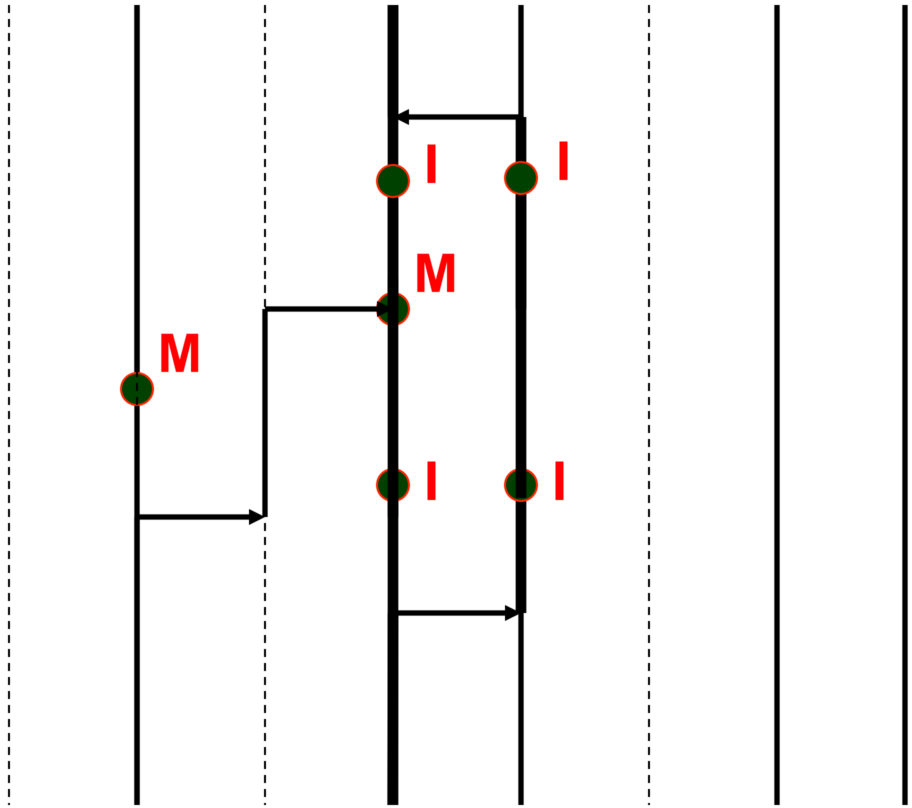


Insert/delete Ira and Masha:

$Z \leftrightarrow G$



connects Z and G configuration spaces


I
I
M
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Worm Algorithm for Other Models

- **XY model (reduced Hamiltonian)**

$$H = -J\sum_{<i,j>} \vec{S}_i \vec{S}_j \qquad \vec{S}_i = (S_i^x, S_i^y) \text{ and } \vec{S}_i^{\,2} = 1$$

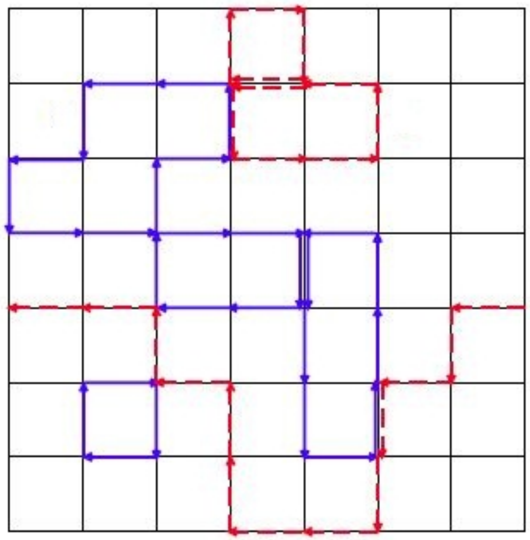
Partition sum

– Spin representation

$$Z_{spin} = \int \prod_{<i,j>} \exp(J\vec{S}_i\vec{S}_j)\prod_k d\vec{S}_k$$

- Graph representation

$$Z_{XY} = \prod_{<i,j>} \sum_{l_{i,j}}{}' I_{l_{i,j}}(\beta)$$



Oriented Loops (current):

Kirchoof law for each site!

- More general current models can be formulated—e.g, Villain model.
- Worm algorithm can be easily formulated.

Worm Algorithm for Other Models

- **N-component loop model on cubic lattices**
  - Spin representation

$$Z_{spin} = \int \prod_{<i,j>} (1 + J\vec{S}_i \cdot \vec{S}_j) \prod_k d\vec{S}_k$$

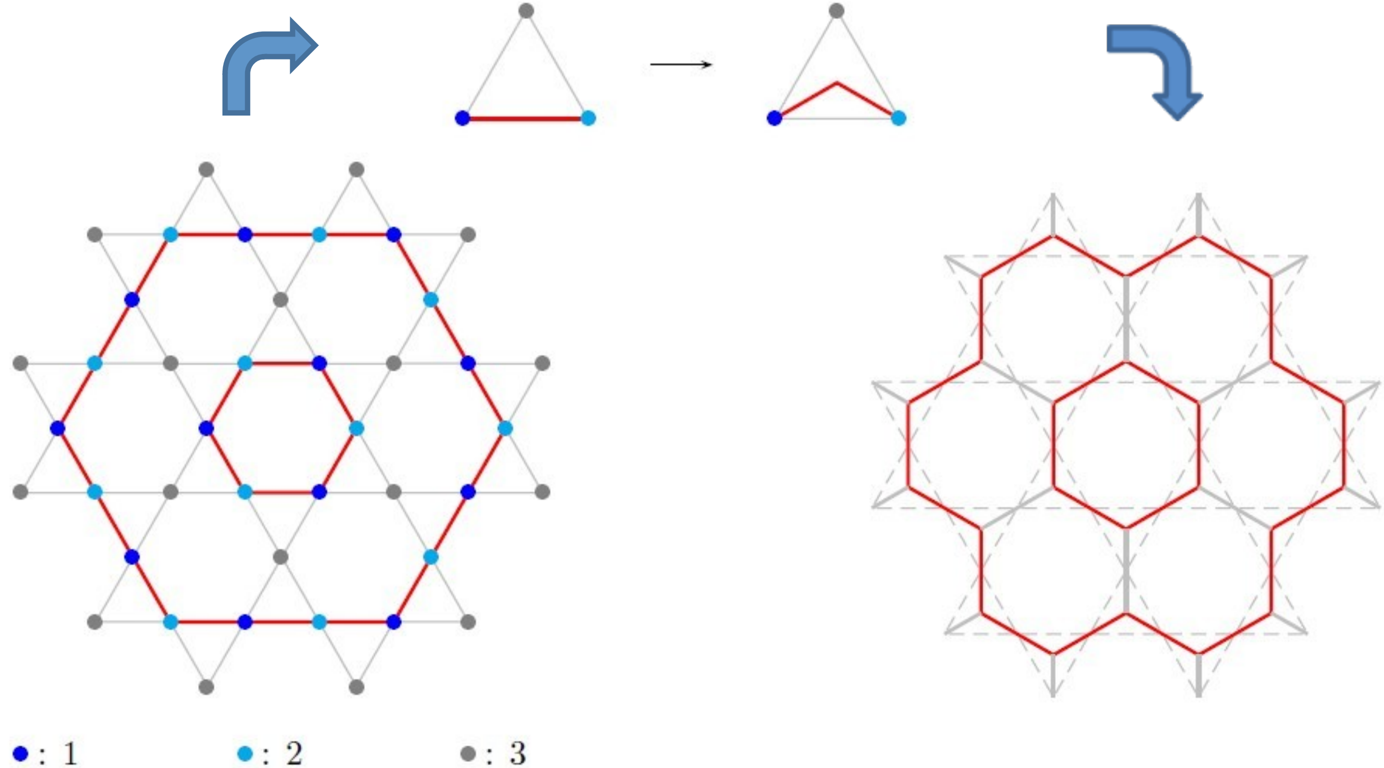
  - Graph representation

$$Z_{loop} = \sum_{\text{Non-intersecting loops}} x^{|A|} n^{|c|} \qquad (x = \tanh J)$$

- Parameter n can be non-integer.
- It plays an important role in the SLE theory in 2D.
- Worm algorithm needs to combine with other computational techniques. (--e.g, coloring technique, efficient search algorithm, rejection-free trick).
- Physics is less well known for D>2.
- Study becomes difficult without worm algorithm.

Worm Algorithm for Other Models

- **Coloring problem (T=0 Potts antiferromagnet)**
  - Ising antiferromagnet on triangular lattice
  - Three-coloring problem on kagome lattice
  - Four-coloring problem on triangular lattice



Worm Algorithm for Other Models

- **Planar/standard q-state Potts models**

  ➔ flow polynomial

- $|\varphi|^4$ **model**

  ➔ J-current model

- **Spin glass?**

Worm Algorithm for Other Models

- **Quantum spin models without sign problem**

  (multi-site interaction is allowed)

- **Fermions in 1D**

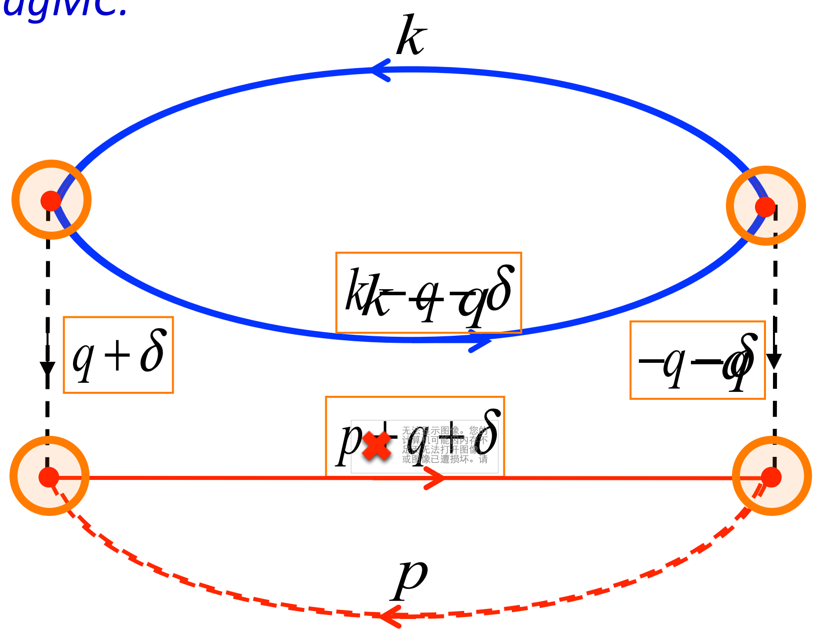
  (No sign problem in 1D)

- **Diagrammatic MC method for Fermionic systems**

Worm Algorithm for Other Models

Move worm in diagMC:

$$\Sigma(p) \mathrel{+}=$$



Now measure Σ

Do not measure Σ

Efficiency of Worm Algorithm

- **Ising model**
  - Near criticality, autocorrelation time $\tau \sim \xi^{z}$
  - D= 2 Ising model
    - Glauber (Metropolis) $z \approx 2$
    - Swendsen-Wang $z \approx 0.2$
    - Worm $z_{|A|} \approx 0.379$
  - D=3 Ising model
    - Worm $z_{|A|} \approx 0.174$
    - Swendsen-Wang $z \approx 0.46$

Efficiency of Worm Algorithm

- **Bosons/quantum spins**

From system sizes

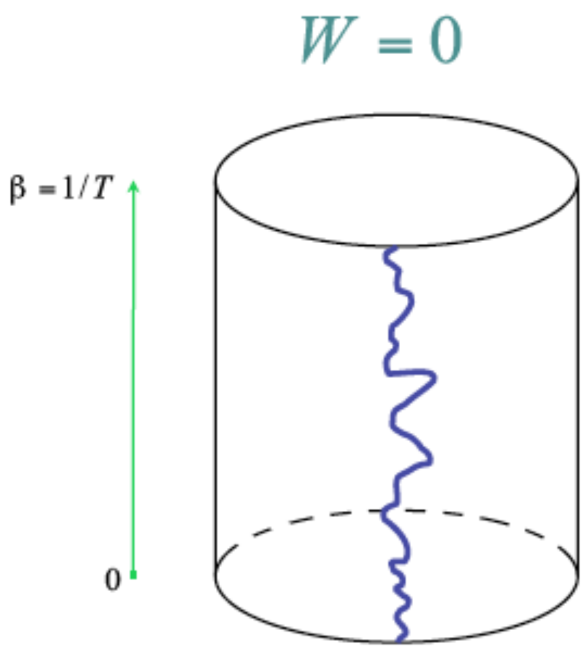
$$L^3 = 8^3$$

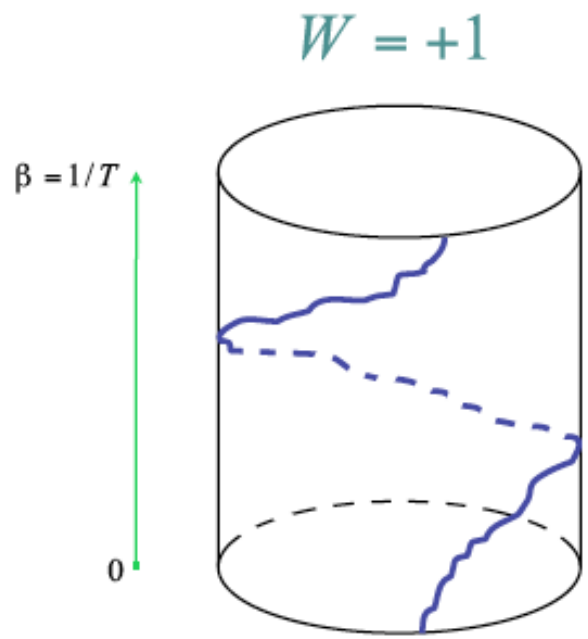
$$L^3 = 200^3$$

To system sizes

Efficiency of Worm Algorithm

- **Why is worm algorithm efficient:**
  - Easy to change topology
  - Capture two-point correlation/Green functions





Application I: probe Higgs resonance

- **Lagrangian in O(2) field theory**

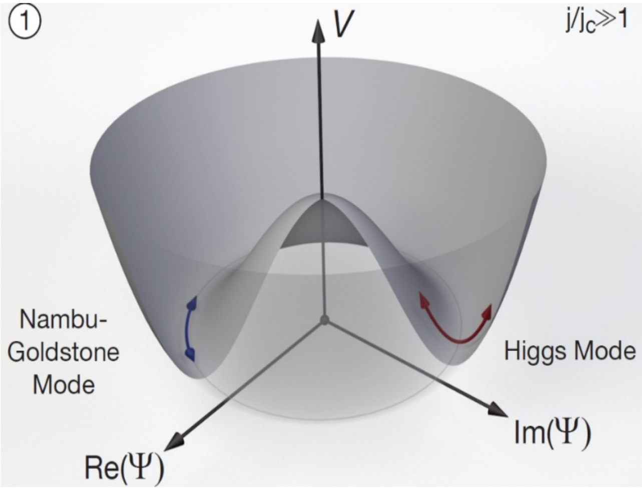
$$L(\psi) = \left|\frac{\partial \psi}{\partial t}\right|^2 - |\nabla \psi|^2 - r\psi^*\psi - \frac{u}{2}(\psi^*\psi)^2$$

ψ is a complex field

r, u: physical parameters

$(d+1)$ space-time; real time

☆ Lorentz invariant



- **Phase transitions in O(2) mean-field theory**

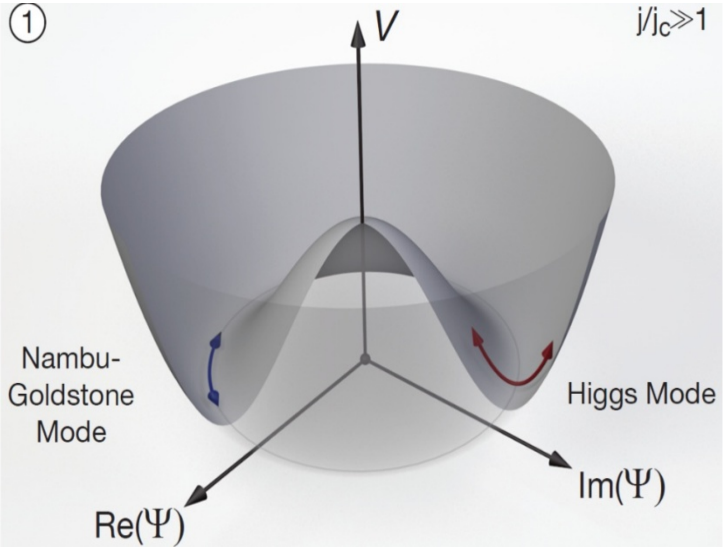
Minimum of potential $V[\psi^*,\psi] = r\psi^*\psi + \frac{u}{2}(\psi^*\psi)^2$

✔ $r > 0 \Rightarrow \psi_0 = 0$: no long-range order exists

✔ $r < 0 \Rightarrow \psi_0 = \sqrt{-r/u}$: long-range order occurs

☆ O(2) symmetry is spontaneously broken!

Application I: probe Higgs resonance



- **Mexican-hat potential**

$$V[\psi^*,\psi]=r\psi^*\psi+\frac{u}{2}\left(\psi^*\psi\right)^2$$

- **Low-energy excitation**

Perturbation near ψ_0 :

$$\psi(x)=e^{i\xi(x)}[\psi_0+\eta(x)]$$

➠ Two decoupled excitation modes

Goldstone mode—oscillation of phase

massless (gapless)

Higgs mode—oscillation of amplitude

massive (gapped)

Application I: probe Higgs resonance

- **Higgs amplitude mode in D=2?**

  – No Higgs mode survives 😩

  ➢ Argument: Higgs mode is overdamped because of strong decay into two Goldstone modes

  ➢ 1/N expansion (up to 2nd order) [Chubukov *et.al.*'94; Altman *et.al.*'02; Zwerger'04; Podolsky *et.al.*'11]

  – **HIGGS MODE SURVIVES** 😆

  ➢ Monte Carlo study [PRL **109**, 010401 (2012); **110**, 140401 (2013); **110**, 170403 (2013)]

  ➢ Ultracold quantum gas [Nature **487**, 454 (2012)]
  ✭ No direct evidence, only onset of resonance

  ➢ Higher-order 1/N expansion [PRB **86**, 054508 (2012)]

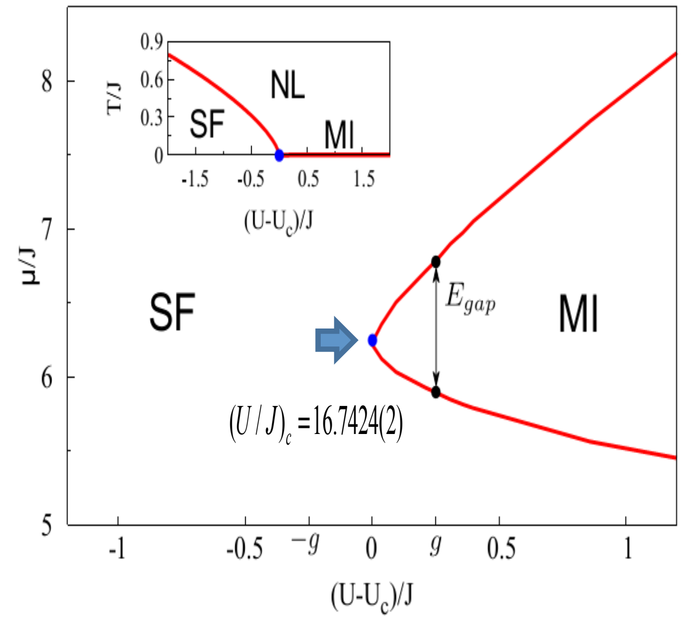
Application I: probe Higgs resonance

- **Bose Hubbard model--a testbed**

$$\hat{H}_{BH} = -J\sum_{<i,j>} b_i^{\dagger} b_j + \frac{U}{2}\sum_i \hat{n}_i(\hat{n}_i - 1) - \sum_i (\mu - V_i)\hat{n}_i$$

  - Efficiently simulated by worm algorithm → Quantum Critical Point (QCP) at U/J =16.7424(2)
  - Emergent Lorentz invariance/particle-hole symmetry near QCP → relativistic O(2) model

Square Lattice



- **Probe for critical dynamics**

  - Measure spectral function $S(\omega)$ as frequency ω varies

    [Energy dissipation/absorption rate $\propto \omega S(\omega)$]

    an excitation mode at $\omega \Leftrightarrow$ a resonance peak at ω

Application I: probe Higgs resonance

- **Monte Carlo probe: kink-kink correlation**

[Fluctuation-dissipation theorem]

Kinetic energy : $\beta K_{MC} = -\sum_{kinks}$

MC measurement:
(Matsubara frequency) $K_{MC}(i\omega_n) = \int_0^\beta d\tau \, e^{i\omega_n \tau} K_{MC}(\tau) = -\sum_{k=kinks} e^{i\omega_n \tau_k}$

$\Downarrow$

Fourier transformation: $\langle K(\tau)K(0)\rangle_{i\omega_n} = \left\langle \left| K_{MC}(i\omega_n) \right|^2 \right\rangle$

$\Downarrow$

Kink-kink correlation : $\chi_{MC}(\tau) = \langle K(\tau)K(0)\rangle$

➢ **But it is in imaginary time domain!**

Application I: probe Higgs resonance

- **Analytical-continuation method**

  – Relation between $\chi_{MC}(\tau)$ and $S(\omega)$

$$\chi_{MC}(\tau) = \int_0^\infty S(\omega)\left(e^{-\omega\tau} + e^{-\omega(\beta-\tau)}\right) d\omega$$

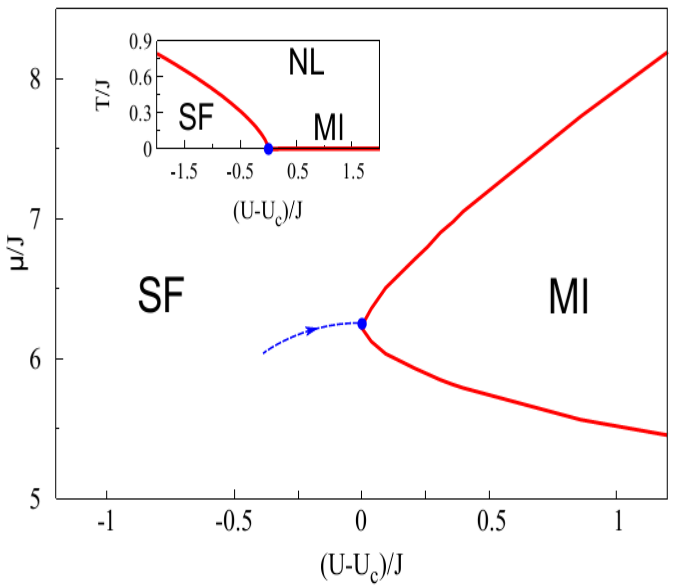
$\chi_{MC}(\tau)$ can be shown to be analytic $\Rightarrow$
$S(\omega)$ can be obtained by reverse transformation via analytical-continuation method (in principle)

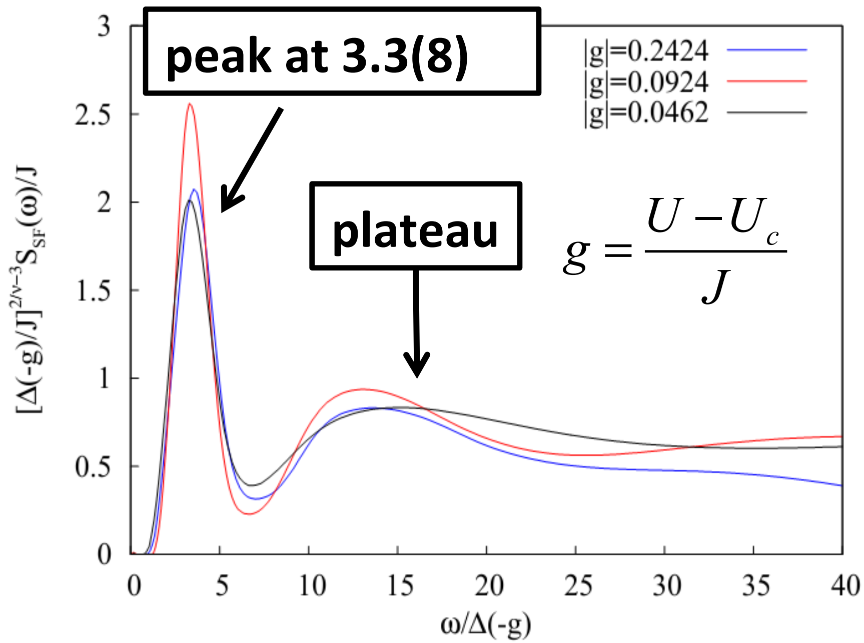
➢ It is an ill-posed problem!

➢ High-precision Monte Carlo data are needed.

Application I: probe Higgs resonance

- **In Superfluid**





Chen, Liu, Deng, Pollet, and Prokof'ev, PRL 110, 170403 (2013)

✯Nice Collapse: universal spectral function!

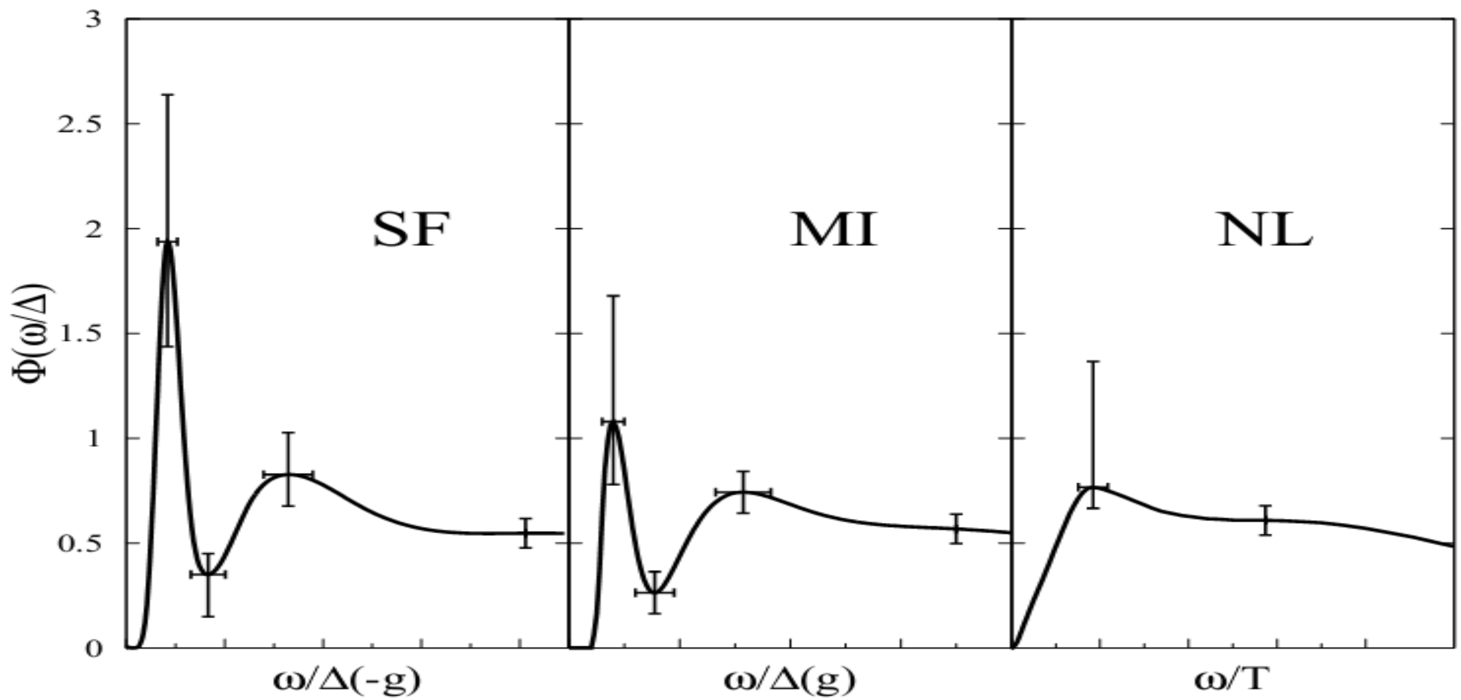
✯Second bump: multi Higgs mode?

✯Good news #3 for analytical condition:

Clear existence of plateau—a must physics condition

Application I: probe Higgs resonance

- **In Mott and Normal Liquid**



☆ Similar shapes in SF and MI.

☆ Resonance peaks in MI and NL? What are they?

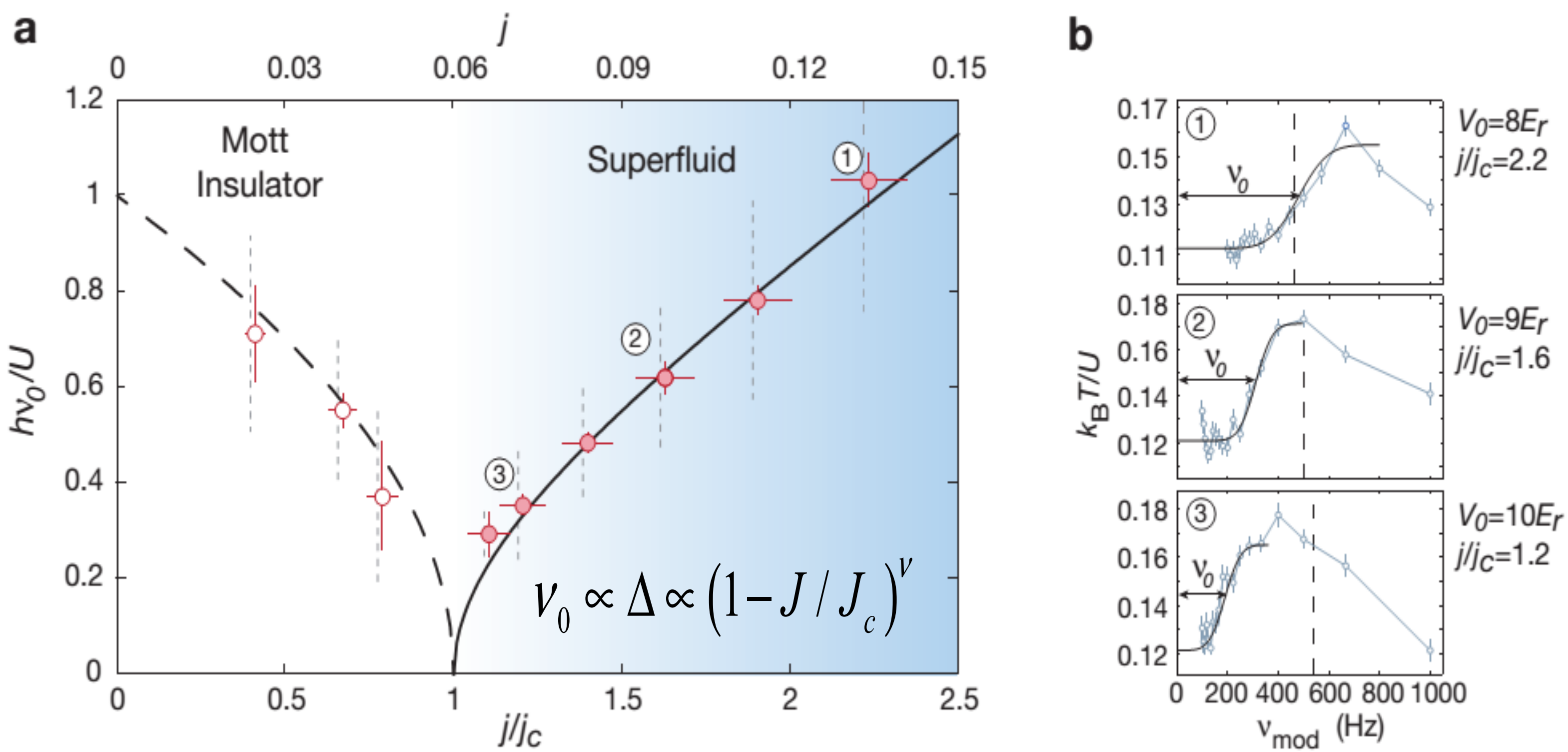
Near QCP, MI, NL, and SF are indistinguishable under ξ .

- MI and NL may have mesoscopic Mexican-hat shape free energy.
- Mesoscopic Higgs resonance is a possible scenario.

Application I: probe Higgs resonance

- **Optical Lattice Emulator for Bose-Hubbard model**

  [Nature **487**, 454 (2012)]



☆ Onset of resonance, but no peak is observed. Why?

Temperature not sufficiently low? Trap effect? Small number of atoms? Monte Caro data support "trap effect".

Application II: probe optical conductivity

- **Frequency-dependent conductivity** $\sigma(\omega)$

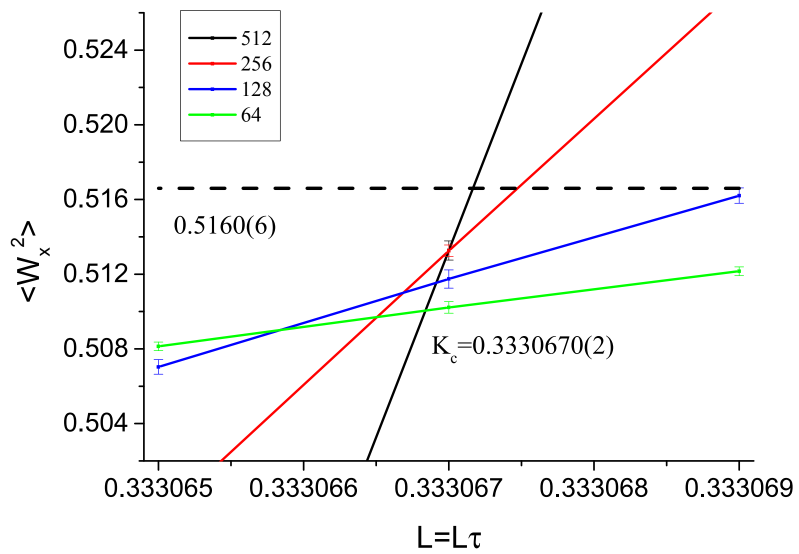
$$\vec{j}(\omega) = \sigma(\omega)\vec{E}(\omega)$$

$E(\omega)$: electronic field; $j(\omega)$: induced current

– A central concept of transport properties.

- **Systems to be studied**
  - Bose-Hubbard model at QCP
  - J-current model (Villain model)

$$H = \frac{1}{2K}\sum_{<ij>}^{\nabla \mathbf{J}=0} J^2_{<ij>}$$



➢ Both can be efficiently simulated by worm algorithm.

➢ Critical points: $(J/U)_c = 16.7424(2)$, $K_c = 0.3330670(2)$

Application II: probe optical conductivity

- **Monte Carlo probe**
  - Frequency-dependent superfluid density:

$$\rho_s(i\omega_n) = -\left\langle E_k \right\rangle / V - \left\langle j(\tau)\,\mathrm{j}(0) \right\rangle_{i\omega_n}$$

  - Kubo formula in Matsubara frequency:

$$\sigma(i\omega_n) = 2\pi\sigma_Q \frac{\rho_s\left(i\omega_n\right)}{\omega_n} \qquad \sigma_Q = 4\frac{e^2}{h} = \frac{2}{\pi} \quad (\mathrm{e}=\hbar=1)$$

- **Universal scaling behavior in critical region**

$$\sigma(\omega,T) = \sigma_Q \Sigma\left(\frac{\omega}{T}\right) \quad \text{with } \sigma\left(\frac{\omega}{T}\to\infty\right) = \sigma(\infty) \quad \text{OR}$$

$$\sigma(\mathrm{i}\omega_n,T) = \sigma_Q \Sigma\left(\frac{\mathrm{i}\omega_n}{T}\right)$$

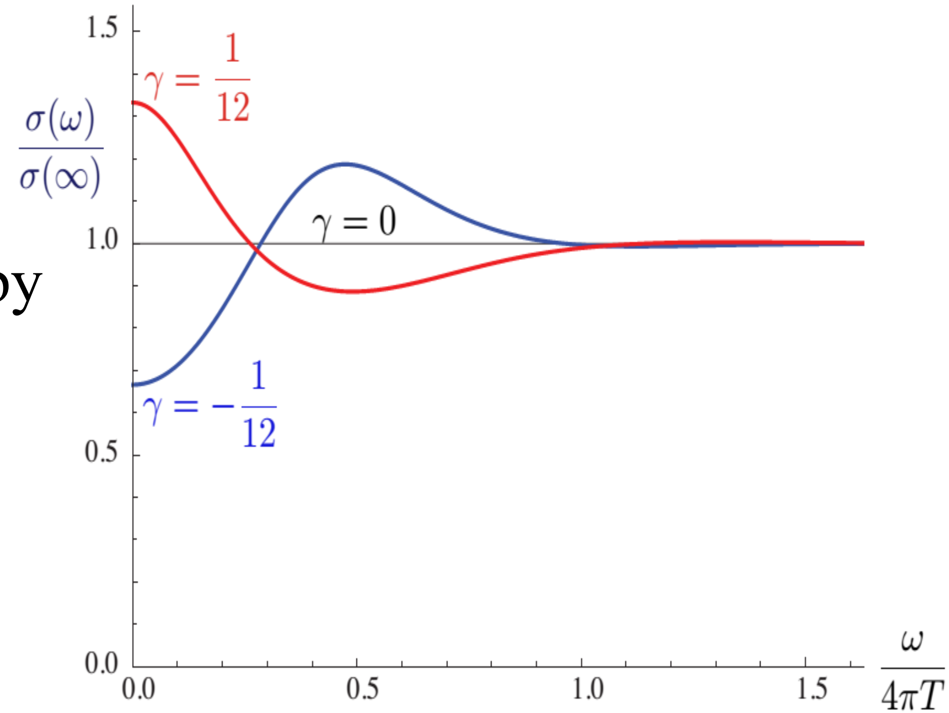
Application II: probe optical conductivity

- **AdS/CFT correspondence from string theory**

Holographic gauge/gravity duality theory predicts:

- Universal conductivity is controlled by two parameters $\sigma(0)$ and $\sigma(\infty)$
- Shape is solely determined by $\gamma = [\sigma(0) - \sigma(\infty)]/4\sigma(\infty)$
- Causality $\Rightarrow$ $|\gamma| \leq 1/12$
- Charge carrier is

$$\begin{cases} \gamma < 0 & \text{vortex-like} \\ \gamma > 0 & \text{particle-like} \end{cases}$$

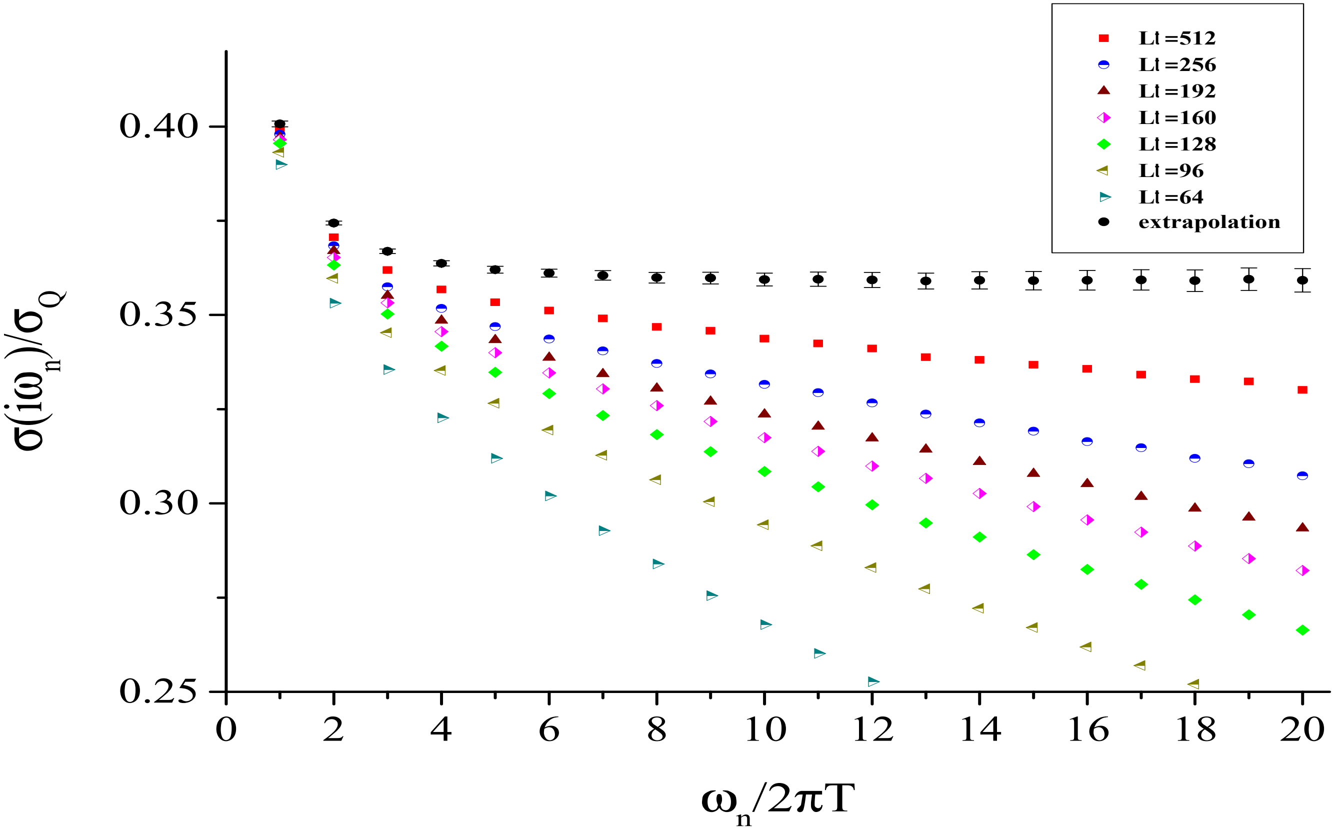


R. C. Myers, S. Sachdev, and A. Singh, *Physical Review D* **83**, 066017 (2011)

- Typos exist in differential equations in the above literature

Application II: probe optical conductivity

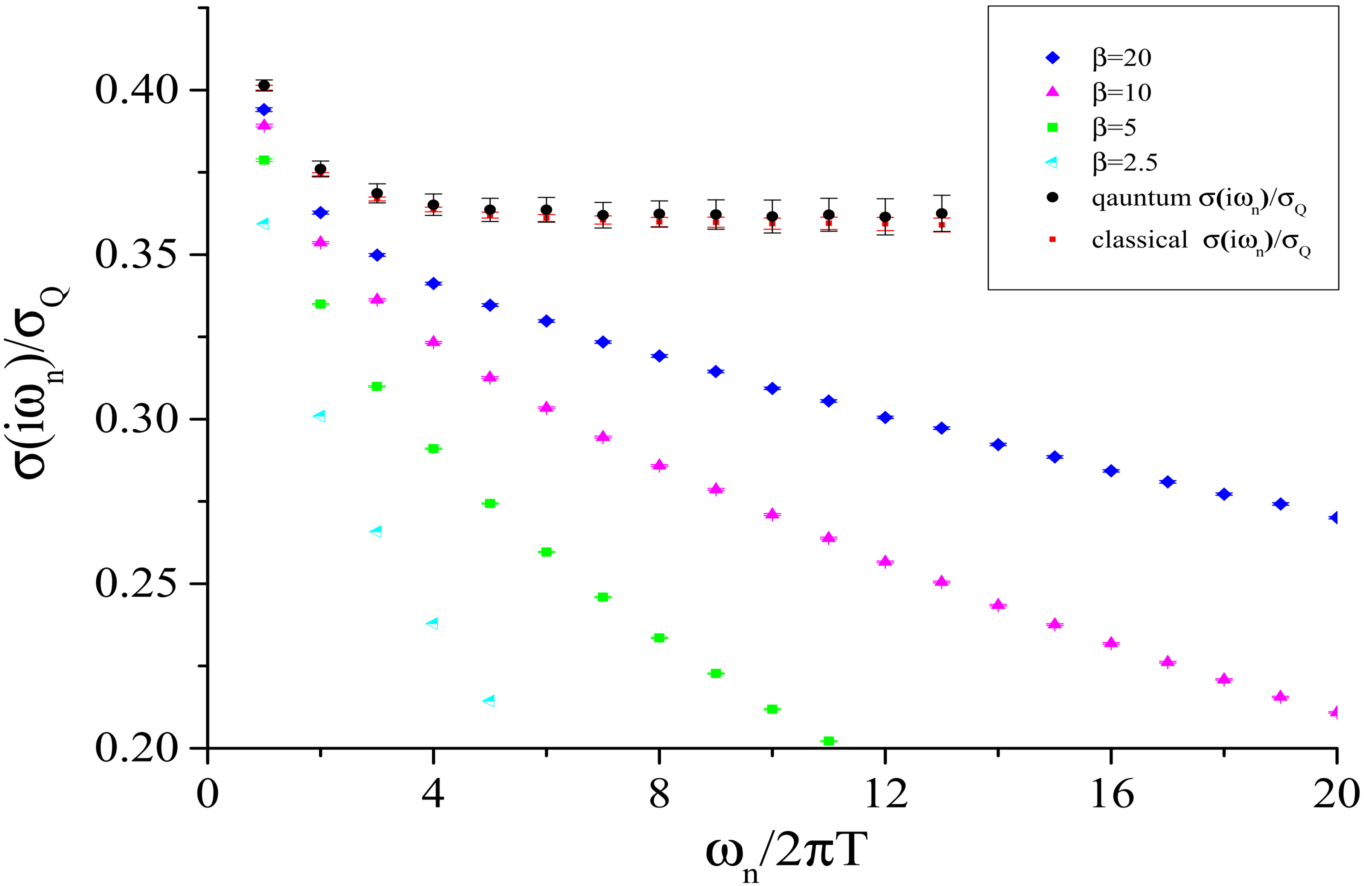
Universal conductivity for Villain model



- Simulations are extensive: high-precision data for system size up to 512 X 1024 X1024

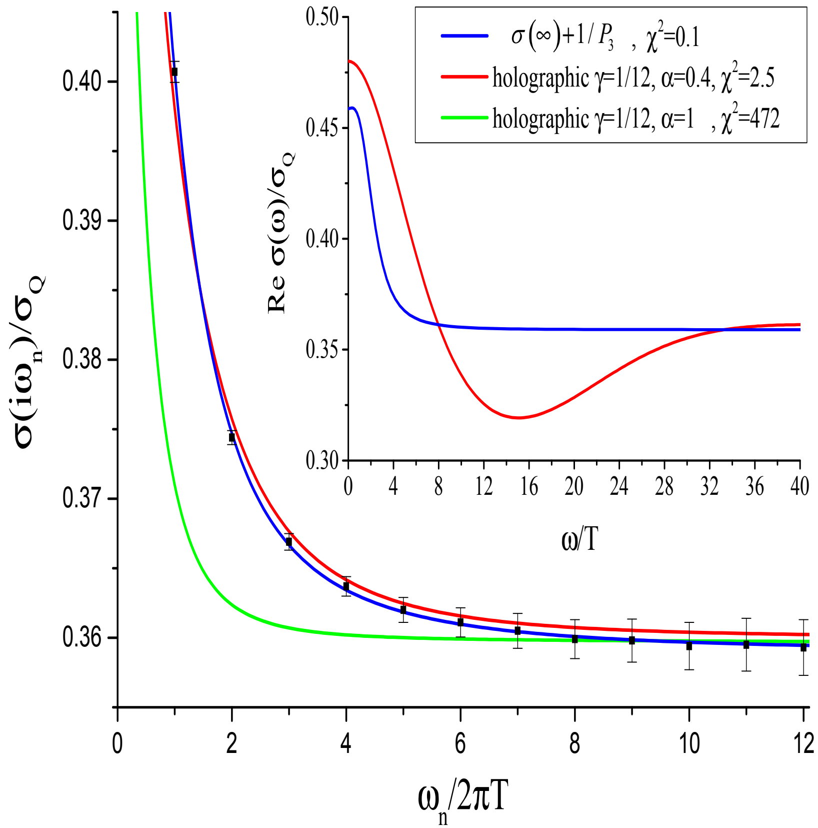
Application I: probe Higgs resonance

- **Universal conductivity for Bose-Hubbard model**



Application I: probe Higgs resonance

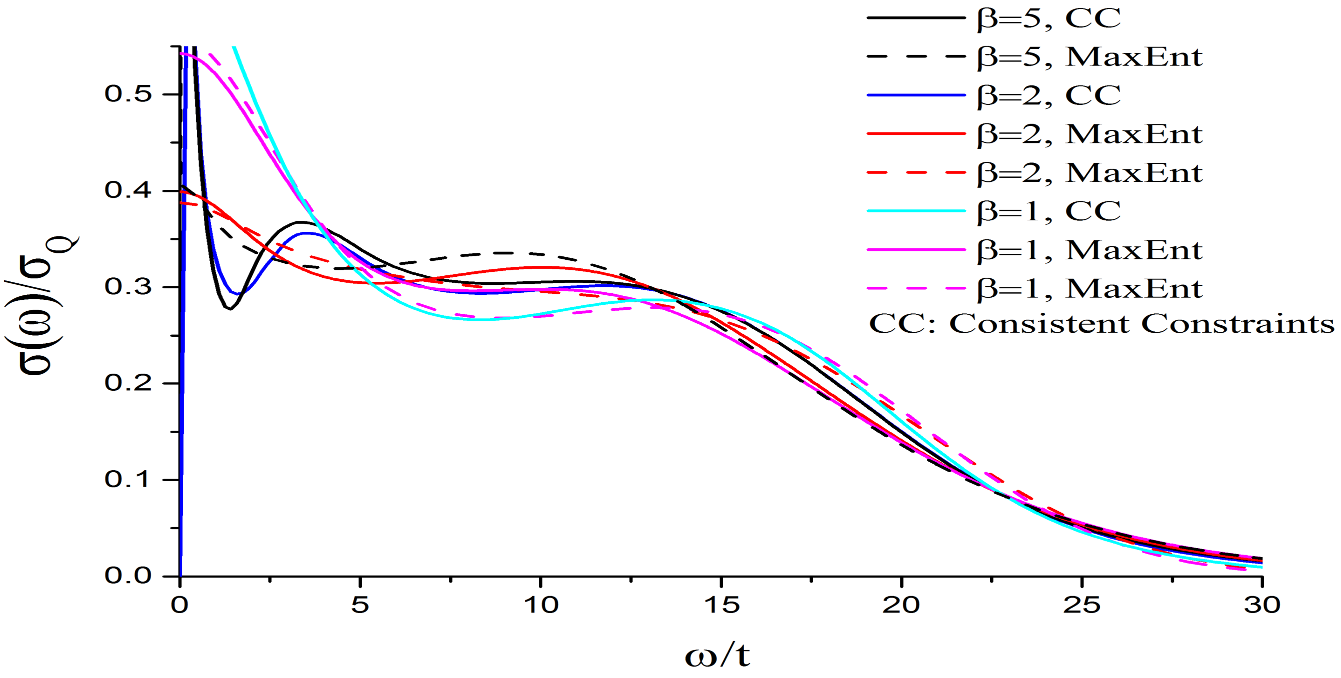
- **Fit by holographic gauge/gravity duality prediction**
  - Universal value: $\sigma(\infty) = 0.359(4)$
  - Particle-like
  - Do not fit in the original prediction even if gamma =1/12 (green line)
  - Holographic prediction is OK if T in CFT is rescaled by 0.4
  - A simple 3rd polynomial works equally well or better



Application II: probe optical conductivity

- **Optical-Lattice Emulator?**

Analytical-continuation results for Bose-Hubbard model:



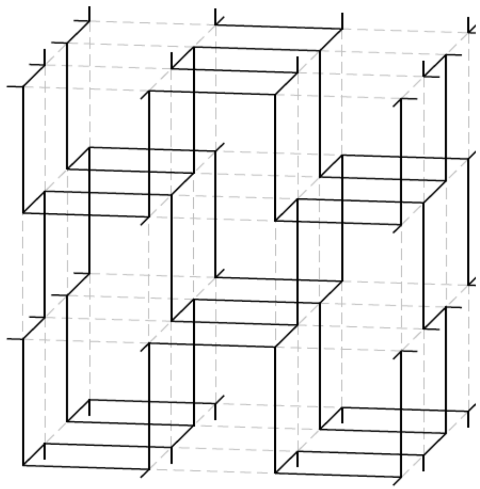
– Stable results for $\omega / T > 2\pi$

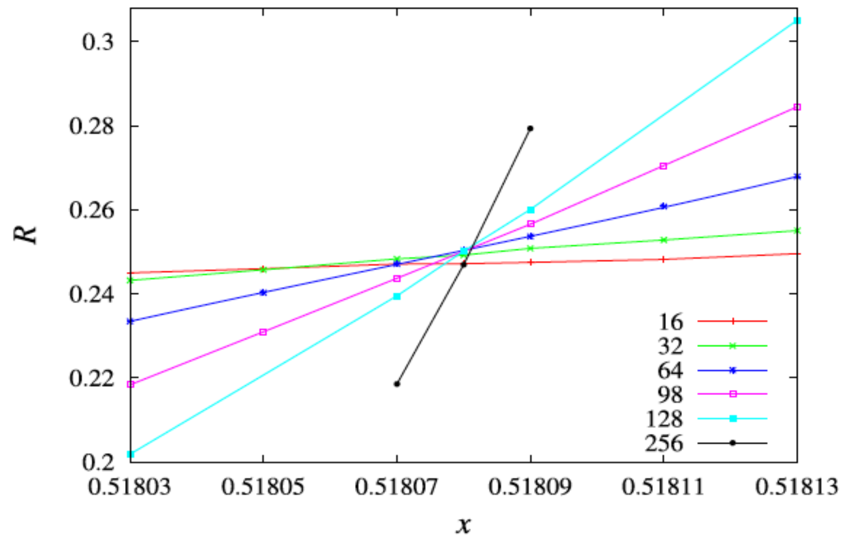
– Experimentally accessible T

– Experiment can measure $\sigma(\infty)$

Application III: O(n) loop model in 3D

- **O(n) loop model in 3D**





(a) R versus x for $n = 1$.

Results:

- Can be efficiently simulated by worm algorithm
- Confirm O(n) universality class in 3D for n=1,2,3,4,5,10

Discussion

- **Worm Algorithm:**
  - Simple but beautiful
  - Highly efficient

- **Broad Applications of Worm Algorithm**
  - Quantum Critical Dynamics

Thank You