Development and Application of worm-type algorithm in classical and quantum lattice models

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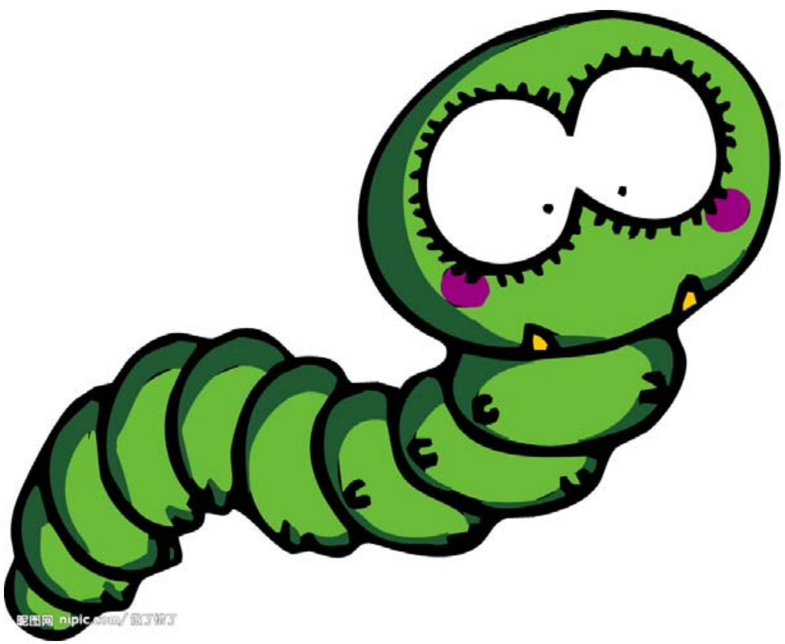
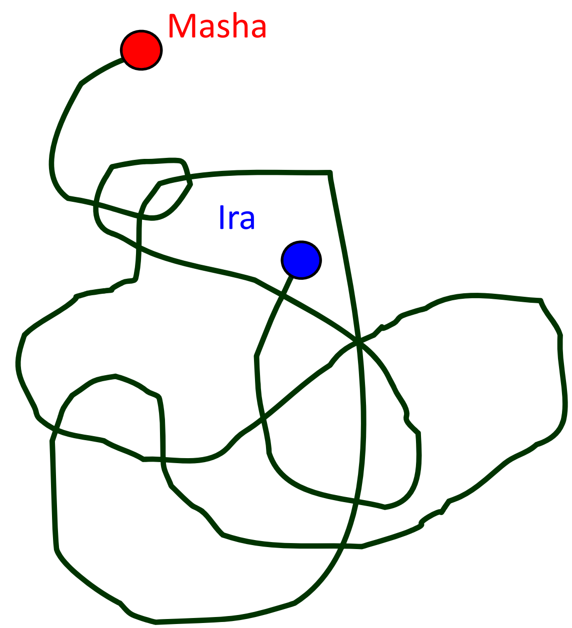
Worm algorithm

- What is worm?
- Application in classical lattice models.
- Application in Bose systems.
- Application in quantum spin systems.
- Application in Fermi systems.
- Other applications.

What is worm?

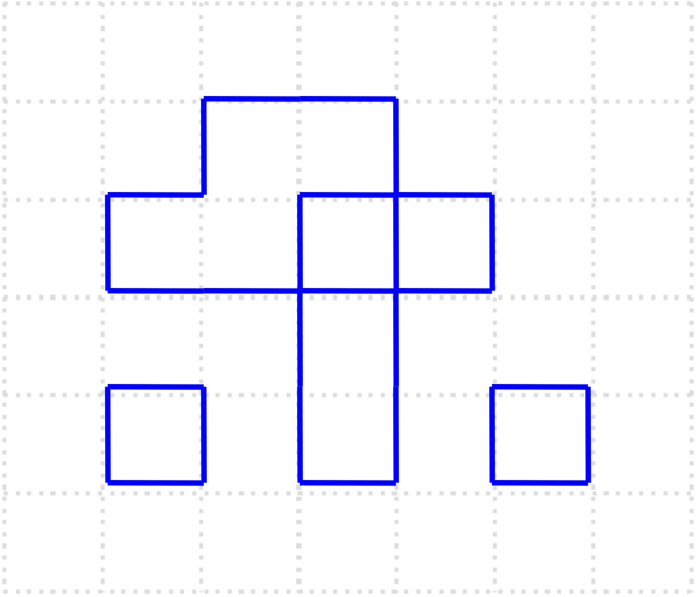


A cartoon picture of a worm

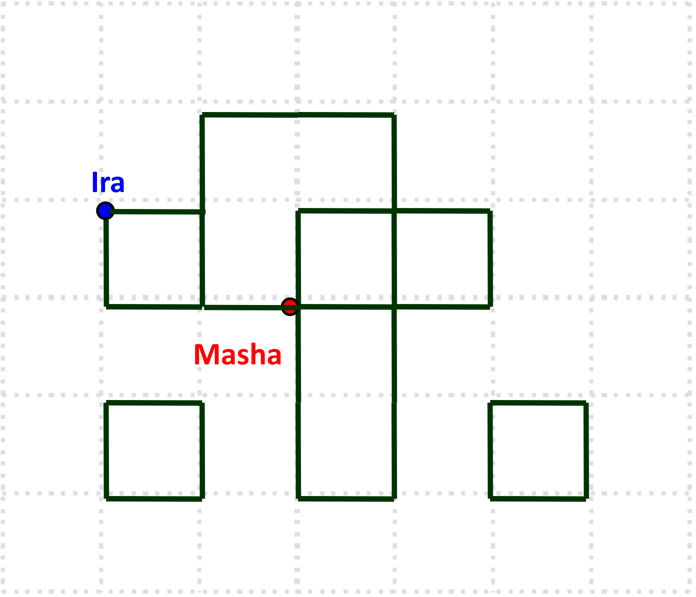


Worm in worm algorithm

Closed loops



Worm state space (A,I,M)



Application in classical lattice models

- Ising model

Consider the Ising model on G

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

The high-temperature expansion is

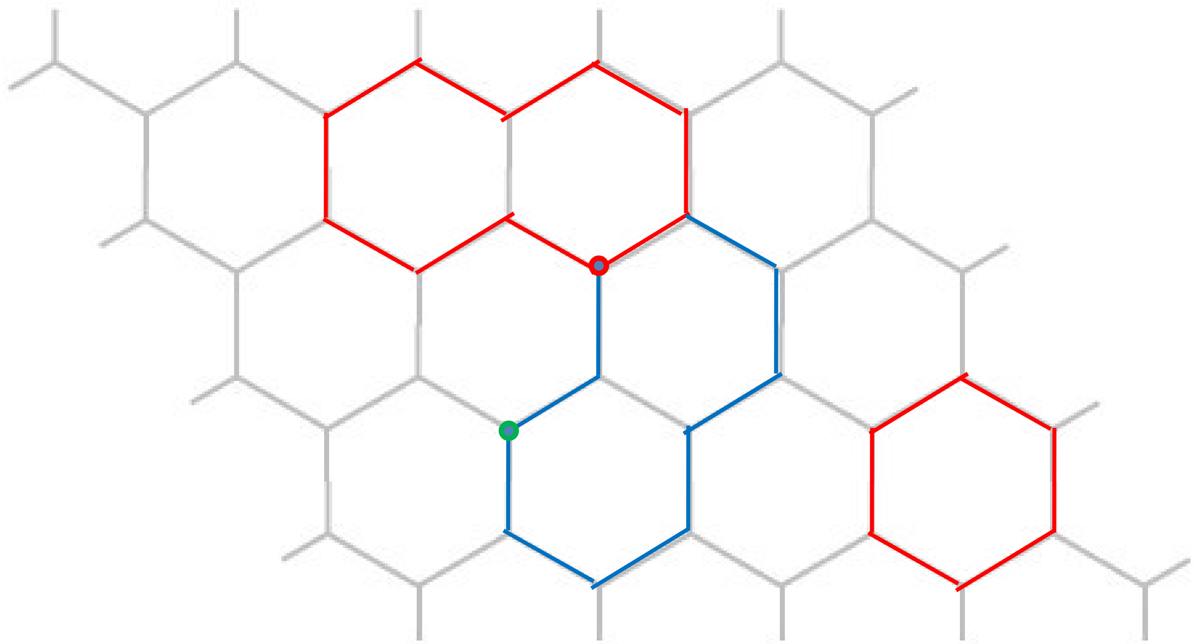
$$Z_{\text{Ising}} = \left(2^{|V|} \cosh^{|E|} \beta\right) \sum_{A \in \mathcal{C}(G)} (\tanh \beta)^{|A|}$$

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

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 $(A, I, M) \rightarrow (A \Delta IL, L, M)$
v) Accept the propose with probability p

- Demonstration



- Efficiency
  - Near a critical point the autocorrelation times typically diverge like $\tau \sim \xi^z$
  - D= 2 Ising model
    - *Glauber (Metropolis) algorithm z ≈ 2*
    - *Swendsen-Wang algorithm z ≈ 0.2*
    - *Worm algorithm* $z_{\mathrm{int},|A|} \approx 0.379$
  - *D=3 Ising model*
    - *Worm algorithm* $z_{\mathrm{int},|A|} \approx 0.174$
    - *Swendsen-Wang algorithm z ≈ 0.46*

- XY model on Square lattice
  - Reduced Hamiltonian $H = -J \sum_{<i,j>} \vec{S}_i \vec{S}_j$

$$\vec{S}_i = (S_i^x, S_i^y) \text{ and } \vec{S}_i^{\,2} = 1$$

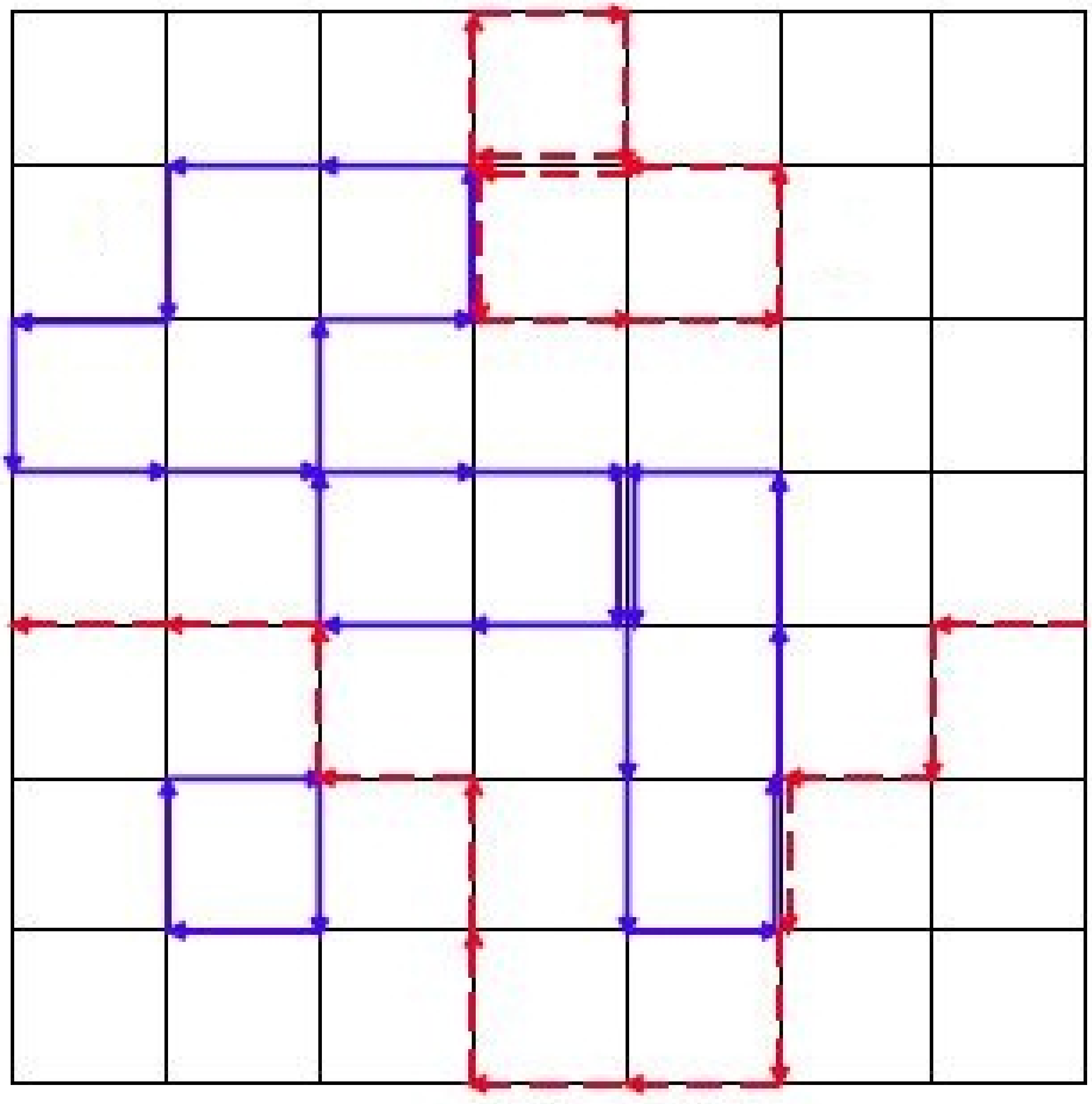
Partition sum

- Spin representation

$$Z_{spin} = \int \prod_{<i,j>} \exp(J \vec{S_i} \vec{S_j}) \prod_k d\vec{S_k}$$

- Graph representation

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



- N-component loop model on honeycomb lattice
  - Partition sum
    - Spin representation

$$Z_{spin} = \int \prod_{<i,j>} (1 + J\overrightarrow{S_i} \cdot \overrightarrow{S_j}) \prod_k d\overrightarrow{S_k}$$

    - Graph representation

$$Z_{loop} = \sum_{\substack{\text{Non-intersecting} \\ \text{loops}}} J^{|A|} n^{|c|}$$

    - Standard worm need non-local connectivity check

- Coloring technique
  - Induced subgraph interpretation

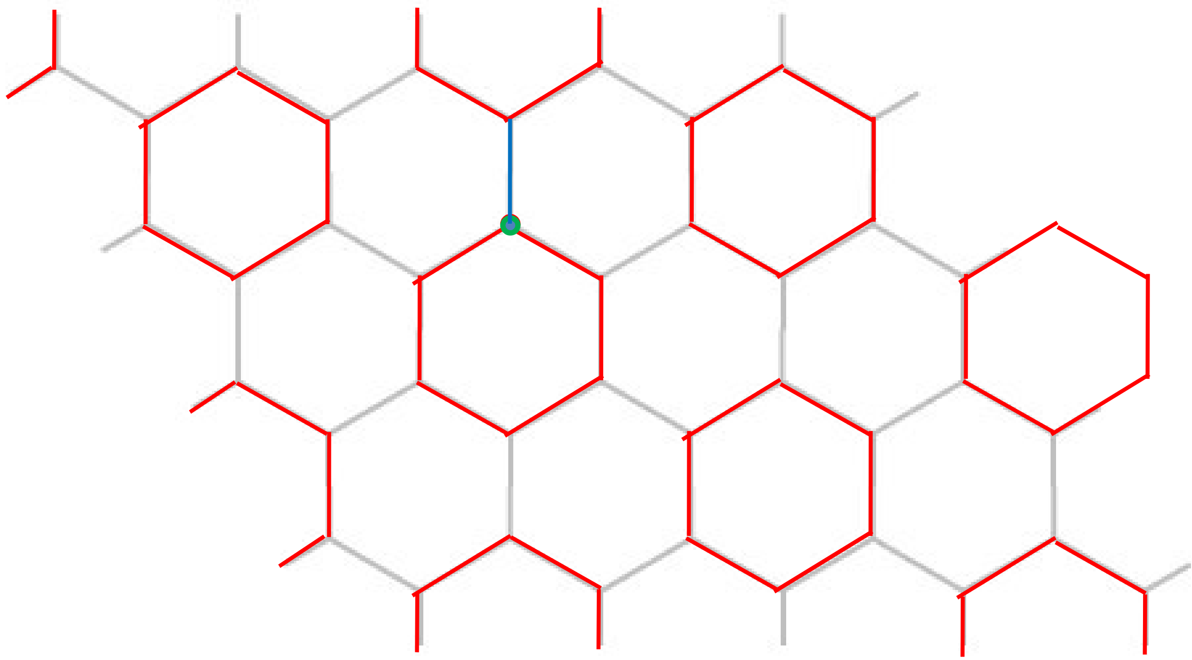
$$Z_{loop} = \sum_{\{b\}} \prod_{k=1}^{c} n J^{b(k)} = \sum_{\{b\}} \prod_{k=1}^{c} [1+(n-1)] J^{b(k)}$$

  - Introduce a color variable

$$Z_{loop} = \sum_{\{b\}} \prod_{k=1}^{c} \sum_{t_k=0}^{1} J^{b(k)t_k} [(n-1) J^{b(k)}]^{1-t_k}$$

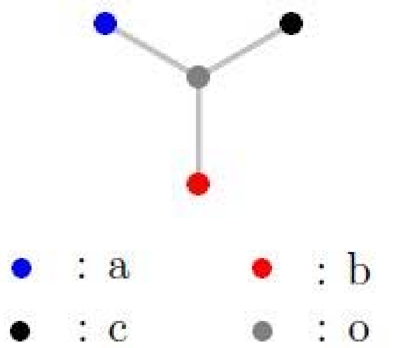
  - Classify vertices to be "active" and "inactive"
  - Define active subgraph, using standard worm

- FPL branch of loop model
  - Standard worm will be frozen in the non-Eulerian configuration.



  - Since we don’t sample in the non-Eulerian configurations, force move.

- FPL branch of loop model
  - Rejection-free technique comes!
  - Original probability



$$p_{oa}, p_{ob}, p_{oc}, p_{oo}$$

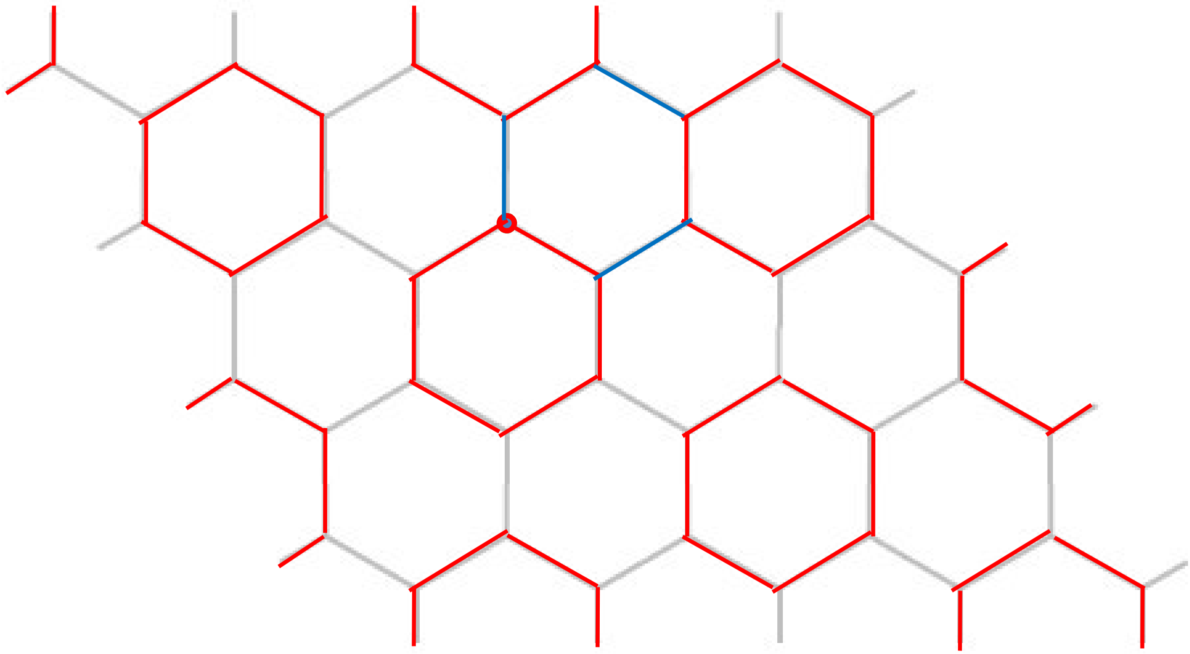
  - Modified probability $p'_{oa}, p'_{ob}, p'_{oc}, p'_{oo}$
  - Rule

$$\frac{p'_{oa}}{p_{oa}} = \frac{p'_{ob}}{p_{ob}} = \frac{p'_{oc}}{p_{oc}}$$

$$p'_{oo} = 0$$

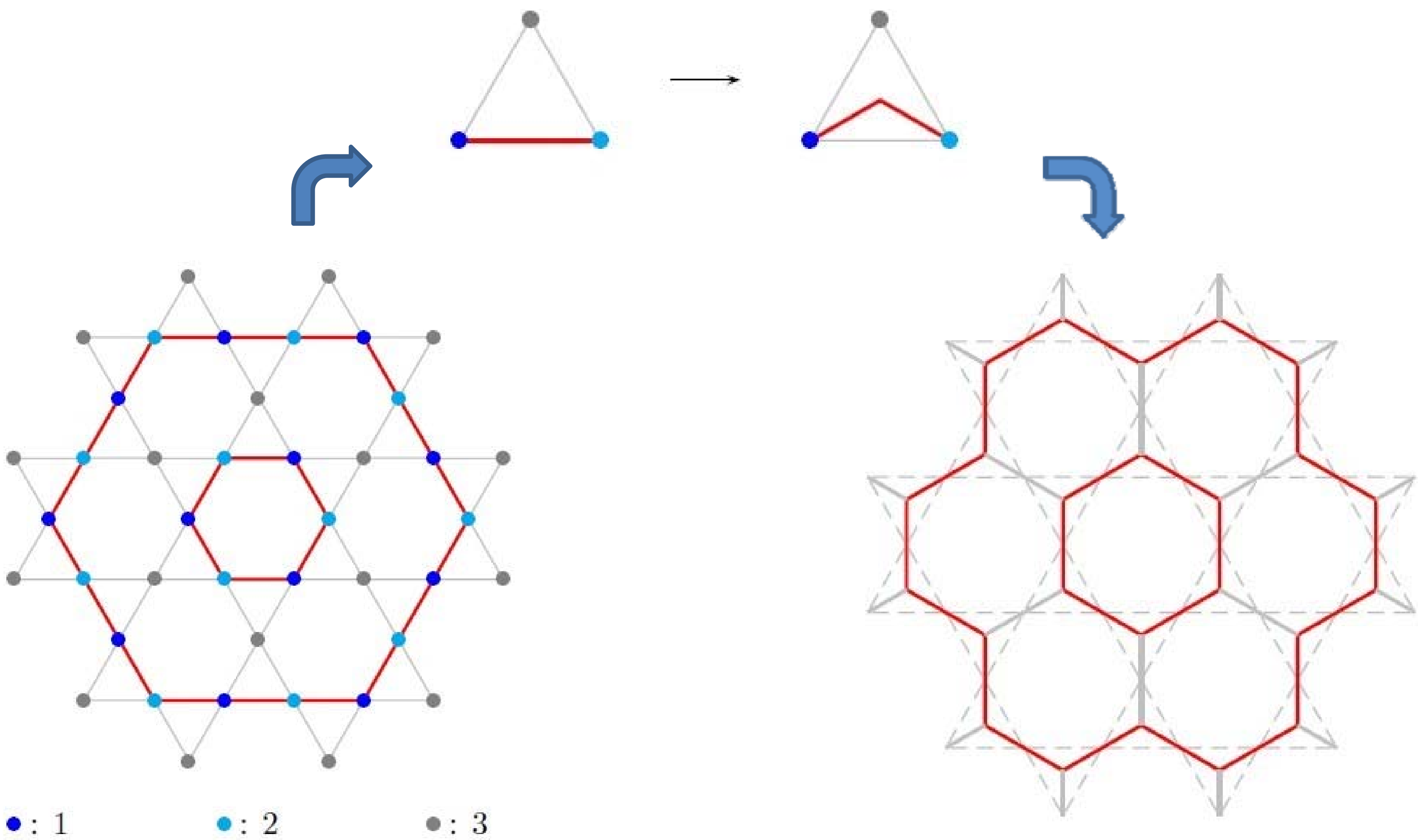
$$p'_{oa} + p'_{ob} + p'_{oc} = 1$$

- FPL branch of loop model
  - Demonstration

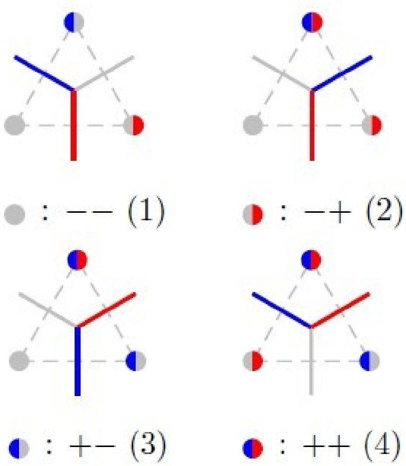


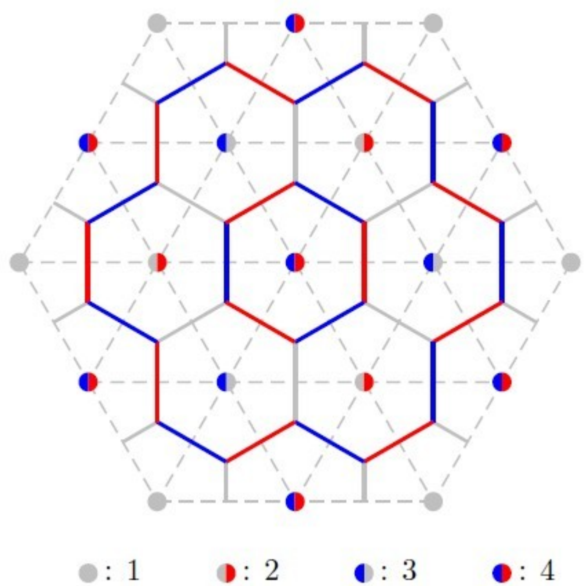
  - Ergodicity is mathematically proved!
  - First valid algorithm for FPL.

- Mapping to the O(2) FPL model
  - Zero temperature 3-state antiferromagnetic Potts model on the kagome lattice



- Mapping to the O(2) FPL mode
  - Zero temperature 4-state antiferromagnetic Potts model on the triangular lattice





- WSK algorithm – Non-ergodic for zero temperature
- Provide the first valid algorithm for these zero temperature antiferromagnetic Potts models

- High-dimensional loop models
- Other applications
  - $|\varphi|^4$ model
  - Extended J-current model
  - Spin glass ???
  - ……

Bosonic mixture on the triangular lattice

$$H = -t_A \sum_{<ij>} a_i^+ a_j - t_B \sum_{<ij>} b_i^+ b_j$$

$$+ V \sum_{<ij>} (n_i^a n_j^a + n_i^b n_j^b) - \mu \sum_i (n_i^a + n_i^b) + U \sum_i n_i^a n_i^b$$

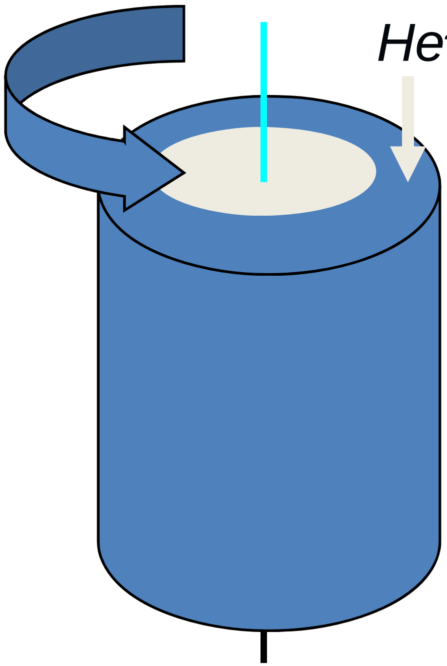
^{87}Rb-^{41}K in an optical lattice;
interactions could be tuned by Feshbach resonance

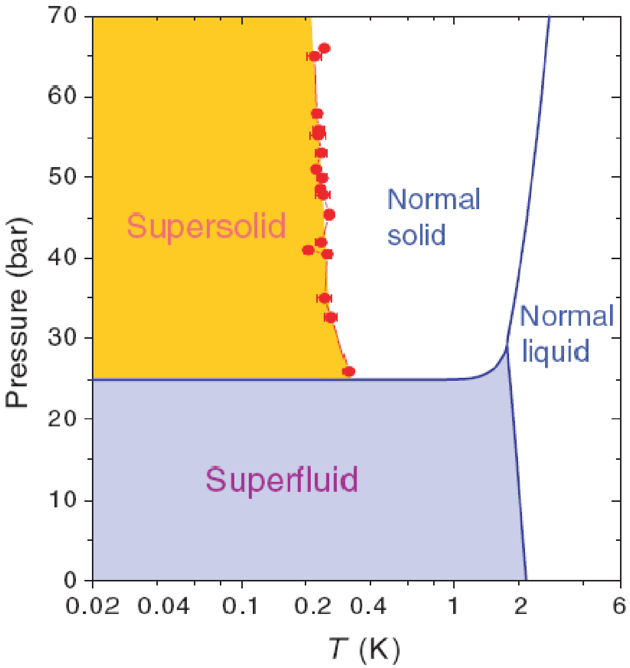
Exist frustration

May exist rich phase diagram

Supersolidity

(Broken lattice symmetries coexisting with superfluidity)





E. Kim and M.Chan, Science (2004)

Also: K. Shirahama, et al (APS 2006)

A.S.C. Rittner, J. Reppy, cond-mat/0604528

Supersolid should show **nonclassical rotational inertia** *due to superfluid component remaining at rest (Leggett, 1970)*

- ***Supersolid?***
- ***Microcrystallites? Superglass? (N. Prokofiev etc.)***

$$H = H_0 + H_1$$

$$H_0 = V \sum_{<ij>} (n_i^a n_j^a + n_i^b n_j^b) - \mu \sum_i (n_i^a + n_i^b) + U \sum_i n_i^a n_i^b$$

$$H_1 = -t_A \sum_{<ij>} a_i^+ a_j - t_B \sum_{<ij>} b_i^+ b_j$$

$H_{0:}$ diagonal

$H_{1:}$ non-diagonal

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

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

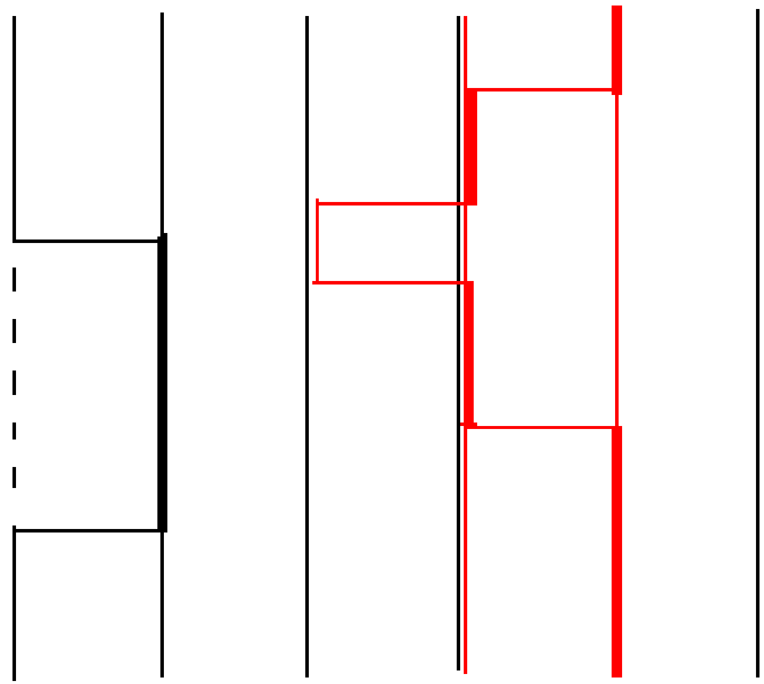
In the diagonal basis set (occupation number, or Fock, representation):

$$\langle \{n_i\} | = \langle \{n_1, n_2, n_3, \ldots\} |$$

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

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

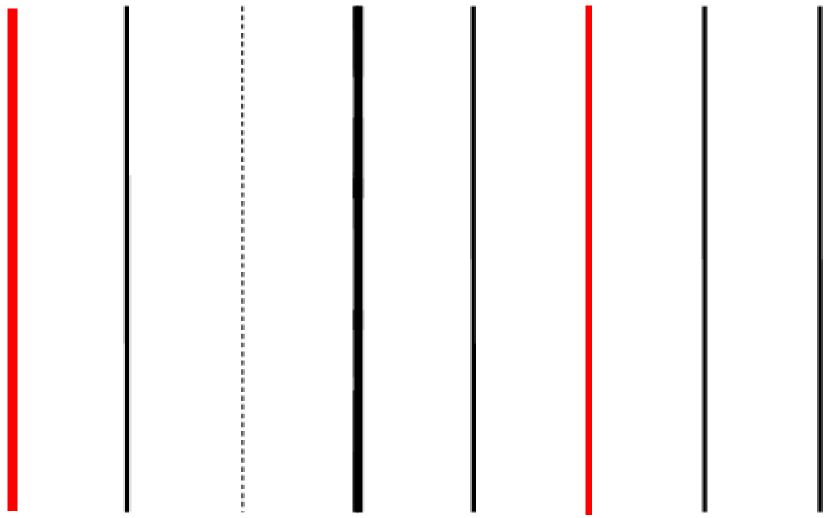
An example of the worldline configuration for the bosonic mixture



$$Z=\sum_{K=0}^{\infty}\iiint_{\tau_K>\ldots>\tau_1}\sum_{\{n\}_\tau} e^{-\int_0^\beta H_0[\{n\}_\tau]d\tau}\prod_{k=1}^{K}\left\langle\{n\}_{\tau_k-0}\,|\,(-H_1\,d\tau)\,|\,\{n\}_{\tau_k+0}\right\rangle$$

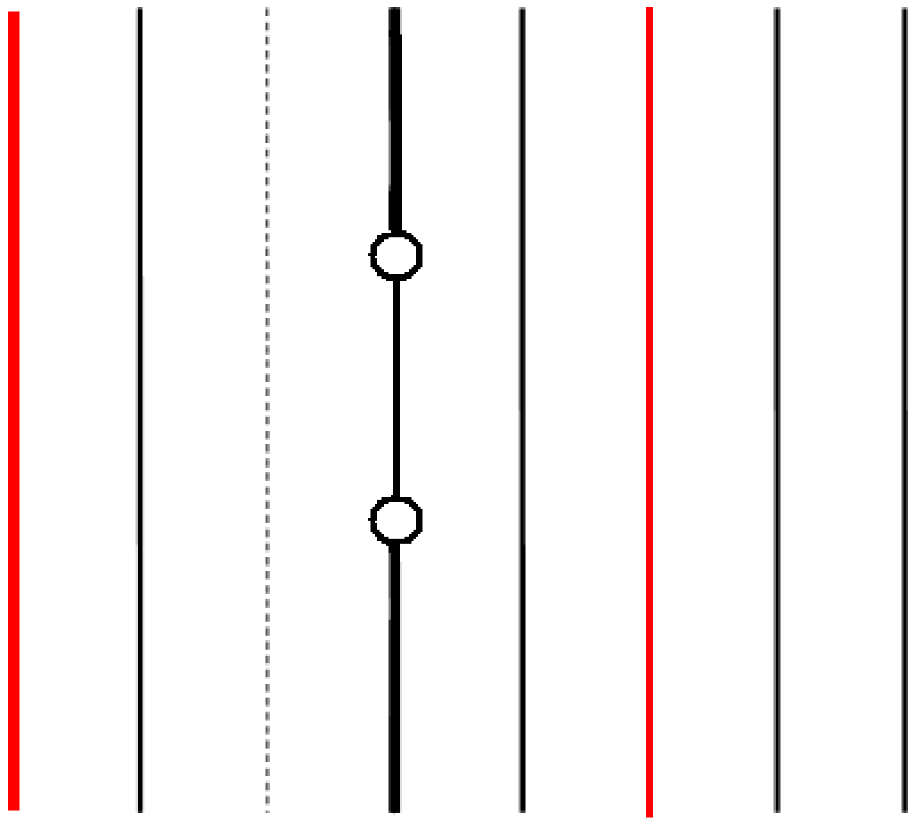
Example: update worldline configuration for bosonic mixture

initial configuration

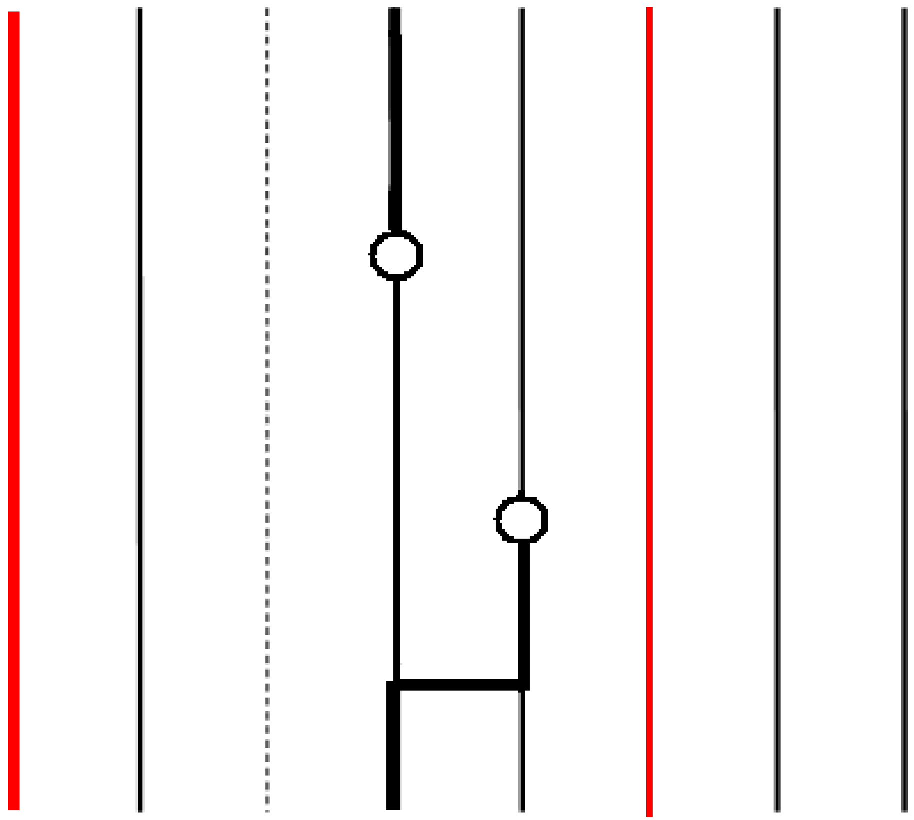


$$\{(n_A,n_B)_{\tau=0}\}= \{(0,2), (1,0), (0,0), (2,0), (1,0), (0,1), (1,0), (1,0)\}$$

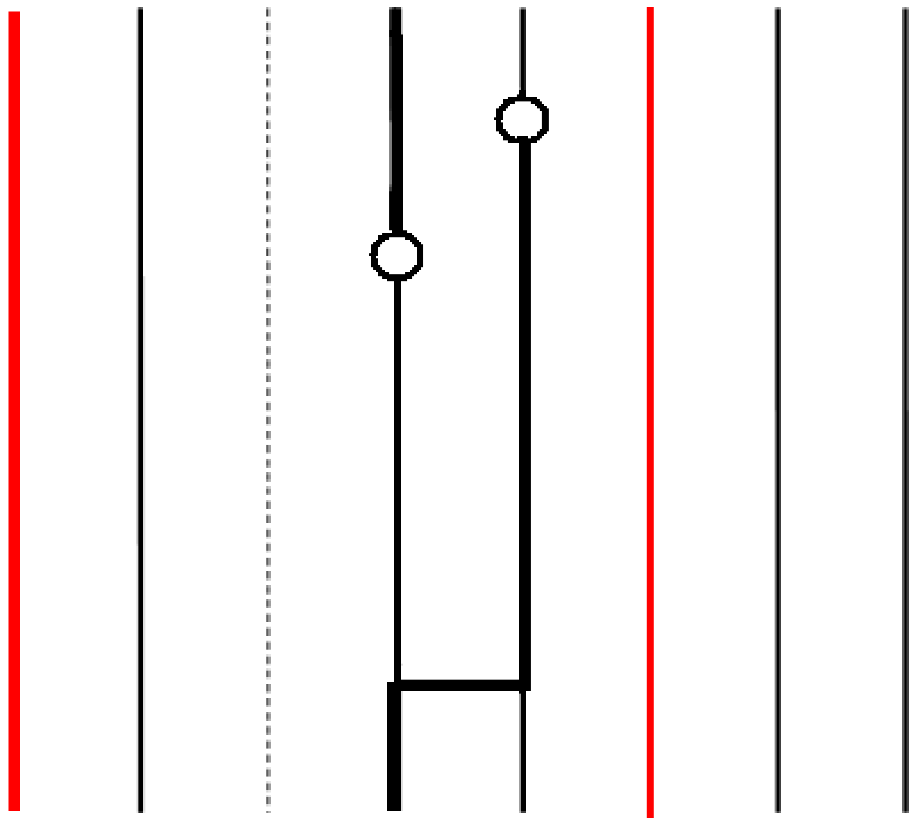
create worm



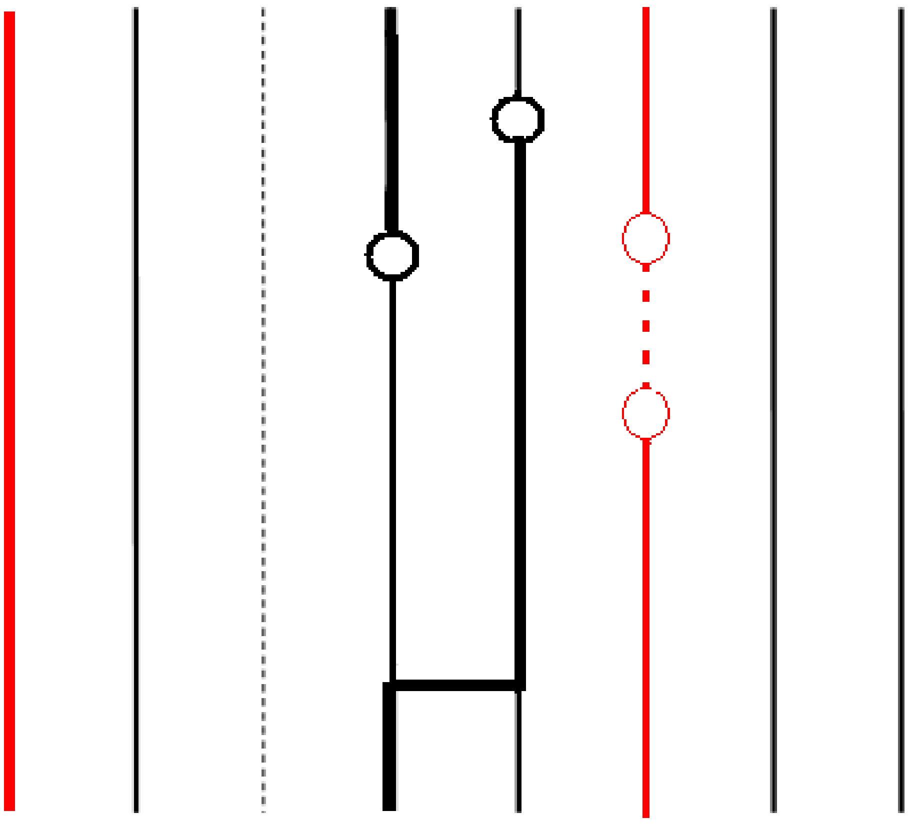
space shift



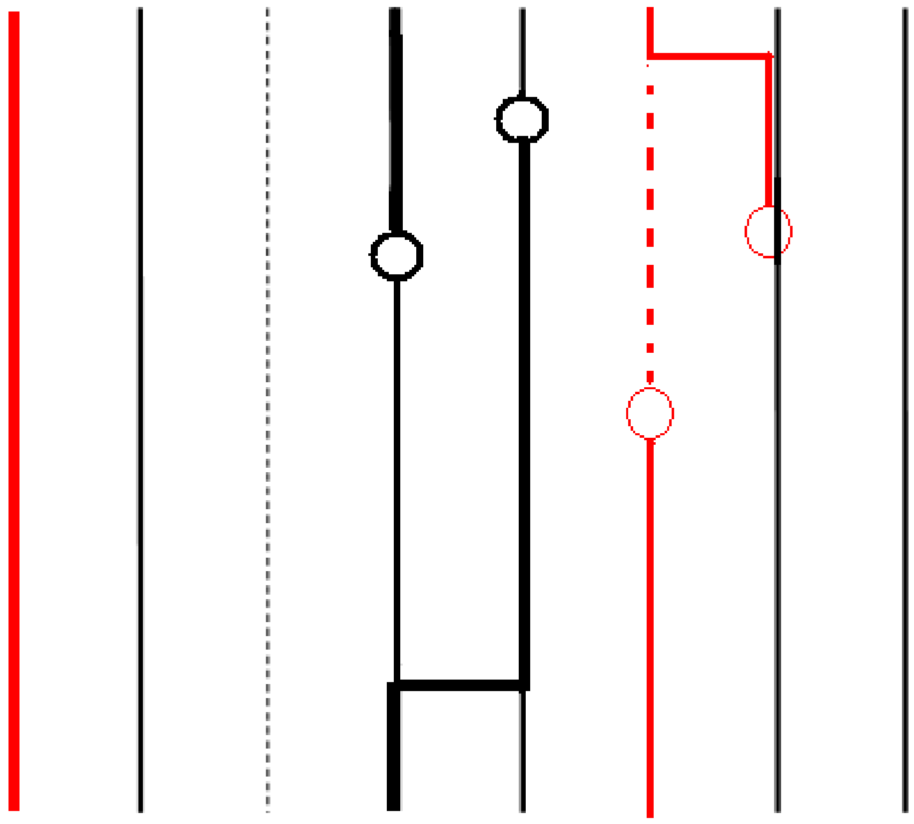
time shift



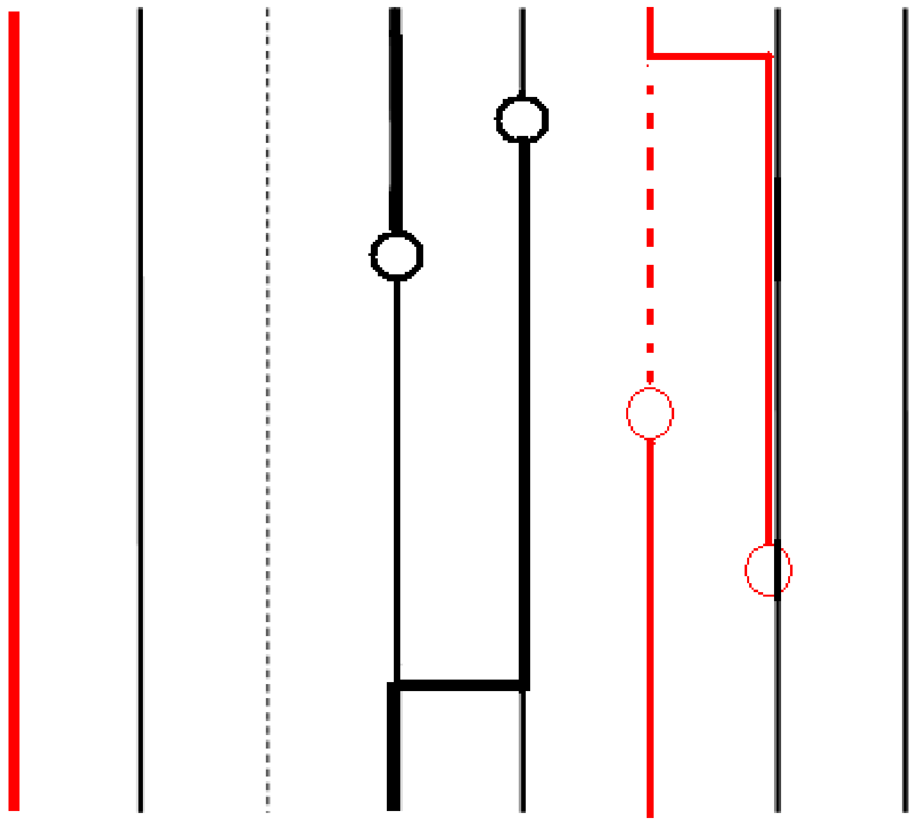
create worm



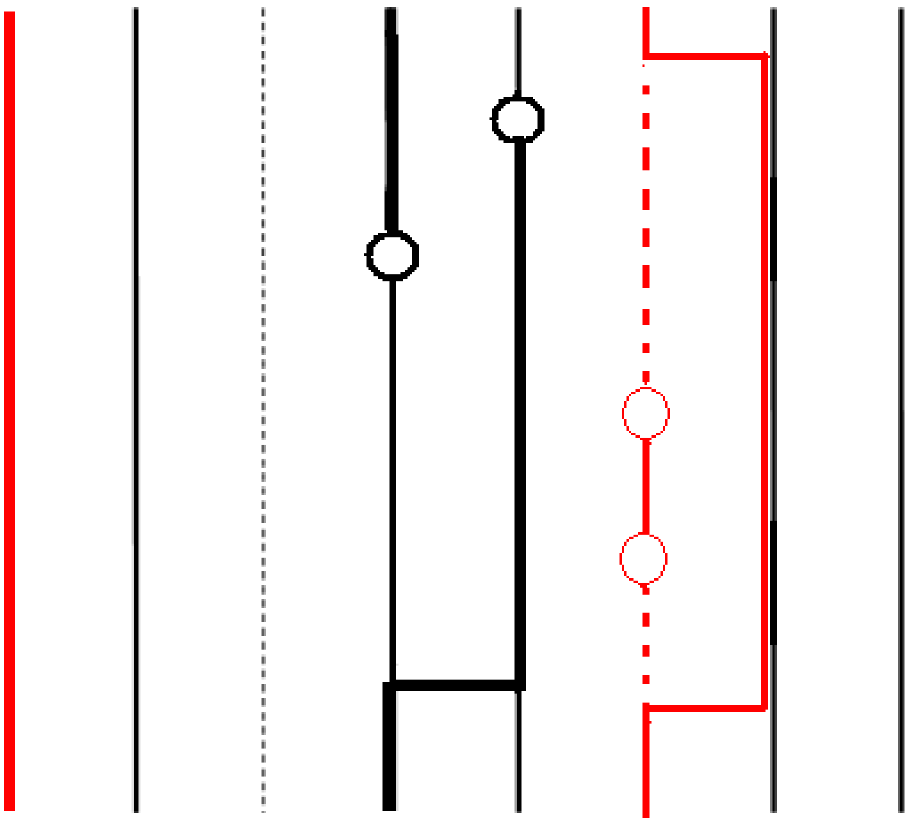
space shift



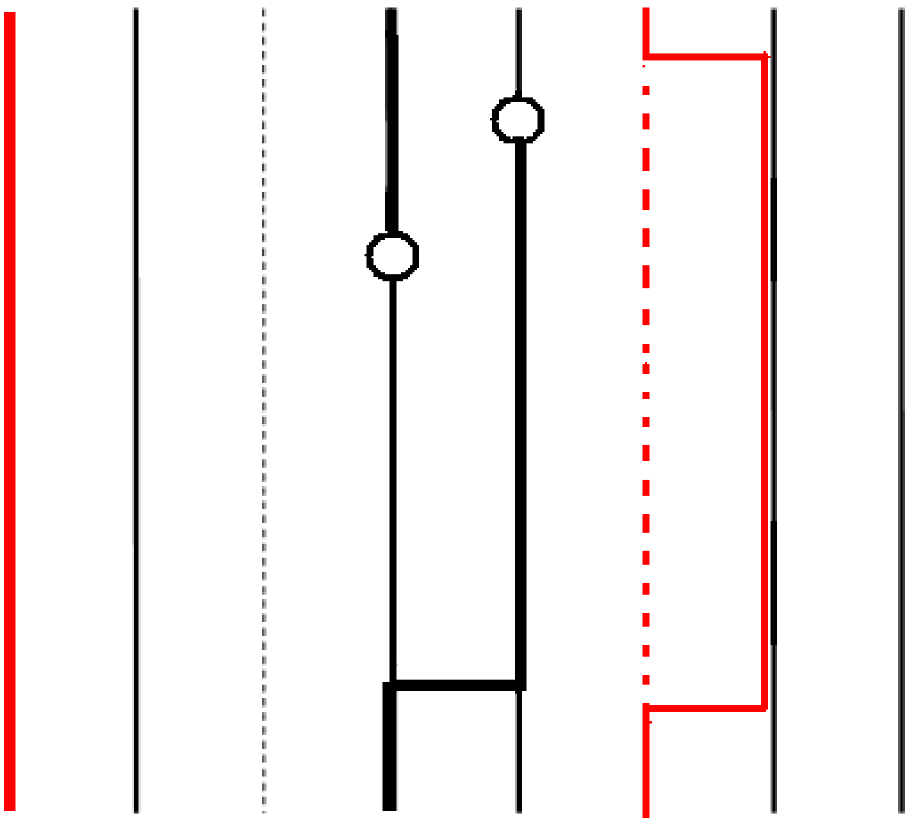
time shift



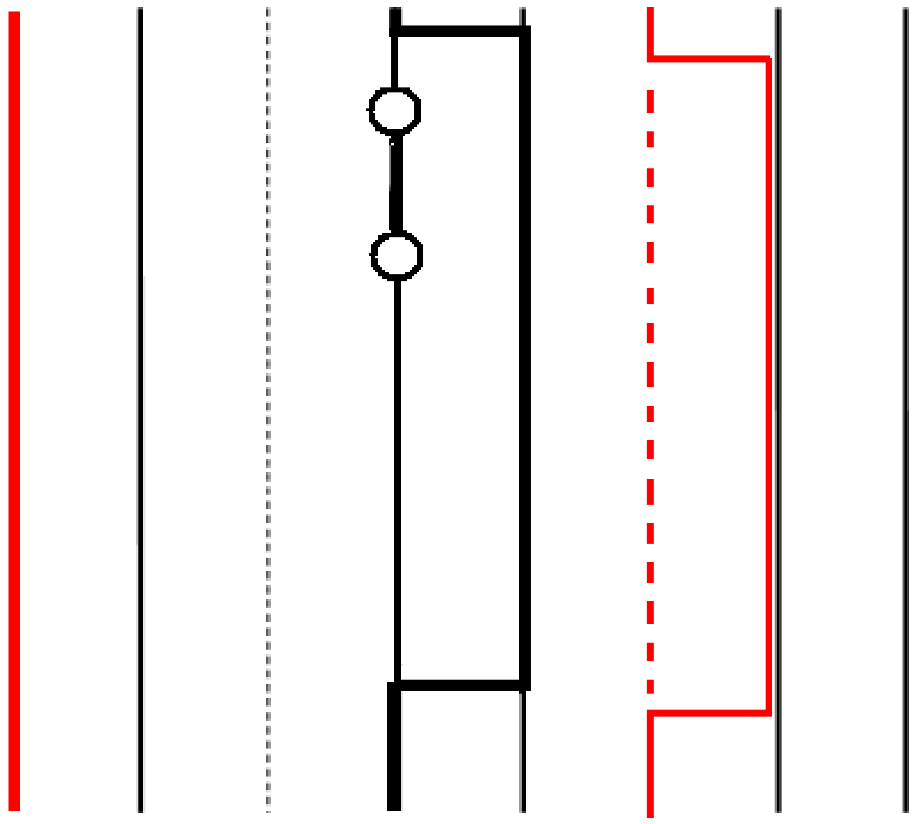
space shift



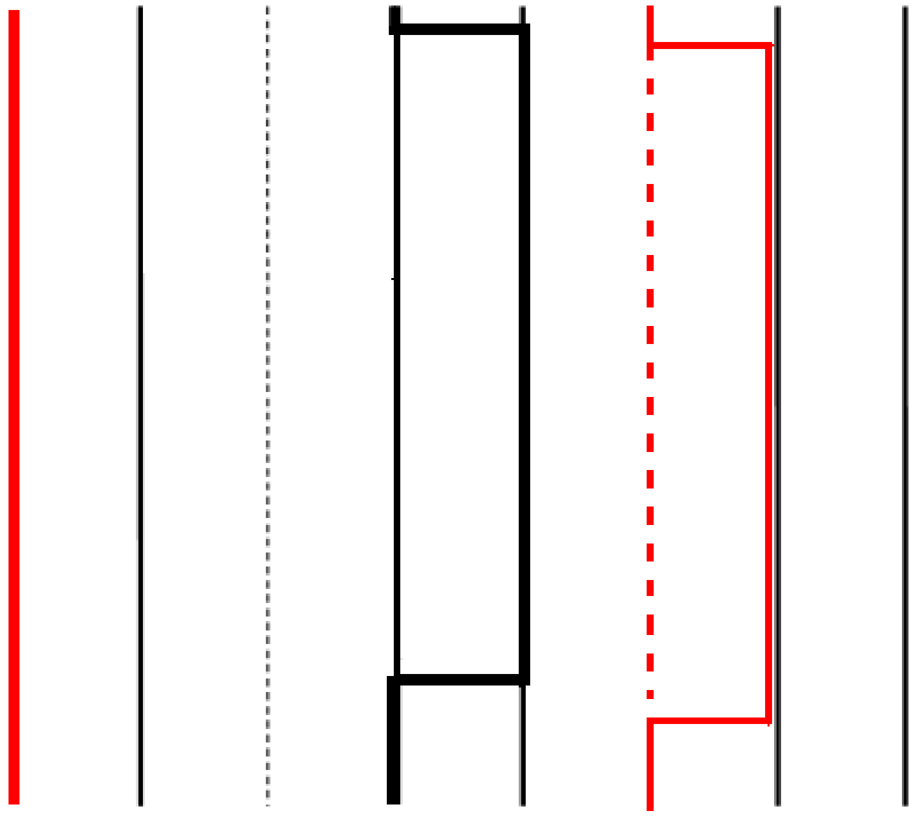
delete worm



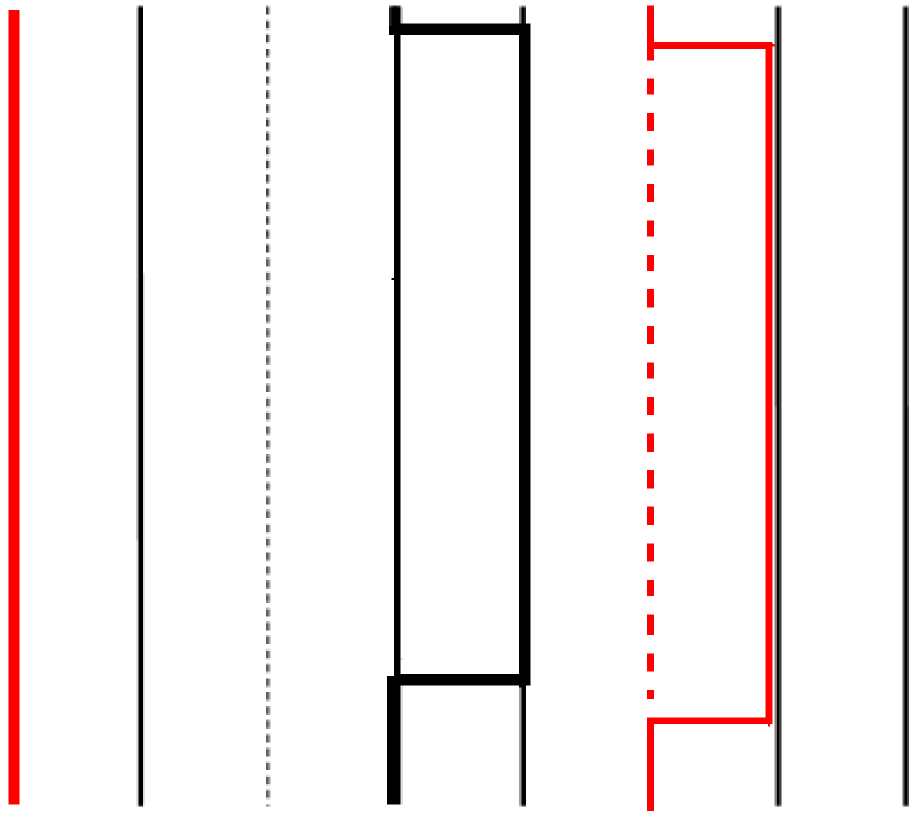
space shift



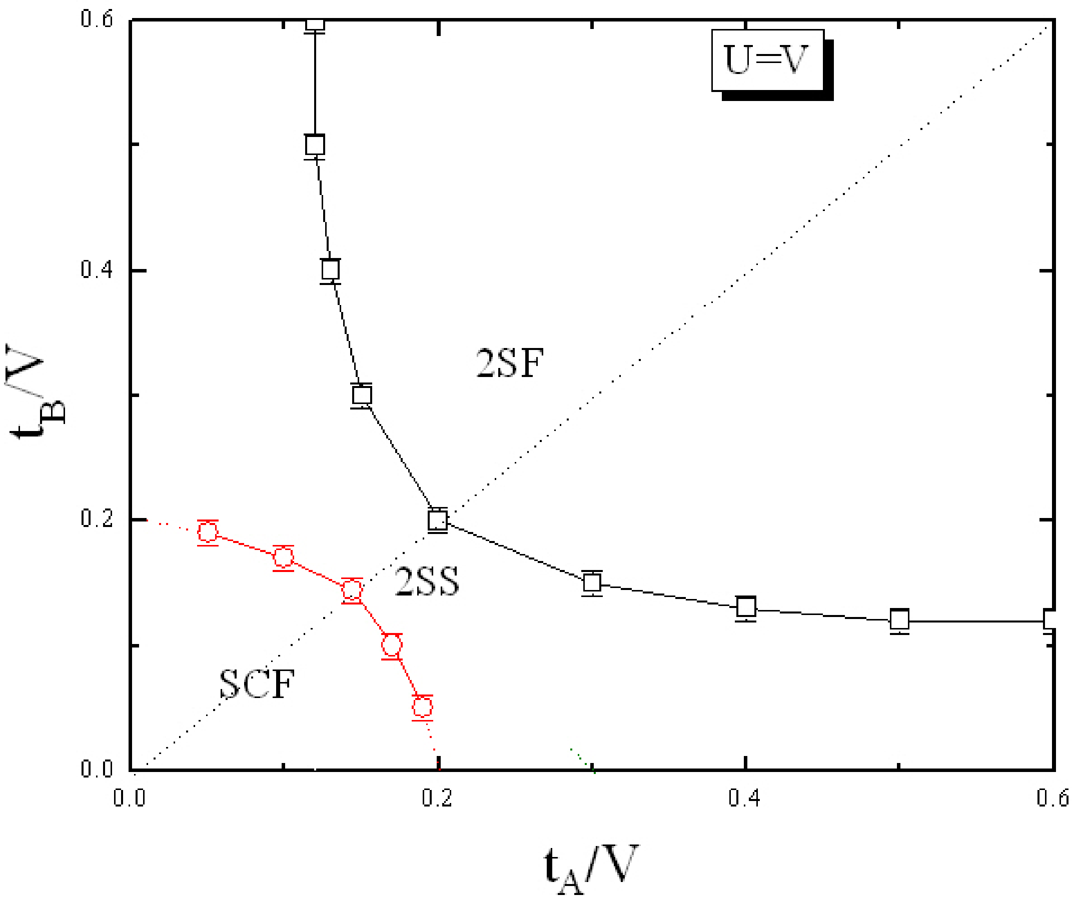
delete worm



New configuration generated



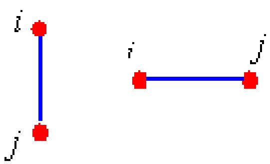
Phase diagram (U=V)

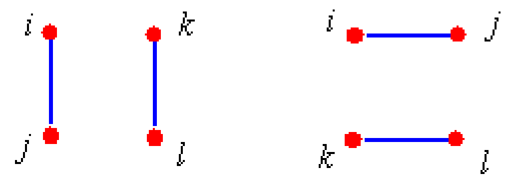


The J-Q model

- Hamiltonian:

$$\hat{H} = J\sum_{<i,j>} \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_j - Q\sum_{<i,j,k,l>} (1-\hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_j)(1-\hat{\mathbf{S}}_k \cdot \hat{\mathbf{S}}_l)$$



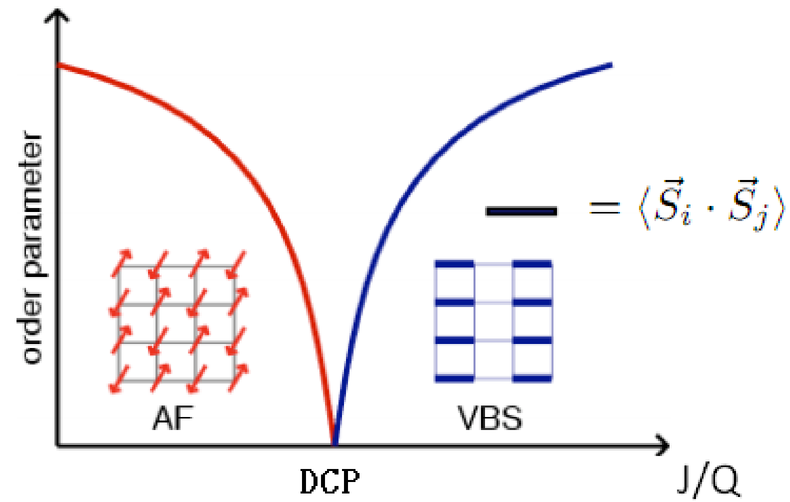


with $S^z = \pm 1$

- Lattice: 2D square lattice
- No sign problems in QMC simulations

Phase diagram & DCP

- AF-VBS transition
- "deconfined" quantum critical: 1^{st} or 2^{nd} ?



1^{st} : ← Landau theory

Kuklov et al, Ann. Phys 321, 1602 (2006);

Jiang et al., JSTAT, P02009 (2008);

Kuklov et al., PRL 101, 050405 (2008)

2^{nd} :

Senthil et al., Science 303, 1490 (2004);

Sandvik, PRL. 98, 227202 (2007), PRL, 104,177201(2010)

Worm algorithm for J-Q model

- Rewrite Hamiltonian as:

$$\hat{H} = \hat{H}_0 + \hat{H}_1 + \hat{H}_2$$

$$\hat{H}_1 \text{ :kink(two-site) interaction}$$

$$\hat{H}_2 \text{ : paired-kink(four-site) interaction}$$

- Four types of operation are needed:
  1. create/annihilate a worm
  2. move(time shift)
  3. kink-creation and kink-annihilation(space shift)
  4. paired-kink-creation and paired-kink-destruction(space shift)
- A more efficient way to simulate J-Q model?
- Our goal: with flowgram method, try to determine the type of AF-VBS transition

More on Quantum spin systems

- 1D
  - Quantum spin chains(with external field)
  - ……
- 2D
  - Heisenberg model (with external field)
  - Toric code model on square lattice
  - …….

Fermi Hubbard

- Fermi Hubbard model

  The **Fermi Hubbard model** was originally proposed (in 1963) to describe electrons in solids and has since been the focus of particular interest as a model for high-temperature superconductivity.

- Our ambiguous goal

  Make a step forward of this 50-year-old problem with Diagrammatic Monte Carlo method.

Fermi Hubbard

- Fermi Hubbard model Hamiltonian

$$H = -t \sum_{<ij>,\sigma} a_{i\,\sigma}\, a_{j\,\sigma}^{\dagger} \; + U \sum_{i} n_{i\uparrow}\, n_{i\downarrow} - \mu \sum_{i,\sigma} n_{i\,\sigma}$$

- Momentum representation

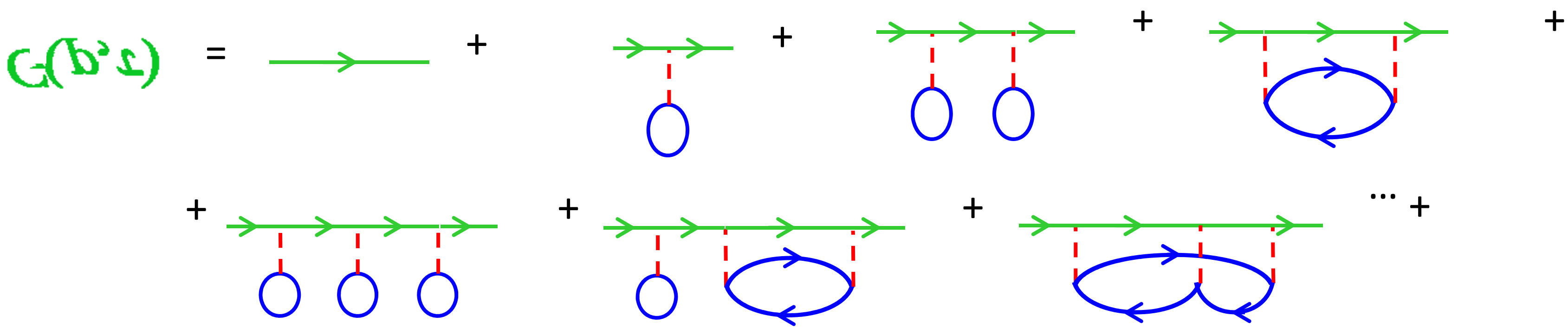
$$H = \sum_{k,\sigma} (\varepsilon_k - \mu) a_{k\sigma}^{\dagger} a_{k\sigma} + \sum_{kpq,\sigma\sigma'} U_q a_{k-q\sigma}^{\dagger} a_{p+q\sigma'}^{\dagger} a_{p\sigma'} a_{k\sigma}$$

Fermi Hubbard

- The full Green's Function:

$$G_{\uparrow,\downarrow}(p,\tau_2-\tau_1) = -\mathrm{Tr}\left[a_{\uparrow,\downarrow p}(\tau_2)\;\; a^{+}_{\uparrow,\downarrow p}(\tau_1)\;\; e^{-H/T} \right]$$

- Diagrammatic expansion



- Sample the diagrams by Monte Carlo !

Sign-problem

Computational complexity
Is exponential : $\exp\{\#\xi\}$

Cluster DMFT

+ universal
- cluster size extrapolation

Cluster DMFT

$$\xi = \left(\frac{\varepsilon_F}{T}\right) L^D$$

linear size

Diagrammatic MC

+ universal
- diagram-order extrapolation

Diagrammatic MC

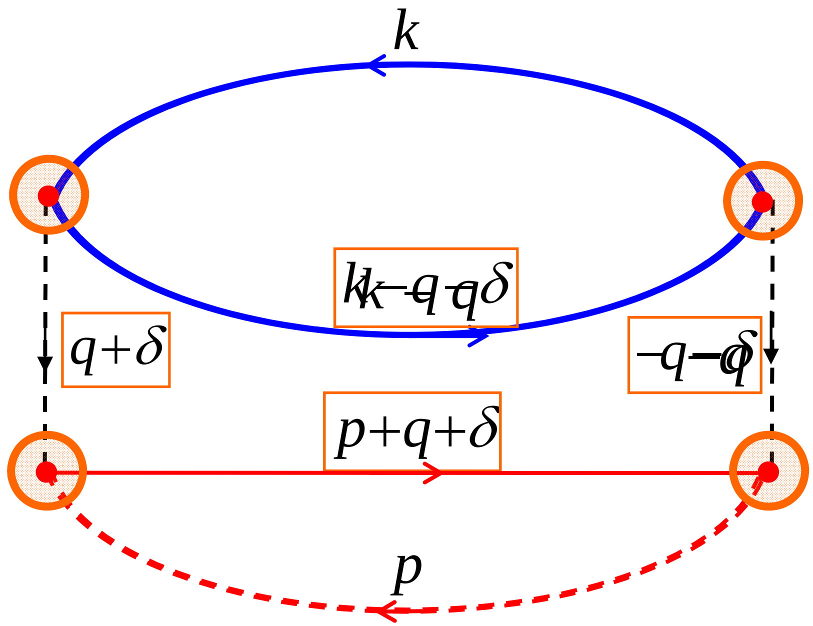
$$\xi = N$$

diagram order

Updates

Move worms:

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



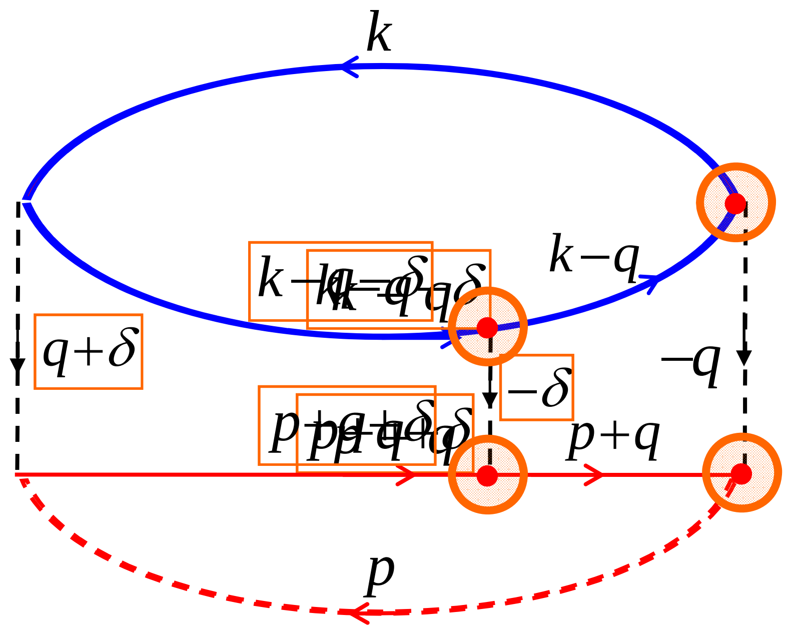
Now measure Σ

Do not measure Σ

Updates

Add a vertex:

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

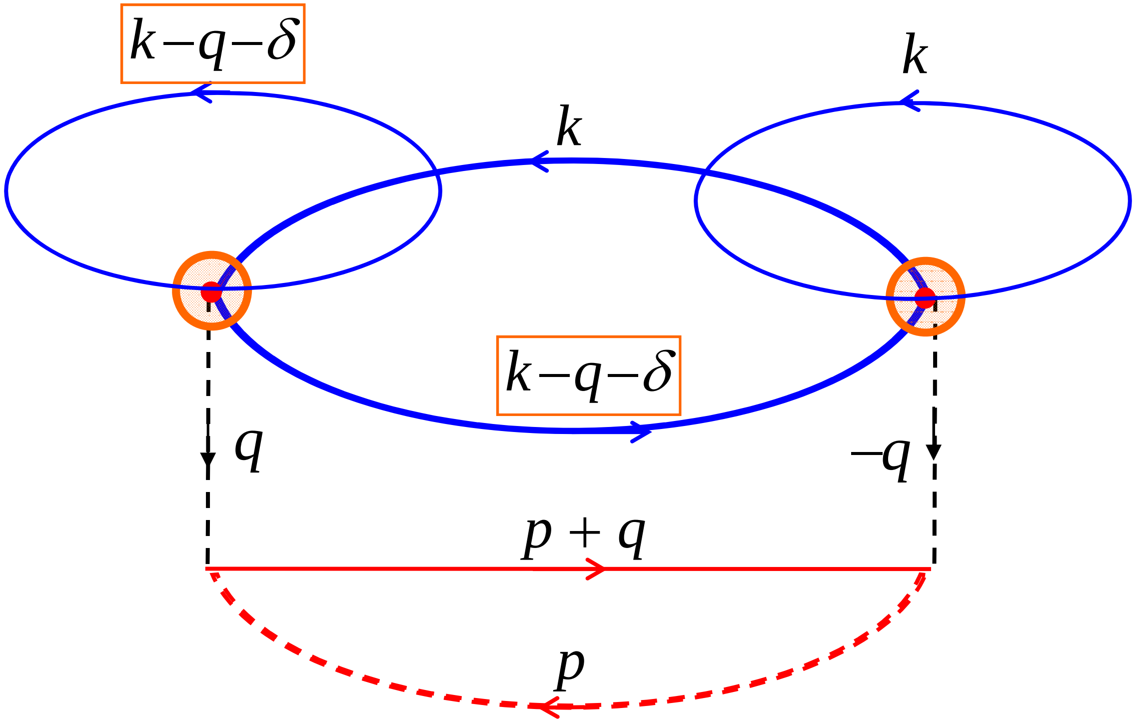


Now measure Σ

Do not measure Σ

Updates

Reconnect:



Do not measure Σ

Fermi Hubbard

- Advantages

(1) Directly work in the thermodynamic limit

(2) Sign problem is less serious.

(3) Sign can be a blessing.

(4) All analytics developed in the past 50 years can be applied.

Fermi Hubbard

- Difficulties (at least for me):

  (1) The coding is very heavy
  (2) Lack of solid mathematical background.
  (3) Lack of solid training in field theory

Unitary gas (BEC-BCS crossover)

- Experiment is done by the Harvard group led by Martin Zwierlein.
- Diagrammatic Monte Carlo is being carried out by the Amherst group led by Nikolay Prokofev and Boris Svistunov.
- Receive high praise at the DARPA-OLE meeting (07/12/2010, Miami).

Others

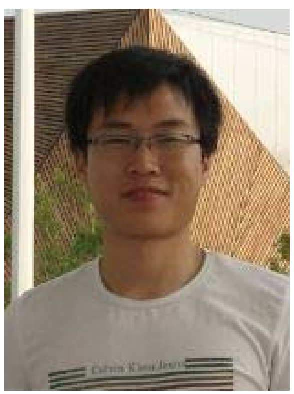
- polaron problem
- impurity solver
- polymer
- graphene
- …

Tim Garoni
Univ. Melbourne

Nikolay Prokof'ev
UMass, Amherst

Boris Svistunov
UMass, Amherst

Felix Werner
ENS, Paris



Qingquan Liu
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Zhejiang Univ.

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USTC

Yuan Huang
USTC

Thank You!