Worm Algorithm for large-scale QMC simulations in continuous space

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Advances in Quantum Monte Carlo techniques
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Collaborators

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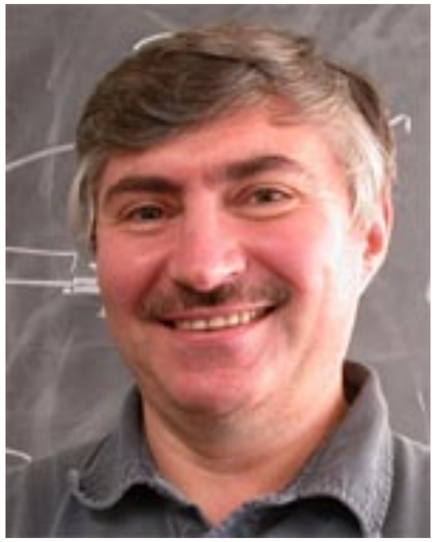
UMass, Amherst



Boris Svistunov
UMass, Amherst

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Powerful approach to Monte Carlo simulations of many-body systems

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  - **Unbiased**: *no* a priori assumption needed (e.g., trial wave function)
  - **Numerically exact** for Bose systems
  - Allows direct computation of most thermodynamic quantities of interest
    - Energetics and structure
    - Superfluid density and condensate fraction
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Worm Algorithm: addresses and solves above issues

Outline

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Basics of Worm Algorithm

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Open Issues

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- **Thermal averages** of physical operators at finite temperature $T = 1/\beta$

$$\langle \hat{\mathcal{O}} \rangle = \frac{\mathrm{Tr}(\hat{\mathcal{O}}\hat{\rho})}{\mathrm{Tr}\hat{\rho}} = \frac{\int dR\ \mathcal{O}(R)\ \rho(R,R,\beta)}{\int dR\ \rho(R,R,\beta)}$$

$$\rho(R,R,\beta) = \langle R|e^{-\beta\hat{K}}|R\rangle \ \textit{many-body density matrix}$$
$$|R\rangle \equiv |\mathbf{r}_1 ... \mathbf{r}_N\rangle \ \ \text{system configuration}$$
$$\hat{K} = \hat{H} - \mu\hat{N} \ \ \textit{grand canonical Hamiltonian}$$
$$Z = \int dR\ \rho(R,R,\beta) \ \text{grand partition function}$$

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  - Obtained through **path integration** (R. P. Feynman, 1953).

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- $u\hbar$ "*imaginary time*" ($k_B = 1$ here)

- **Integration** over all possible continuous, β-periodic many-particle paths

$$S[R(u)] = \int_0^{\beta\hbar} du \left\{ \sum_{i=1}^{N} \frac{m}{2\hbar^2}\left(\frac{d\mathbf{r}_i}{du}\right)^2 + V(R(u)) \right\}$$

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- **Euclidean Action** S associated to path balance between *kinetic* (path curvature) and *potential* energy (depends on interactions) along path
  - **Smooth**, straight paths have generally **higher** probability
  - Paths of **high potential energy** have **low** probability

Quantum Statistics

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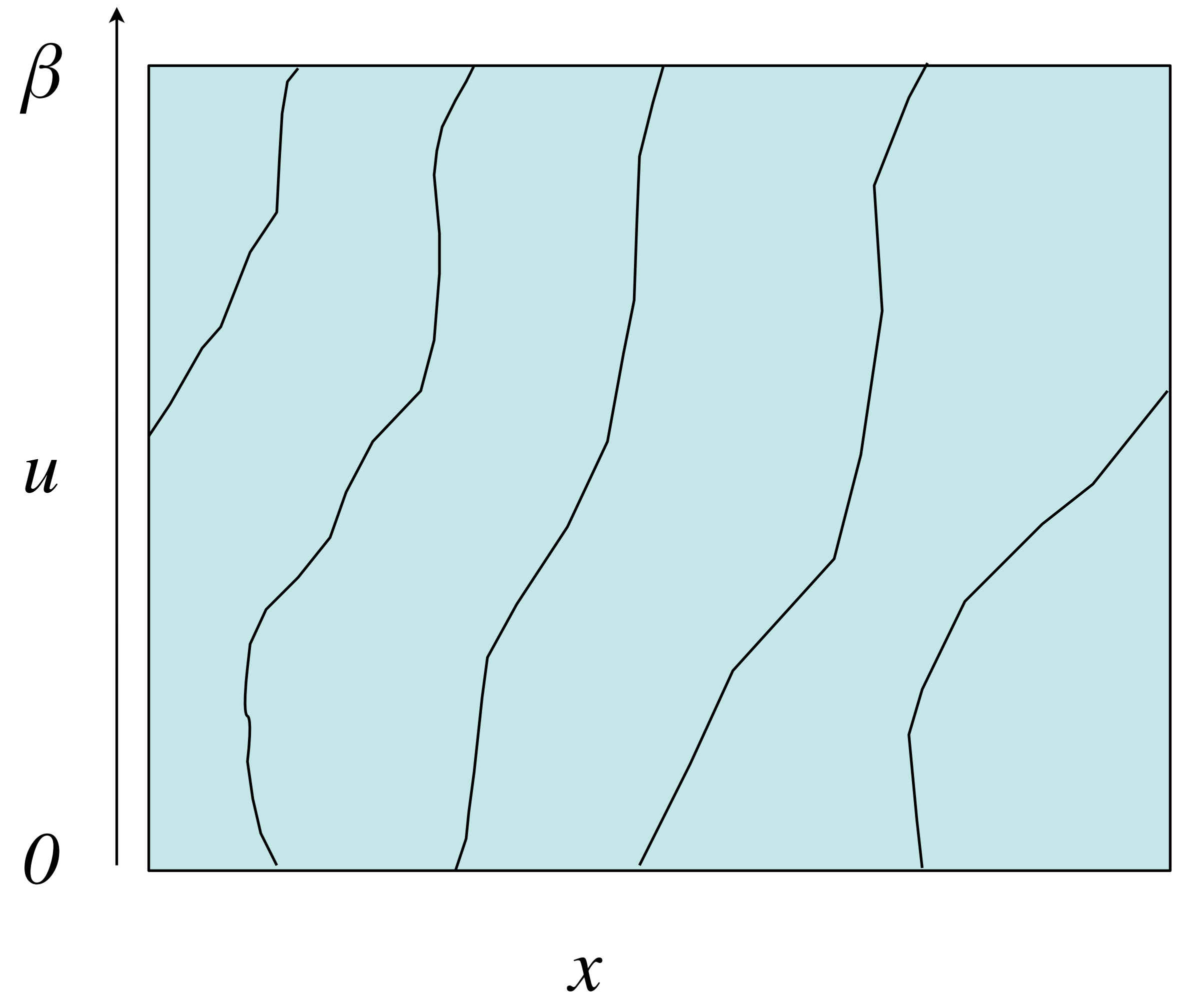

Example
4 particles in 1d

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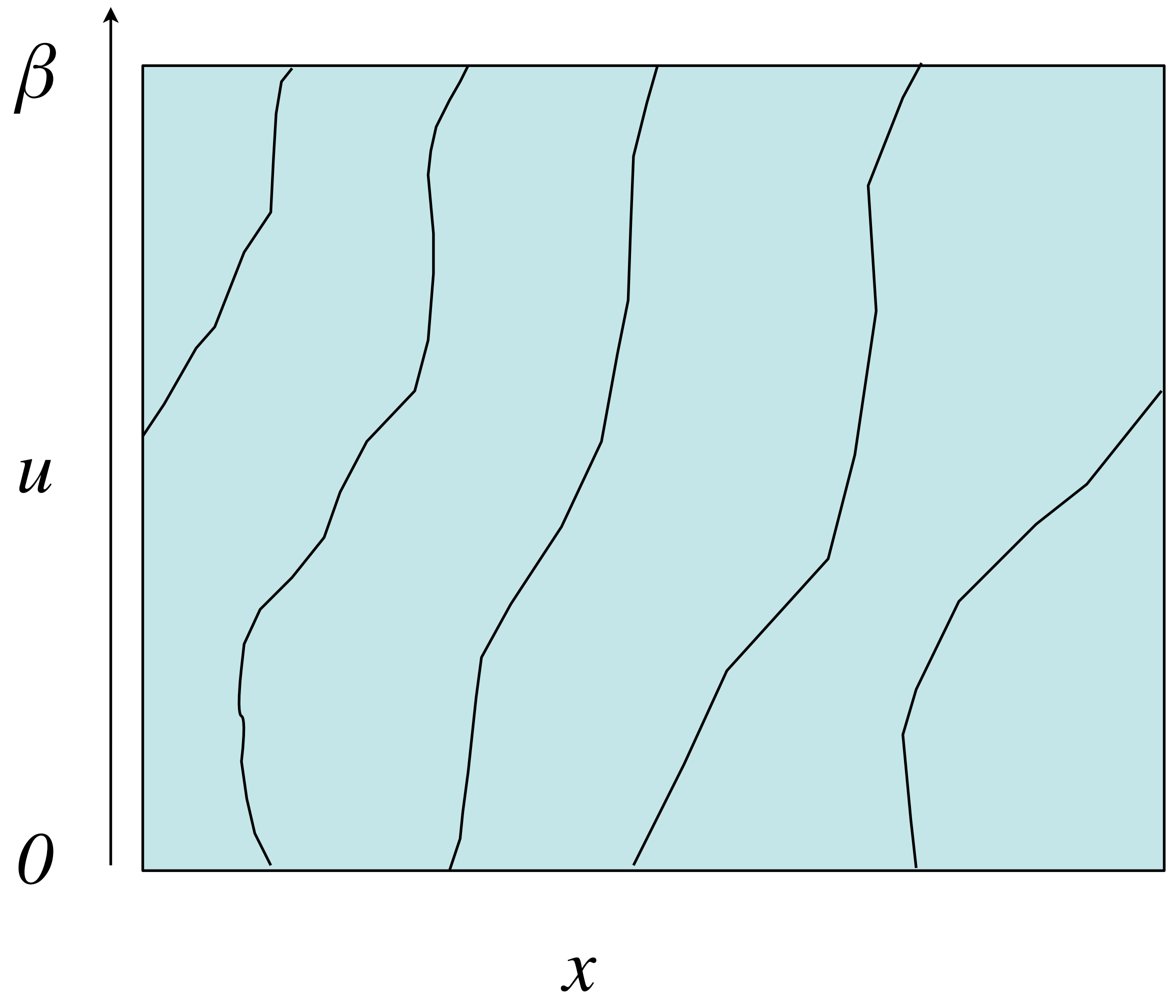

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- **Paths** are β-periodic, i.e., $R(\beta)=R(0)$
  - However, individual particle positions can undergo **exchanges**
  - **Crucial** ingredient of the physics of ensembles of indistinguishable particles
  - Underlie phenomena such as **BEC and Superfluidity**
  - Ascribing ***physical content*** to paths is tempting but ***dangerous***

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Discretization: $R(u) \equiv \{R_0, R_1, ..., R_{M-1}\}$, $R_M \equiv PR_0$
(P *permutation of particle labels*)
$M\tau = \beta$, τ is the *time step*
Simplest approximate action (we can do better but it is not needed now):

$$S[R(u)] \approx \sum_{i=1}^{N} \sum_{l=0}^{P-1} \frac{m(\mathbf{r}_{il} - \mathbf{r}_{il+1})^2}{2\tau\hbar^2} + \tau \sum_{l} V(R_l)$$

(*Note*: in the absence of interaction any discretized form is *exact*)

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$$P \propto \exp\left[-S[R(u)]\right] = \prod_{i=1}^{N} \prod_{l=0}^{M-1} \rho_\circ(\mathbf{r}_{il}, \mathbf{r}_{il+1}, \tau) \times \prod_{l=0}^{M-1} e^{-\tau V(R_l)}$$

where

$$\rho_\circ(\mathbf{r}, \mathbf{r}', \tau) = \left(2\pi\hbar^2\tau/m\right)^{-1/d} \exp\left[-\frac{m(\mathbf{r}-\mathbf{r}')^2}{2\hbar^2\tau}\right]$$

is the density matrix of a *free particle*, and

$$V(R) = U(R, \tau) - \mu N$$

In the simplest version, U is the *total potential energy*, does not depend on τ (In some approximations, it does)

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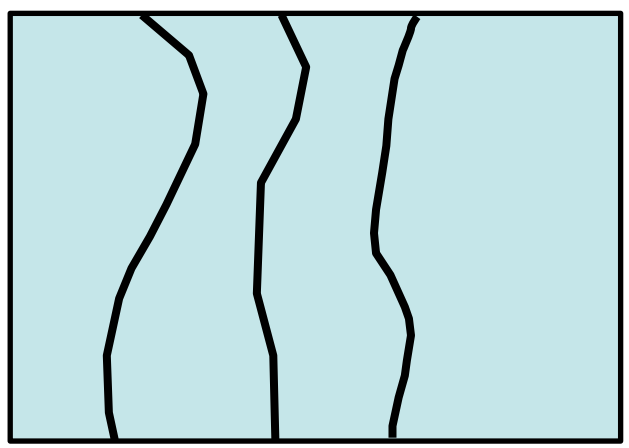
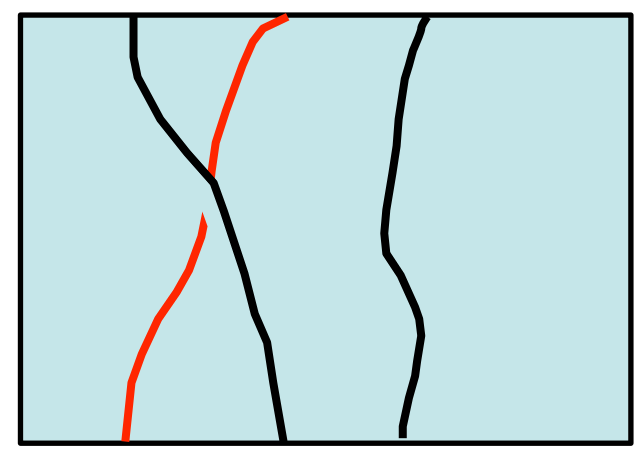
  - Permutations are sampled by *explicit construction of permutation cycles*





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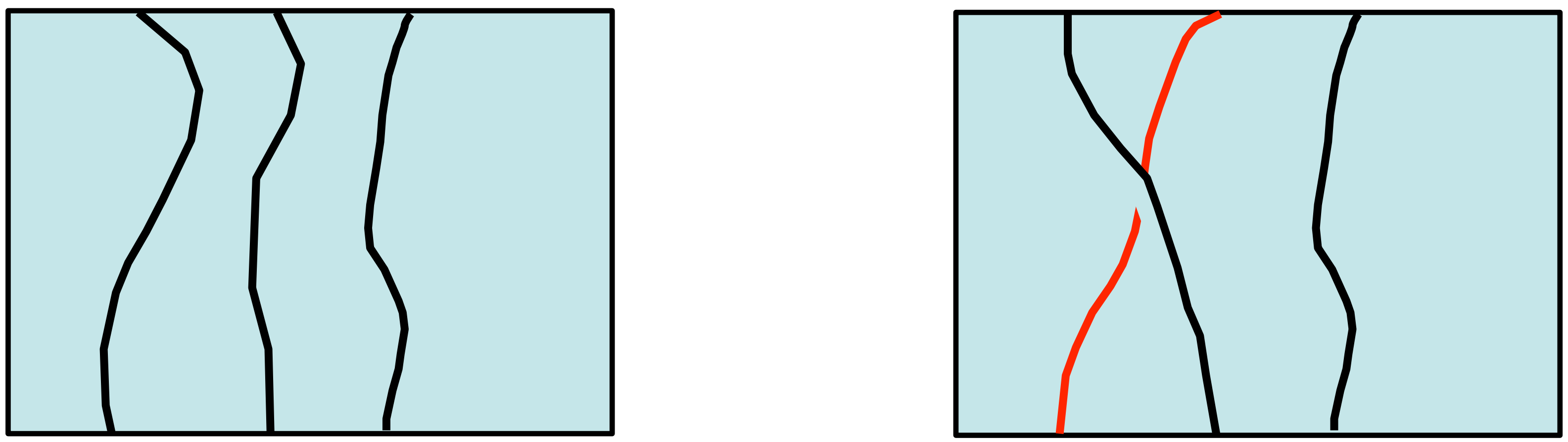

- **Sampling issues**
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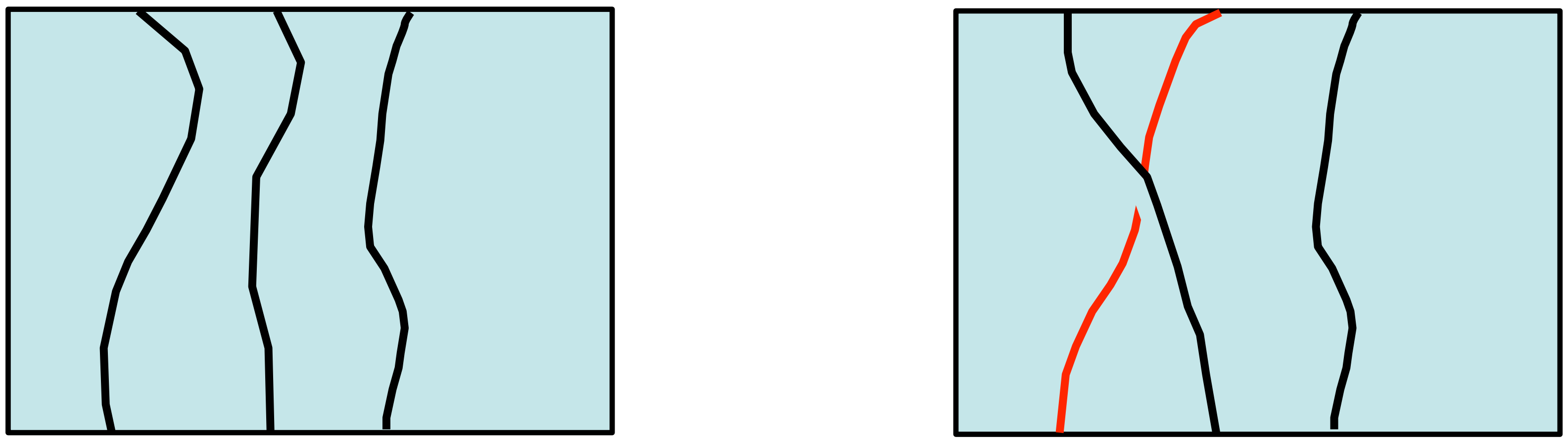

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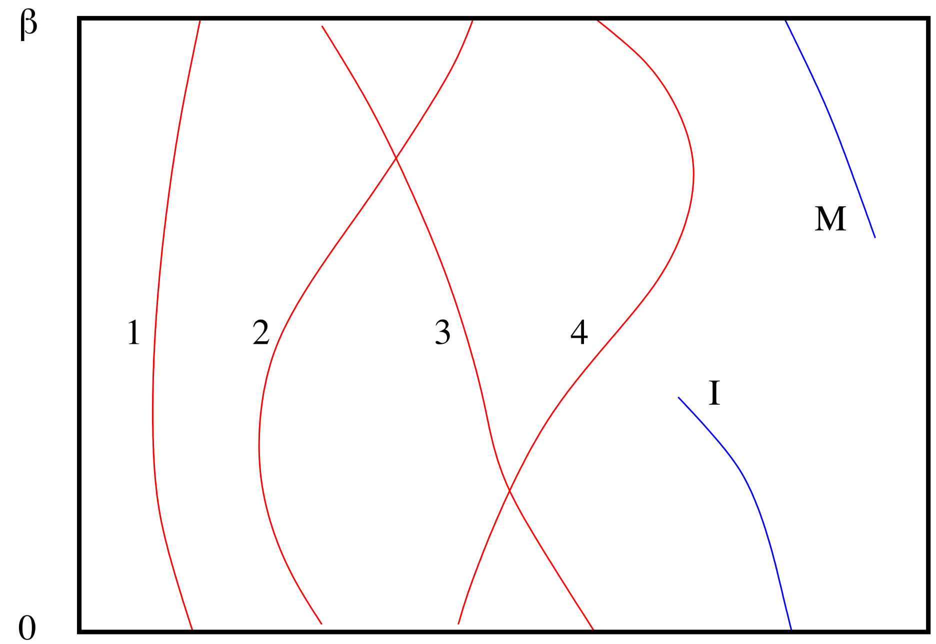
- **Problems**
  - **Superfluid fraction** connected to *winding* of paths through boundaries
  - Occurrence of *nonzero* winding requires *macroscopic* permutation cycles (length ~ $N^{1/d}$)
  - Effort required to sample macroscopic permutation cycles scales **exponentially** with N
  - Extrapolation of results to thermodynamic limit problematic
  - Even for finite systems (quantum droplets), efficient sampling of permutations can be crucial
  - Ambiguous interpretation of results (*no* superfluidity *or* ergodicity problem ?)

Worm Algorithm (of *Ira* and *Masha*)



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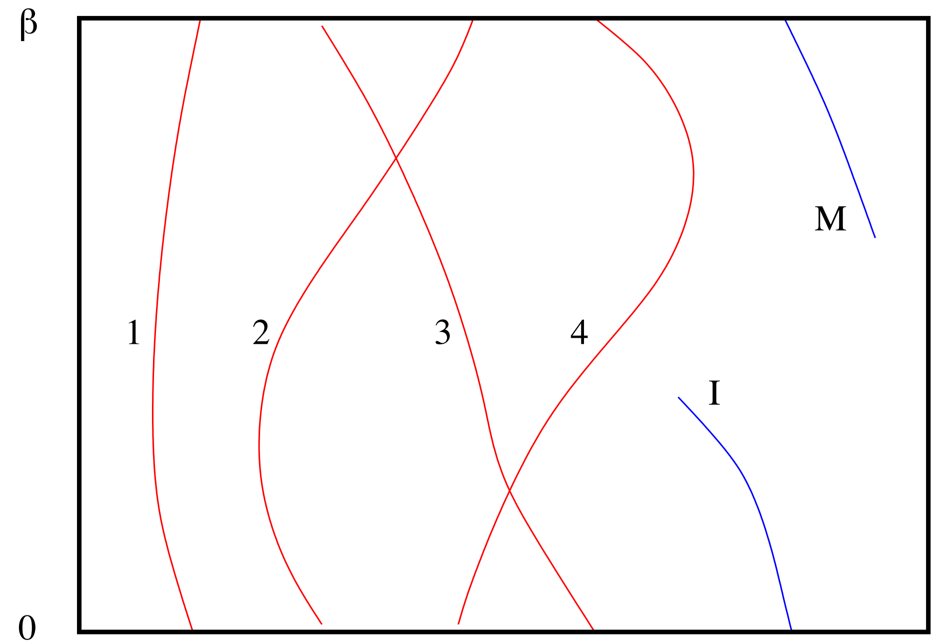

- Generalize configuration space, from that of the partition function to that of the **Matsubara Green function**

$$G(\mathbf{r}_1,\mathbf{r}_2,t) = \frac{g(\mathbf{r}_1,\mathbf{r}_2,t)}{Z} = -\langle \hat{\mathcal{T}}[\hat{\psi}(\mathbf{r}_1,t)\ \hat{\psi}^\dagger(\mathbf{r}_2,0)]\rangle$$

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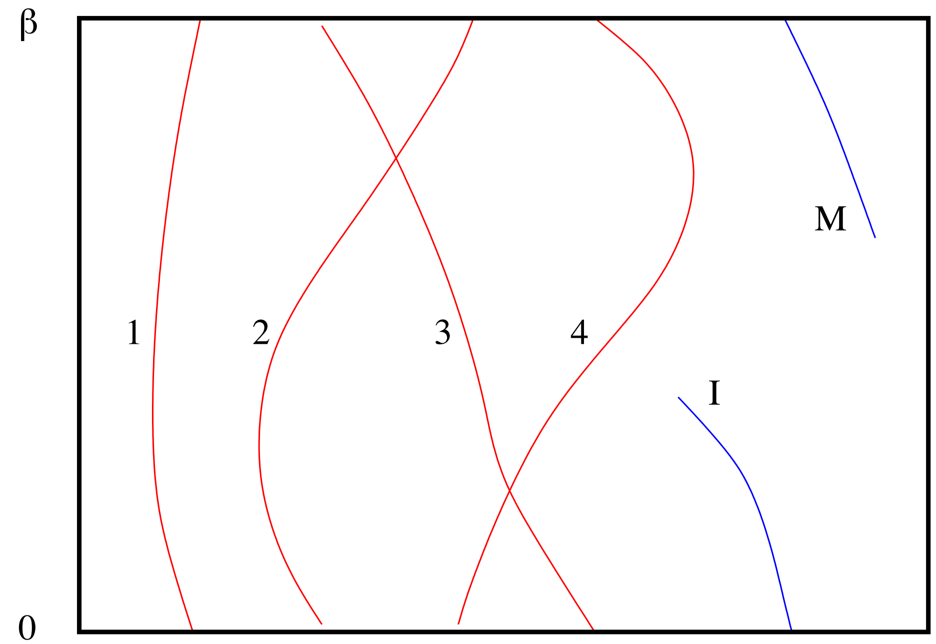

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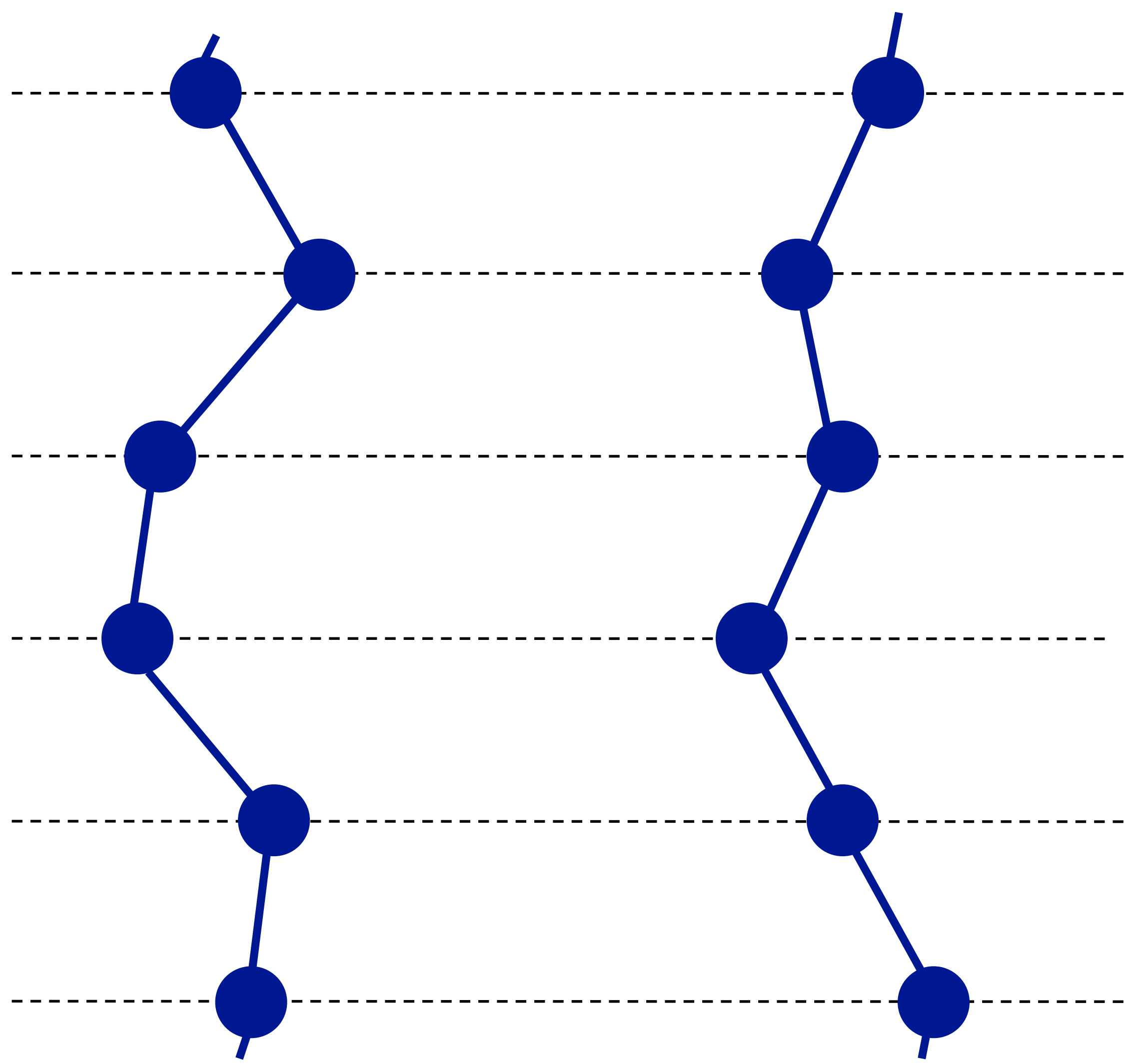
- **One open world line** with two dangling ends (*worm*)
  - ***Z***- and ***G***-sectors are identified
  - Sampling of paths occurs through simple set of complementary moves

Z



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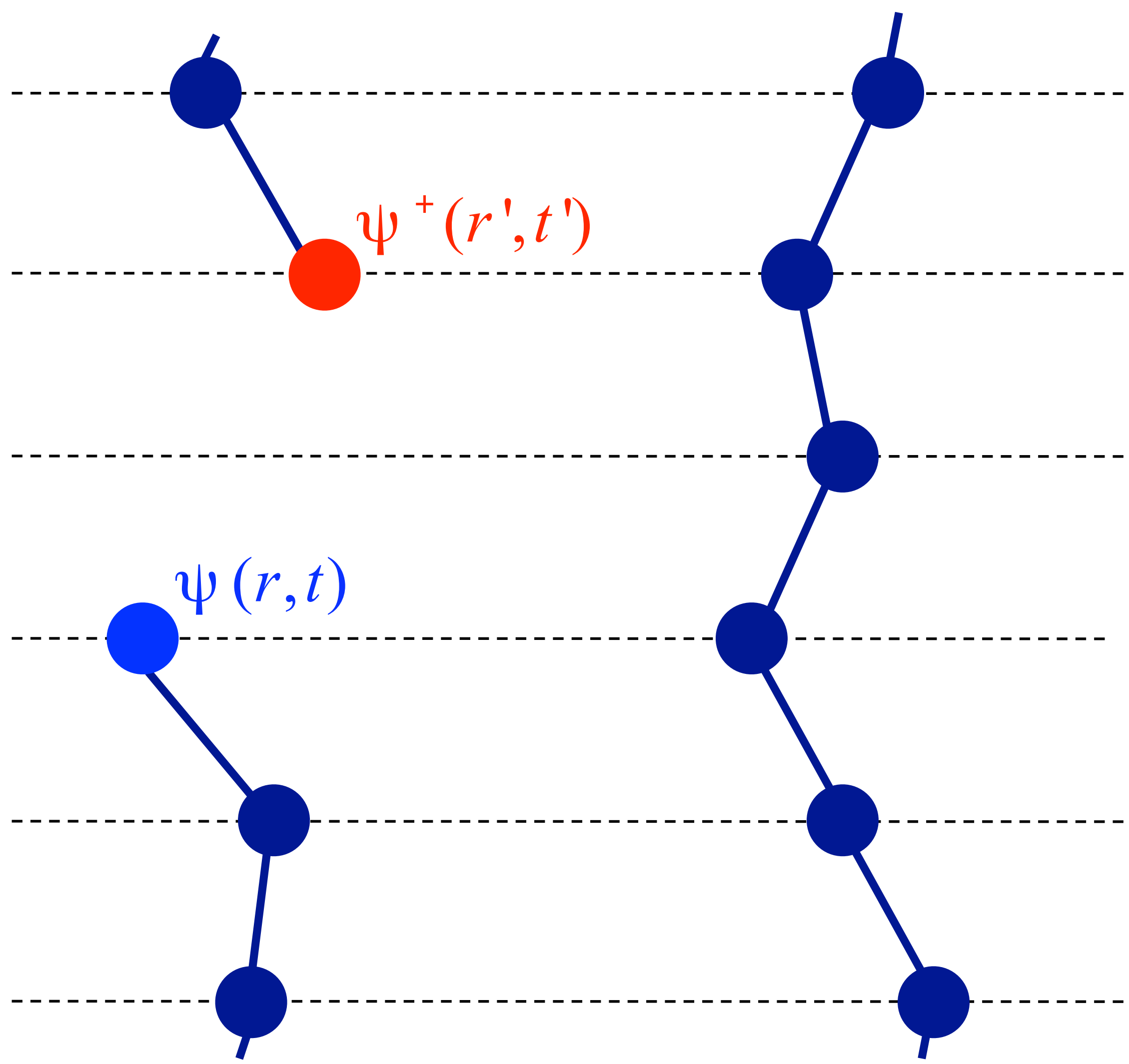

(open/close update)

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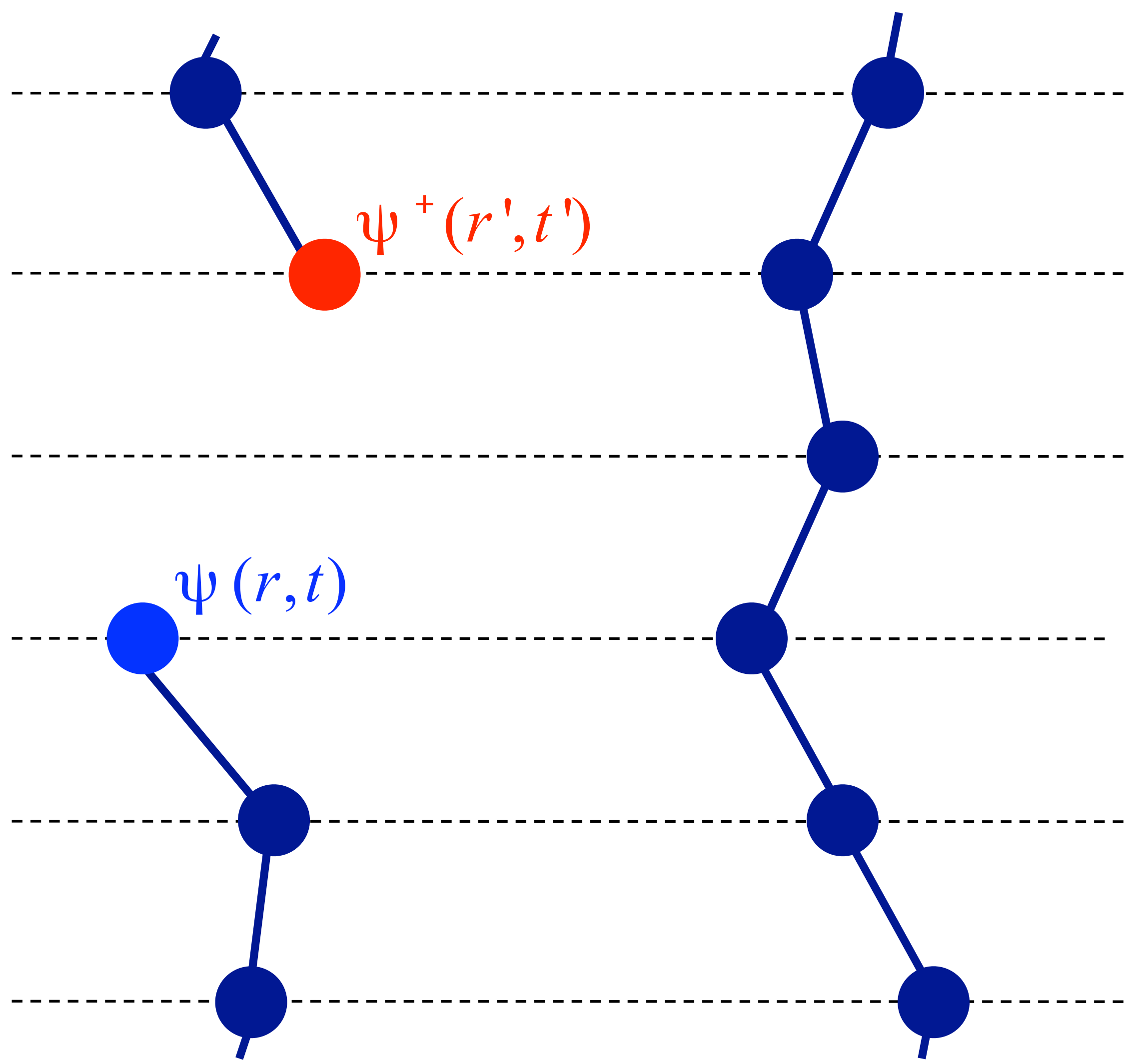
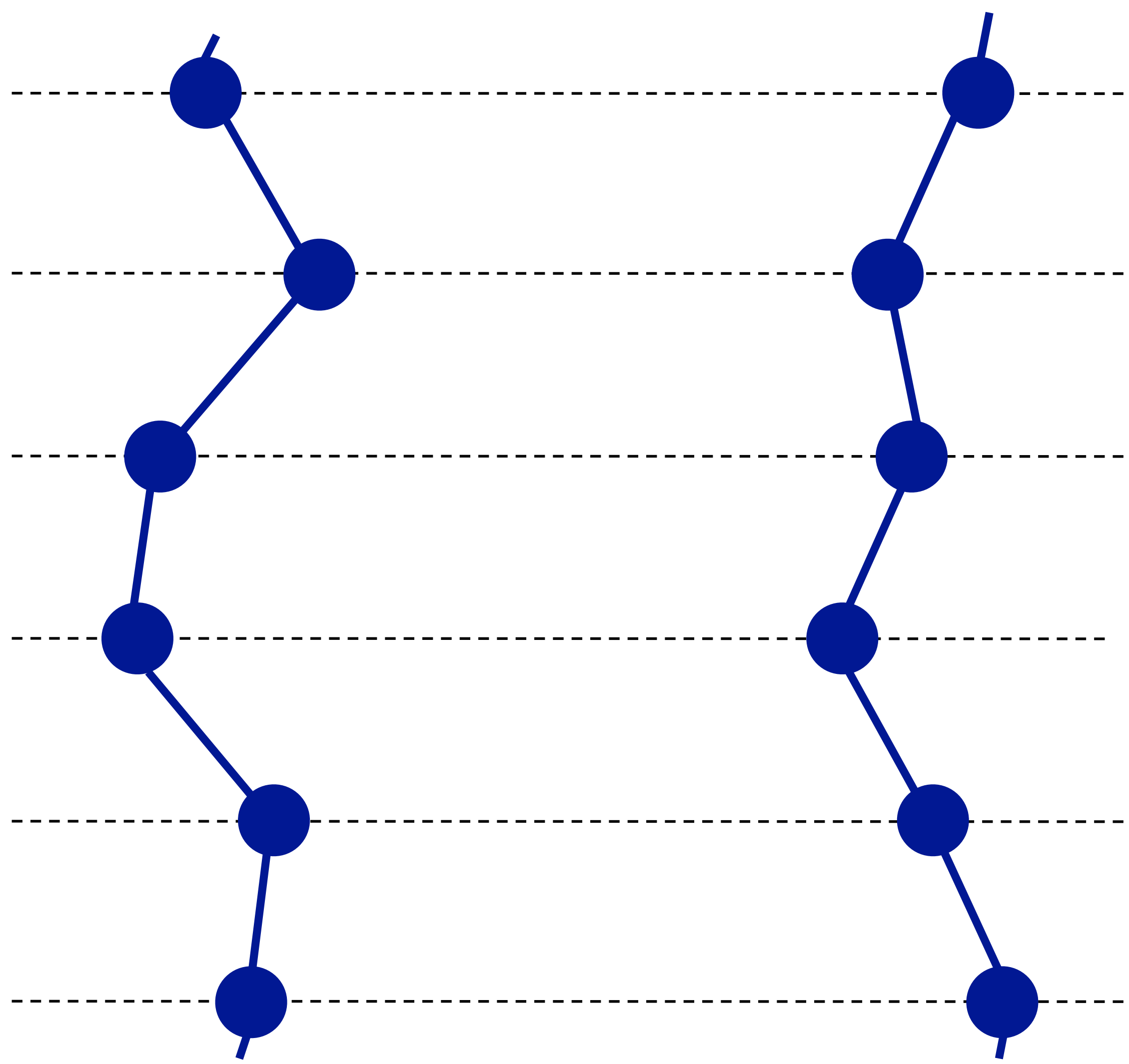


(open/close update)

$$P_{\rm op} = \min\left\{1,\ \frac{C\, m_\circ N M\ \mathrm{e}^{\Delta U - \mu m \tau}}{\rho_\circ(\mathbf{r}_I, \mathbf{r}_M, m\tau)}\right\}$$

$$P_{\rm cl} = \min\left\{1,\ \frac{\rho_\circ(\mathbf{r}_I, \mathbf{r}_M, m\tau) e^{\Delta U + \mu m \tau}}{C m_\circ N M}\right\}$$

Z



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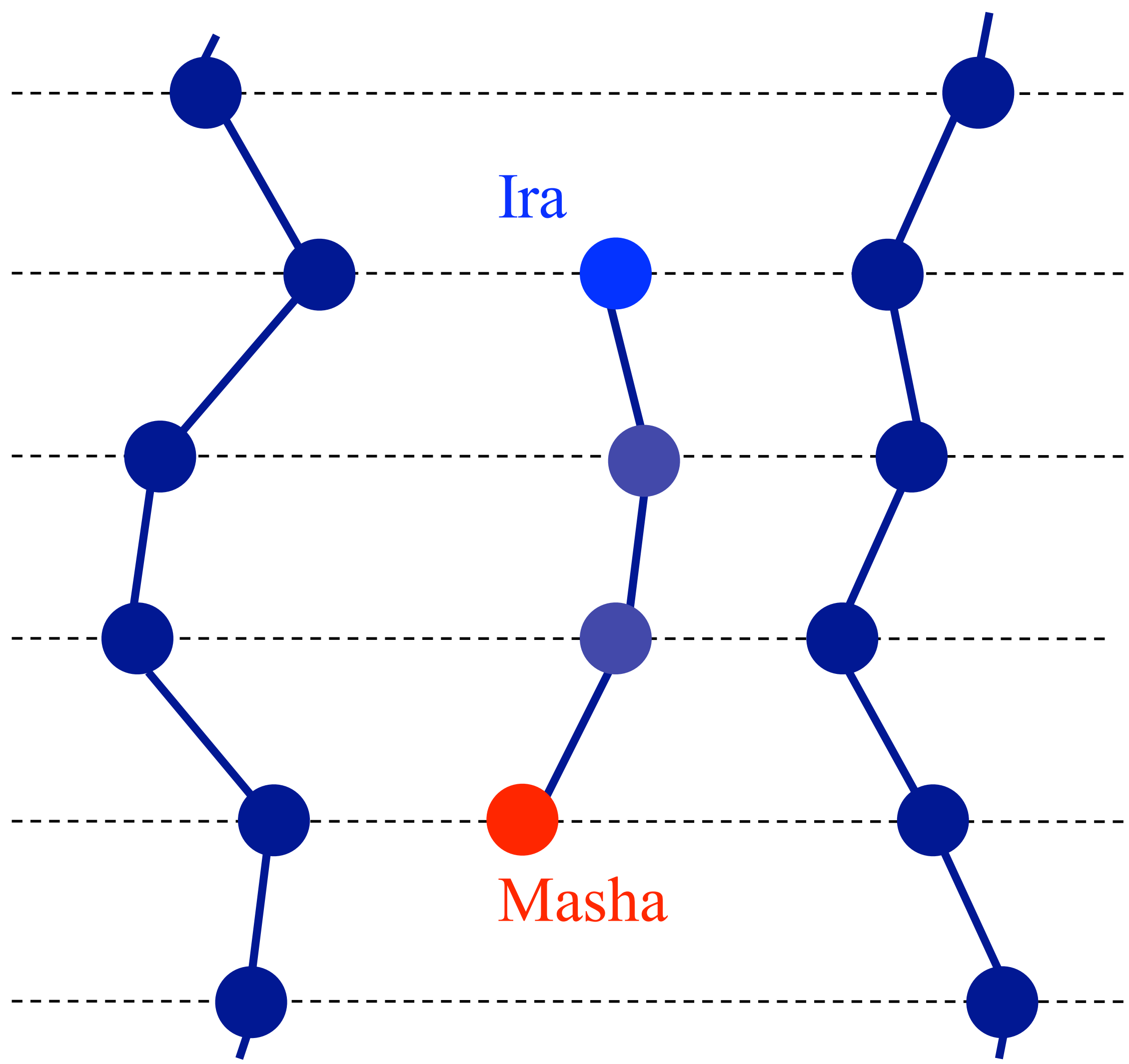

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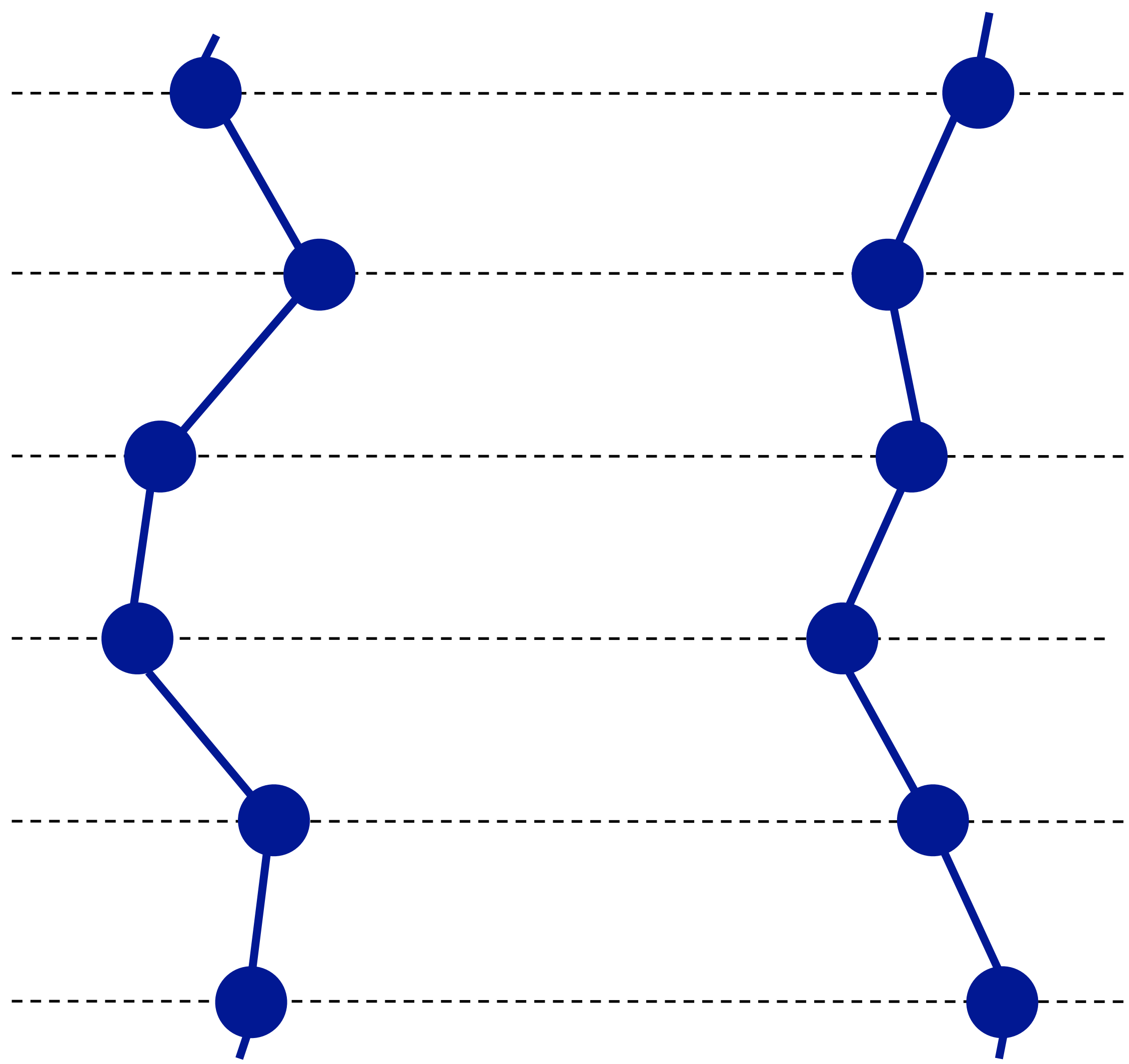

(insert/remove update)

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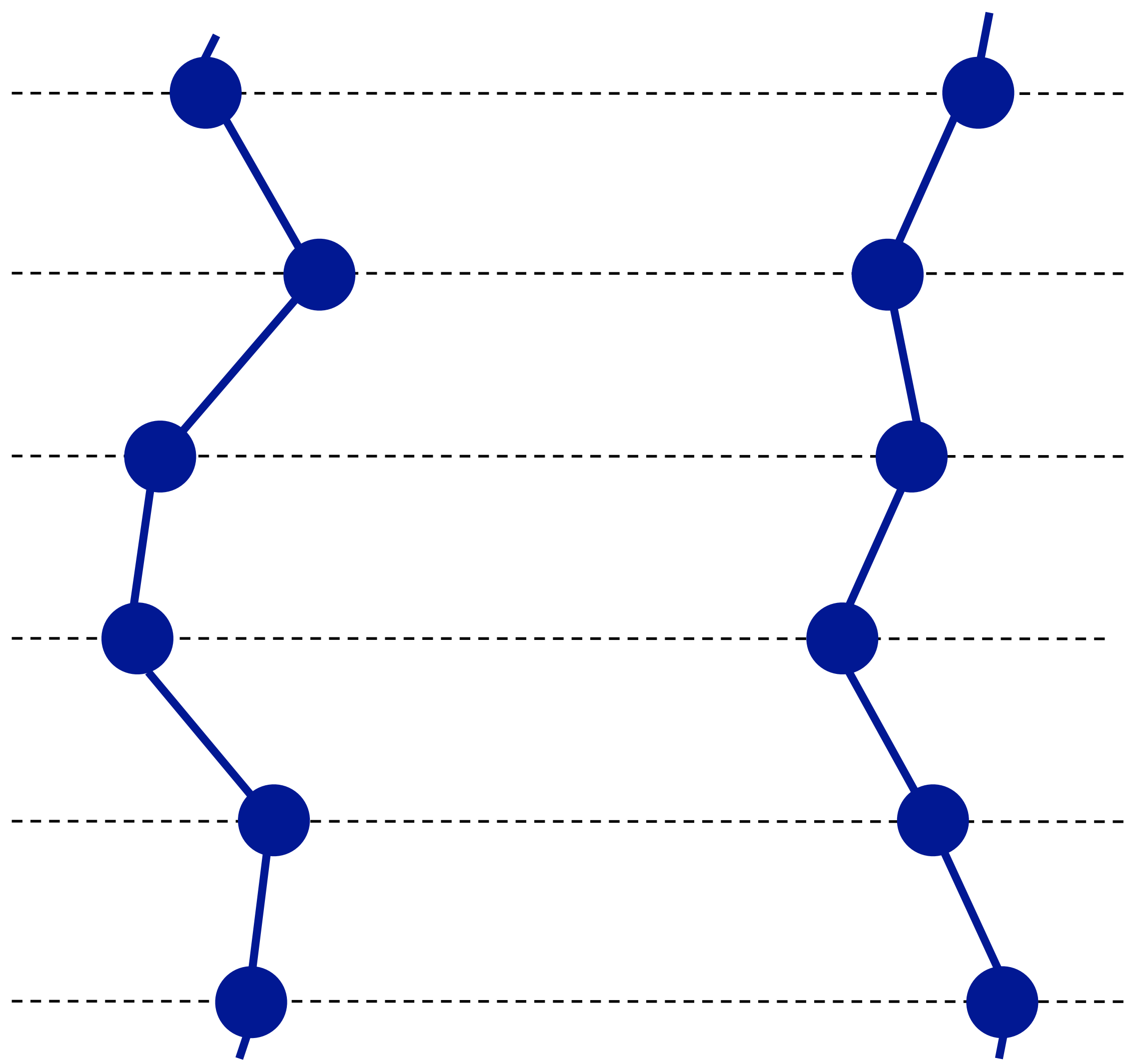
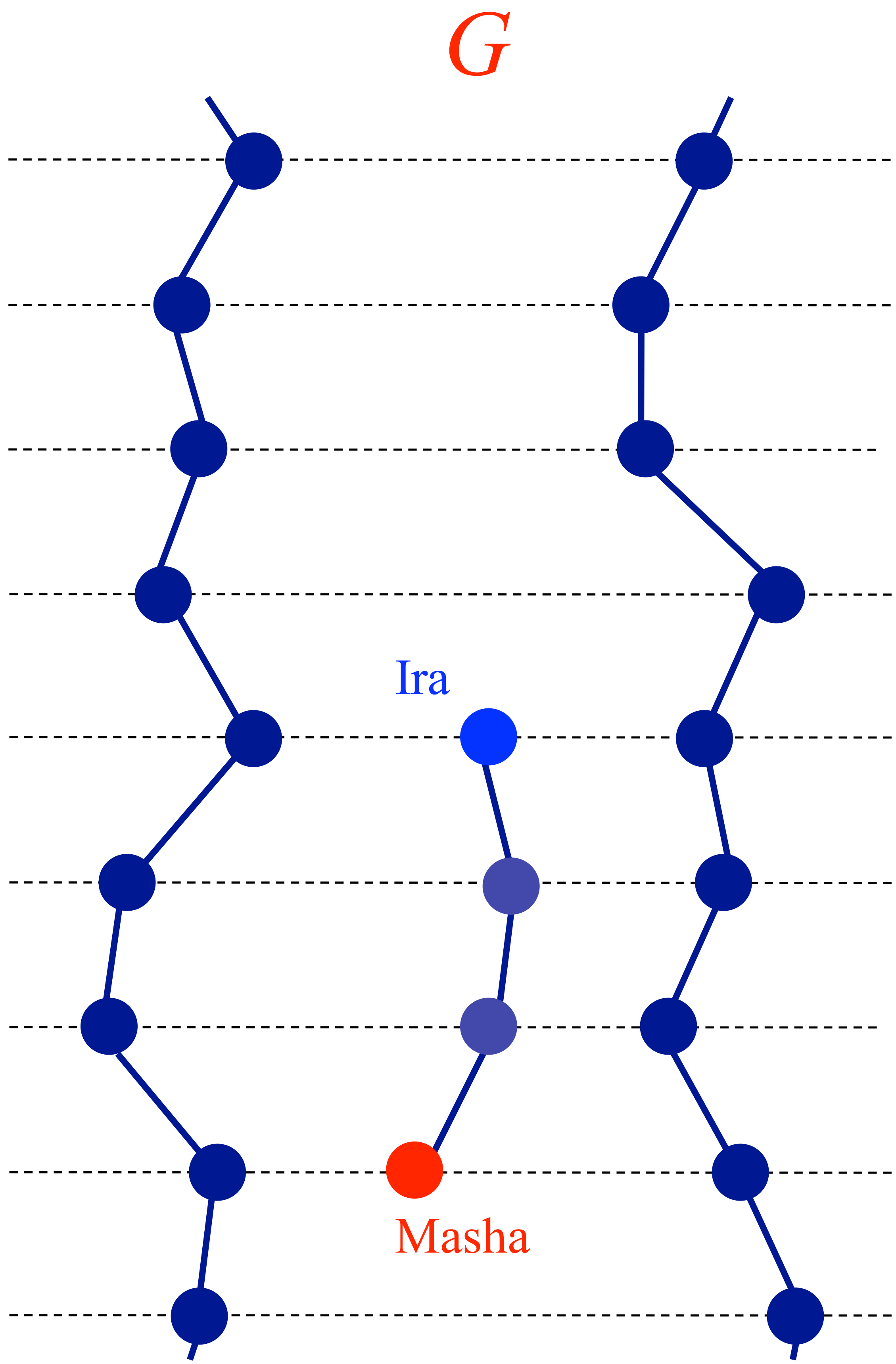


(insert/remove update)

$$P_{\text{in}} = \min\left\{1, e^{\Delta U + \mu m \tau} C\Omega M m_{\circ}\right\} \qquad P_{\text{rm}} = \min\left\{1, \frac{e^{\Delta U - \mu m \tau}}{C\Omega M m_{\circ}}\right\}$$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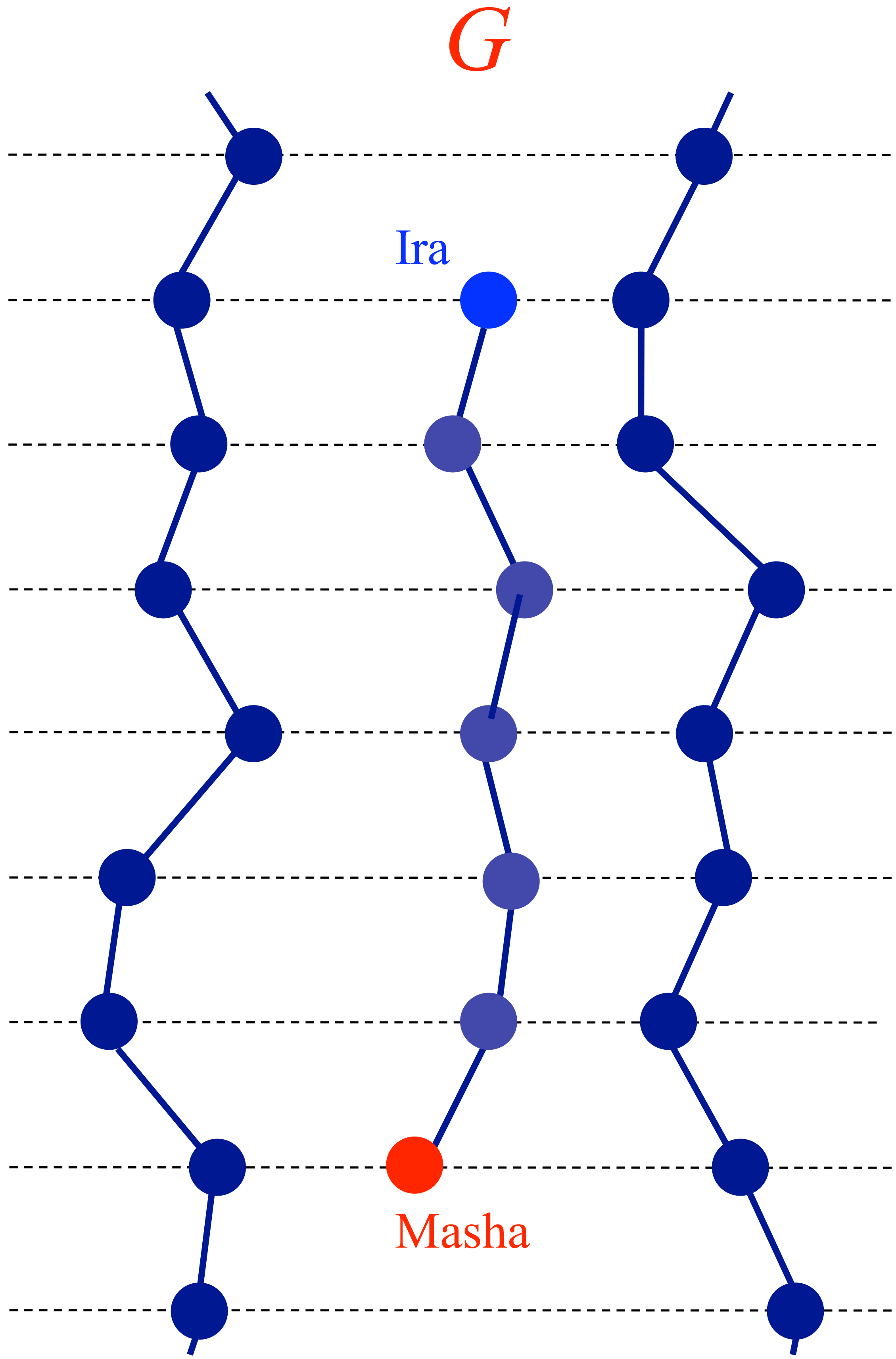
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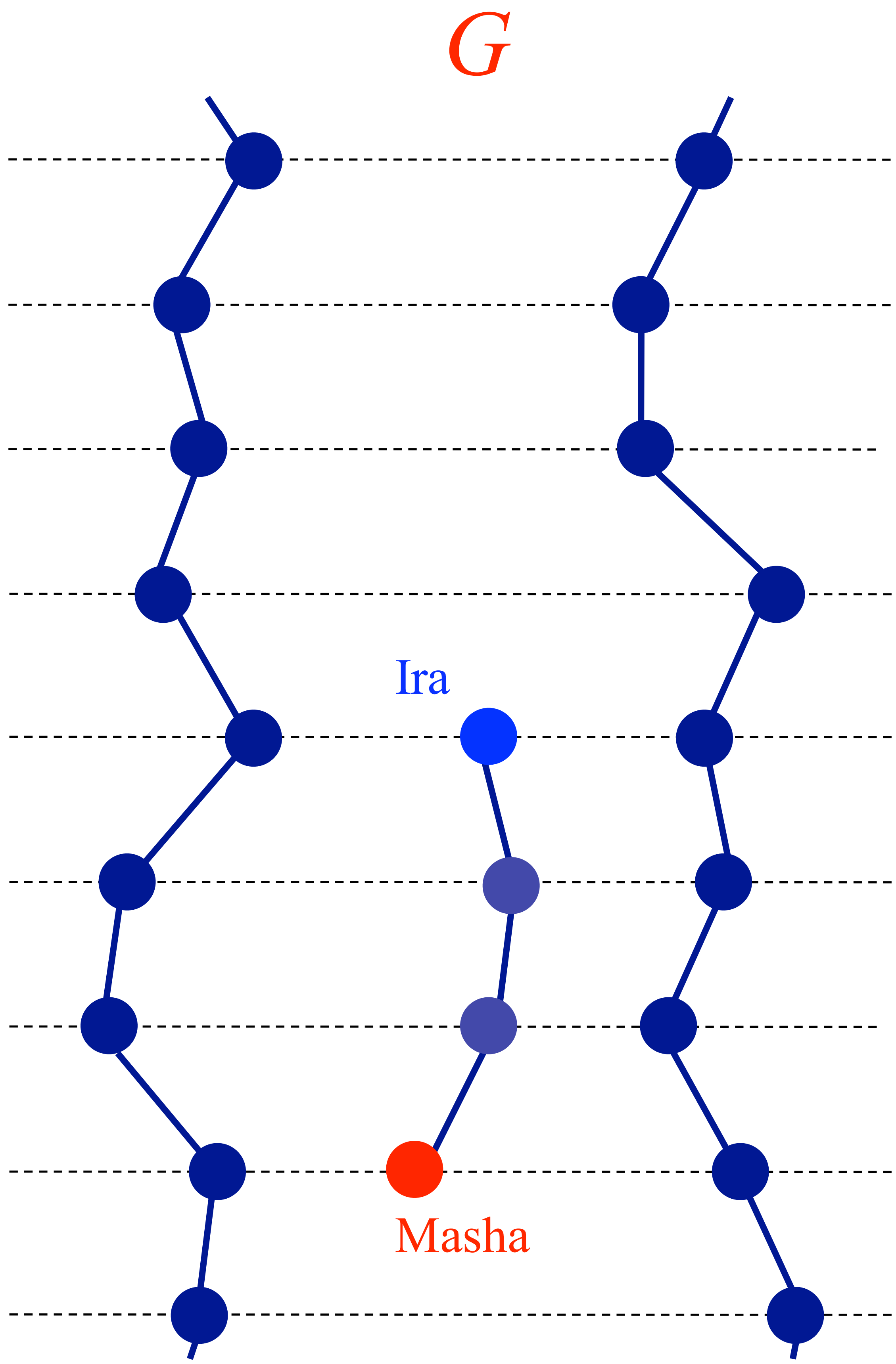
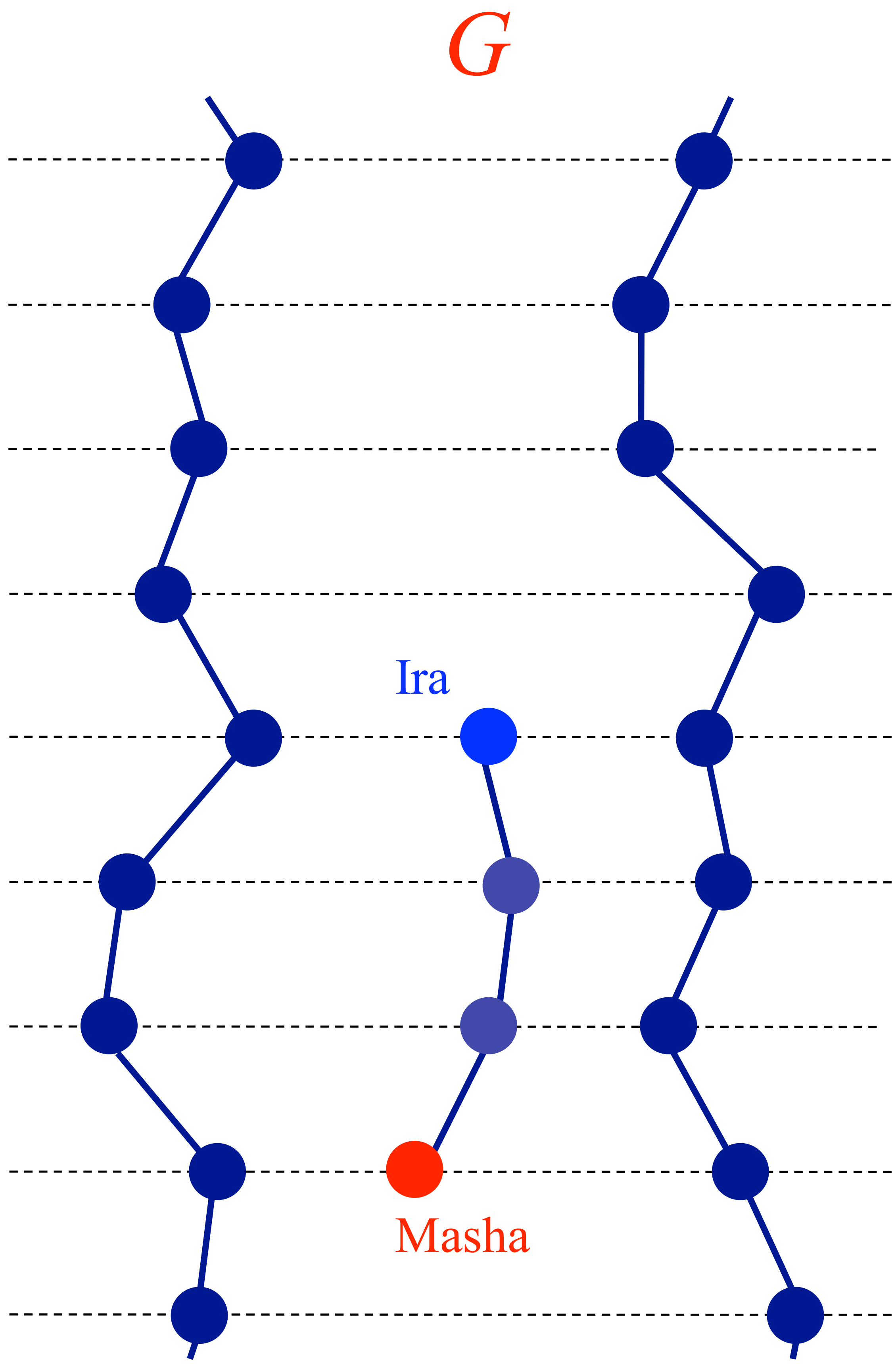


(advance/recede update)



All new positions sampled *directly* from $\rho_\circ$

$$P_{\rm ad} = \min\left\{1,\ \mathrm{e}^{\Delta U + \mu m \tau}\right\}$$

$$P_{\rm re} = \min\left\{1,\ \mathrm{e}^{\Delta U - \mu m \tau}\right\}$$

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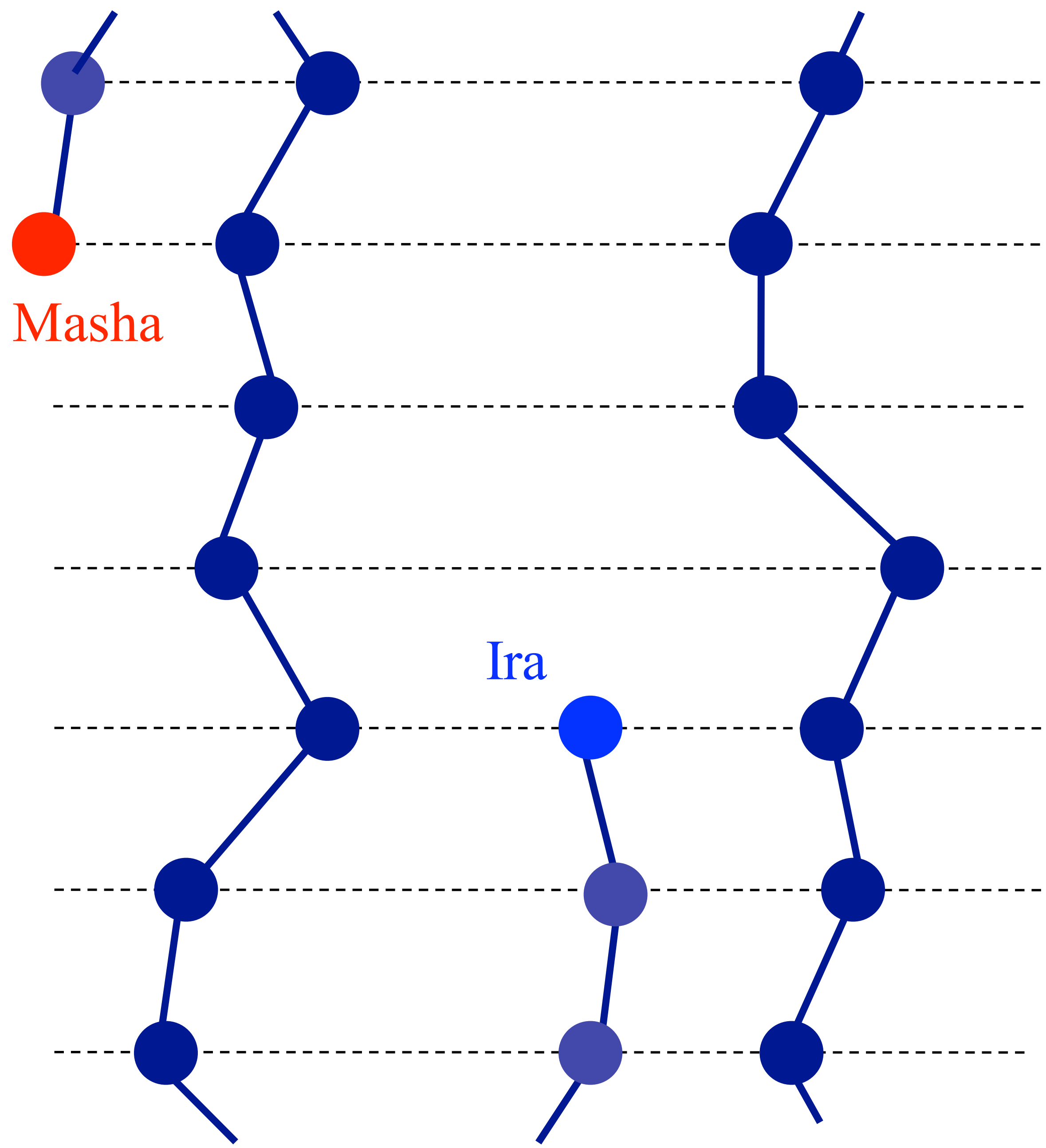

swap update (self-complementary)

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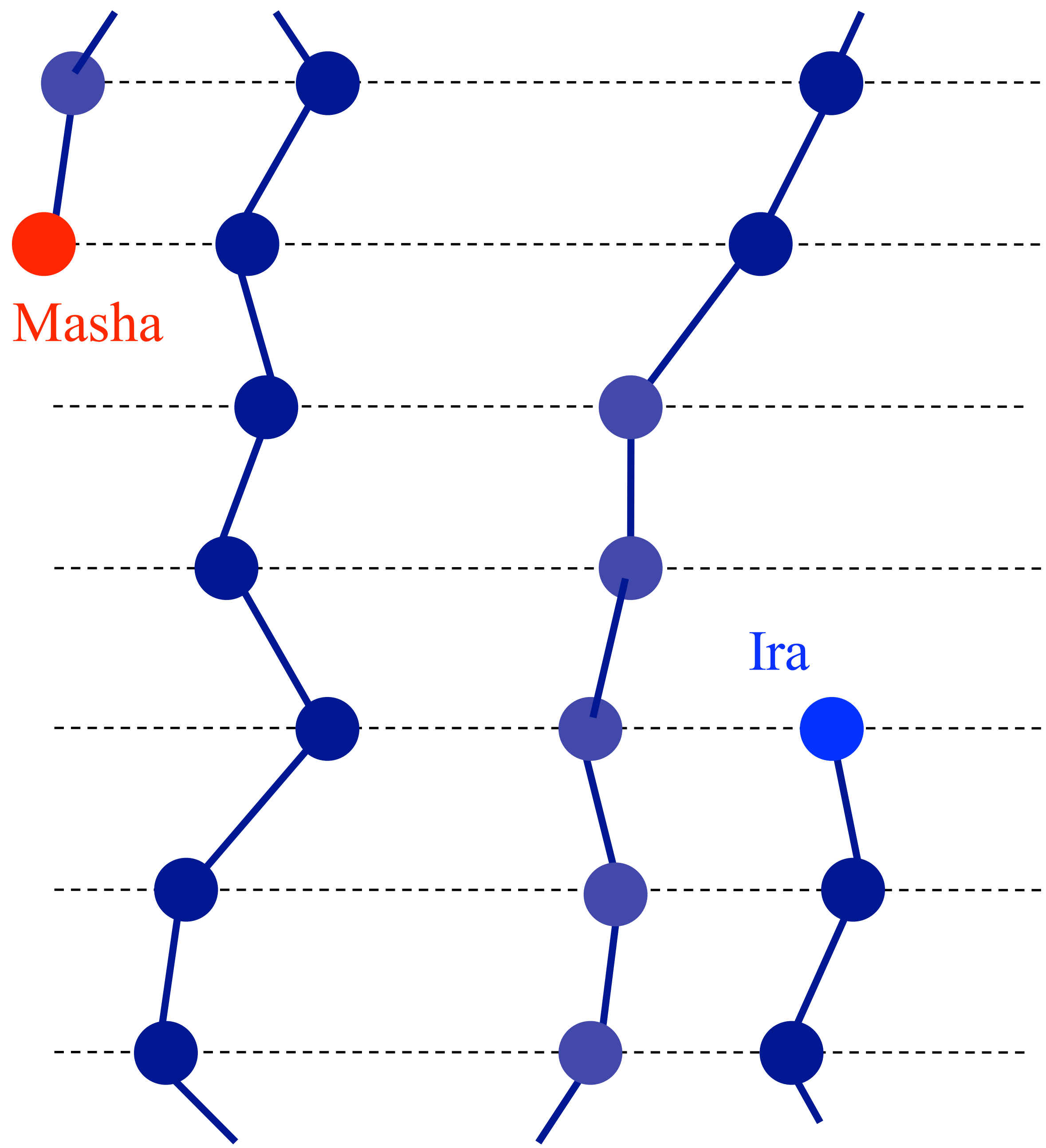

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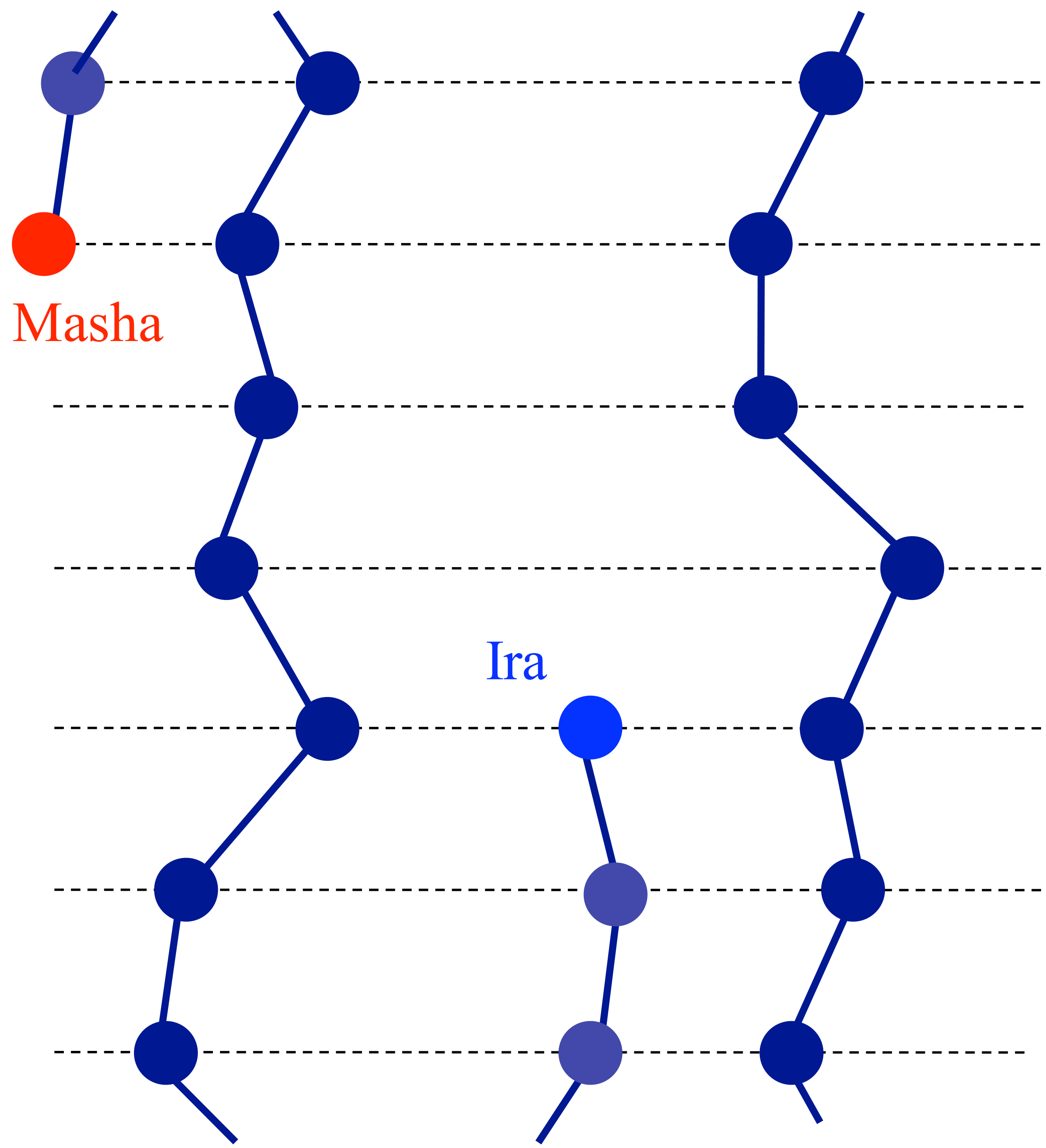

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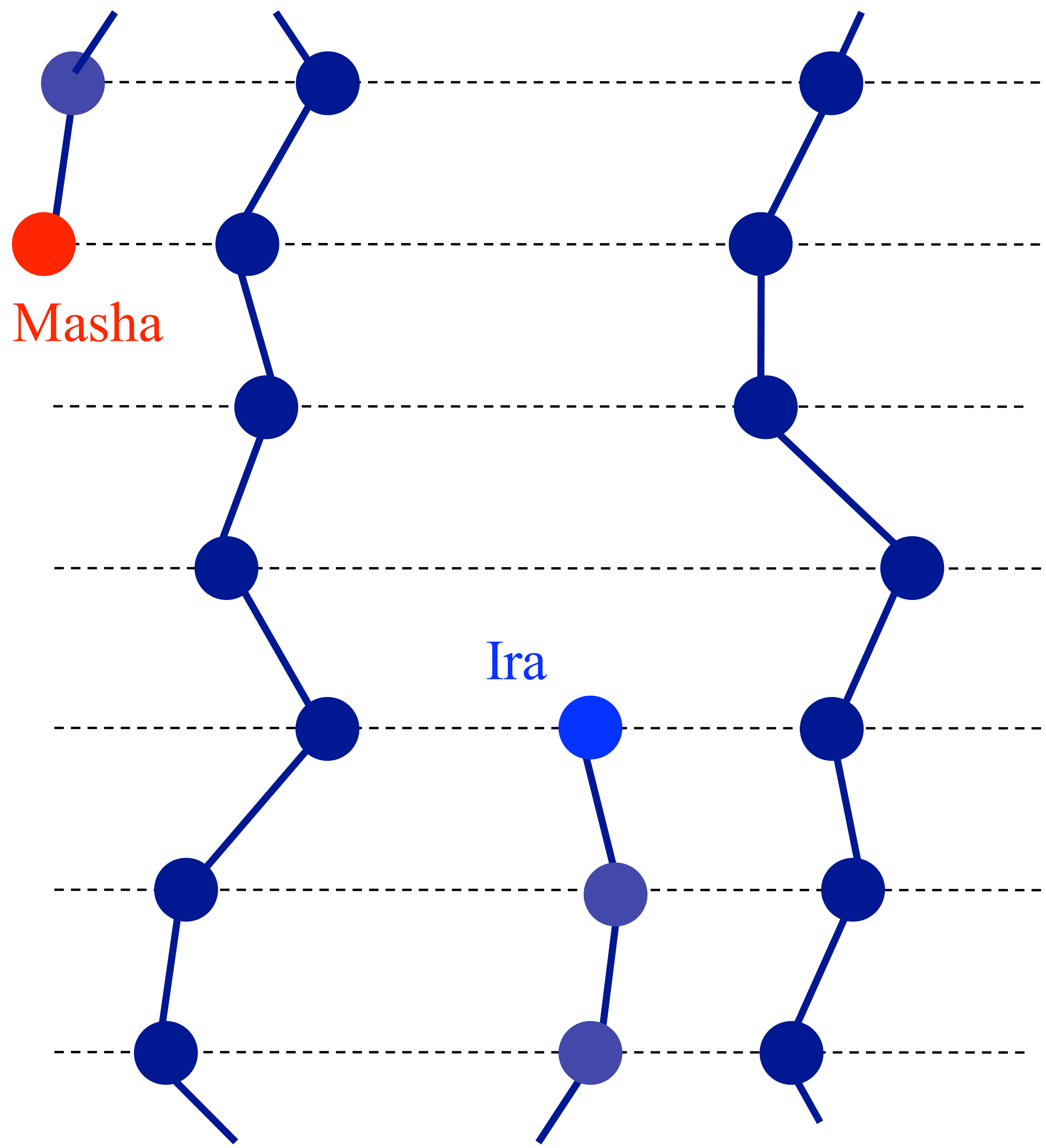

$$P_{\rm sw} = \min\left\{1, e^{\Delta U} Z_i / Z_l\right\}$$

Z probability table of possible swaps

swap update (self-complementary)

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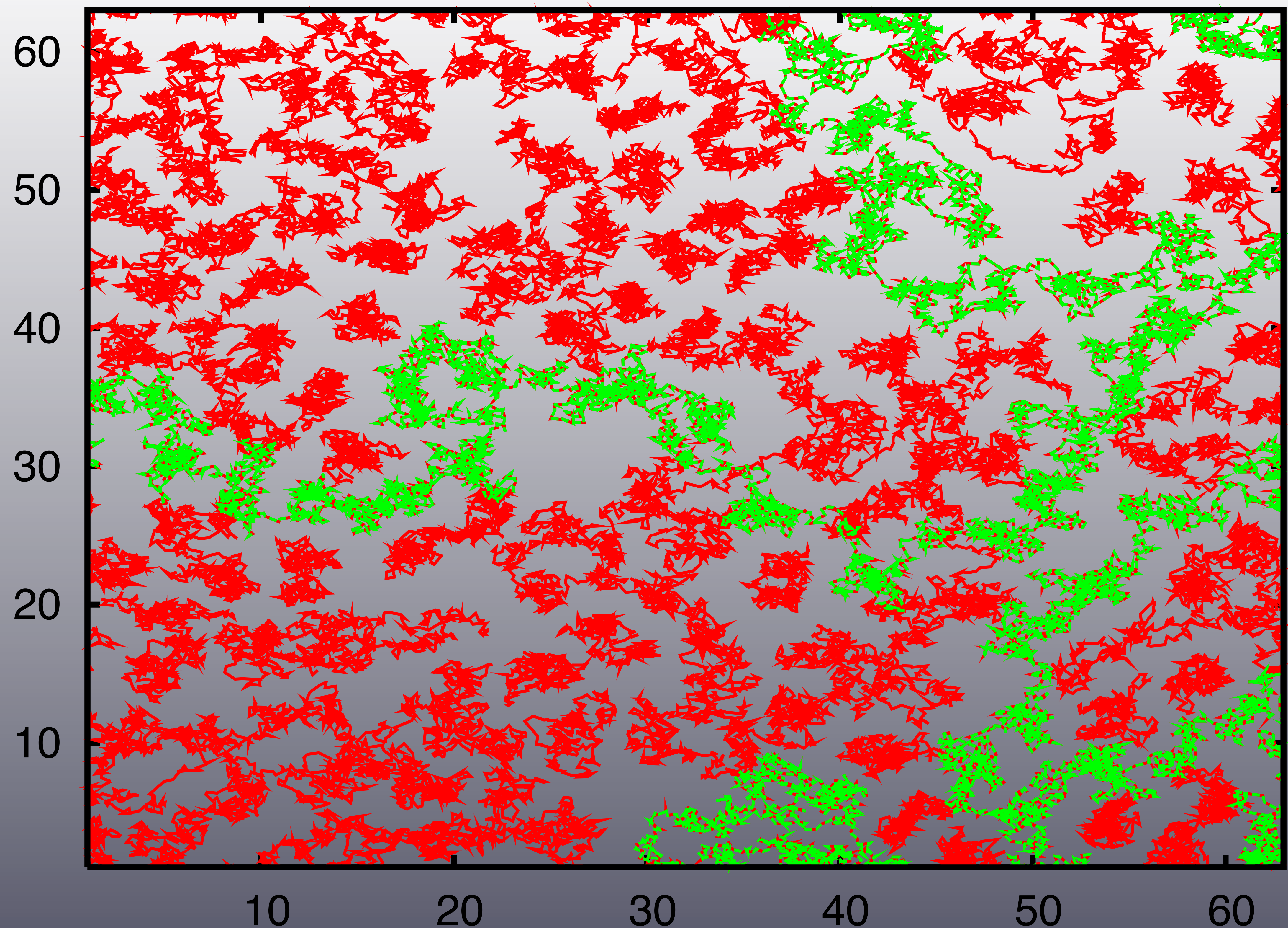
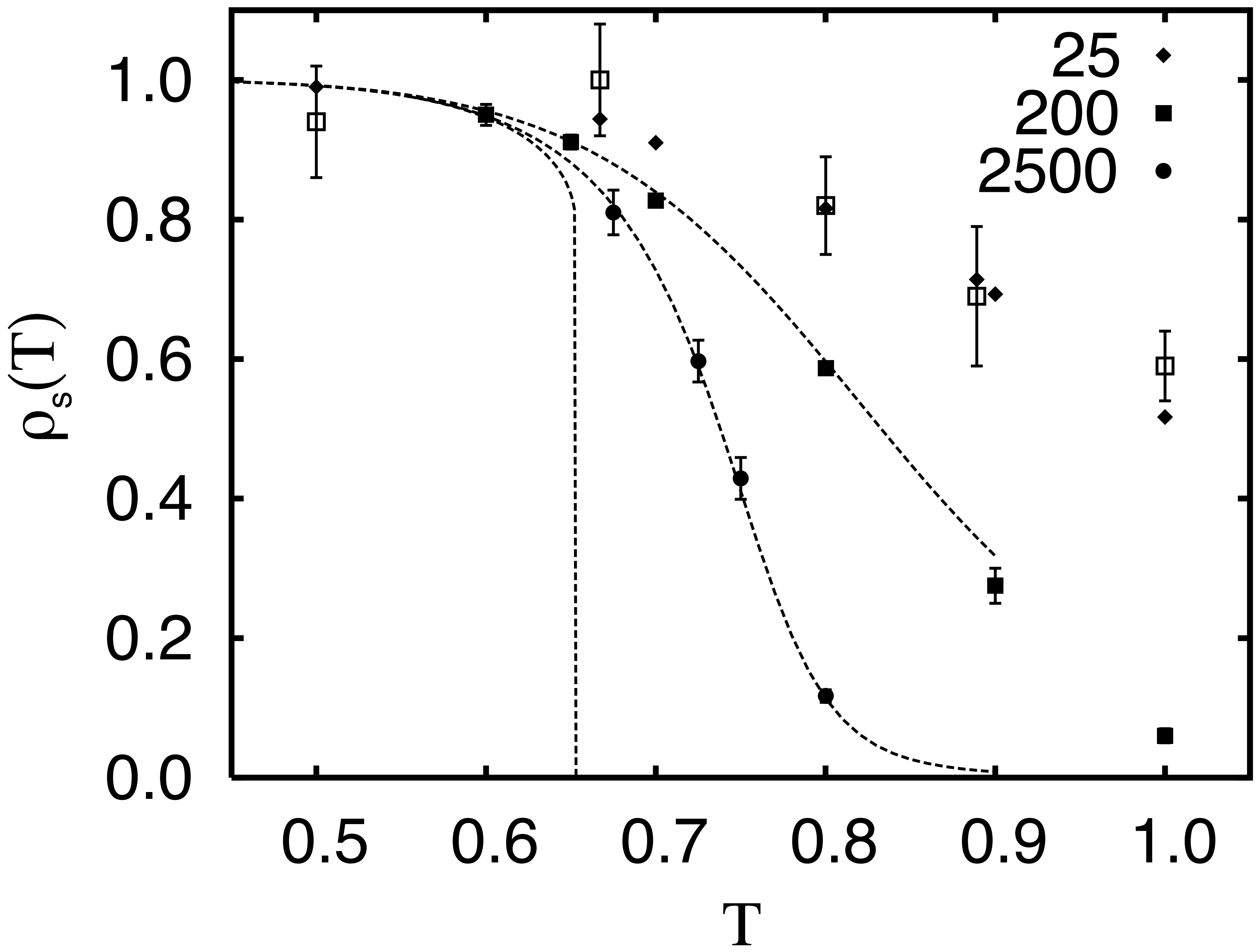
Can I and M get "stuck" away from each other?

- Statistics of spatial distances between *I* and *M* given by *one-body density matrix*
  - Decaying exponentially in a non-BEC
  - Going to a constant in a BEC (but high acceptance probability of reconnection)

Example: ^{4}He in two dimensions, T=0.6 K



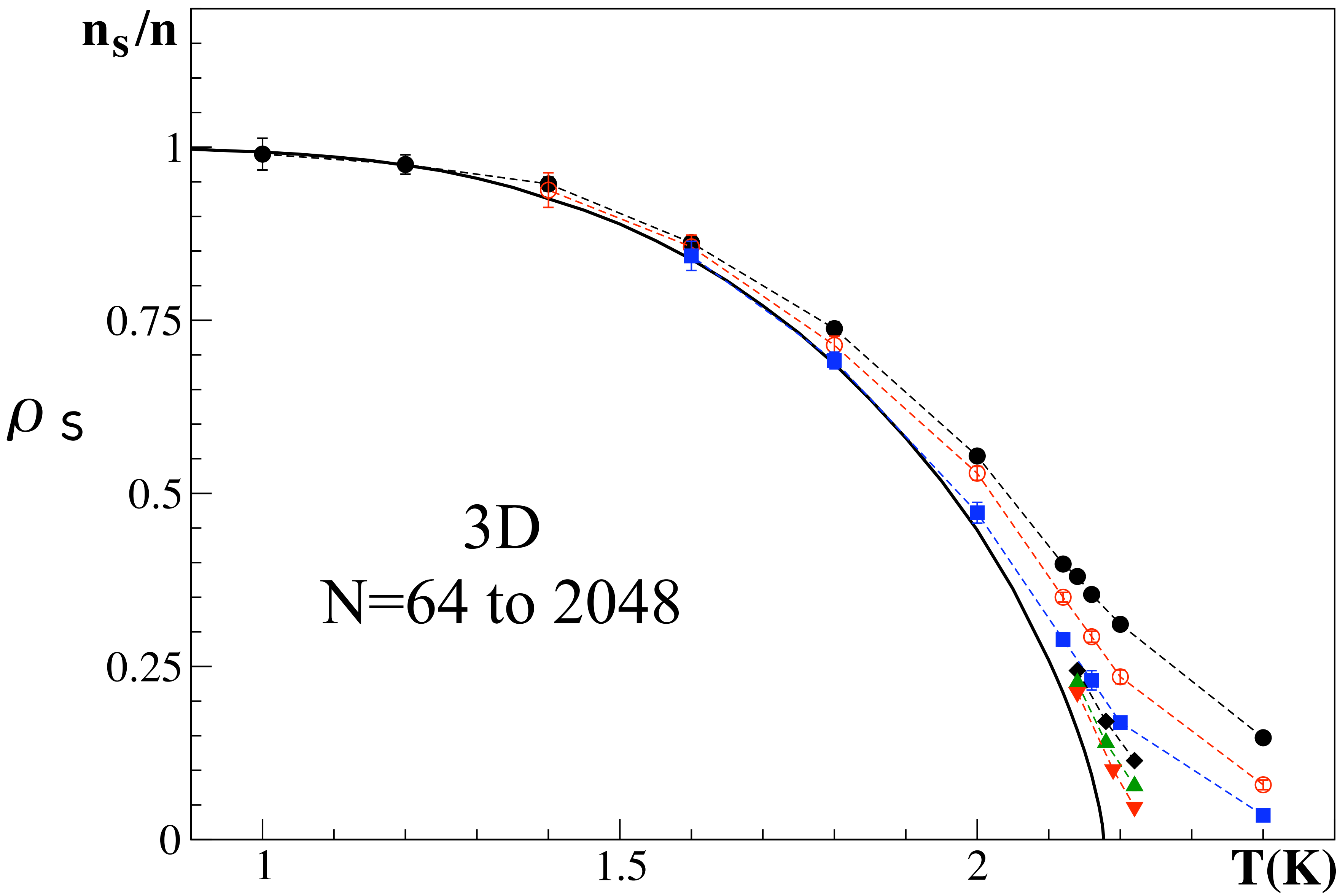
Application: Superfluid Transition in ^4He



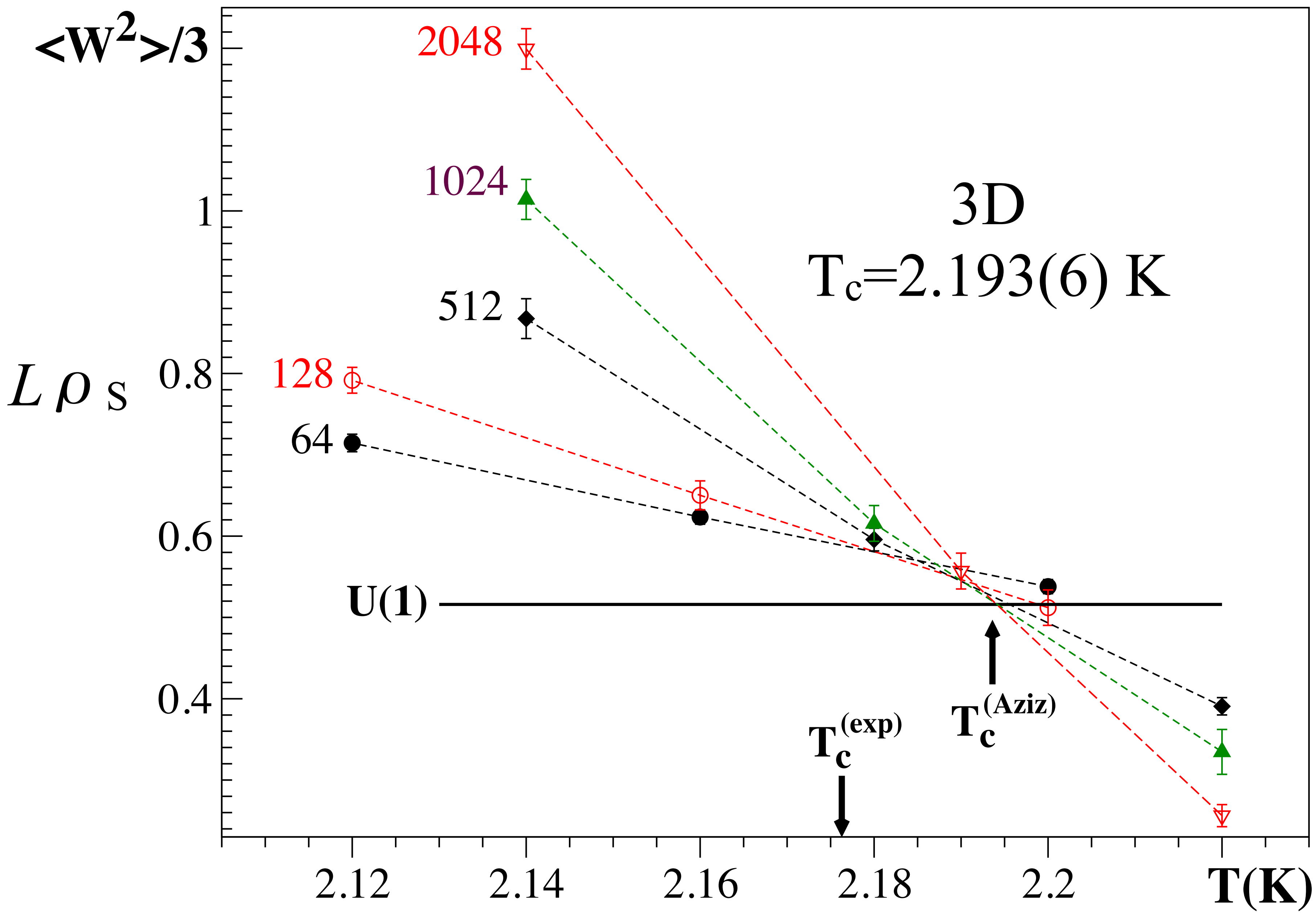
2D

T_c = 0.655 (10) K

Superfluid Transition in ^{4}He (cont'd)



Superfluid Transition in ^{4}He (cont'd)



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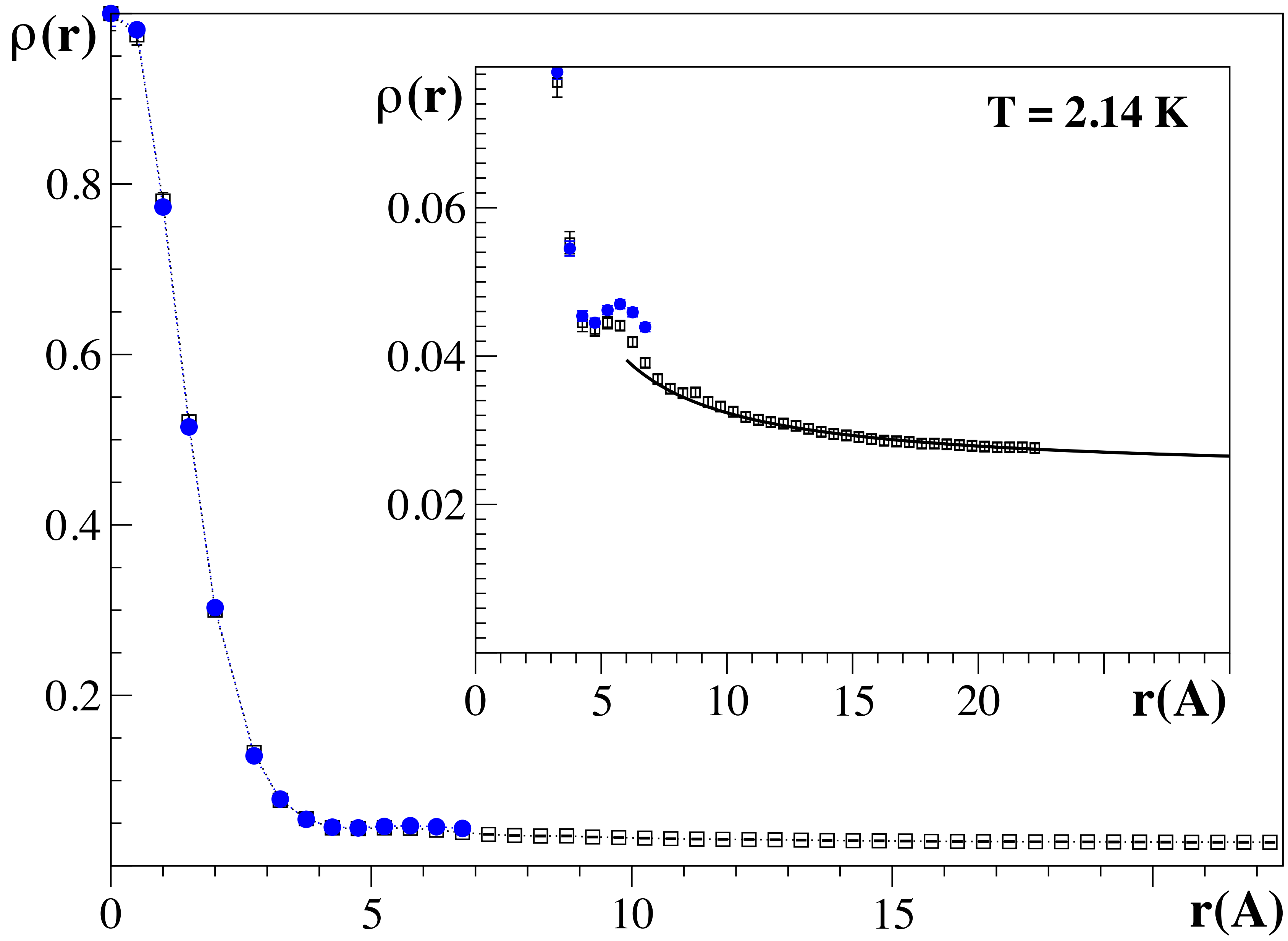
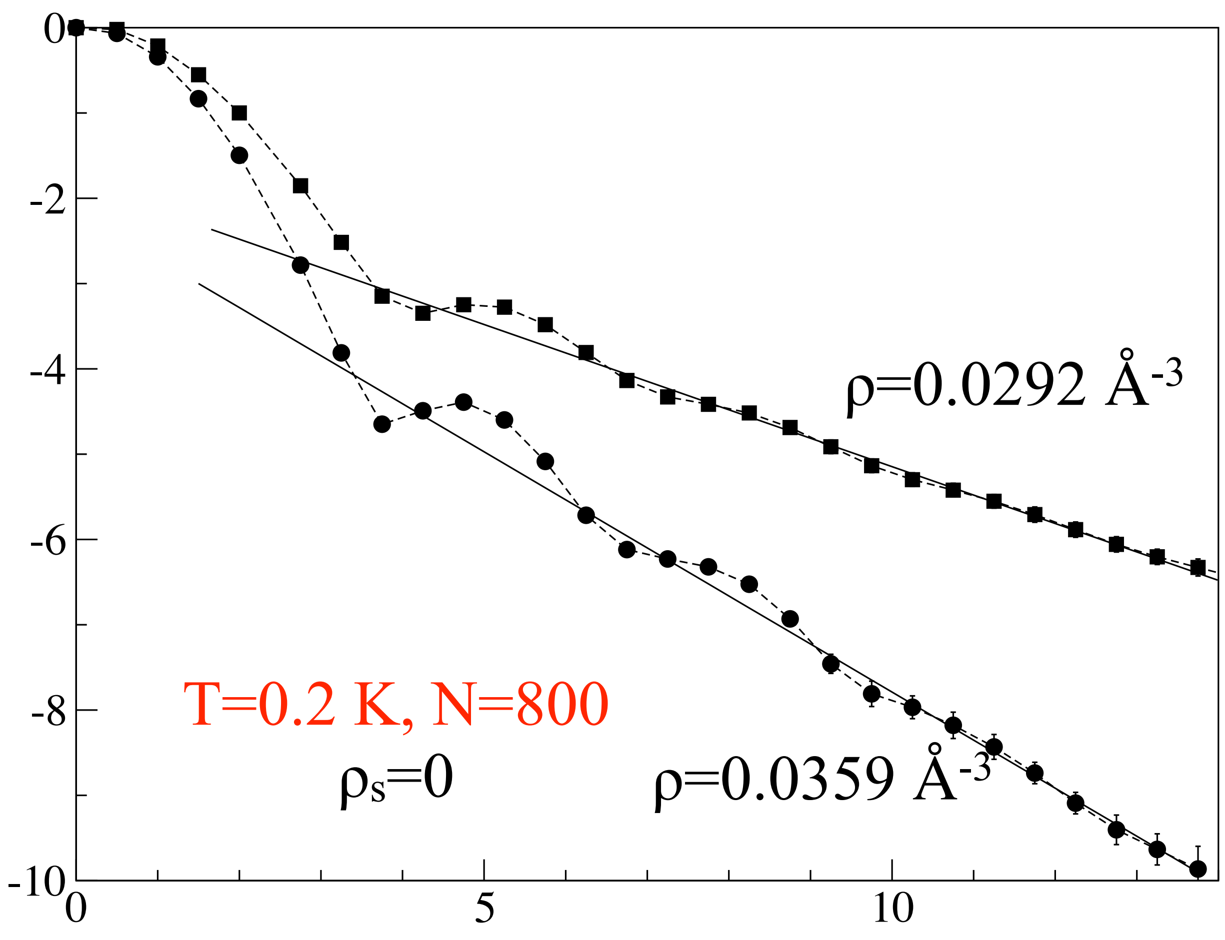


Application: Search for BEC in Solid ^{4}He

MB, N. Prokof'ev and B. Svistunov, Phys. Rev. Lett. **96**, 105301 (2006)



Exponential decay of one-body density matrix seen at low T, large r for perfect hcp ^{4}He crystal

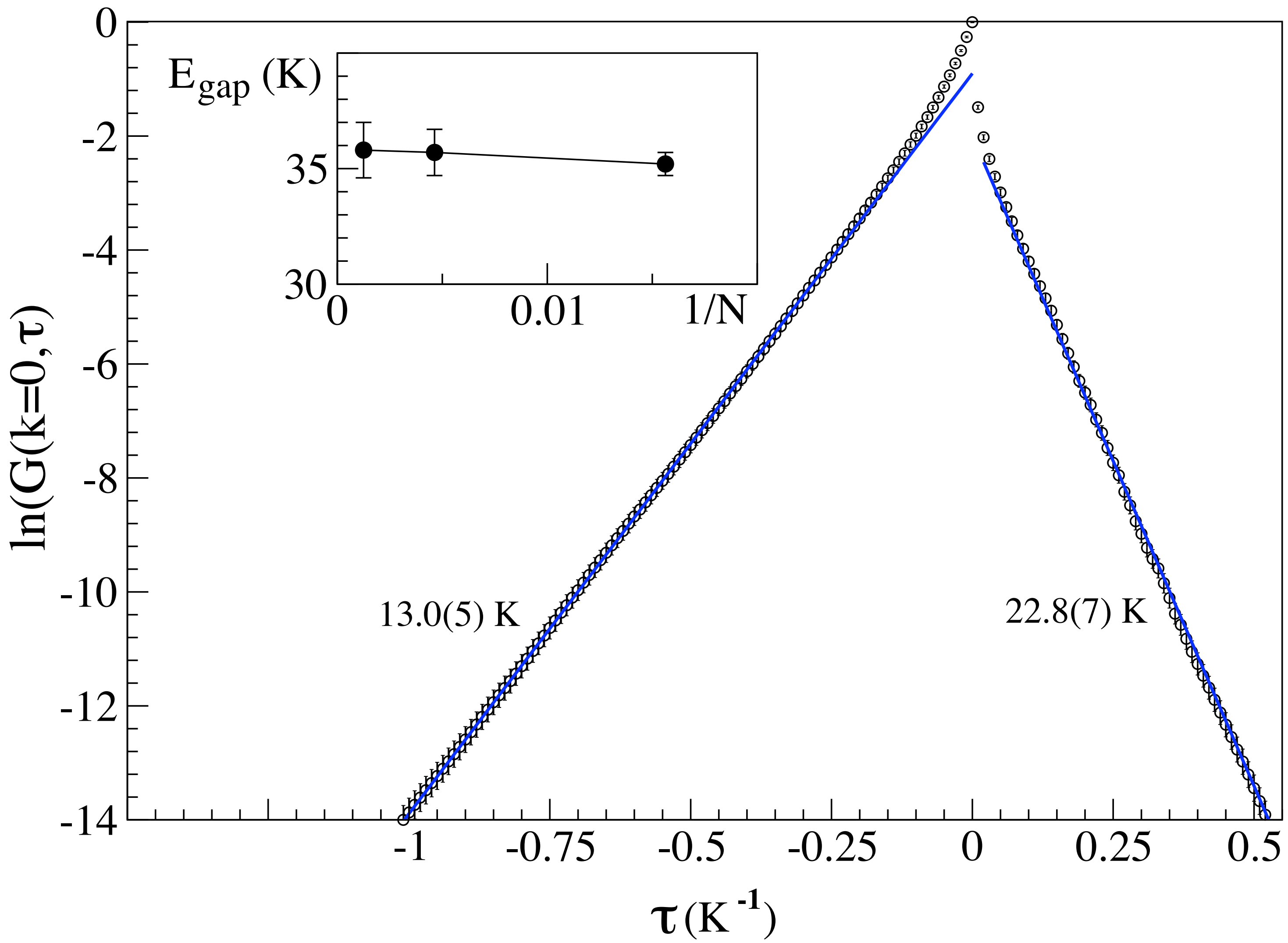
Absence of BEC
Independent of pressure

Absence of SF
No long permutation cycles

Application: vacancies in Solid ^{4}He

MB, A. Kuklov, L. Pollet, N. Prokof'ev, B. Svistunov and M. Troyer, PRL **97**, 080401 (2006)

Activation energy for vacancies and interstitials can be obtained straightforwardly from **exponential decay** of **Matsubara Green function**



$G(\mathbf{k}=0,\tau) \sim e^{-|\tau|\Delta}$, long τ

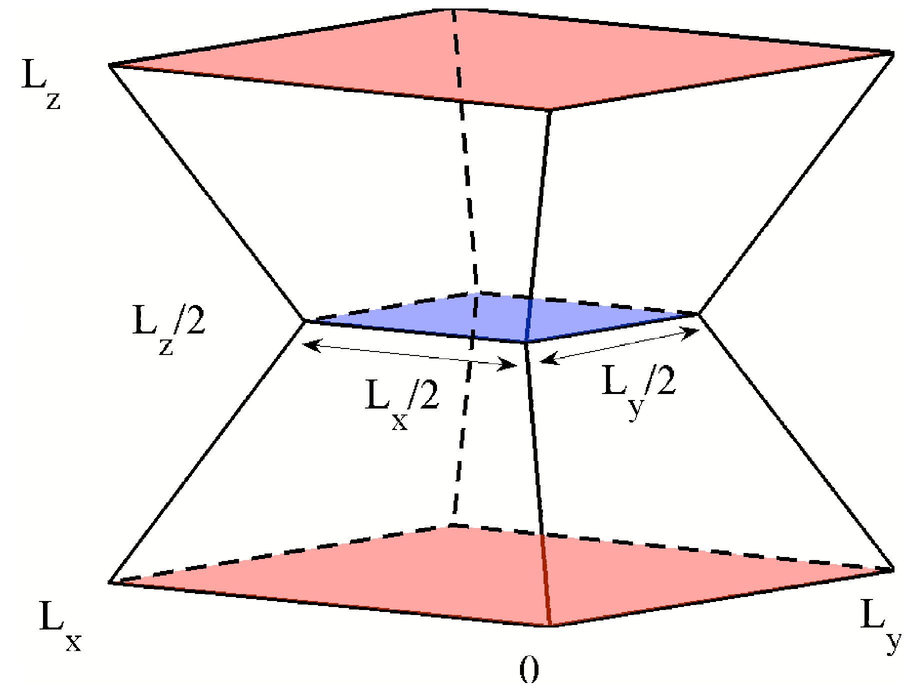
Matsubara too large for thermal activation at $T < 1$ K

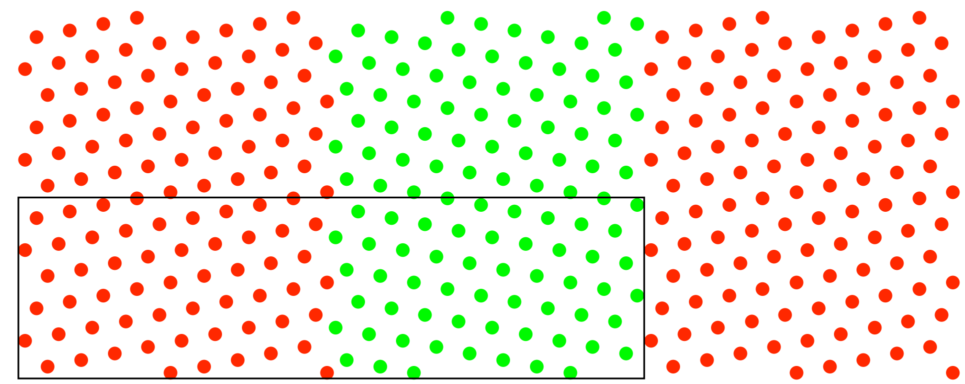
Consistent with **no** vacancies (nor interstitials) in solid He

Application: Possible superfluidity at grain boundaries in solid ^{4}He

L. Pollet, MB, A. Kuklov, N. Prokof'ev, B. Svistunov and M. Troyer, Phys. Rev. Lett. **98**, 135301 (2007).

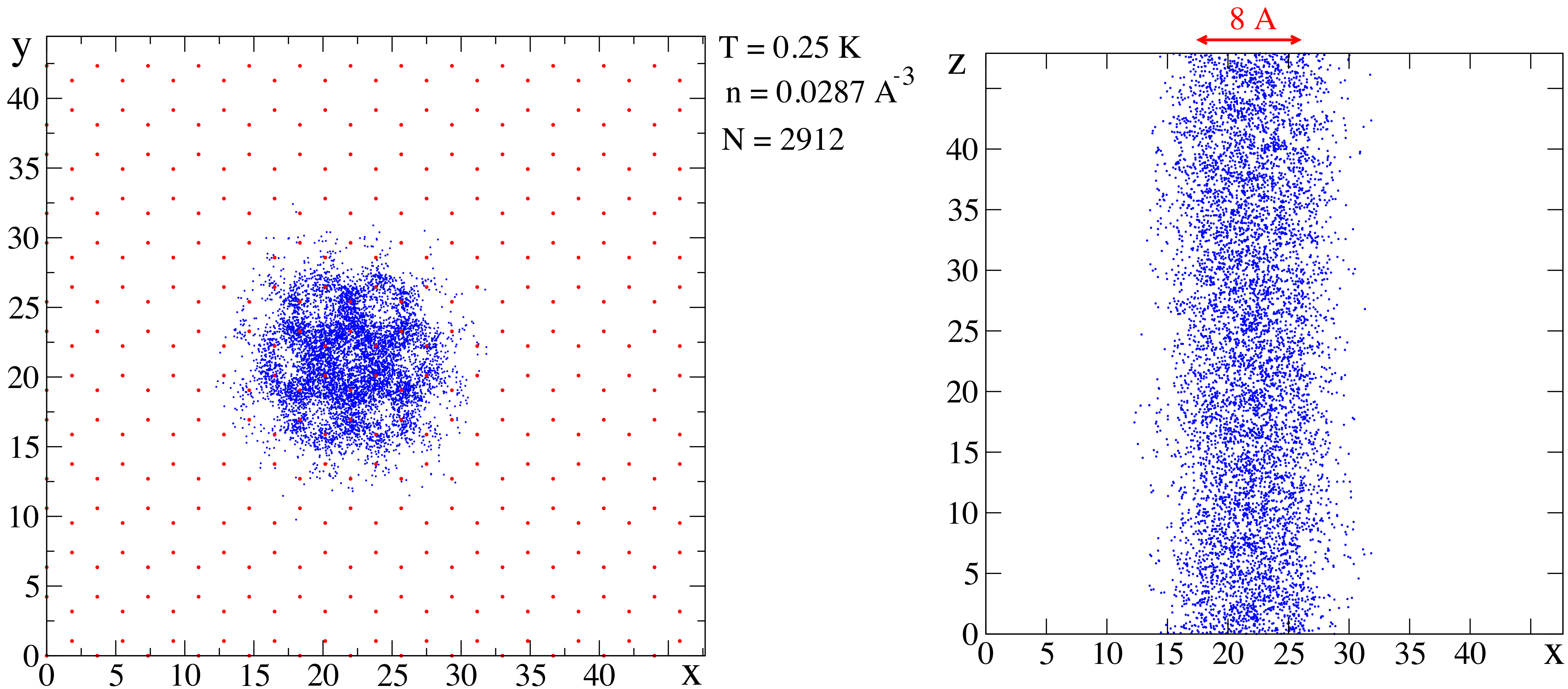
- By direct simulation, evidence is obtained that a grain boundary in direct contact with a superfluid at the melting pressure is **thermodynamically stable**.
- Superfluid behavior of a generic GB at temperatures of the order of 0.5 K is observed. Indeed, a **generic GB is found to be superfluid**, although insulating GBs exist as well, for particular relative orientations of the crystallites.
- Simulations performed on systems including as many as **13,000** particles (*yes, that many are needed*)





Application: Possible superfluidity in the core of a screw dislocation in solid ^{4}He

MB, A. Kuklov, L. Pollet, N. Prokof'ev, B. Svistunov and M. Troyer, Phys. Rev. Lett. **99**, 035301 (2007).



Simulations of single screw dislocation inside hcp ^{4}He crystal show evidence of spatially modulated ***Luttinger liquid*** (1d supersolid ?)

Importance of long exchanges near melting

MB, L. Pollet, N. Prokof'ev and B. Svistunov, Phys. Rev. Lett. **109**, 025302 (2012).

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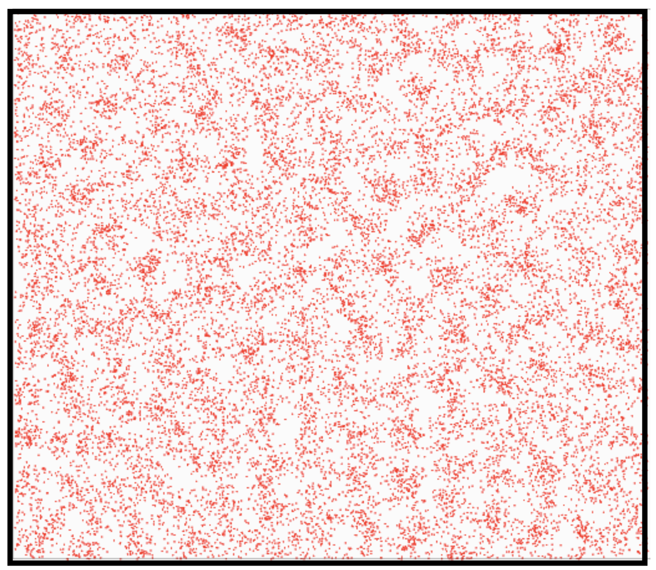

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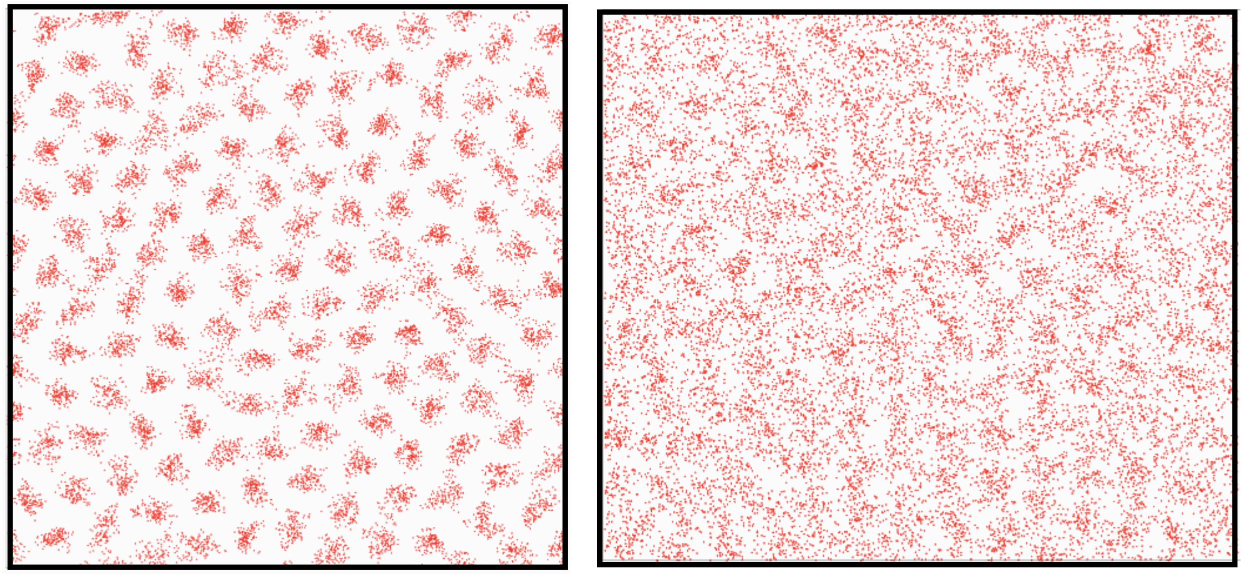

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Thermodynamic equilibrium structure *crucially* depends on quantum statistics
System can lower its energy by forming a *quasi*-BEC and losing *solid* order

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- Standard microscopic model, based on Aziz pair potential

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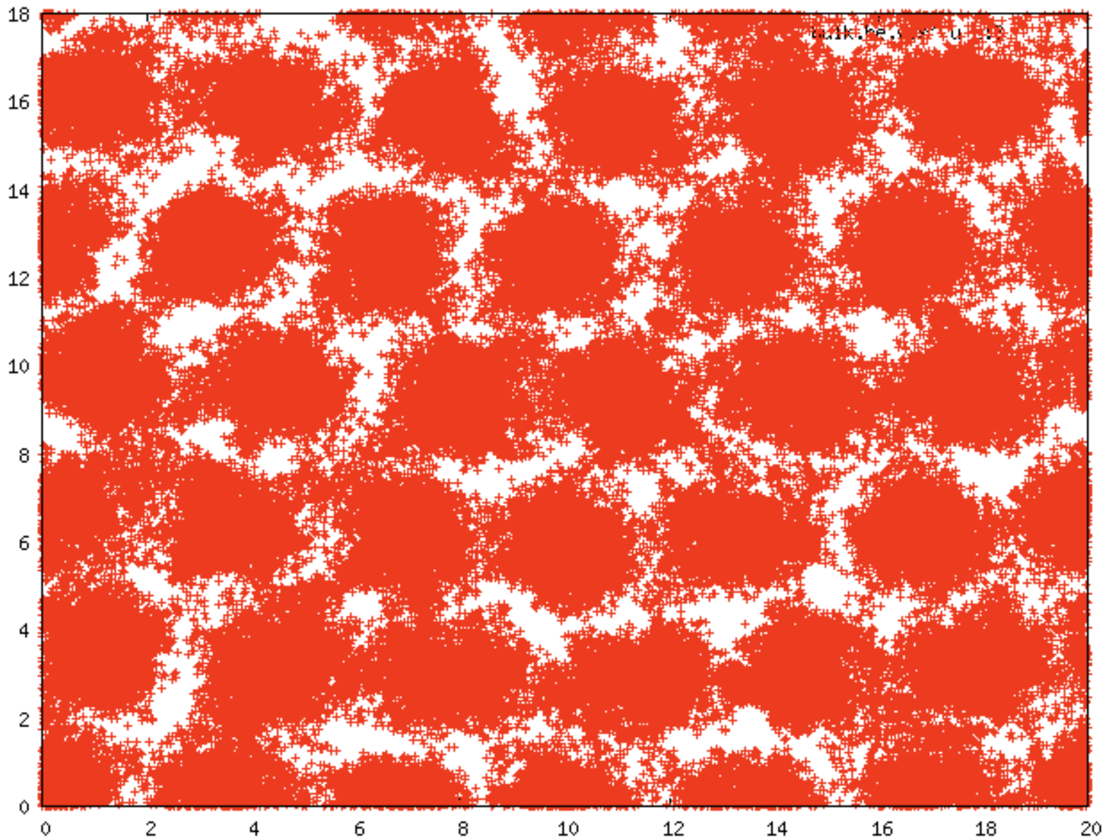

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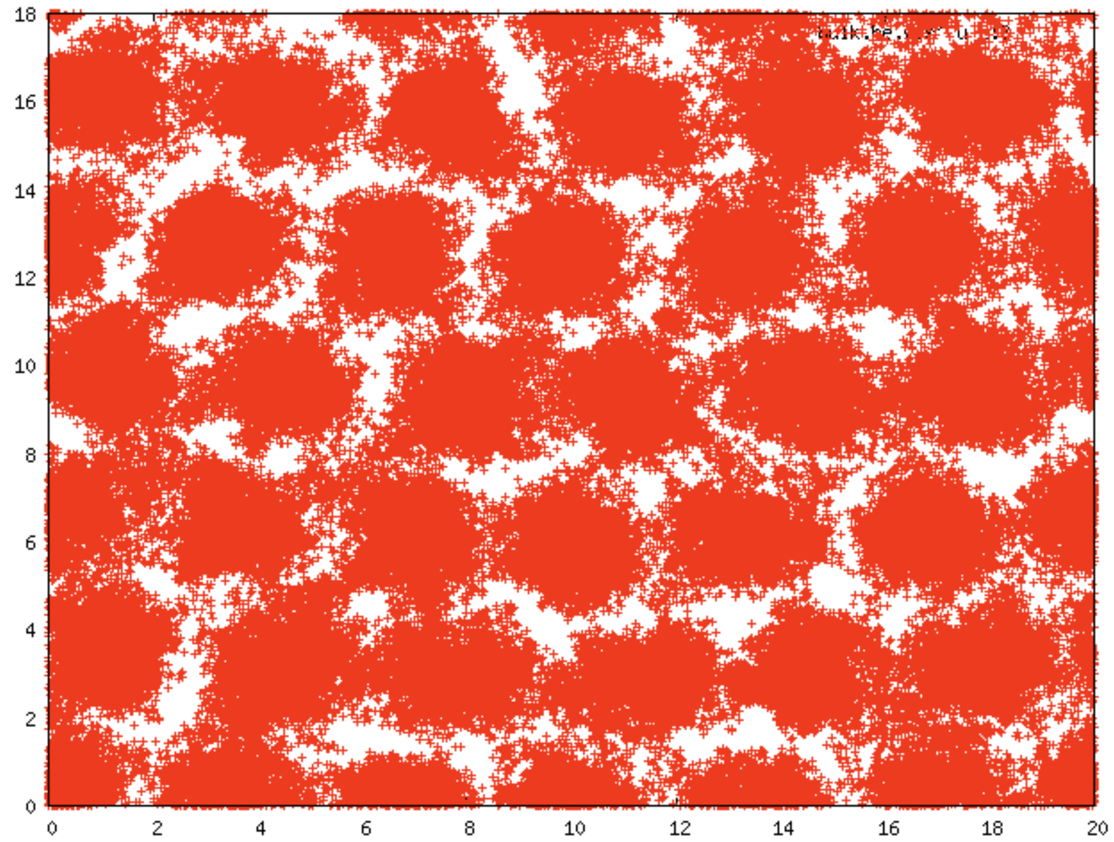

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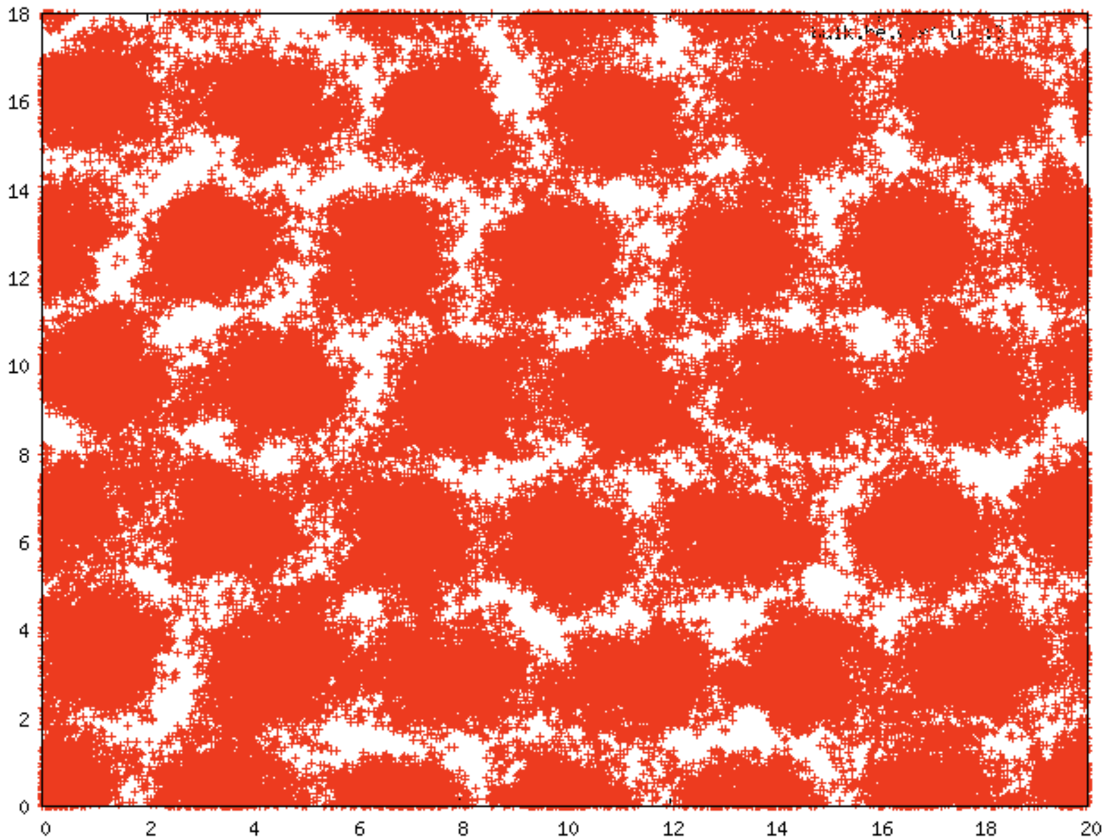

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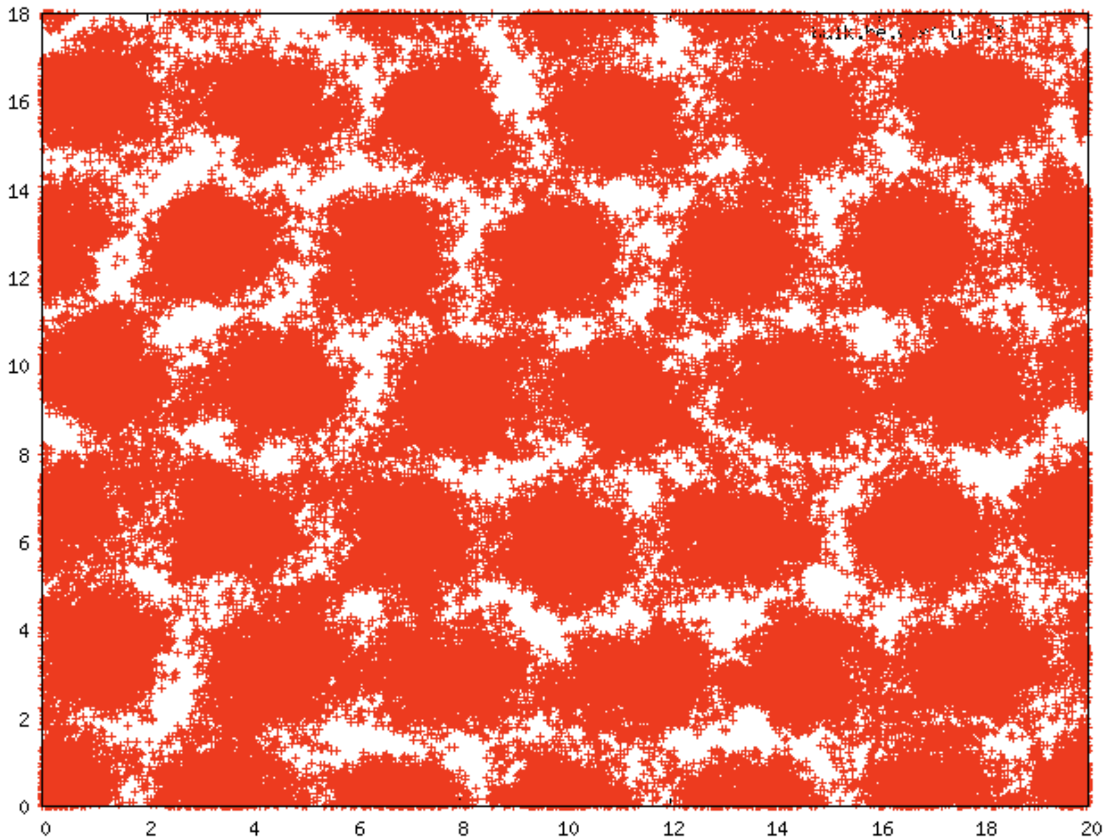

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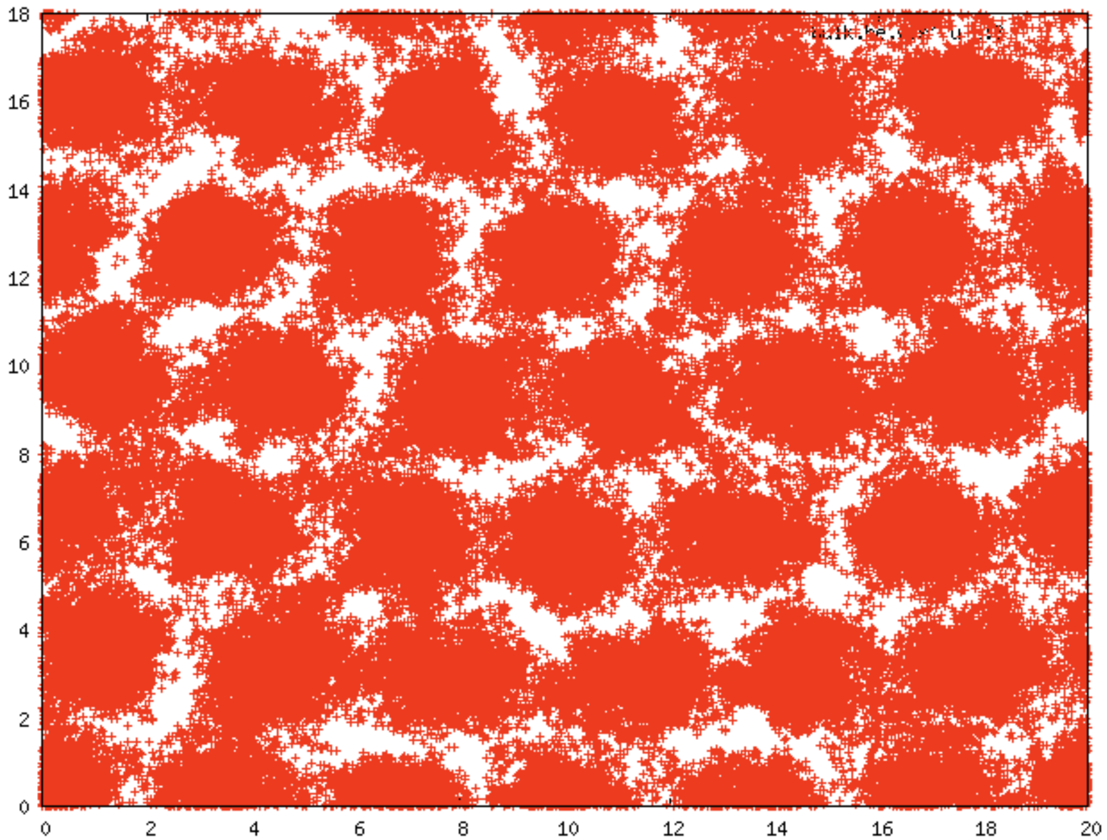

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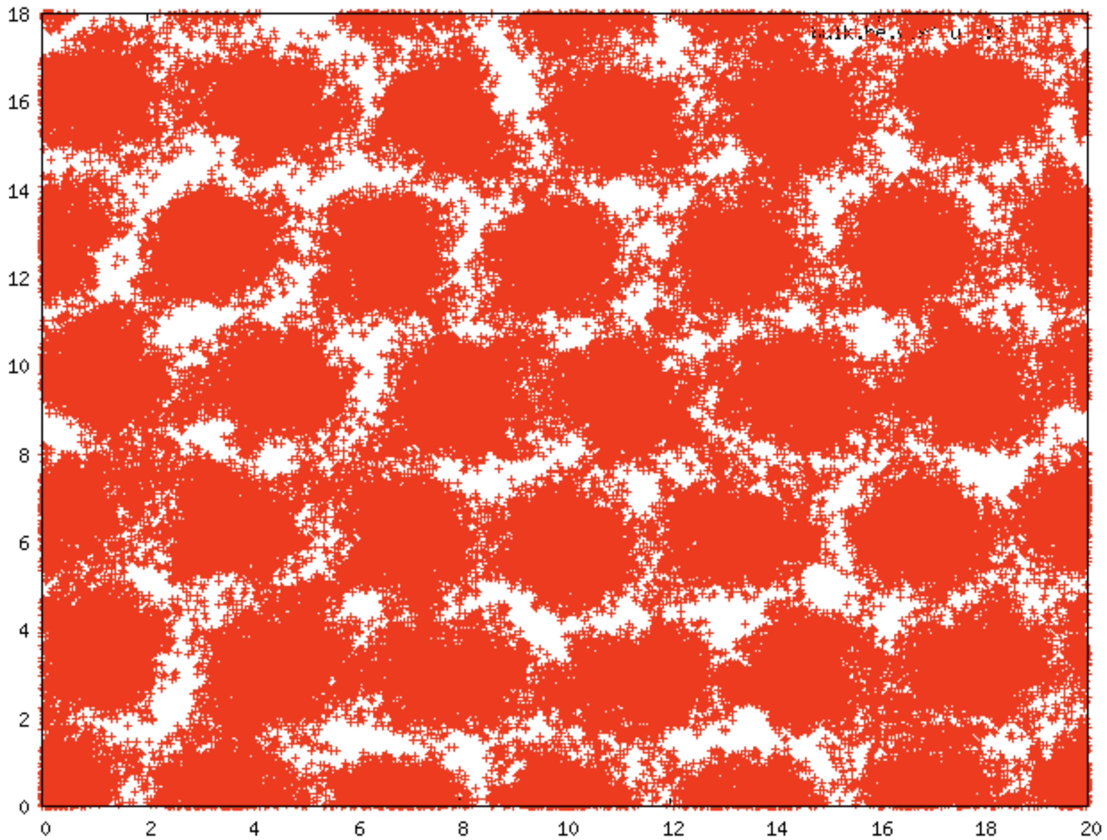

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Simulation results strongly suggest that ^{4}He *would be a crystal* at this *T*, if its atoms were indeed *distinguishable*. Here too, Bose statistics strongly affects the phase diagram of this Bose system, *not just at the liquid-solid phase boundary*.

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Thank you !