The Abdus Salam International Centre for Theoretical Physics

United Nations Educational, Scientific and Cultural Organization

IAEA International Atomic Energy Agency

1959-7

Workshop on Supersolid 2008

18 - 22 August 2008

The solid state of Helium-4: to flow or not to flow

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binding of a He-3 impurity to the screw dislocation in Helium-4

Phys. Rev. Lett. **97**, 080401 (2006).

Phys. Rev. Lett. **98**, 135301 (2007).

Phys. Rev. Lett. **99**, 035301 (2007).

http://arxiv.org/abs/0805.3713 (PRL)

Philippe Corboz (ETH)
Lode Pollet (ETH)
Nikolay Prokof'ev (Amherst)
Matthias Troyer (ETH)

http://arxiv.org/abs/0807.4021

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Boris Svistunov (Amherst)

Outline

1. by general request : Path Integral Monte Carlo
2. binding of a ^{3}He atom to the core of a screw dislocation

How to find the properties of Helium-4

$$Z = \mathrm{Tr}\exp(-\beta H) \qquad H = -\frac{\hbar^2\nabla^2}{2m} + U_{\mathrm{Aziz}}$$

$$Z = \int dR_0 \langle R_0 | exp(-\beta H) | R_0 \rangle = \int dR_0 \rho(R_0, R_0; \beta)$$

$$\exp(-\beta(T+U)) \neq \exp(-\beta T)\exp(-\beta U) \quad \text{if} \quad [T, V] \neq 0$$

$$\delta = \beta/M \qquad \exp(-\beta H) = \exp(-\delta H)^M$$

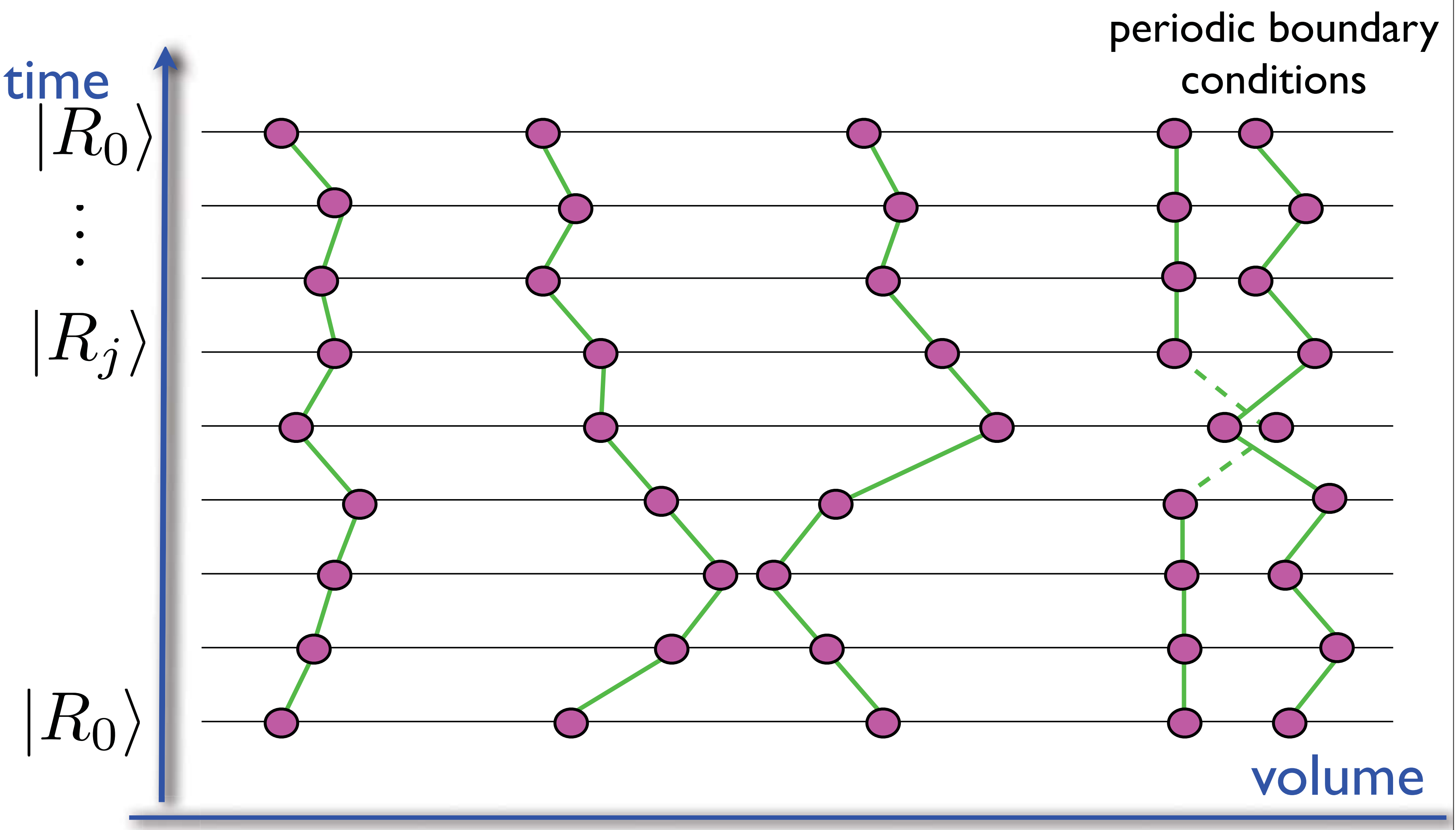
$$\exp(-\delta(T+U)) \approx \exp(-\delta T)\exp(-\delta U) + \mathcal{O}(\delta^2)$$

$$
\begin{aligned}
Z &= \int dR_0 \langle R_0 | exp(-\beta H) | R_0 \rangle \\
&= \lim_{M \to \infty} \int dR_0 \langle R_0 | \left[e^{-\delta T} e^{-\delta U} \right]^M | R_0 \rangle \\
&= \lim_{M \to \infty} \int dR_0 \ldots dR_M \\
& \langle R_0 | e^{-\delta T} | R_1 \rangle \langle R_1 | e^{-\delta U} | R_1 \rangle \ldots \\
& < R_M | e^{-\delta T} | R_0 \rangle \langle R_0 | e^{-\delta U} | R_0 \rangle
\end{aligned}
$$

diagonal

diagonal

Path integral and worldlines



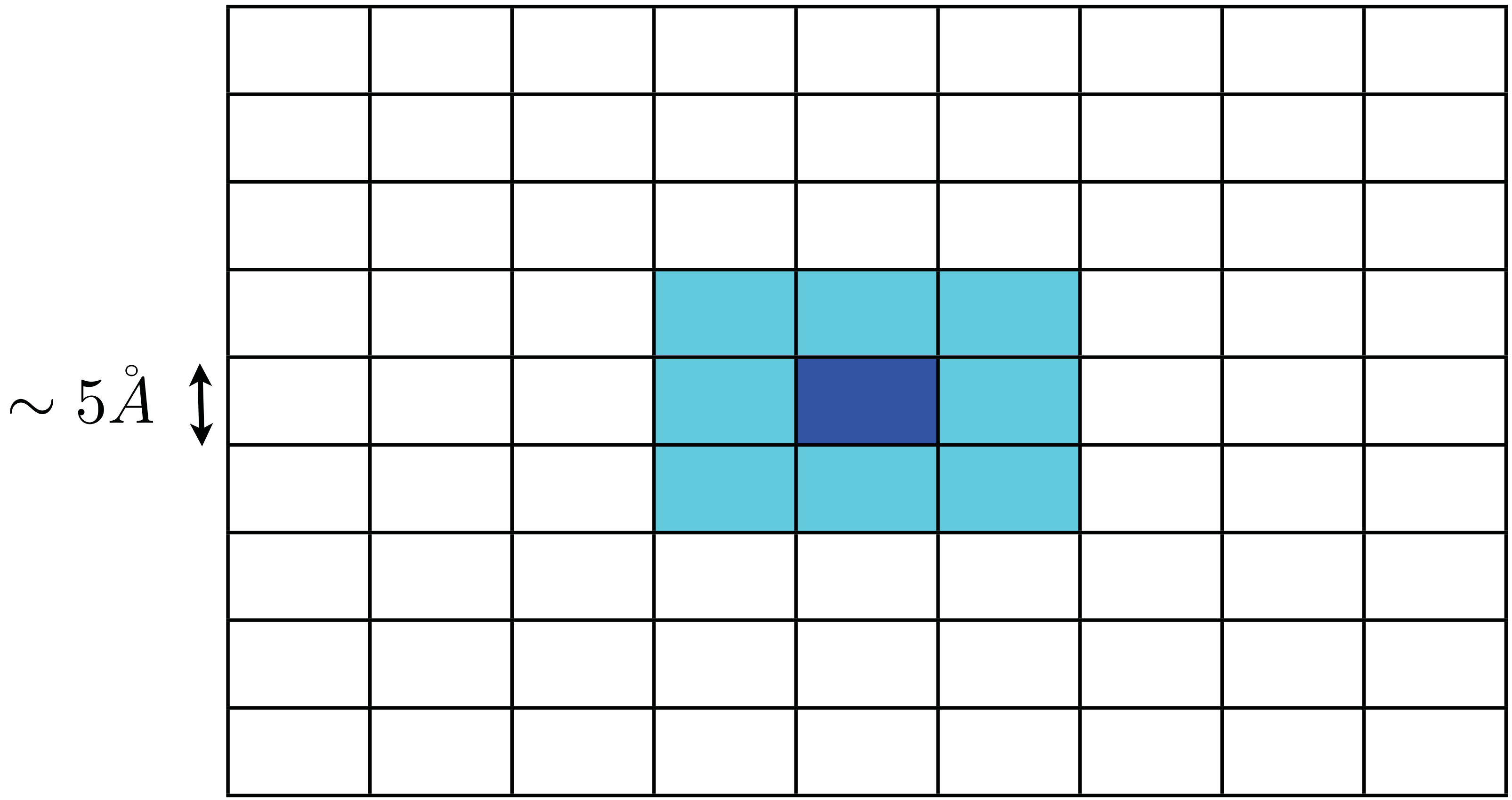
$$\langle R_0|e^{-\delta T}|R_1\rangle = (4\pi\lambda\delta)^{-3N/2} \exp\left[-\frac{(R_0 - R_1)^2}{4\lambda\delta}\right]$$

$$\lambda = \hbar^2/(2m) = 6.0596 A^2 K$$

$$\rho(R_{i-1}, R_i, \delta) = (4\pi\lambda\delta)^{-3N/2} \exp\left(-\left[\frac{(R_{i-1} - R_i)^2}{4\lambda\delta} + \delta U(R_i)\right]\right)$$

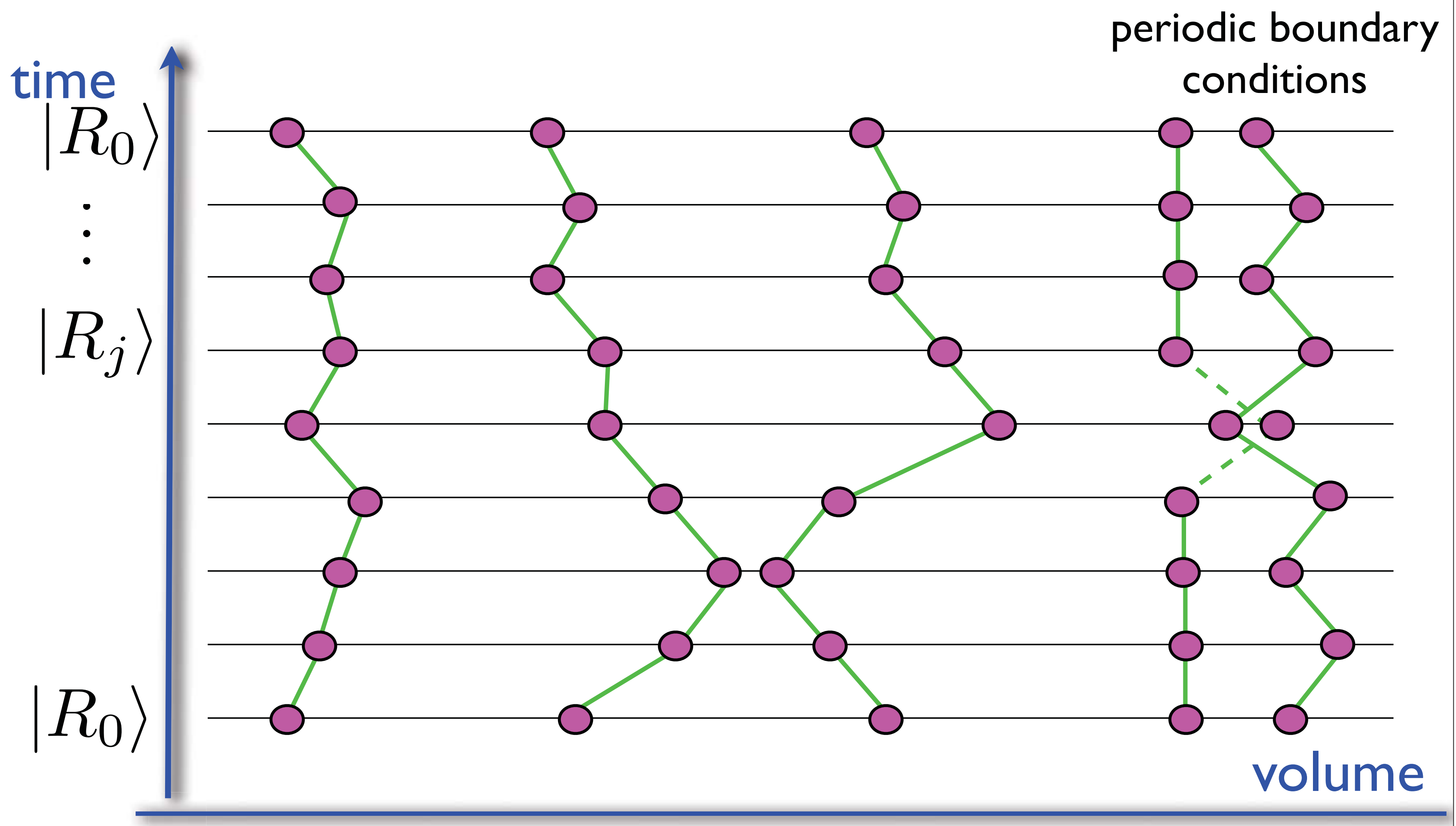
bosons are indistinguishable particles; we need to sum over all possible permutations

Aziz potential is long-range : work with cells

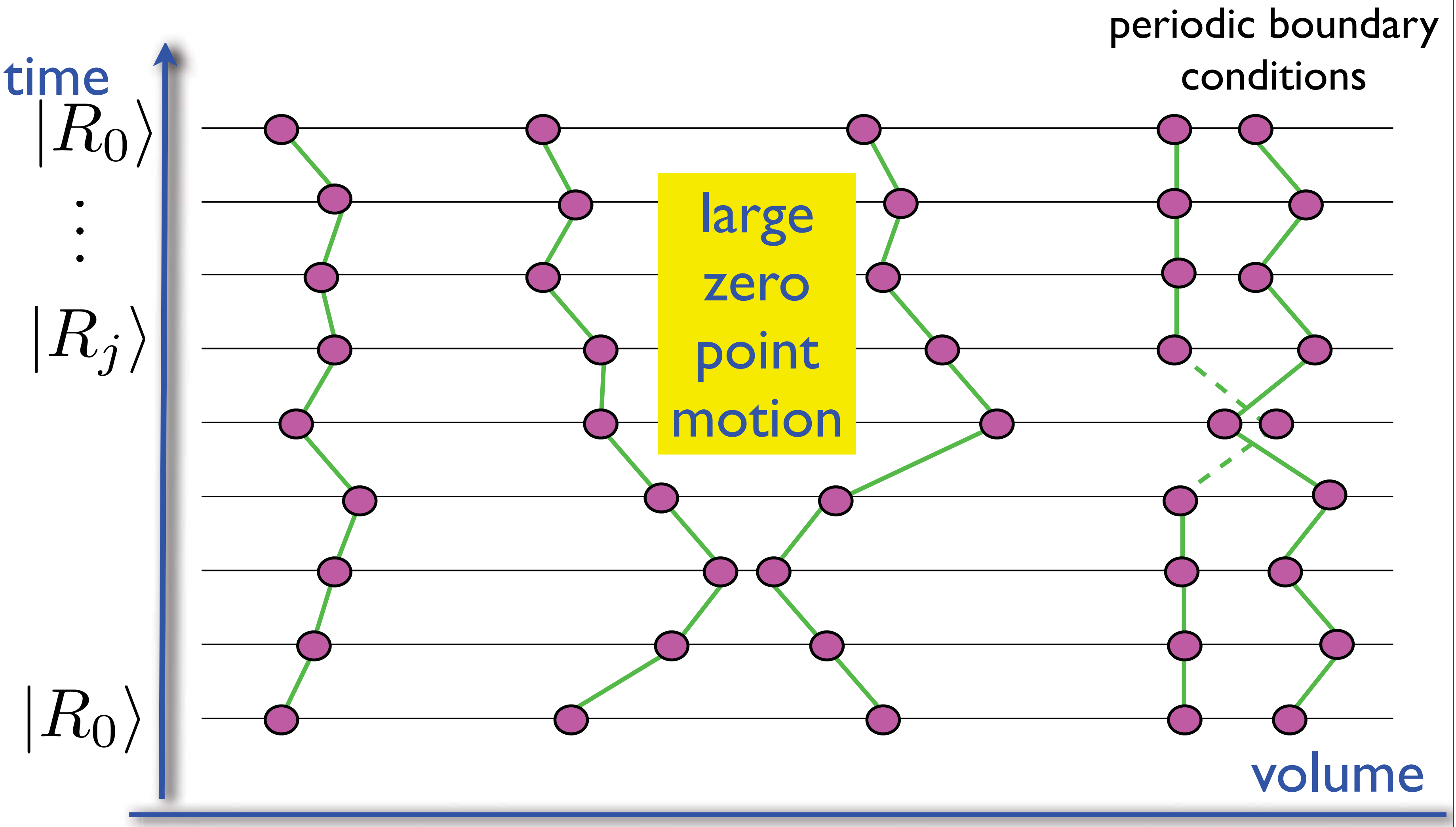


N. B. part of the potential outside the cut-off can be taken care of exactly because it is attractive (trick !)

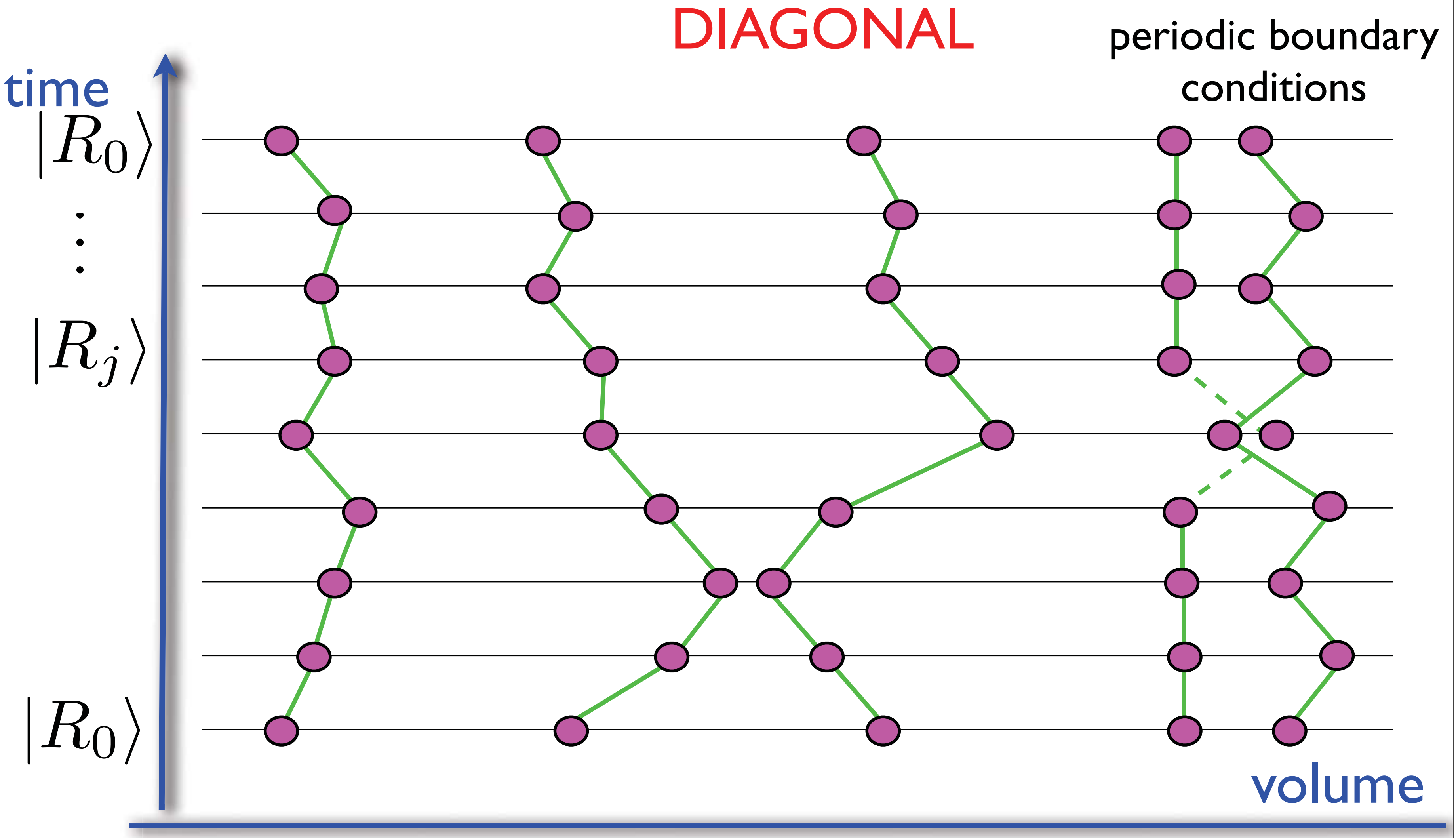
Path integral and worldlines



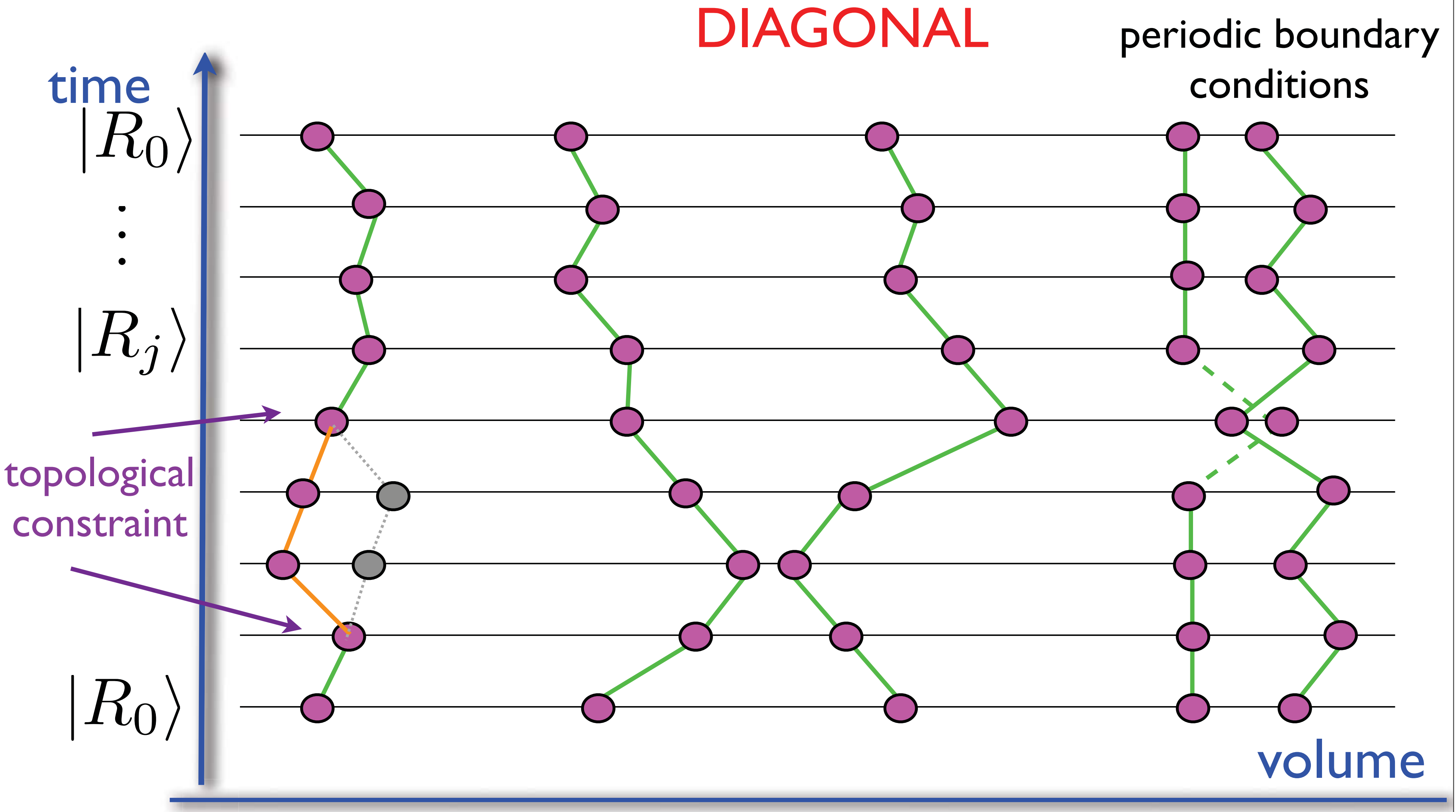
Path integral and worldlines

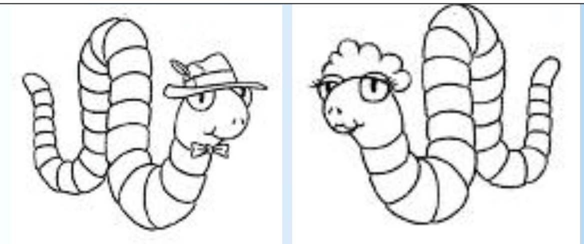


Path integral and worldlines

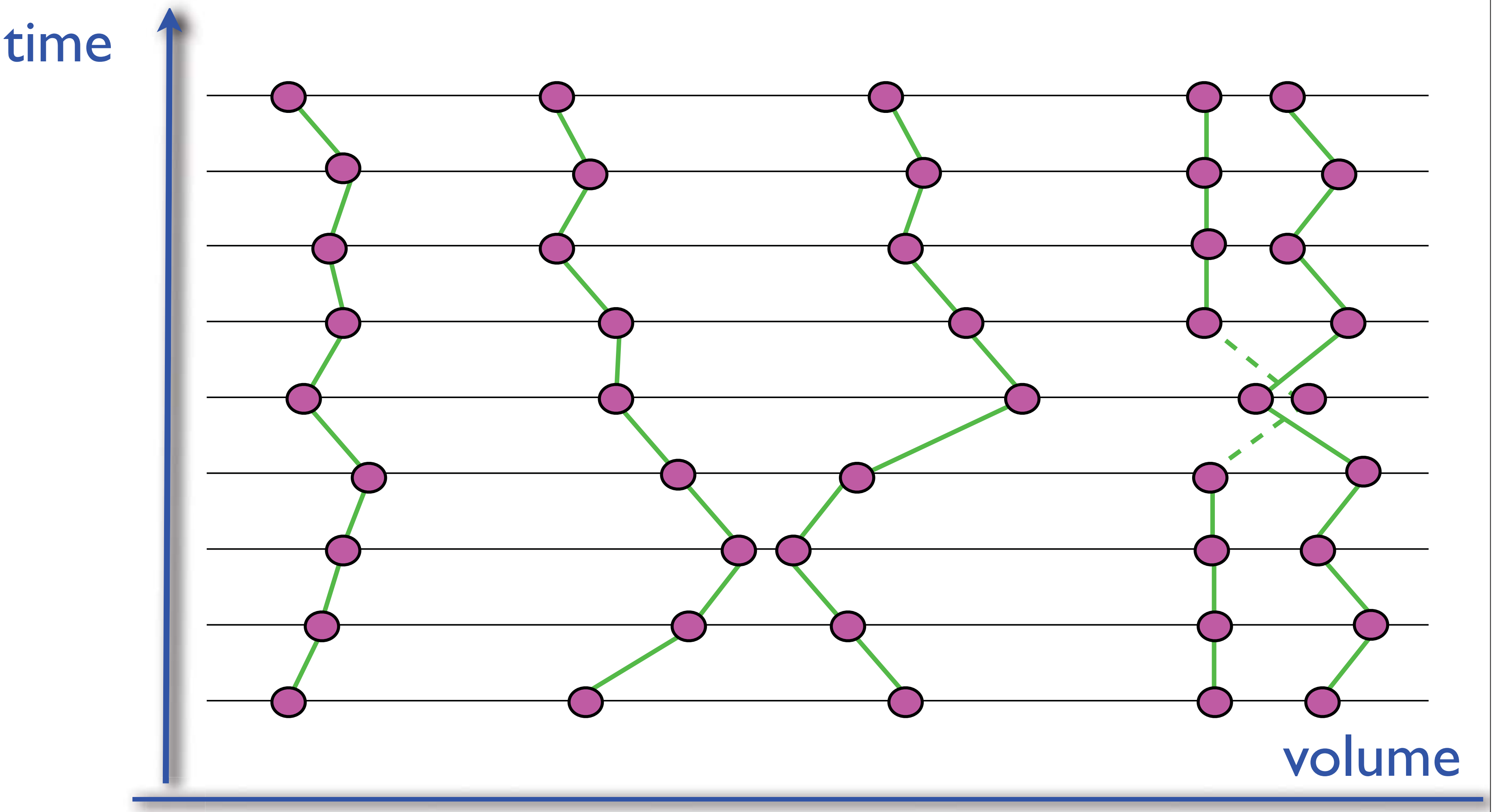


Path integral and worldlines

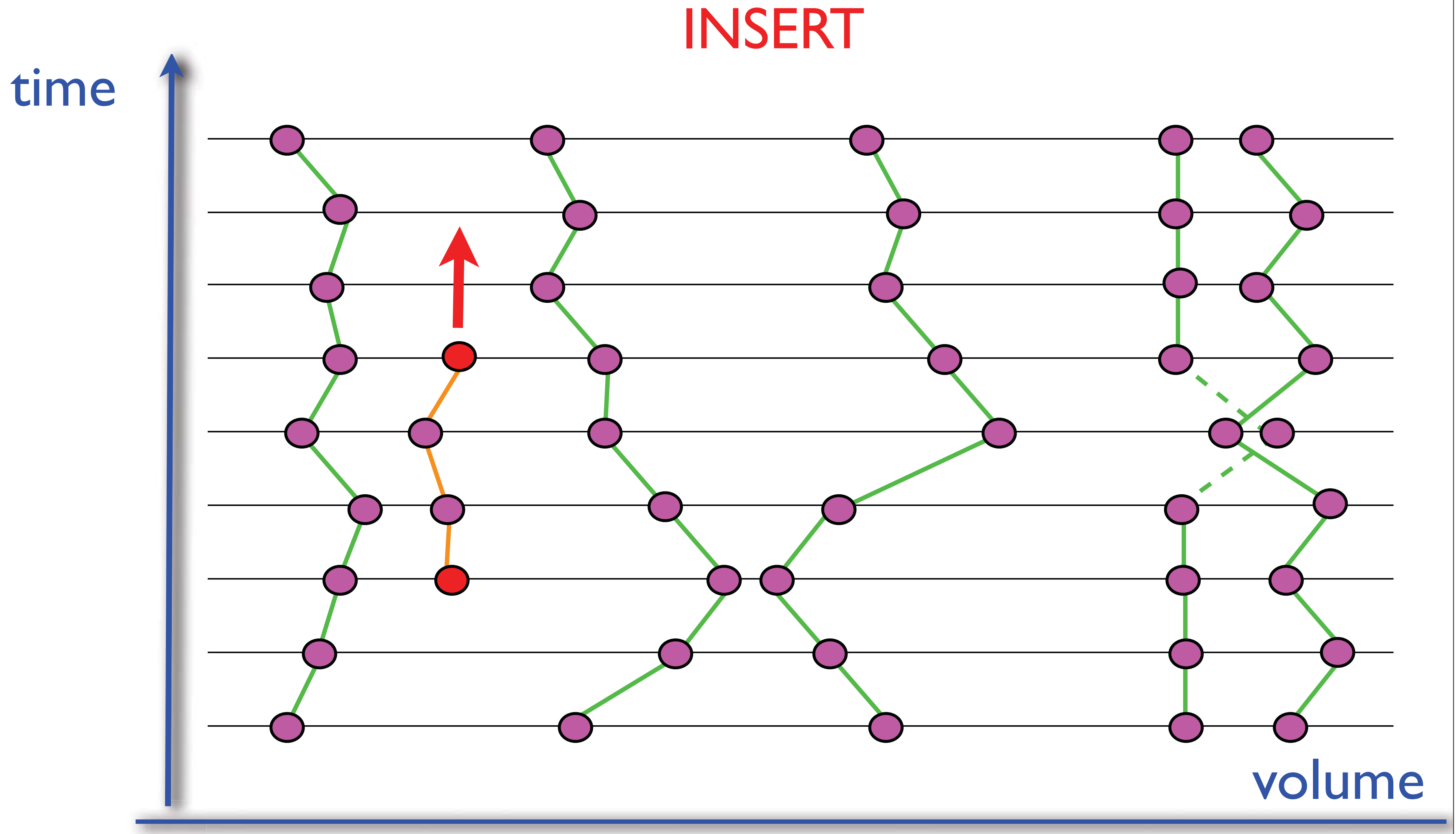


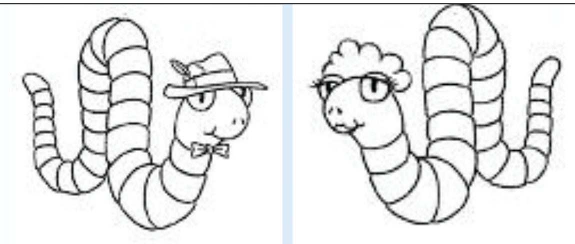


Path integral and worms



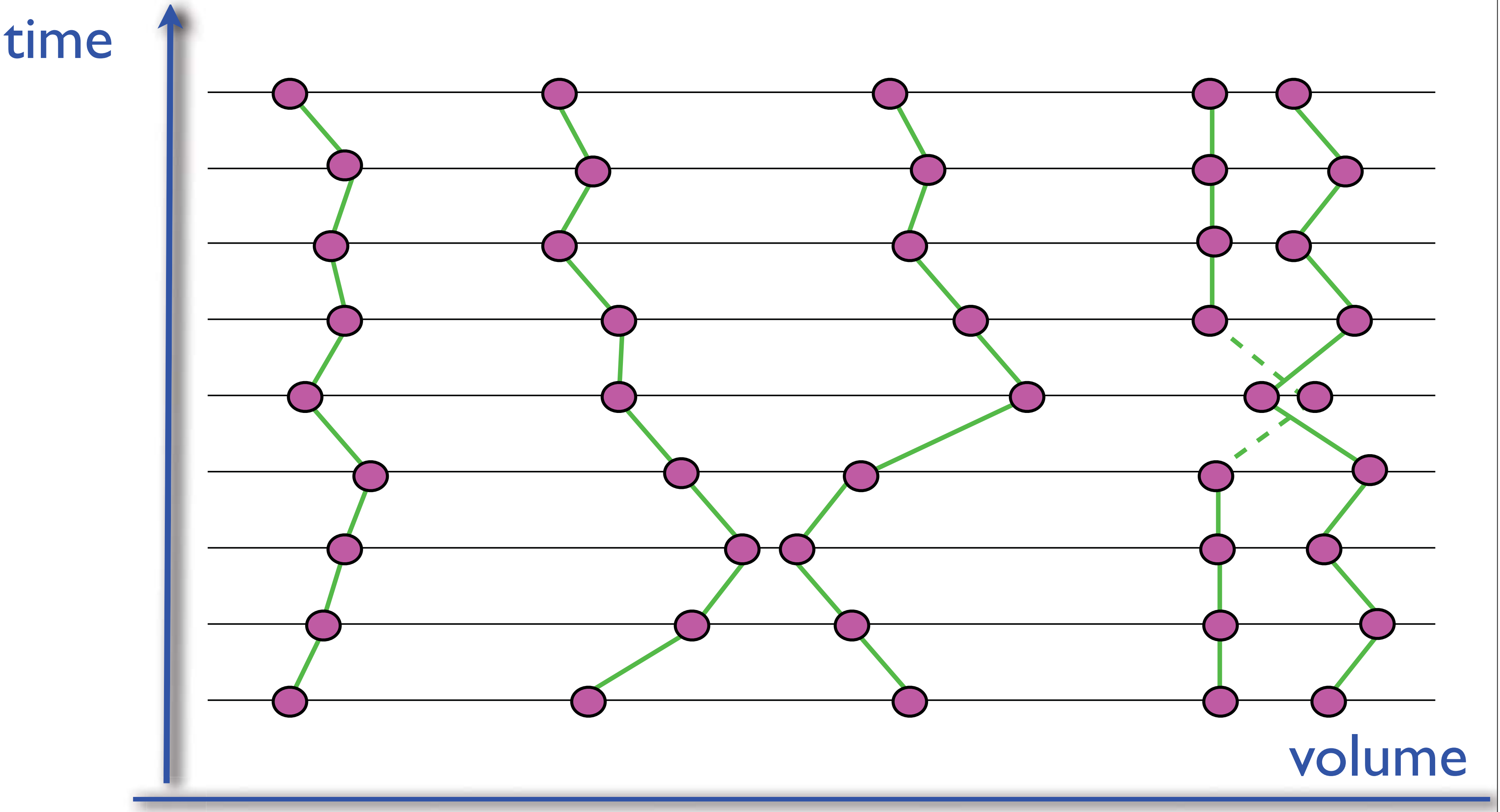
Path integral and worms



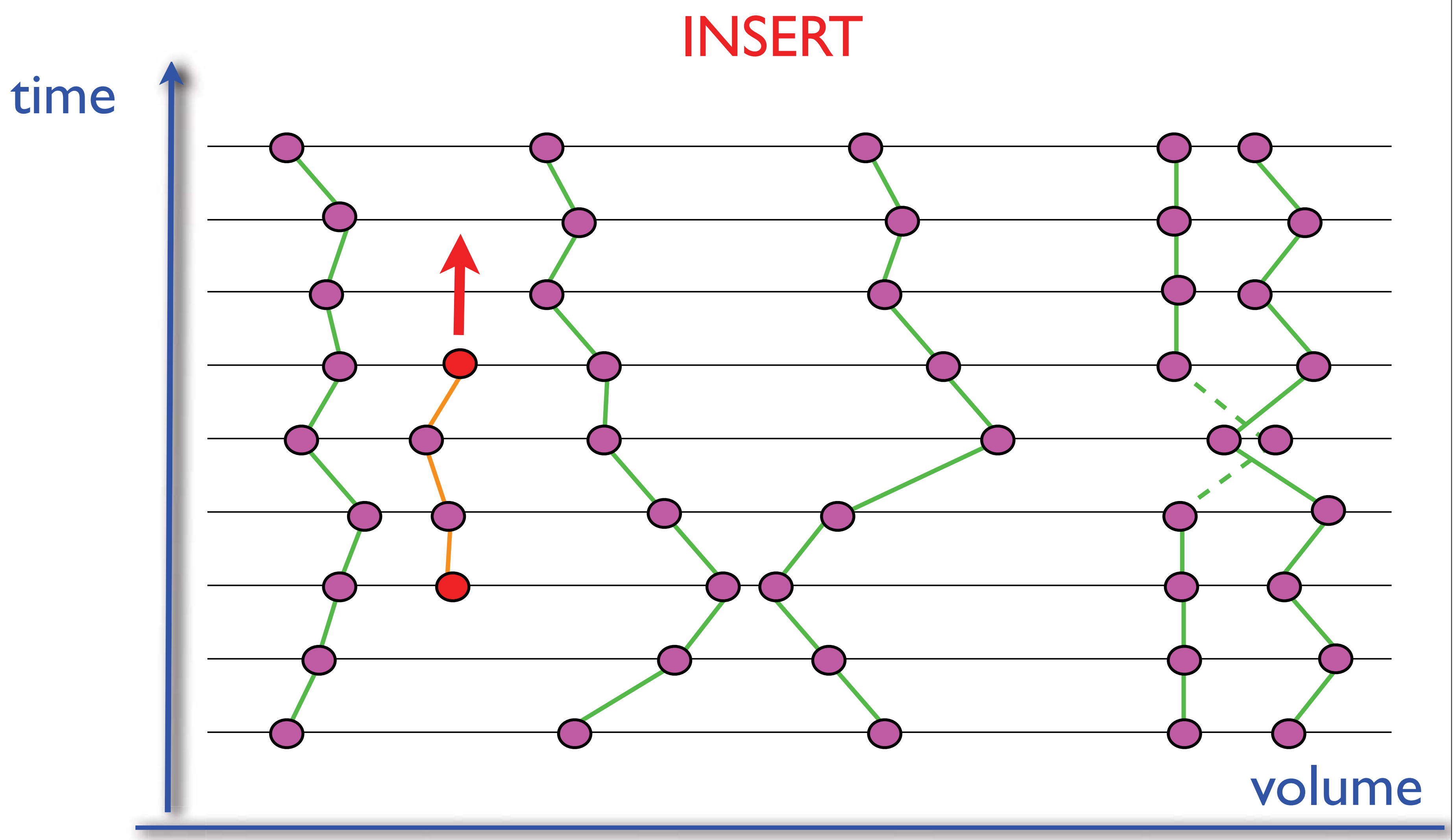


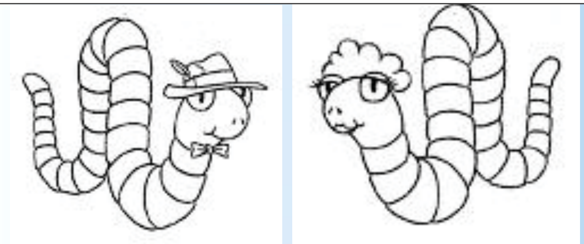
Path integral and worms

REMOVE



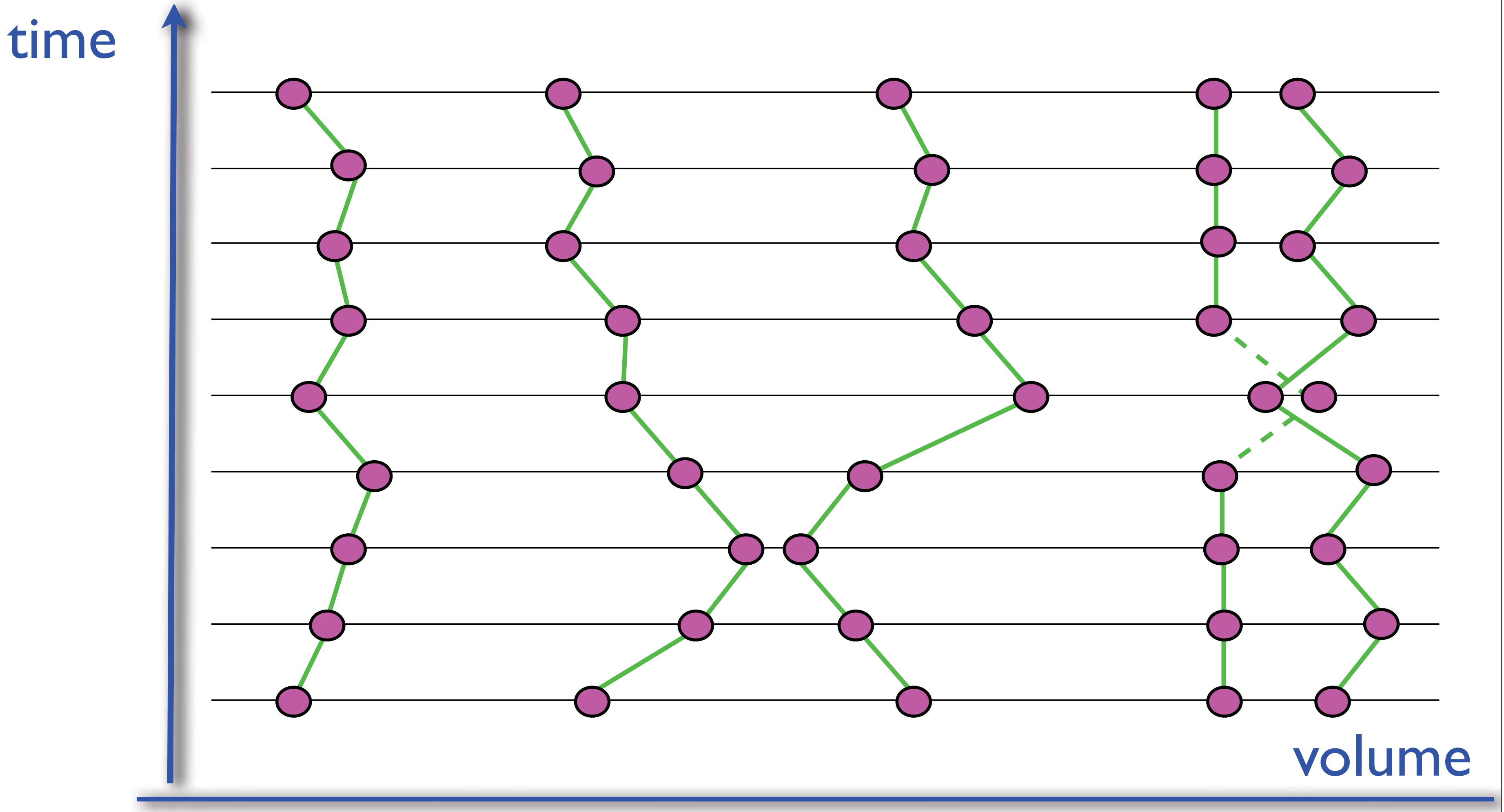
Path integral and worms



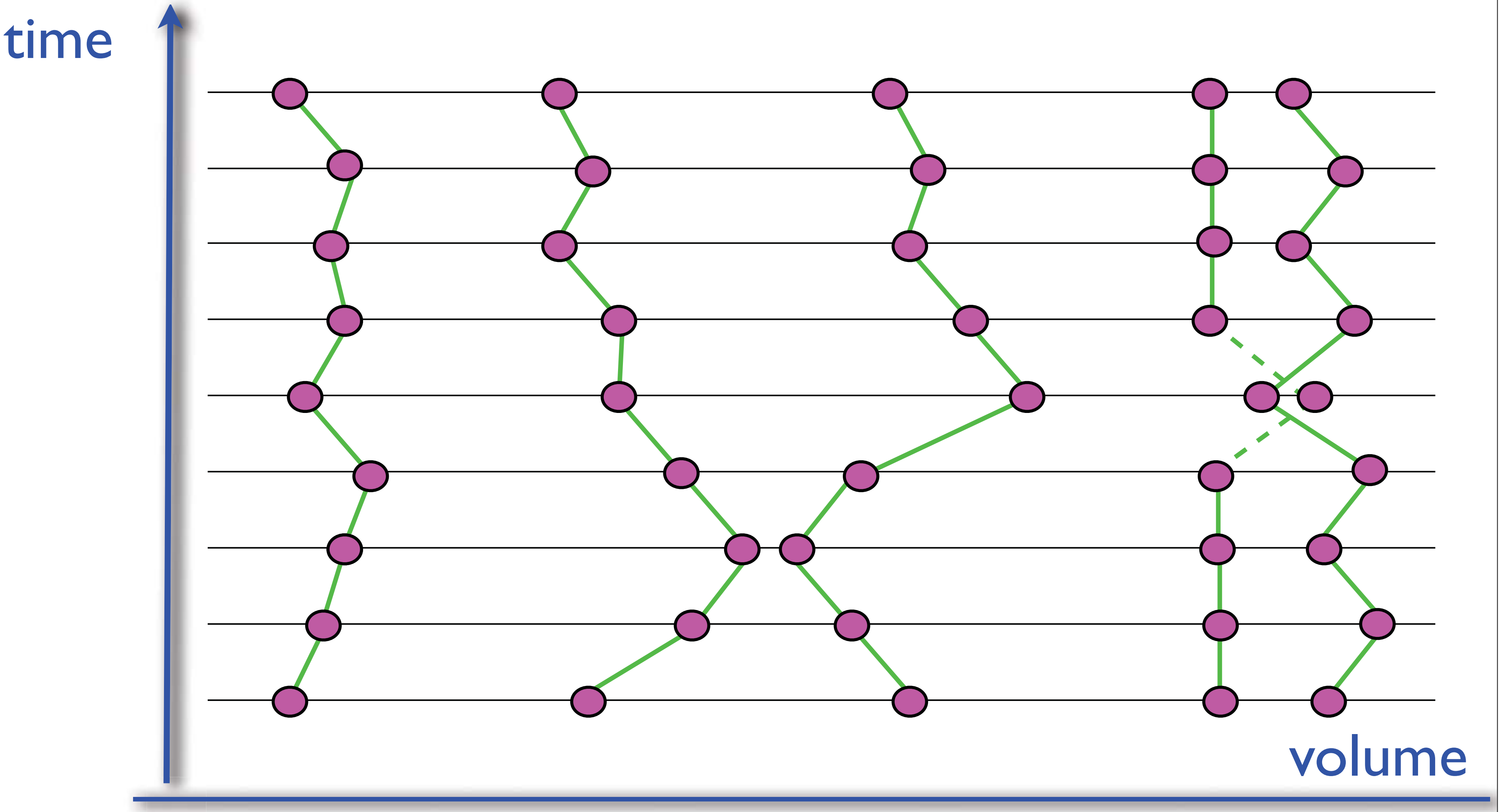


Path integral and worms

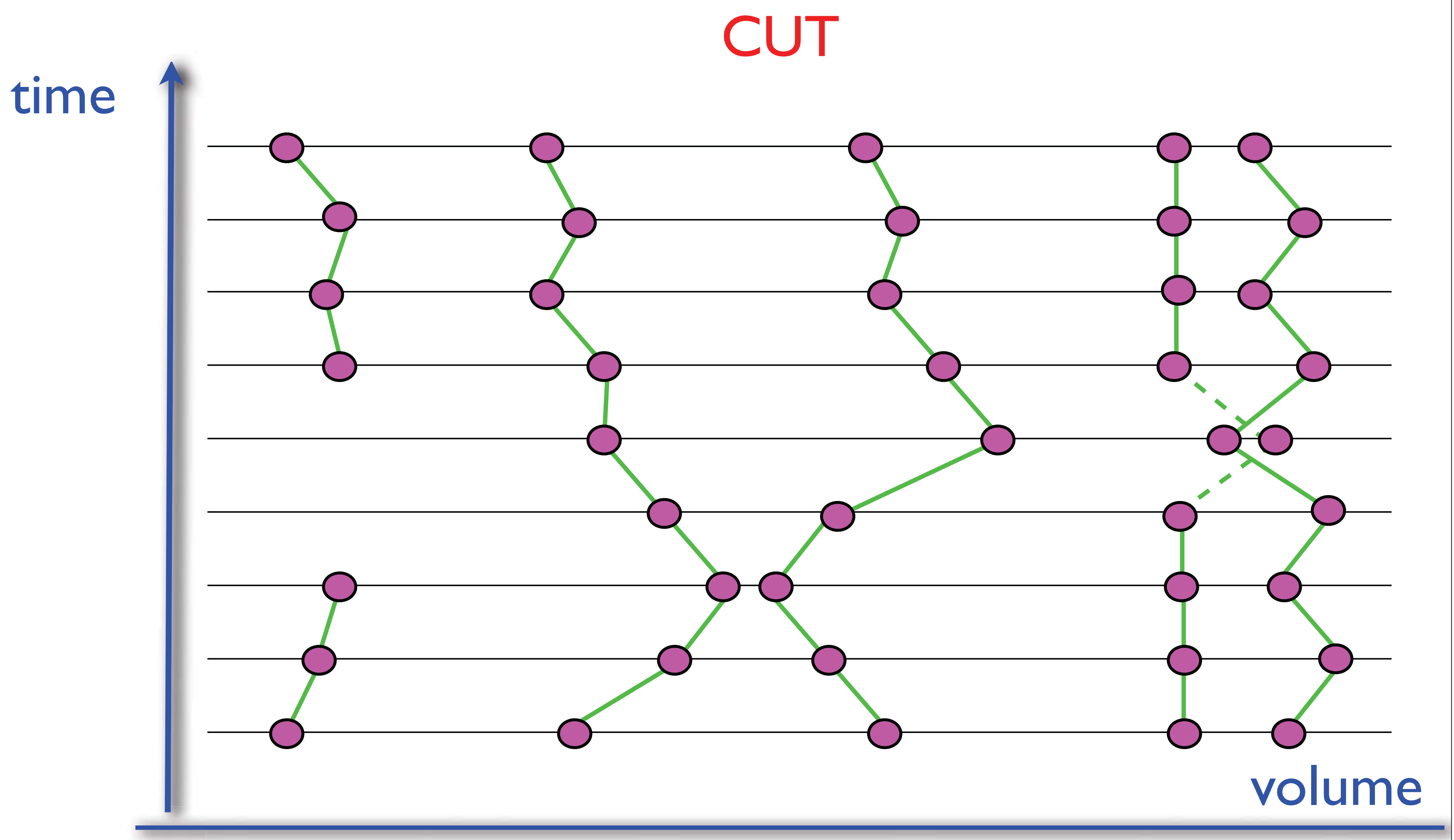
REMOVE



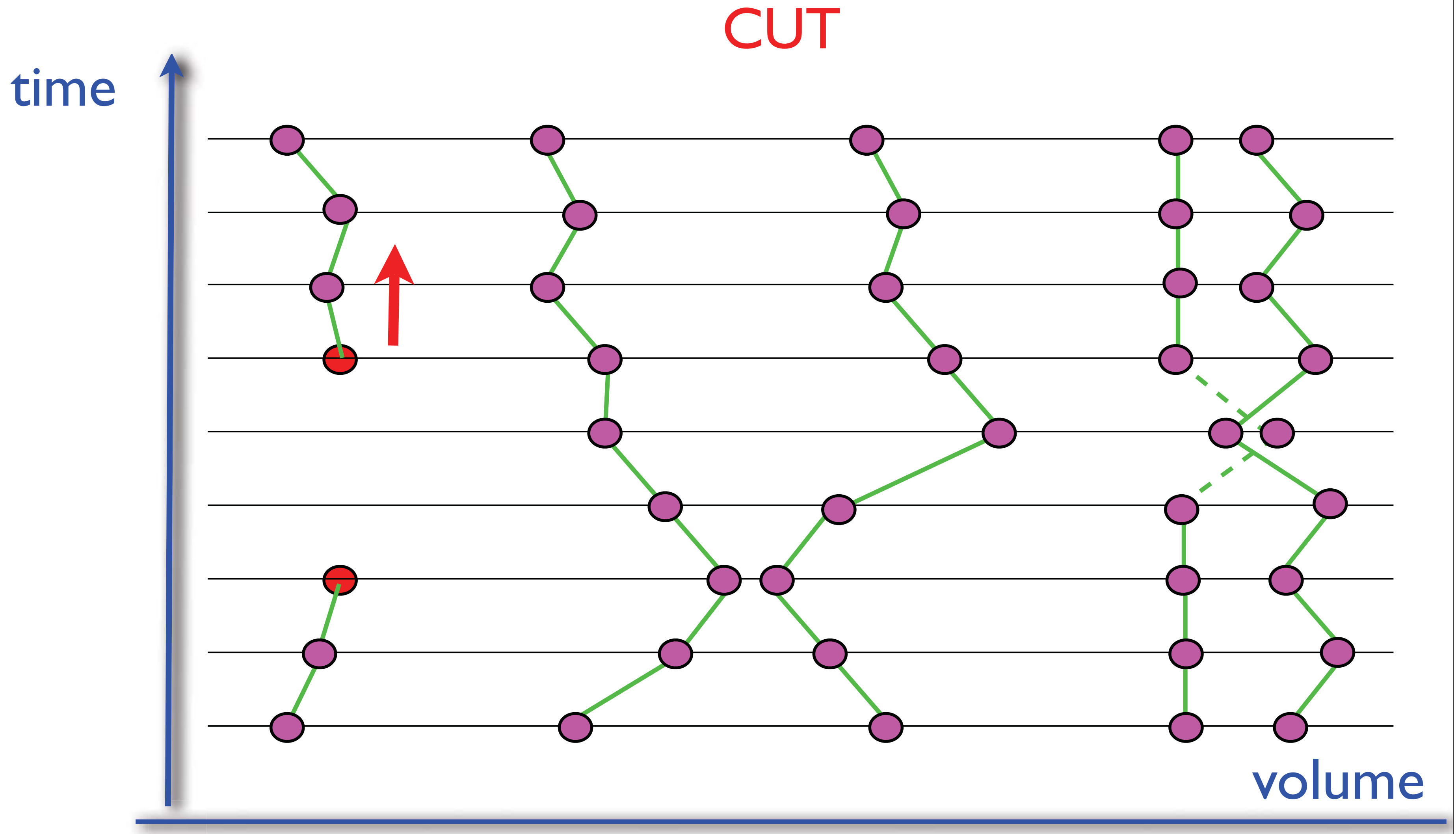
Path integral and worms



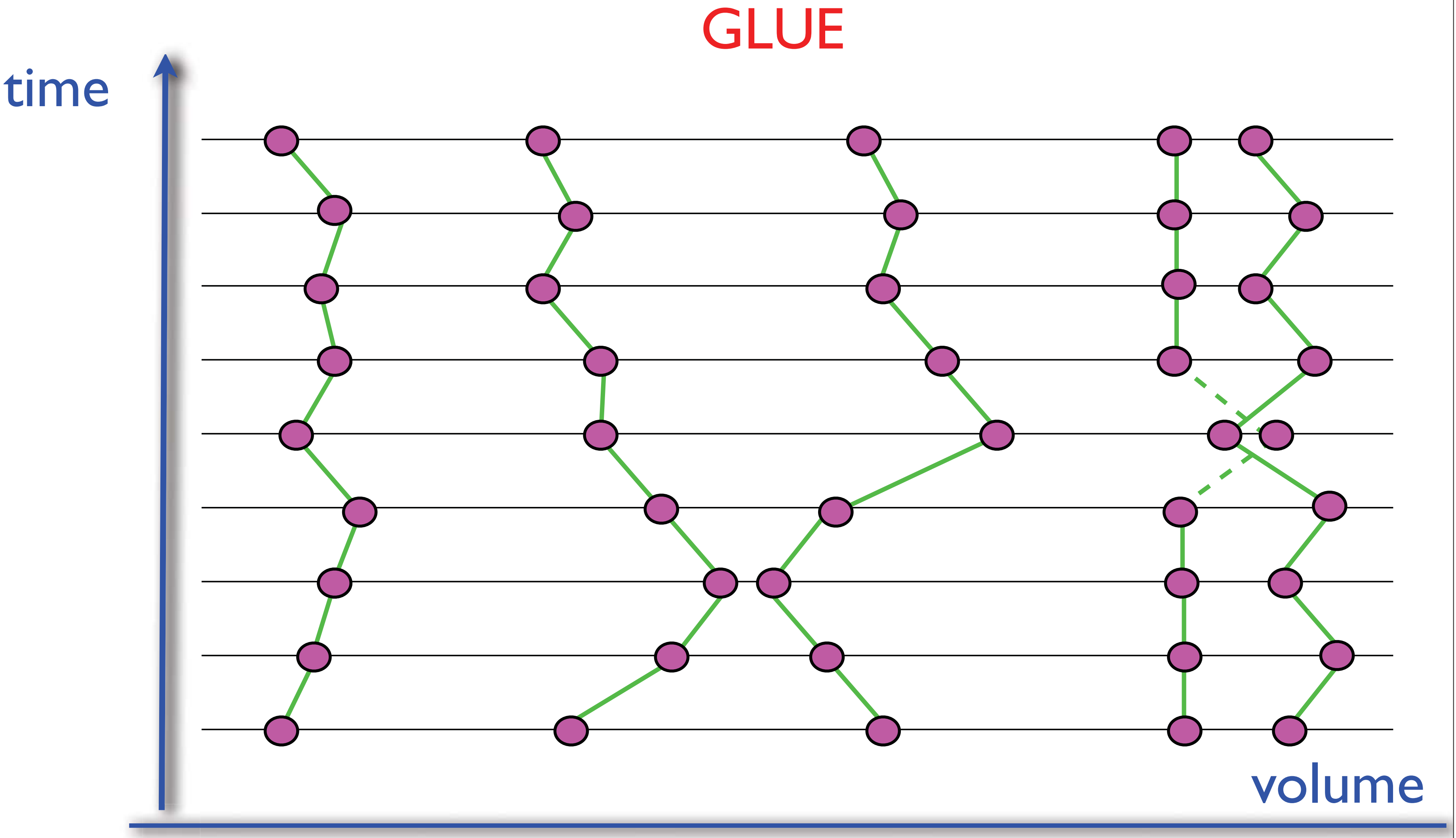
Path integral and worms



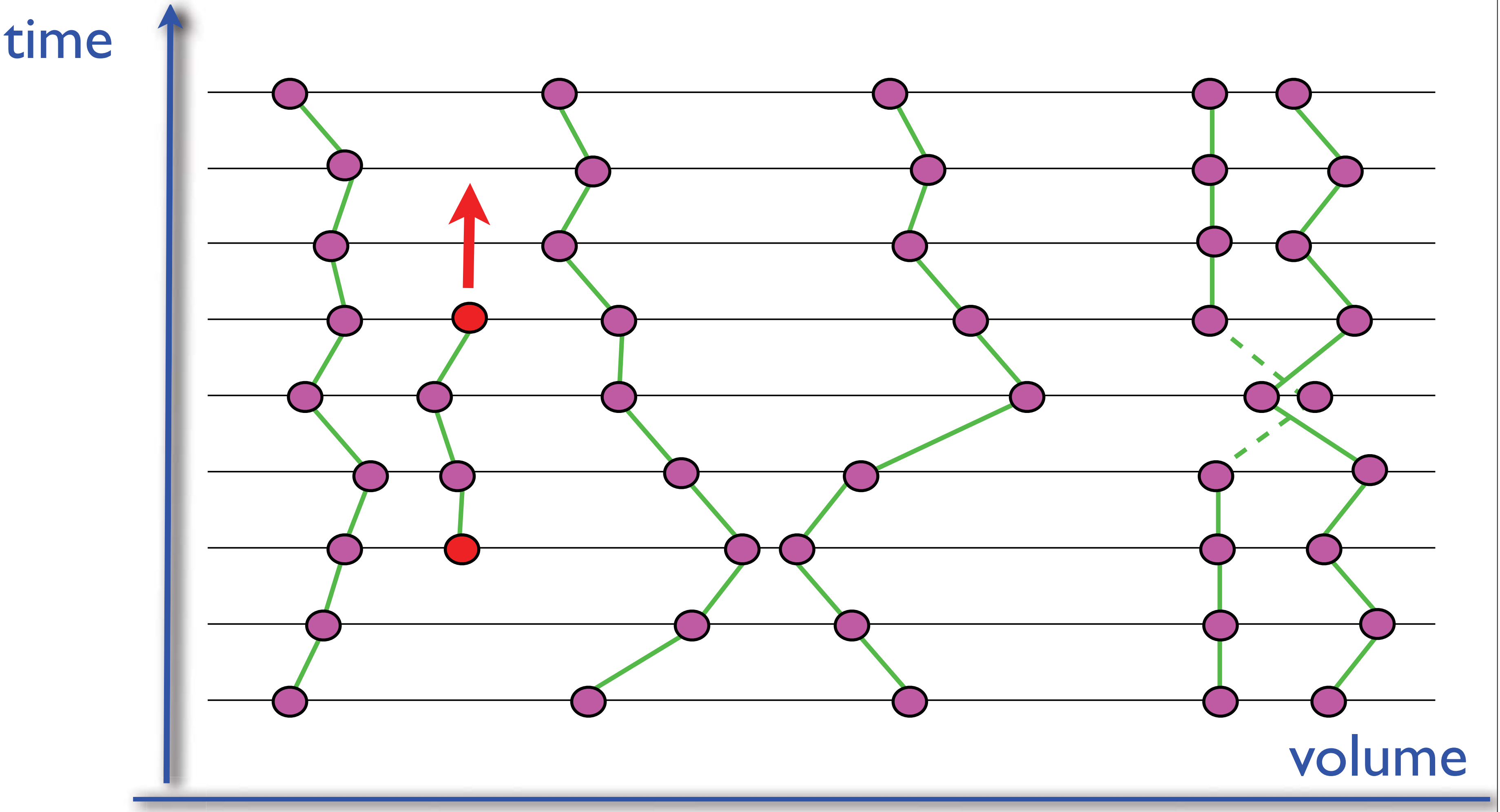
Path integral and worms



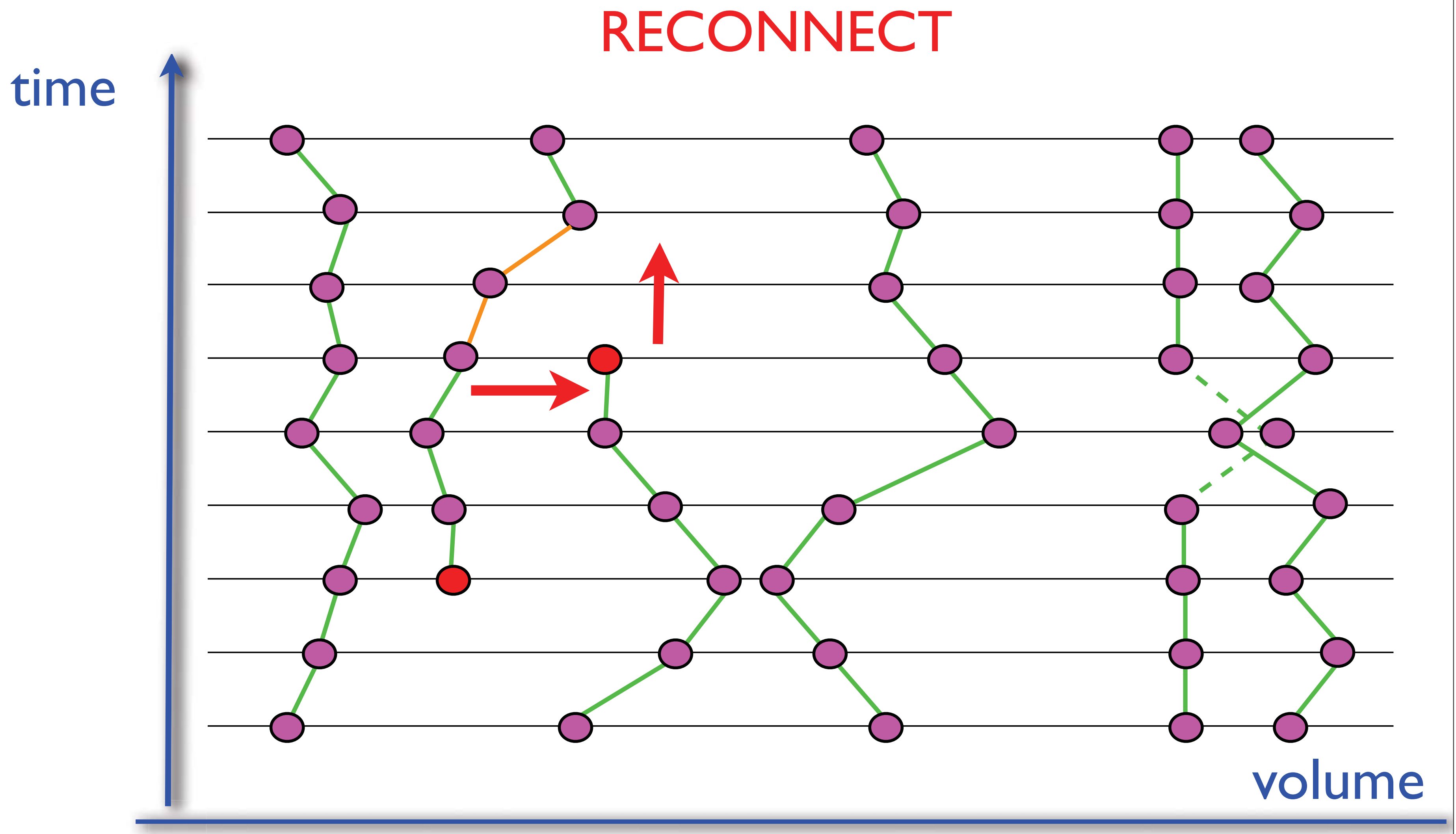
Path integral and worms



Path integral and worms



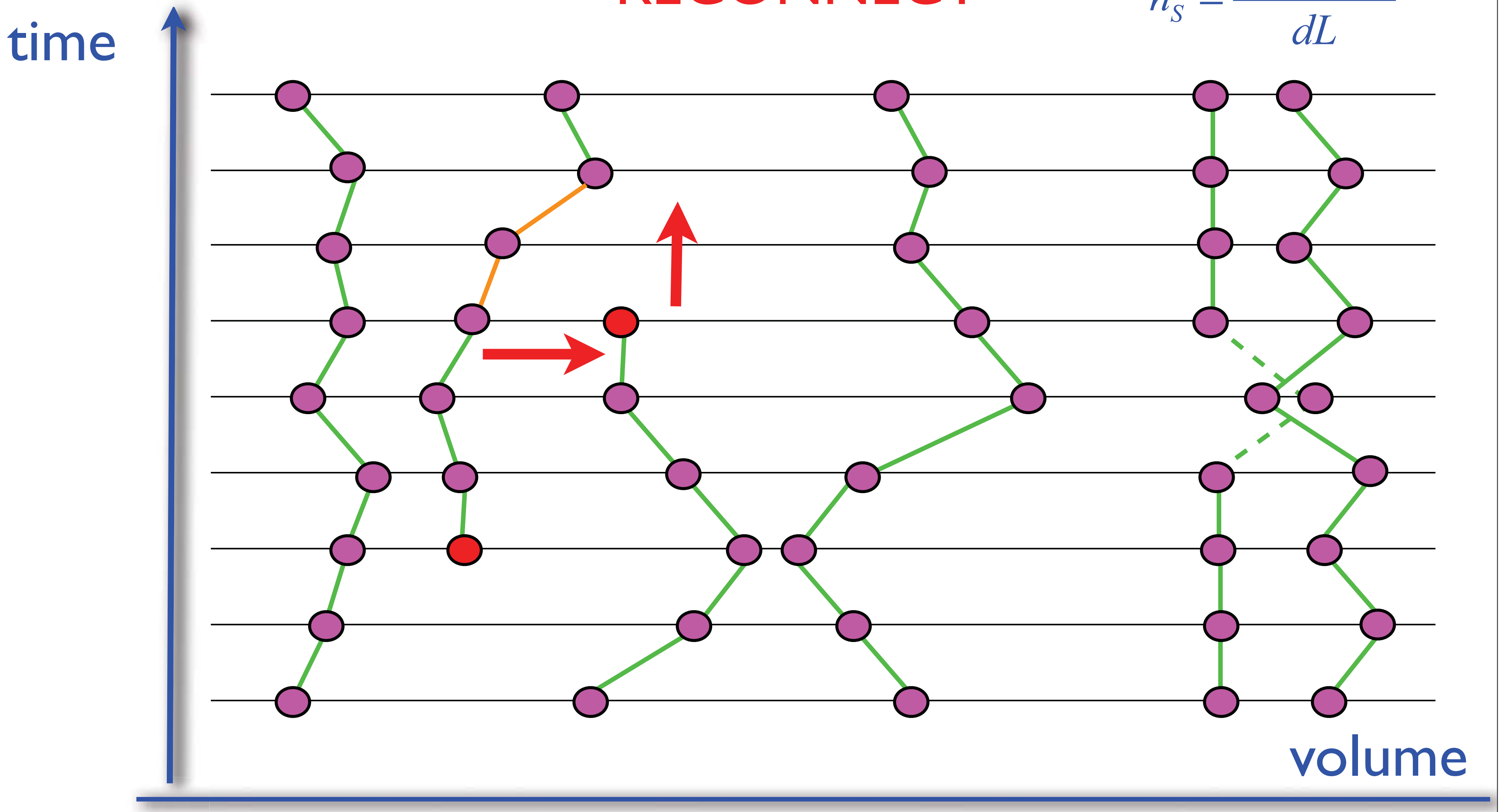
Path integral and worms



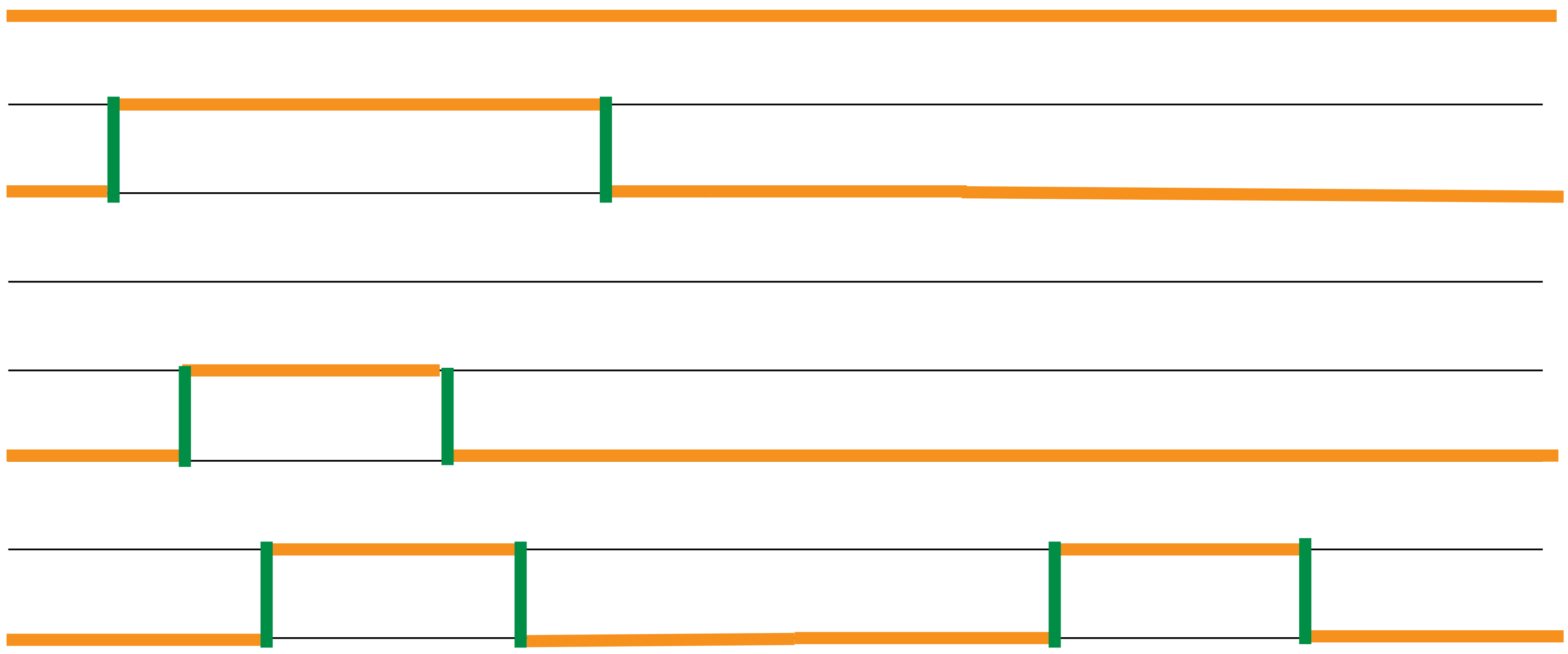
Path integral and worms

RECONNECT

$$n_S = \frac{mT\langle W^2\rangle}{dL}$$

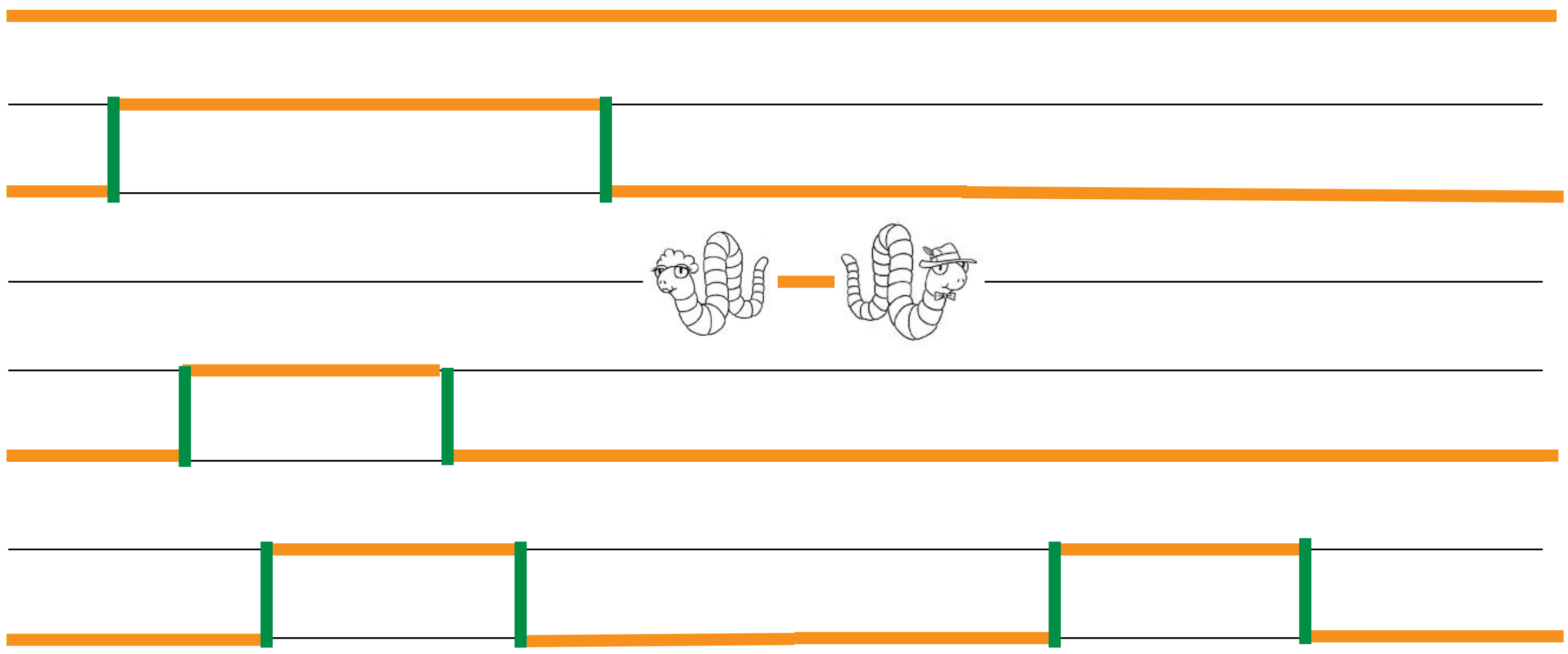


Worm updates



N.V. Prokof'ev, B.V. Svistunov and I. Tupitsyn, Sov. Phys. JETP **87**, 310 (1998).

Worm updates



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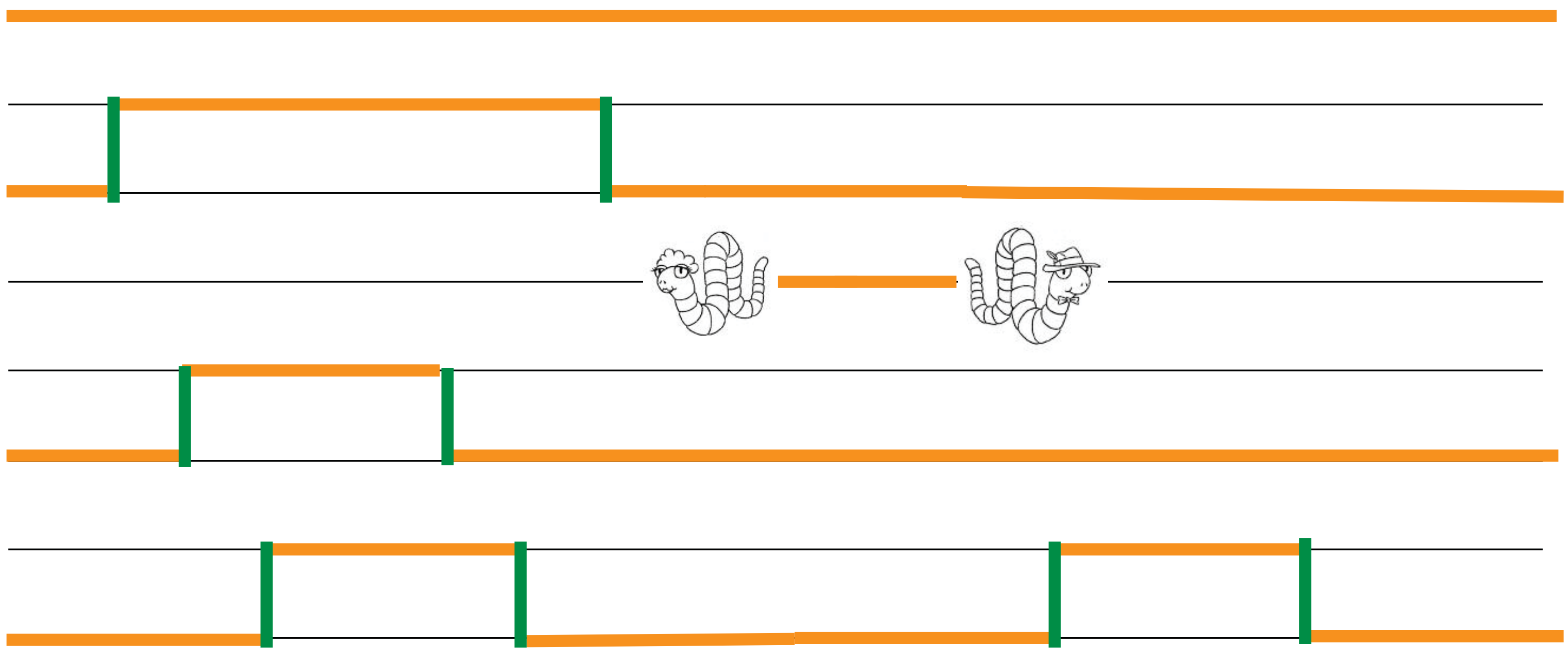
Worm updates



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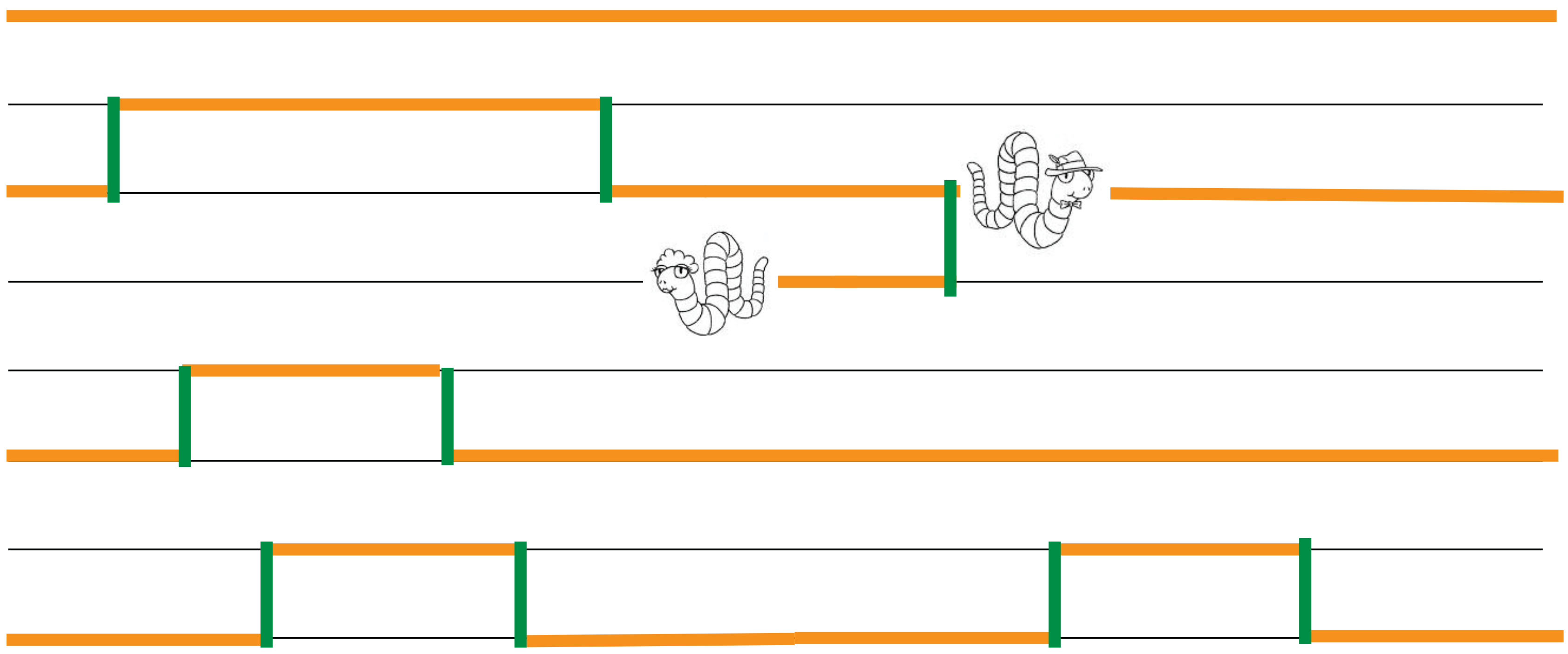

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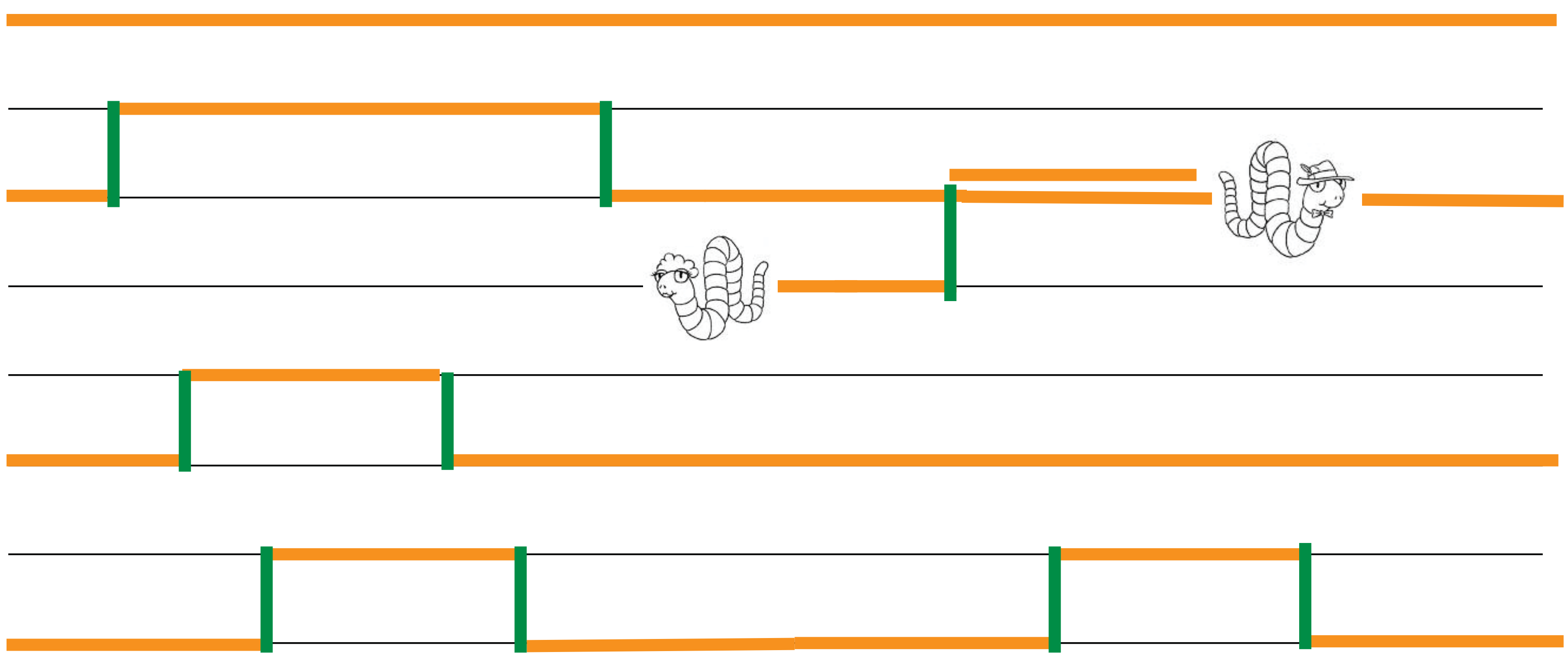

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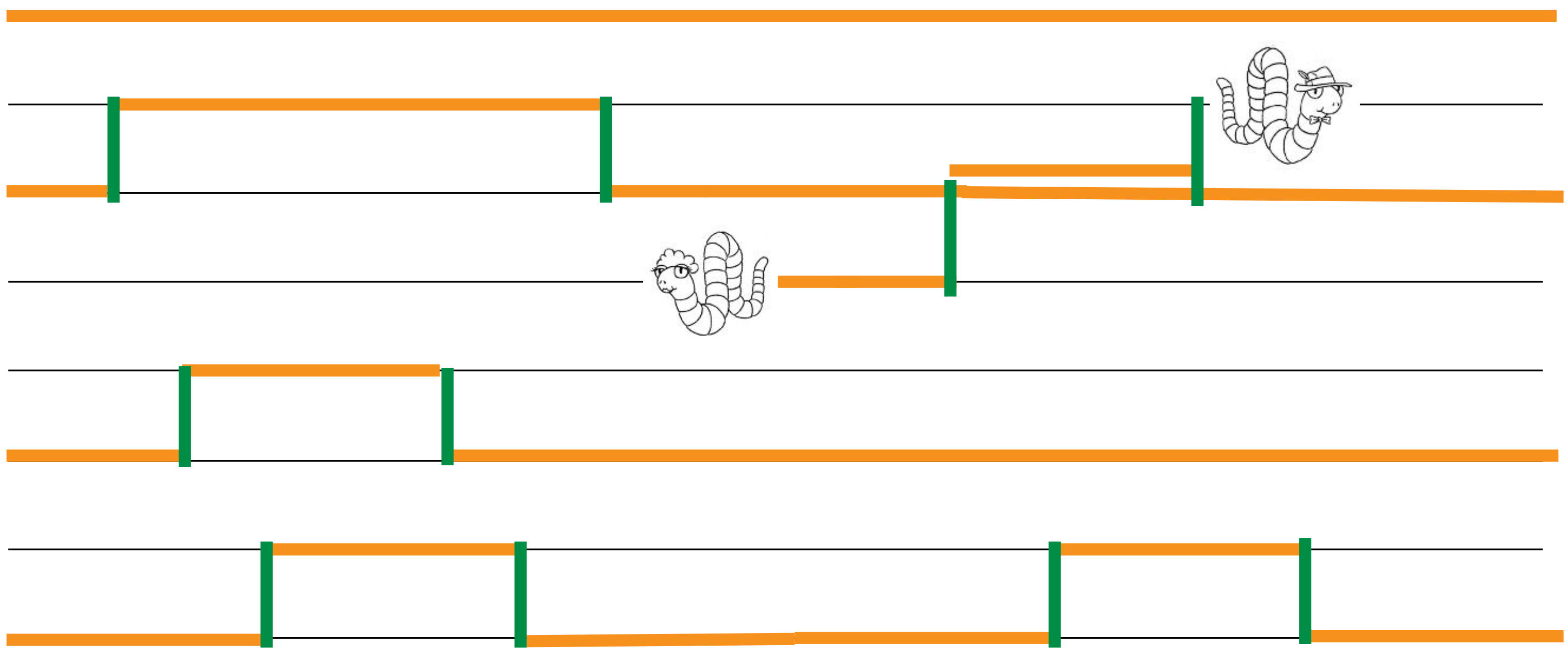

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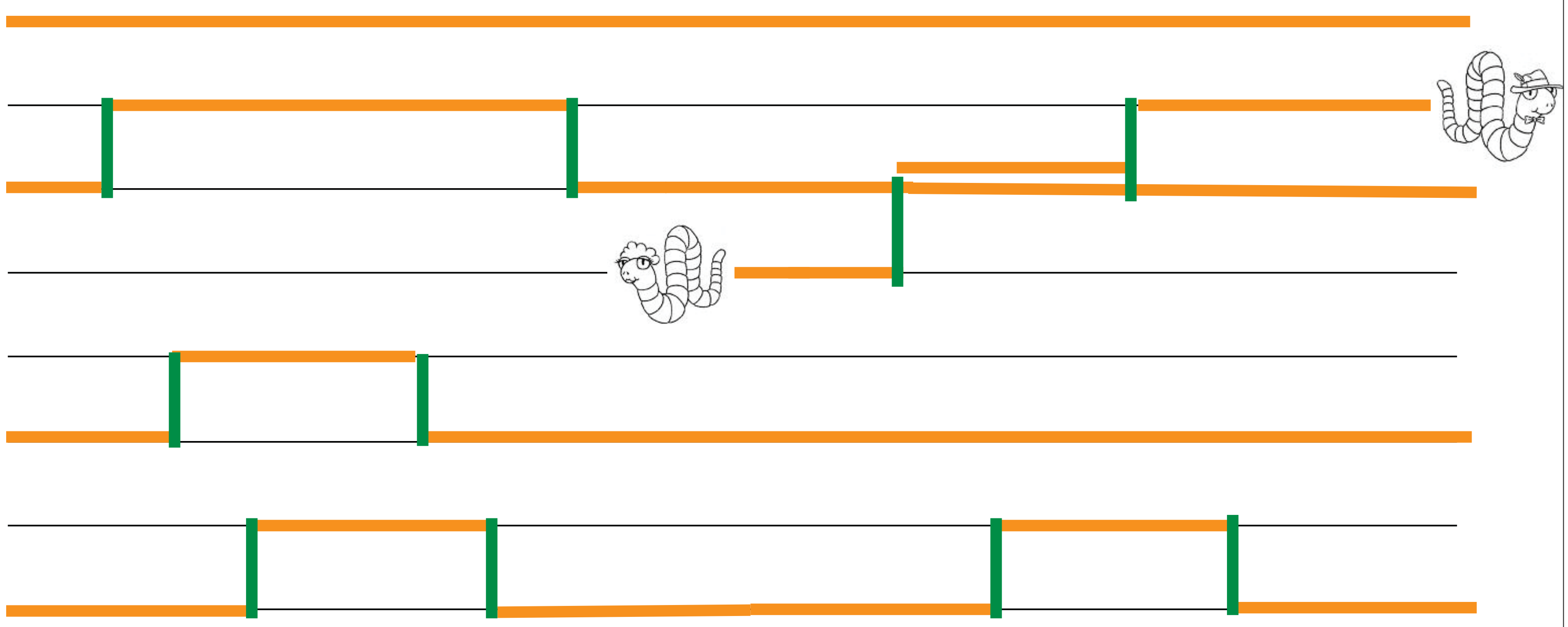

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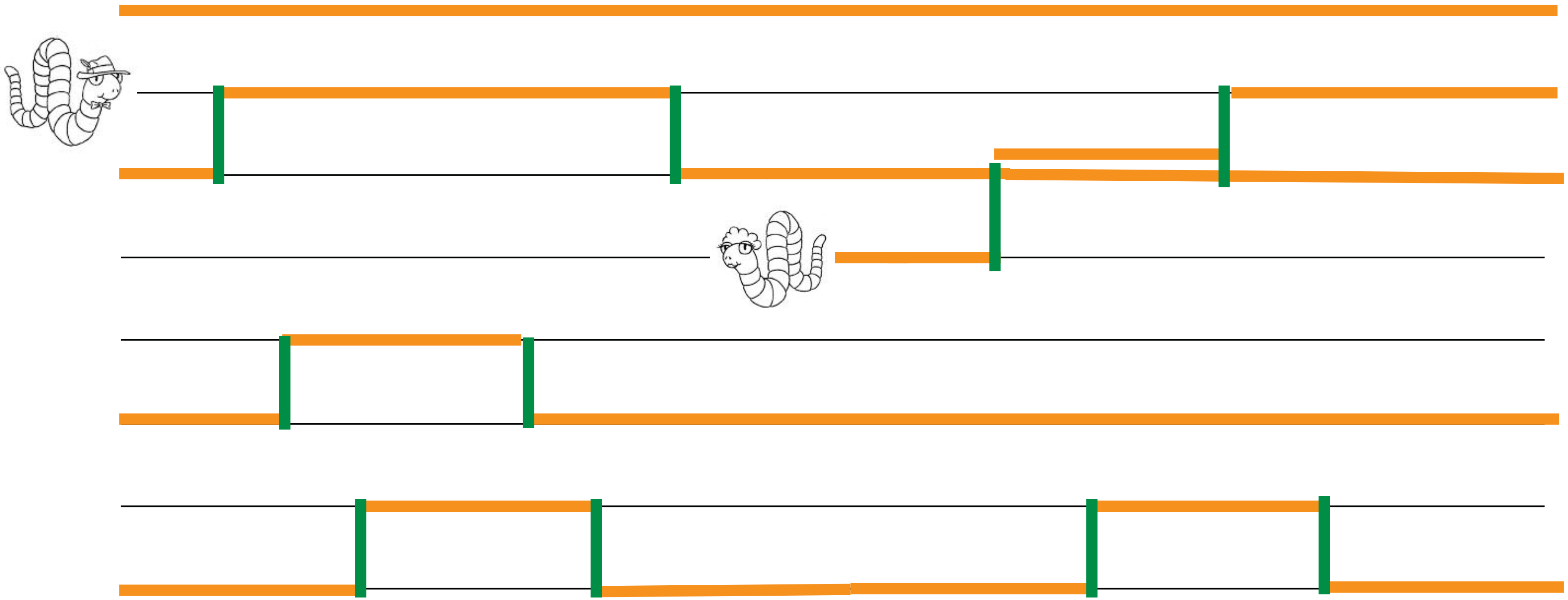

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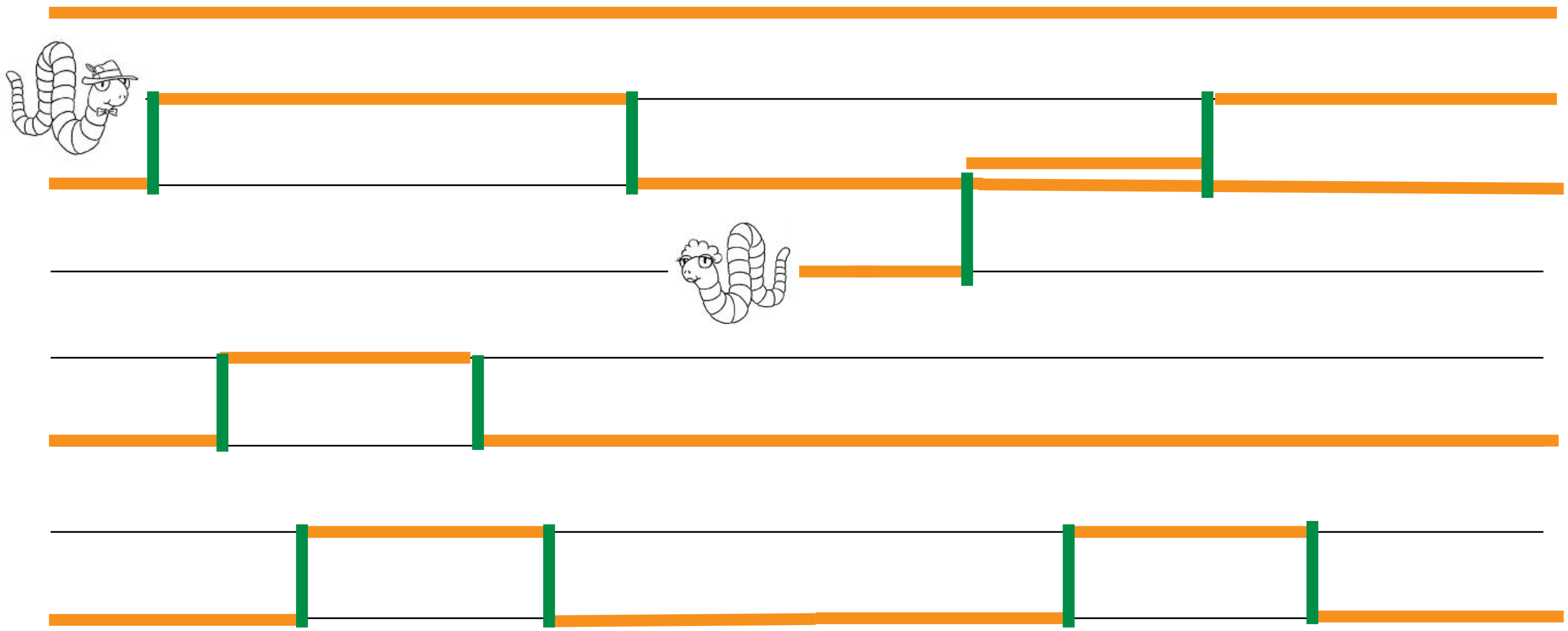

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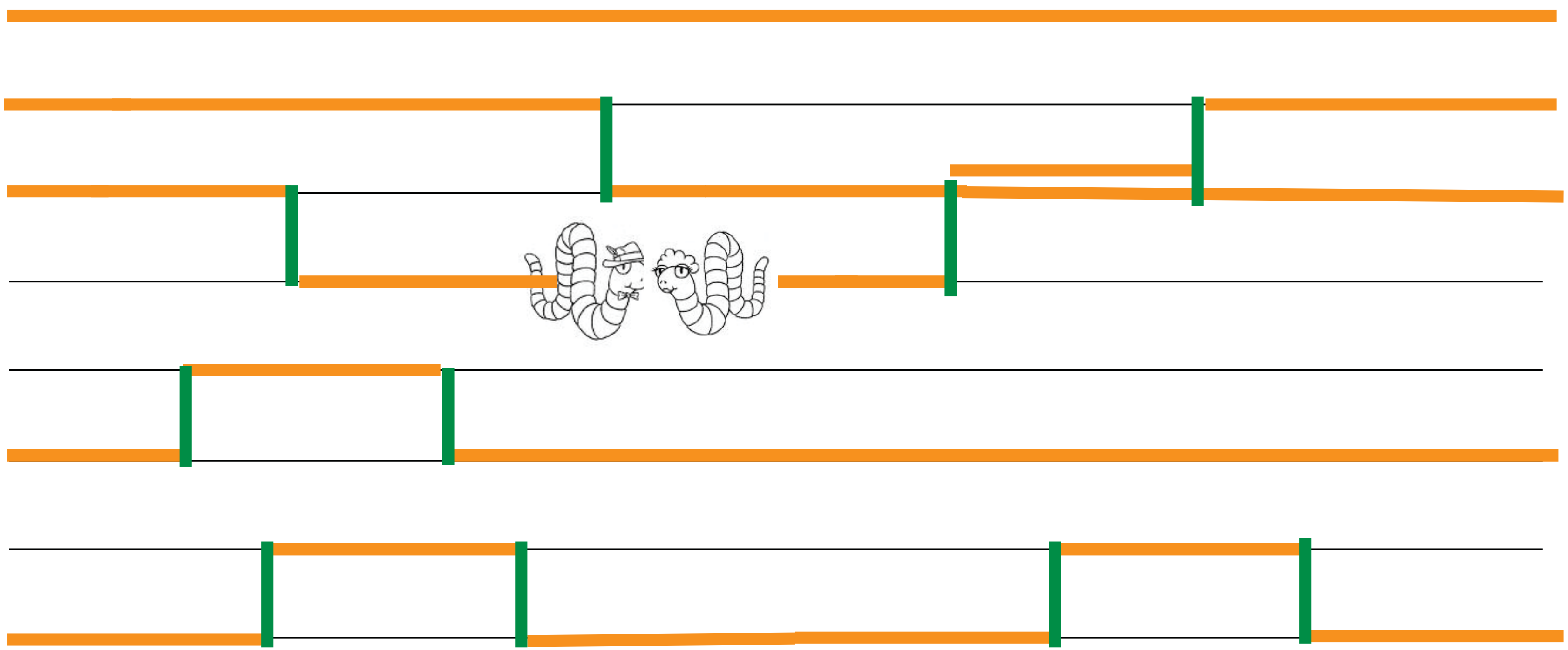

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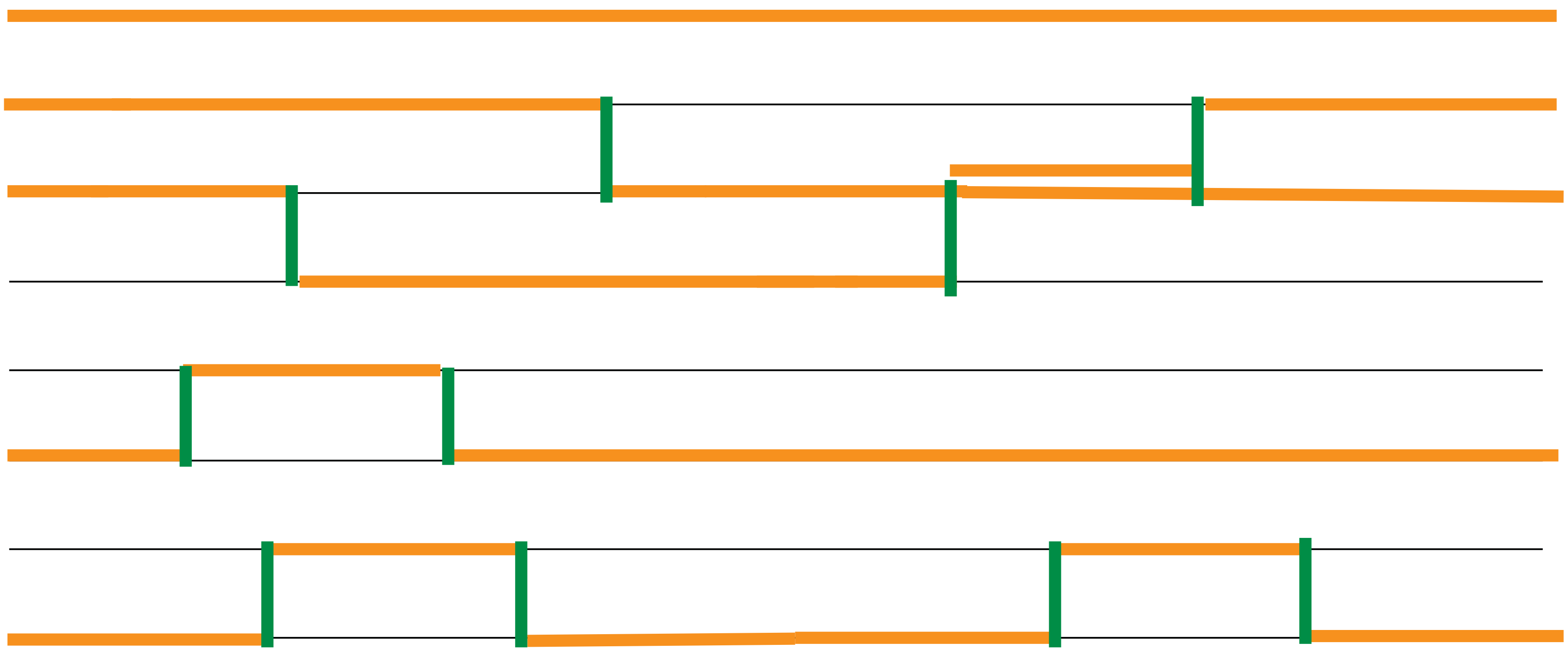
Worm updates



grand-canonical

bosonic exchange

N.V. Prokof'ev, B.V. Svistunov and I. Tupitsyn, Sov. Phys. JETP **87**, 310 (1998).

How powerful is the worm algorithm (PIMC)

+

- bosonic permutations
- superfluid properties (are 'easier' than insulating one)

- big system sizes
- all static thermodynamic quantities
- numerically exact
- first principles, no priori assumptions
- calculating eff param. of models

-

- no fermions
- periodic boundary conditions required, which might lead to the introduction of inert particles; unclear how to treat inert particles
- mesoscopic sizes : single defects
- no dynamics
- hard to get good statistics on energy, specific heat is impossible, ...
- QMC process is not real-time process
- time discretization

Outline

1. by general request : Path Integral Monte Carlo
2. binding of a ^{3}He atom to the core of a screw dislocation

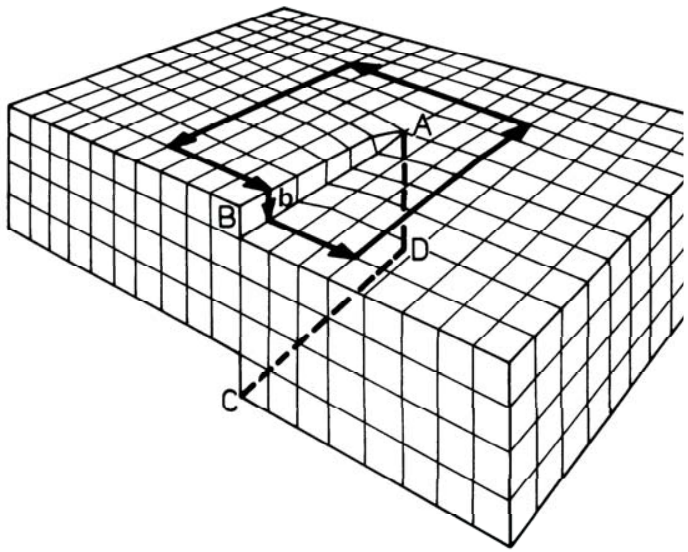
screw dislocation

Defects are important in torsional oscillator experiments.
One particular example is the screw dislocation

b : Burger's vector

µ : shear modulus

stress : $$\tau_r = -\frac{\mu b}{2\pi r}$$



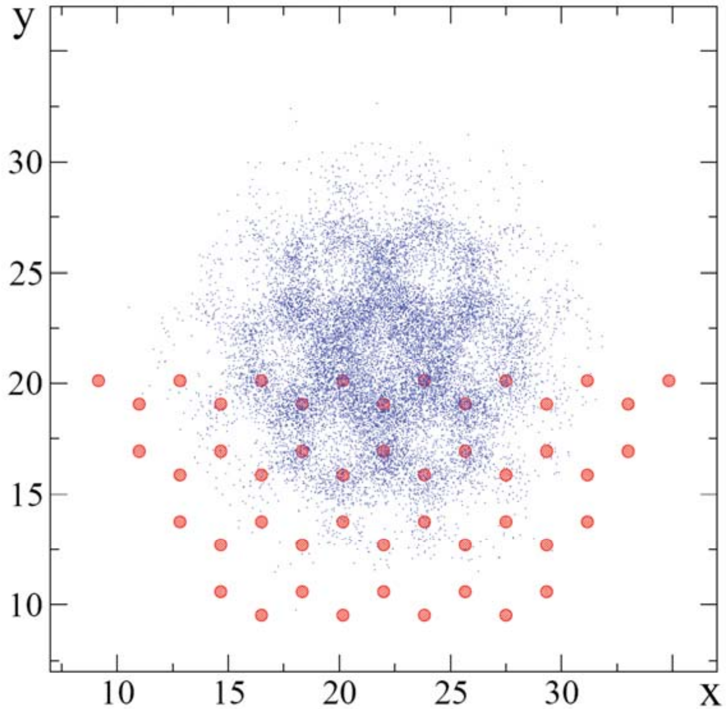
Screw dislocation

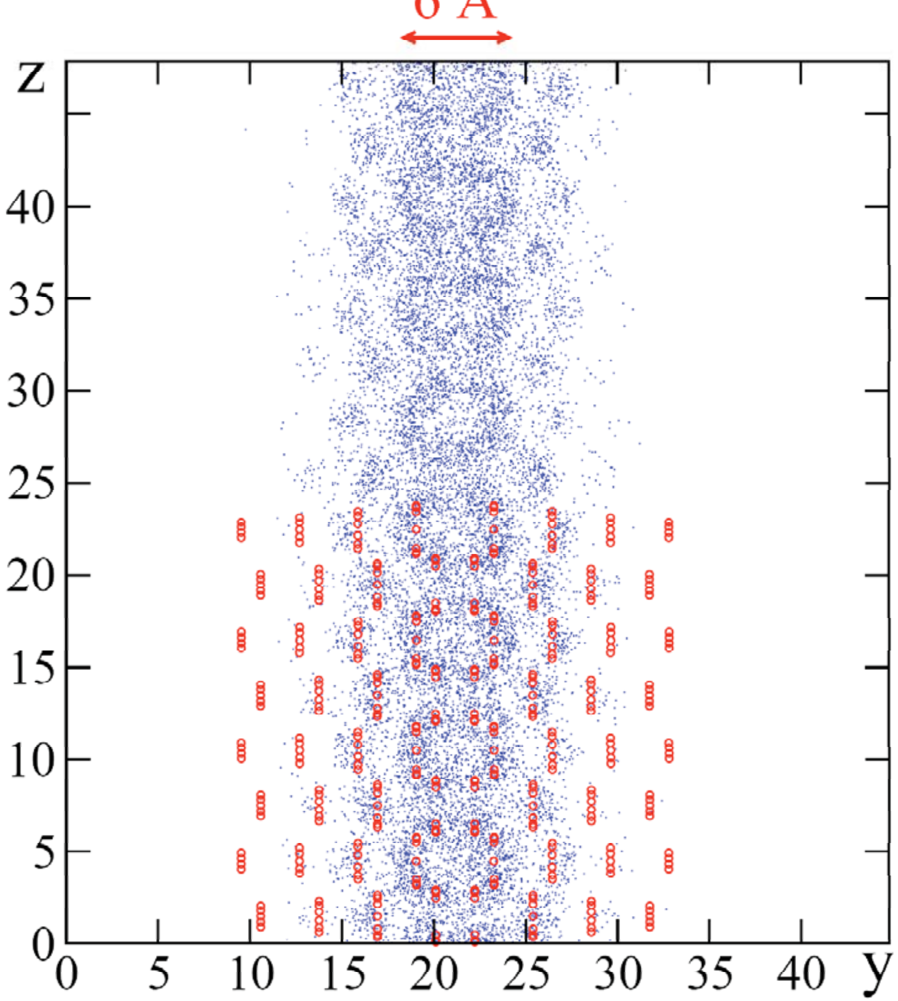
Shevchenko state

$$\tau = (T_*/T)^{2/K_\mathrm{L}-1}/T_*$$

$$n_s \approx 1\mathring{A}^{-1}, K_\mathrm{L} = 0.205(20)$$

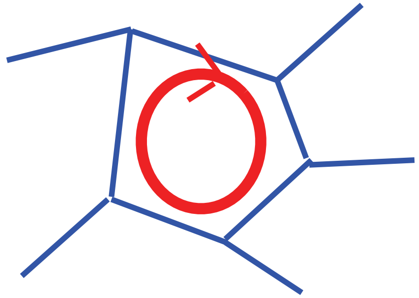
$$T_c \sim T_* a/l \ll T_*$$





Shevchenko model

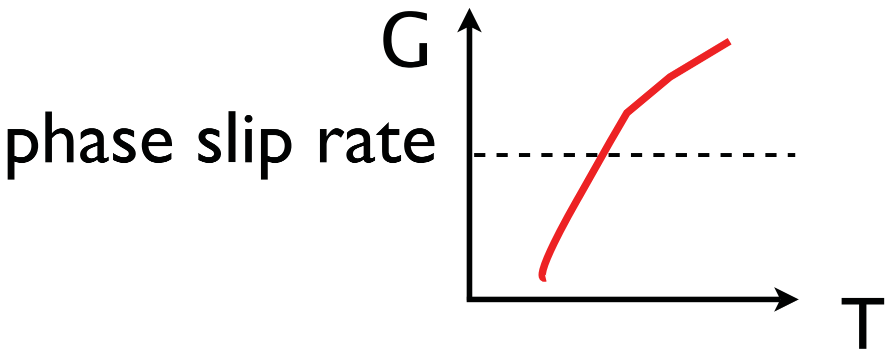
$T^* = 1$ K
$T_c = T^*\, a/l$



$J_i \sim 1/l$

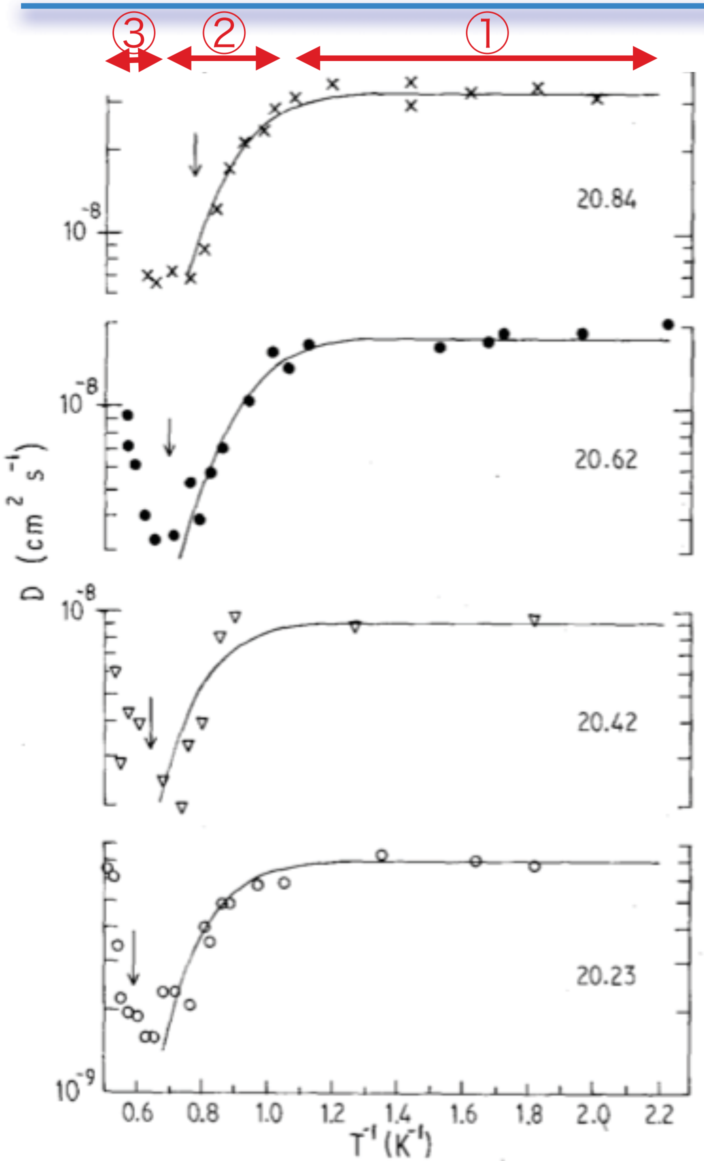
1. $T < T_c$: 3d condensation or vortex glass
2. $T_c < T < T^*$: all properties we want from 'vortex liquid'

- $w\tau \ll 1$: normal
- $w\tau \gg 1$: indistinguishable from superfluid



S. I. Shevchenko, Sov. J. Low. Temp. Phys. **14**, 553 (1988).
V.A. Kashurnikov, V. I. Podlivaev, N.V. Prokof'ev, and B.V. Svistunov, Phys. Rev. B **53**, 13091 (1996).
Yu. Kagan, N.V. Prokof'ev, and B.V. Svistunov, Phys. Rev. A **61**, 045601 (2000).

NMR of spin diffusion



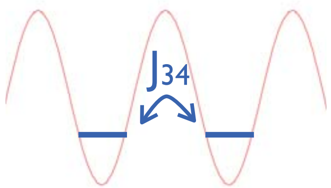
A. R. Allen, M. G. Richards, and J. Schratter, J Low Temp Phys, Vol. **47**, Nos. 3/4, p. 289 (1982).

x_3=500 ppm

1) low concentrations, low temperature, ^{3}He-^{3}He scattering

temperature independent, 0.5K <T < 0.8K

ballistic motion in narrow band



$$J_{^3He} \sim 10^{-4} K$$

2) higher temperatures, scattering with phonons

$$D = C\hbar J_{34}^2 a^2 \Theta_{\mathrm{D}}^8 / k_{\mathrm{B}} T^9$$

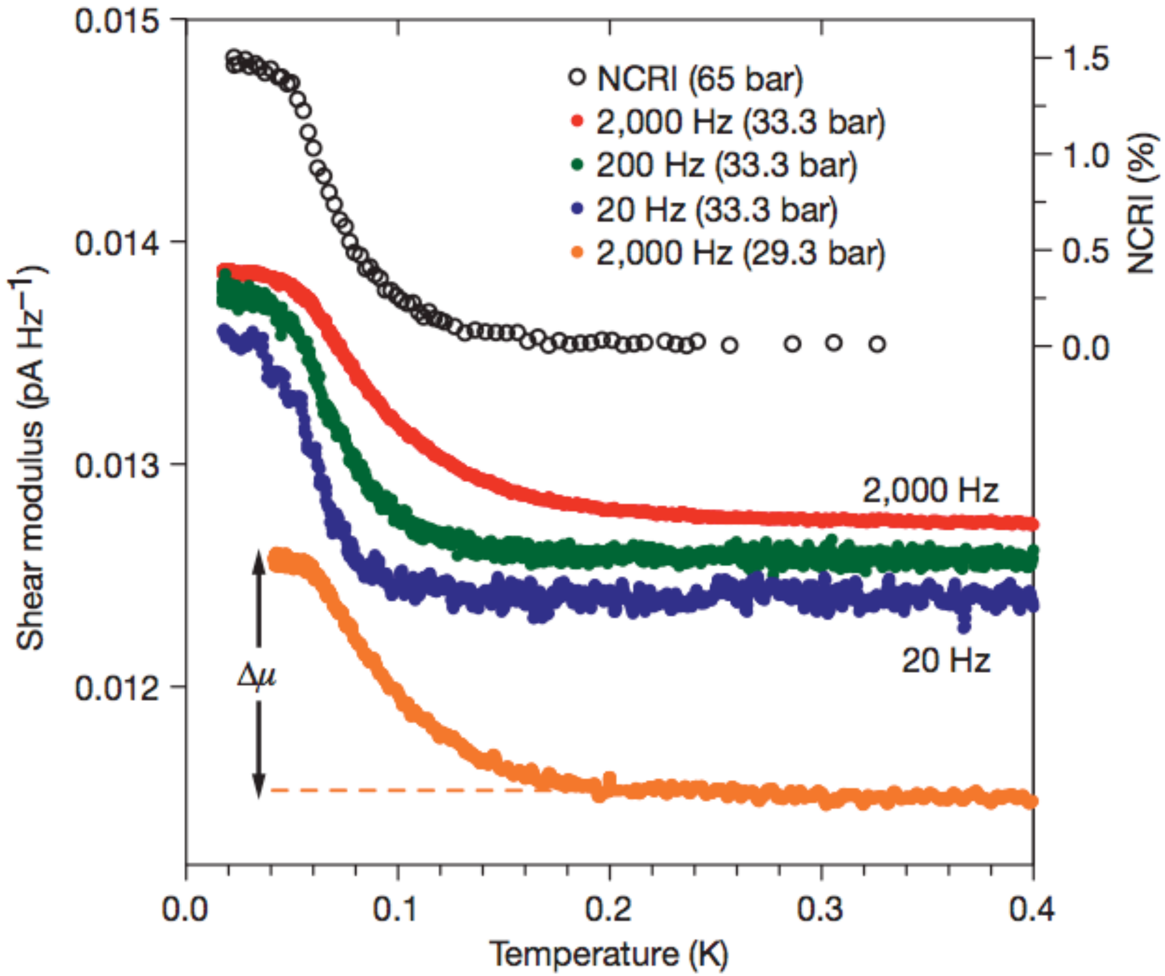
3) high temperatures,incoherent scattering with vacancies

$$D = D_0 \exp(-W/k_{\mathrm{B}}T)$$

(data do not allow to rule out phonon-assisted tunneling)

The Day-Beamish conundrum

The Alberta group observed stiffening of the ^{4}He crystal, with the same hysteretic, temperature, frequency, ^{3}He dependence as in the TO



J. Day and J. Beamish, Nature **450**, 853 (2007).

stiffening origins

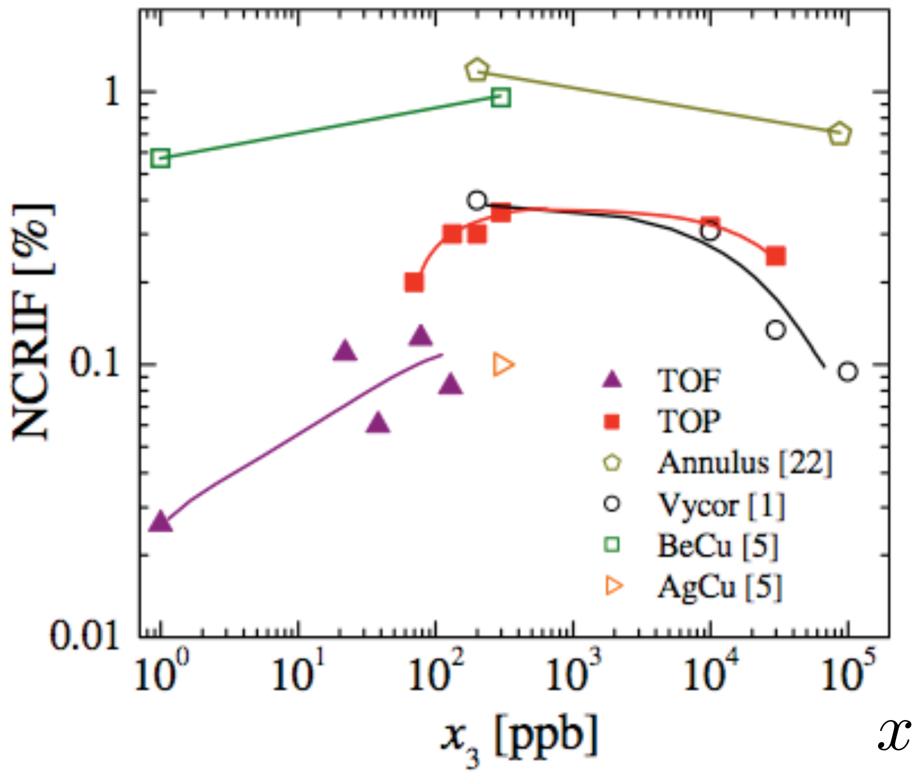
- pinning of dislocations, distance L_N between pinning sites
- stiffening is independent of frequency according to the Granato-Lücke theory, up to 30% reduction in shear modulus
- with impurities, the impurity pinning length L_{IP} can become smaller than L_N

$$T_P \sim -(E_B/k_B)[\ln(xL_N/a)]^{-1}$$

T_P : pinning temperature,
E_B : binding energy,
a : interparticle distance.

He-3 & NCRIF

E. Kim et al., Phys. Rev. Lett. **100**, 065301 (2008).



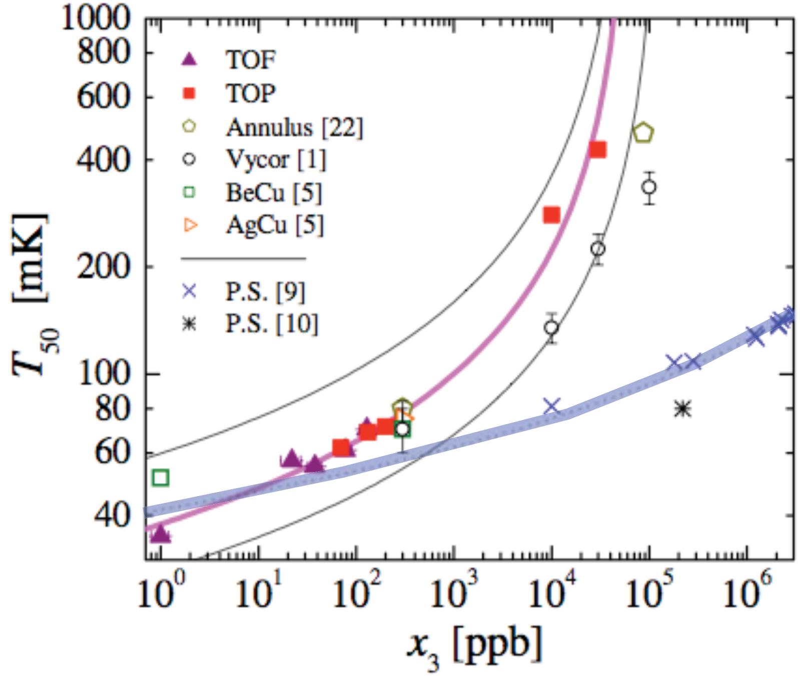
minimum value required?
maximum around 0.5 ppm
sample dependent

$$x_3 = 10\text{ppm} \quad : \quad T_F = 3\text{mK}$$

$$x_3 = 30\text{ppm} \quad : \quad T_F = 6\text{mK}$$

He-3 & NCRIF

E. Kim et al., Phys. Rev. Lett. **100**, 065301 (2008).



solid lines : $T_{IP} = T_x$

phase separation (in blue) *not* consistent with data, at least above T > 50 mK

(elasticity change cannot fully account for observed NCRIF)

A. C. Clark, J. D. Maynard, and M. H. W. Chan, Phys. Rev. B **77**, 184513 (2008).

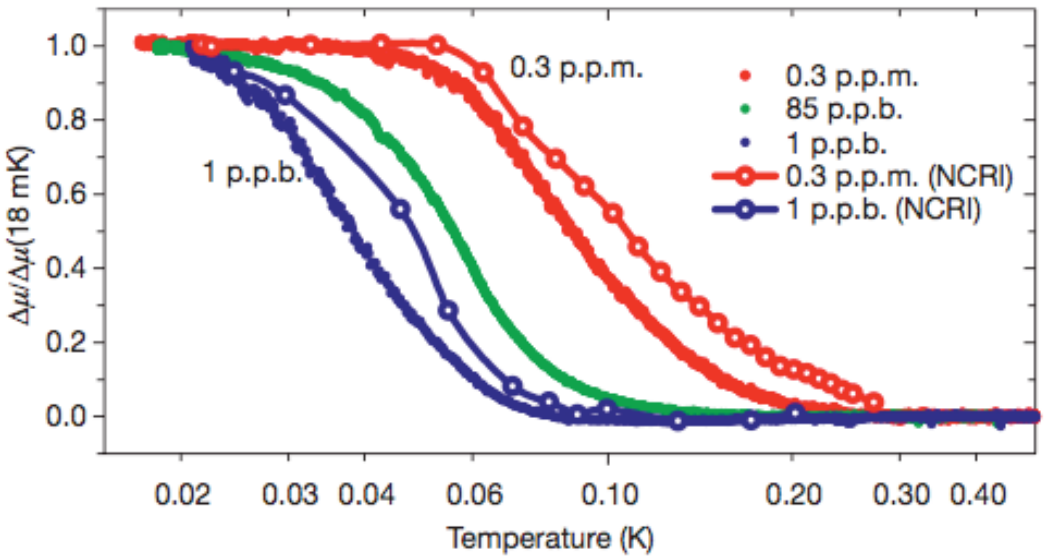
T_x [K]	E_B [K]	L_{IP} [μm]	Λ [10^6 cm^{-2}]
T_{10}	0.66	1.7	7
T_{50}	0.42	1.9	6
T_{90}	0.33	1.3	12

dislocation densities calculated by setting $L_{IP} = L_N$ and $\Lambda L_N^2 = 0.2$

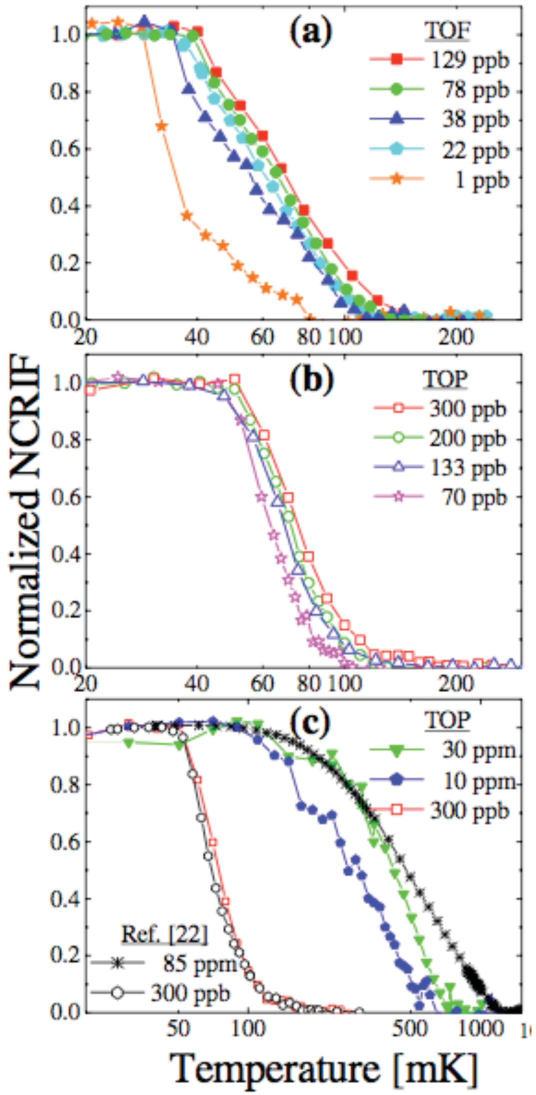
observed x_3 correlated with impurity-pinning of dislocations

Shear modulus vs He-3

J. Day and J. Beamish, Nature **450**, 853 (2007).

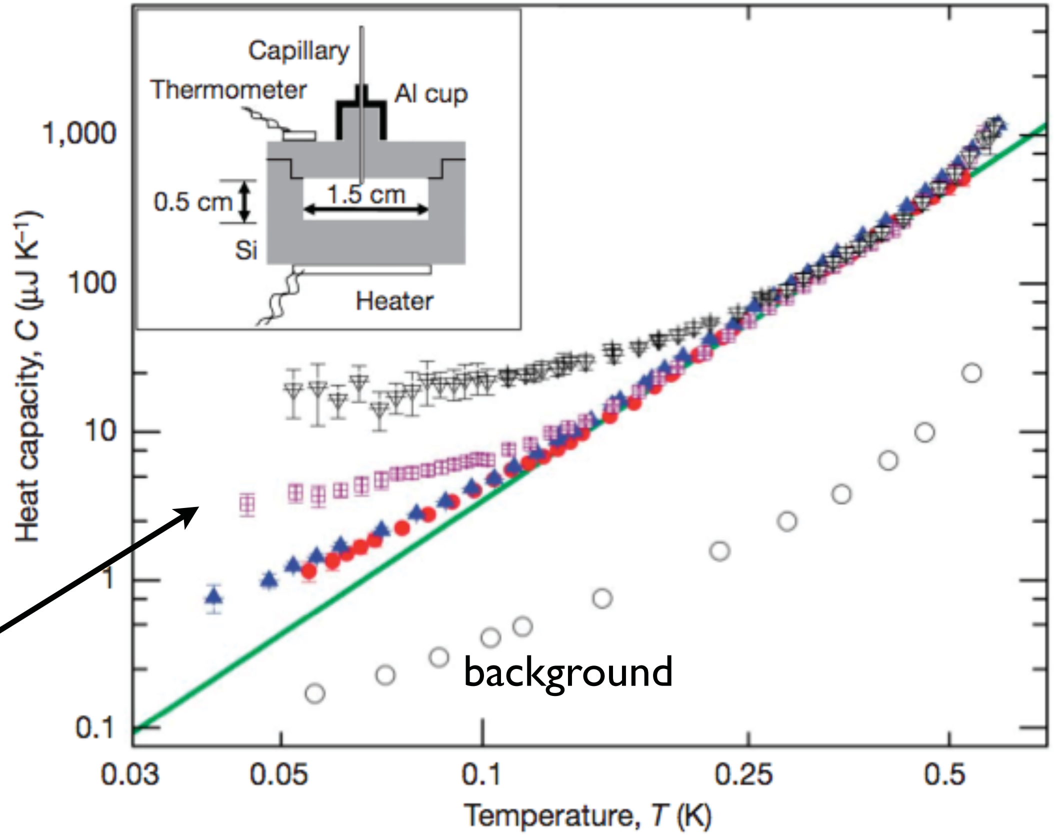


E. Kim et al., Phys. Rev. Lett. **100**, 065301 (2008).



specific heat measurements

X. Lin, A. C. Clark, and M. W. H. Chan, Nature **449**, 1025 (2007).



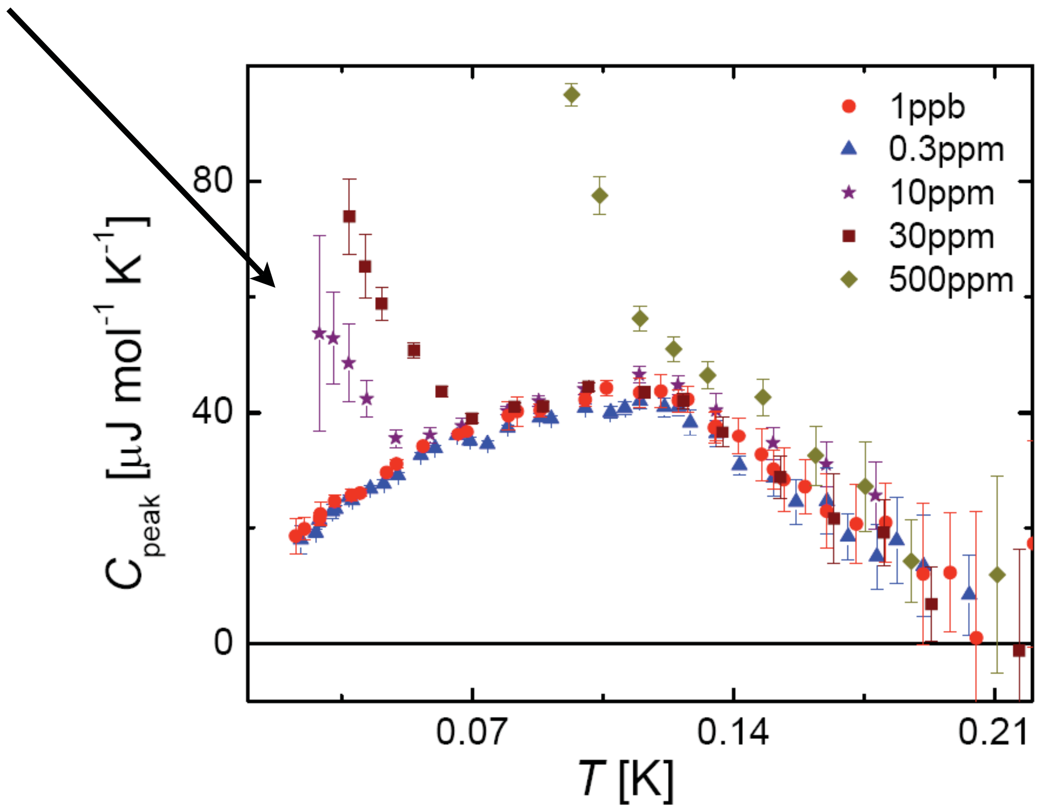
scales with x_3

- 30 ppm
- 10 ppm
- 0.3 ppm
- 1 ppb
- T^3

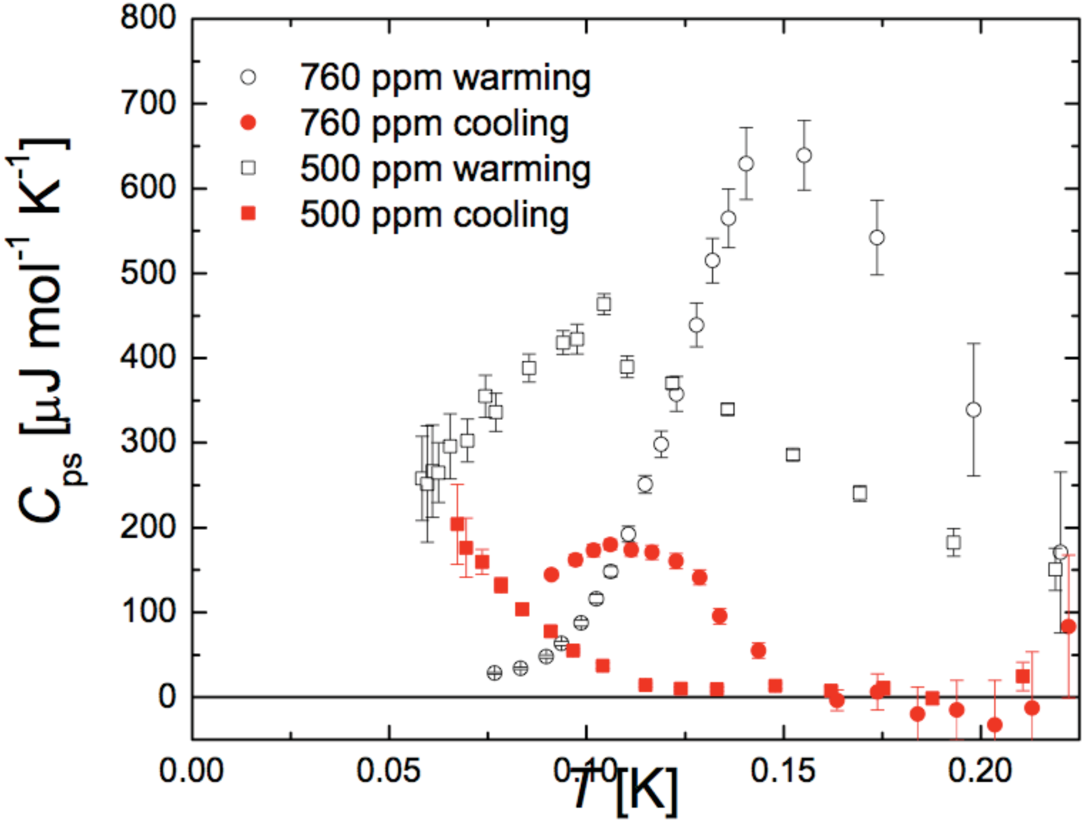
new data from PennState

after subtraction of phonon contribution :

He-3 independent peak



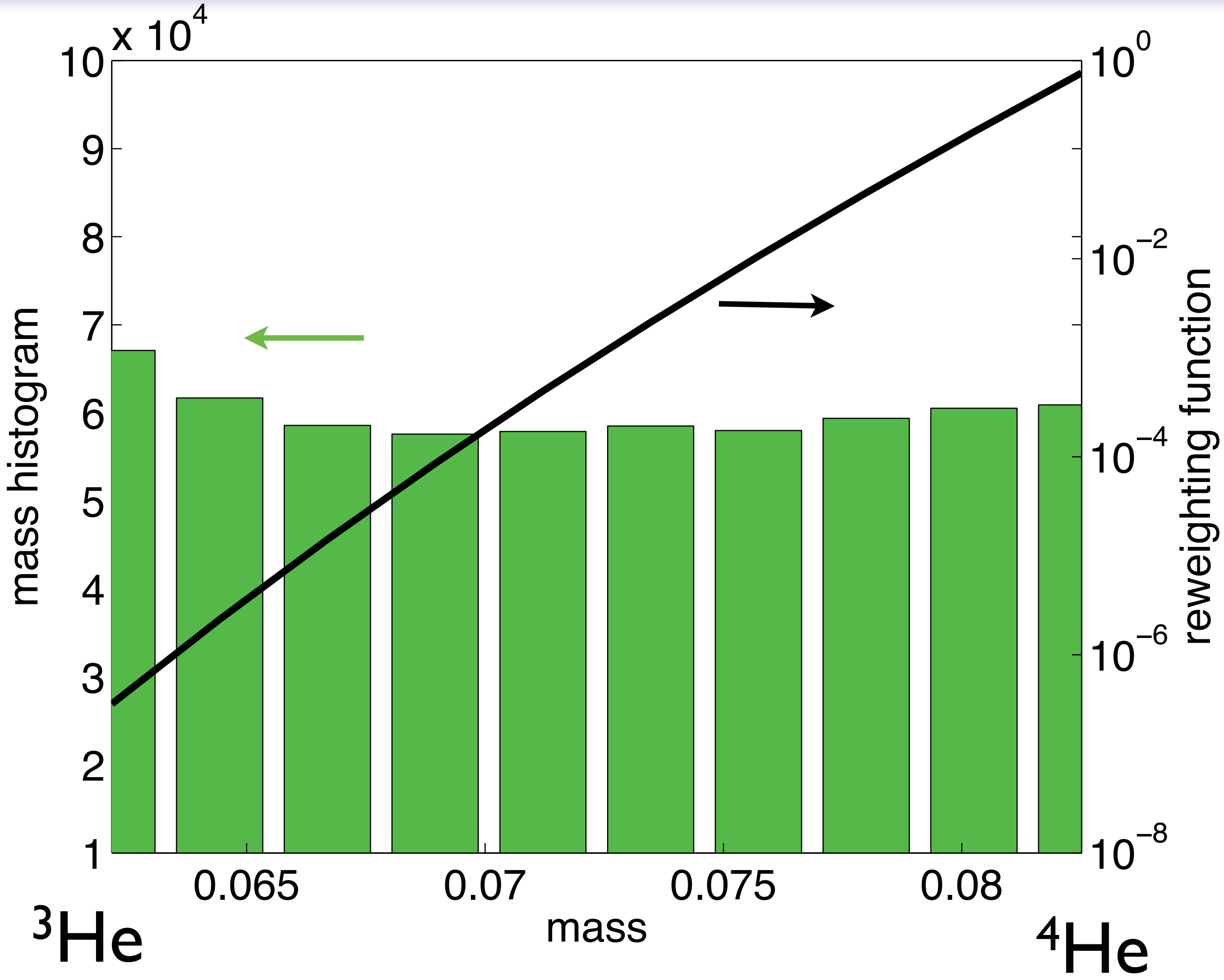
new data from PennState



signatures of phase separation

hysteresis, time dependent

^3He binding to the screw dislocation



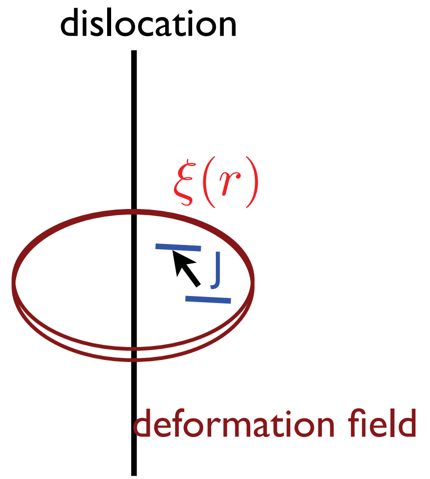
all interactions are given by the bare Aziz potential, no effective interaction for ^3He is assumed

replacing ^4He by ^3He has a too low acceptance ratio

solution : gradual mass reweighing, make the histogram flat and measure only in the 3He sector

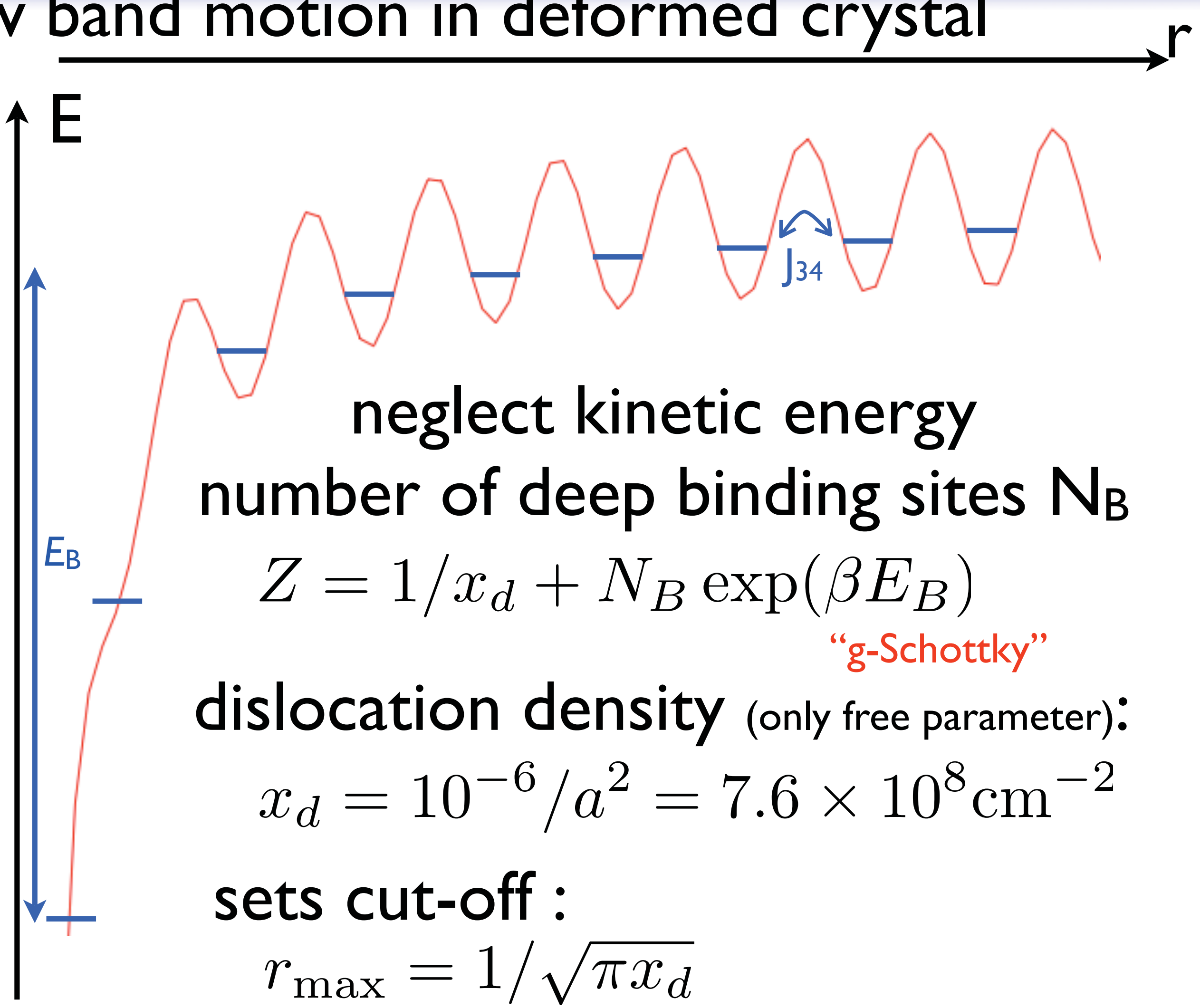
binding mechanism, T < 0.8K

narrow band motion in deformed crystal



$$u_z(r,\phi) = \frac{b\phi}{2\pi}$$

$$\tau_r = -\frac{\mu b}{2\pi r}$$



neglect kinetic energy

number of deep binding sites N_B

$$Z = 1/x_d + N_B \exp(\beta E_B)$$

"g-Schottky"

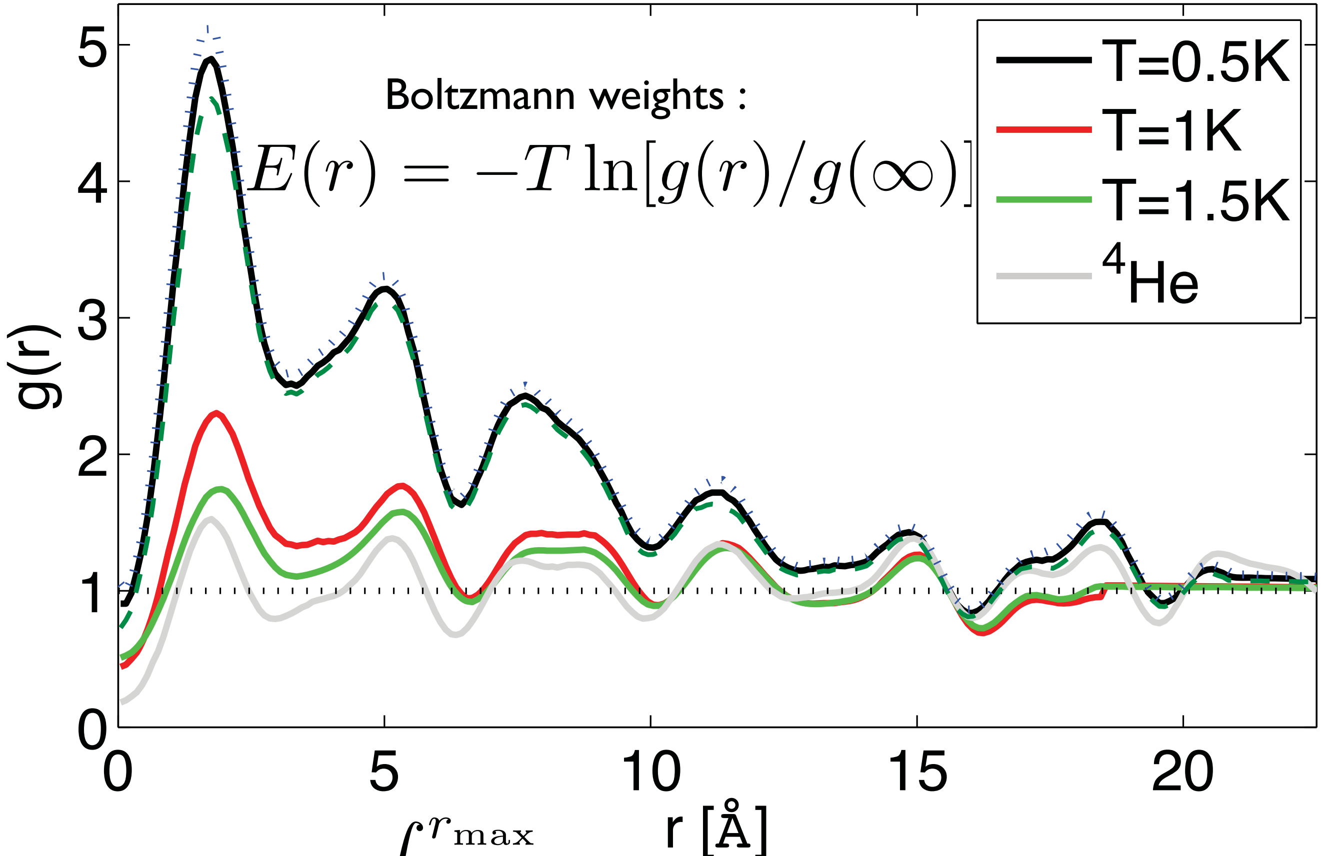
dislocation density (only free parameter):

$$x_d = 10^{-6}/a^2 = 7.6 \times 10^8 \mathrm{cm}^{-2}$$

sets cut-off :

$$r_{\max} = 1/\sqrt{\pi x_d}$$

^{3}He binding to the screw dislocation



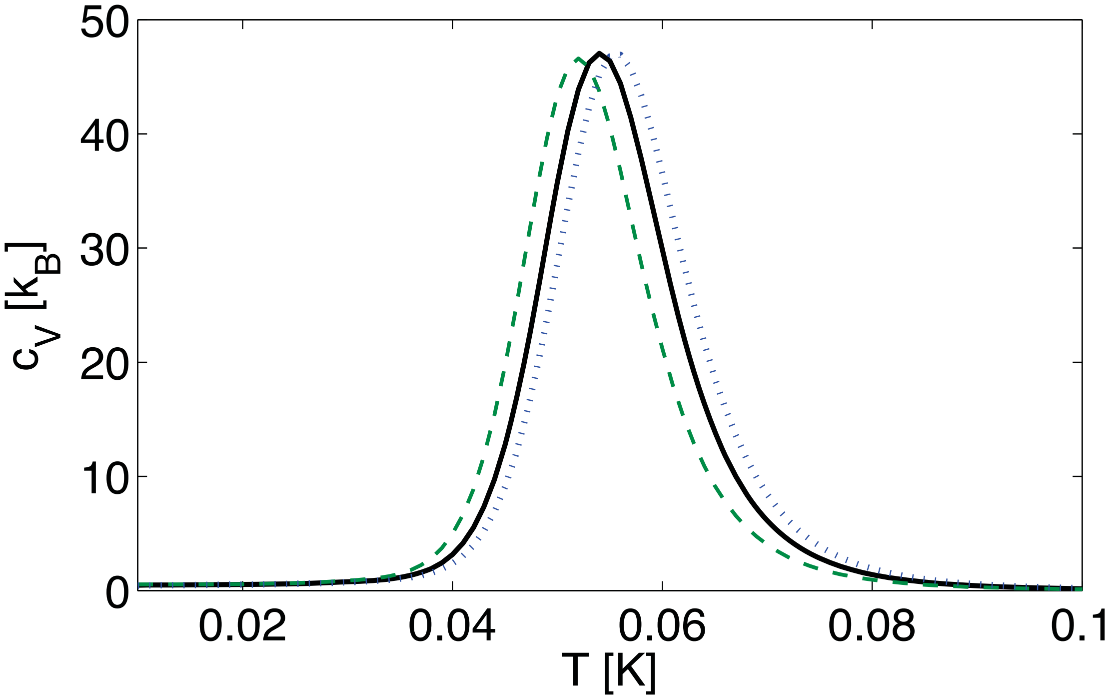
$$Z(T) = 2\pi \int_0^{r_{\max}} r \exp(-E(r)/T)dr$$

$$E_B \approx -T \ln[g_{\max}/g_\infty] = 0.8 \pm 0.1\text{K}$$

self-consistent for all temperatures

g-Schottky anomaly

at much lower $T \leq T_F$:
different behavior



scales with 3He concentration binding to the dislocation

$$T_{\max} \approx \frac{E_{\mathrm{B}}}{\ln(1/N_B x_d)}$$

$$\approx 55\mathrm{mK}$$

assumed dislocation density

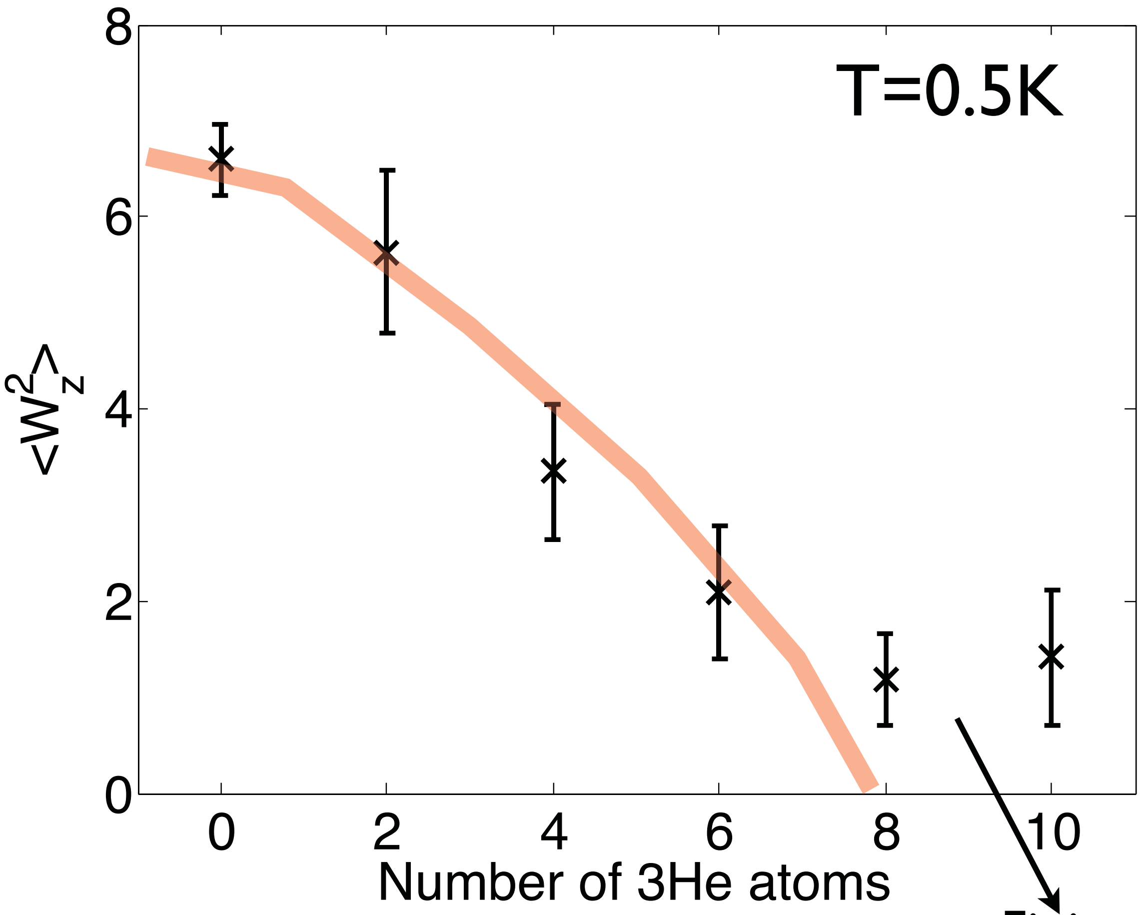
$$x_d = 10^{-6}/a^2 = 7.6 \times 10^8 \mathrm{cm}^{-2}$$

only *logarithmically* dependent on x_d

$$S \approx \log x_d = \int_0^{T_{\mathrm{high}}} \frac{C}{T'} dT'$$

$$c_V^{\max} \approx \log x_d \frac{T_{\max}}{\Delta T} \approx 40\mathrm{k_B}$$

Blocking the superfluid path



Finite size effects
1d systems

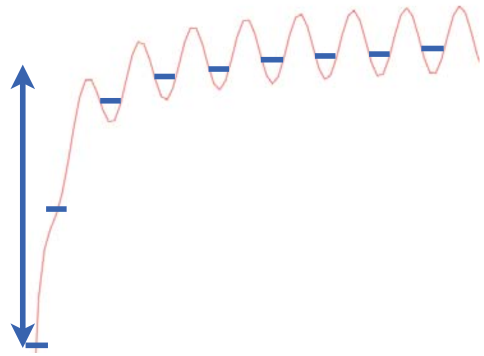
^{3}He is very hot vs. Fermi temperature and behaves mostly like a 'Boltzmannon'. Very small sign problem.

quantum diffusion/ relaxation problem

thermodynamics so far!

Problems :

- spin diffusion T-independent, 0.5K < T < 0.8K, ballistic motion ⟷ binding
- level spacing due to strain of screw is much larger than the bandwidth of the ^{3}He : how can the ^{3}He get closer to the core?



slow kinetic relaxation,
quantum diffusion problem

incoherent one-phonon assisted hopping is dominant at *large* distances and low temperatures (assume fixed the dislocation)

$$\tau^{-1} = J_{34}^2 \xi^2 T / \Theta_{\mathrm{D}}^4 \qquad \xi = a(dE/dr) \gg zJ_{34}$$

(~many years)

⟶ time dependent effects (cf. specific heat)

conclusion

The ‘*homeopathic*’ role of ^{3}He is now better understood:

indisputable result when thermodynamics are valid, but connection with experiment might be unclear

- Binding of ^{3}He to a screw dislocation
- E_B = 0.8(1) K , Tmax = E_B / log(disloc.dens. x # binding sites)
- produces bump in specific heat around 60 mK through mapping on a Schottky model with *degenerate* levels
- produces stiffening in the same temperature range
- quantum diffusion problem, slow relaxation
- in line with most recent (?) NMR data for spin diffusion coefficient at low temperature
- other mechanisms for dislocation transitions/crossovers at lower temperature?
- link with NCRIF in torsional oscillators is unclear, there is no known model/experiment that relates ^{3}He to dislocations during crystal growth, ... → sample quality influence unknown, link with Shevchenko state unclear