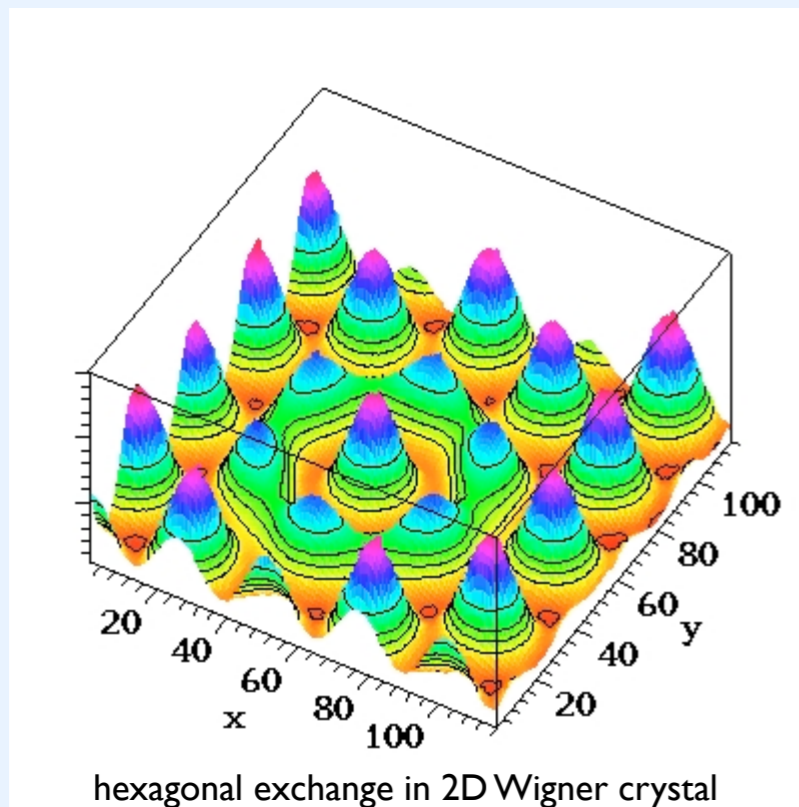


# Ring Exchanges in a Perfect solids of $^4\text{He}$

*David Ceperley, NCSA, UIUC, USA*

*Bernard Bernu, LPTMC(LPTL), CNRS-Paris VI*



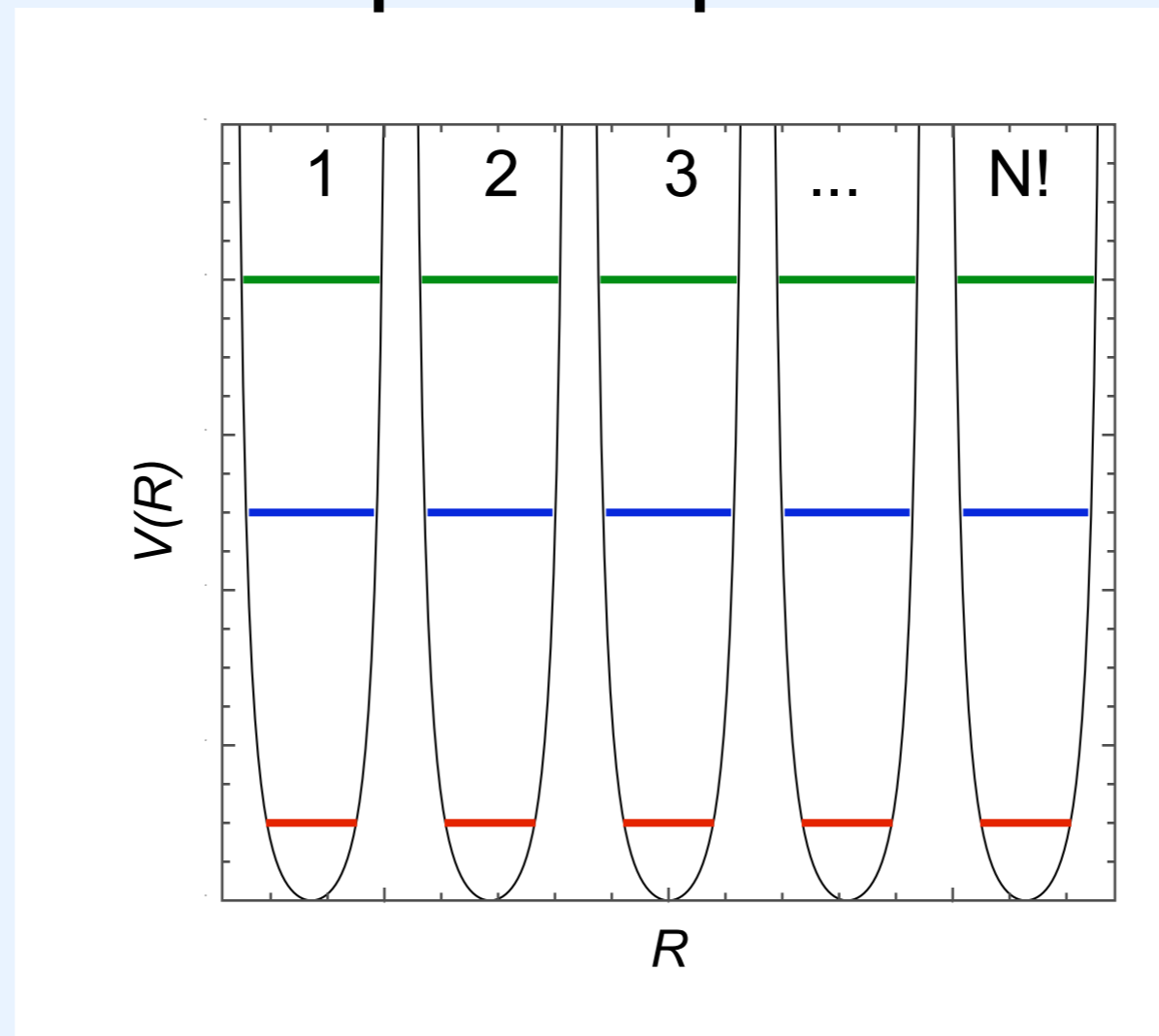
Ring Exchanges are  
Evaluated by PIMC

# outline

- Thouless Theory:
  - For spin  $1/2$  fermions
  - Extension to bosons
- Exchanges of  $n$  particles:
  - Energies **decrease exponentially** with  $n$
  - Number **increases exponentially** with  $n$
- Large  $n$  extrapolation

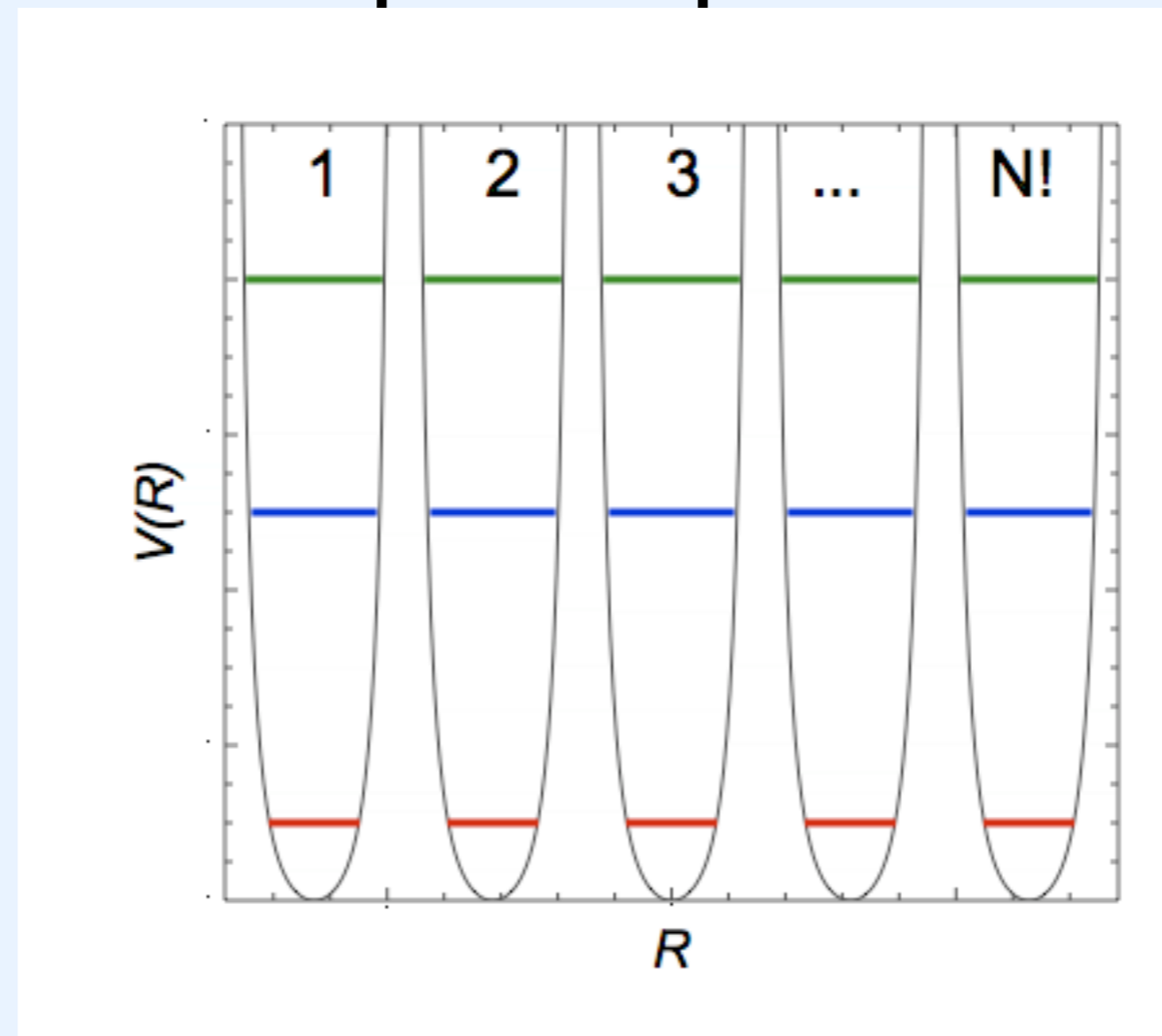
# Thouless Theory (I)

- $N!$  potential wells in phase space



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- $N!$  potential wells in phase space



← phonons, ...

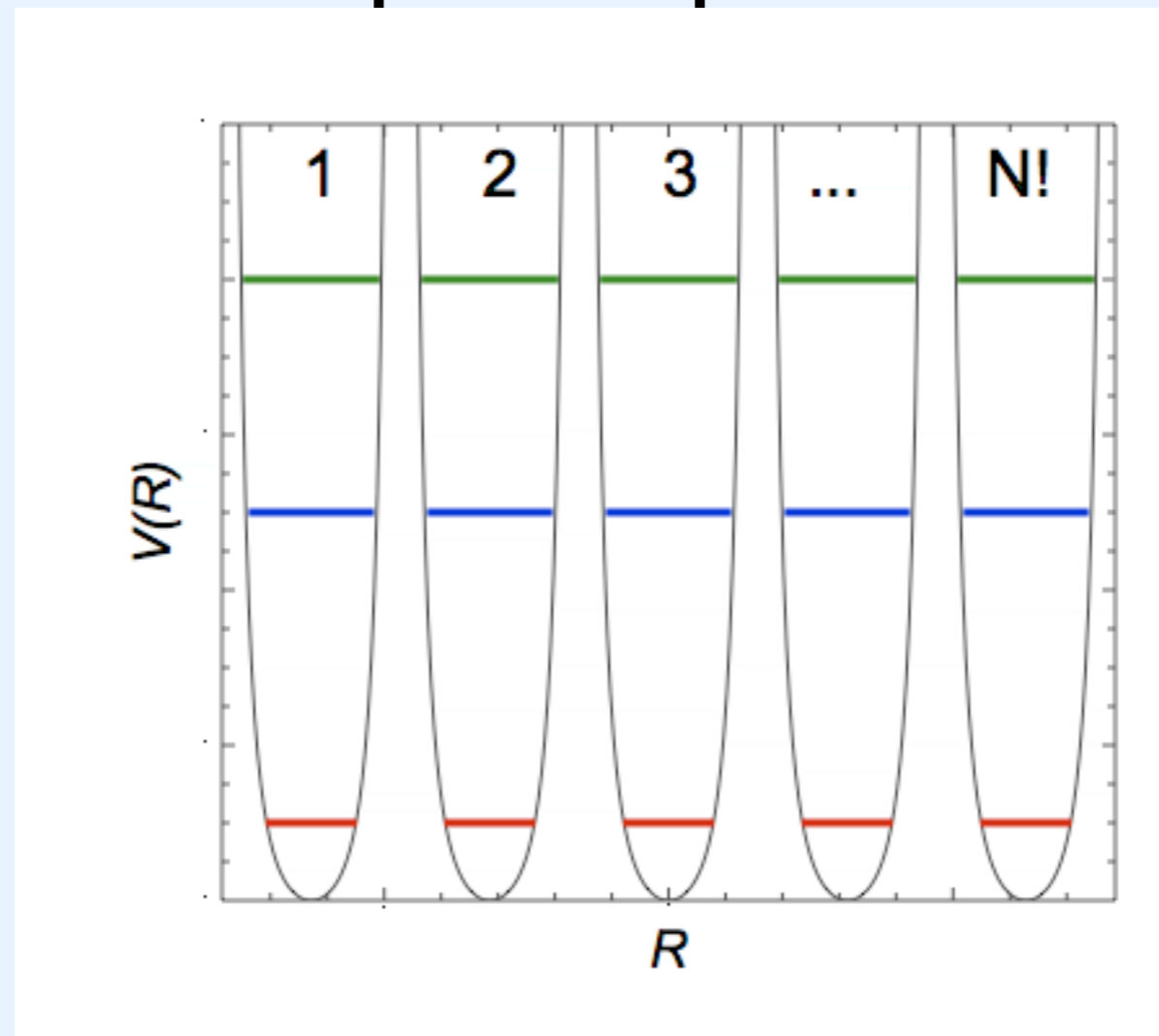
←

← groundstate manifold



# Thouless Theory (I)

- $N!$  potential wells in phase space



← phonons, ...

← groundstate manifold

- Which states to keep depends on spin particles?

# Thouless Theory (II)

- wave function :  $\Psi(R, S) = \Psi(R)\Psi(S)$
- $\Psi(R)$  ground state : symmetric
- spin 1/2 :  $\Psi(S)$  antisymmetric

$$N! \longrightarrow 2^N$$

$$H(S) = - \sum_P (-1)^P J_P \hat{P}(S)$$

# Exchange in fermionic solids

Thouless Theory: spin degrees of freedom decoupled from space degrees of freedom

Free spins : phonons ( $\sim T^D$ )

“Frozen” phonons spin exchanges

$$H^{\text{eff}} = - \sum_P (-1)^P J_P P$$

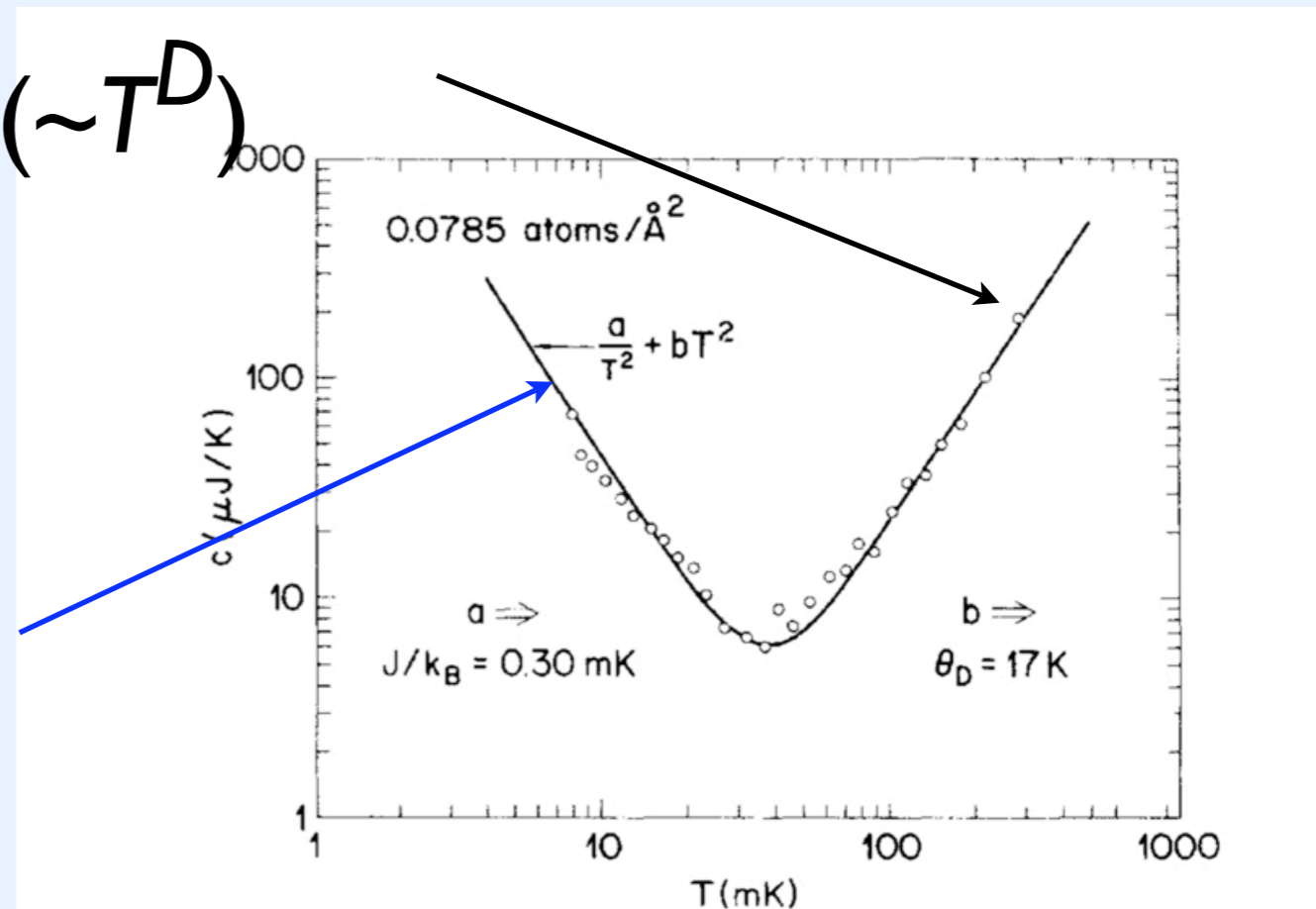


FIG. 8. Log-log plot of the heat capacity of an incommensurate solid  $^3\text{He}$  monolayer. Below 30 mK the heat capacity is dominated by the nuclear spins and at higher temperatures by the phonons.

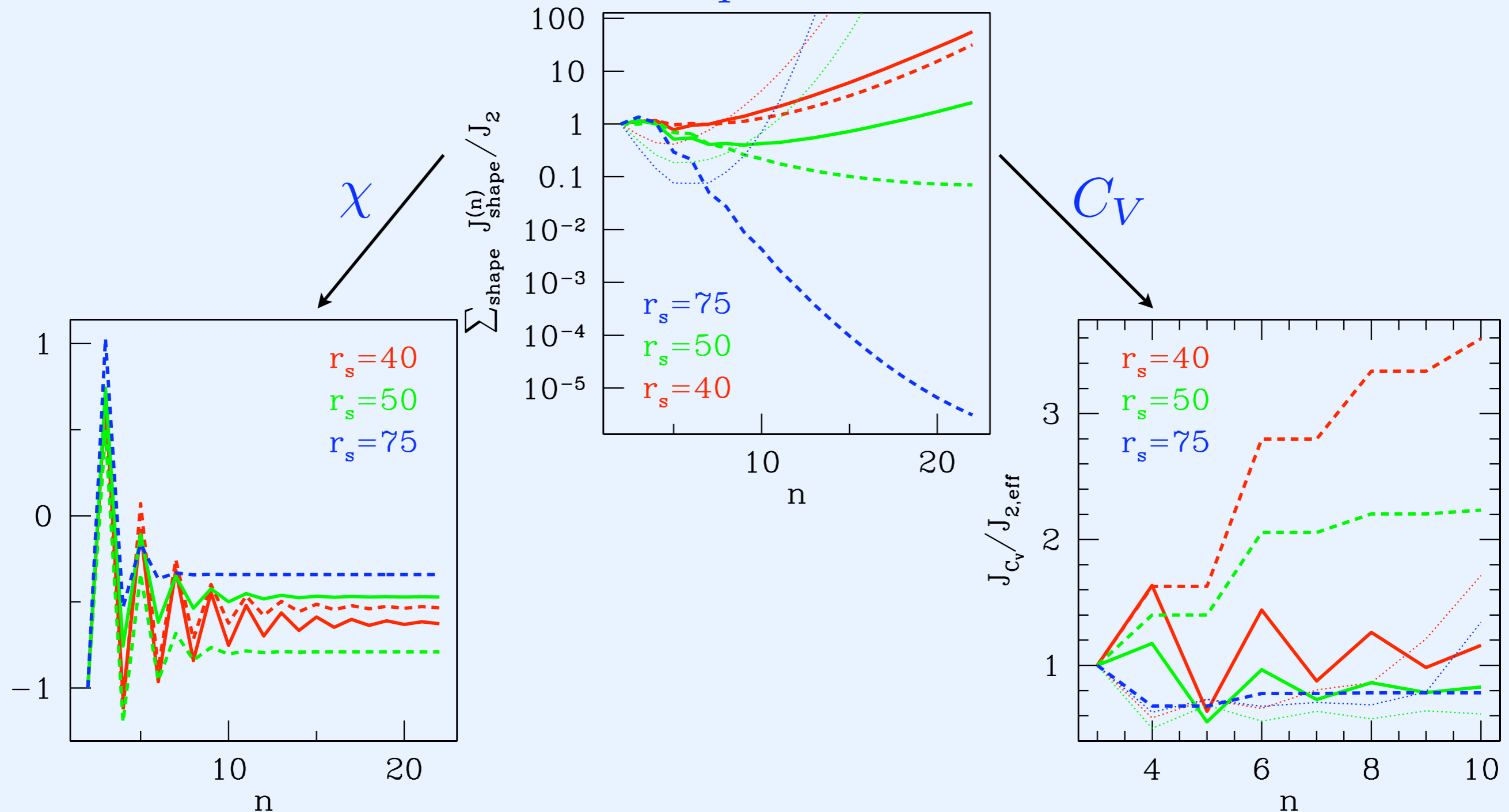
$^3\text{He}$  on graphite (D. Greywall, PRL 1990)

# Exchange in fermionic solids

Wigner crystal in two dimension:

Bernu, B. and D. M. Ceperley *cond-mat/0310309, J. Phys.: Condens. Matter* 16 (2004) p701-707

$$H^{\text{eff}} = - \sum_P (-1)^P J_P P$$





# Thouless Theory (II)

- wave function :  $\Psi(R, S) = \Psi(R)\Psi(S)$
- $\Psi(R)$  ground state : symmetric
- spin 1/2 :  $\Psi(S)$  antisymmetric

$$N! \longrightarrow 2^N \qquad H(S) = - \sum_P (-1)^P J_P \hat{P}(S)$$

- spin 0 :  $\Psi(S)$  symmetric (one single state)

$$\Psi_N(R) = \frac{1}{N!} \sum_P \Psi_{Z_0}(PR)$$
$$\delta E \simeq \sum_{P \neq 1} J_p$$

# Path Integral

- Trotter Formula

$$e^{-\beta(T+V)} = \lim_{M \rightarrow \infty} \left[ e^{\beta T/M} e^{\beta V/M} \right]^M$$

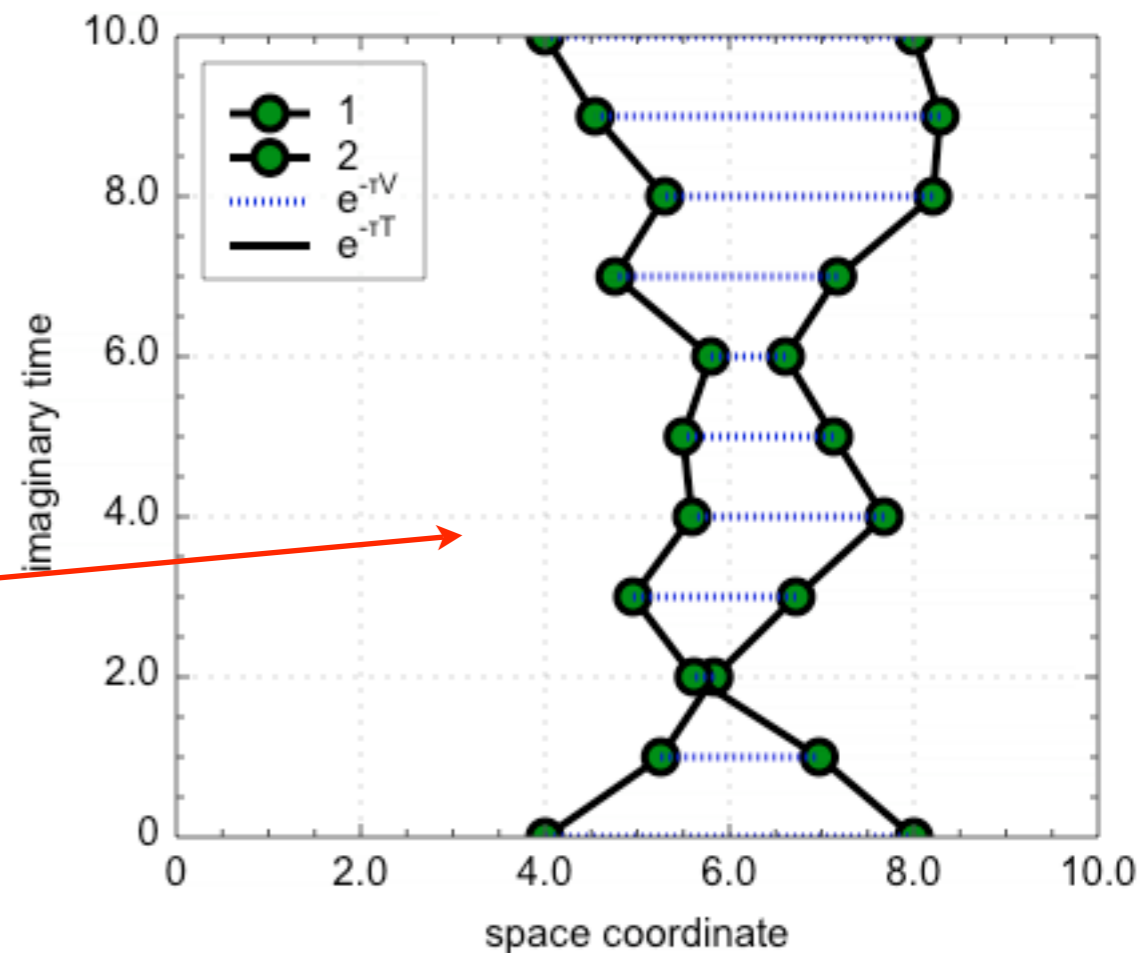
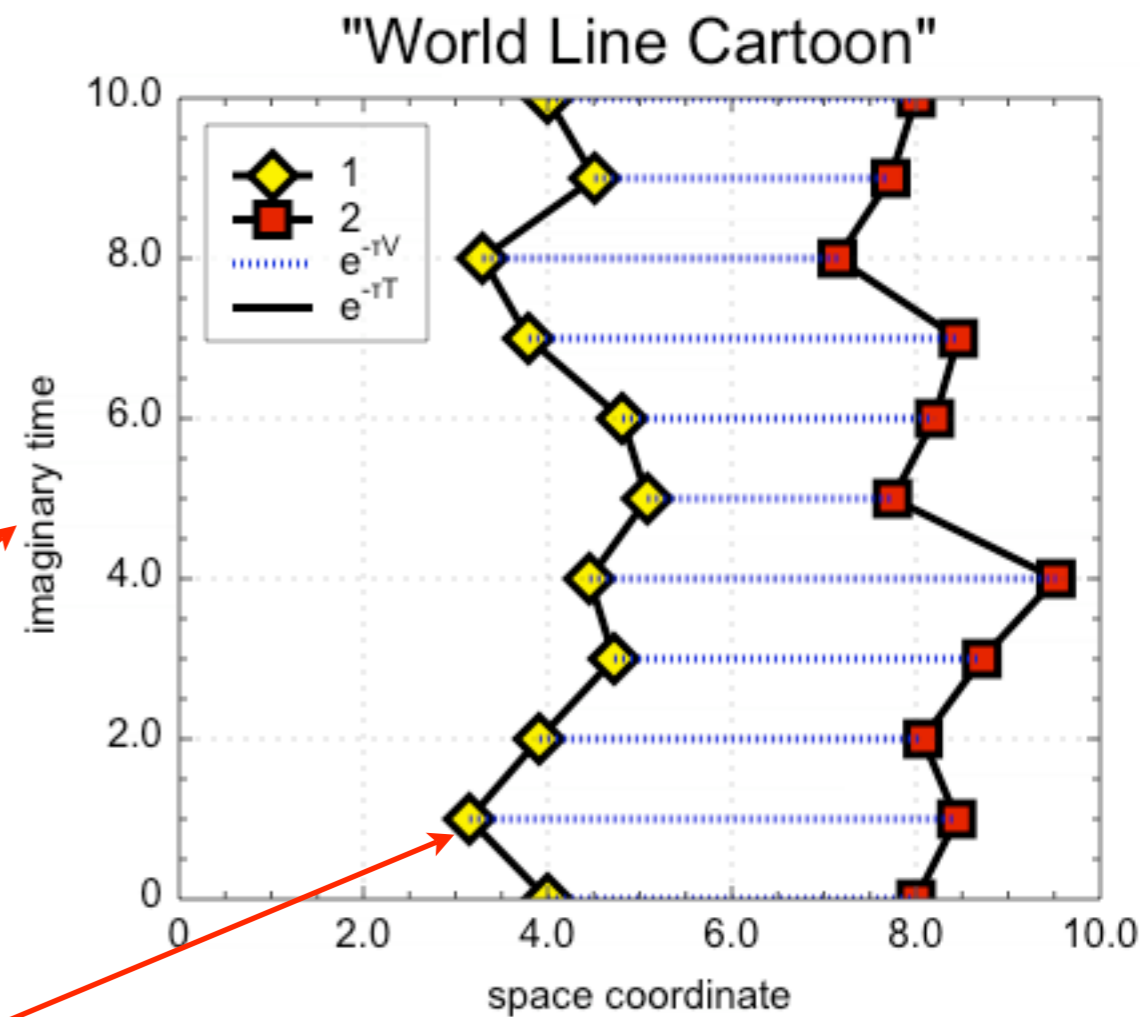
- Exact mapping to a classical system (also true for bosons and fermions)

- a particle : a polymer

- an exchange of  $p$  particles : one single bigger polymer from

$p$ -polymers

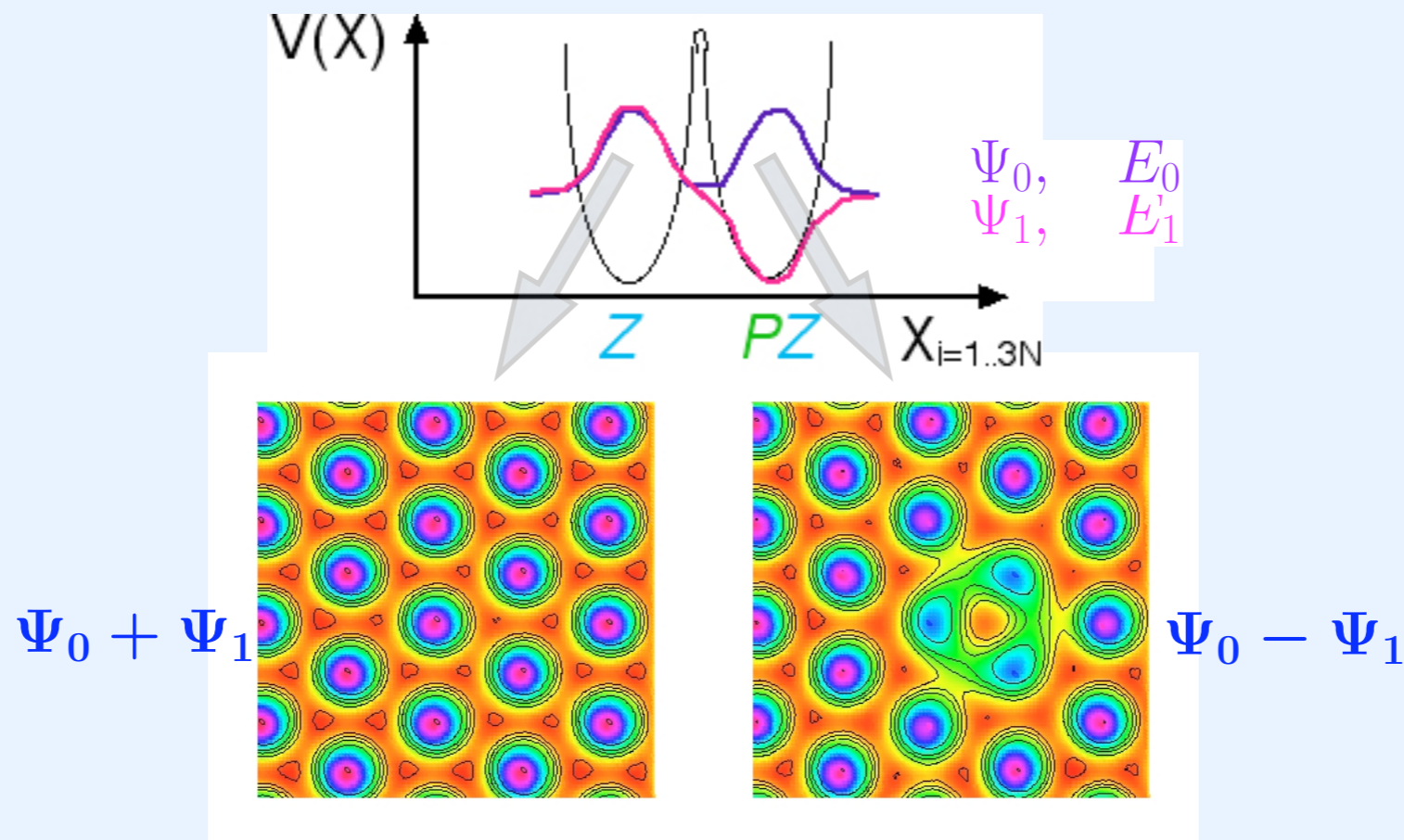
- equilibrium : closed polymers





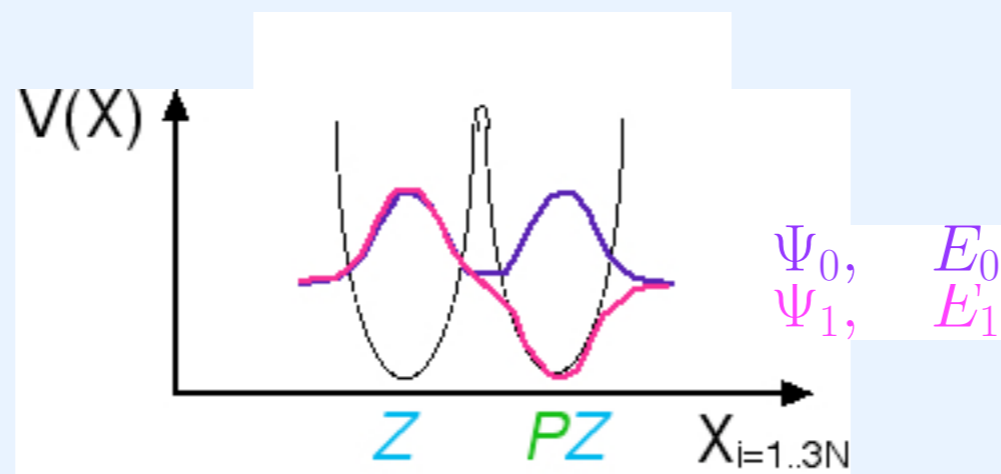
# Thouless theory : from $V(r)$ to $P_{ij}$

- $N!$  wells in configuration space
- For a given  $P$  : 2 wells in configuration space



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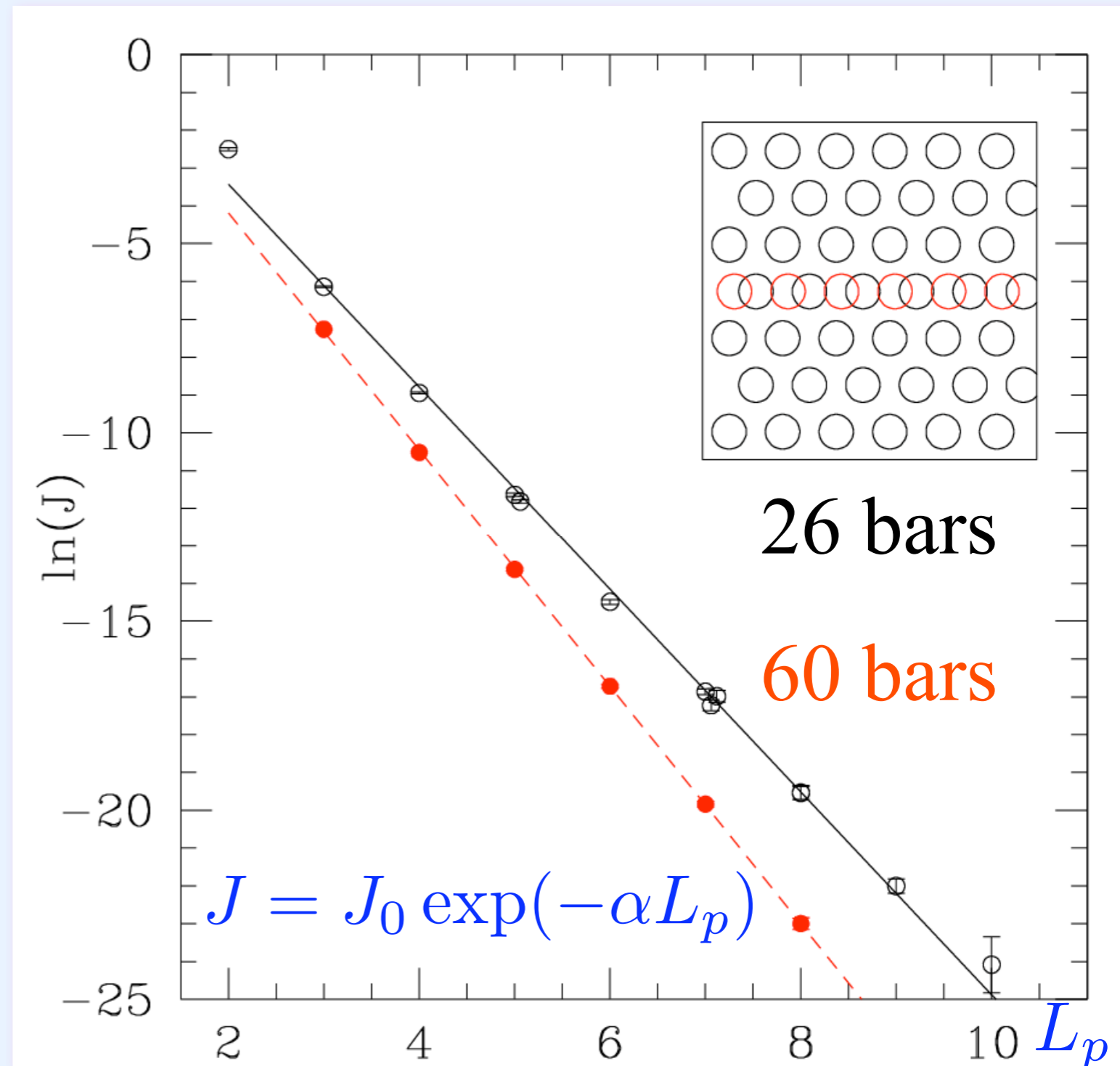


$$F_P(\beta) = \frac{\langle Z | \exp(-\beta H) | PZ \rangle}{\langle Z | \exp(-\beta H) | Z \rangle} = \tanh(J_P(\beta - \beta_0))$$

$$J_P = (E_1 - E_0)/2 \quad \beta_0 = \ln |\psi_1(Z)/\psi_0(Z)|$$

# Feynman-Kikuchi Model

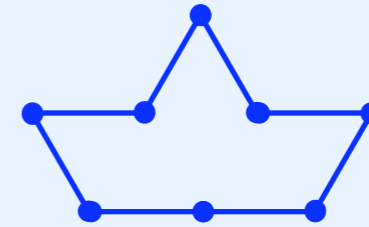
- $J$  decreases exponentially with the cycle length  $L_p$
- linear exchange :



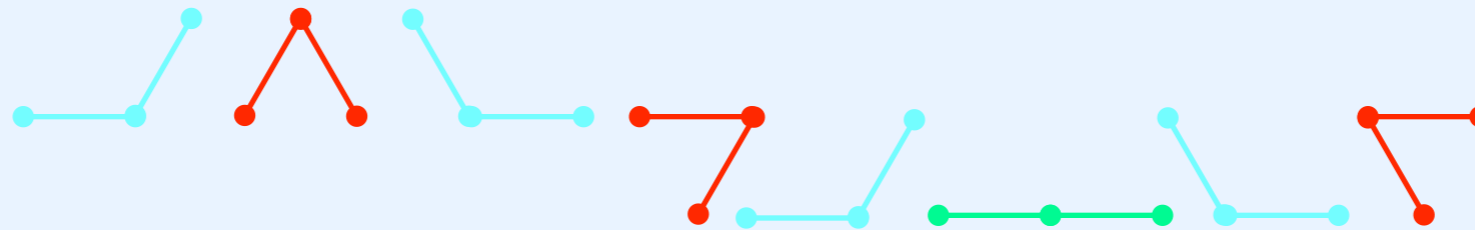
# Geometrical effects:

$$J_{n,s} = e^{\alpha_0 + \alpha_n n + \alpha_p p_s + \sum_v \alpha_v N_{s,v}}$$

- Exchanges do depend on geometry :

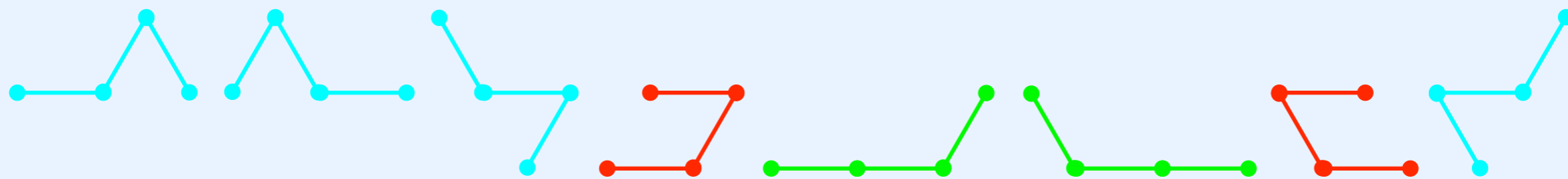


2 links pattern



$$\ln J_{\text{graph}} = 4\alpha_{\text{cyan}} + 3\alpha_{\text{red}} + 1\alpha_{\text{green}}$$

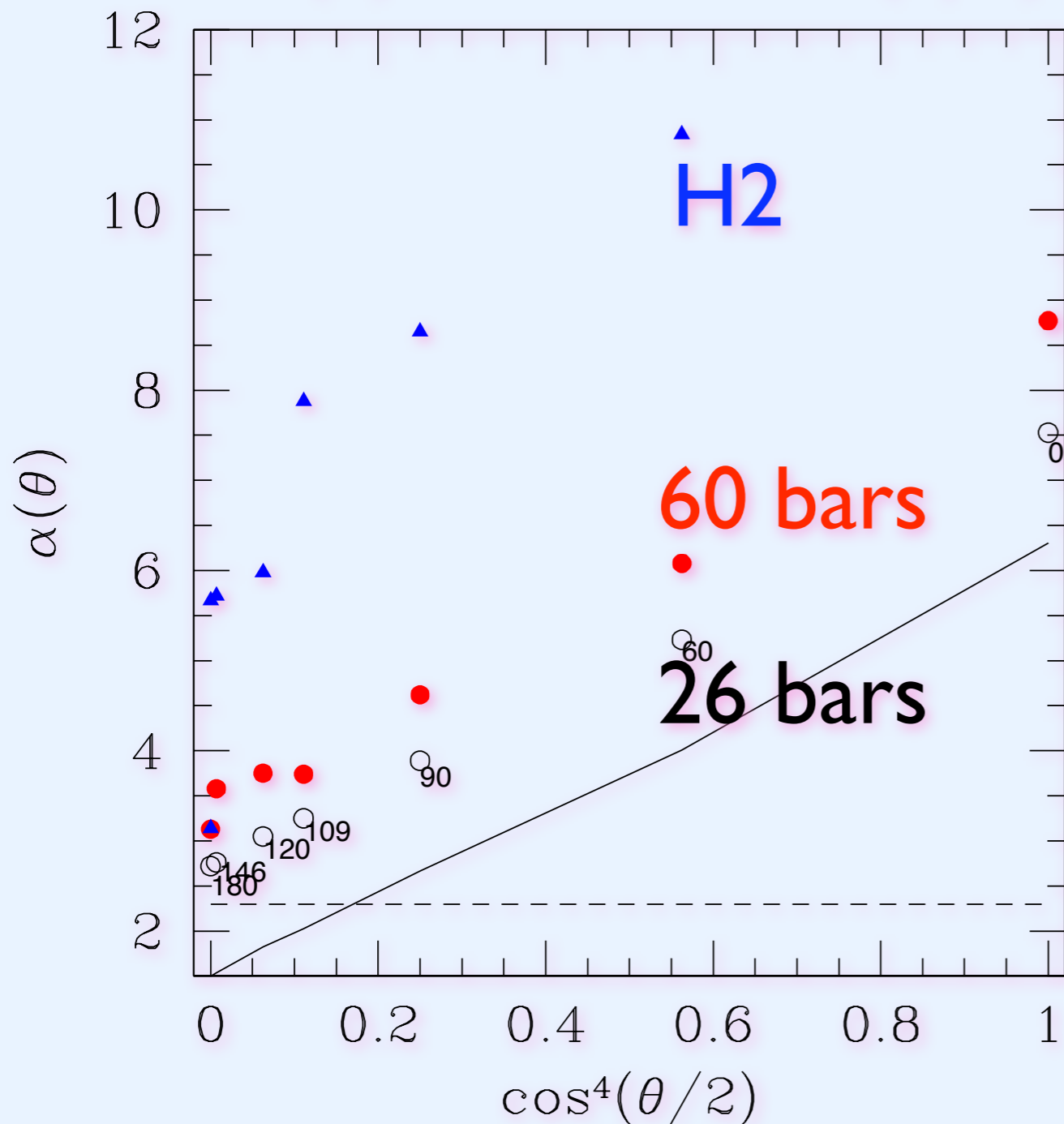
3 links pattern



$$\ln J_{\text{graph}} = 4\alpha_{\text{cyan}} + 2\alpha_{\text{red}} + 2\alpha_{\text{green}}$$

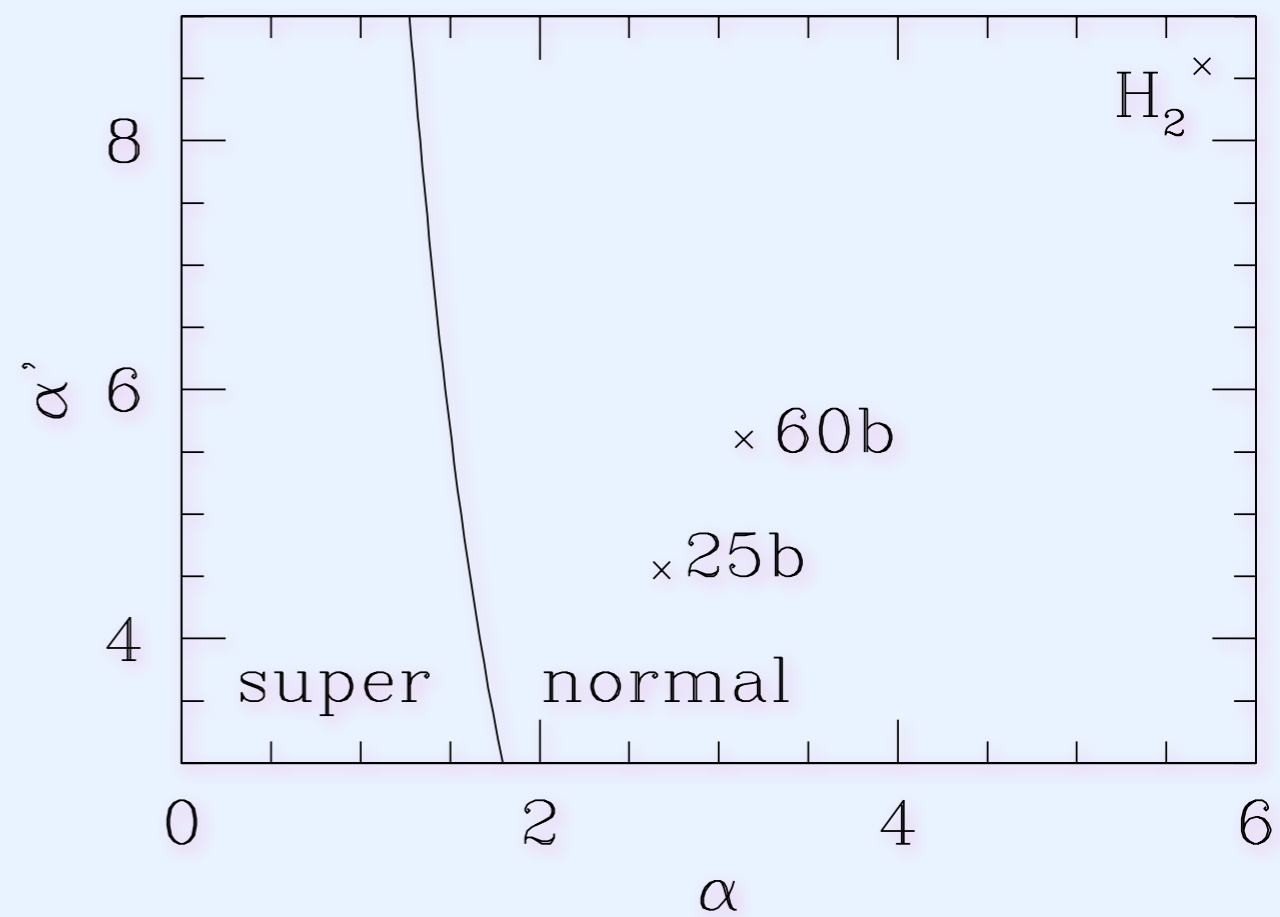
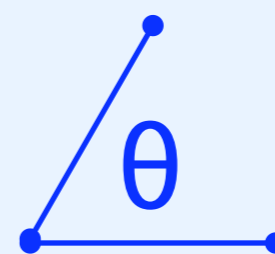
● **Fit:**

$$\alpha(\theta) = \alpha + \alpha' \cos^4(\theta/2)$$



$$J = J_0 \exp \left[ - \sum_{k=1}^{L_p} \alpha(\theta_k) \right]$$

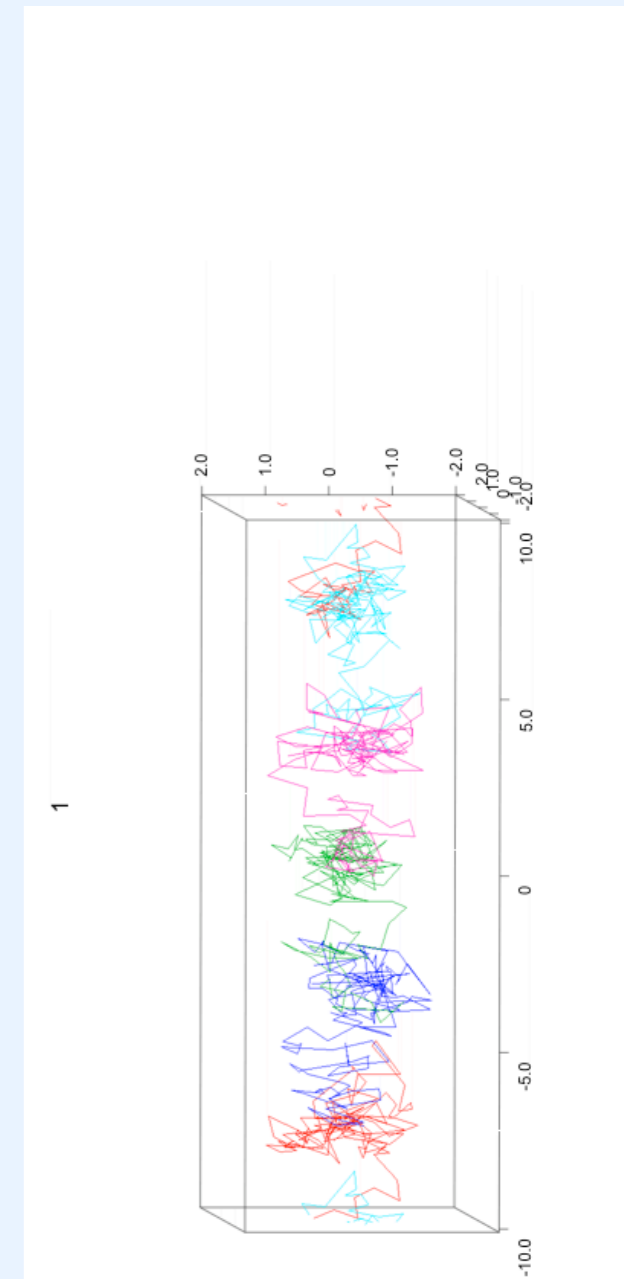
$$J_0 \simeq 7.2K$$





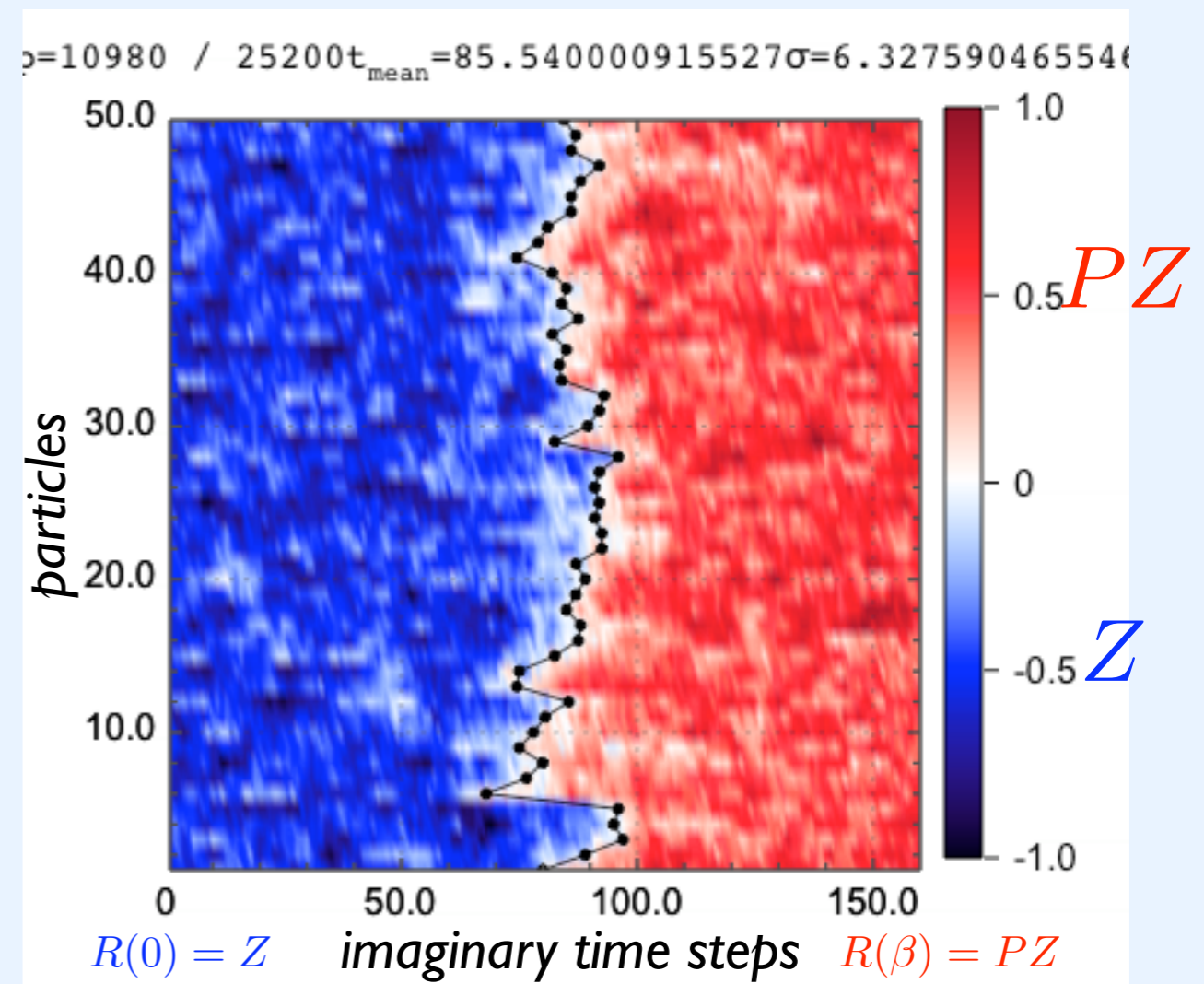
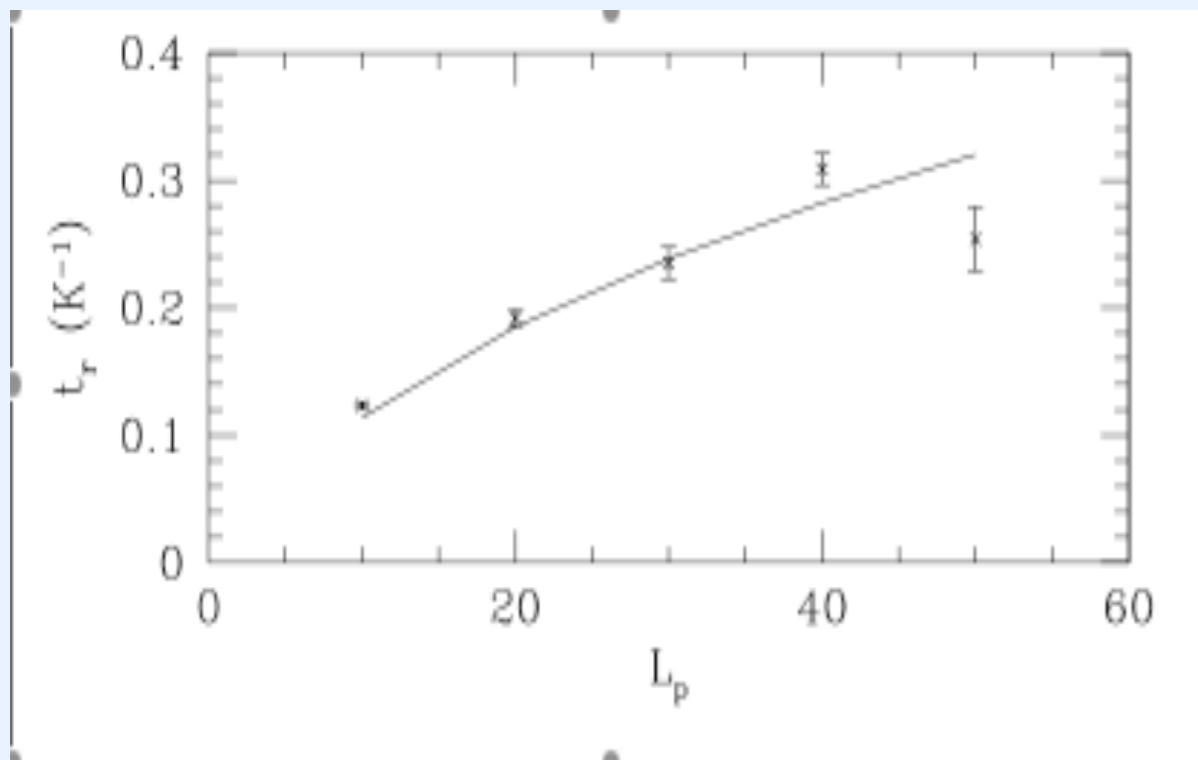
# Exchange Mechanism

- “small” exchanges : all particles “must” exchange at the “same” imaginary time : instanton.



# Exchange Mechanism

- “small” exchanges : all particles “must” exchange at the “same” imaginary time : instanton.
- What happens for longer ring exchanges



# Conclusions

☑ Exchanges are localized in perfect crystal of  $^4\text{He}$

📍 more complicated type of exchanges

> exchange of a few plans

## \* Questions

- In perfect crystals, can exchanges give a supersolid ?

