Title: Quantum Spin Simulations - Lecture 11

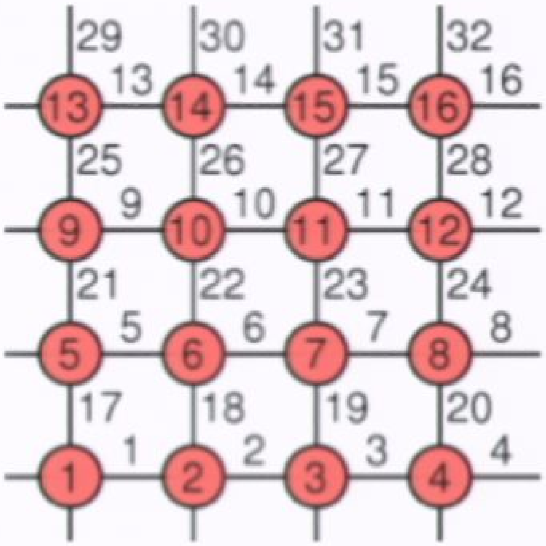
Date: Apr 19, 2010 11:00 AM

URL: http://pirsa.org/10040053

Abstract:

Exact diagonalization of 2D systems (simple square lattice)

- Label lattice sites and bonds
- hamiltonian construction very similar to 1D chains using site and bond maps



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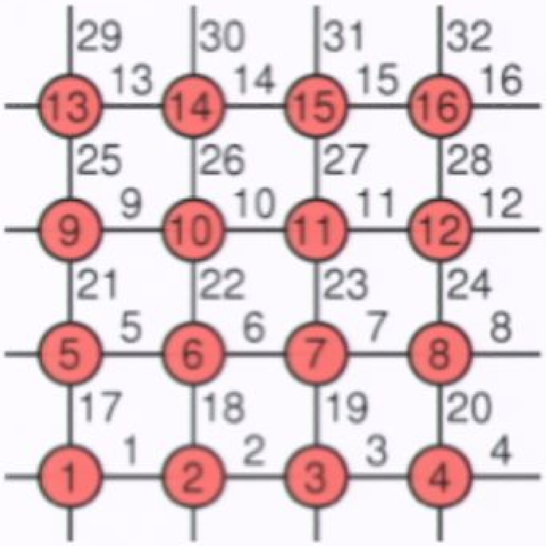

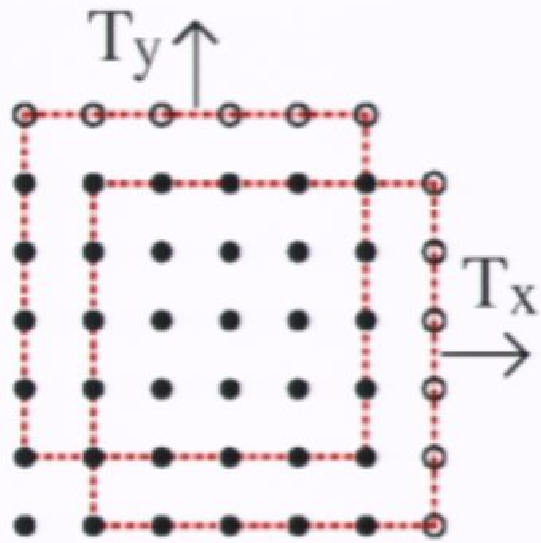

2D momentum states ($L_x \times L_y$ lattice)

$$|a(\mathbf{k})\rangle = |a(k_x, k_y)\rangle = \frac{1}{\sqrt{N_a}} \sum_{x=1}^{L_x} \sum_{y=1}^{L_y} \mathrm{e}^{-i(k_x x + k_y y)} T_y^y T_x^x |a\rangle$$

$$k_\gamma = \frac{2\pi}{L_\gamma} m_\gamma, \quad m_\gamma = 0, 1, \ldots, L_\gamma - 1, \quad \gamma = x, y$$

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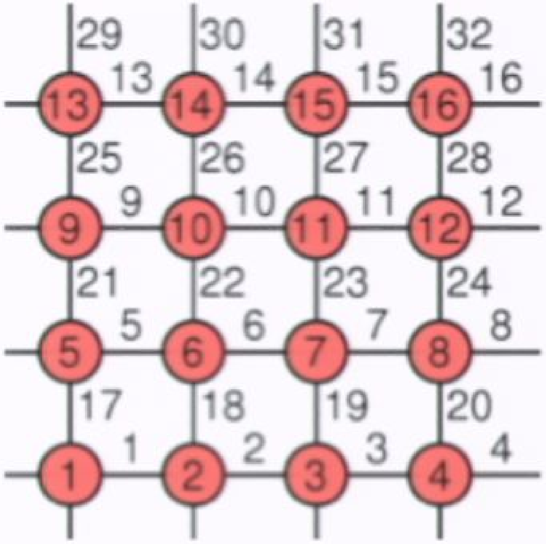

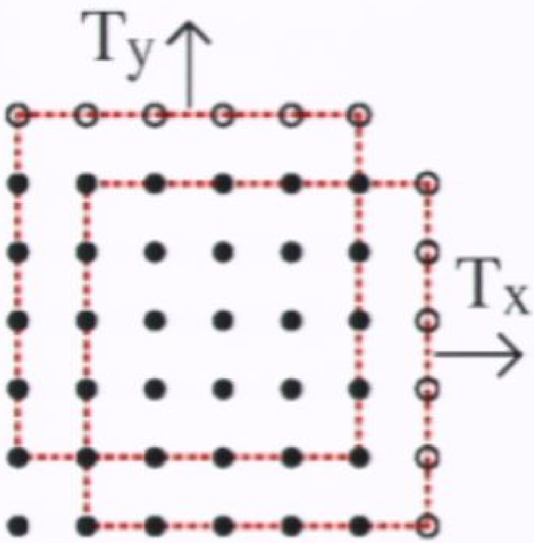

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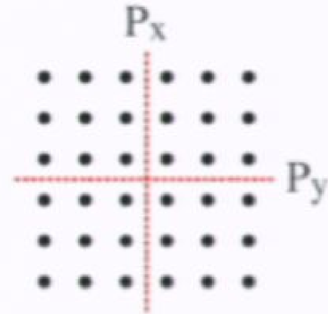
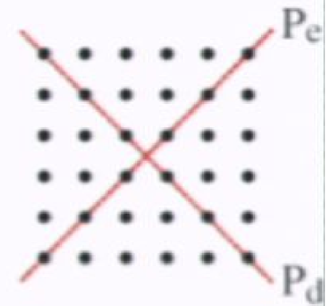
In this case it is very difficult to construct a real-valued basis

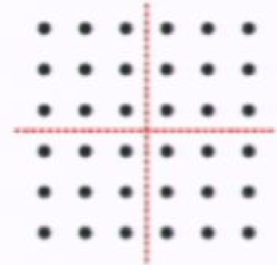
Jsing reflection symmetries (L×L lattice)

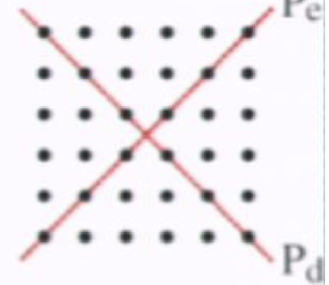




Using reflection symmetries (L×L lattice)

There are 8 different transformations of a square
- combination of reflections and rotations
- can choose the most convenient operations





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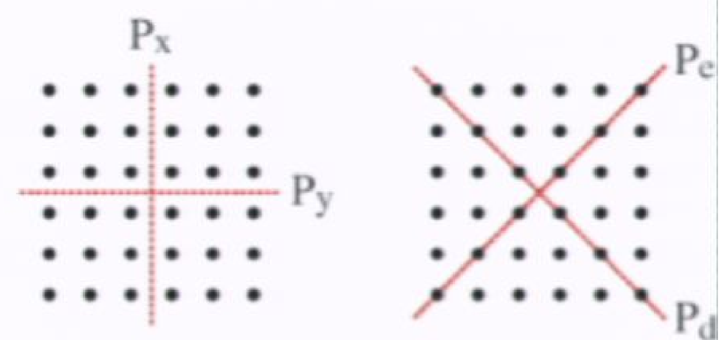

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General form of the momentum state with other symmetries

$$|a^{\sigma}(\mathbf{k}, \{q\})\rangle = \frac{1}{\sqrt{N_a}} \sum_{r_x=1}^{L_x} \sum_{r_x=1}^{L_x} \mathrm{e}^{-i(k_x x + k_y y)} T_y^{r_y} T_x^{r_x} Q |a\rangle$$

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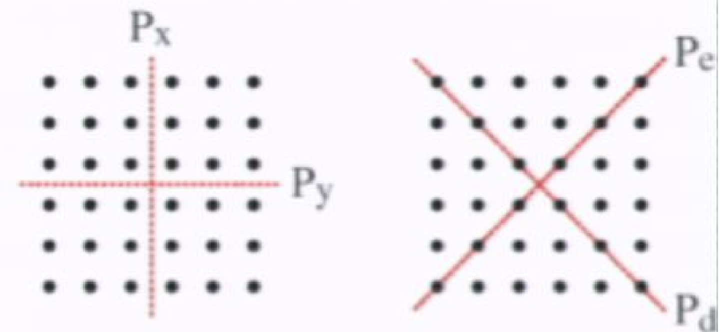

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Using three reflections; P_x, P_y, P_d

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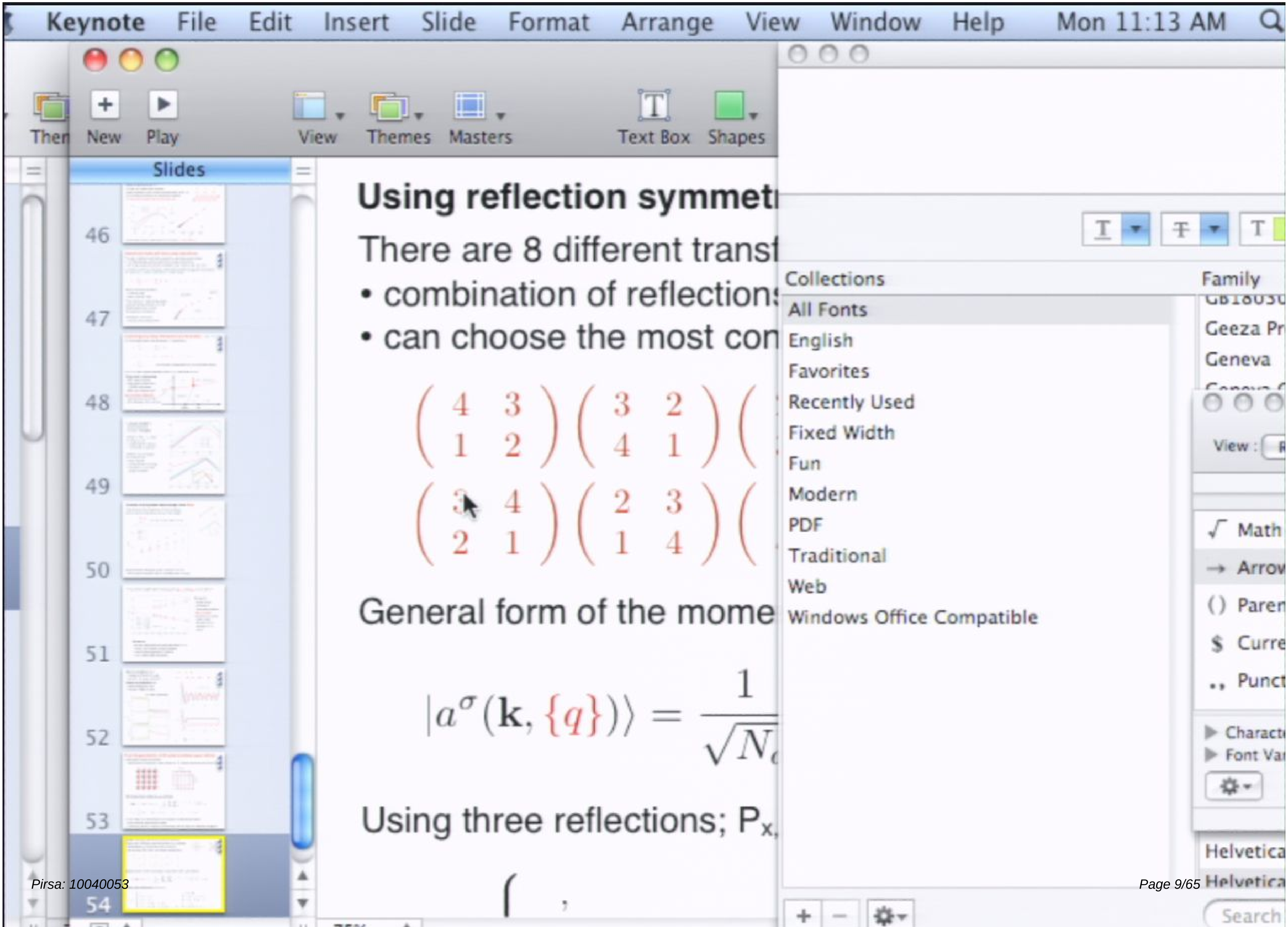
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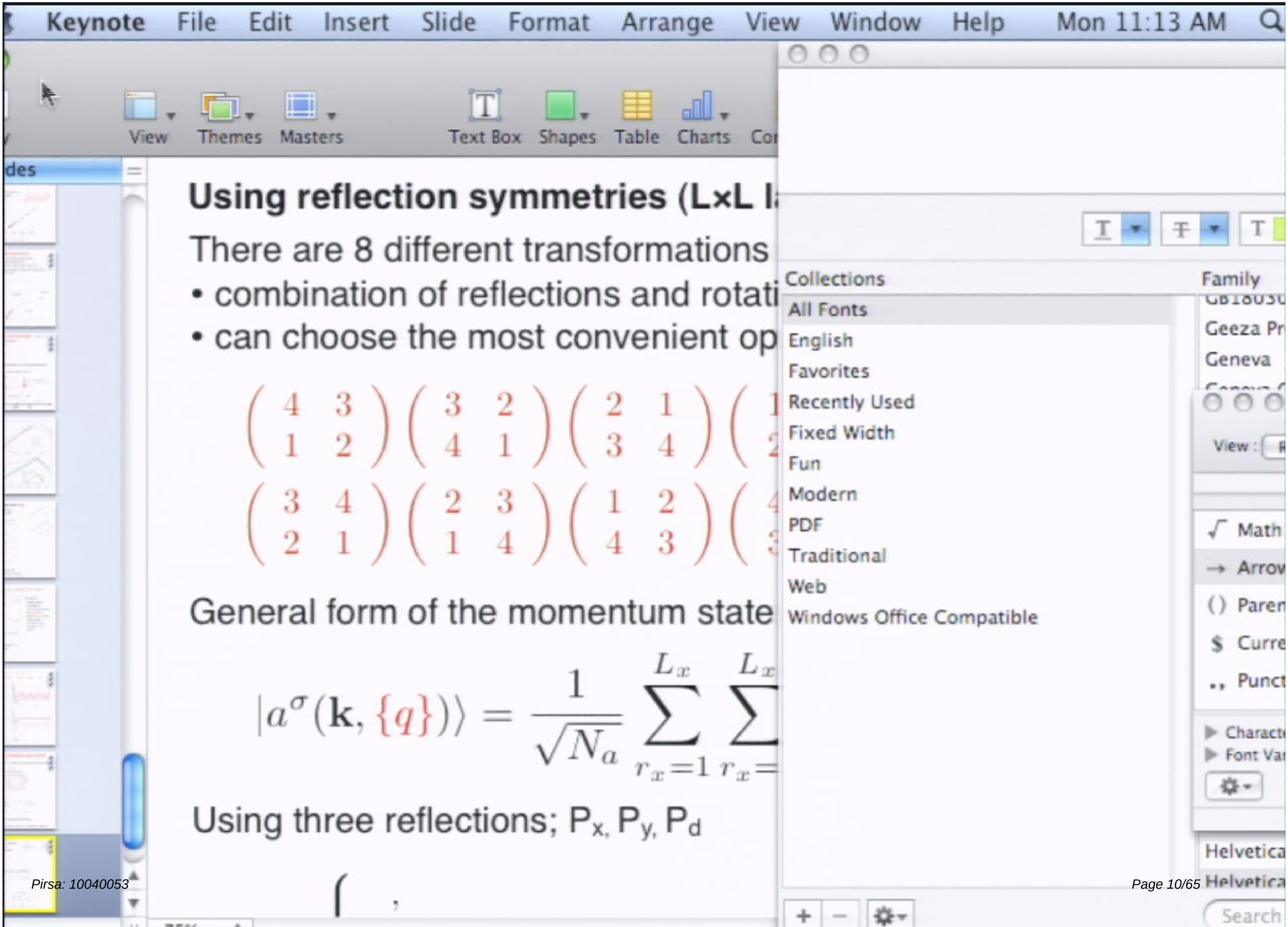
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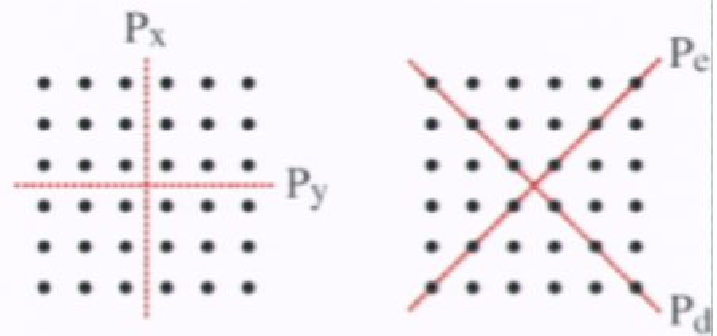

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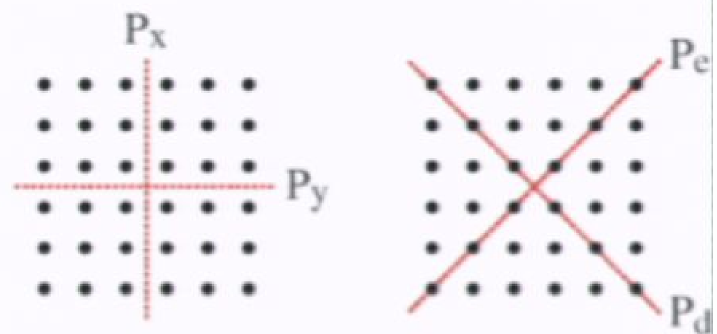

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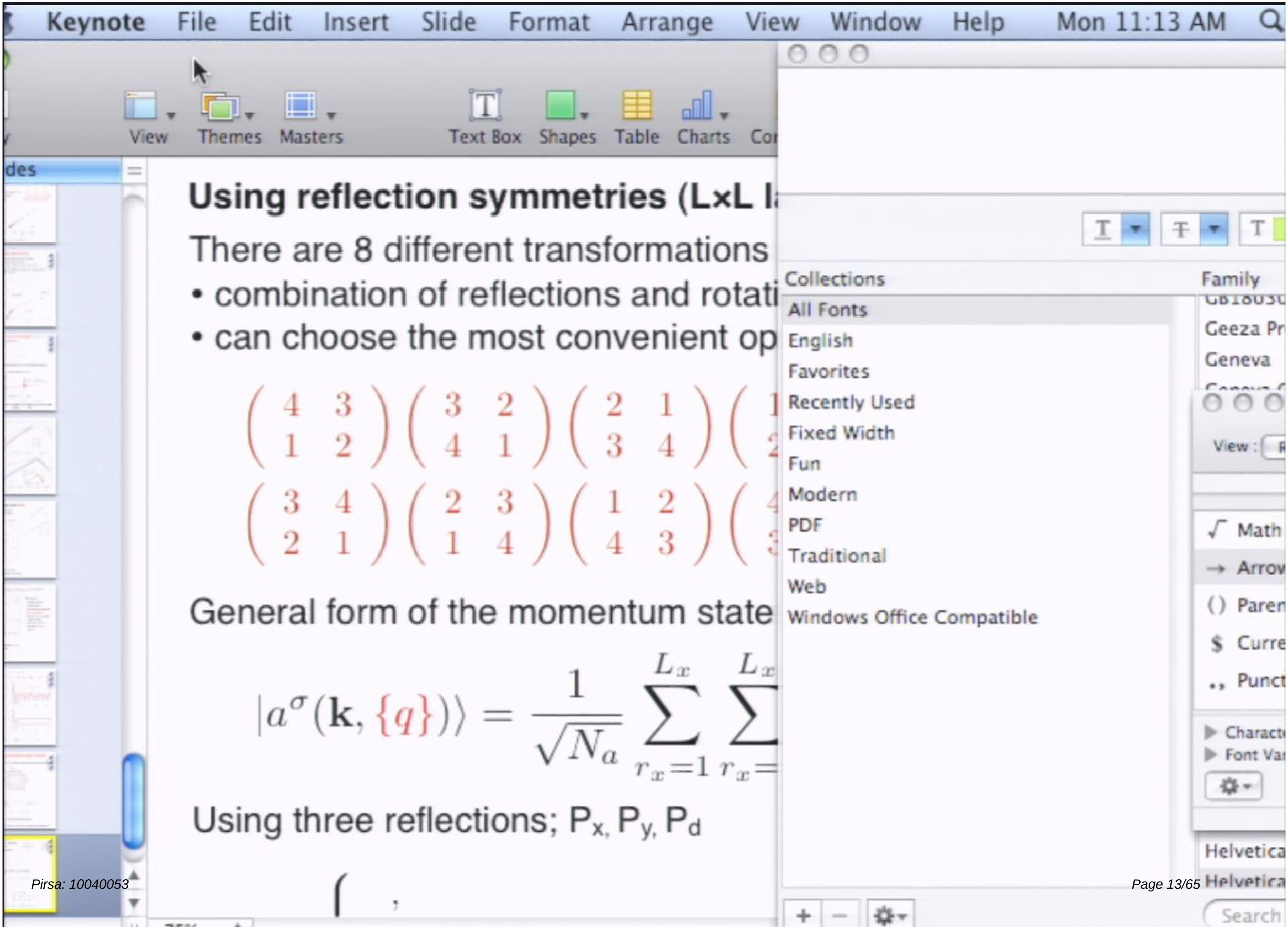
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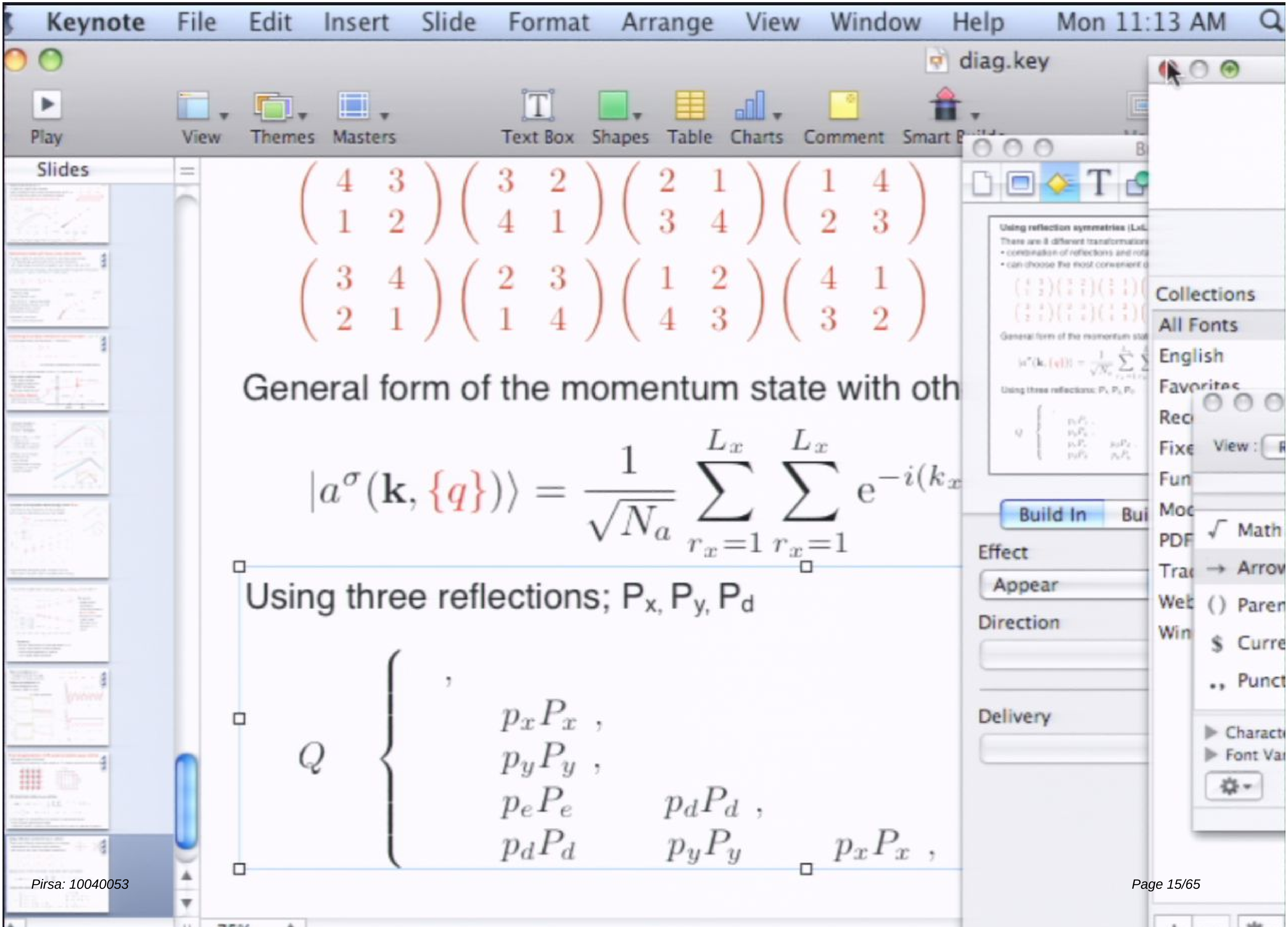
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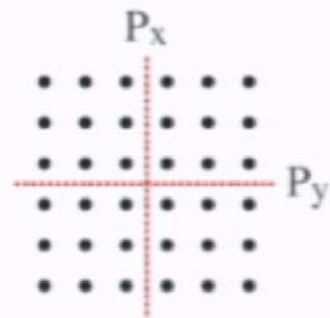

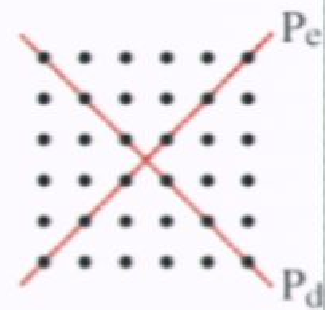

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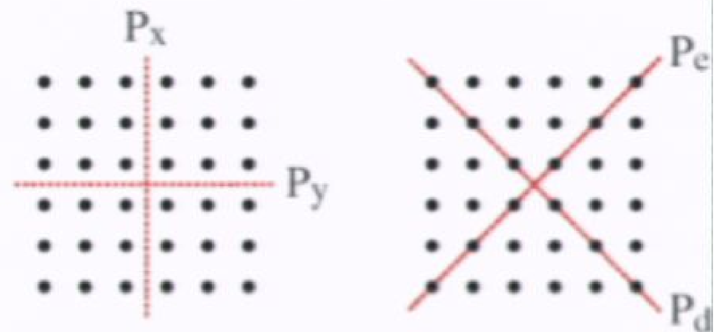

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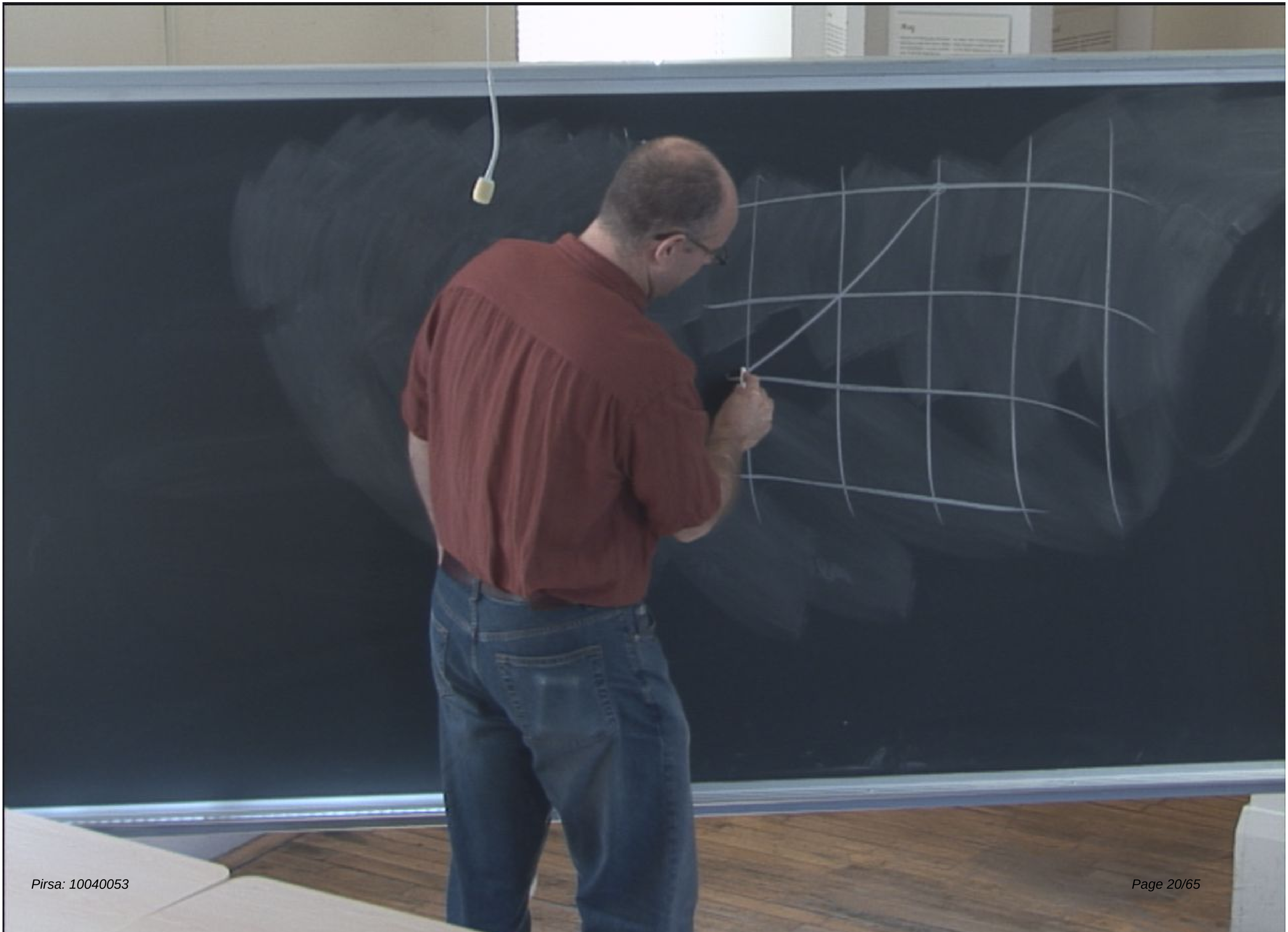
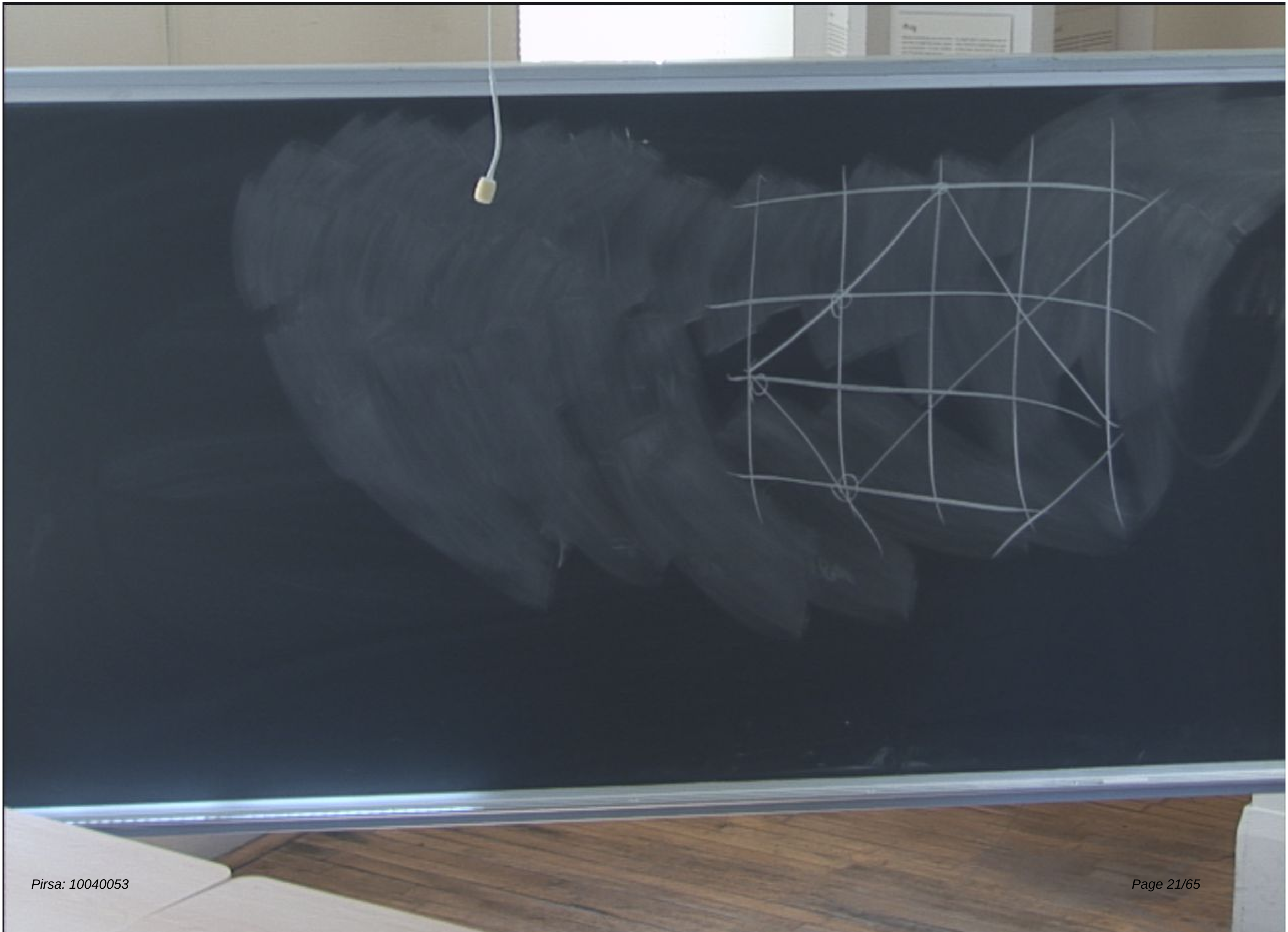
Lanczos results for the 2D Heisenberg model

Ground state and lowest spin-S excitations on 4×4 and 6×6 lattices





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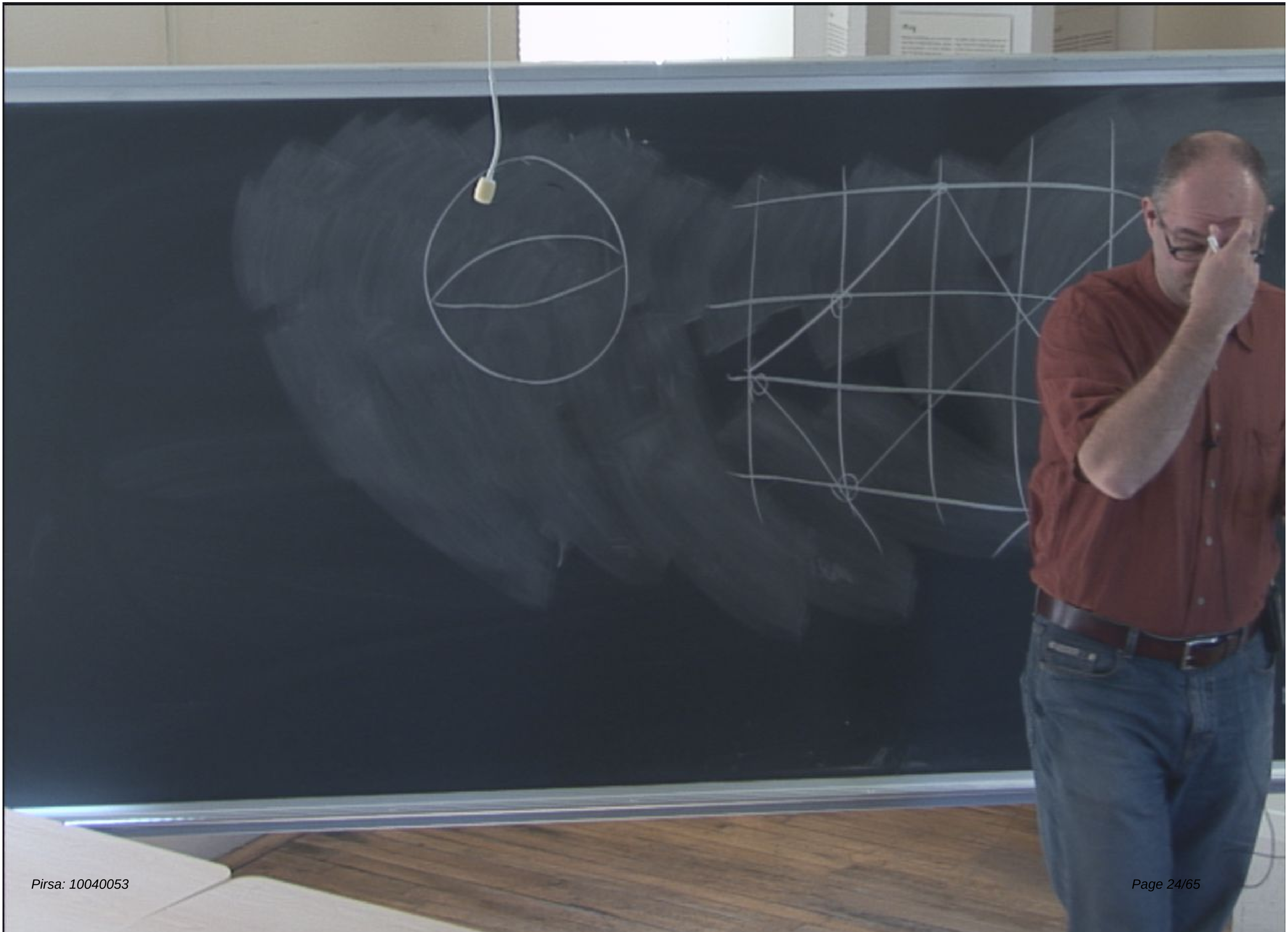
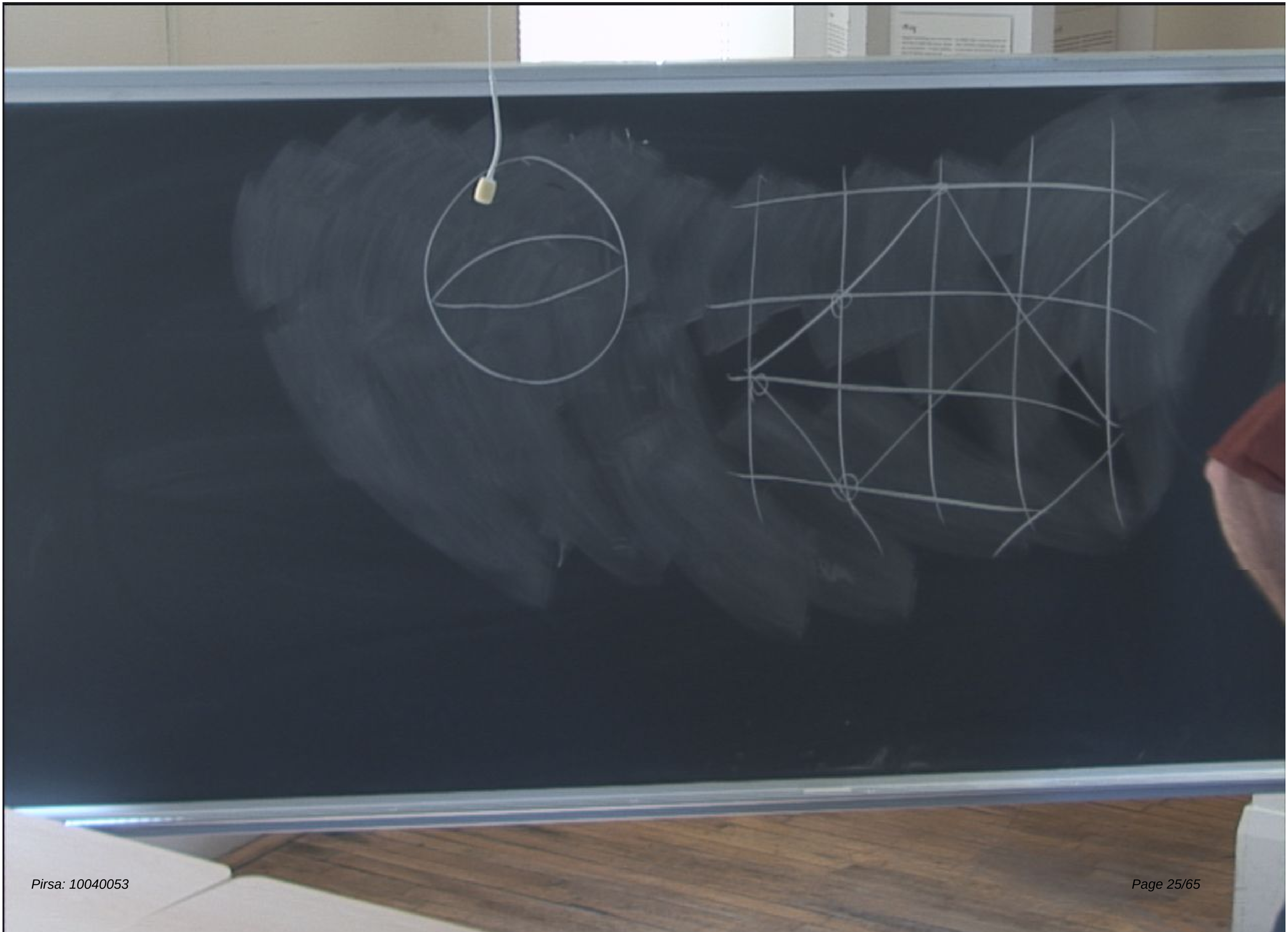
A fundamental aspect of the Néel state: **Quantum-rotor excitations**

- lowest-energy excitations of finite lattices
- not captured by spin-wave theory
- correspond to global rotations of the Neel order (frozen in spin-wave theory)





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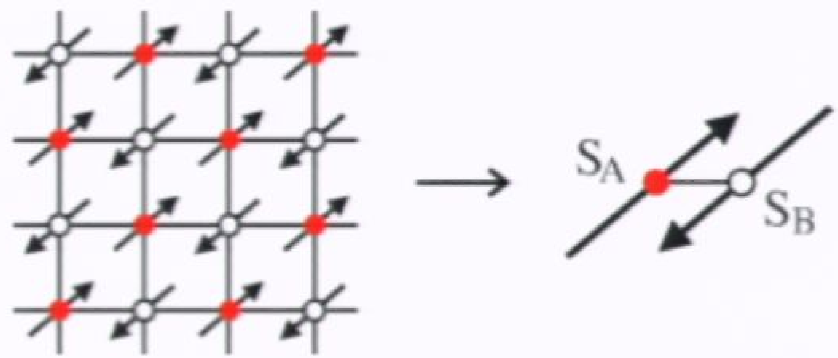
<u>Consider sublattices as two big spins</u>

- $S_A, S_B \sim N/2$
- effective interactions $\mathbf{J_{AB} \sim S_A \cdot S_B / N}$
- leads to $\Delta_S = E_S - E_0 \sim S(S+1)/N$
- S = total spin of the excitation



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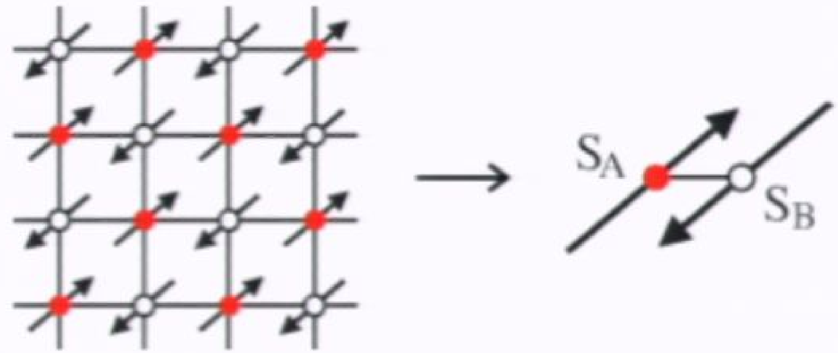

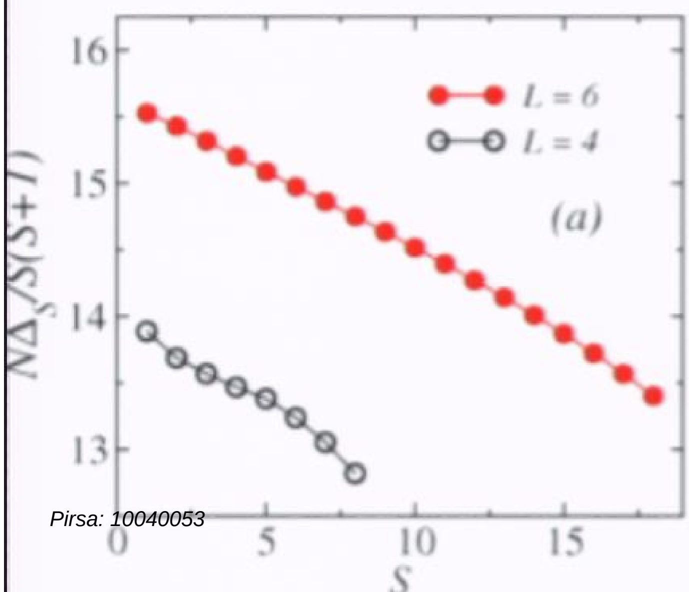

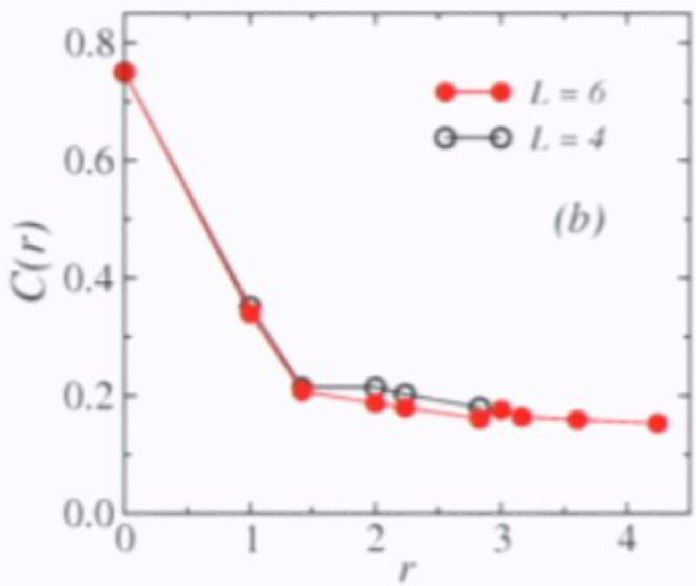

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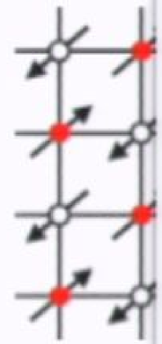
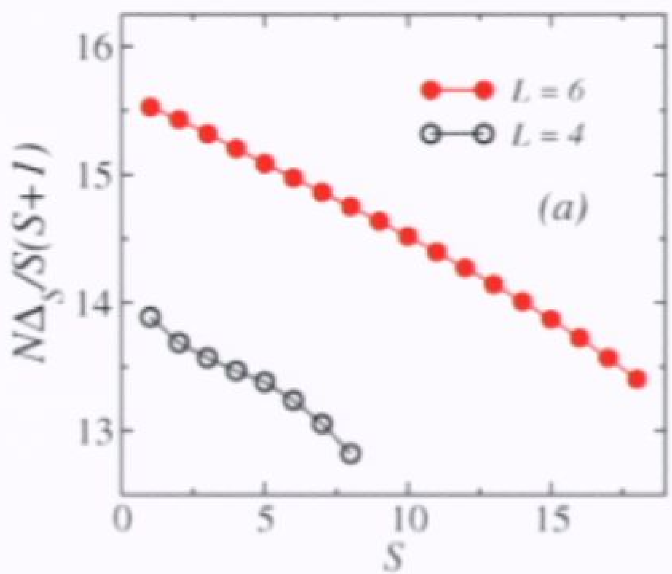
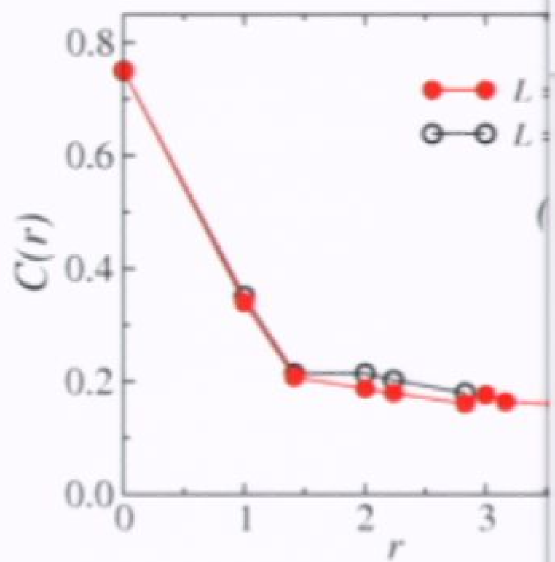
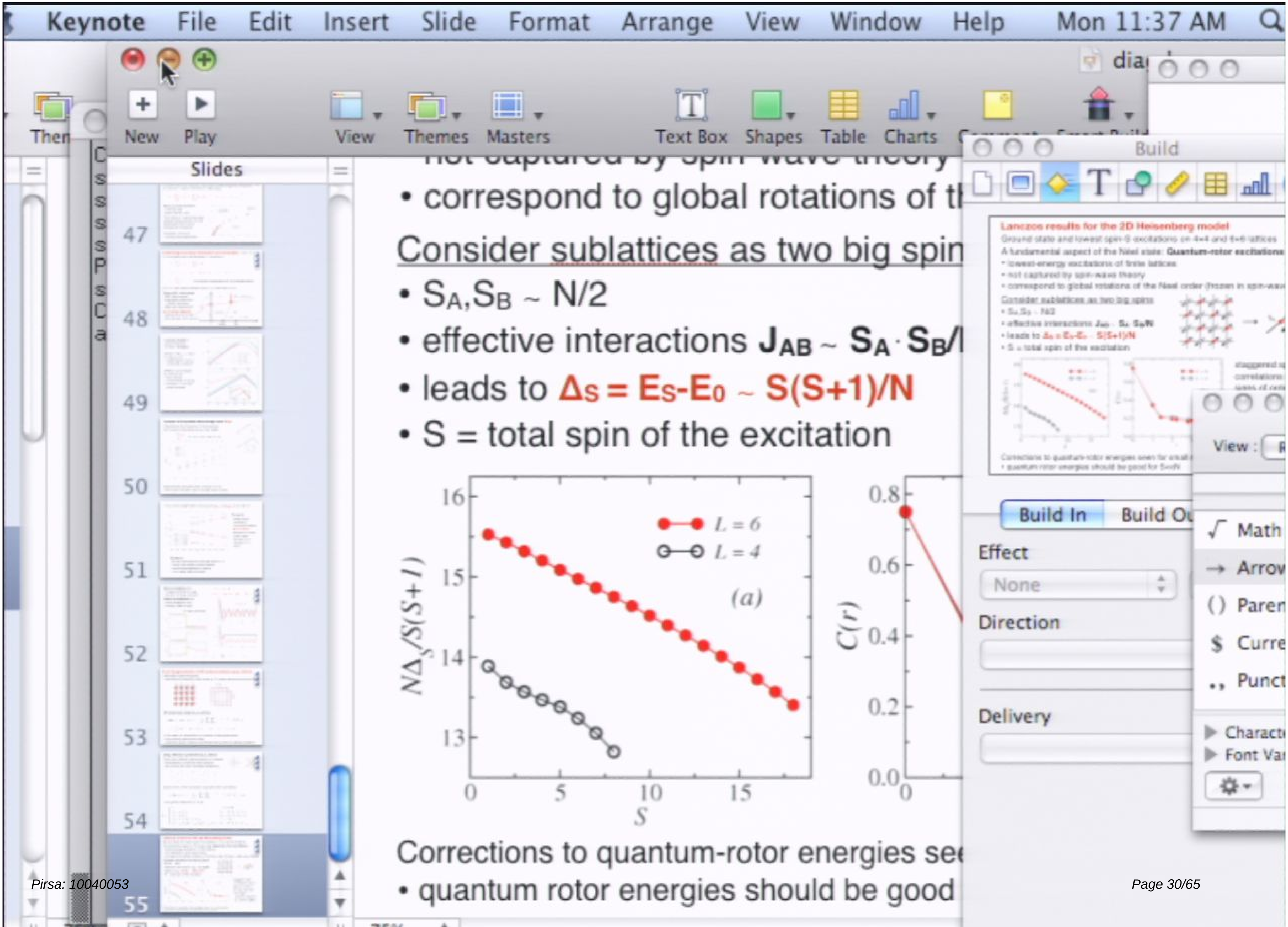






Corrections to quantum-rotor energies seen for small sys

• quantum rotor energies should be good for S<<N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• correspond to global rotations of t
Consider sublattices as two big spin
• SA,SB ~ N/2
• effective interactions JAB ~ SA · SB/
• leads to ΔS = ES-E0 ~ S(S+1)/N
• S = total spin of the excitation
NΔS/S(S+1)
C(r)
L = 6
L = 4
(a)
S
Corrections to quantum-rotor energies se
• quantum rotor energies should be good
Build
Lanczos results for the 2D Heisenberg model
Build In Build Ou
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PERIMETER SCHOLARS INTERNATIONAL
April 5-23, 2010, Course on "Quantum Spin Simulations"

Anders W. Sandvik, Boston University

PART3: Quantum Monte Carlo Methods

Introduction; path integrals and series representation

SSE algorithm for the S=1/2 Heisenberg model

- some details needed to make a simple but very efficient program
- essentially lattice-independent (bipartite) formulation

Examples: properties of chains, ladders, planes

- critical state of the Heisenberg chain and odd number of coupled chains
- gapped (quantum diordered) state of even number of coupled chains
- long-range order in 2D

The valence-bond basis and resonating valence-bond states

- alternative to single-spin ↑,↓ basis; properties of the basis
- exact solution of the frustrated chain at the "Majumdar-Ghosh" point
- amplitude-product states
- projector QMC method

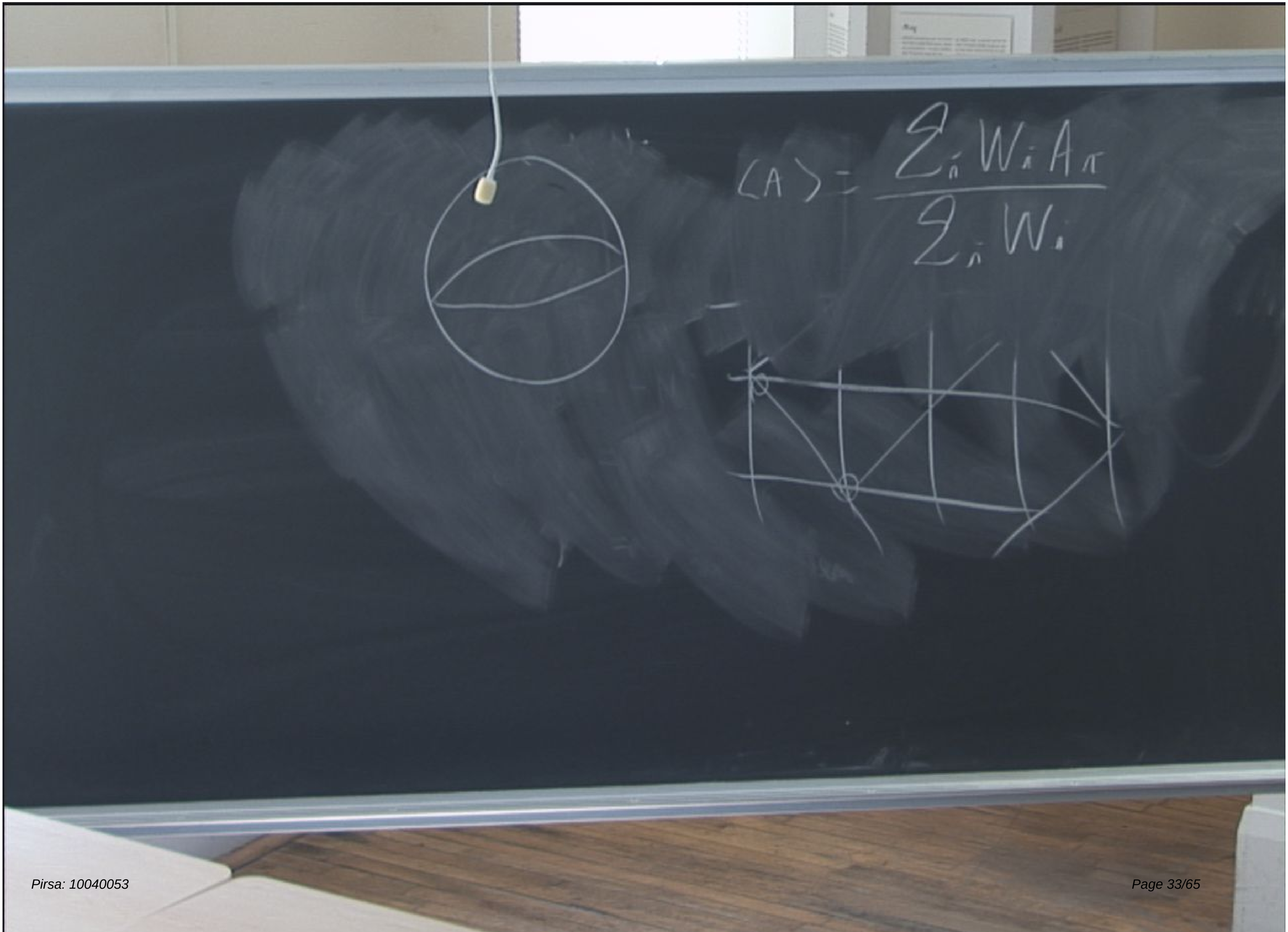
Néel to VBS quantum phase transition

Path integrals in quantum statistical mechanics

We want to compute a thermal expectation value

$$\langle A \rangle = \frac{1}{Z} \mathrm{Tr}\{ A e^{-\beta H} \}$$

where $\beta=1/T$ (and possibly $T \to 0$). How to deal with the exponential operator?


$\langle A \rangle = \frac{\sum_n W_n A_n}{\sum_n W_n}$

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"Time slicing" of the partition function

$$Z = \mathrm{Tr}\{\mathrm{e}^{-\beta H}\} = \mathrm{Tr}\left\{\prod_{l=1}^{L}\mathrm{e}^{-\Delta_\tau H}\right\} \qquad \Delta_\tau = \beta/L$$

Choose a basis and insert complete sets of states;

$$Z = \sum_{\alpha_0}\sum_{\alpha_1}\cdots\sum_{\alpha_L-1}\langle\alpha_0|\mathrm{e}^{-\Delta_\tau H}|\alpha_{L-1}\rangle\cdots\langle\alpha_2|\mathrm{e}^{-\Delta_\tau H}|\alpha_1\rangle\langle\alpha_1|\mathrm{e}^{-\Delta_\tau H}|\alpha_0\rangle$$

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Use approximation for imaginary time evolution operator. Simplest way

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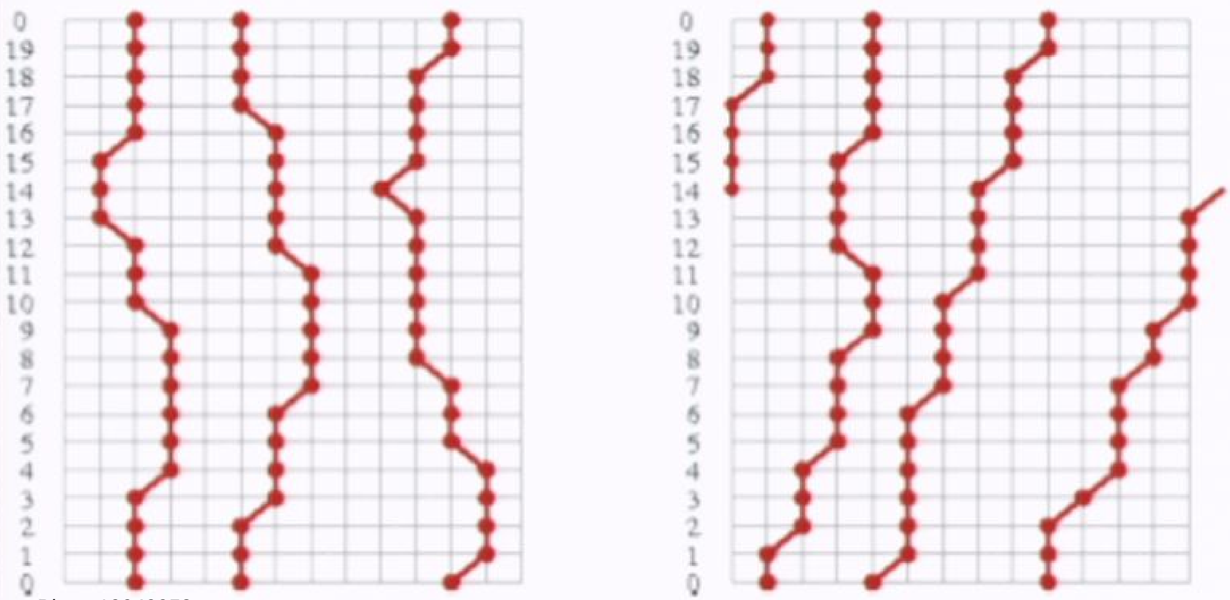

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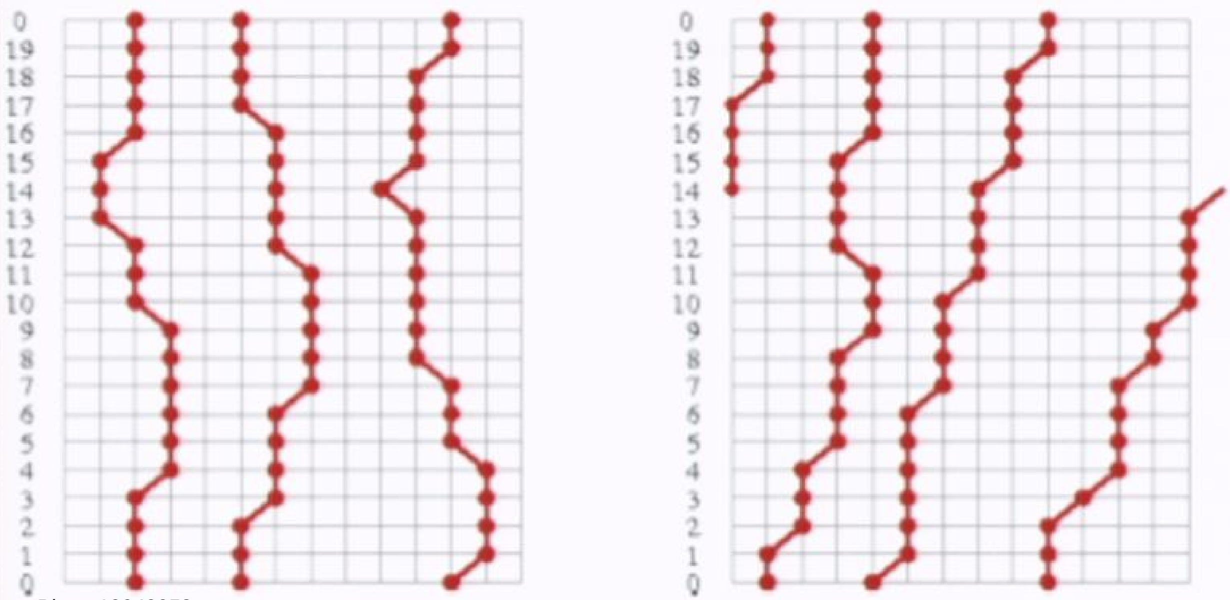

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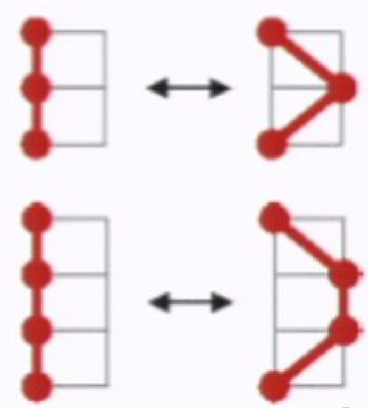

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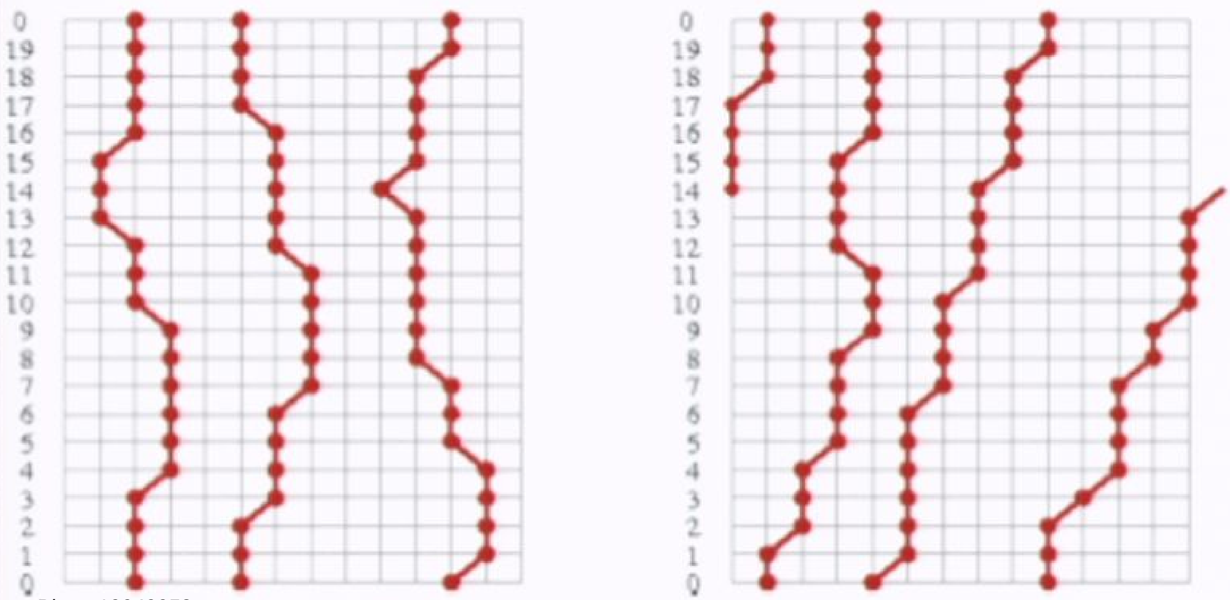

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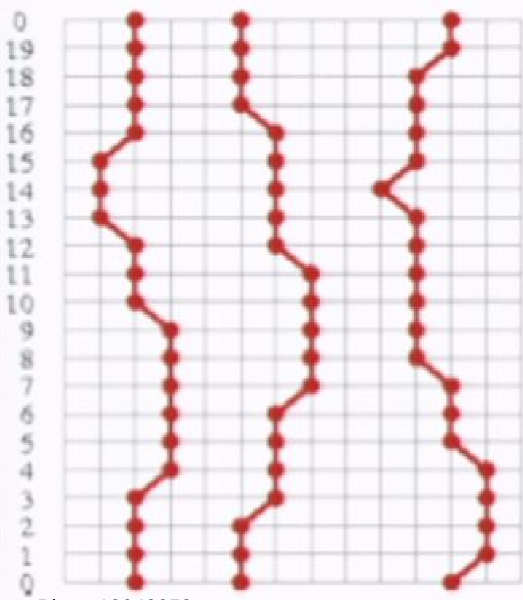

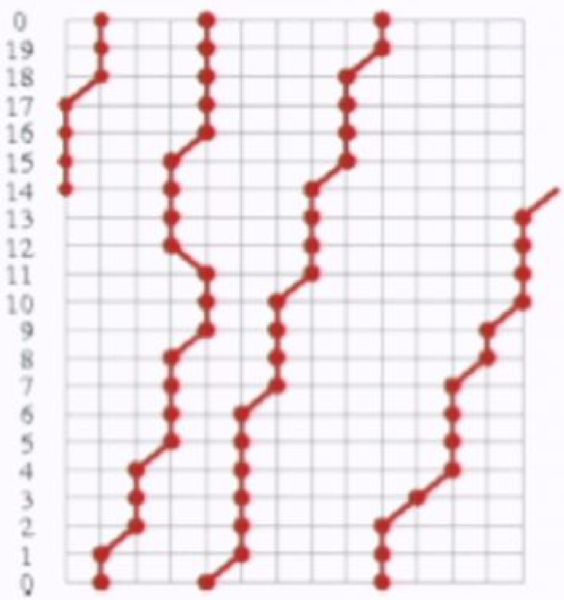

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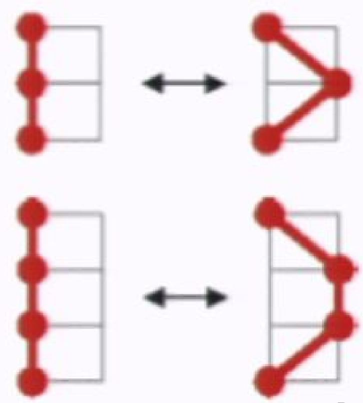

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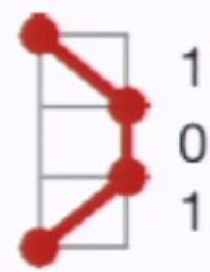

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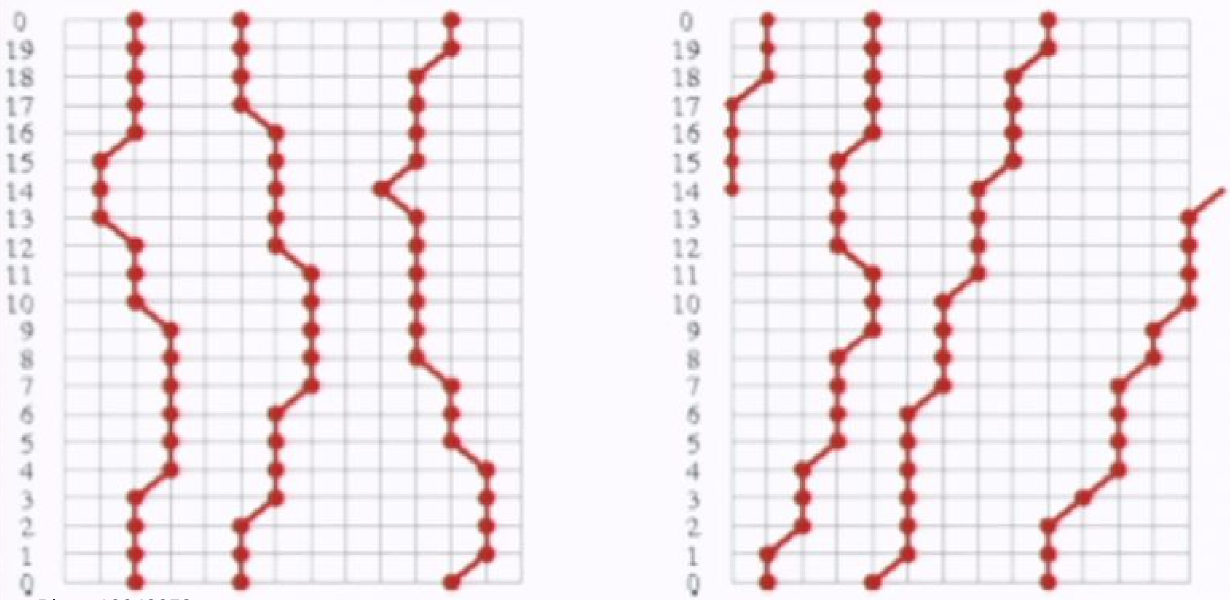

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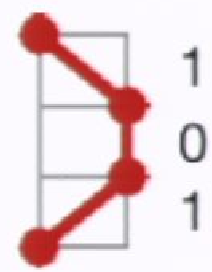

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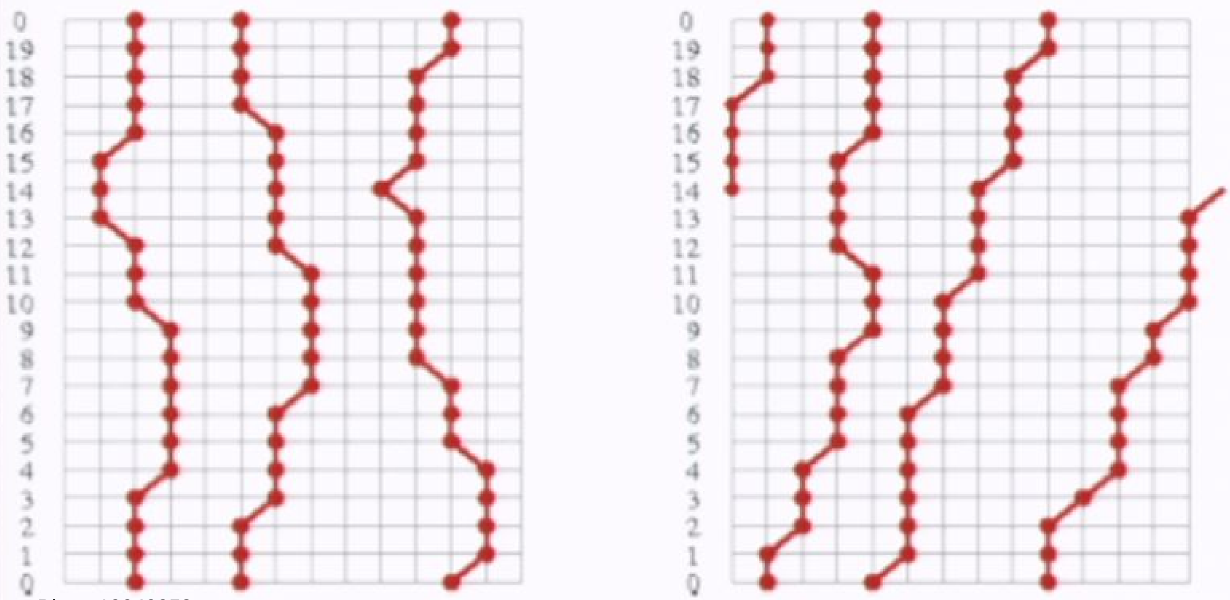

$Z = \sum W(\{\alpha\})$ $\quad W(\{\alpha\}) = \Delta^{n_K}$ $\quad n_K$ = number of "jumps"

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$$H = K = -\sum_{\langle i,j\rangle} K_{ij} = -\sum_{\langle i,j\rangle} (a_j^\dagger a_i + a_i^\dagger a_j) \qquad n_i = a_i^\dagger a_i \in \{0,1\}$$

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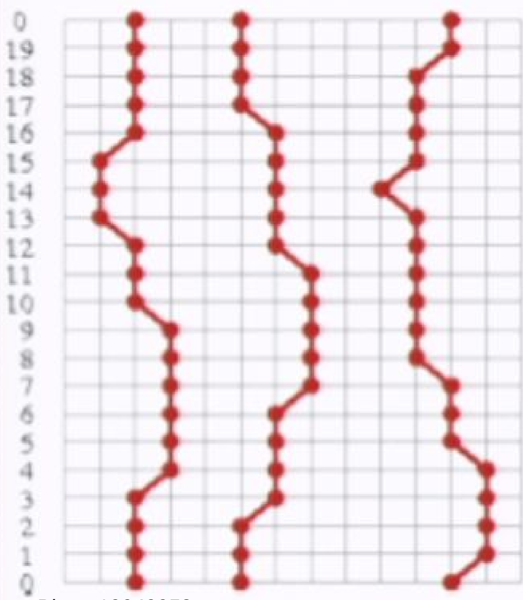
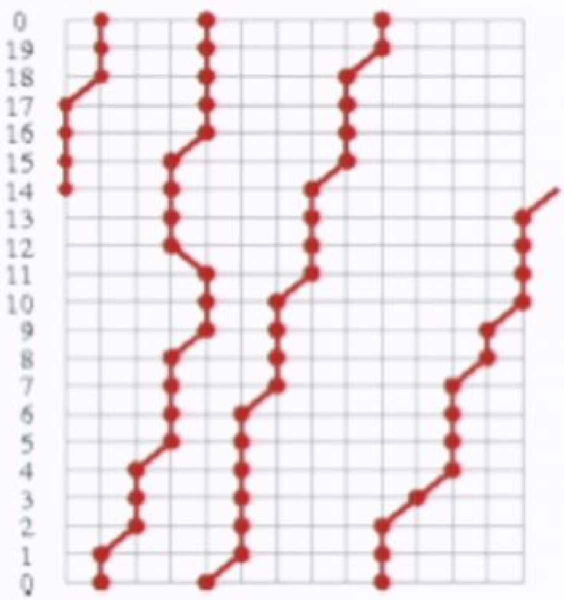
$$H = -2\sum_{\langle i,j\rangle}(S_i^x S_j^x + S_i^y S_j^y) = -\sum_{\langle i,j\rangle}(S_i^+ S_j^- + S_i^- S_j^+), \quad S^z = \pm\frac{1}{2} \sim n_i = 0, 1$$

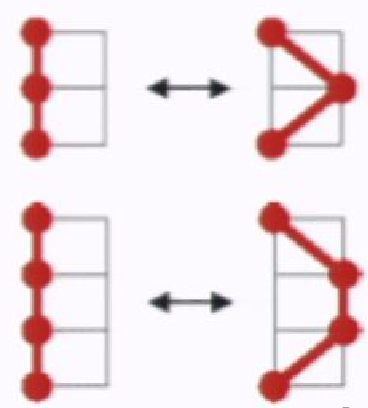
"World line" representation of

$$Z \approx \sum_{\{\alpha\}} \langle \alpha_0 | 1 - \Delta_\tau H | \alpha_{L-1}\rangle \cdots \langle \alpha_2 | 1 - \Delta_\tau H | \alpha_1 \rangle \langle \alpha_1 | 1 - \Delta_\tau H | \alpha_0 \rangle$$





world line moves for Monte Carlo sampling



Expectation values

$$\langle A \rangle = \frac{1}{Z} \sum_{\{\alpha\}} \langle \alpha_0 | \mathrm{e}^{-\Delta_\tau} | \alpha_{L-1} \rangle \cdots \langle \alpha_2 | \mathrm{e}^{-\Delta_\tau H} | \alpha_1 \rangle \langle \alpha_1 | \mathrm{e}^{-\Delta_\tau H} A | \alpha_0 \rangle$$

We want to write this in a form suitable for MC importance sampling

$$\langle A \rangle = \frac{\sum_{\{\alpha\}} A(\{\alpha\}) W(\{\alpha\})}{\sum_{\{\alpha\}} W(\{\alpha\})} \quad \longrightarrow \quad \langle A \rangle = \langle A(\{\alpha\}) \rangle_W$$

$$\begin{aligned} W(\{\alpha\}) &= \text{weight} \\ A(\{\alpha\}) &= \text{estimator} \end{aligned}$$

Expectation values

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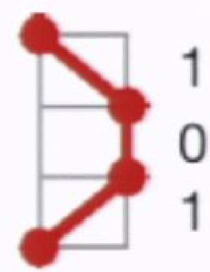
For any quantity diagonal in the occupation numbers (spin z):

$$A(\{\alpha\}) = A(\alpha_n) \quad\text{or}\quad A(\{\alpha\}) = \frac{1}{L}\sum_{l=0}^{L-1} A(\alpha_l)$$

Kinetic energy (here full energy). Use

$$K\mathrm{e}^{-\Delta_\tau K} \approx K \qquad K_{ij}(\{\alpha\}) = \frac{\langle\alpha_1|K_{ij}|\alpha_0\rangle}{\langle\alpha_1|1-\Delta_\tau K|\alpha_0\rangle} \in \{0, \frac{1}{\Delta_\tau}\}$$



Average over all slices → count number of kinetic jumps

$$\langle K_{ij}\rangle = \frac{\langle n_{ij}\rangle}{\beta}, \qquad \langle K\rangle = -\frac{\langle n_K\rangle}{\beta} \qquad \langle K\rangle \propto N \rightarrow \langle n_K\rangle \propto \beta N$$

Expectation values

$$\langle A \rangle = \frac{1}{Z} \sum_{\{\alpha\}} \langle \alpha_0 | e^{-\Delta_\tau} | \alpha_{L-1} \rangle \cdots \langle \alpha_2 | e^{-\Delta_\tau H} | \alpha_1 \rangle \langle \alpha_1 | e^{-\Delta_\tau H} A | \alpha_0 \rangle$$

We want to write this in a form suitable for MC importance sampling

$$\langle A \rangle = \frac{\sum_{\{\alpha\}} A(\{\alpha\}) W(\{\alpha\})}{\sum_{\{\alpha\}} W(\{\alpha\})} \longrightarrow \langle A \rangle = \langle A(\{\alpha\}) \rangle_W$$

$$W(\{\alpha\}) = \text{weight}$$
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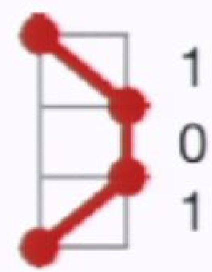

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