Title: Quantum Spin Simulations (PHYS 7380) - Lecture 12

Date: Apr 20, 2010 11:00 AM

URL: http://pirsa.org/10040054

Abstract:

Example: hard-core bosons

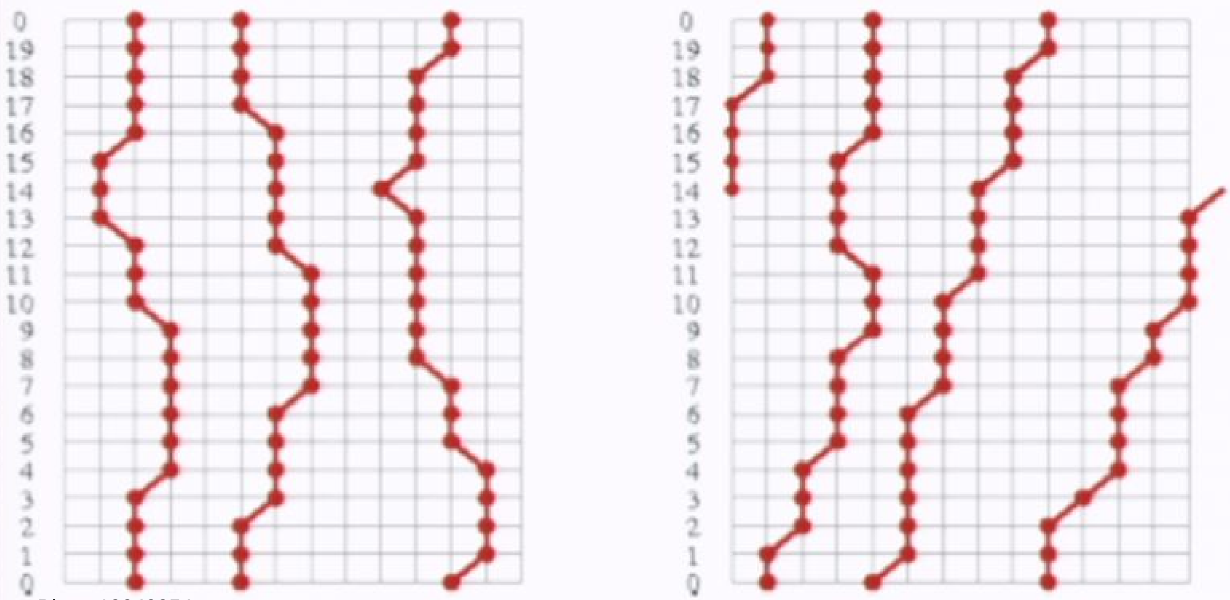
$$H = K = -\sum_{\langle i,j \rangle} K_{ij} = -\sum_{\langle i,j \rangle} (a_j^\dagger a_i + a_i^\dagger a_j) \qquad n_i = a_i^\dagger a_i \in \{0,1\}$$

Equivalent to S=1/2 XY model

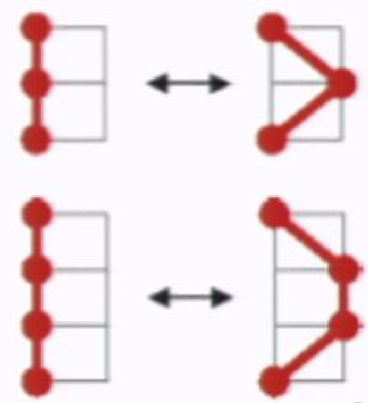
$$H = -2\sum_{\langle i,j \rangle} (S_i^x S_j^x + S_i^y S_j^y) = -\sum_{\langle i,j \rangle} (S_i^+ S_j^- + S_i^- S_j^+), \quad S^z = \pm\frac{1}{2} \sim n_i = 0,1$$

"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

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

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

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

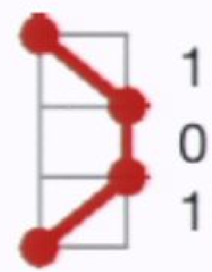
$$W(\{\alpha\}) = \text{weight}$$
$$A(\{\alpha\}) = \text{estimator}$$

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

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



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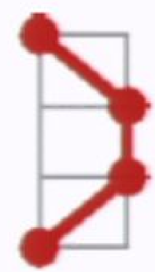

Average over all slices → count number of kinetic jumps

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

Expectation values

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

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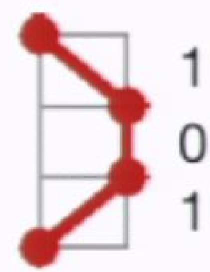

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ncluding interactions

For any diagonal interaction V (Trotter, or split-operator, approximation)

$$e^{-\Delta_\tau H} = e^{-\Delta_\tau K} e^{-\Delta_\tau V} + \mathcal{O}(\Delta_\tau^2) \to \langle \alpha_{l+1} | e^{-\Delta_\tau H} | \alpha_l \rangle \approx e^{-\Delta_\tau V_l} \langle \alpha_{l+1} | e^{-\Delta_\tau K} | \alpha_l \rangle$$

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Product over all times slices →

$$W(\{\alpha\}) = \Delta_\tau^{n_K} \exp\left(-\Delta_\tau \sum_{l=0}^{L-1} V_l \right)$$

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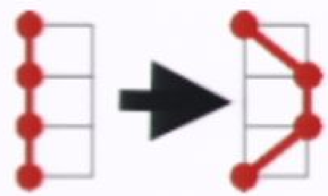

$$P_{\mathrm{acc}} = \min\left[\Delta_\tau^2 \frac{V_{\mathrm{new}}}{V_{\mathrm{old}}}, 1\right]$$

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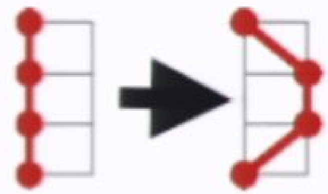

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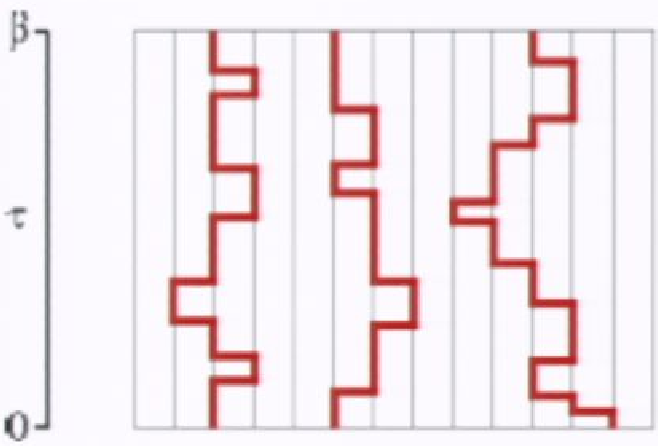
The continuous time limit

Limit $\Delta_\tau \rightarrow 0$: number of kinetic jumps remains finite, store events only



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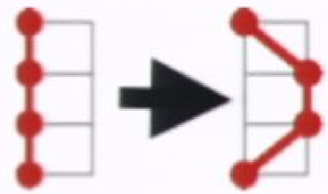

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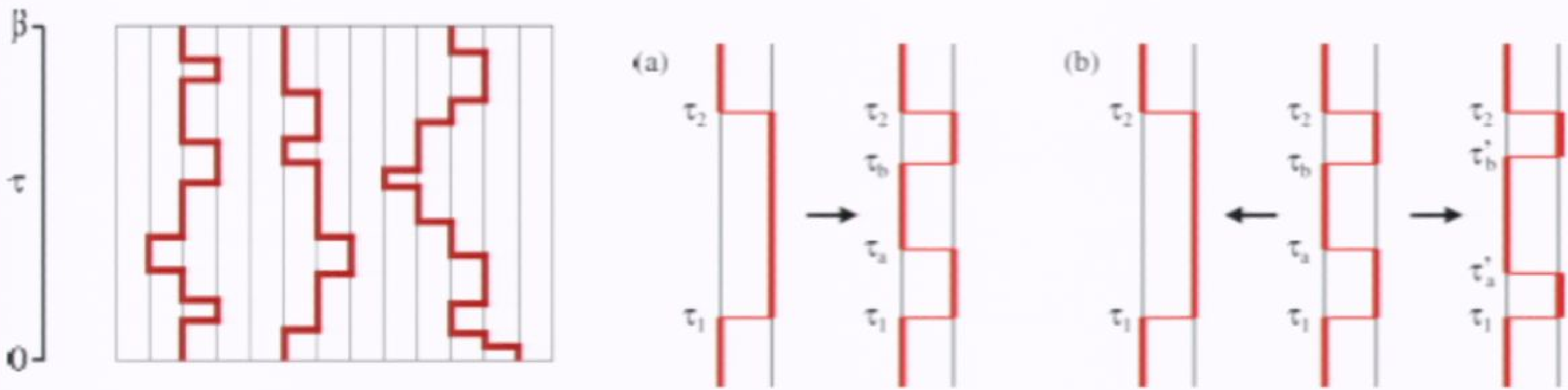

local updates (problem when $\Delta_\tau \rightarrow 0$?)

- consider probability of inserting/removing events within a time window

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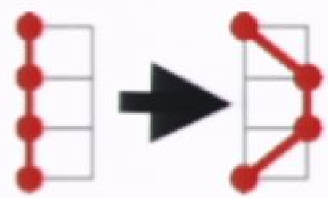

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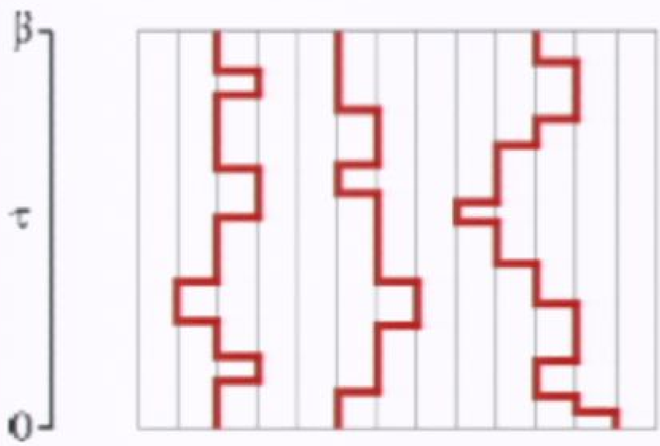
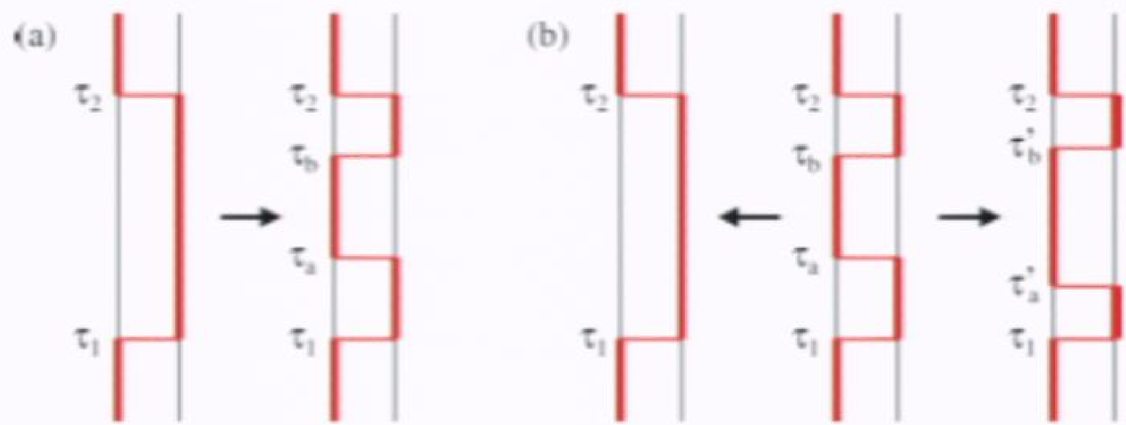




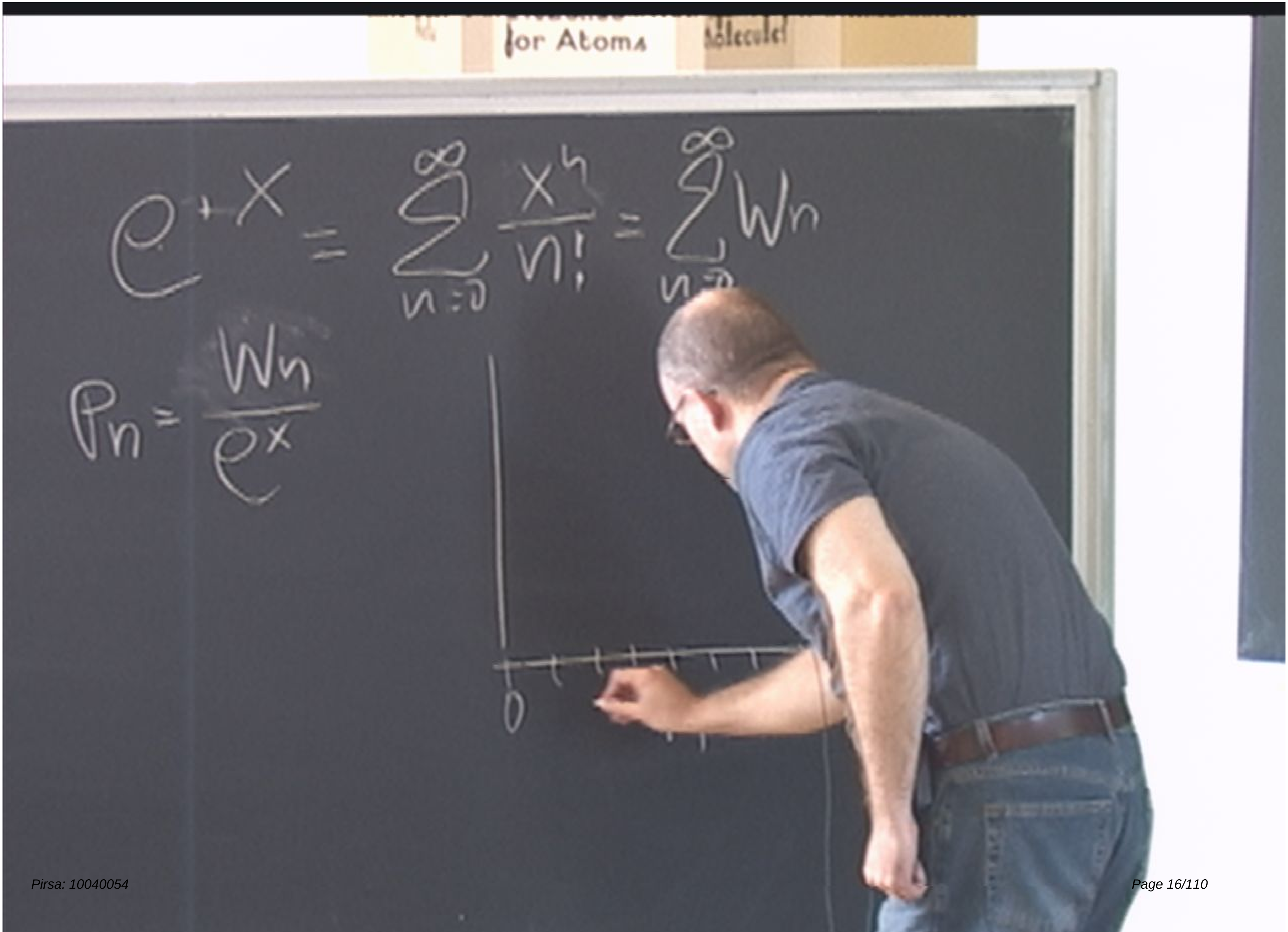
Special methods (**loop and worm updates**) developed for efficient

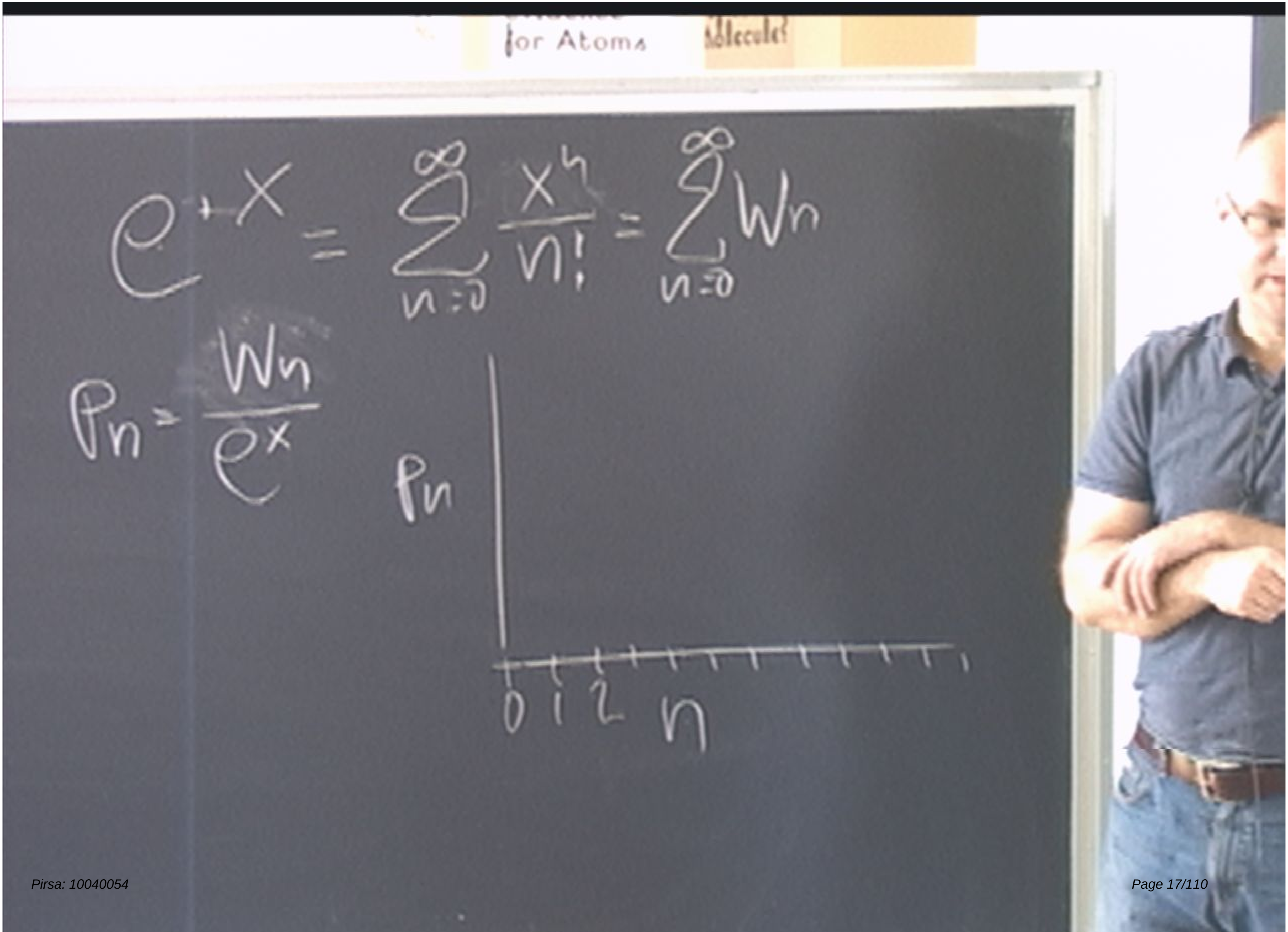
local updates (problem when $\Delta_\tau \rightarrow 0$?)

- consider probability of inserting/removing events within a time window

Series expansion representation

Start from the Taylor expansion $e^{-\beta H} = \sum_{n=0}^{\infty} \frac{(-\beta)^n}{n!} H^n$ (approximation-free method from the outset)


for Atoms
$e^{+x} = \sum_{n=0}^{\infty} \frac{x^n}{n!} = \sum_{n=0}^{\infty} W_n$
$P_n = \frac{W_n}{e^x}$
0


for Atoms
Molecule?
$e^{x} = \sum_{n=0}^{\infty} \frac{x^n}{n!} = \sum_{n=0}^{\infty} W_n$
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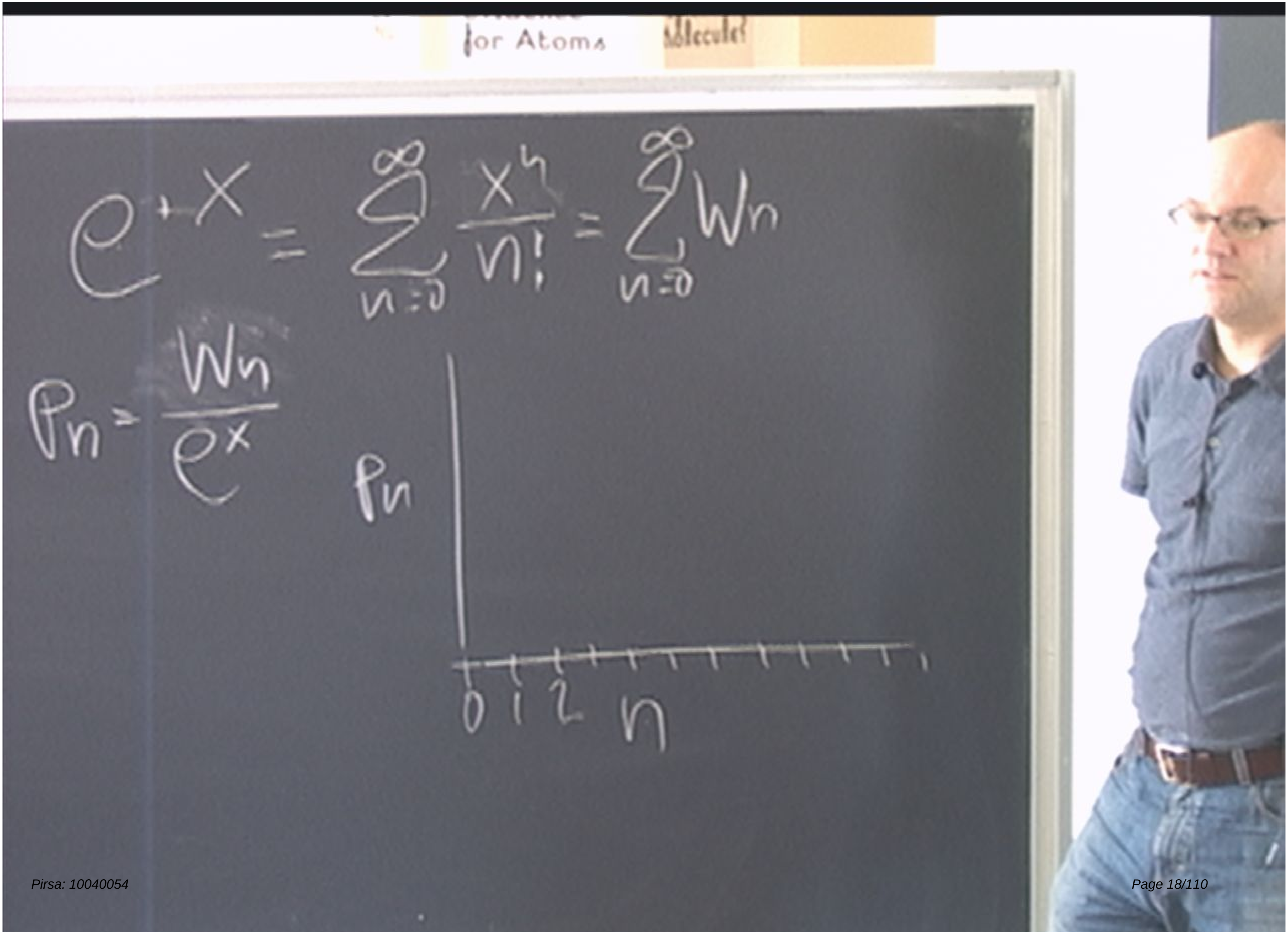
P_n
0 1 2 n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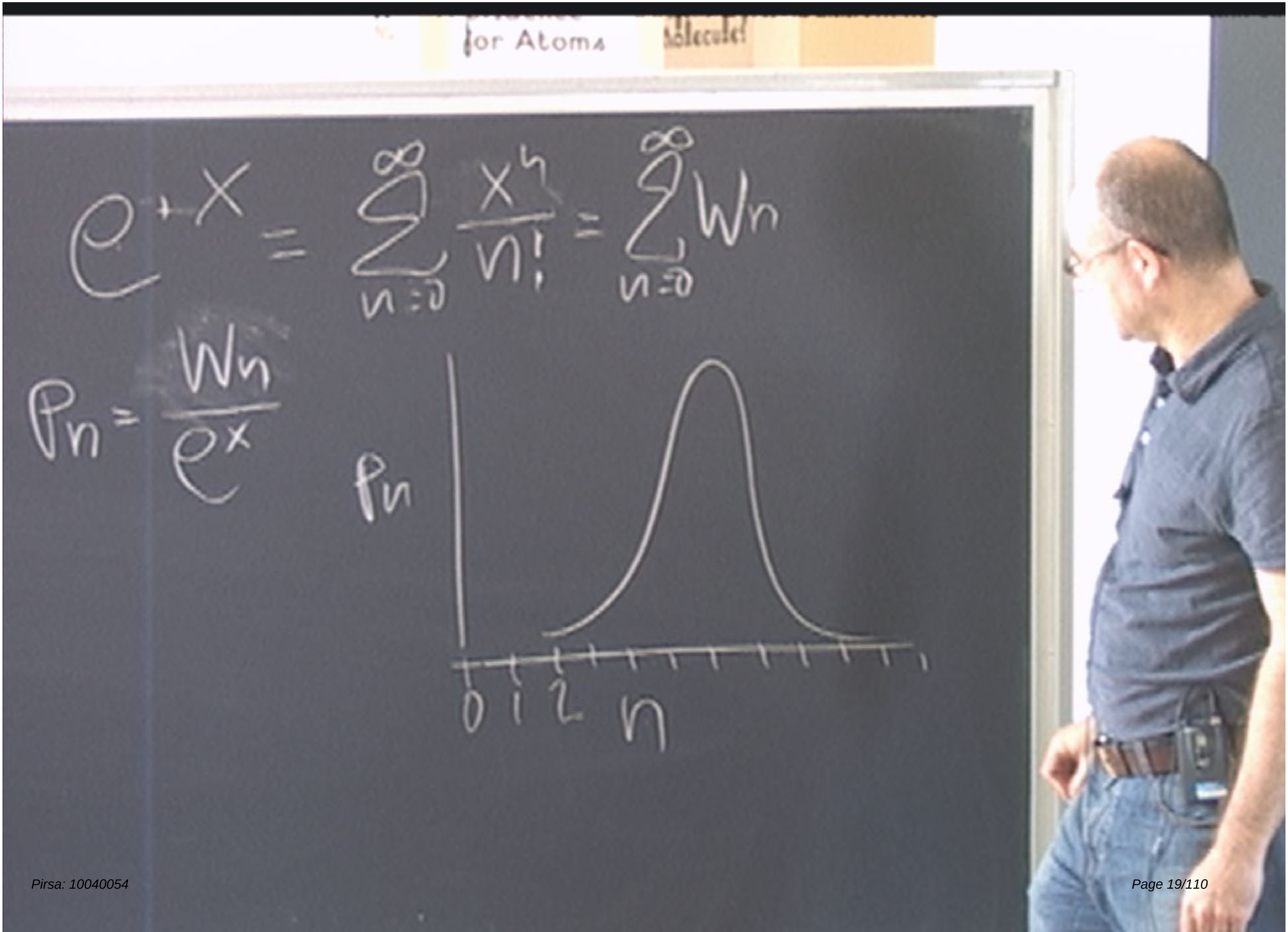
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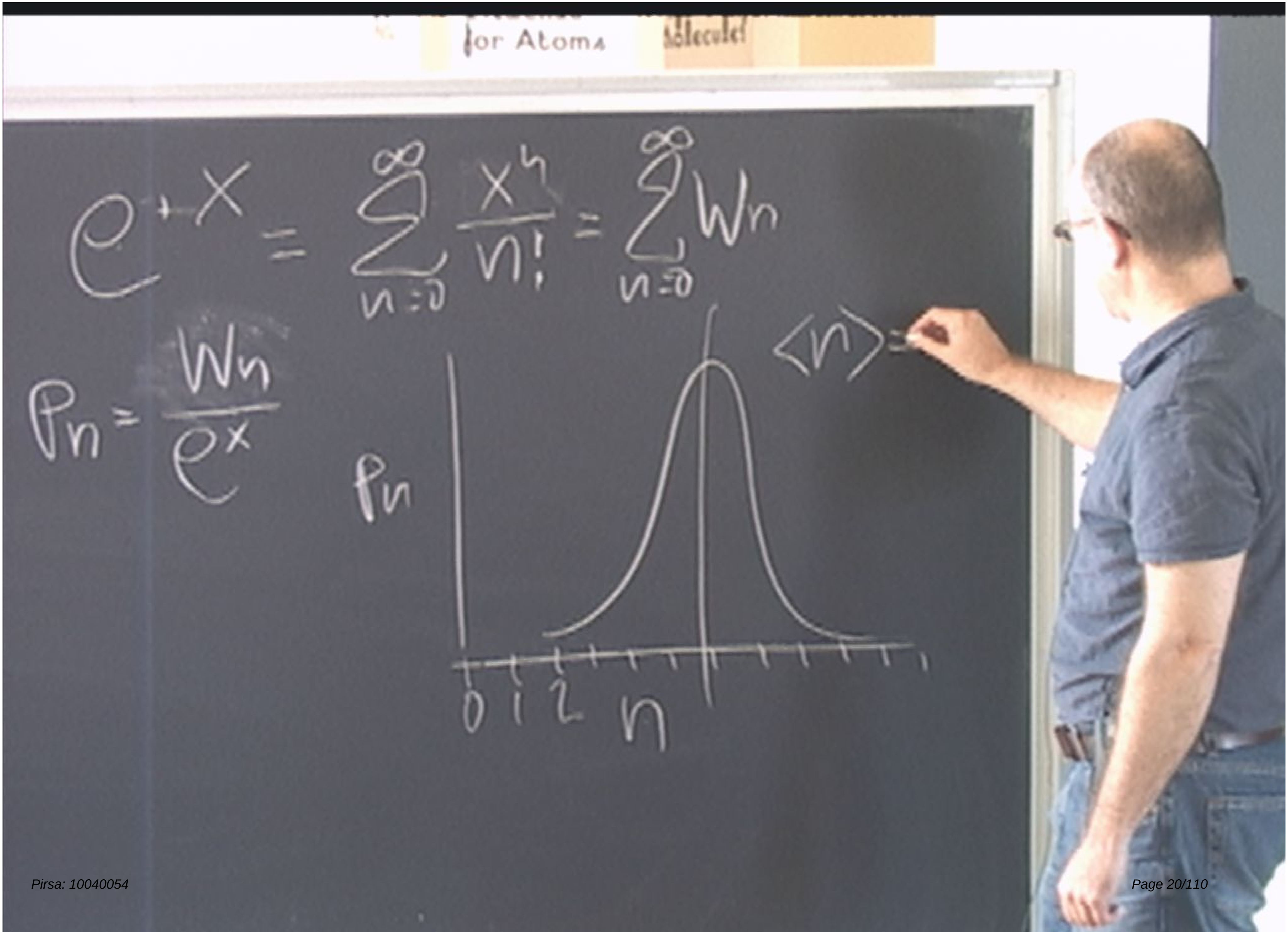
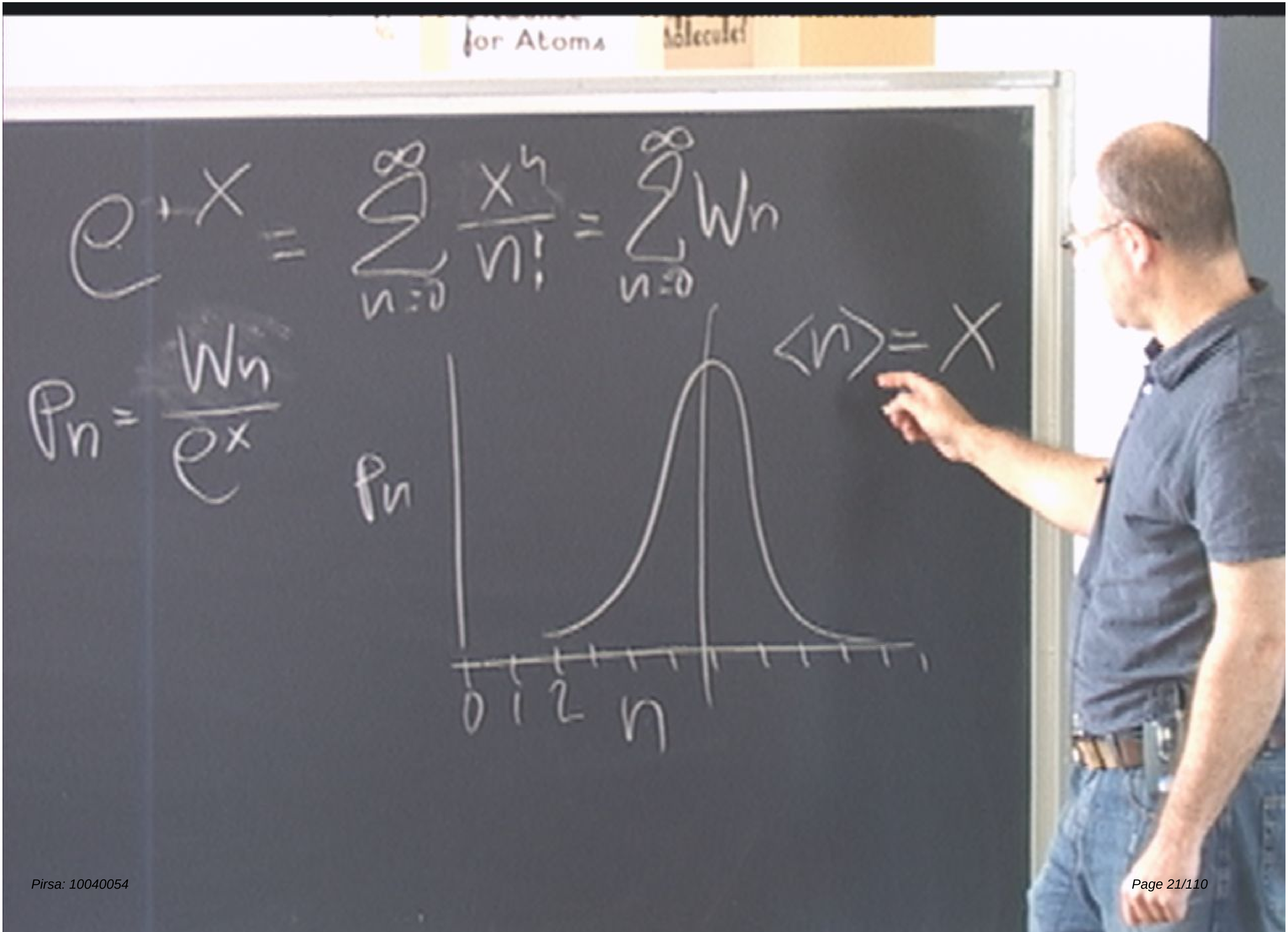

for Atoms
Molecule
e^{+x} = Σ_{n=0}^∞ x^n/n! = Σ_{n=0}^∞ W_n
P_n = W_n / e^x
P_n
0 1 2
n
⟨n⟩ =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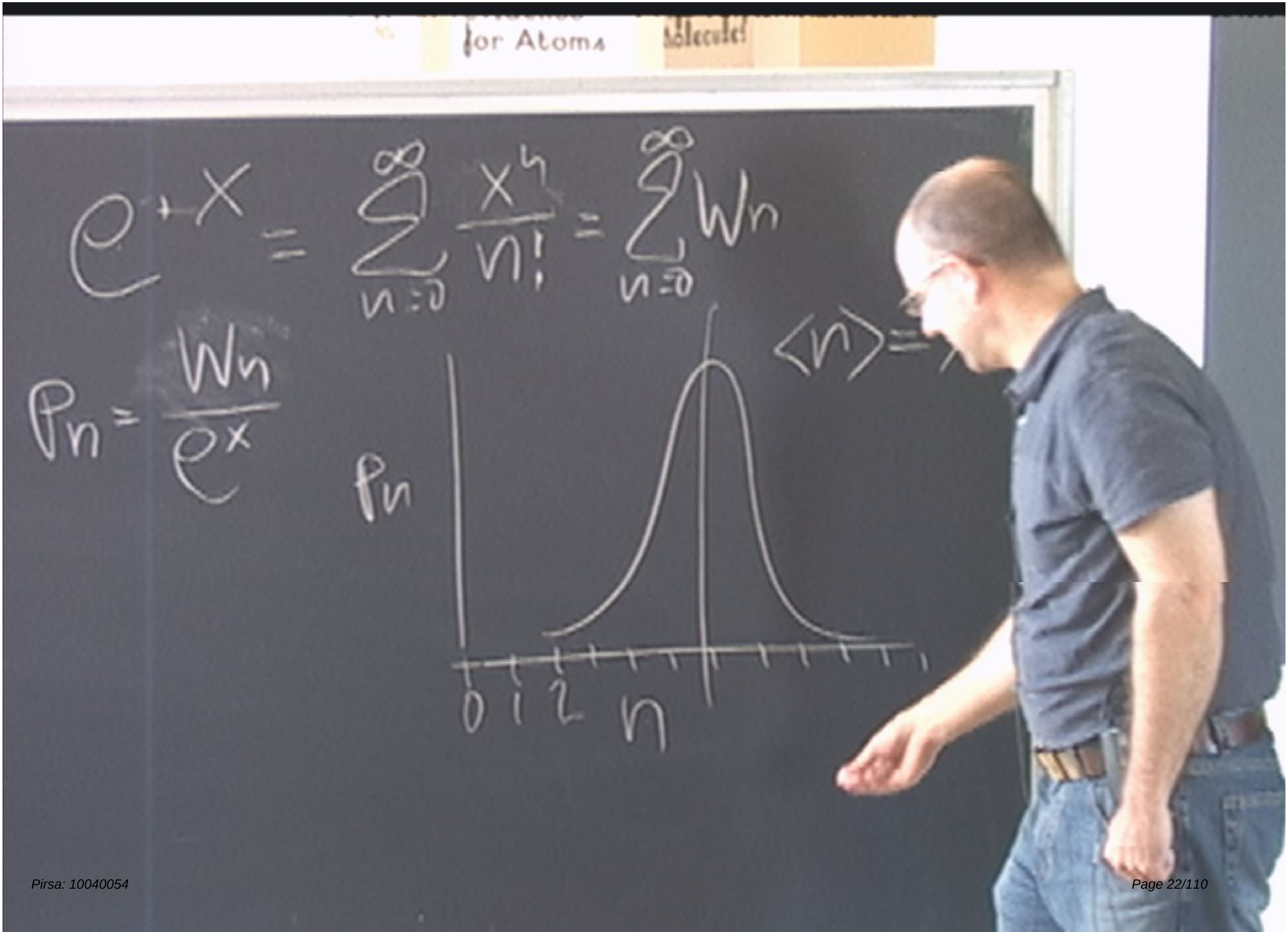
$P_n = \frac{W_n}{e^x}$
$\langle n \rangle = x$
P_n
0 1 2 n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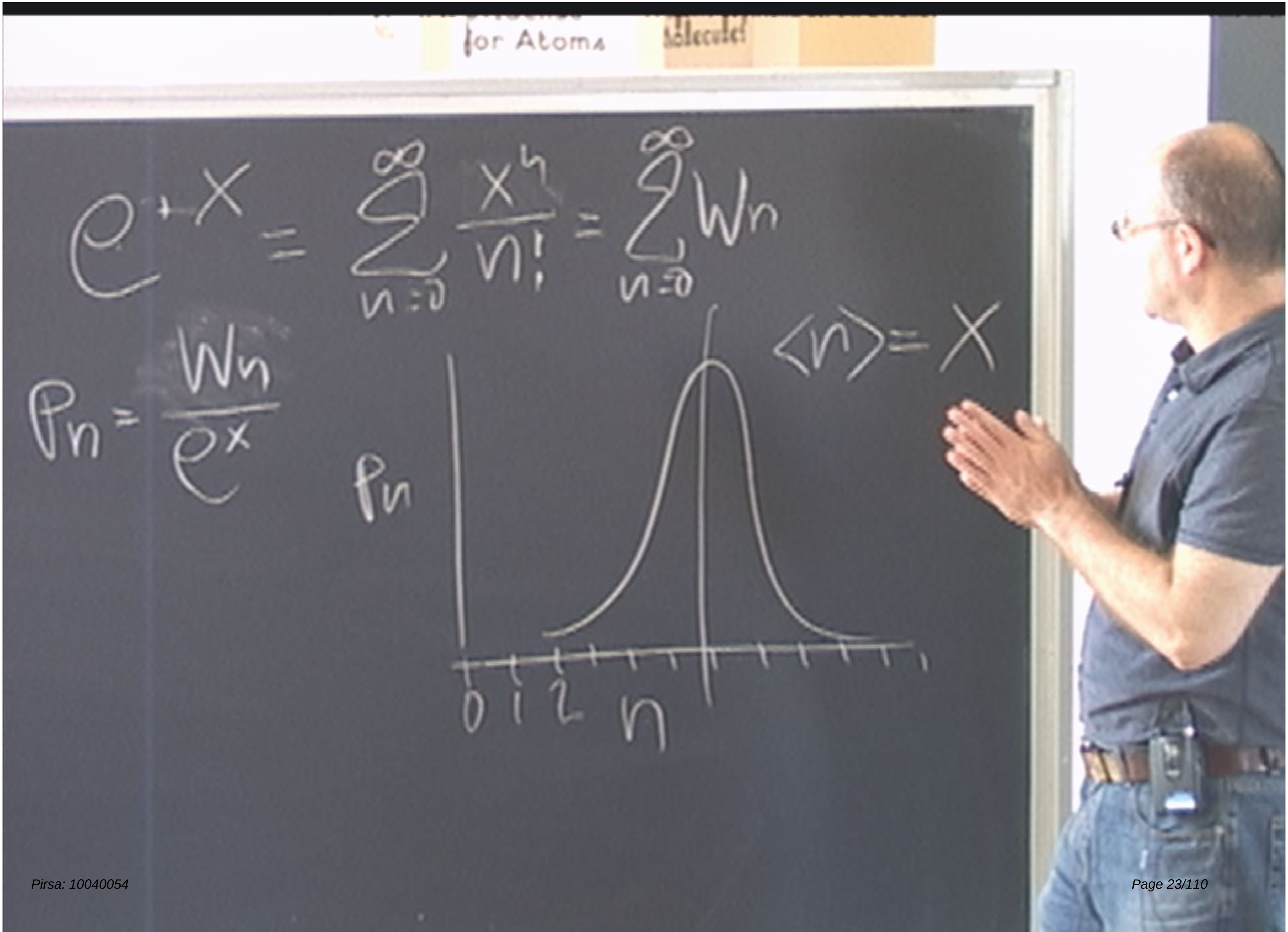
P_n
0 1 2
n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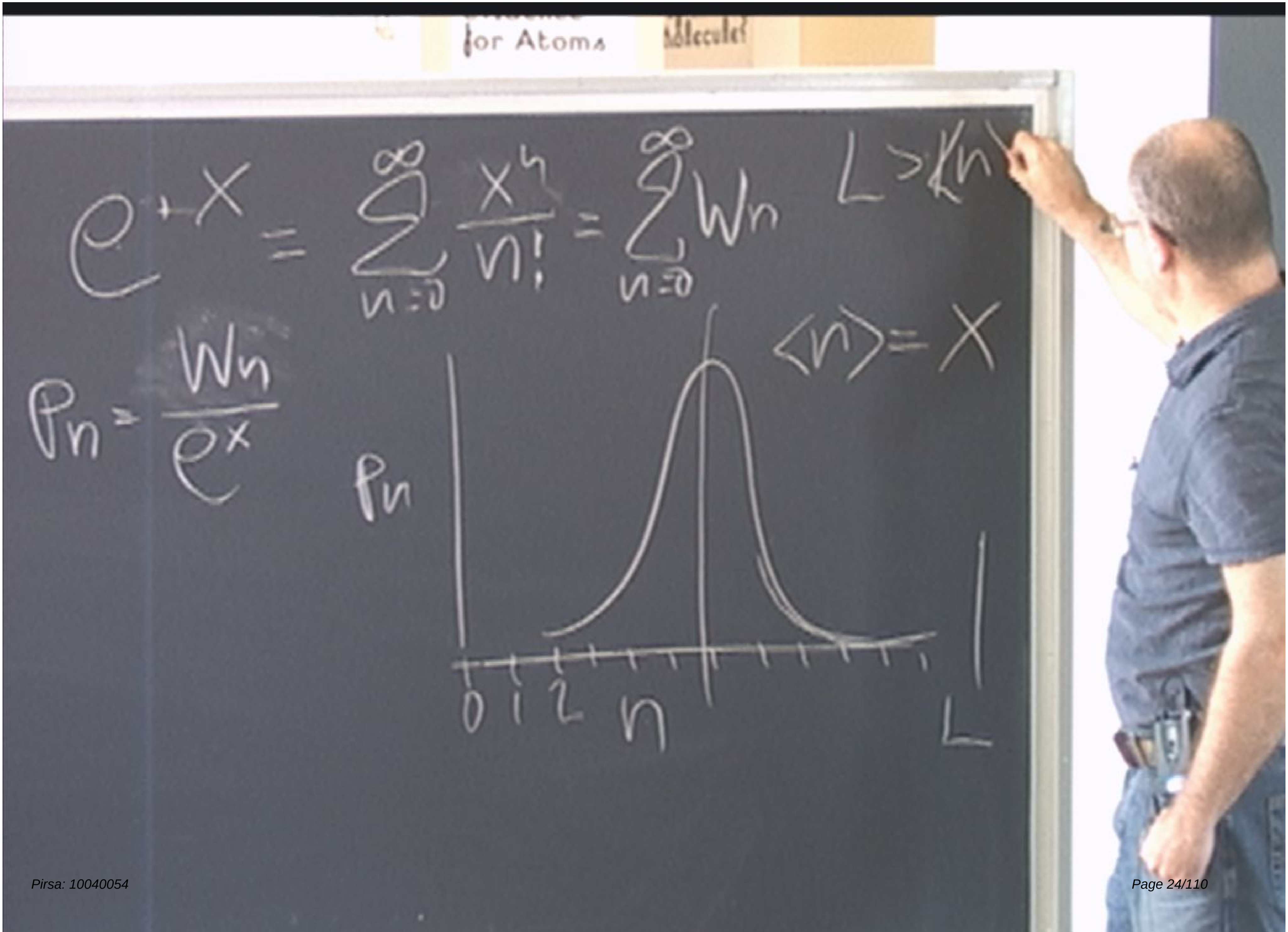
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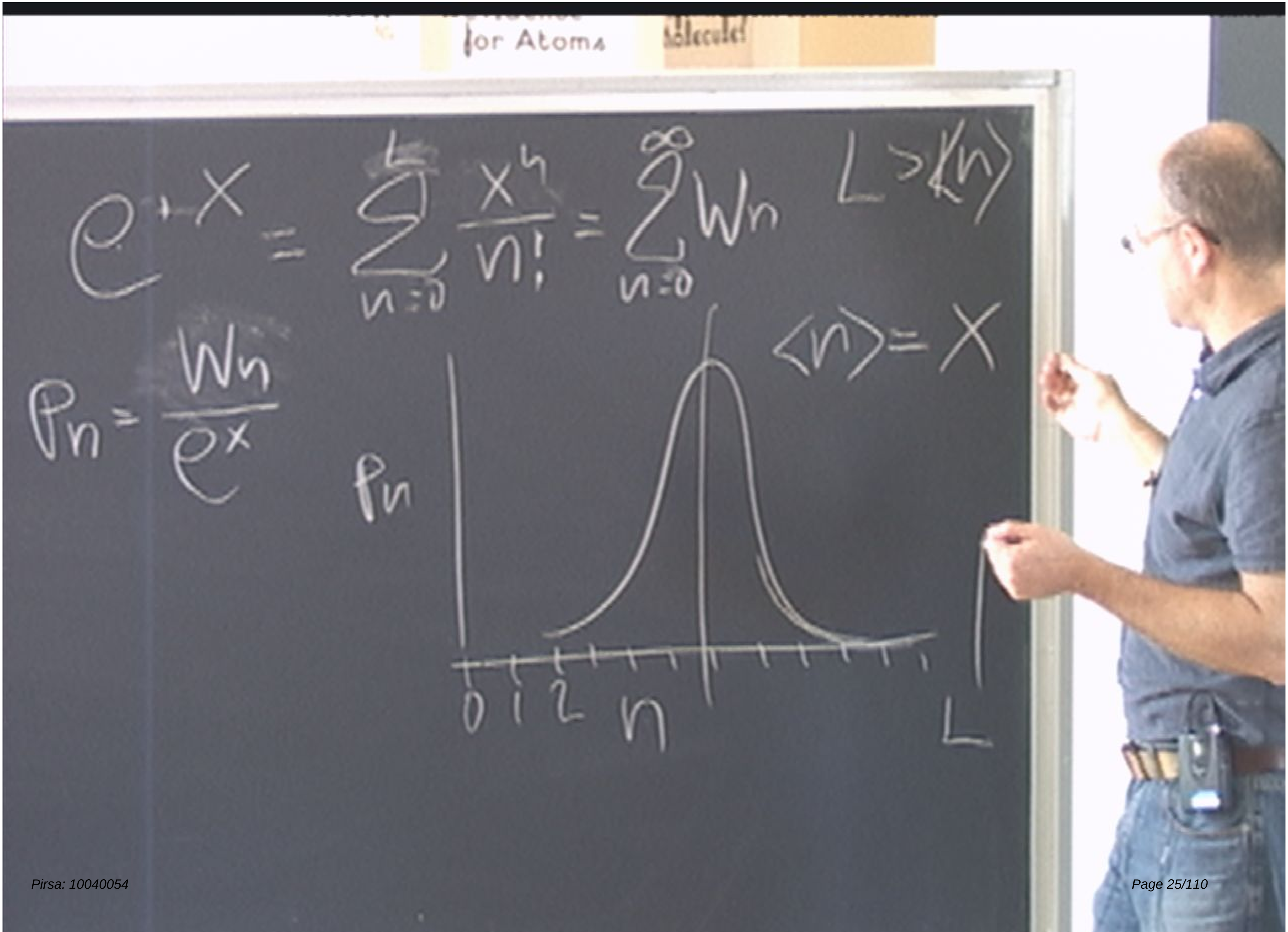
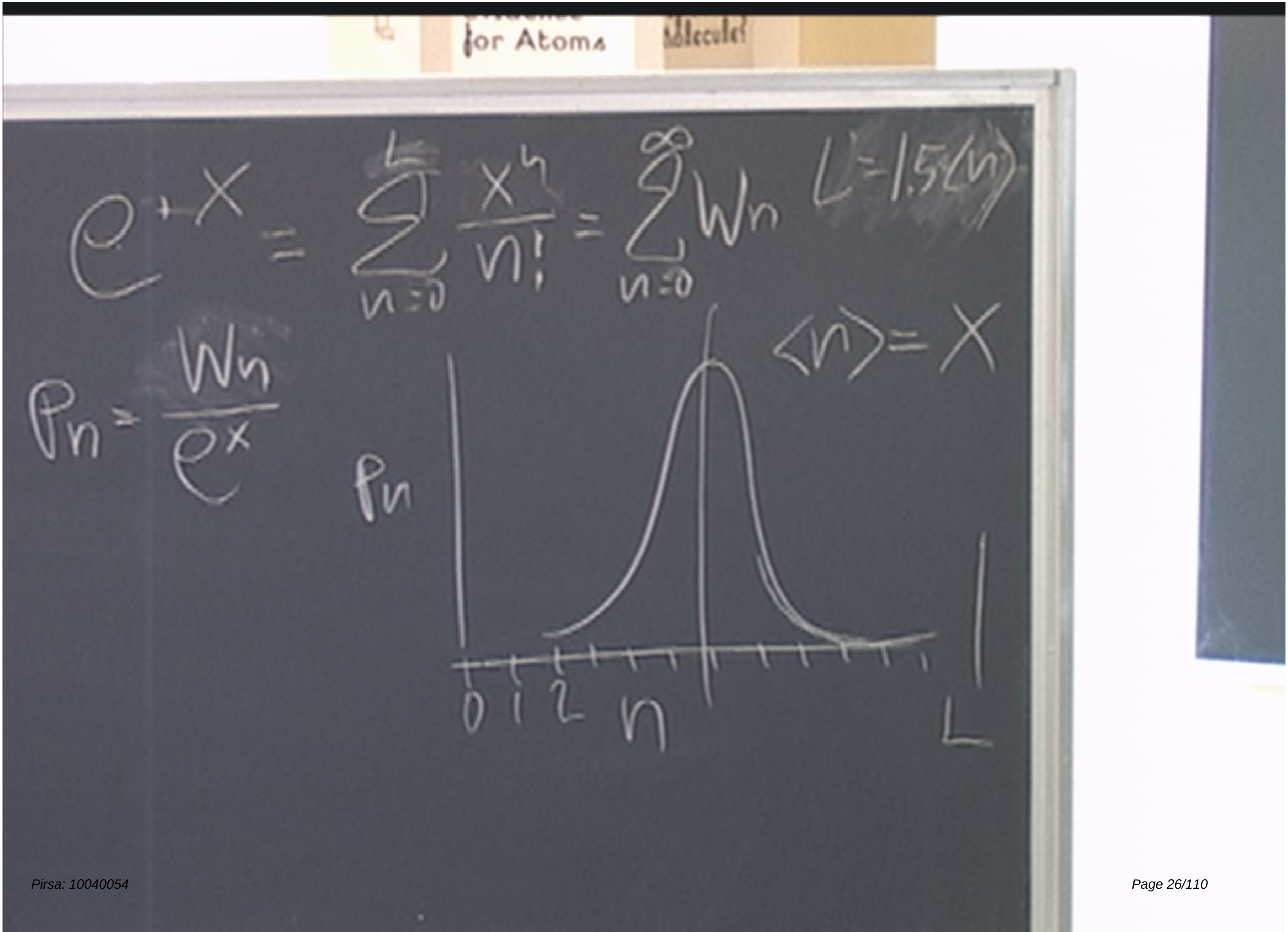

for Atoms
Molecule!
e^x = Σ_{n=0}^{L} x^n/n! = Σ_{n=0}^{∞} W_n
L > ⟨n⟩
P_n = W_n / e^x
⟨n⟩ = X
P_n
0 1 2 n
L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$\langle n \rangle = x$
P_n
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L

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$$Z = \sum_{n=0}^{\infty} \frac{(-\beta)^n}{n!} \sum_{\{\alpha\}_n} \langle \alpha_0 | H | \alpha_{n-1} \rangle \cdots \langle \alpha_2 | H | \alpha_1 \rangle \langle \alpha_1 | H | \alpha_0 \rangle$$

Similar to the path integral; $1 - \Delta\tau H \to H$ and weight factor outside

Example: hard-core bosons

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

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?

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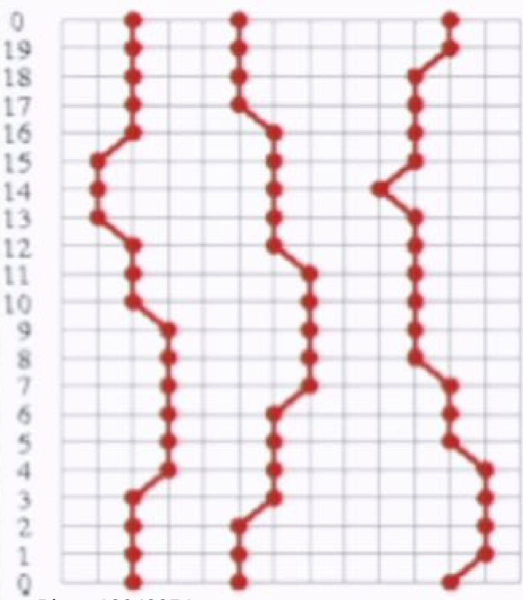

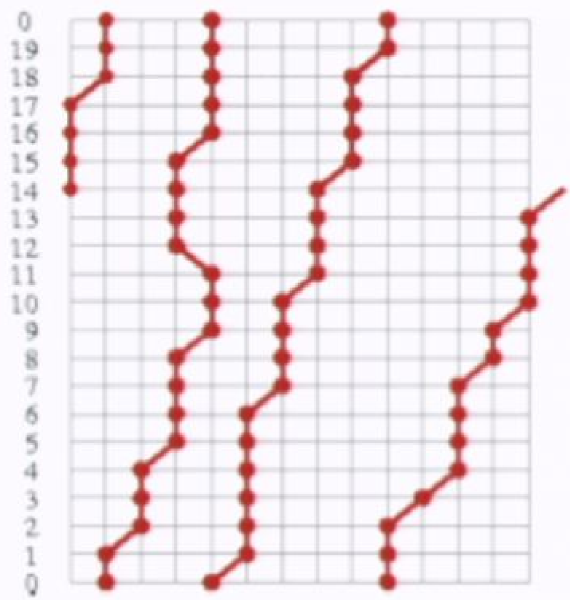

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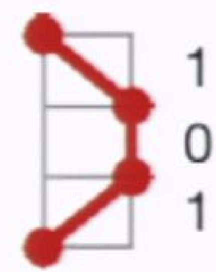

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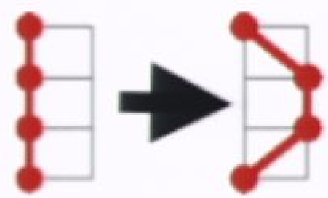
Product over all times slices →

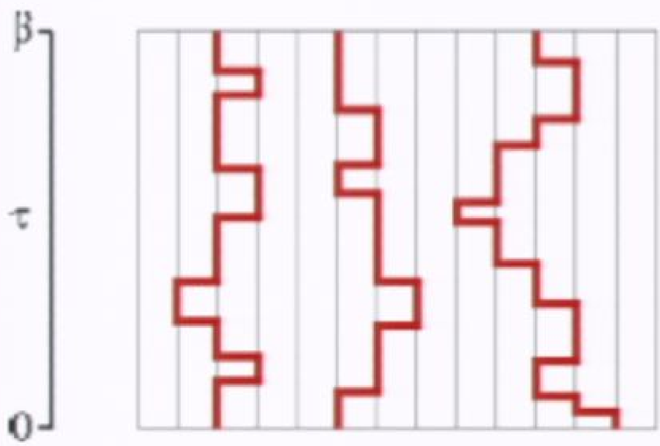
$$W(\{\alpha\}) = \Delta_\tau^{n_K} \exp\left(-\Delta_\tau \sum_{l=0}^{L-1} V_l \right)$$

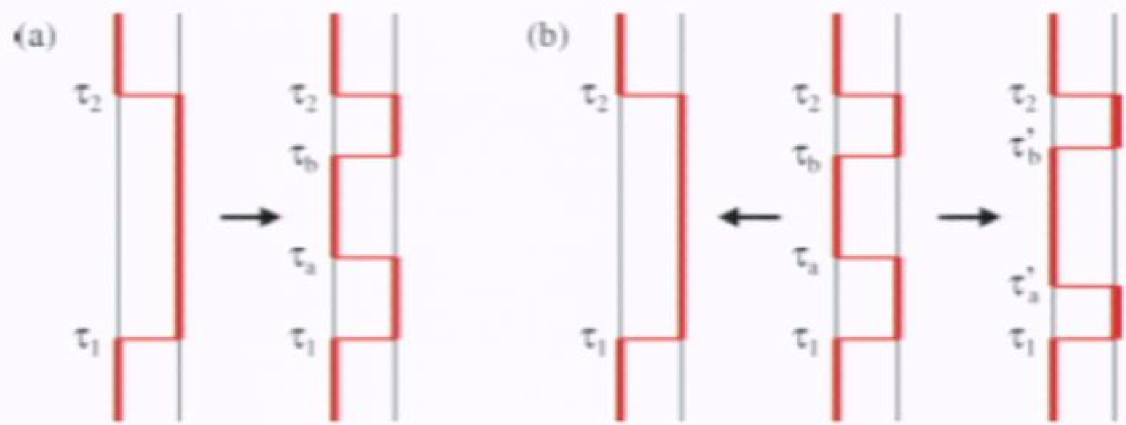


$$P_{\text{acc}} = \min\left[\Delta_\tau^2 \frac{V_{\text{new}}}{V_{\text{old}}}, 1 \right]$$

The continuous time limit

Limit $\Delta_\tau \rightarrow 0$: number of kinetic jumps remains finite, store events only





local updates (problem when $\Delta_\tau \rightarrow 0$?)

- consider probability of inserting/removing events within a time window

Series expansion representation

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relabel terms to "get rid of" extra slice

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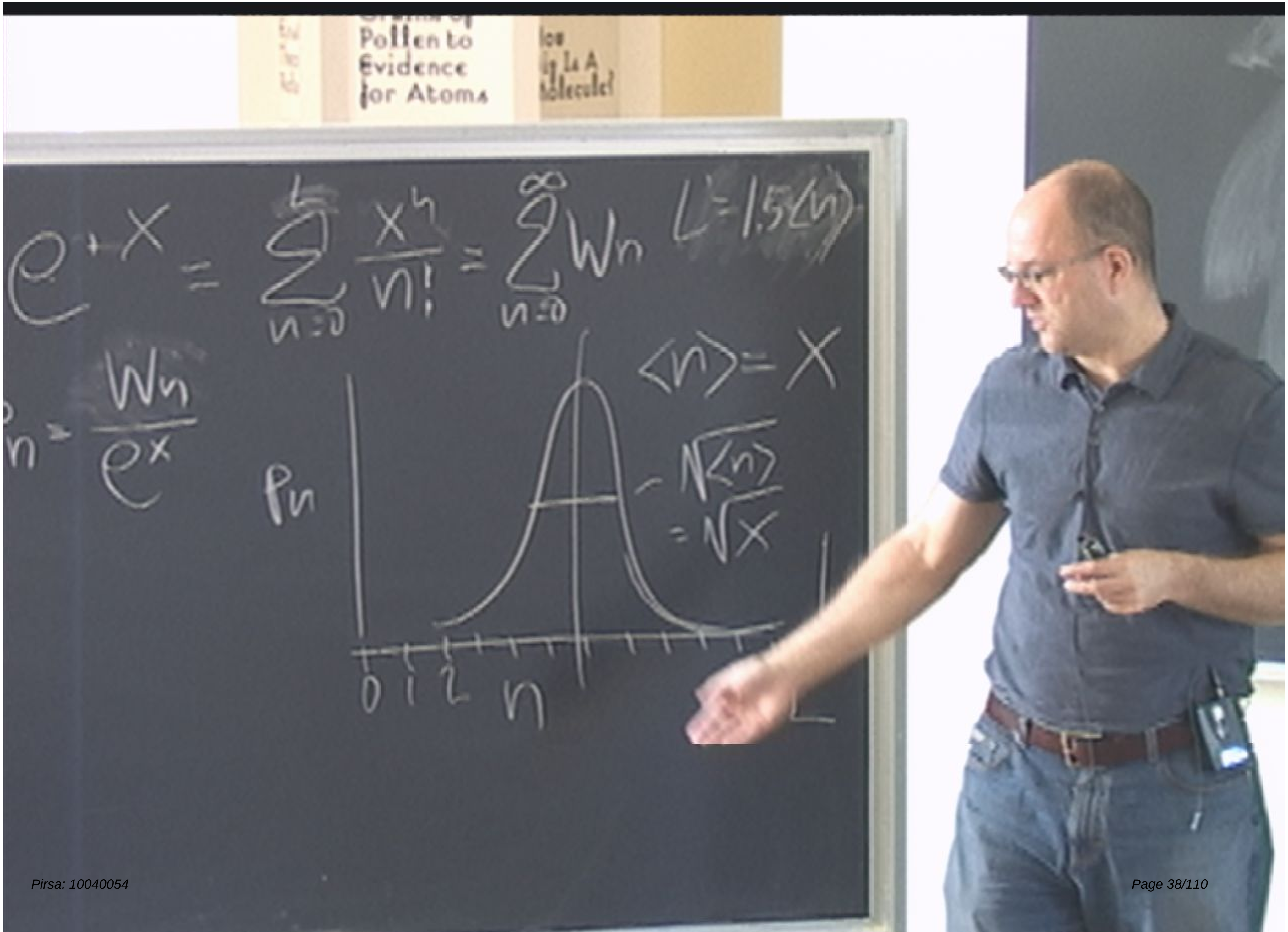
Pollen to
Evidence
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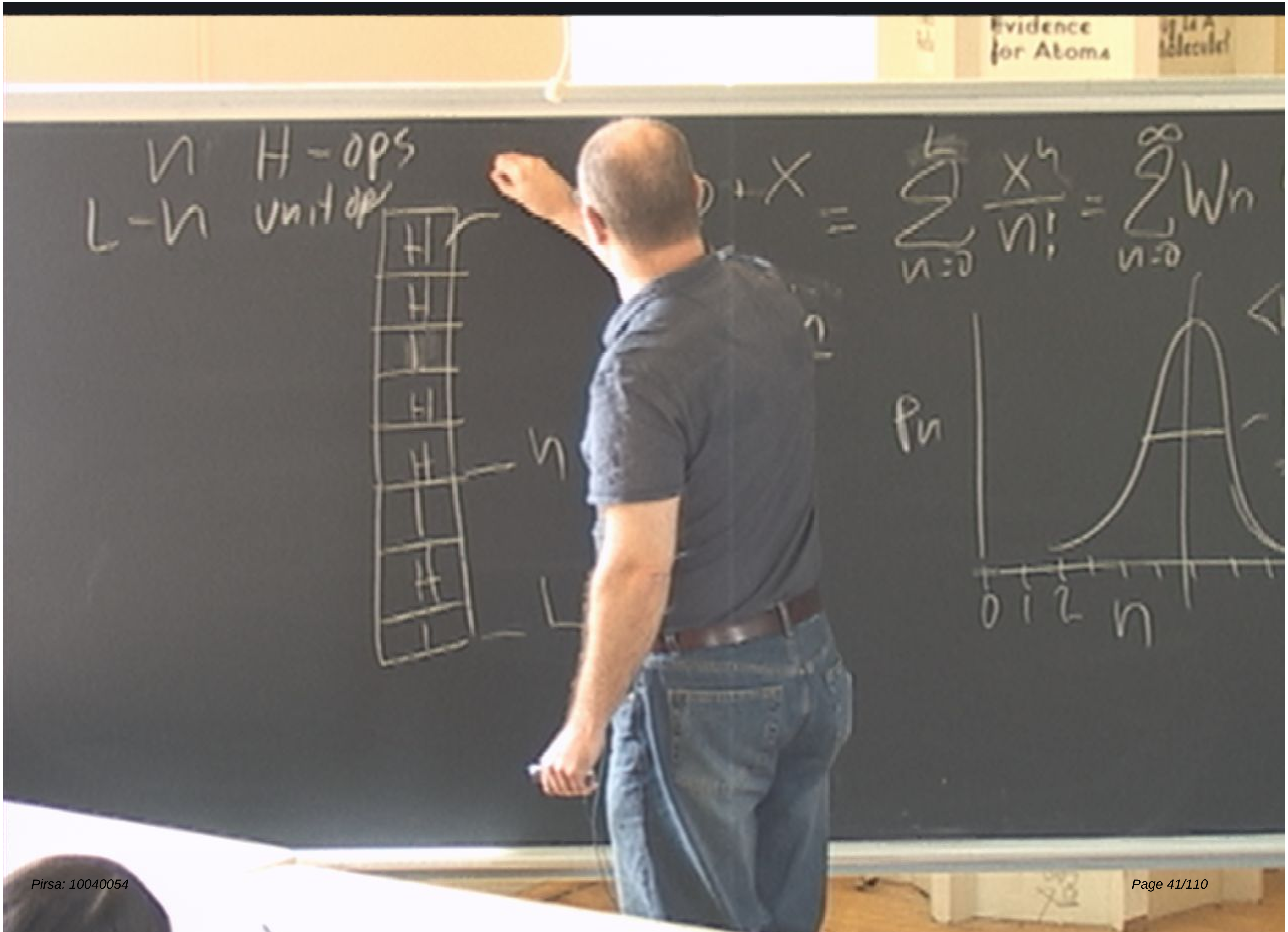
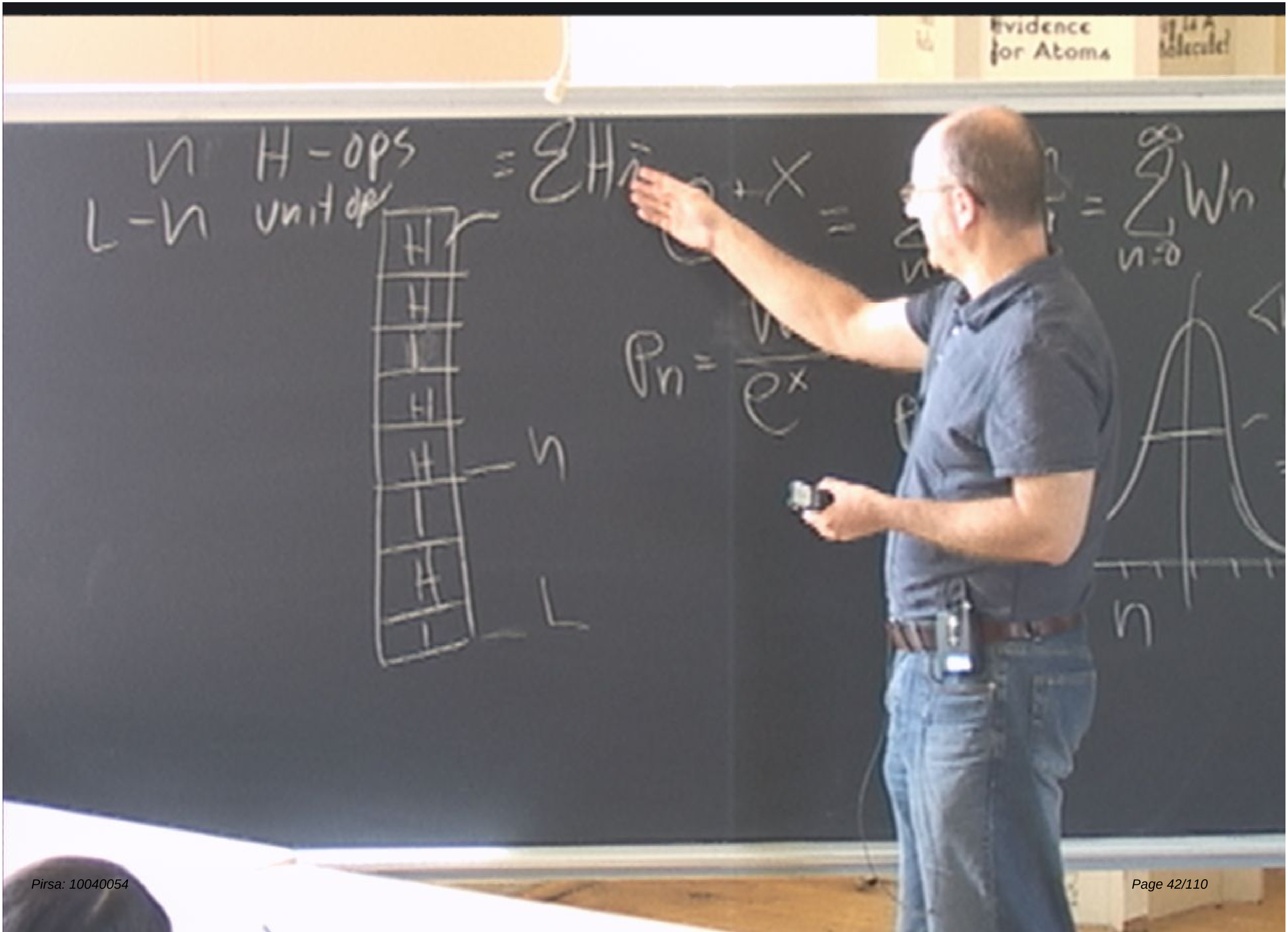

Evidence
for Atoms
n H-ops
L-n unit op
n
L
Pn
0 1 2 n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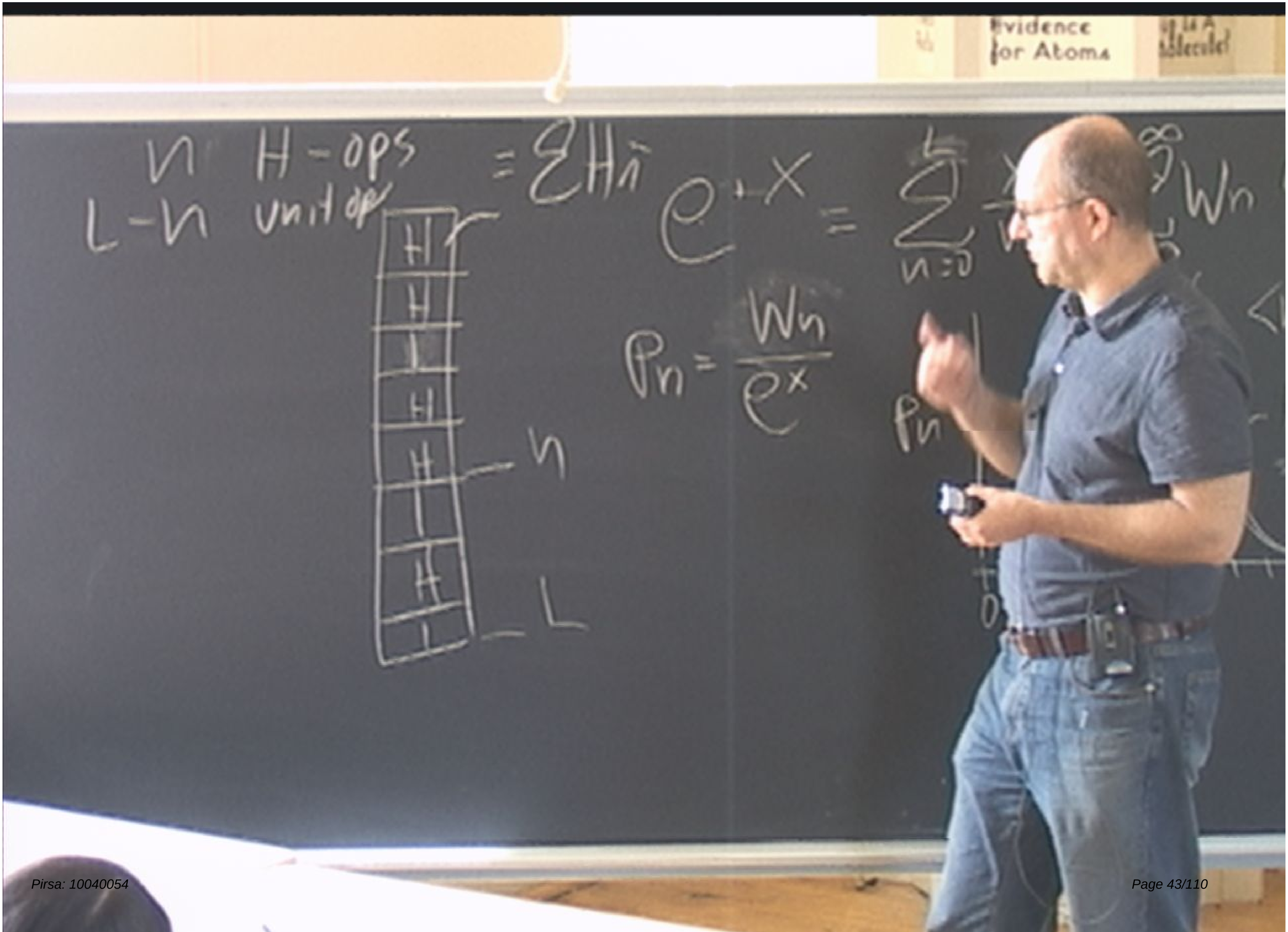
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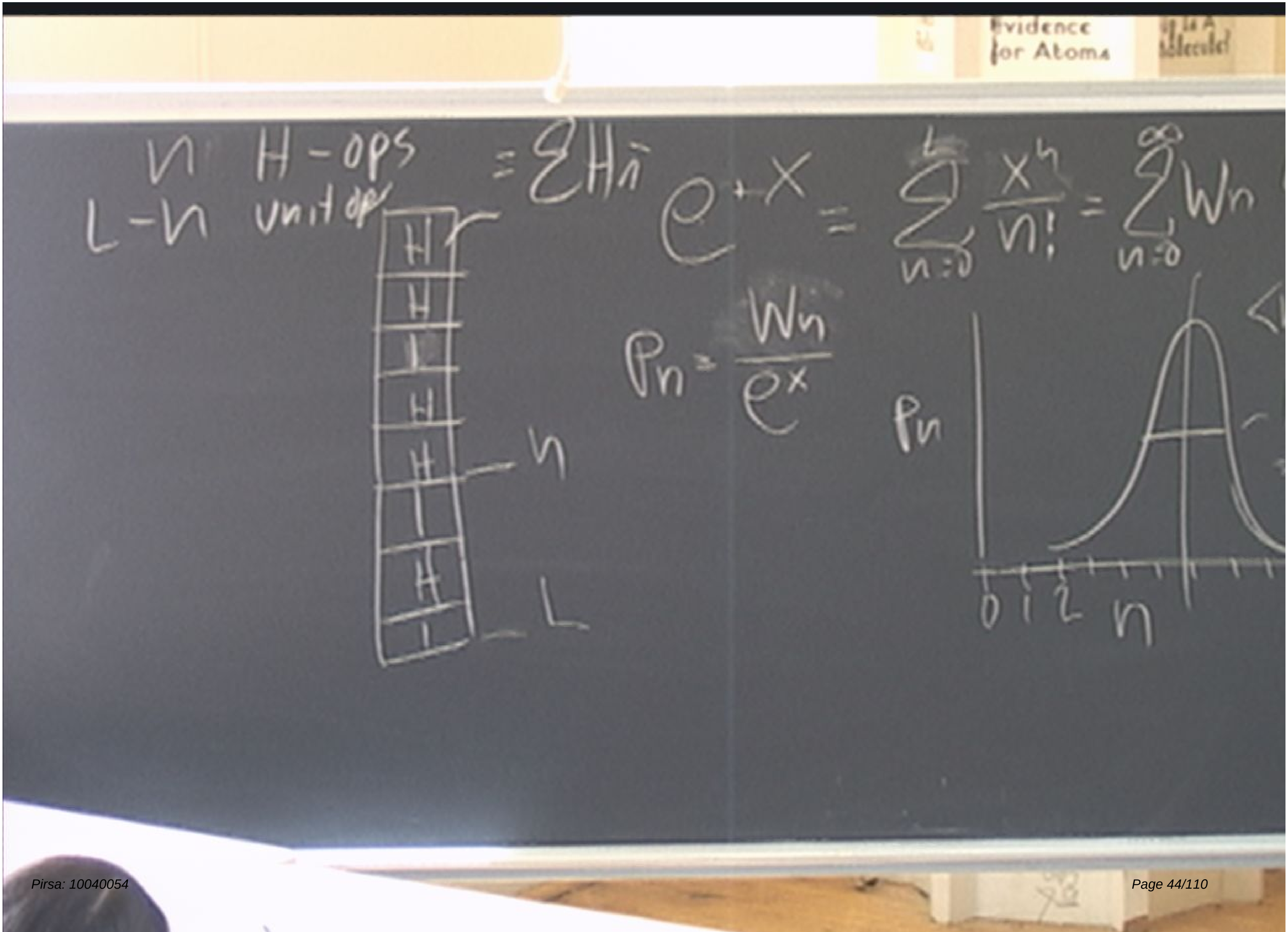
Evidence
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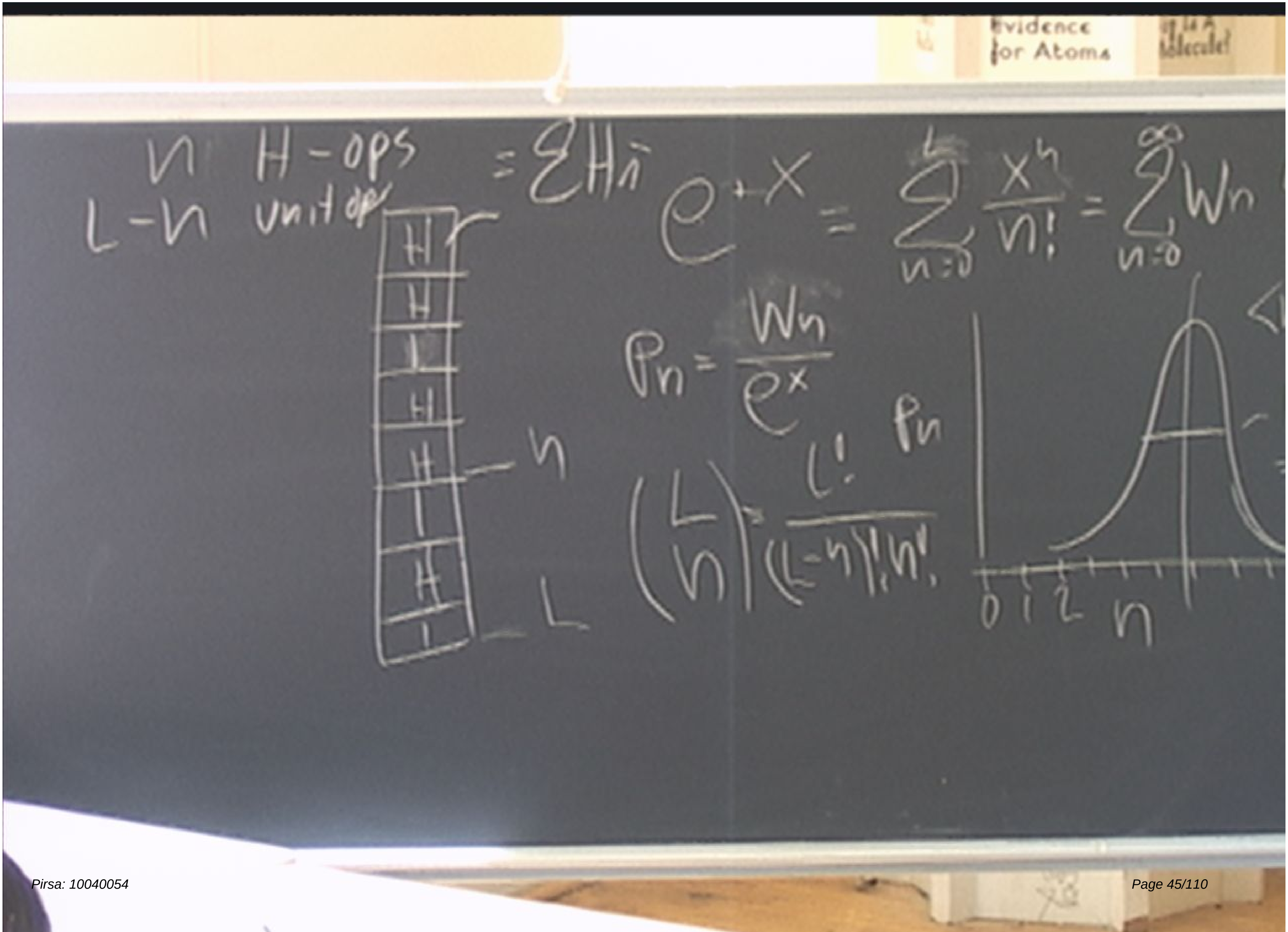
n H-ops
L-n unit op
= ΣH_n
e^{+x} = Σ_{n=0}^{L} x^n/n! = Σ_{n=0}^{∞} W_n
P_n = W_n / e^x
P_n
0 1 2 n
n
L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Pn = Wn / e^x
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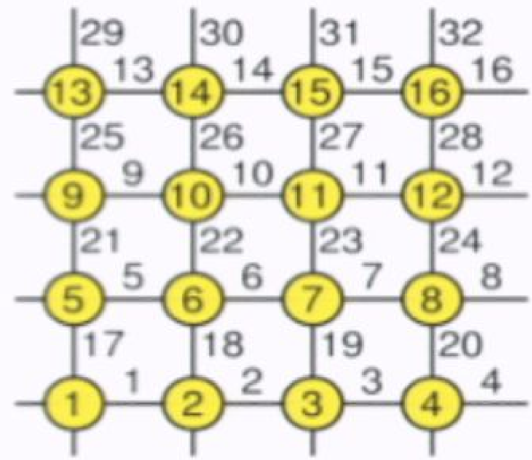
Stochastic Series expansion (SSE): S=1/2 Heisenberg model

Write H as a bond sum for arbitrary lattice

$$H = J \sum_{b=1}^{N_b} \mathbf{S}_{i(b)} \cdot \mathbf{S}_{j(b)},$$

2D square lattice
bond and site labels



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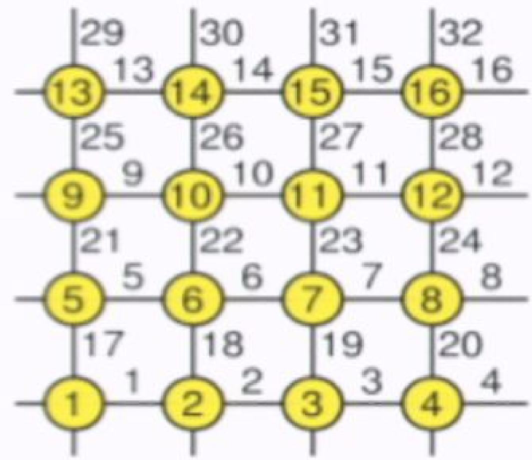

Diagonal (1) and off-diagonal (2) bond operators

$$\begin{aligned} H_{1,b} &= \tfrac{1}{4} - S^z_{i(b)} S^z_{j(b)}, \\ H_{2,b} &= \tfrac{1}{2}(S^+_{i(b)} S^-_{j(b)} + S^-_{i(b)} S^+_{j(b)}). \end{aligned}$$

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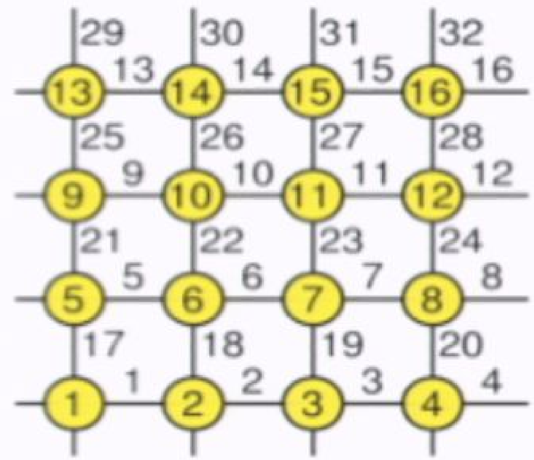

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Four non-zero matrix elements

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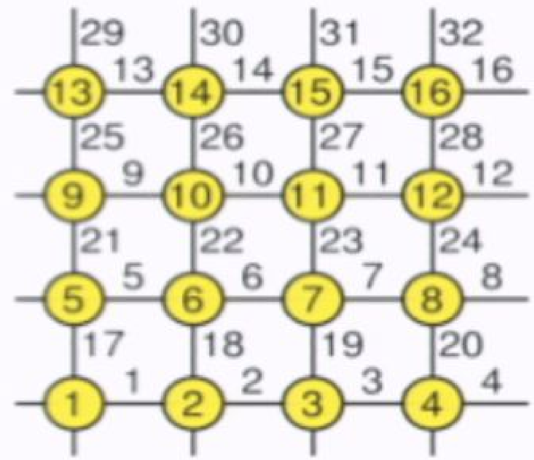

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Partition function

$$Z = \sum_{\alpha}\sum_{n=0}^{\infty}(-1)^{n_2}\frac{\beta^n}{n!}\sum_{S_n}\left\langle \alpha \left| \prod_{p=0}^{n-1} H_{a(p),b(p)} \right| \alpha \right\rangle$$

n_2 = number of a(i)=2 (off-diagonal operators) in the sequence

For fixed-length scheme

$$Z = \sum_{\alpha} \sum_{S_L} (-1)^{n_2} \frac{\beta^n (L-n)!}{L!} \sum_{S_L} \left\langle \alpha \left| \prod_{p=0}^{L-1} H_{a(p),b(p)} \right| \alpha \right\rangle \qquad W(\alpha, S_L) = \left(\frac{\beta}{2}\right)^n \frac{(L-n)!}{L!}$$

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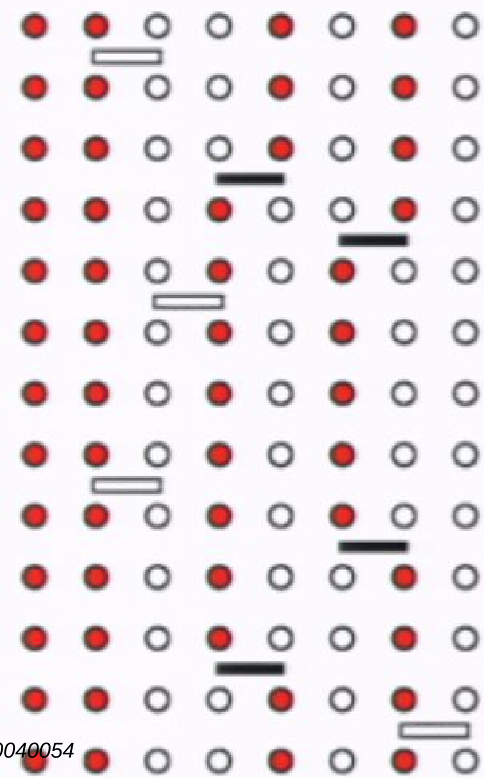
i = 1 2 3 4 5 6 7 8

$\sigma(i)$ = -1 +1 -1 -1 +1 -1 +1 +1



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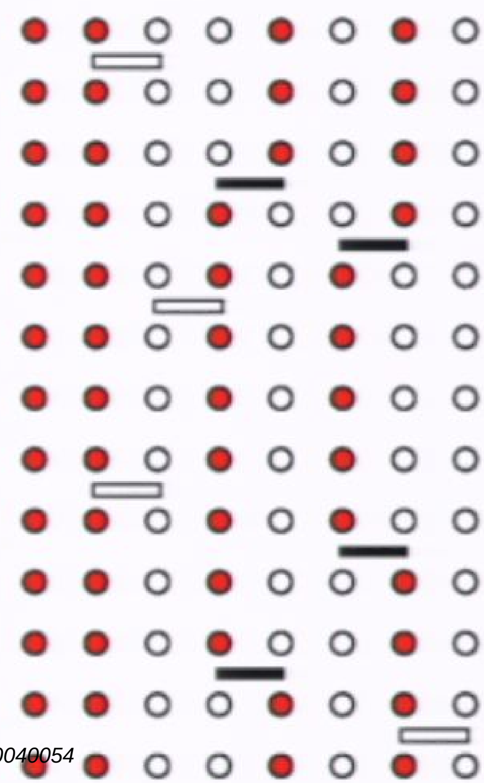

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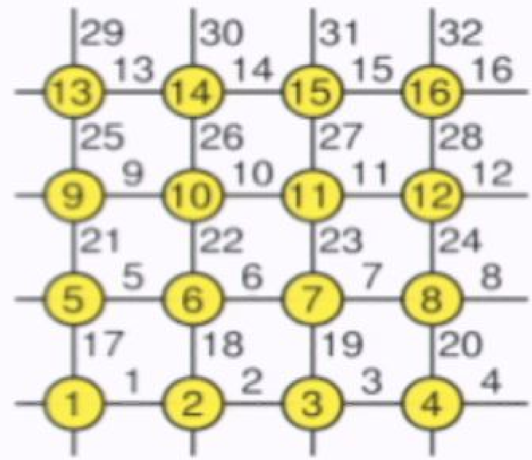
Stochastic Series expansion (SSE): S=1/2 Heisenberg model

Write H as a bond sum for arbitrary lattice

$$H = J \sum_{b=1}^{N_b} \mathbf{S}_{i(b)} \cdot \mathbf{S}_{j(b)},$$

2D square lattice
bond and site labels



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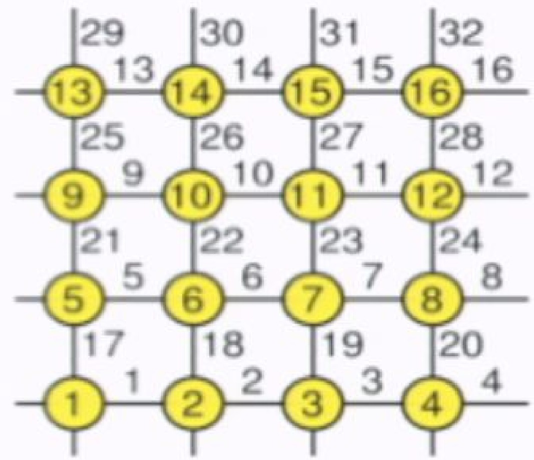

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Four non-zero matrix elements

$$\langle \uparrow_{i(b)} \downarrow_{j(b)} | H_{1,b} | \uparrow_{i(b)} \downarrow_{j(b)} \rangle = \tfrac{1}{2} \qquad \langle \downarrow_{i(b)} \uparrow_{j(b)} | H_{2,b} | \uparrow_{i(b)} \downarrow_{j(b)} \rangle = \tfrac{1}{2}$$

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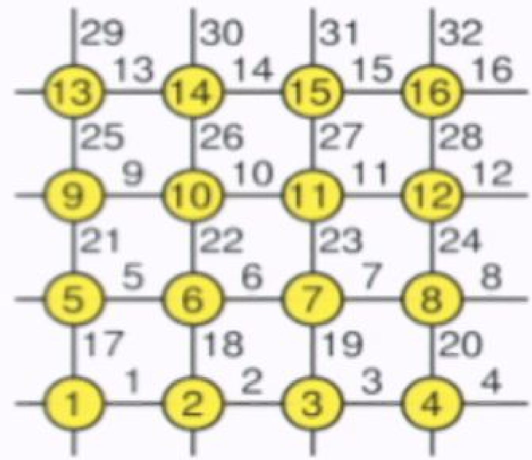

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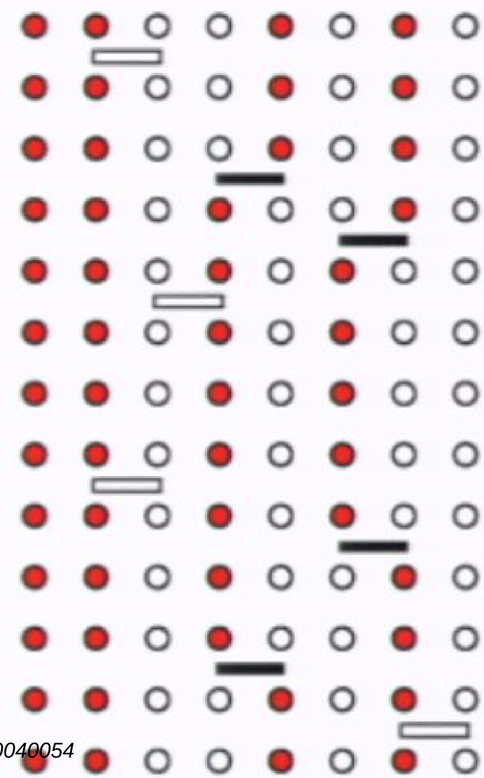

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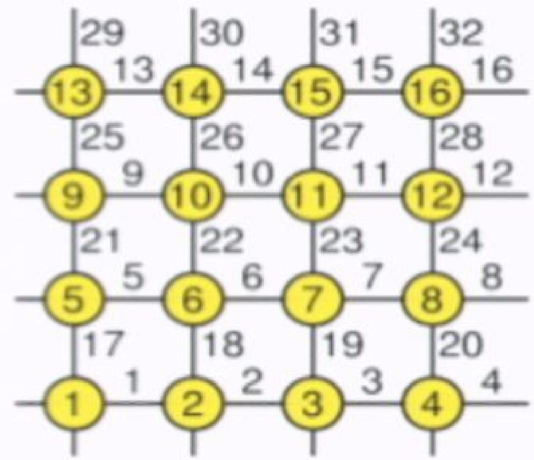

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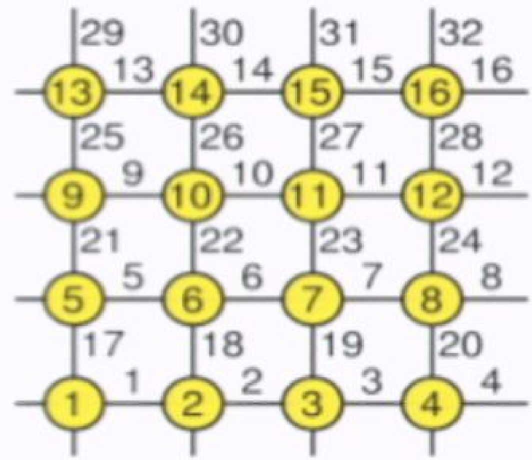

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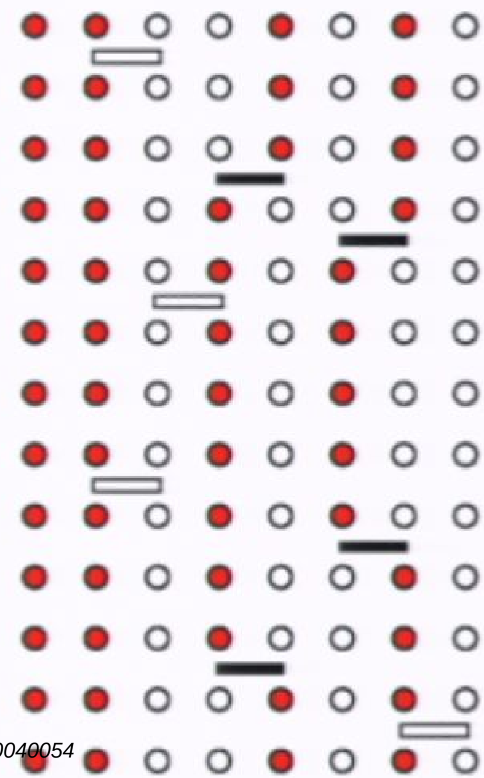

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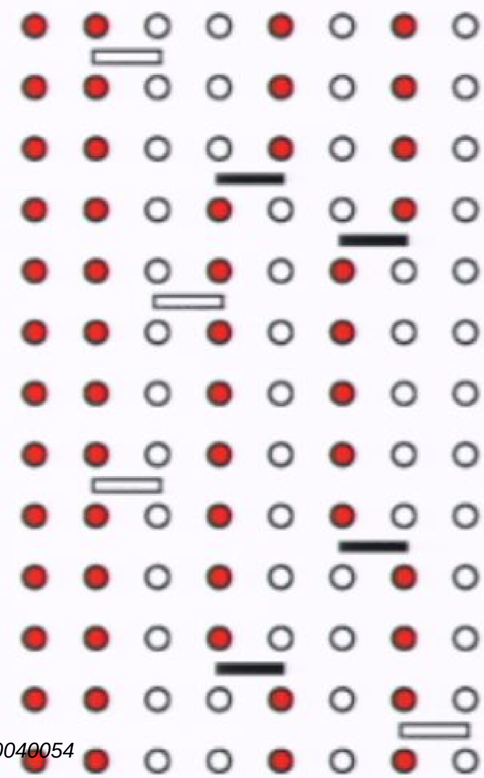

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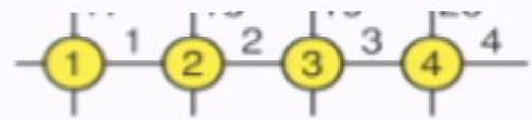

Expectation values

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

Example: hard-core bosons

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

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Equivalent to S=1/2 XY model

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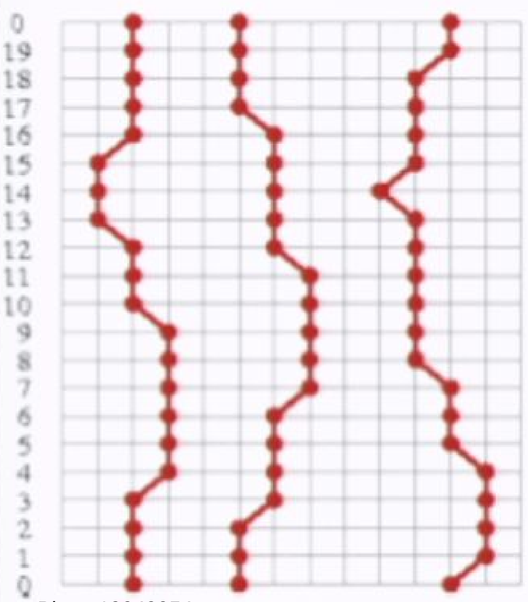
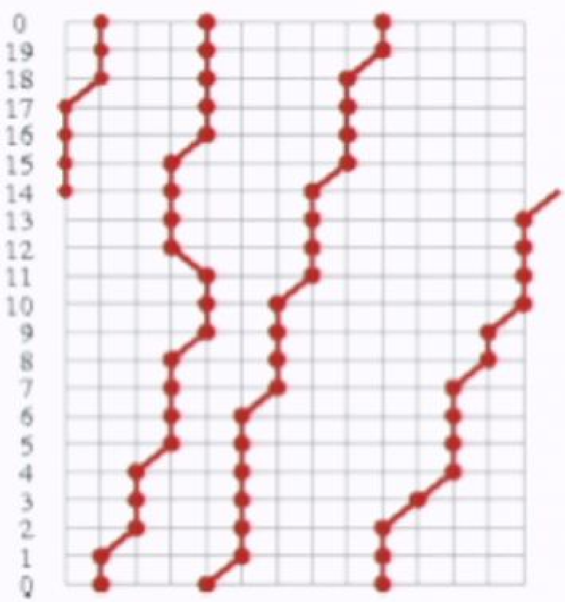
"World line" representation of

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





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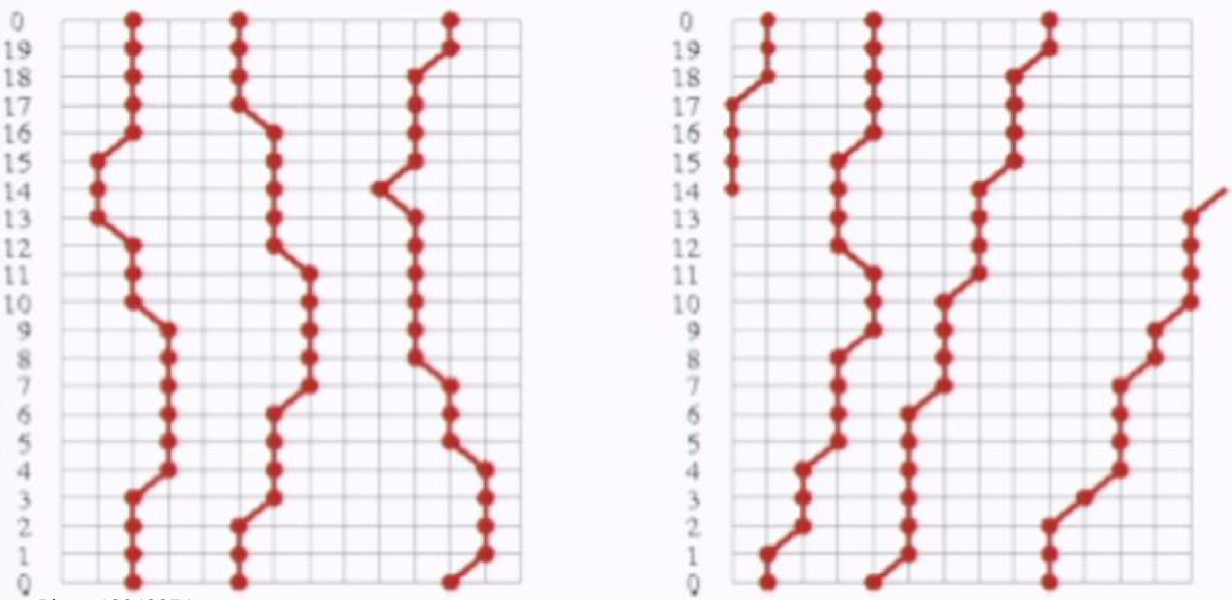
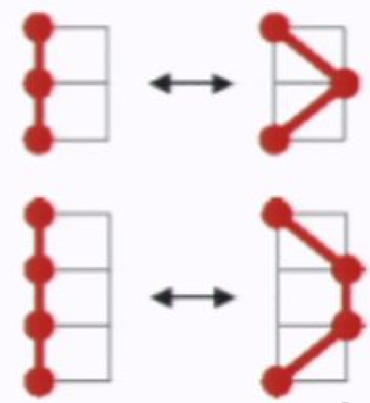


world line moves for Monte Carlo sampling



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

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

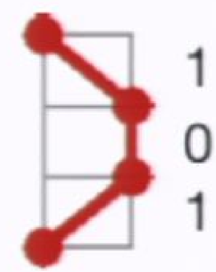
$$W(\{\alpha\}) = \text{weight}$$
$$A(\{\alpha\}) = \text{estimator}$$

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

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

Kinetic energy (here full energy). Use

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



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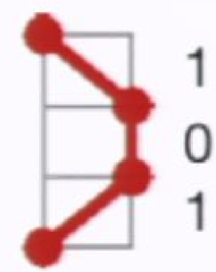

Average over all slices → count number of kinetic jumps

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

ncluding interactions

For any diagonal interaction V (Trotter, or split-operator, approximation)

$$e^{-\Delta_\tau H} = e^{-\Delta_\tau K} e^{-\Delta_\tau V} + \mathcal{O}(\Delta_\tau^2) \rightarrow \langle \alpha_{l+1} | e^{-\Delta_\tau H} | \alpha_l \rangle \approx e^{-\Delta_\tau V_l} \langle \alpha_{l+1} | e^{-\Delta_\tau K} | \alpha_l \rangle$$

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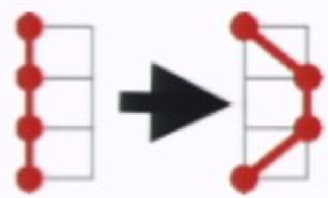
Product over all times slices →

$$W(\{\alpha\}) = \Delta_\tau^{n_K} \exp\left(-\Delta_\tau \sum_{l=0}^{L-1} V_l\right)$$



$$P_{\mathrm{acc}} = \min\left[\Delta_\tau^2 \frac{V_{\mathrm{new}}}{V_{\mathrm{old}}}, 1\right]$$

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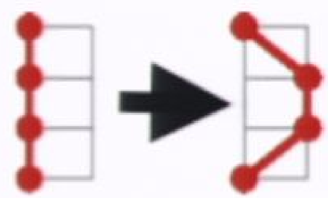
$$e^{-\Delta_\tau H} = e^{-\Delta_\tau K} e^{-\Delta_\tau V} + \mathcal{O}(\Delta_\tau^2) \rightarrow \langle \alpha_{l+1} | e^{-\Delta_\tau H} | \alpha_l \rangle \approx e^{-\Delta_\tau V_l} \langle \alpha_{l+1} | e^{-\Delta_\tau K} | \alpha_l \rangle$$

Product over all times slices →

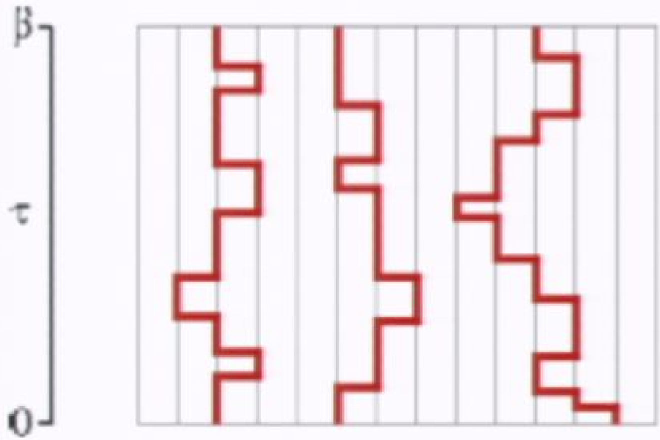
$$W(\{\alpha\}) = \Delta_\tau^{n_K} \exp\left(-\Delta_\tau \sum_{l=0}^{L-1} V_l \right)$$



$$P_{\text{acc}} = \min\left[\Delta_\tau^2 \frac{V_{\text{new}}}{V_{\text{old}}}, 1 \right]$$

The continuous time limit

Limit $\Delta_\tau \rightarrow 0$: number of kinetic jumps remains finite, store events only



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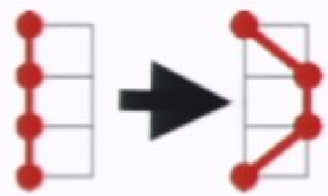

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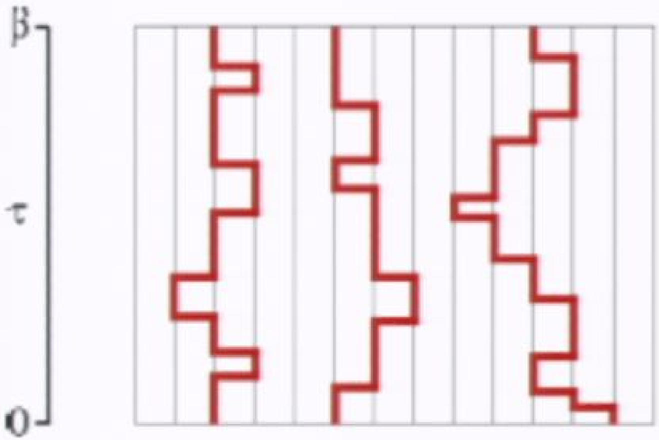

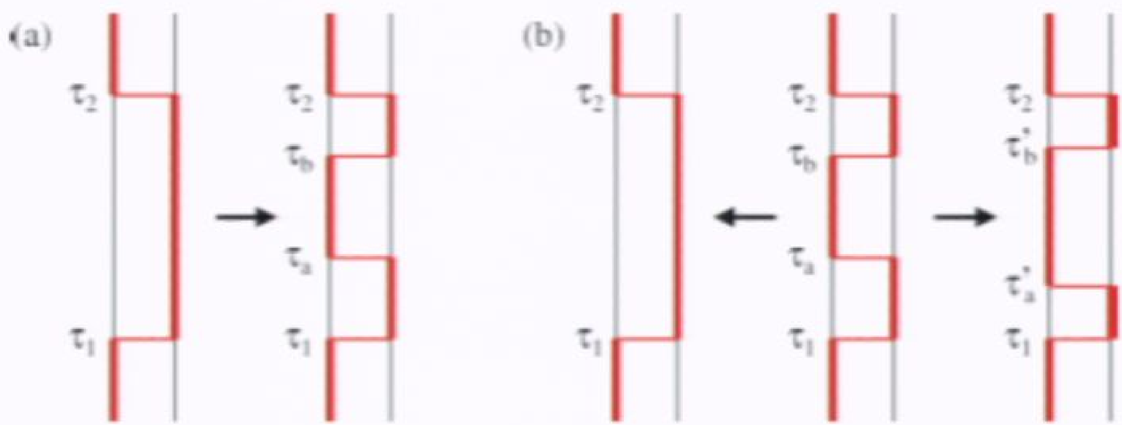

Special methods (**loop and worm updates**) developed for efficient

local updates (problem when $\Delta_\tau \rightarrow 0$?)

- consider probability of inserting/removing events within a time window

Series expansion representation

Start from the Taylor expansion $e^{-\beta H} = \sum_{n=0}^{\infty} \frac{(-\beta)^n}{n!} H^n$ (approximation-free method from the outset)

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Similar to the path integral; $1 - \Delta\tau H \to H$ and weight factor outside

For hard-core bosons the (allowed) path weight is $W(\{\alpha\}_n) = \beta^n / n!$

For any model, the energy is

this is the operator we "measure"

$$E = \frac{1}{Z} \sum_{n=0}^{\infty} \frac{(-\beta)^n}{n!} \sum_{\{\alpha\}_{n+1}} \langle \alpha_0 | H | \alpha_n \rangle \cdots \langle \alpha_2 | H | \alpha_1 \rangle \langle \alpha_1 | H | \alpha_0 \rangle$$

one more "slice" to sum over here

$$= -\frac{1}{Z} \sum_{n=1}^{\infty} \frac{(-\beta)^n}{n!} \frac{n}{\beta} \sum_{\{\alpha\}_n} \langle \alpha_0 | H | \alpha_{n-1} \rangle \cdots \langle \alpha_2 | H | \alpha_1 \rangle \langle \alpha_1 | H | \alpha_0 \rangle = \frac{\langle n \rangle}{\beta}$$

relabel terms to "get rid of" extra slice

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$$C = \langle n^2 \rangle - \langle n \rangle^2 - \langle n \rangle$$

From this follows: narrow n-distribution with $\langle n \rangle \propto N\beta, \quad \sigma_n \propto \sqrt{N\beta}$

Fixed-length scheme: cut-off at N=L, fill in with unit operators $H_0=1$

$$Z = \sum^{L} \frac{(-\beta)^n (L-n)!}{L!} \sum \sum \langle \alpha_0 | H_{i(L)} | \alpha_{L-1} \rangle \cdots \langle \alpha_2 | H_{i(2)} | \alpha_1 \rangle \langle \alpha_1 | H_{i(1)} | \alpha_0 \rangle$$

For fixed-length scheme

$$Z = \sum_{\alpha} \sum_{S_L} (-1)^{n_2} \frac{\beta^n (L-n)!}{L!} \sum_{S_L} \left\langle \alpha \left| \prod_{p=0}^{L-1} H_{a(p),b(p)} \right| \alpha \right\rangle \qquad W(\alpha, S_L) = \left(\frac{\beta}{2}\right)^n \frac{(L-n)!}{L!}$$

Propagated states: $|\alpha(p)\rangle \propto \prod_{i=0}^{p-1} H_{a(i),b(i)} |\alpha\rangle$

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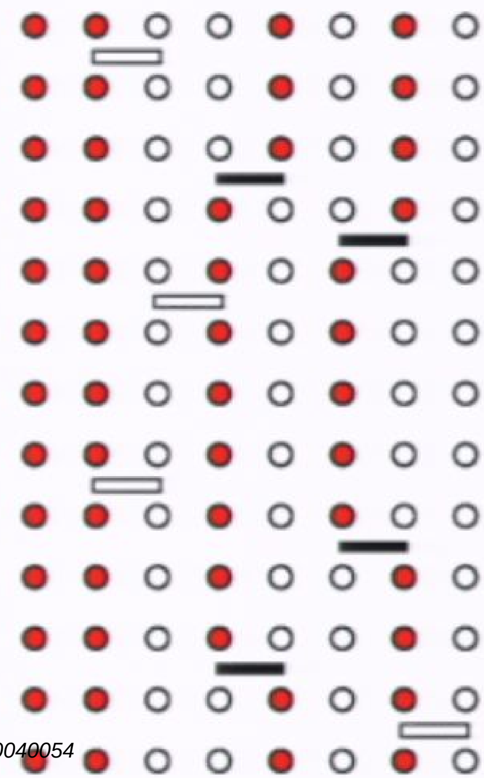
i = 1 2 3 4 5 6 7 8

$\sigma(i)$ = -1 +1 -1 -1 +1 -1 +1 +1



p	$a(p)$	$b(p)$	$s(p)$
11	1	2	4
10	0	0	0
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W>0 (n_2 even) for bipartite lattice

Frustration leads to **sign problem**

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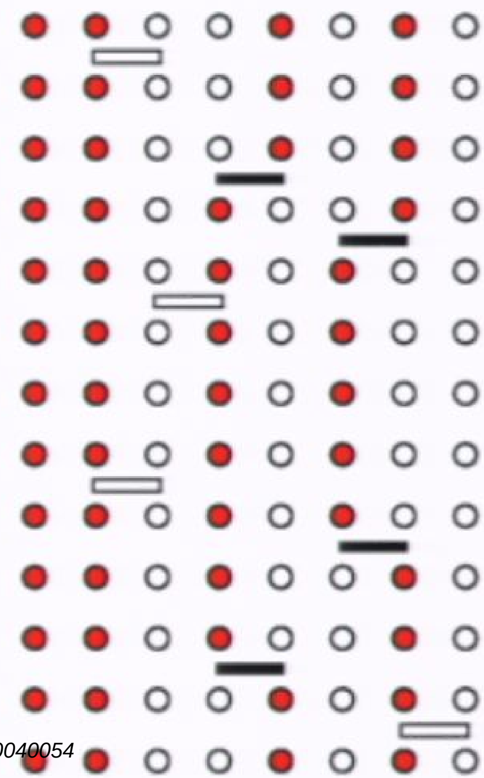

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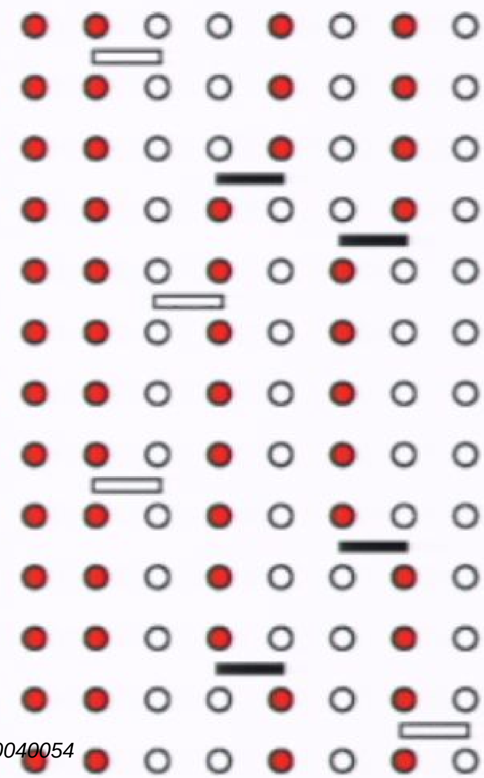

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In a program:

s(p) = operator-index string
- **s(p) = 2*b(p) + a(p)-1**
- diagonal; s(p) = even
- off-diagonal; s(p) = off

σ(i) = spin state, i=1,...,N
- only one has to be stored

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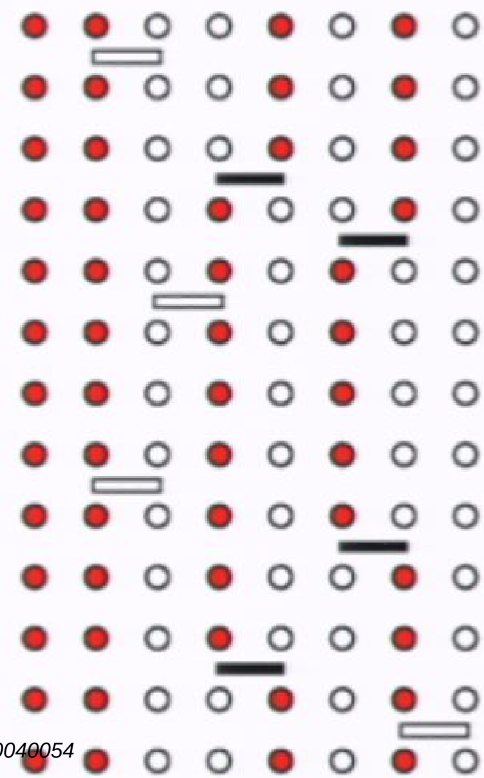

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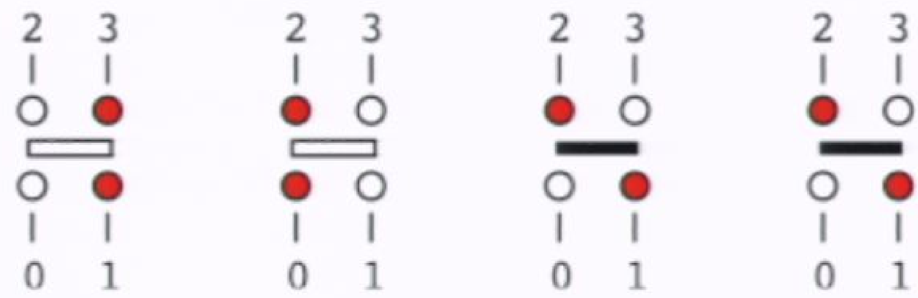
Linked vertex storage

The "legs" of a vertex represents the spin states before (below) and after (above) an operator has acted



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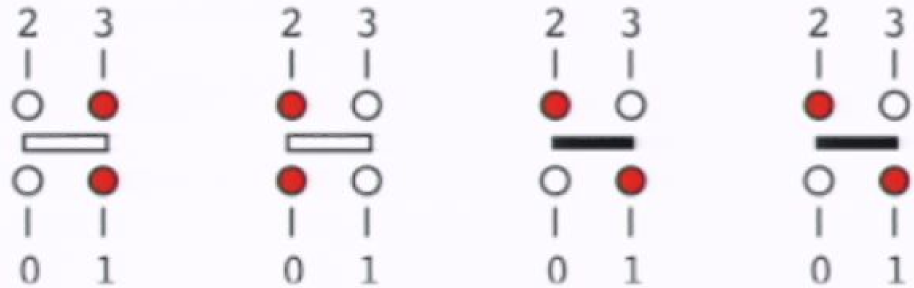

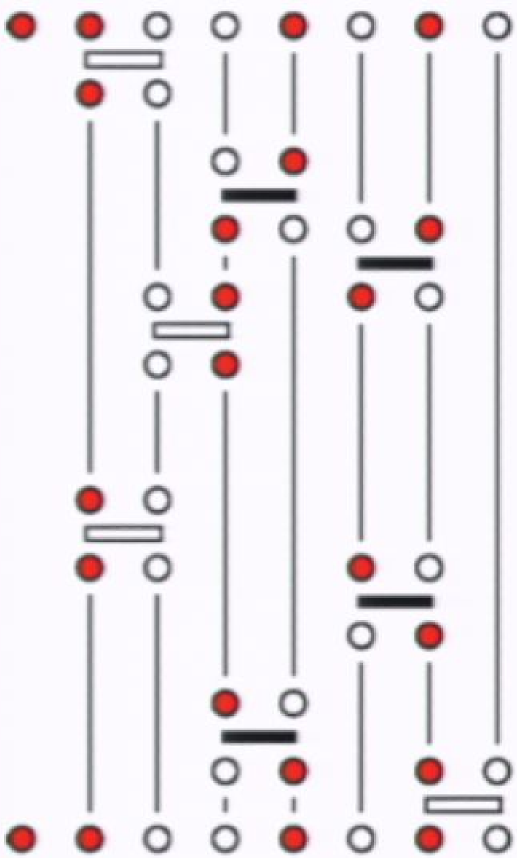

p	v	X(v)	v	X(v)	v	X(v)	v	X(v)
11	44	18	45	30	46	16	47	17
10	40	-	41	-	42	-	43	-
9	36	31	37	7	38	4	39	5
8	32	14	31	15	34	12	35	0
7	28	19	29	6	30	45	31	36
6	24	-	25	-	26	-	27	-
5	20	-	21	-	22	-	23	-
4	16	46	17	47	18	44	19	28
3	12	34	13	2	14	32	15	33
2	8	-	9	-	10	-	11	-
1	4	38	5	39	6	29	7	37
0	0	35	1	3	2	13	3	1
	l=0		l=1		l=2		l=3	

Spin states between operations are redundant; represented by links

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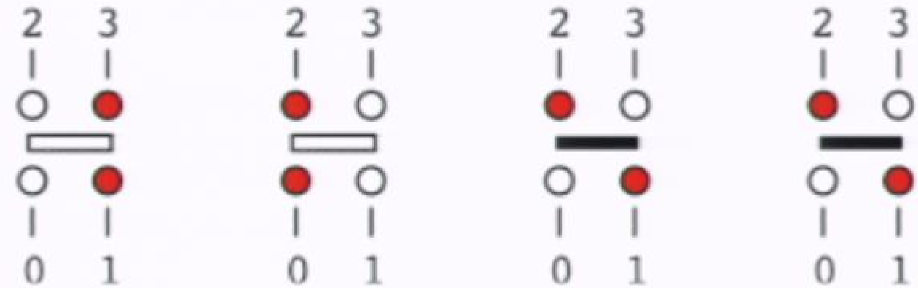

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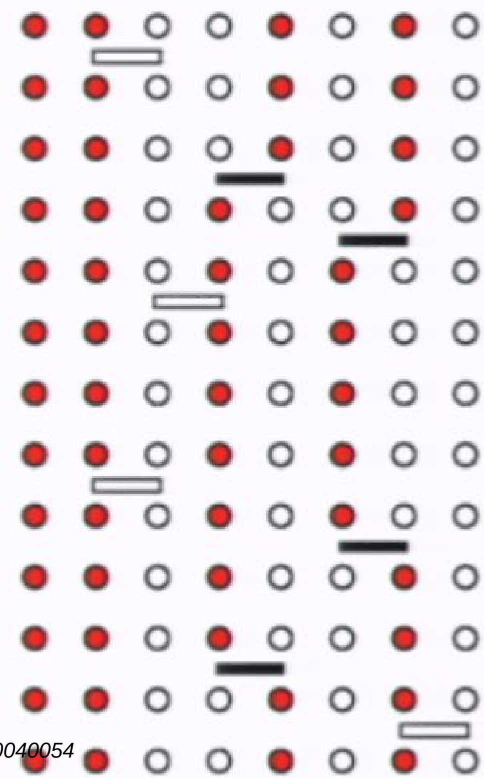

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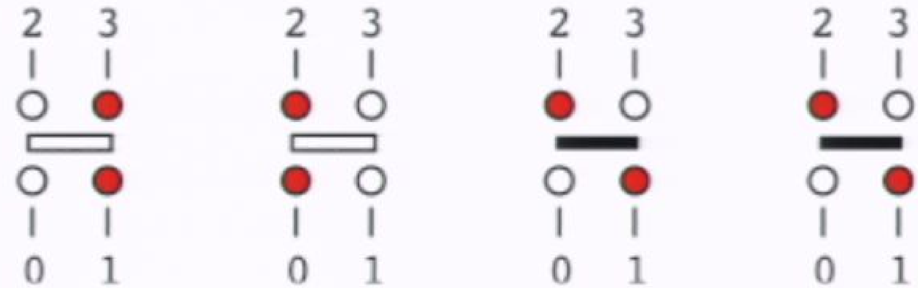

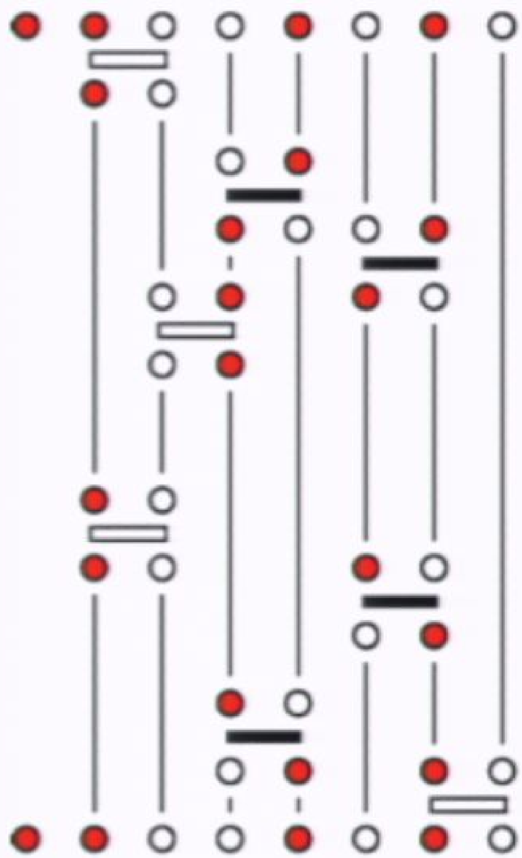

p	v (l=0)	X(v) (l=0)	v (l=1)	X(v) (l=1)	v (l=2)	X(v) (l=2)	v (l=3)	X(v) (l=3)
11	44	18	45	30	46	16	47	17
10	40	-	41	-	42	-	43	-
9	36	31	37	7	38	4	39	5
8	32	14	31	15	34	12	35	0
7	28	19	29	6	30	45	31	36
6	24	-	25	-	26	-	27	-
5	20	-	21	-	22	-	23	-
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2	8	-	9	-	10	-	11	-
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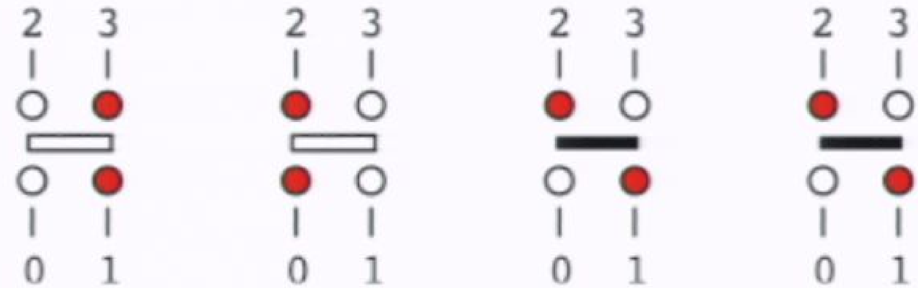

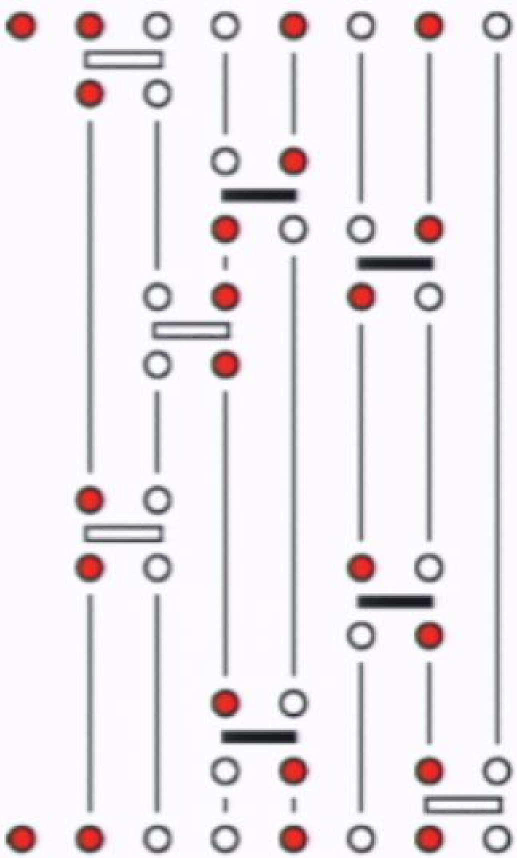

p	v (l=0)	X(v) (l=0)	v (l=1)	X(v) (l=1)	v (l=2)	X(v) (l=2)	v (l=3)	X(v) (l=3)
11	44	18	45	30	46	16	47	17
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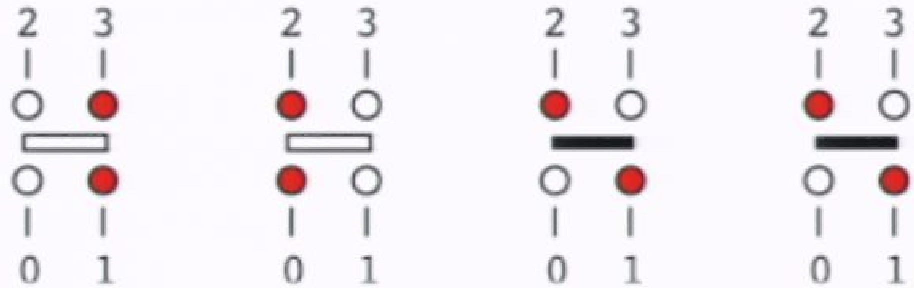

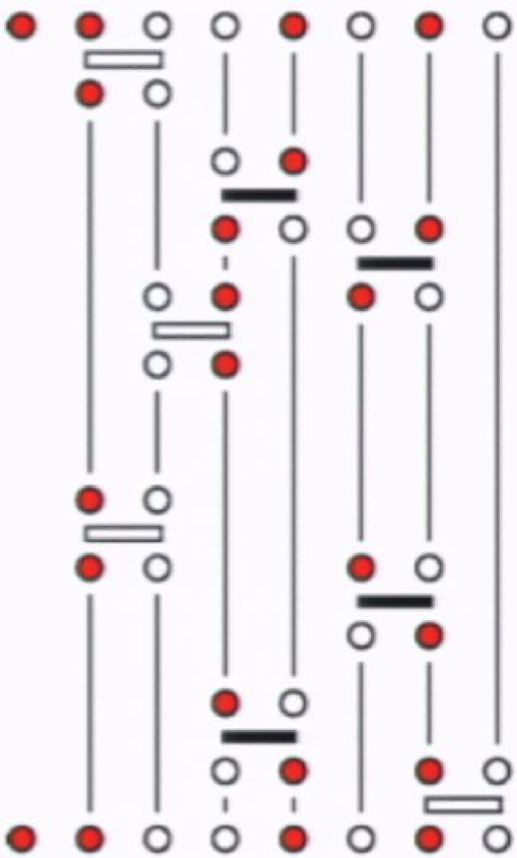

p	v	X(v)	v	X(v)	v	X(v)	v	X(v)
11	44	18	45	30	46	16	47	17
10	40	-	41	-	42	-	43	-
9	36	31	37	7	38	4	39	5
8	32	14	31	15	34	12	35	0
7	28	19	29	6	30	45	31	36
6	24	-	25	-	26	-	27	-
5	20	-	21	-	22	-	23	-
4	16	46	17	47	18	44	19	28
3	12	34	13	2	14	32	15	33
2	8	-	9	-	10	-	11	-
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0	0	35	1	3	2	13	3	1
	$l=0$		$l=1$		$l=2$		$l=3$	

X( ) = vertex list

- operator at p→X(v)
  v=4p+l, l=0,1,2,3
- links to next and previous leg

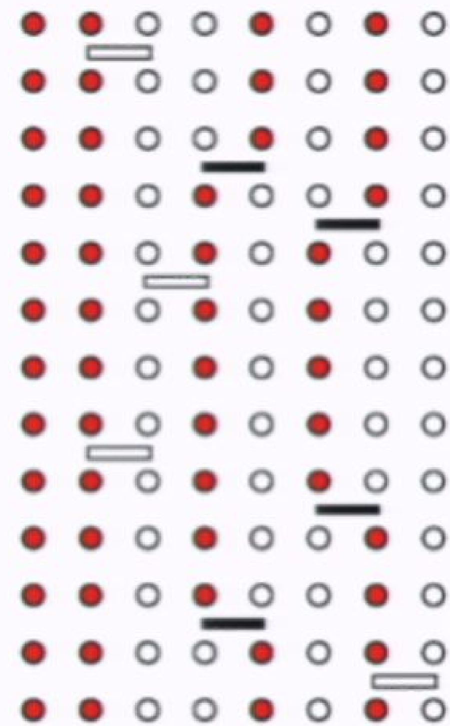
Spin states between operations are redundant; represented by links

Monte Carlo sampling scheme

Change the configuration; $(\alpha, S_L) \to (\alpha', S_L')$

$$W(\alpha, S_L) = \left(\frac{\beta}{2}\right)^n \frac{(L-n)!}{L!}$$

$$P_{\text{accept}} = \min\left[\frac{W(\alpha', S_L)}{W(\alpha, S_L)} \frac{P_{\text{select}}(\alpha', S_L' \to \alpha, S_L)}{P_{\text{select}}(\alpha, S_L \to \alpha', S_L')}, 1\right]$$



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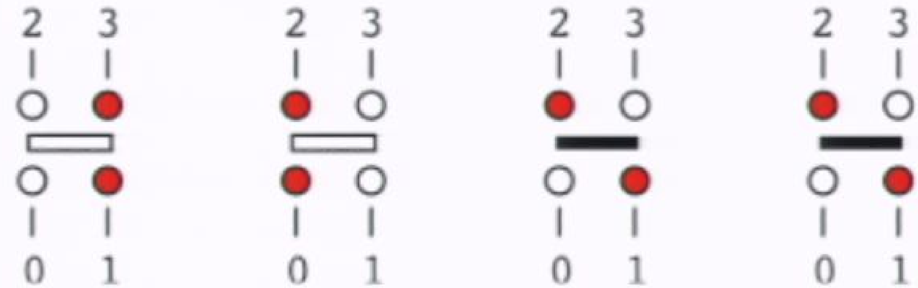

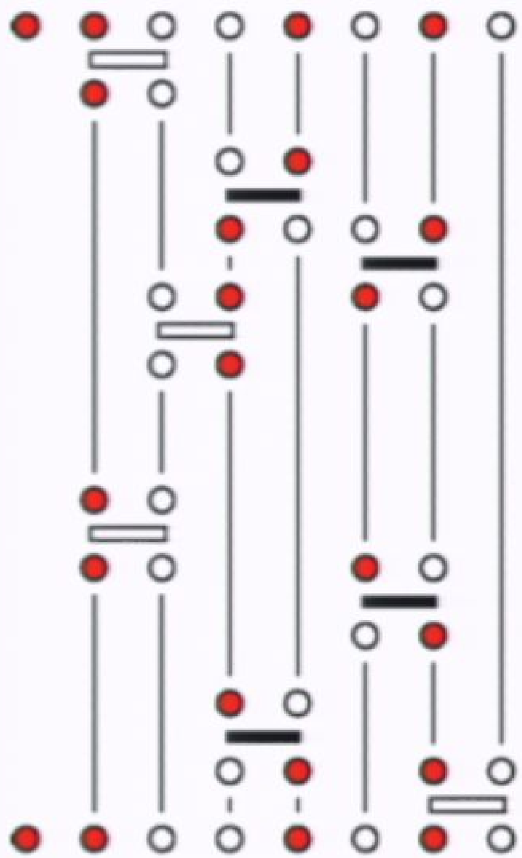

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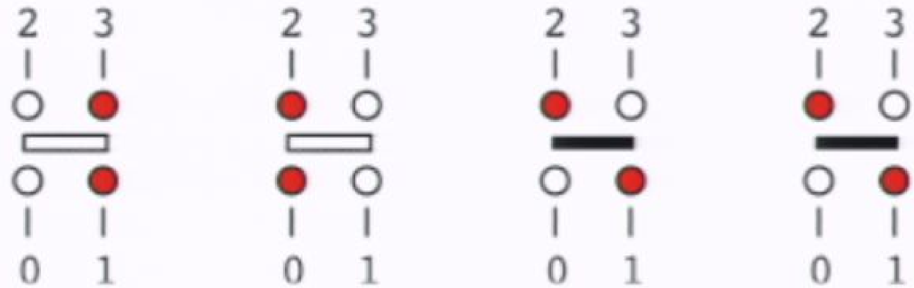
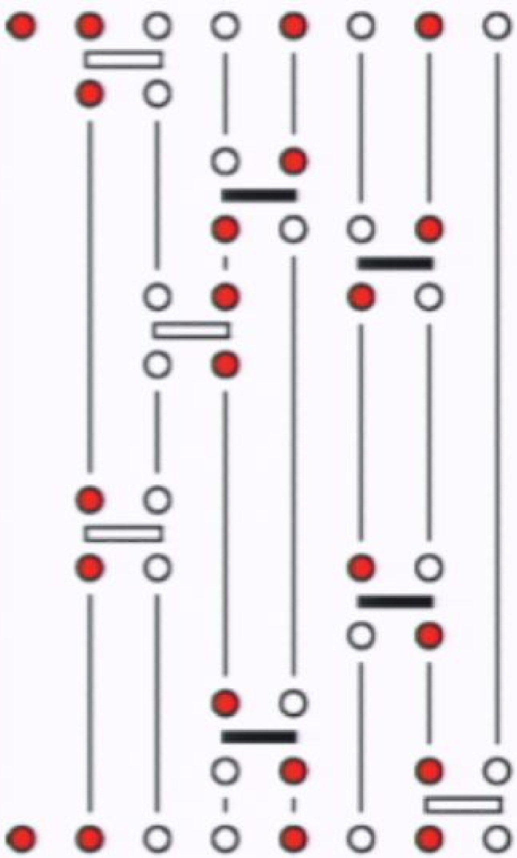
0	0	35	1	3	2	13	3	1
	l=0		l=1		l=2		l=3	

Spin states between operations are redundant; represented by links

Linked vertex storage

The "legs" of a vertex represents the spin states before (below) and after (above) an operator has acted





p	v	X(v)	v	X(v)	v	X(v)	v	X(v)
11	44	18	45	30	46	16	47	17
10	40	-	41	-	42	-	43	-
9	36	31	37	7	38	4	39	5
8	32	14	31	15	34	12	35	0
7	28	19	29	6	30	45	31	36
6	24	-	25	-	26	-	27	-
5	20	-	21	-	22	-	23	-
4	16	46	17	47	18	44	19	28
3	12	34	13	2	14	32	15	33
2	8	-	9	-	10	-	11	-
1	4	38	5	39	6	29	7	37
0	0	35	1	3	2	13	3	1
	$l=0$		$l=1$		$l=2$		$l=3$	

X( ) = vertex list

- operator at p→X(v)
  v=4p+l, l=0,1,2,3
- links to next and previous leg

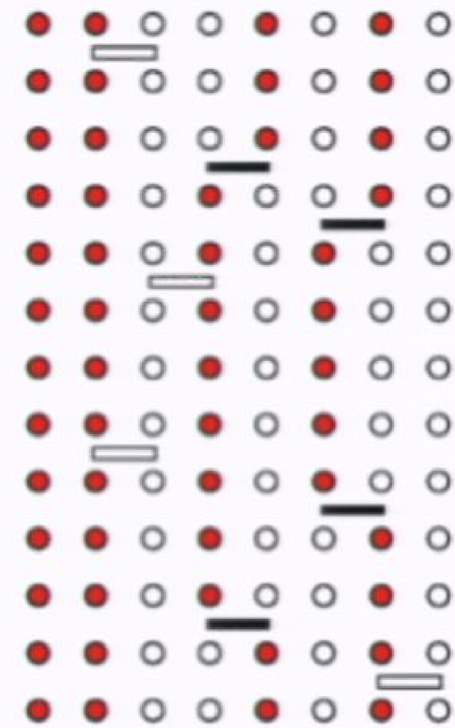
Spin states between operations are redundant; represented by links

Monte Carlo sampling scheme

Change the configuration; $(\alpha, S_L) \rightarrow (\alpha', S'_L)$

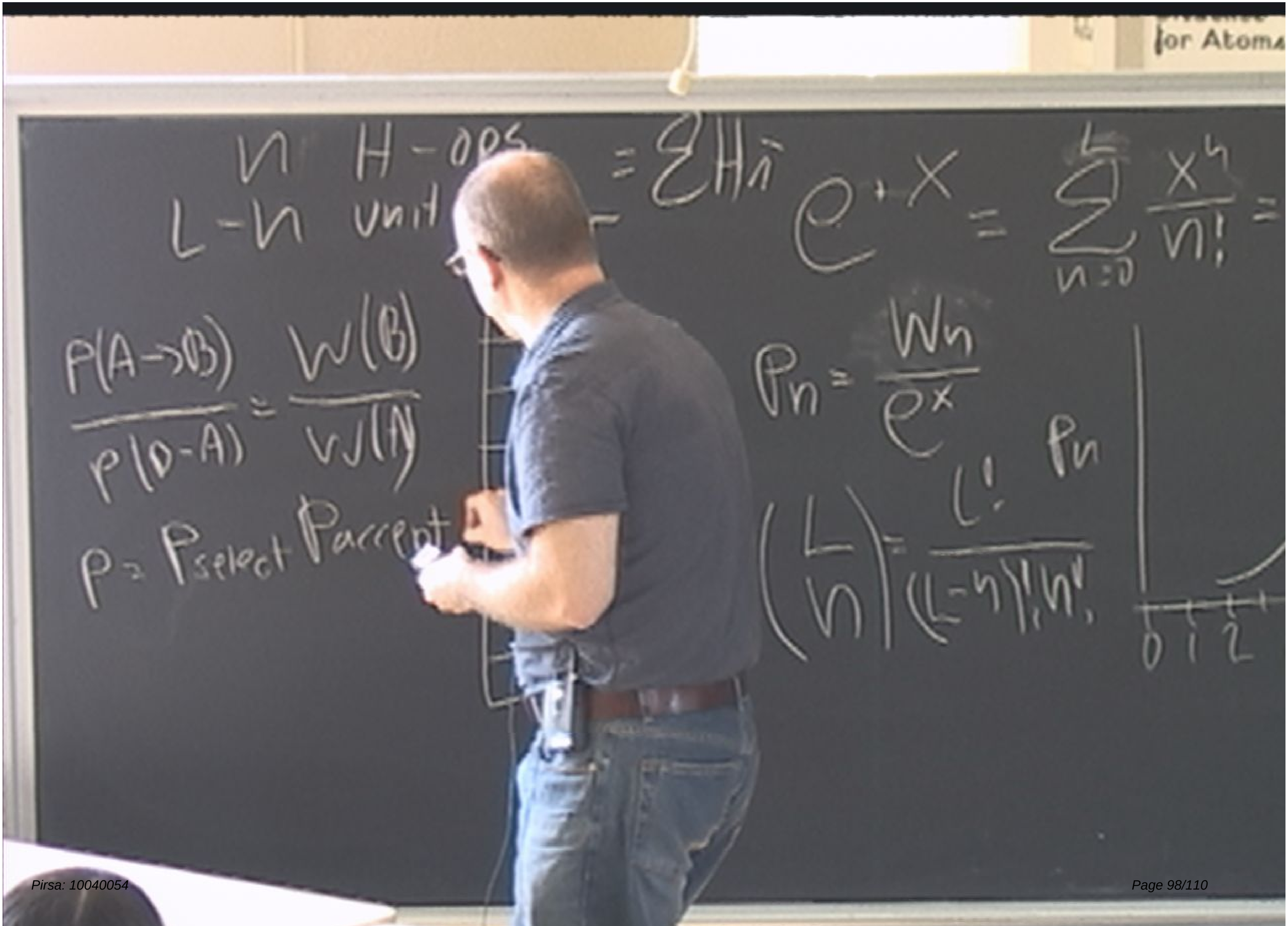
$$W(\alpha, S_L) = \left(\frac{\beta}{2}\right)^n \frac{(L-n)!}{L!}$$

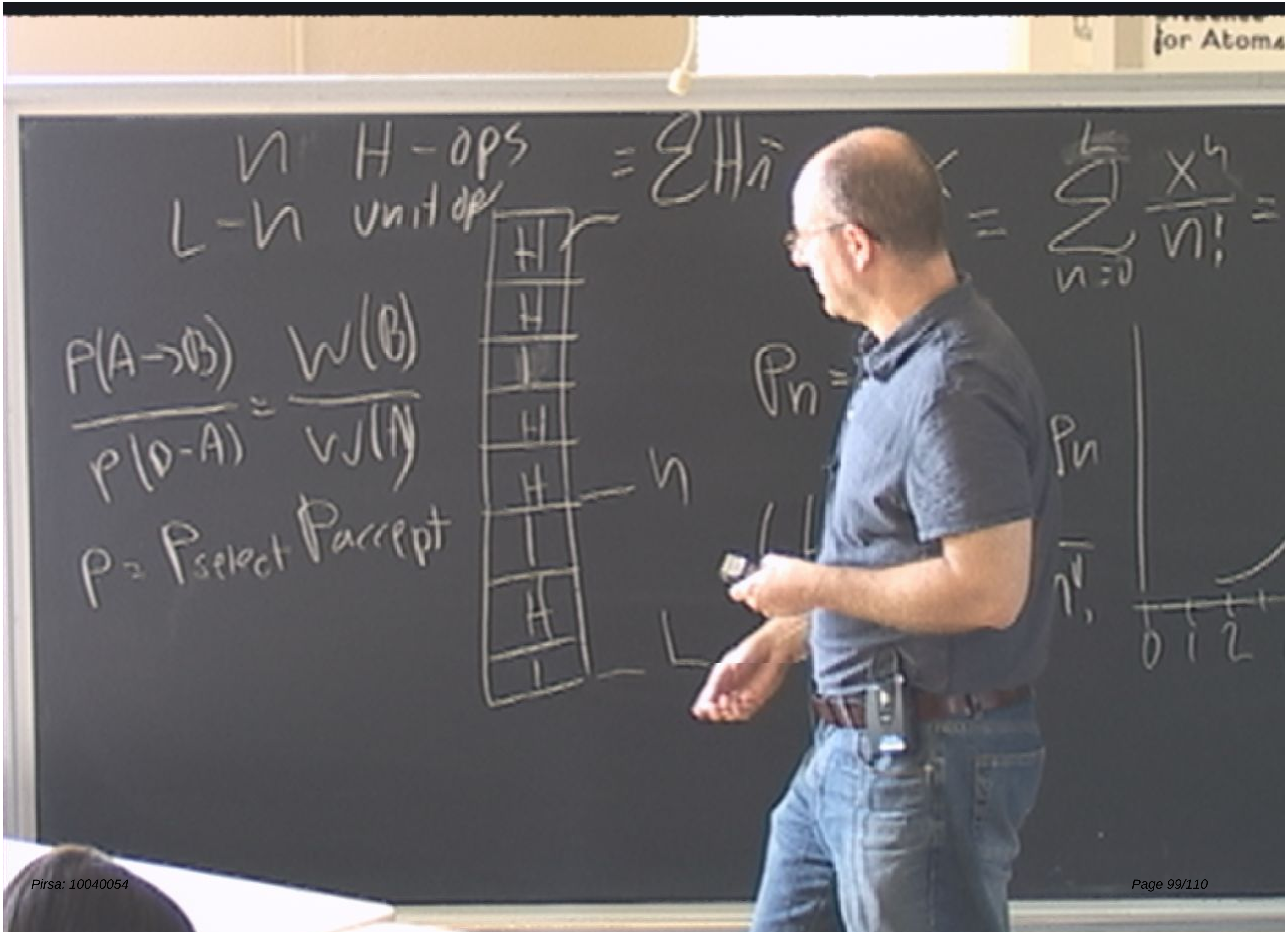
$$P_{\text{accept}} = \min\left[\frac{W(\alpha', S_L)}{W(\alpha, S_L)} \frac{P_{\text{select}}(\alpha', S'_L \rightarrow \alpha, S_L)}{P_{\text{select}}(\alpha, S_L \rightarrow \alpha', S'_L)}, 1\right]$$



Diagonal update: $[0,0]_p \leftrightarrow [1,b]_p$

Attempt at p=0,...,L-1. Need to know |α(p)>
- generate by flipping spins when off-diagonal operator


for Atom
n H-ops
L-n unit
= ΣHi
e^x = Σ x^n / n!
P(A→B) / P(B→A) = W(B) / W(A)
P = Pselect Paccept
Pn = Wn / e^x
(L n) = L! / ((L-n)! n!)
0 1 2



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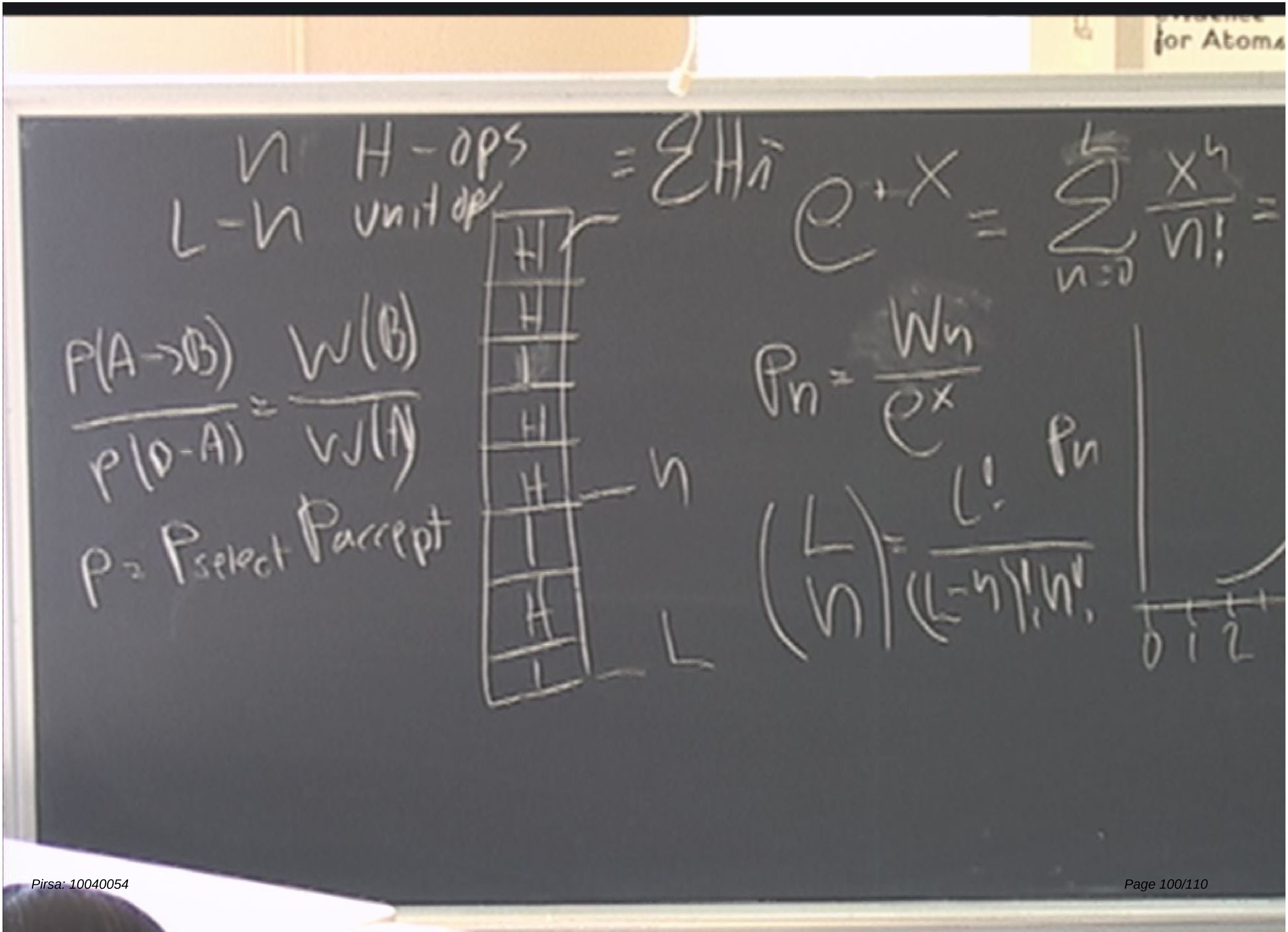
for Atom
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P(A→B)/P(B→A) = W(B)/W(A)
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n
L
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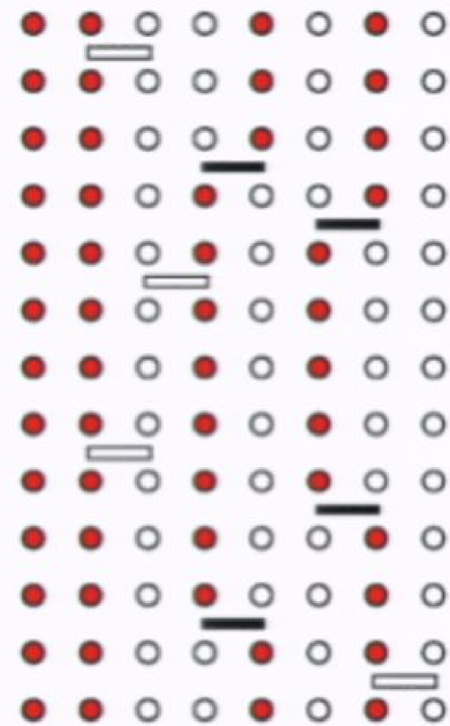

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Change the configuration; $(\alpha, S_L) \to (\alpha', S_L')$

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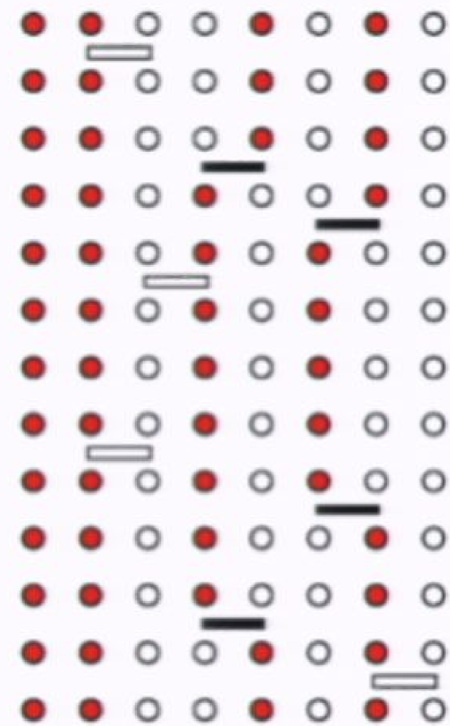

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n is the current power

- n → n+1 (a=0 → a=1)
- n → n-1 (a=1 → a=0)

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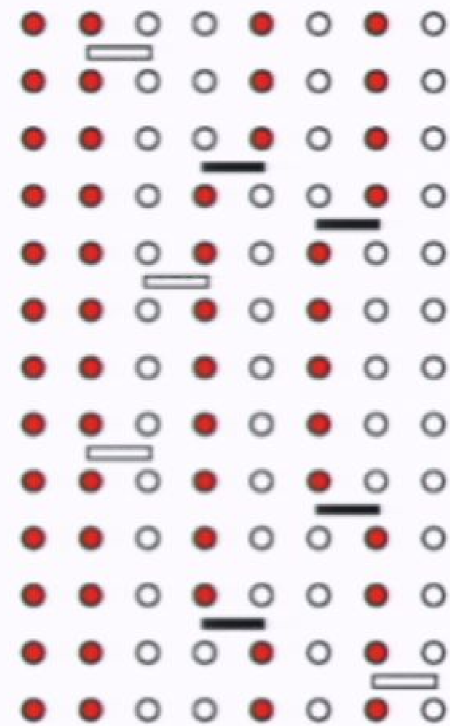

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Acceptance probabilities

$$P_{\text{accept}}([0,0] \to [1,b]) = \min\left[\frac{\beta N_b}{2(L-n)}, 1\right]$$

Diagonal update; pseudocode implementation

do $p = 0$ **to** $L-1$
  if $(s(p) = 0)$ **then**
    $b =$ **random**$[1, \dots, N_b]$; **if** $\sigma(i(b)) = \sigma(j(b))$ **cycle**
    if (**random**$[0-1] < P_{\text{insert}}(n)$) **then** $s(p) = 2b$; $n = n + 1$ **endif**
  elseif (**mod**$[s(p), 2] = 0$) **then**
    if (**random**$[0-1] < P_{\text{remove}}(n)$) **then** $s(p) = 0$; $n = n - 1$ **endif**
  else
    $b = s(p)/2$; $\sigma(i(b)) = -\sigma(i(b))$; $\sigma(j(b)) = -\sigma(j(b))$
  endif
enddo

i(b),j(b) sites on bond b

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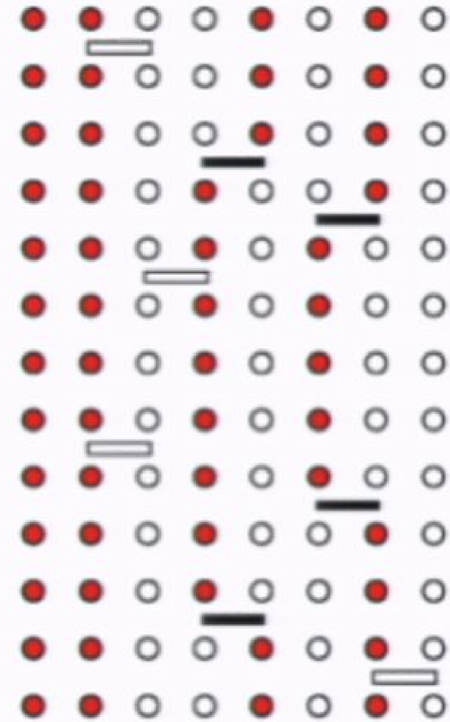

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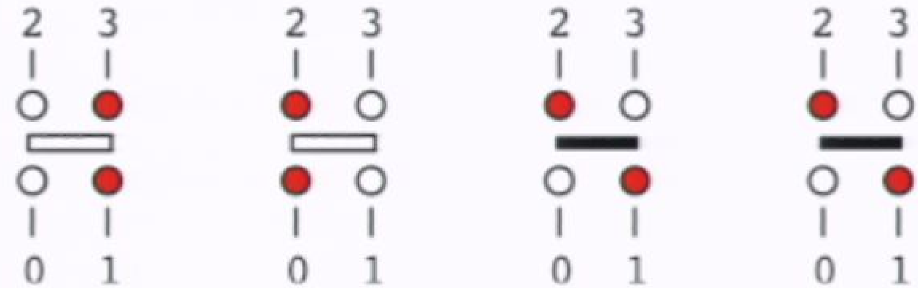


For fixed-length scheme

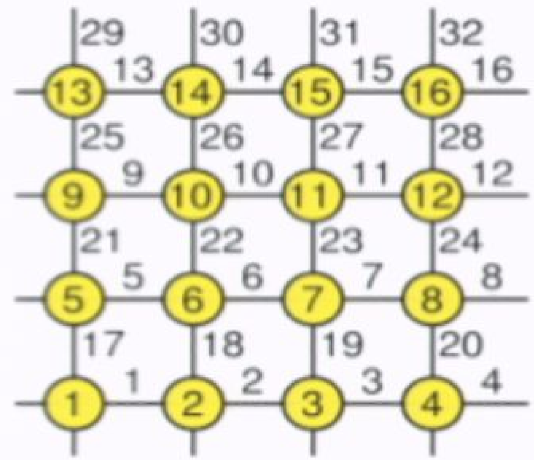
$$Z = \sum_{\alpha} \sum_{S_L} (-1)^{n_2} \frac{\beta^n (L-n)!}{L!} \sum_{S_L} \left\langle \alpha \left| \prod_{p=0}^{L-1} H_{a(p),b(p)} \right| \alpha \right\rangle \qquad W(\alpha, S_L) = \left(\frac{\beta}{2}\right)^n \frac{(L-n)!}{L!}$$

Stochastic Series expansion (SSE): S=1/2 Heisenberg model

Write H as a bond sum for arbitrary lattice

$$H = J \sum_{b=1}^{N_b} \mathbf{S}_{i(b)} \cdot \mathbf{S}_{j(b)},$$

2D square lattice bond and site labels



Series expansion representation

Start from the Taylor expansion $e^{-\beta H} = \sum_{n=0}^{\infty} \frac{(-\beta)^n}{n!} H^n$ (approximation-free method from the outset)

$$Z = \sum_{n=0}^{\infty} \frac{(-\beta)^n}{n!} \sum_{\{\alpha\}_n} \langle \alpha_0 | H | \alpha_{n-1} \rangle \cdots \langle \alpha_2 | H | \alpha_1 \rangle \langle \alpha_1 | H | \alpha_0 \rangle$$

Similar to the path integral; $1 - \Delta\tau H \to H$ and weight factor outside

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Similar to the path integral; $1 - \Delta\tau H \to H$ and weight factor outside

For hard-core bosons the (allowed) path weight is $W(\{\alpha\}_n) = \beta^n / n!$