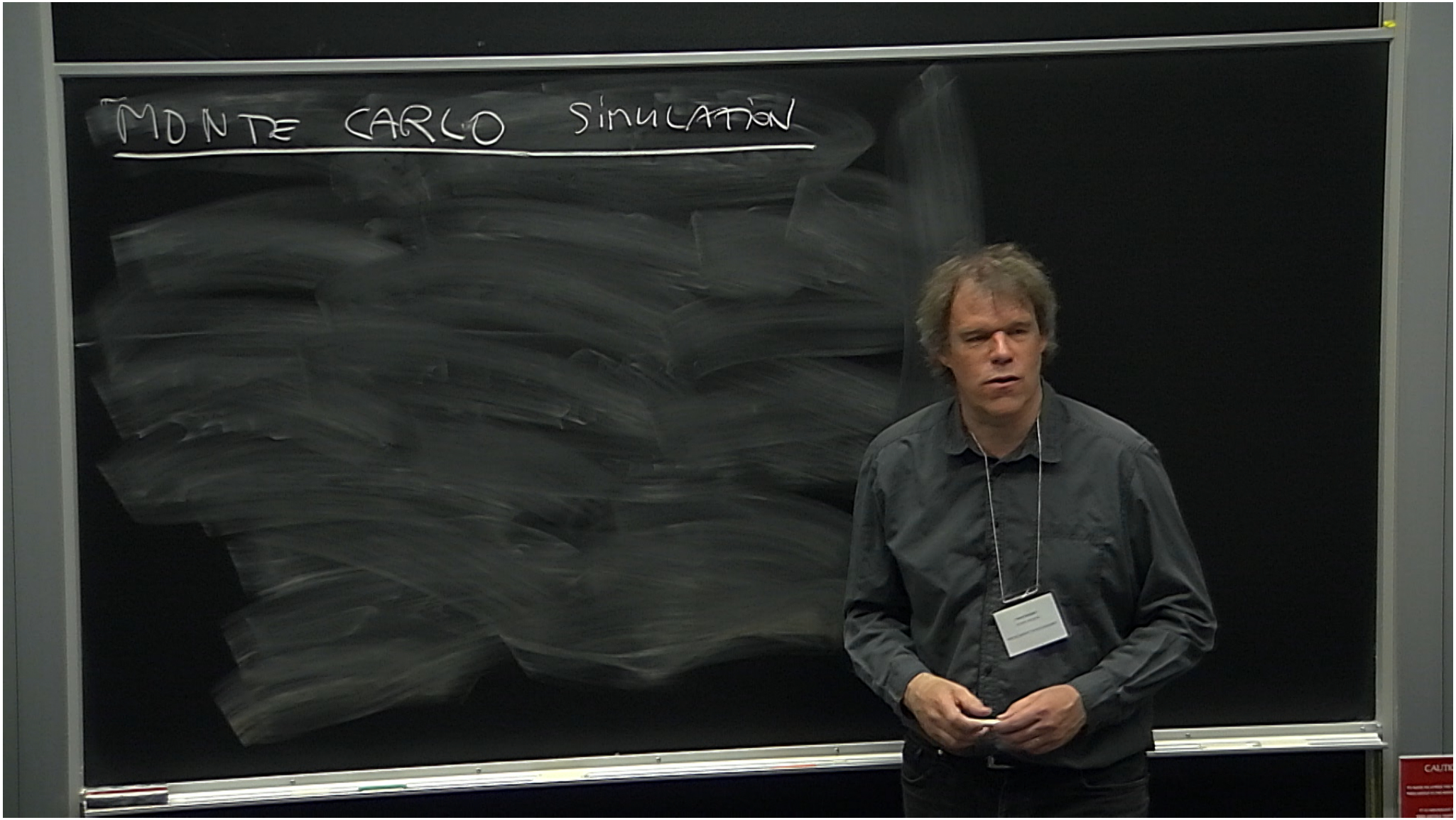
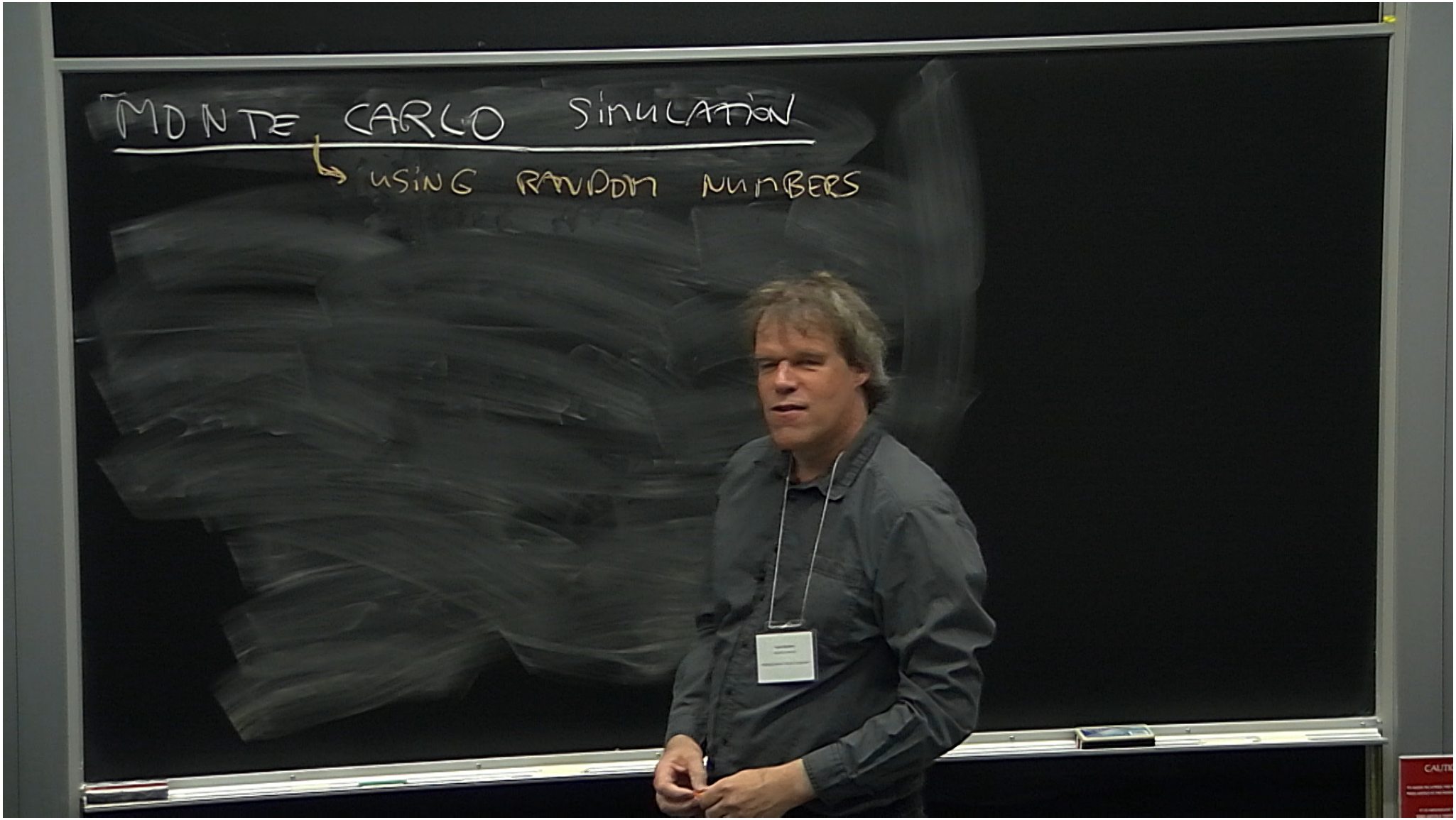
Title: Introduction to Monte Carlo methods - 2

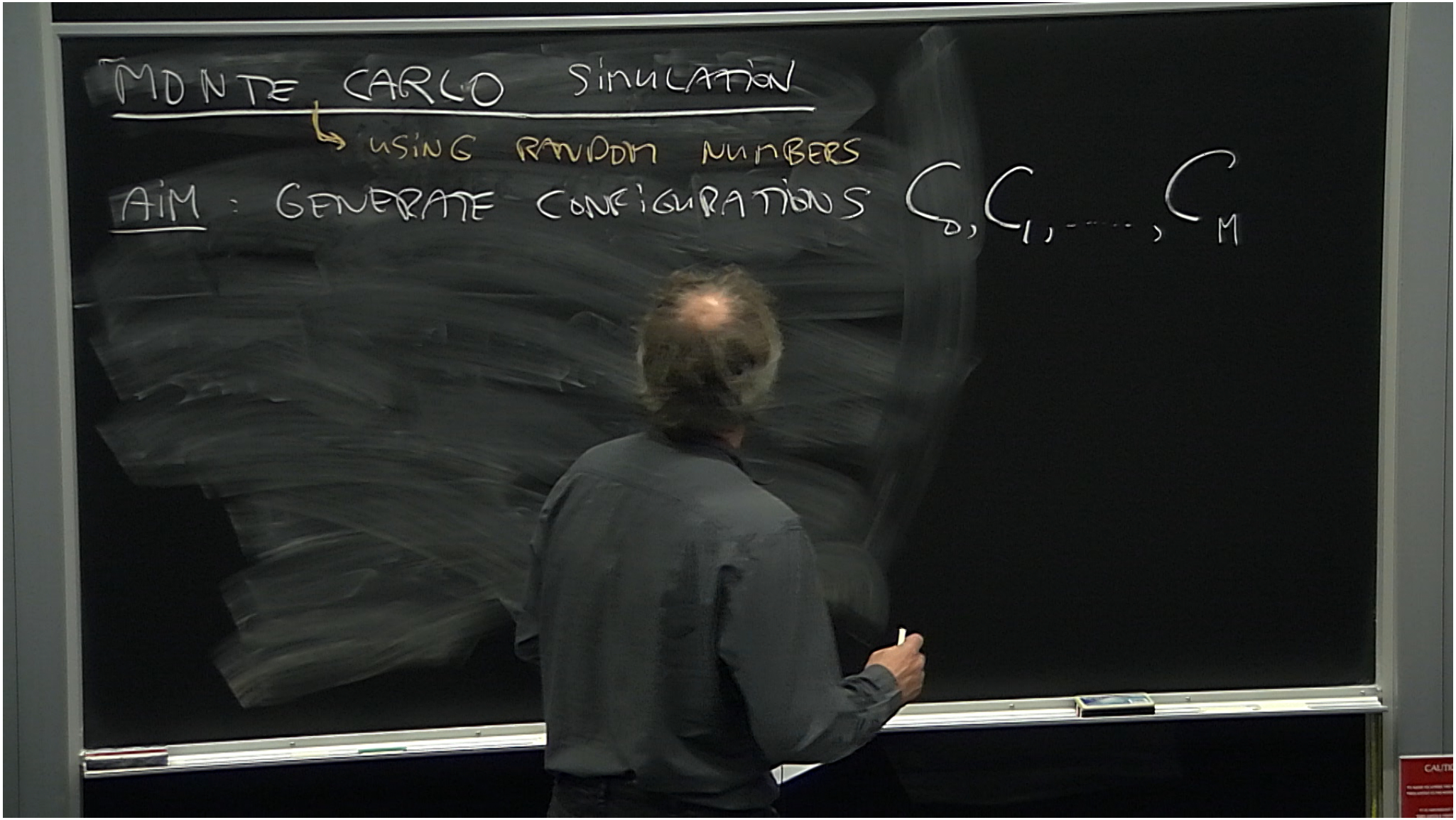
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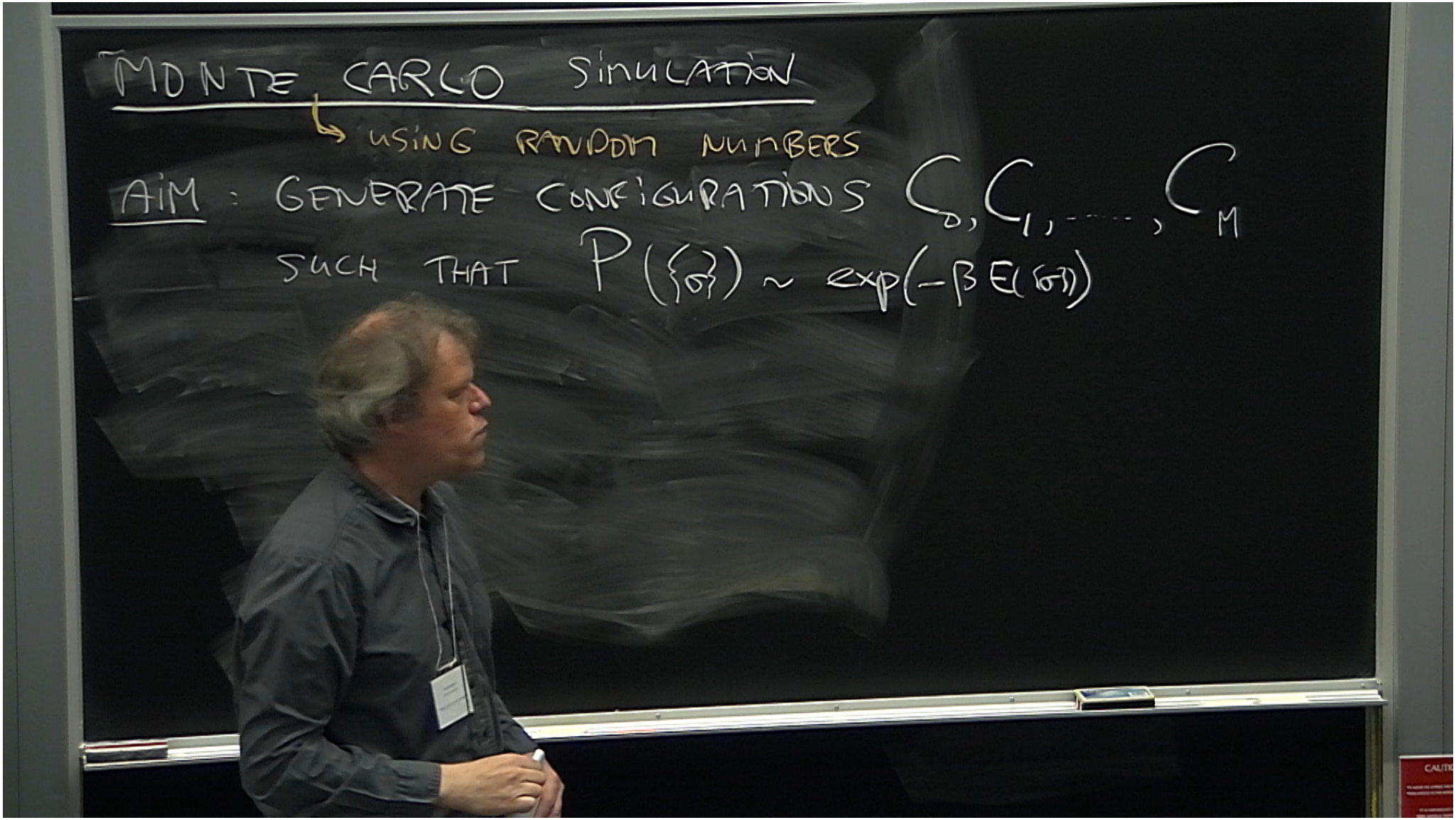
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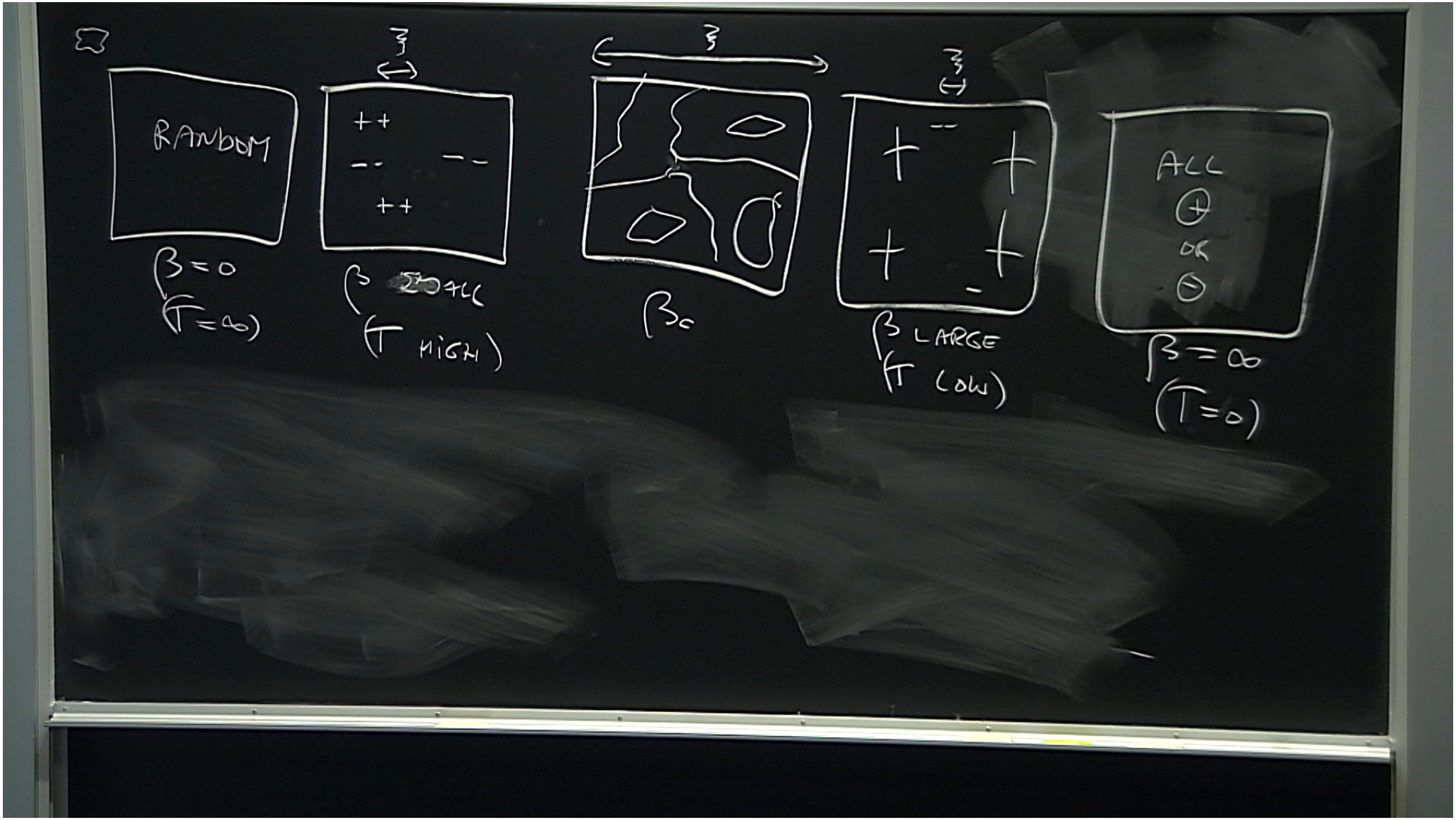
Abstract:

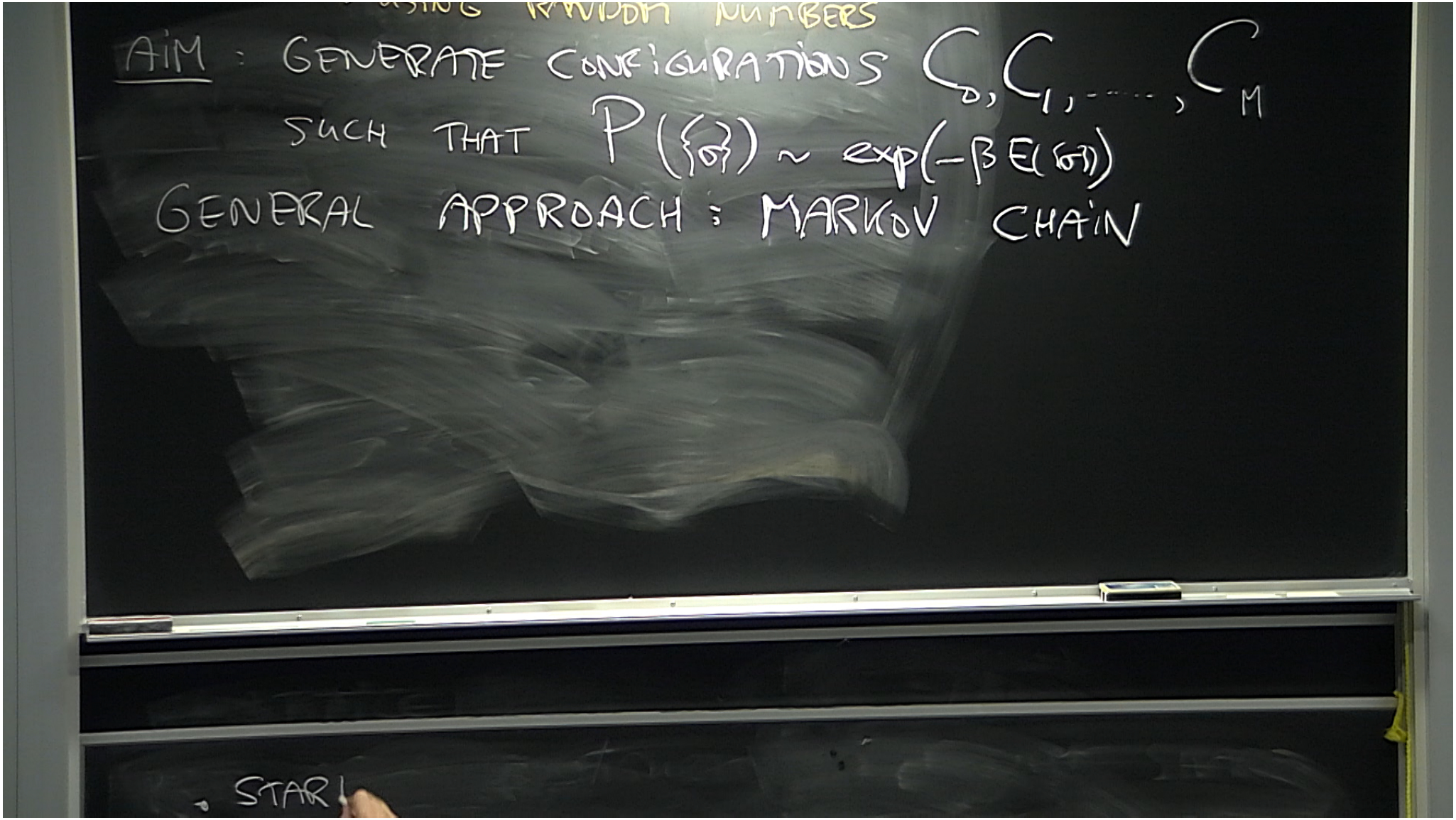

MONTE CARLO SIMULATION

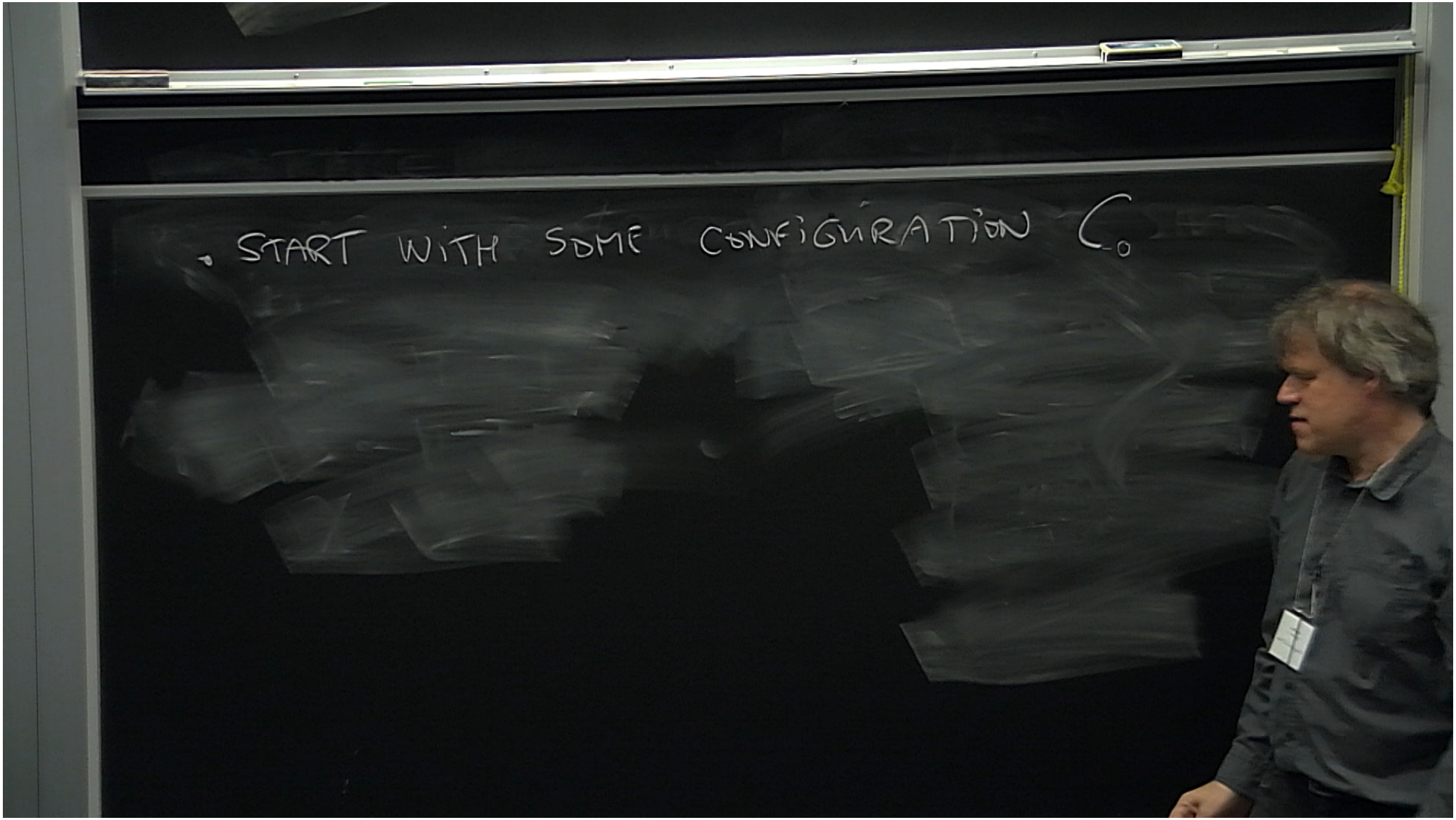

MONTE CARLO SIMULATION
USING RANDOM NUMBERS

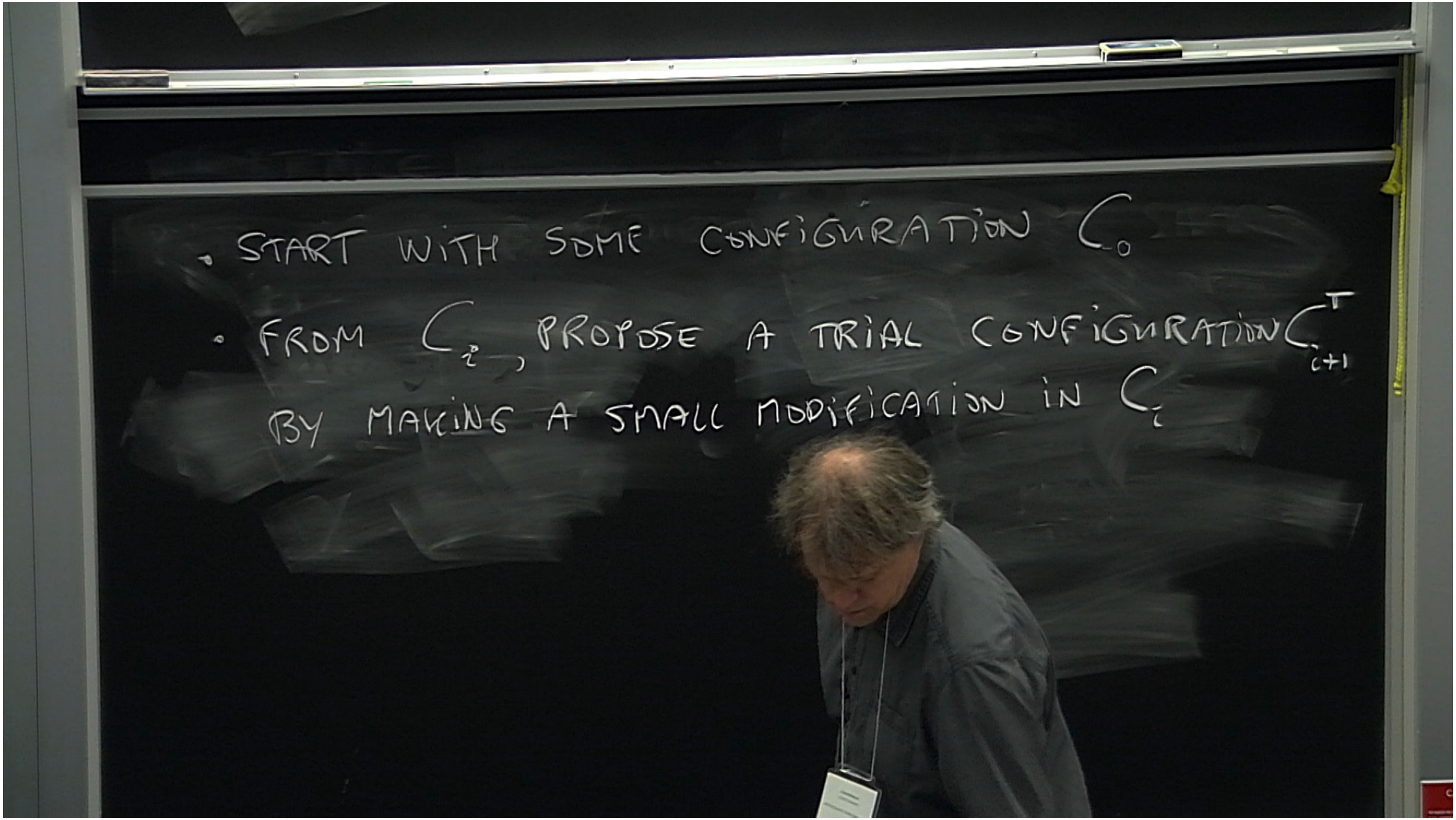

MONTE CARLO SIMULATION
↳ USING RANDOM NUMBERS
AIM : GENERATE CONFIGURATIONS $C_0, C_1, \ldots, C_M$


MONTE CARLO SIMULATION
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SUCH THAT $P(\{\sigma_i\}) \sim \exp(-\beta E(\sigma_i))$

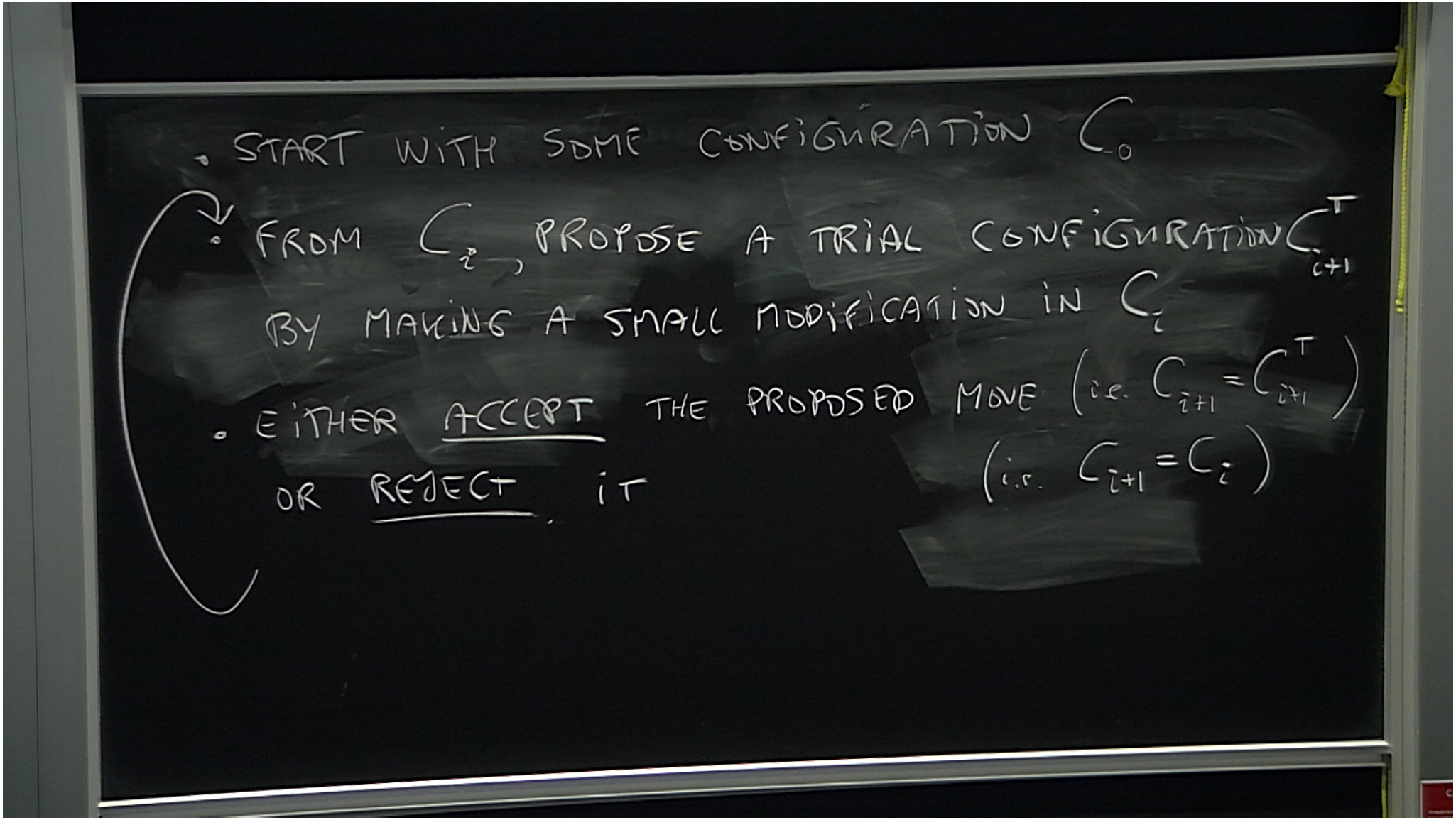

RANDOM
β = 0
(T = ∞)
++
−−
−−
++
(T HIGH)
β_c
LARGE
(T LOW)
ALL
⊕
OR
⊖
β = ∞
(T = 0)

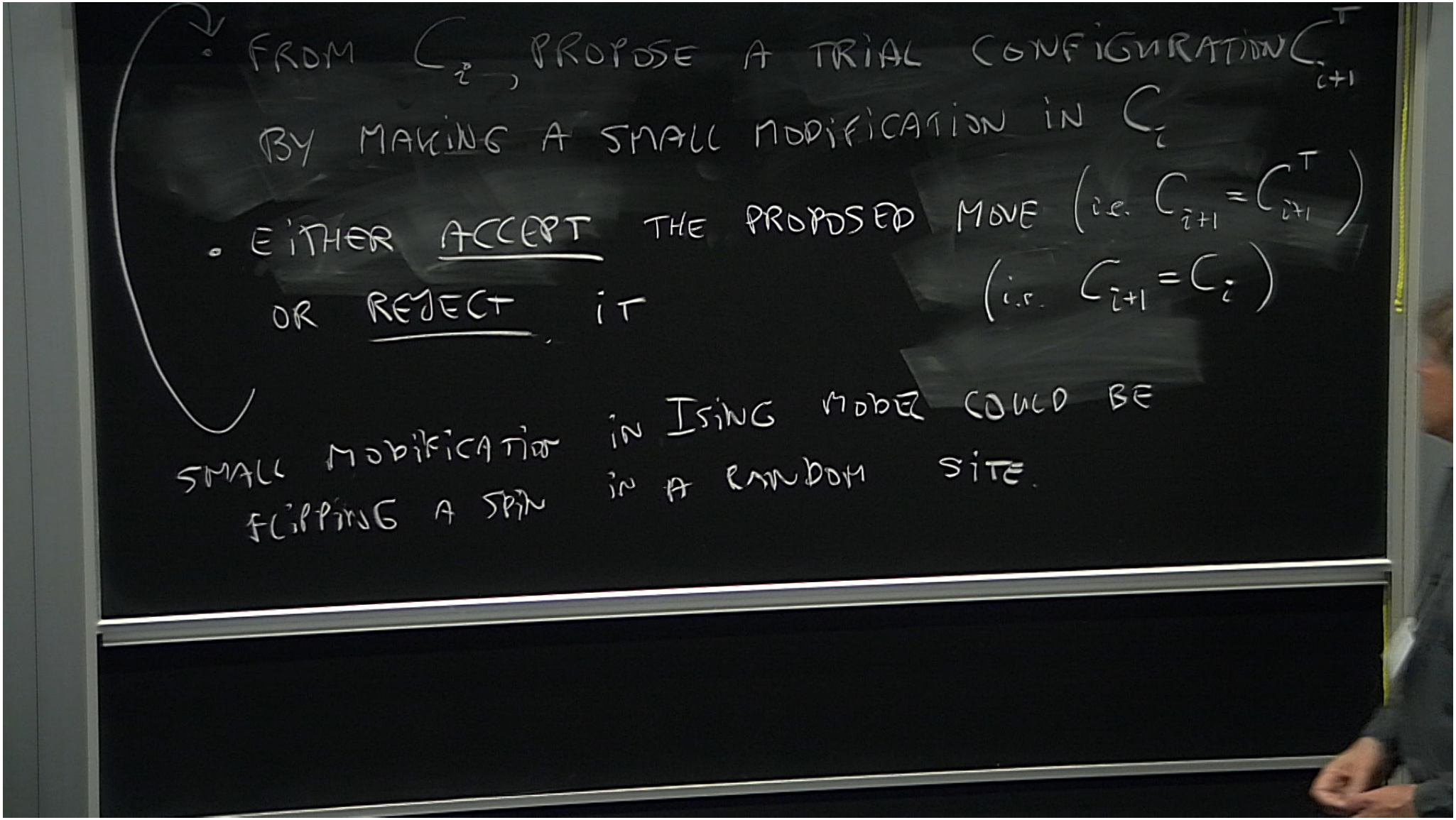

RANDOM NUMBERS
AIM : GENERATE CONFIGURATIONS $C_0, C_1, \ldots, C_M$
SUCH THAT $P(\{\sigma\}) \sim \exp(-\beta E(\{\sigma\}))$
GENERAL APPROACH : MARKOV CHAIN
START

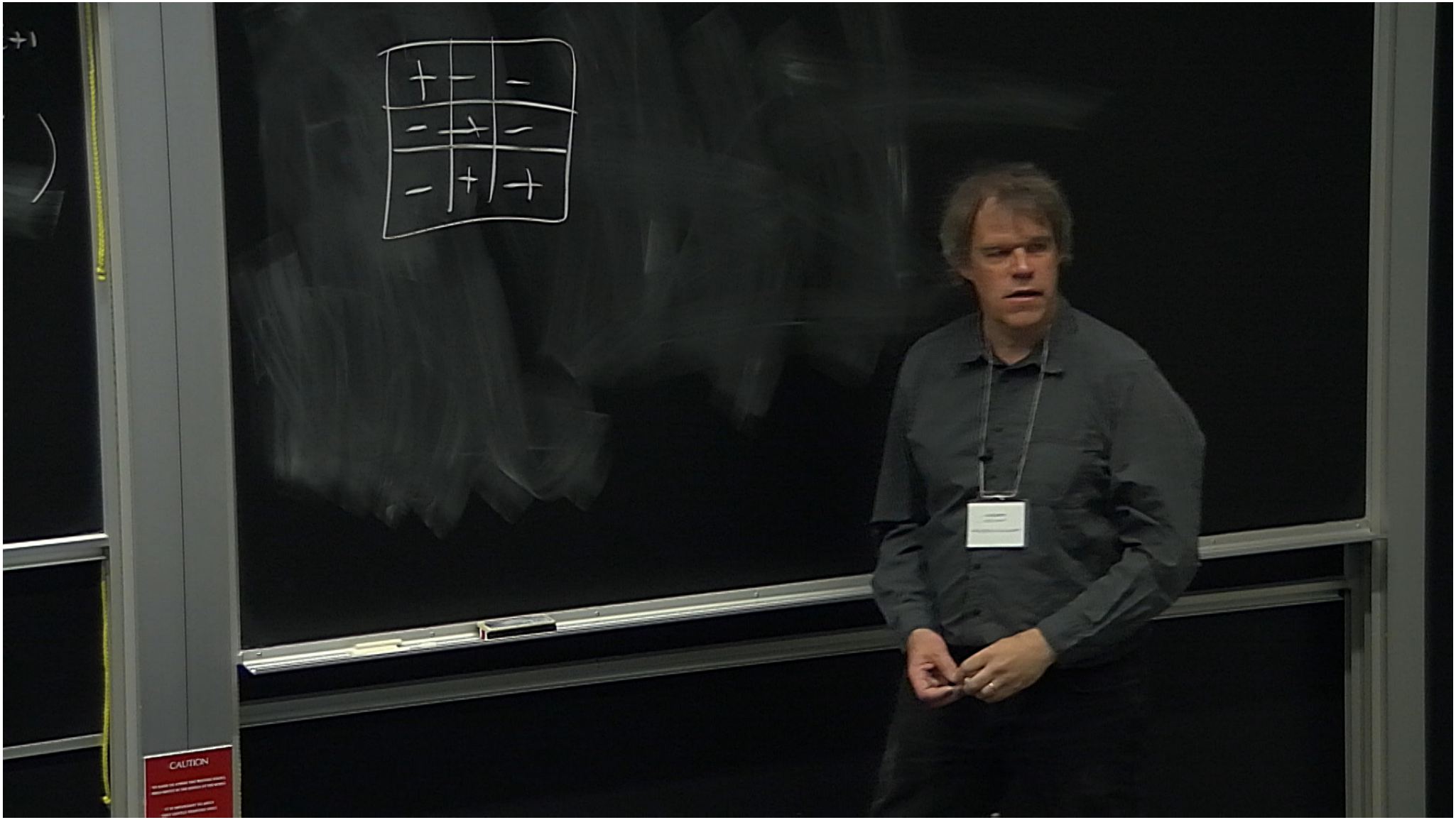

• START WITH SOME CONFIGURATION C_0

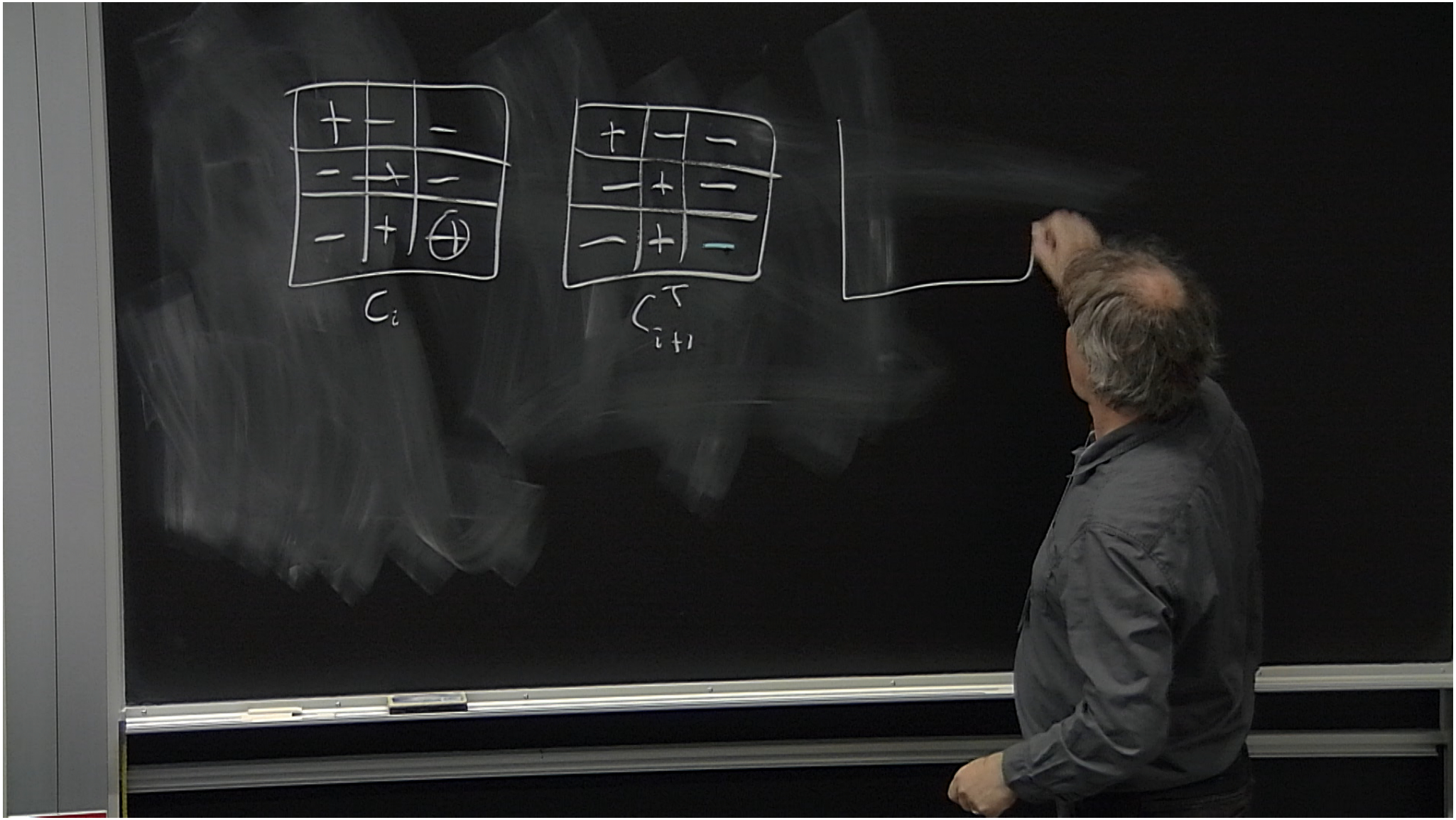

• START WITH SOME CONFIGURATION C_0
• FROM C_i, PROPOSE A TRIAL CONFIGURATION C_{i+1}^T
BY MAKING A SMALL MODIFICATION IN C_i

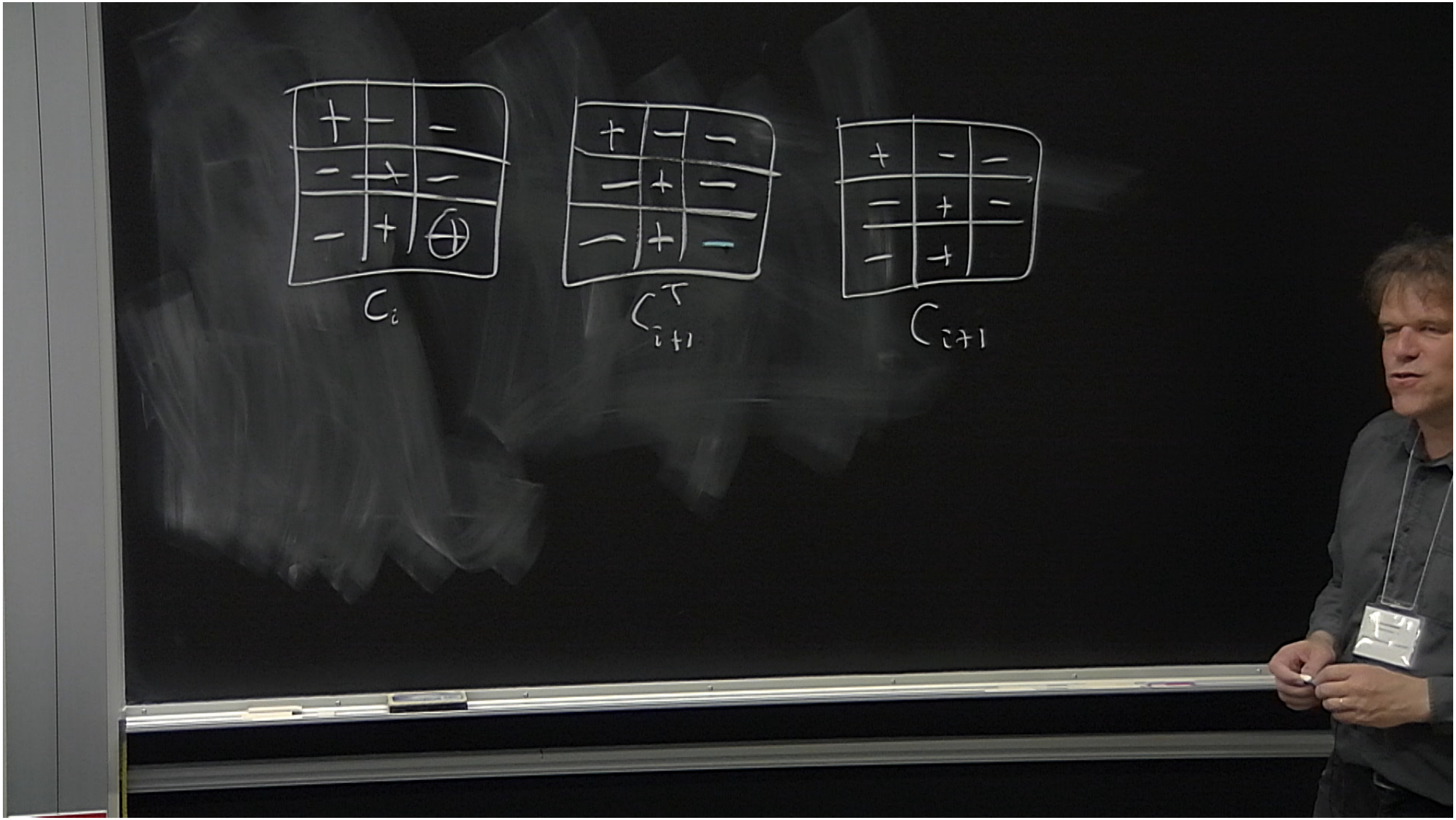
- START WITH SOME CONFIGURATION C_0
- FROM C_i, PROPOSE A TRIAL CONFIGURATION C_{i+1}^T BY MAKING A SMALL MODIFICATION IN C_i
- EITHER ACCEPT THE PROPOSED MOVE (i.e. $C_{i+1} = C_{i+1}^T$)
  OR REJECT IT (i.e. $C_{i+1} = C_i$)

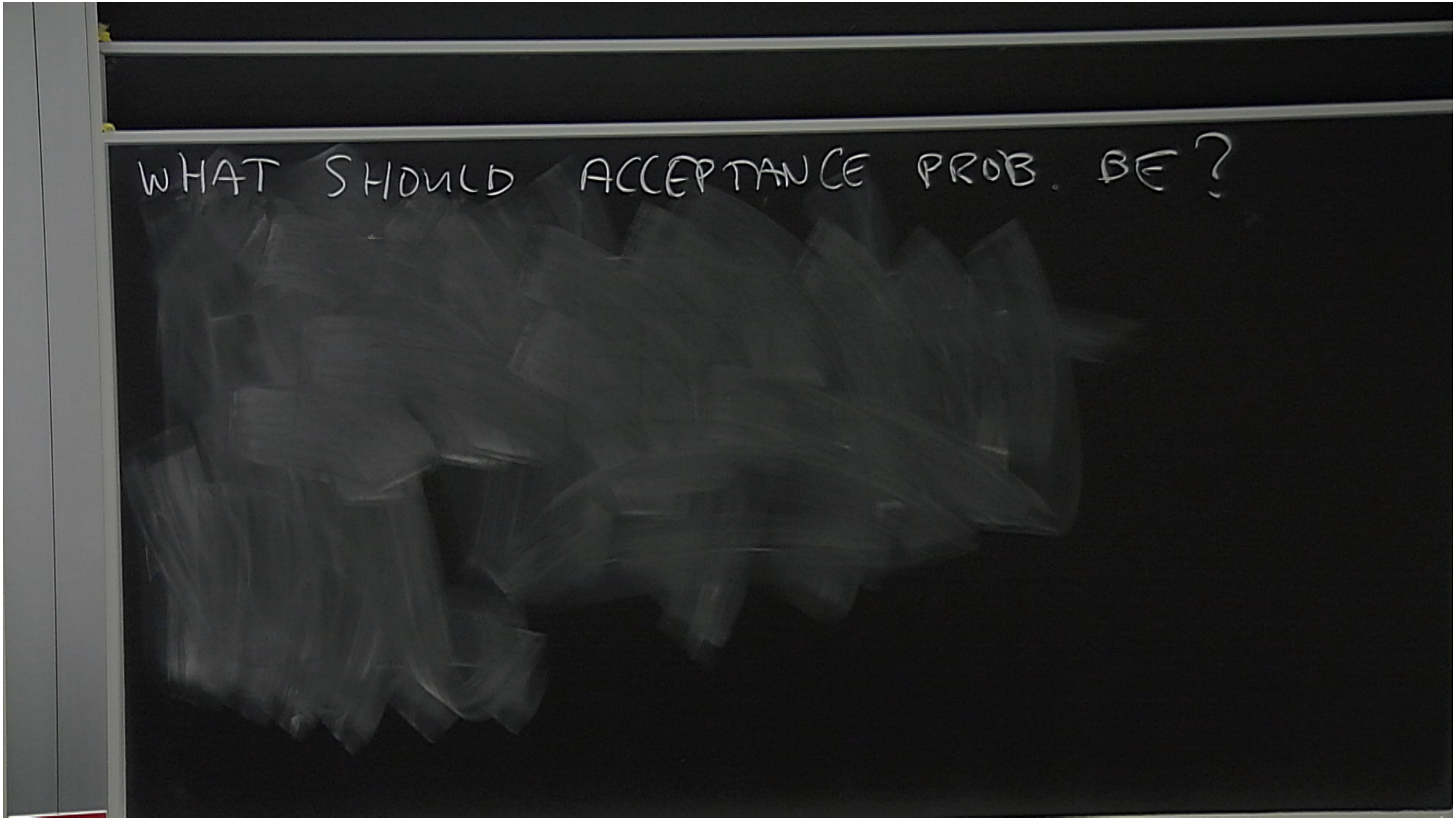

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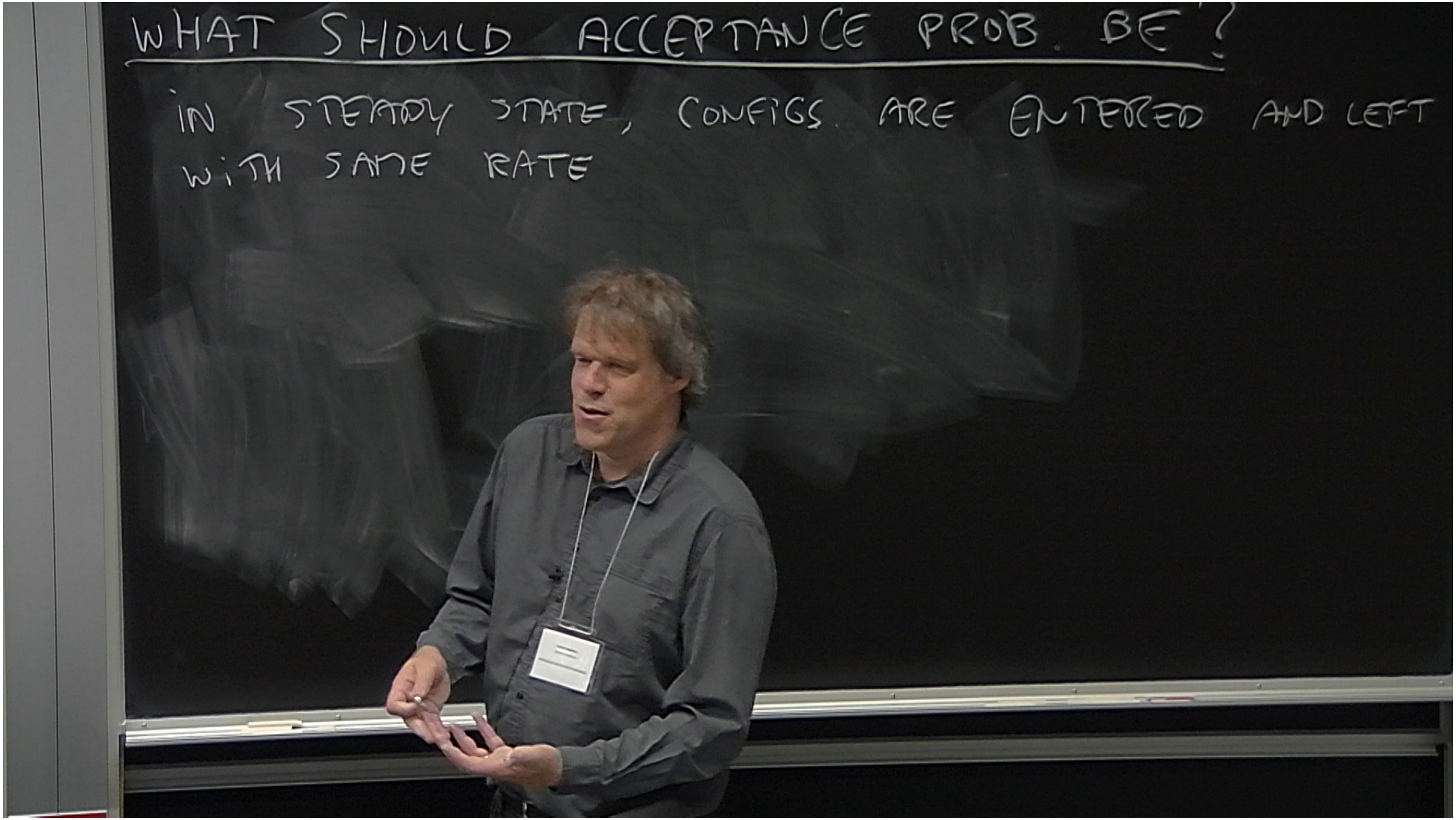

FROM C_i, PROPOSE A TRIAL CONFIGURATION C_{i+1}^T
BY MAKING A SMALL MODIFICATION IN C_i
EITHER ACCEPT THE PROPOSED MOVE (i.e. $C_{i+1} = C_{i+1}^T$)
OR REJECT IT (i.e. $C_{i+1} = C_i$)
SMALL MODIFICATION IN ISING MODEL COULD BE
FLIPPING A SPIN IN A RANDOM SITE.

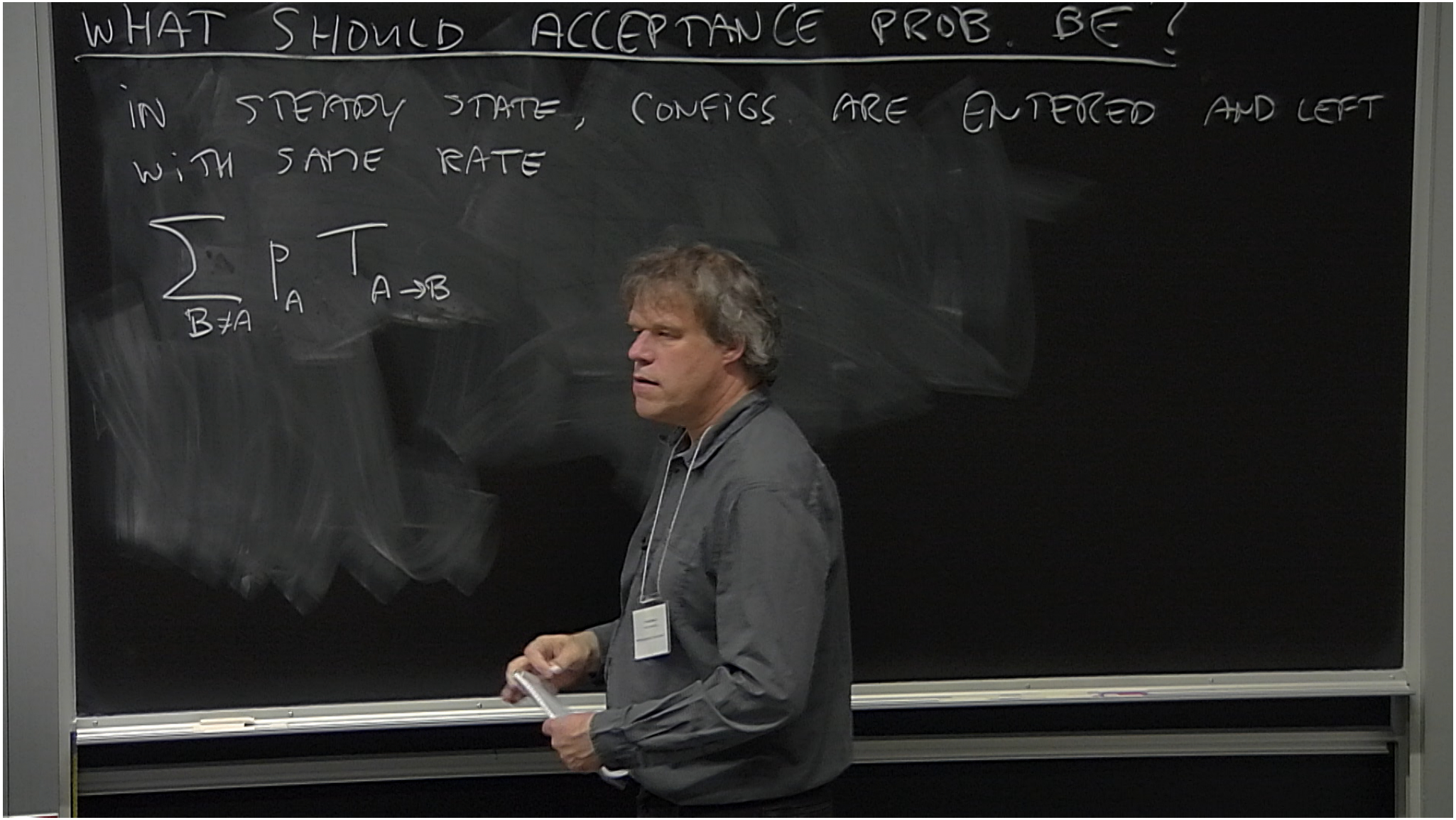

CAUTION

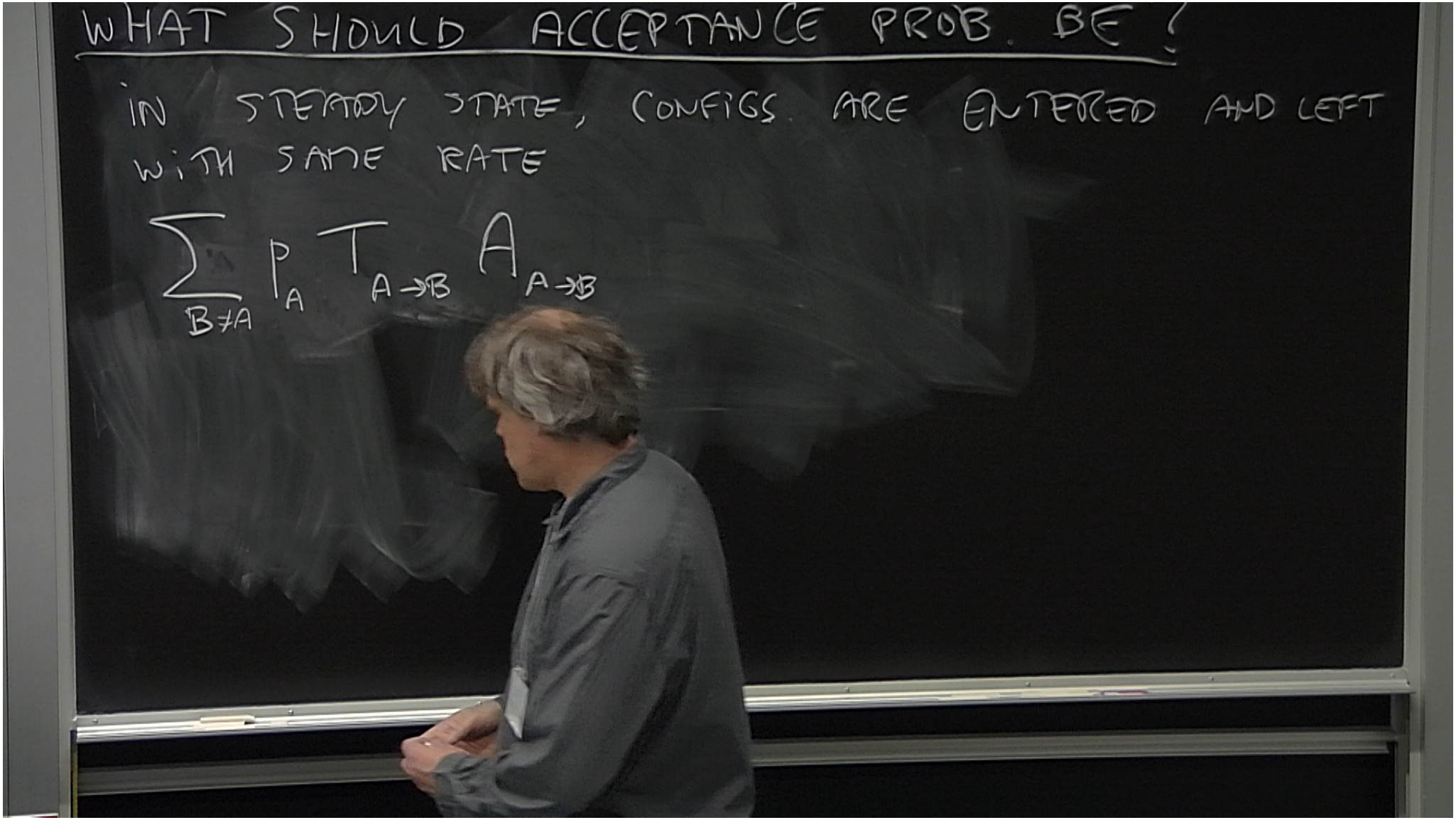

C_i
C_{i+1}^T

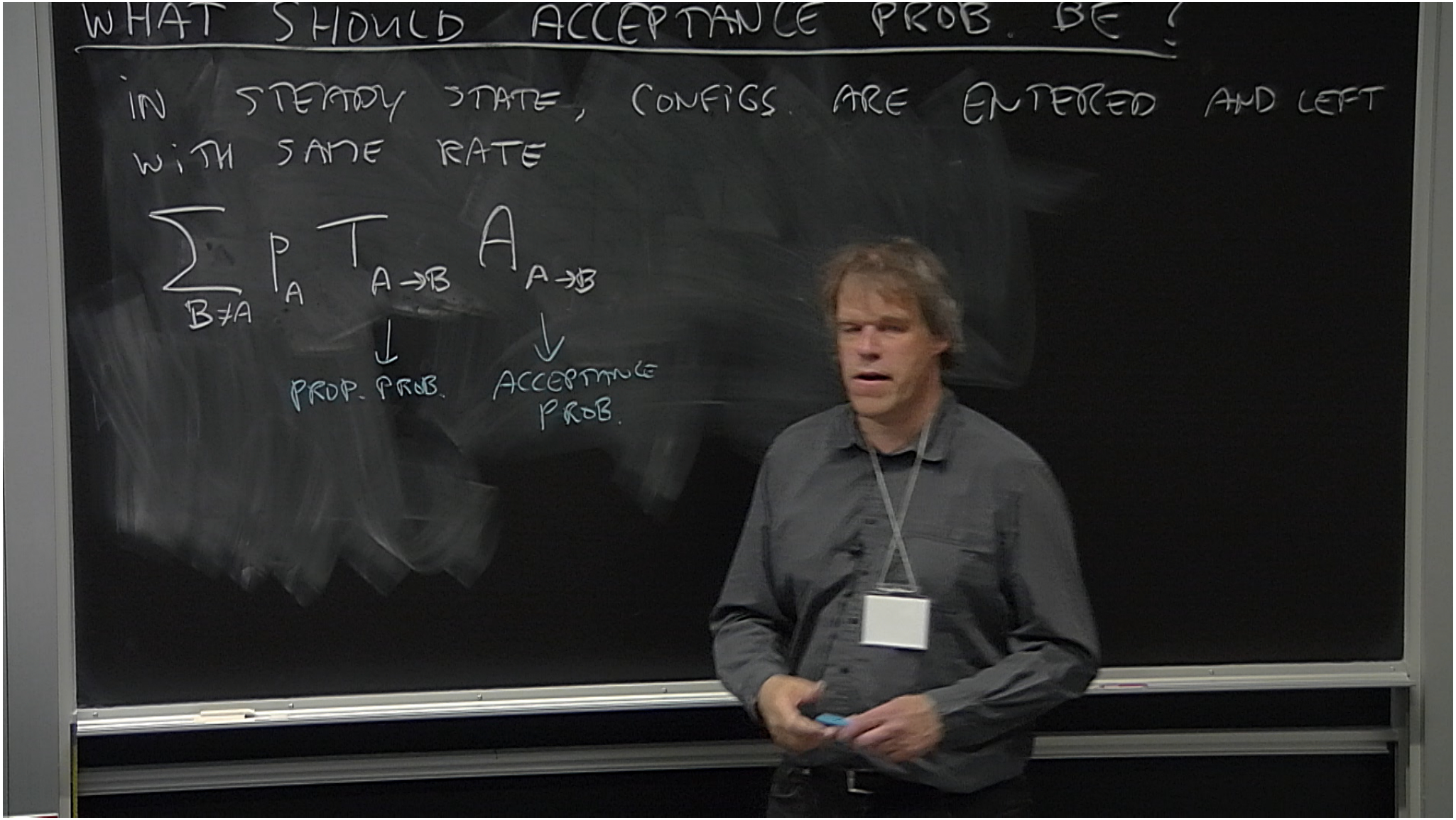

C_i
C_{i+1}^T
C_{i+1}

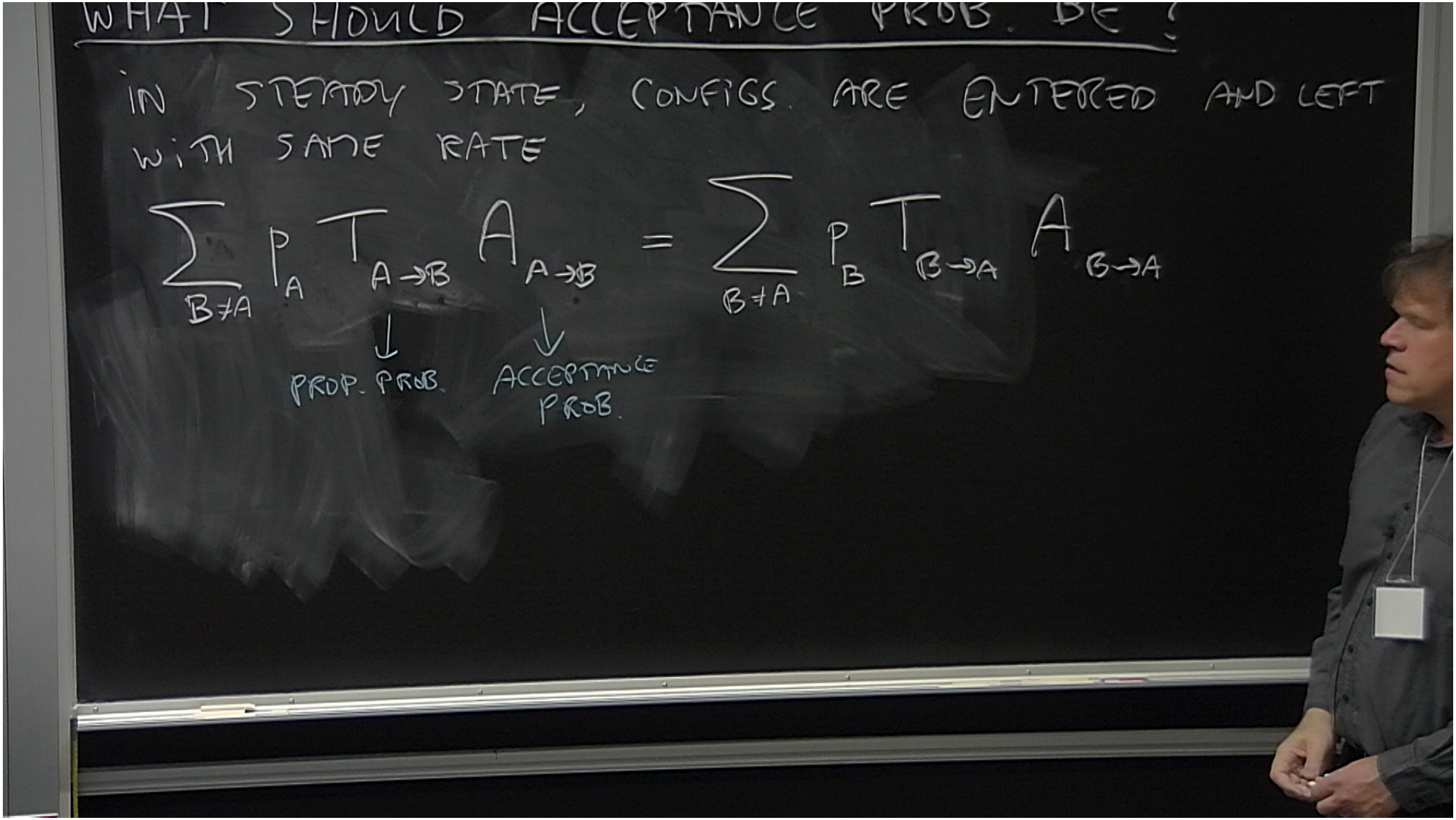

WHAT SHOULD ACCEPTANCE PROB. BE?

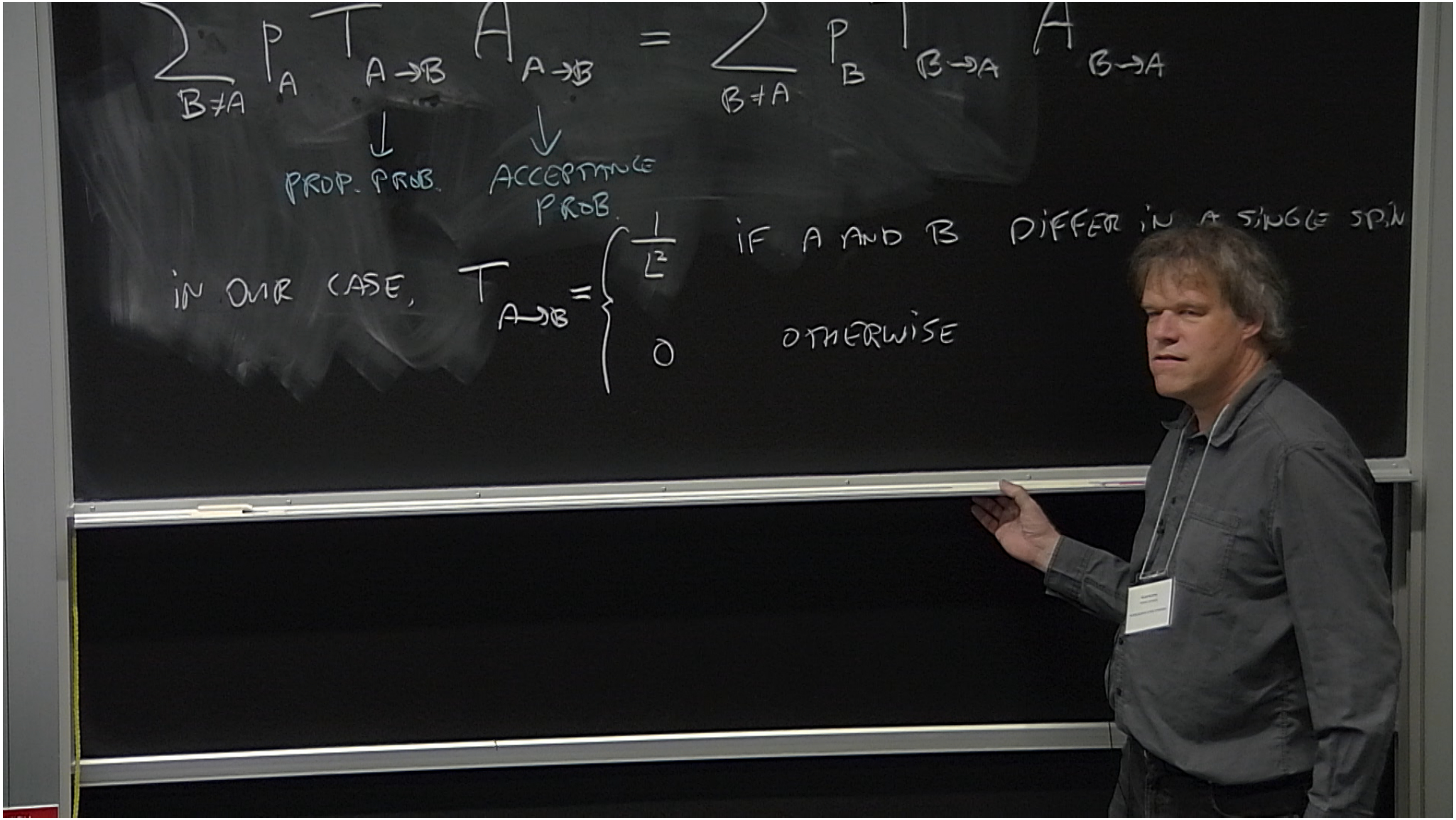

WHAT SHOULD ACCEPTANCE PROB BE?
IN STEADY STATE, CONFIGS ARE ENTERED AND LEFT
WITH SAME RATE

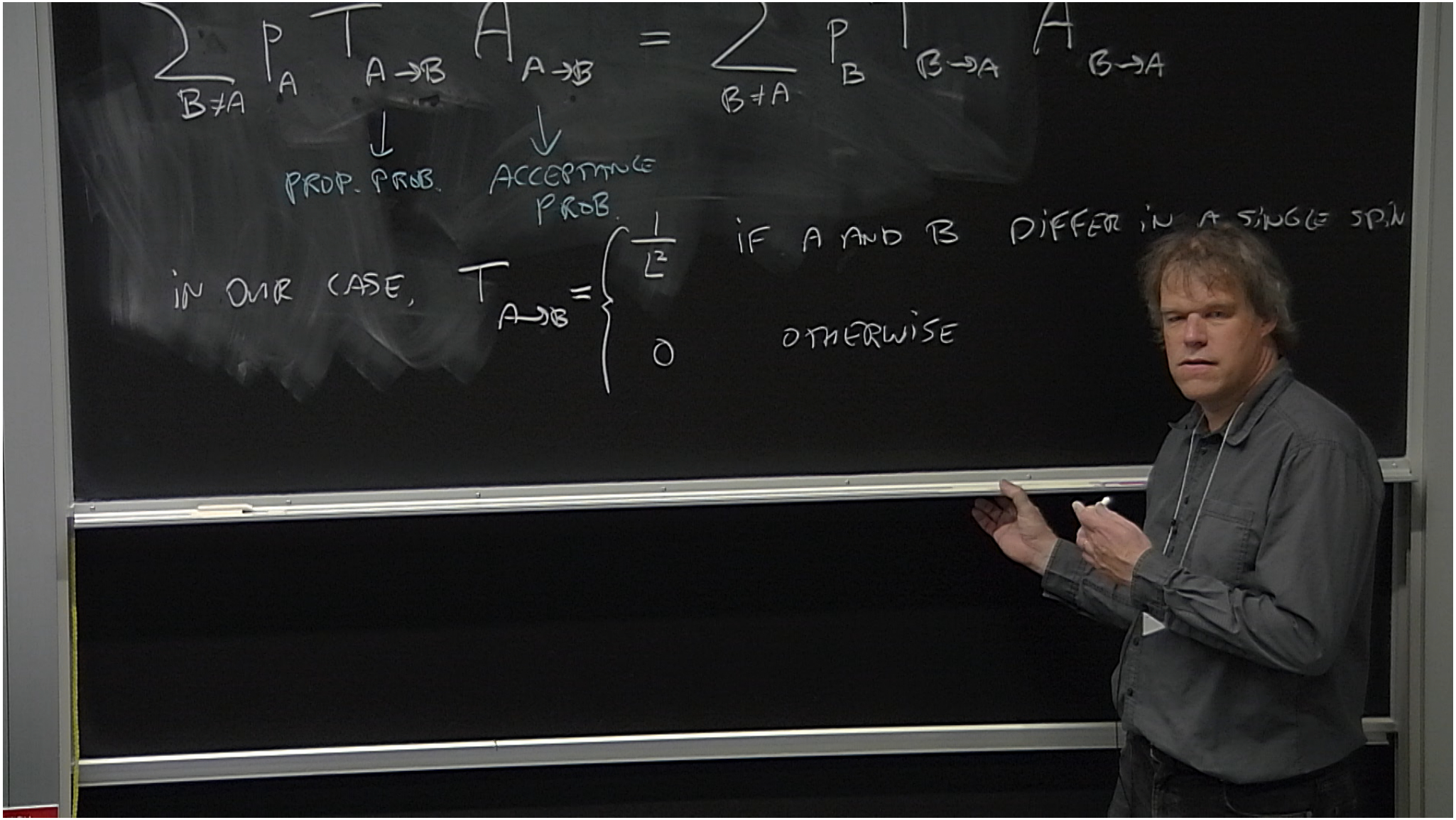

WHAT SHOULD ACCEPTANCE PROB. BE?
IN STEADY STATE, CONFIGS ARE ENTERED AND LEFT WITH SAME RATE
$\sum_{B \neq A} P_A T_{A \to B}$

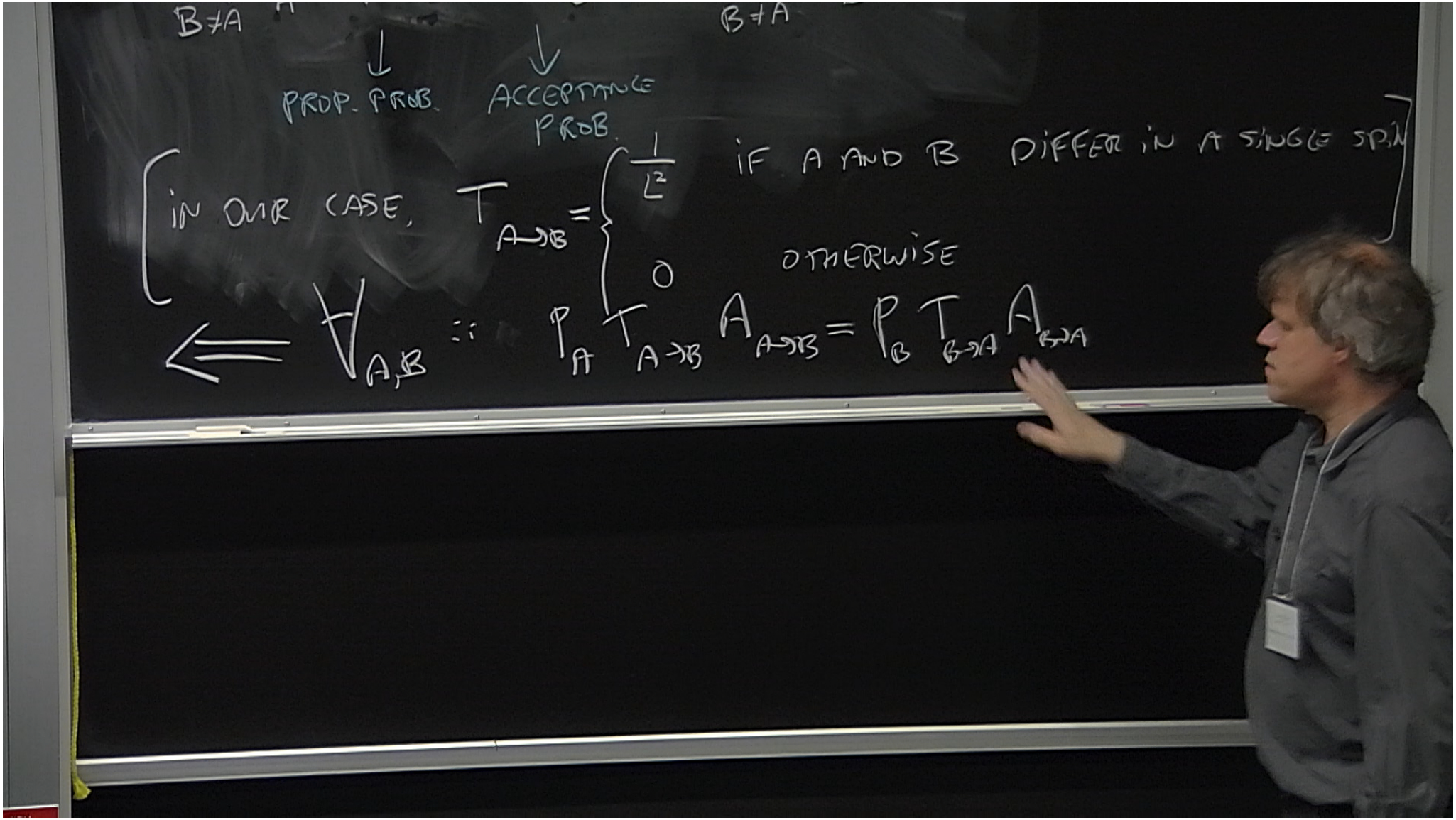

WHAT SHOULD ACCEPTANCE PROB. BE?
IN STEADY STATE, CONFIGS ARE ENTERED AND LEFT WITH SAME RATE
$\sum_{B \neq A} p_A T_{A \to B} A_{A \to B}$

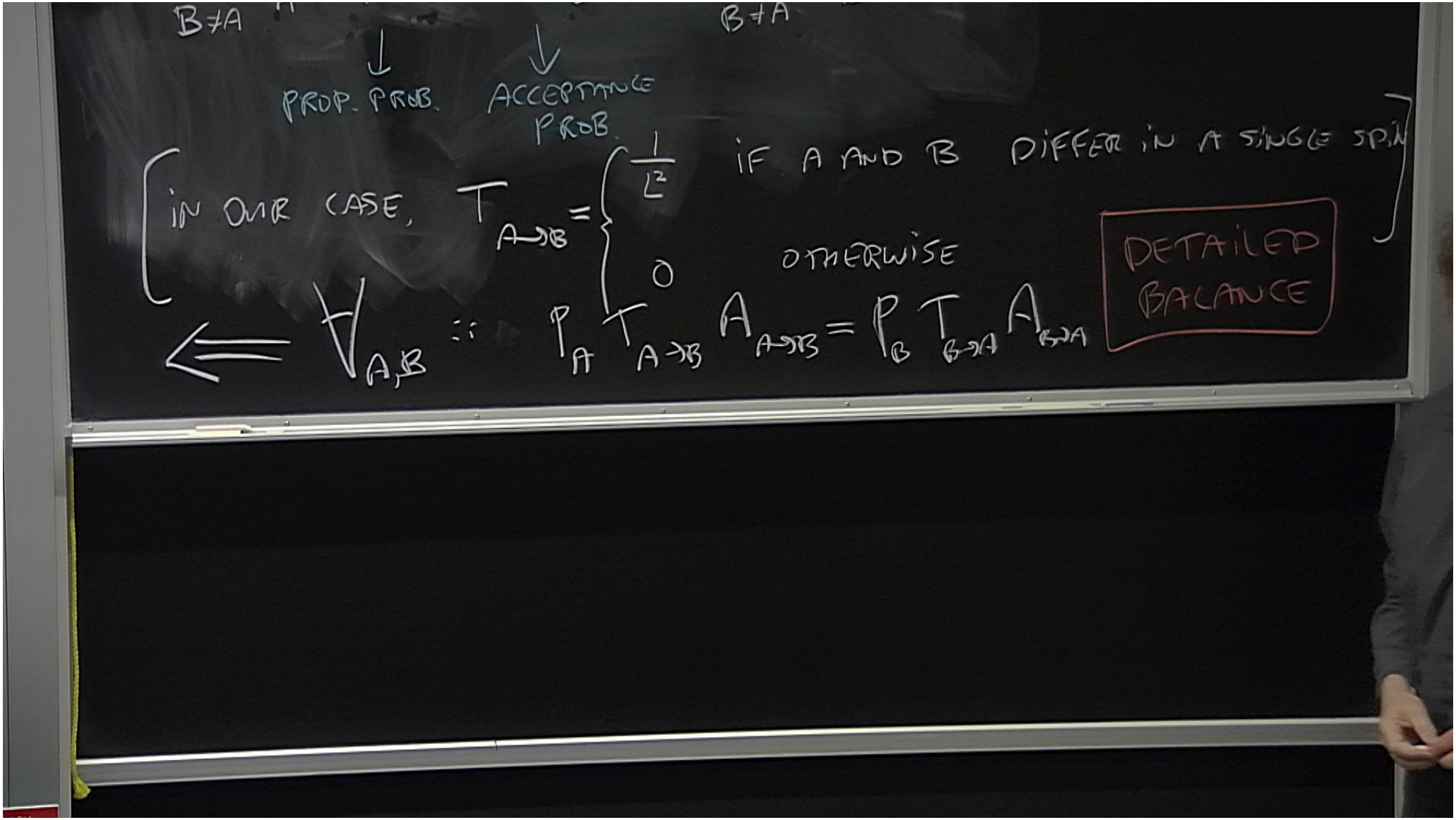

WHAT SHOULD ACCEPTANCE PROB. BE ?
IN STEADY STATE, CONFIGS. ARE ENTERED AND LEFT WITH SAME RATE
$\sum_{B \neq A} p_A T_{A \to B} A_{A \to B}$
PROP. PROB.
ACCEPTANCE PROB.

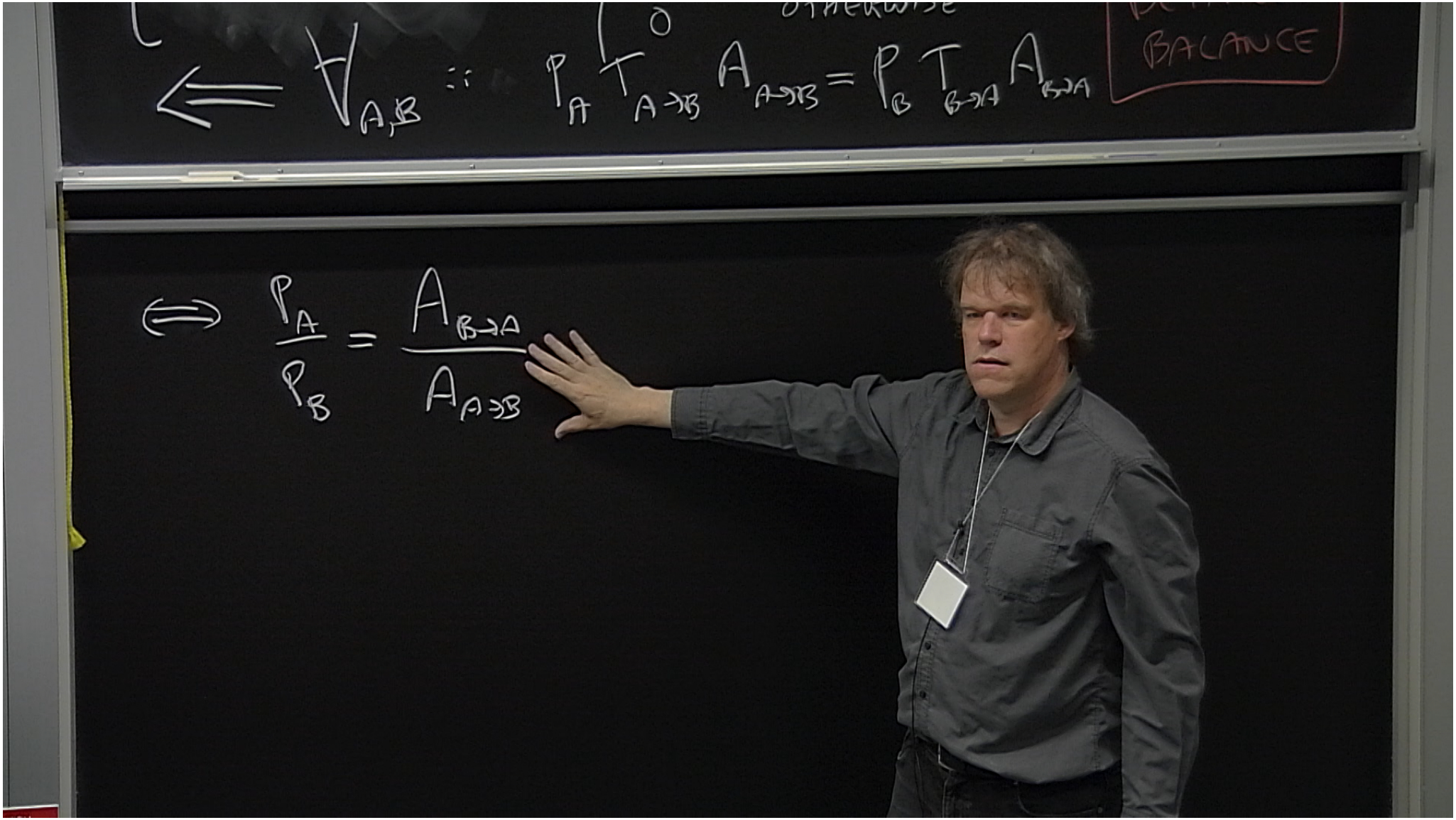

WHAT SHOULD ACCEPTANCE PROB. BE?
IN STEADY STATE, CONFIGS. ARE ENTERED AND LEFT WITH SAME RATE
$\sum_{B \neq A} p_A T_{A \to B} A_{A \to B} = \sum_{B \neq A} p_B T_{B \to A} A_{B \to A}$
PROP. PROB.
ACCEPTANCE PROB.

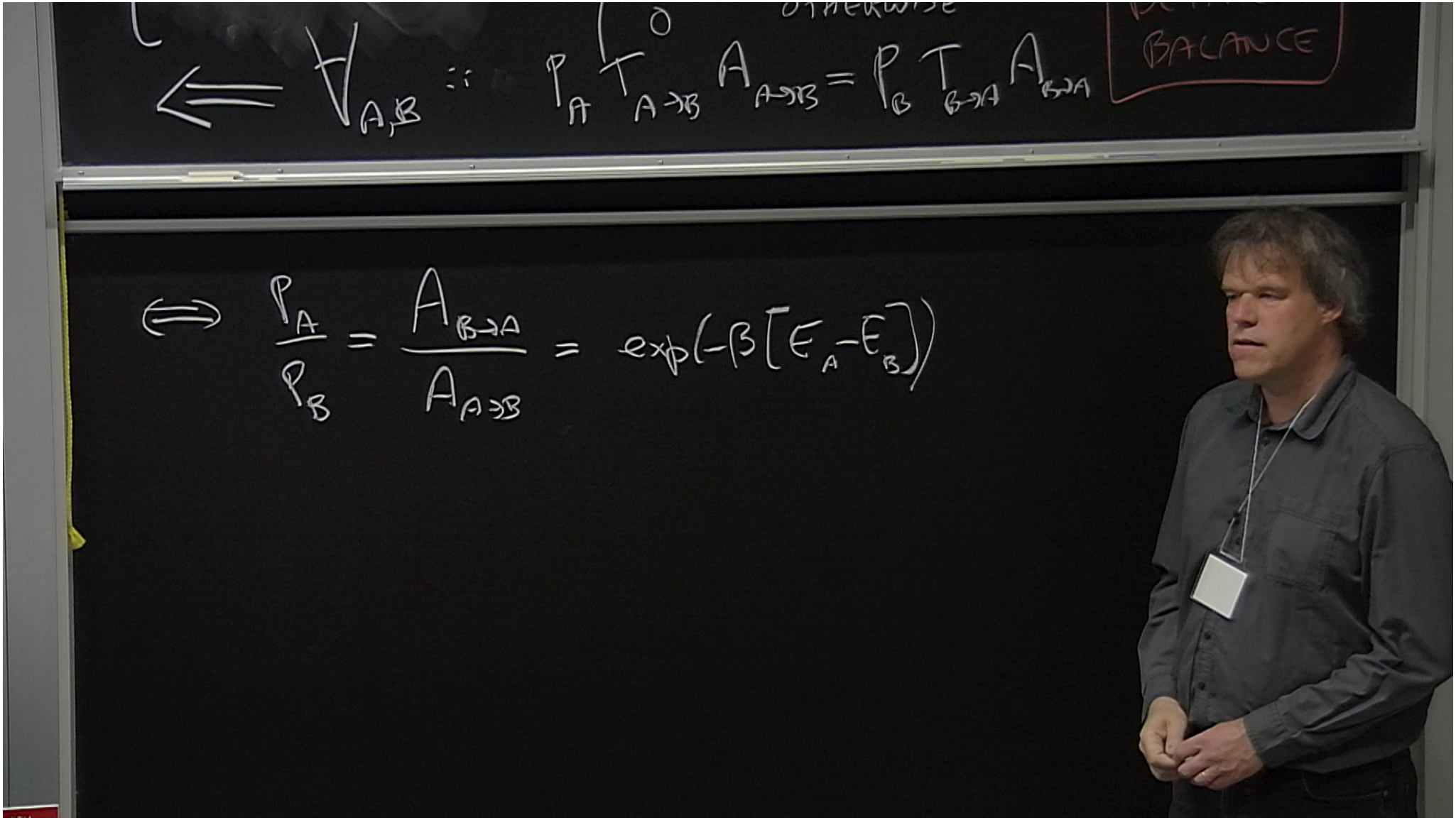

$\sum_{B \neq A} P_A T_{A \to B} A_{A \to B} = \sum_{B \neq A} P_B T_{B \to A} A_{B \to A}$
PROP. PROB.
ACCEPTANCE PROB.
IN OUR CASE, $T_{A \to B} = \begin{cases} \frac{1}{L^2} & \text{IF A AND B DIFFER IN A SINGLE SPIN} \\ 0 & \text{OTHERWISE} \end{cases}$


$\sum_{B \neq A} P_A T_{A \to B} A_{A \to B} = \sum_{B \neq A} P_B T_{B \to A} A_{B \to A}$
PROP. PROB.
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IN OUR CASE, $T_{A \to B} = \begin{cases} \frac{1}{L^2} & \text{IF A AND B DIFFER IN A SINGLE SPIN} \\ 0 & \text{OTHERWISE} \end{cases}$


B≠A
B≠A
PROP. PROB.
ACCEPTANCE PROB.
IN OUR CASE, $T_{A\to B} = \begin{cases} \frac{1}{L^2} & \text{IF A AND B DIFFER IN A SINGLE SPIN} \\ 0 & \text{OTHERWISE} \end{cases}$
$\Longleftarrow \forall_{A,B} :: P_A T_{A\to B} A_{A\to B} = P_B T_{B\to A} A_{B\to A}$


B≠A
B≠A
PROP. PROB.
ACCEPTANCE PROB.
IN OUR CASE, $T_{A\to B} = \begin{cases} \frac{1}{L^2} & \text{IF A AND B DIFFER IN A SINGLE SPIN} \\ 0 & \text{OTHERWISE} \end{cases}$
$\Longleftarrow \forall_{A,B} :: P_A T_{A\to B} A_{A\to B} = P_B T_{B\to A} A_{B\to A}$
DETAILED BALANCE


$\Leftarrow \forall_{A,B} :: P_A T_{A\to B} A_{A\to B} = P_B T_{B\to A} A_{B\to A}$
otherwise
0
BALANCE
$\Leftrightarrow \frac{P_A}{P_B} = \frac{A_{B\to A}}{A_{A\to B}}$

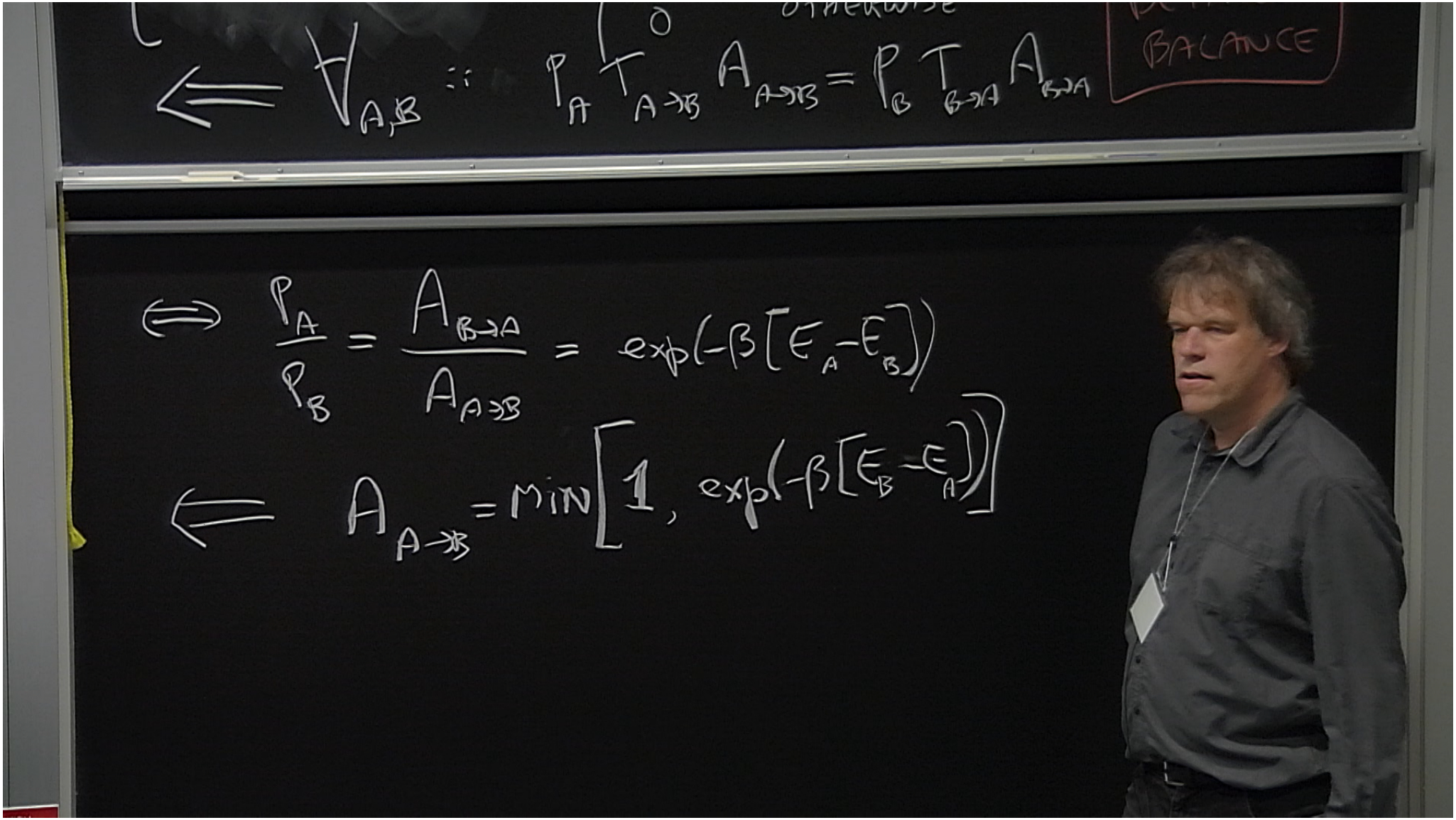

$\Leftarrow \forall_{A,B} :: p_A T_{A\to B} A_{A\to B} = p_B T_{B\to A} A_{B\to A}$
otherwise
BALANCE
$\Leftrightarrow \frac{p_A}{p_B} = \frac{A_{B\to A}}{A_{A\to B}} = \exp(-\beta[E_A - E_B])$

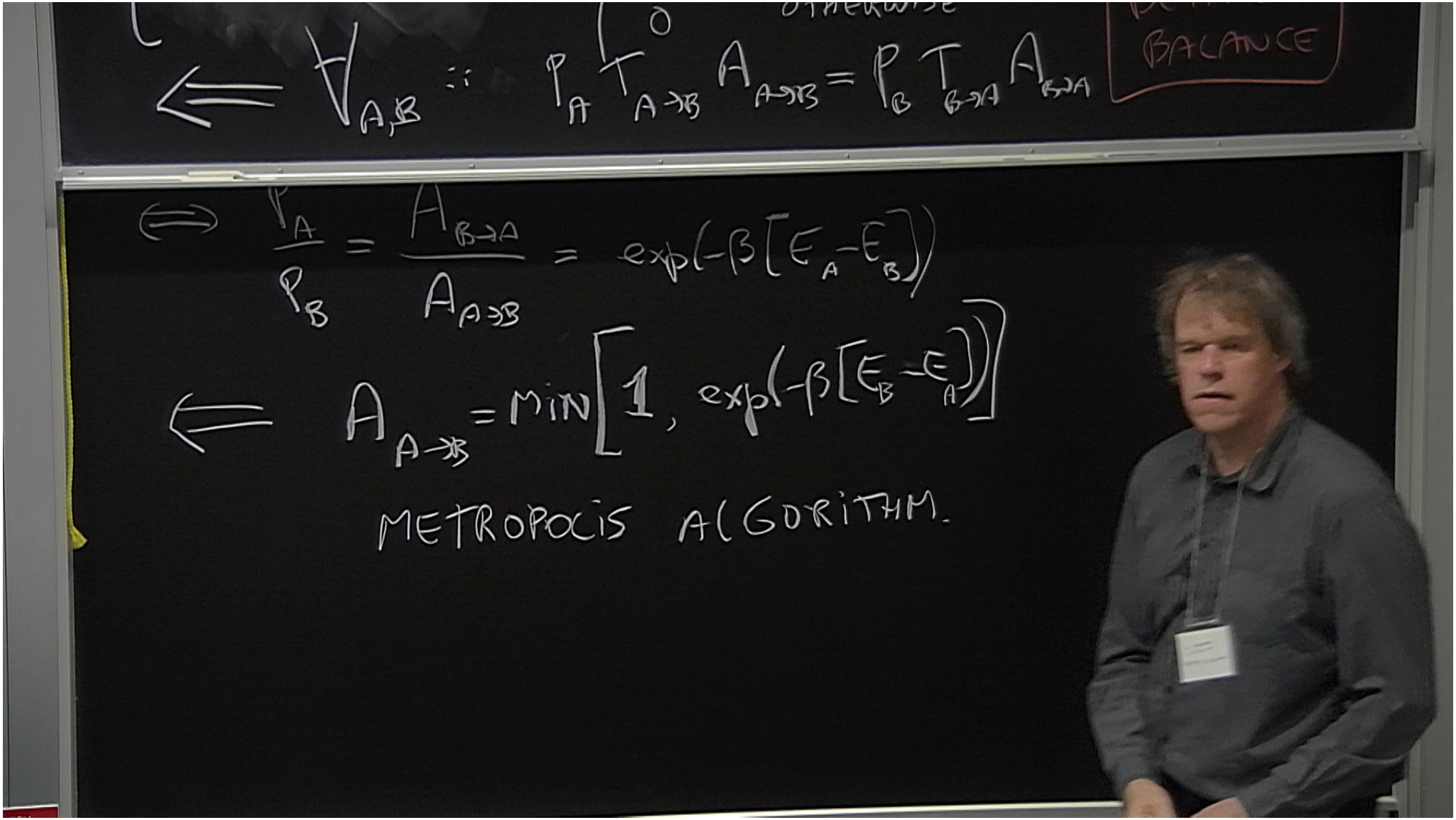
$$\Leftarrow \forall_{A,B} :: P_A \begin{cases} T_{A\to B} & \\ 0 & \text{otherwise} \end{cases} A_{A\to B} = P_B T_{B\to A} A_{B\to A}$$

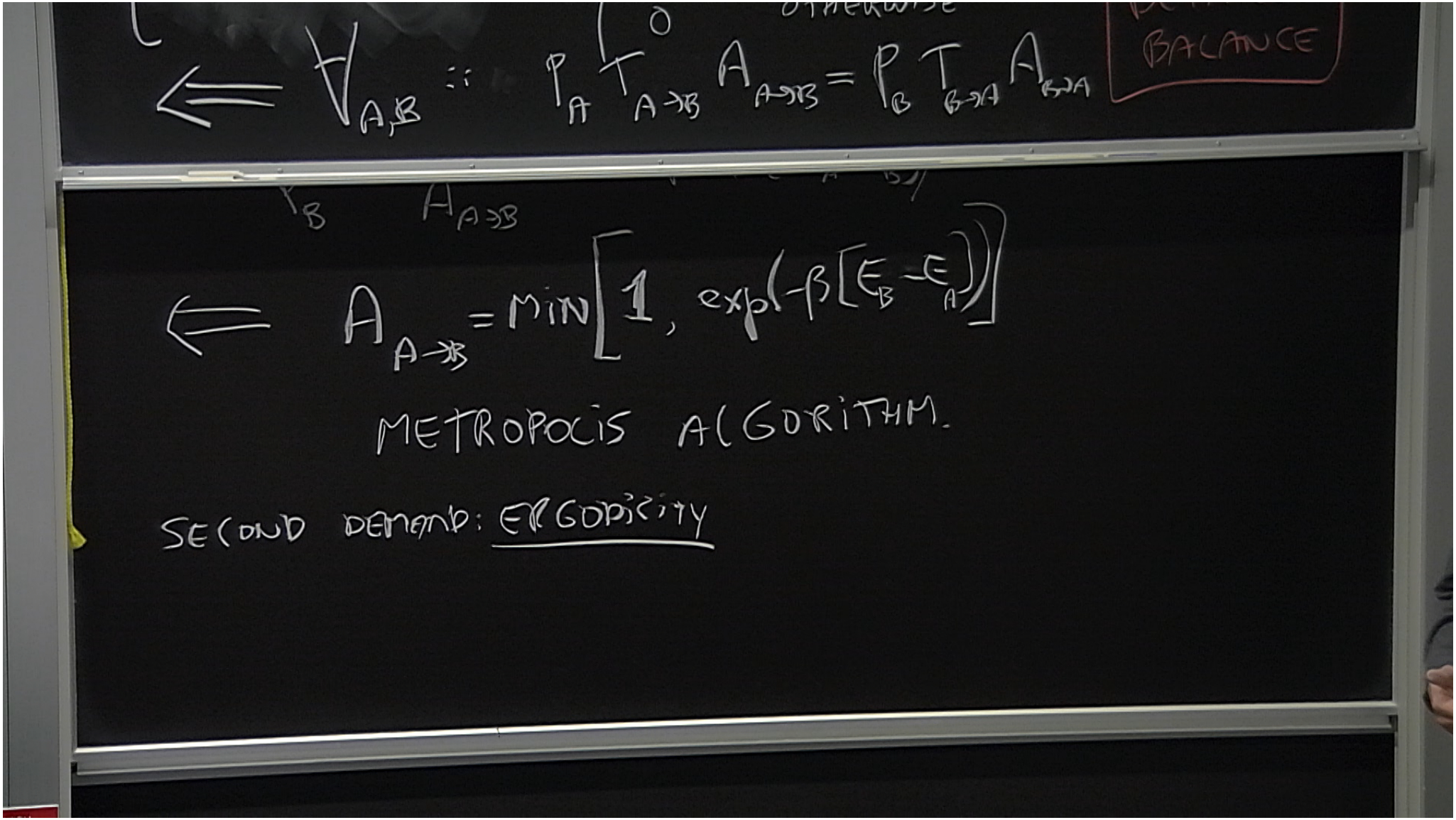
DETAILED BALANCE

$$\Leftrightarrow \frac{P_A}{P_B} = \frac{A_{B\to A}}{A_{A\to B}} = \exp(-\beta[E_A - E_B])$$

$$\Leftarrow A_{A\to B} = \min\left[1, \exp(-\beta[E_B - E_A])\right]$$


$\Leftarrow \forall_{A,B} :: P_A T_{A\to B} A_{A\to B} = P_B T_{B\to A} A_{B\to A}$
otherwise
0
BALANCE
$\Leftrightarrow \frac{P_A}{P_B} = \frac{A_{B\to A}}{A_{A\to B}} = \exp(-\beta[E_A - E_B])$
$\Leftarrow A_{A\to B} = \min\left[1, \exp(-\beta[E_B - E_A])\right]$


$\Leftarrow \forall_{A,B} :: P_A T_{A\to B} A_{A\to B} = P_B T_{B\to A} A_{B\to A}$
BALANCE
$\Leftrightarrow \frac{P_A}{P_B} = \frac{A_{B\to A}}{A_{A\to B}} = \exp(-\beta[E_A - E_B])$
$\Leftarrow A_{A\to B} = \min\left[1, \exp(-\beta[E_B - E_A])\right]$
METROPOLIS ALGORITHM.


$\Leftarrow \forall_{A,B} :: P_A T_{A\to B} A_{A\to B} = P_B T_{B\to A} A_{B\to A}$
BALANCE
$\Leftarrow A_{A\to B} = \min\left[1, \exp(-\beta[E_B - E_A])\right]$
METROPOLIS ALGORITHM.
SECOND DEMAND: ERGODICITY

$$\Longleftarrow \forall_{A,B} :: P_A \begin{cases} T_{A\to B} A_{A\to B} = P_B T_{B\to A} A_{B\to A} \\ 0 \quad \text{otherwise} \end{cases}$$

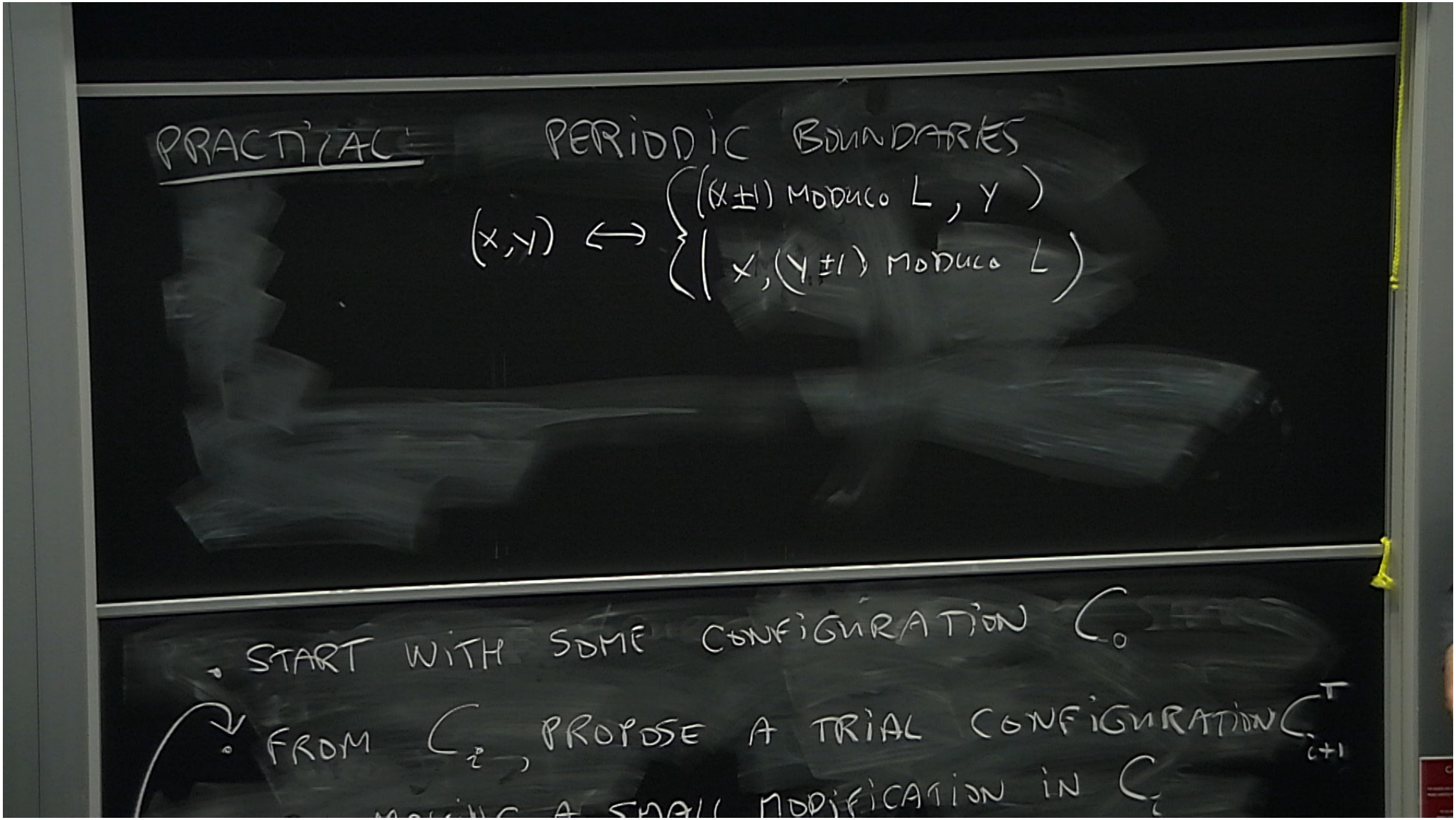
DETAILED BALANCE

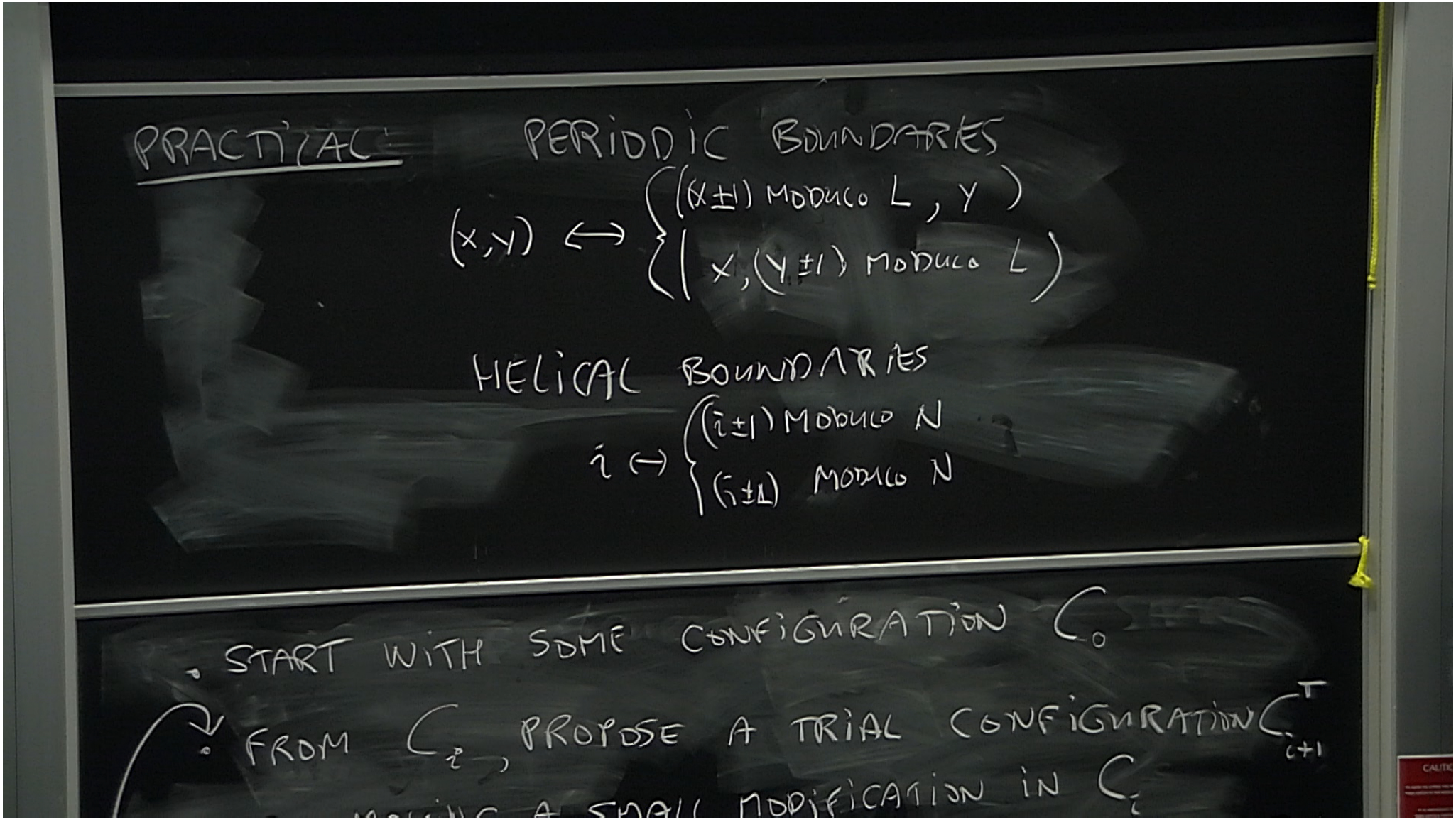
$$P_B \quad A_{A\to B}$$

$$\Longleftarrow A_{A\to B} = \text{MIN}\left[1, \exp\left(-\beta\left[E_B - E_A\right]\right)\right]$$

METROPOLIS ALGORITHM.

SECOND DEMAND: ERGODICITY. FROM ANY A, ANY OTHER CONF. B CAN BE REACHED


PRACTICAL: PERIODIC BOUNDARIES
$(x,y) \leftrightarrow \begin{cases} ((x \pm 1) \text{ MODULO } L, y) \\ (x, (y \pm 1) \text{ MODULO } L) \end{cases}$
• START WITH SOME CONFIGURATION C_0
• FROM C_i, PROPOSE A TRIAL CONFIGURATION C_{i+1}^T
MODIFICATION IN C_i

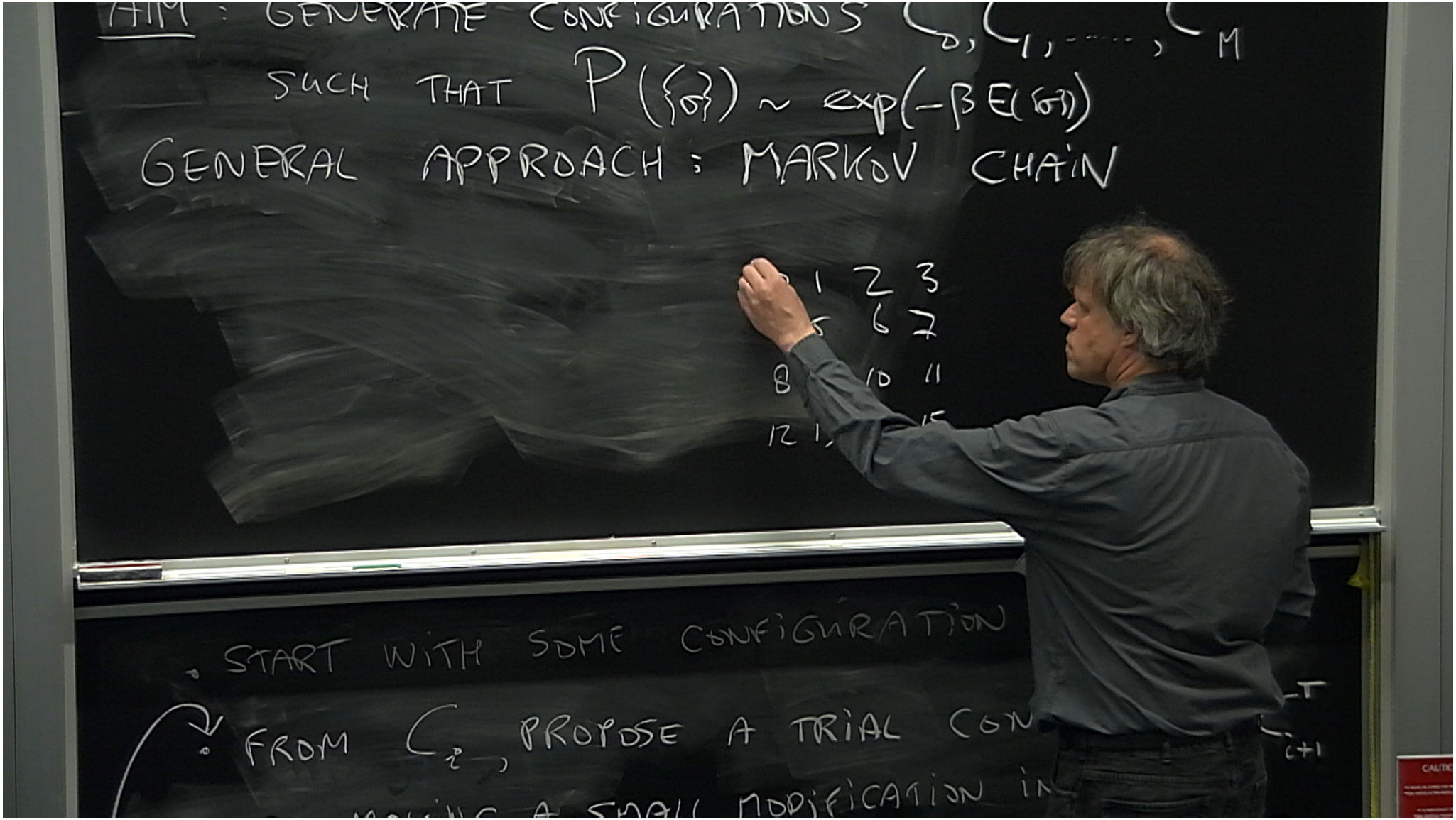

PRACTICAL: PERIODIC BOUNDARIES
$(x,y) \leftrightarrow \begin{cases} ((x \pm 1) \text{ MODULO } L, y) \\ (x, (y \pm 1) \text{ MODULO } L) \end{cases}$
HELICAL BOUNDARIES
$i \leftrightarrow \begin{cases} (i \pm 1) \text{ MODULO } N \\ (i \pm L) \text{ MODULO } N \end{cases}$
• START WITH SOME CONFIGURATION C_0
• FROM C_i, PROPOSE A TRIAL CONFIGURATION C_{i+1}^T
MODIFICATION IN C_i

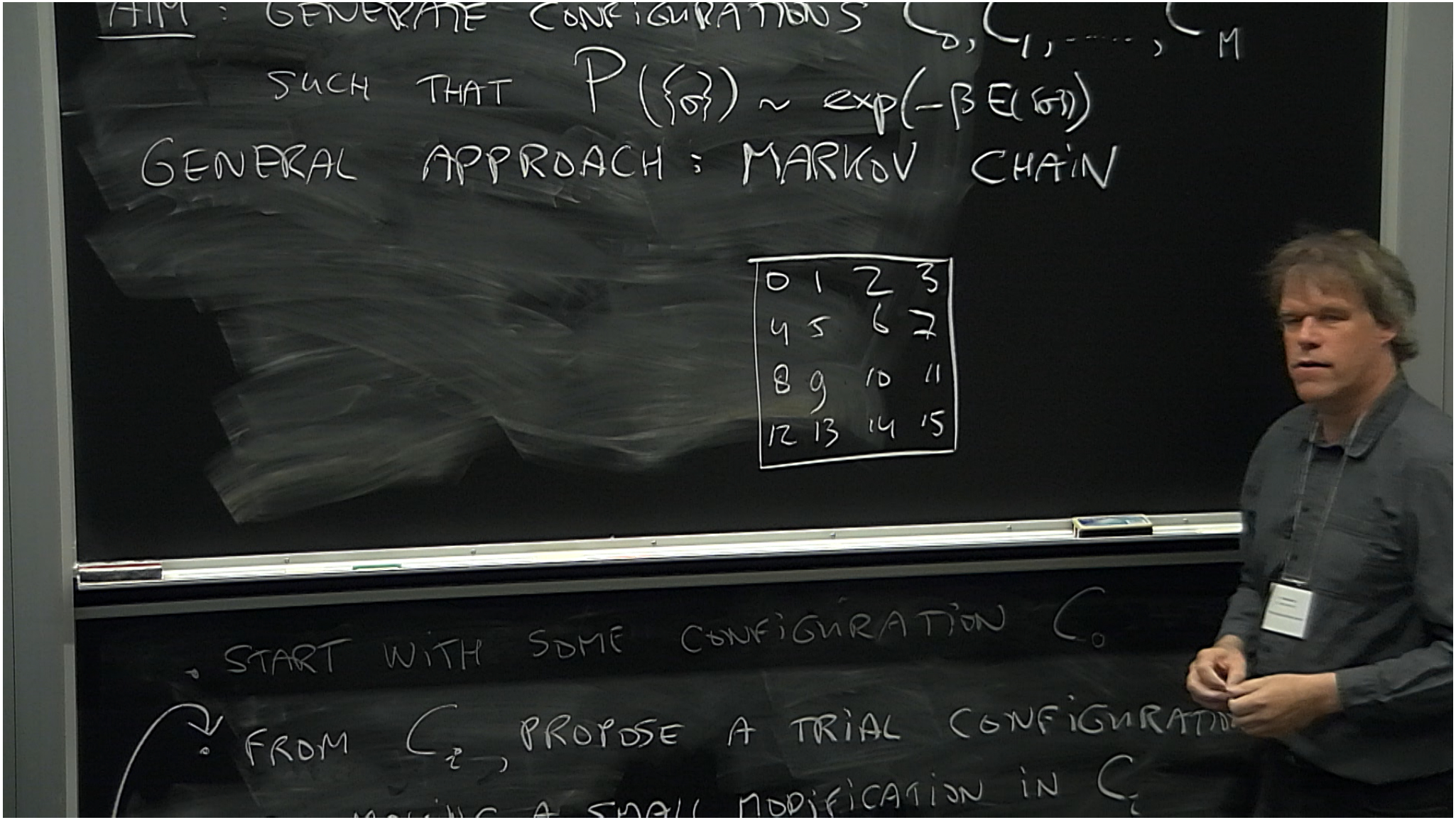
$$(x,y) \hookrightarrow \begin{cases} ((x \pm 1) \text{ MODULO } L,\ y) \\ (x,\ (y \pm 1) \text{ MODULO } L) \end{cases}$$

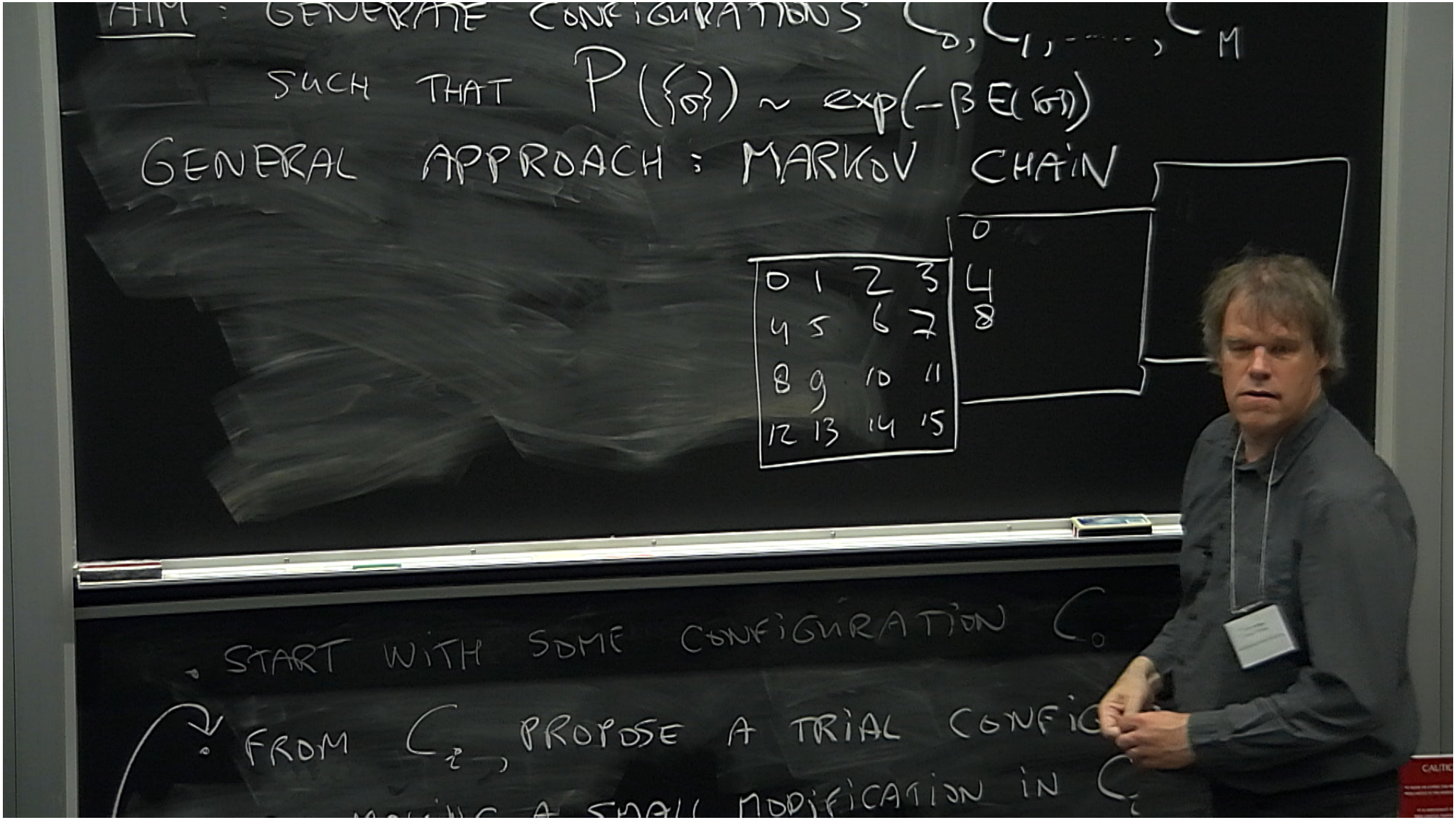
OR HELICAL BOUNDARIES

$$i \hookrightarrow \begin{cases} (i \pm 1) \text{ MODULO } N \\ (i \pm L) \text{ MODULO } N \end{cases}$$

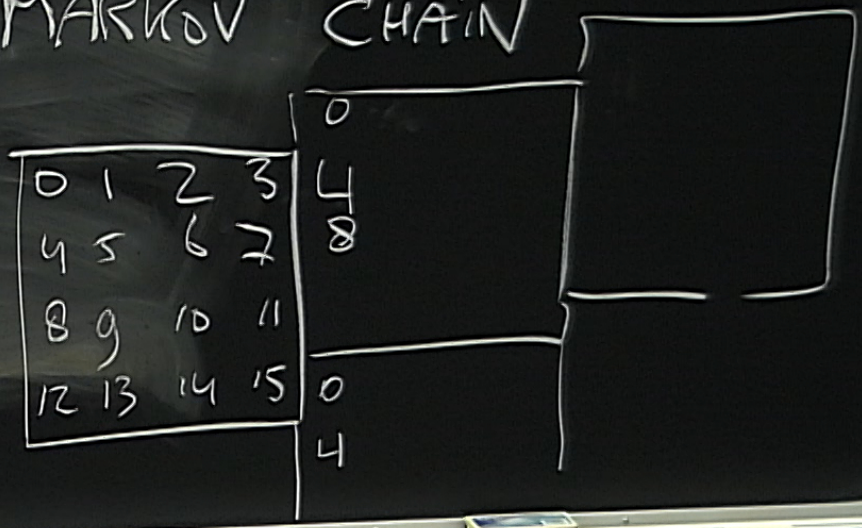
... WITH SOME CONFIGURATION C_0


AIM : GENERATE CONFIGURATIONS $C_0, C_1, \ldots, C_M$
SUCH THAT $P(\{\sigma_i\}) \sim \exp(-\beta E(\{\sigma_i\}))$
GENERAL APPROACH : MARKOV CHAIN
0 1 2 3
4 5 6 7
8 9 10 11
12 13 14 15
START WITH SOME CONFIGURATION
FROM C_i, PROPOSE A TRIAL CON
C_{i+1}


AIM : GENERATE CONFIGURATIONS $C_0, C_1, \ldots, C_M$
SUCH THAT $P(\{\sigma\}) \sim \exp(-\beta E(\{\sigma\}))$
GENERAL APPROACH : MARKOV CHAIN
0 1 2 3
4 5 6 7
8 9 10 11
12 13 14 15
START WITH SOME CONFIGURATION C_0
FROM C_i, PROPOSE A TRIAL CONFIGURATION
MODIFICATION IN C_i


AIM : GENERATE CONFIGURATIONS $C_0, C_1, \ldots, C_M$
SUCH THAT $P(\{\sigma\}) \sim \exp(-\beta E(\{\sigma\}))$
GENERAL APPROACH : MARKOV CHAIN
0 1 2 3
4 5 6 7
8 9 10 11
12 13 14 15
0
4
8
START WITH SOME CONFIGURATION C_0
FROM C_i, PROPOSE A TRIAL CONFIG
MODIFICATION IN C_i

AIM : GENERATE CONFIGURATIONS $C_0, C_1, \ldots, C_M$
SUCH THAT $P(\{\sigma\}) \sim \exp(-\beta E(\sigma))$
GENERAL APPROACH : MARKOV CHAIN

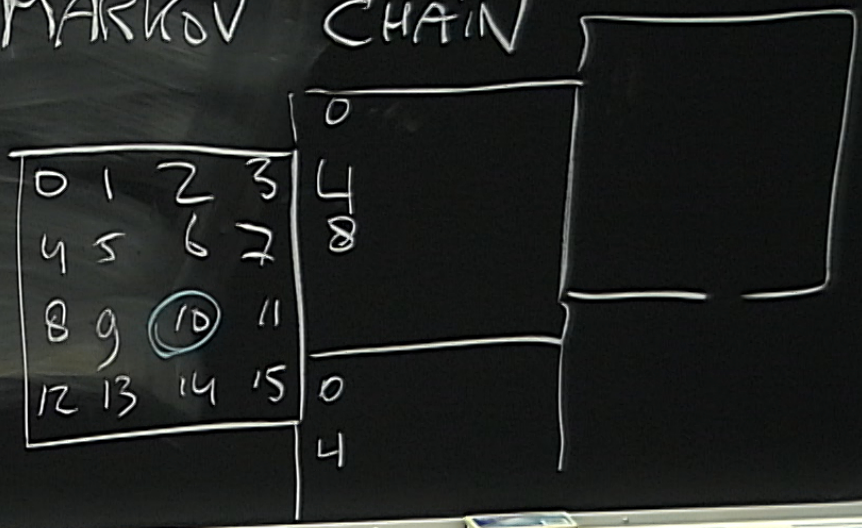


- START WITH SOME CONFIGURATION C_0
- FROM C_i, PROPOSE A TRIAL CONFIGURATION C_{i+1}^T
BY MAKING A SMALL MODIFICATION IN C_i

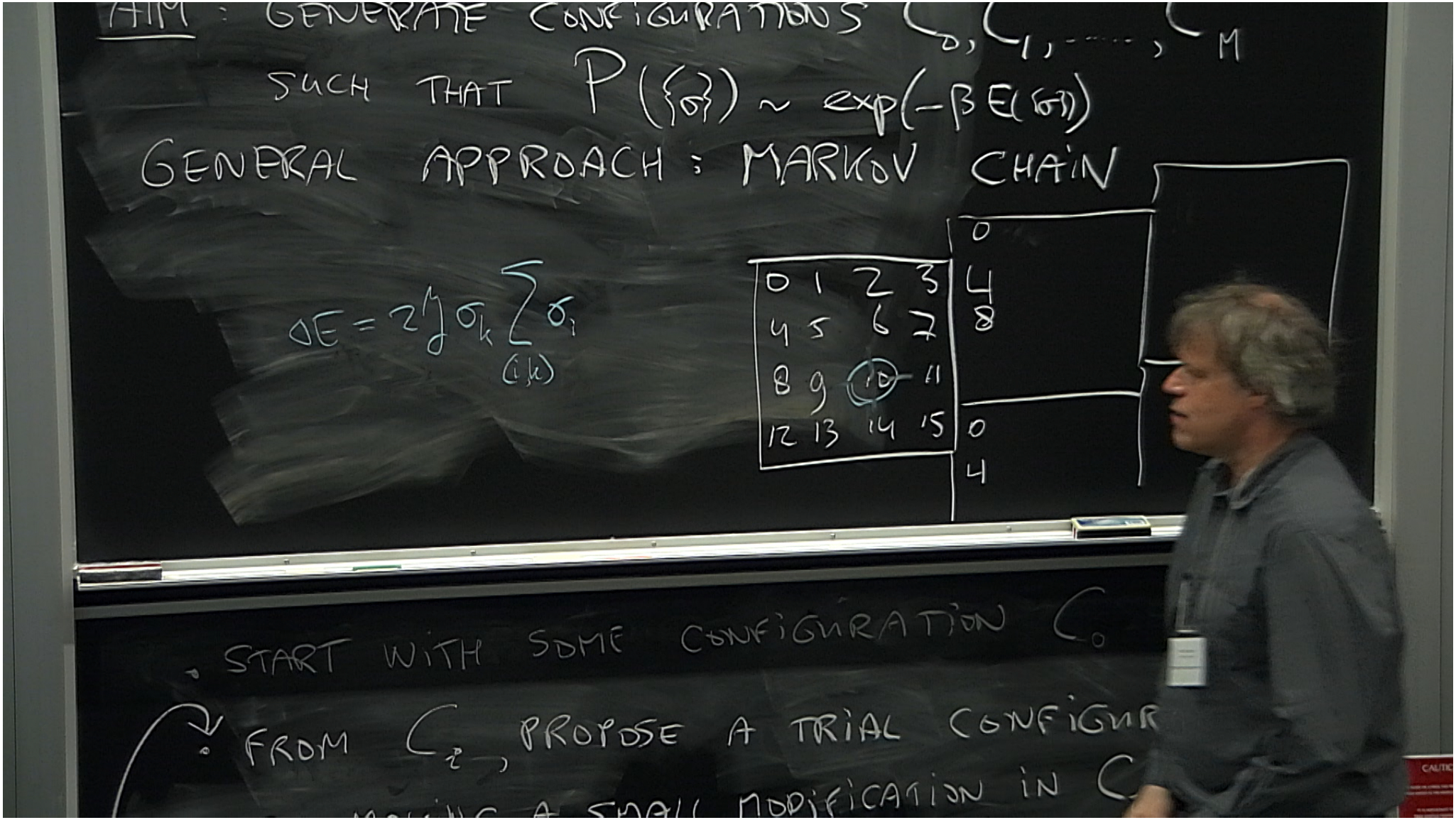
AIM : GENERATE CONFIGURATIONS $C_0, C_1, \ldots, C_M$

SUCH THAT $P(\{\sigma\}) \sim \exp(-\beta E(\sigma))$

GENERAL APPROACH : MARKOV CHAIN



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AIM : GENERATE CONFIGURATIONS $C_0, C_1, \ldots, C_M$
SUCH THAT $P(\{\sigma\}) \sim \exp(-\beta E(\{\sigma\}))$
GENERAL APPROACH : MARKOV CHAIN
$\Delta E = 2J\sigma_k \sum_{(i,k)} \sigma_i$
0 1 2 3
4 5 6 7
8 9 10 11
12 13 14 15
0
4
8
0
4
START WITH SOME CONFIGURATION C_0
FROM C_i, PROPOSE A TRIAL CONFIGUR
MODIFICATION IN C