Title: How Difficult is Quantum Many-Body Theory?

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Abstract: The basic problem of much of condensed matter and high energy physics, as well as quantum chemistry, is to find the ground state properties of some Hamiltonian. Many algorithms have been invented to deal with this problem, each with different strengths and limitations. Ideas such as entanglement entropy from quantum information theory and quantum computing enable us to understand the difficulty of various problems. I will discuss recent results on area laws and use these to prove that we can use matrix product states to efficiently represent ground states for one-dimensional systems with a spectral gap, while certain other one-dimensional problems, without the gap assumption, almost certainly have no efficient way for us to even represent the ground state on a classical computer. I will also discuss recent results on higher-dimensional matrix product states, in an attempt to extend the remarkable success of matrix product algorithms beyond one dimension.

How Hard is Quantum Many-Body Theory?

M. B. Hastings
T-13, Complex Systems Group
Los Alamos National Laboratory

Thanks: X.-G. Wen, F. Verstraete, T. Koma, S. Bravyi

Outline:

- Algorithm overview: perturbation theory, DMRG (matrix product), exact diagonalization.
- Computational complexity classes. Difficulty of the problem depends on entanglement.
- Easy problems (P or almost polynomial): perturbing a system. Can find efficient representation of ground state.
- Harder problems: (NP) 1d gapped systems. Area laws for quantum entanglement imply an efficient representation exists.
- Very hard: (QMA-complete) 1d gapless.

Some common algorithms:

Exact diagonalization:

Requires exponentially long time. Even finding ground state is typically limited to 30-40 spin-1/2 spins.

Perturbation theory:

$$H = H_0 + \lambda V$$

$$E_n = E_n^{(0)} + \lambda \langle \Psi_n^{(0)} | V | \Psi_n^{(0)} \rangle + \lambda^2 \sum_{k \neq n} \frac{|\langle \Psi_k^{(0)} | V | \Psi_n^{(0)} \rangle|^2}{E_n^{(0)} - E_k^{(0)}} + ...$$

Different ways to compute the terms.
Feynman diagrams (physics). Moller-Plesset (quantum chemistry).
Convergence of series?

Matrix product methods (including DMRG):

Based on ground state ansatz of the form:

$$\Psi(s_1, s_2, s_3, ...) = \sum_{\alpha,\beta,\gamma,\delta,...} A^{(1)}_{\alpha\beta}(s_1) A^{(2)}_{\beta\gamma}(s_2) A^{(3)}_{\gamma\delta}(s_3)....$$

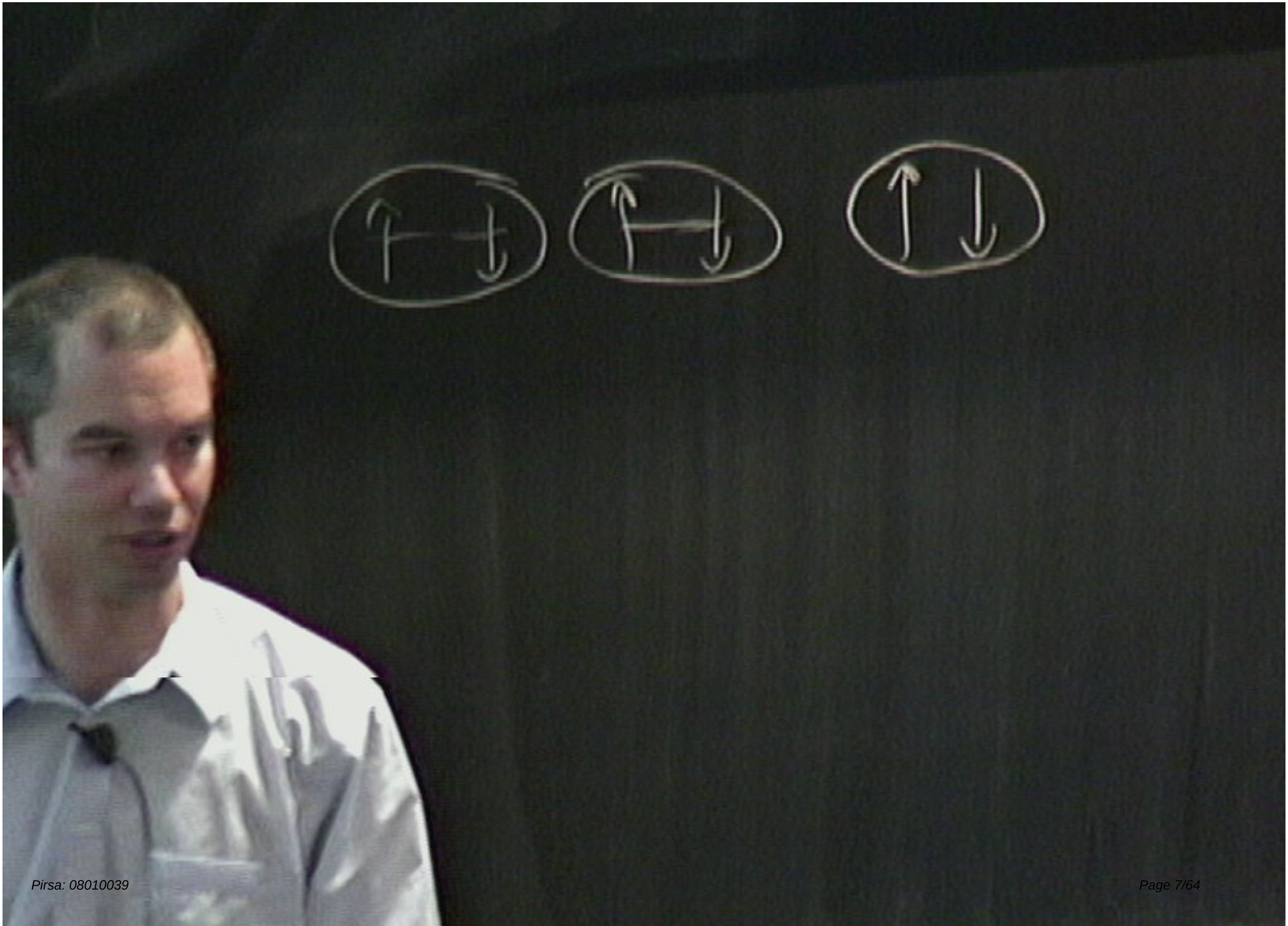
Spin 1: $s_i = -1, 0, 1$

$\alpha, \beta, \gamma = 1...k$

Spin 1/2: $s_i = -1/2, 1/2$

Matrices A are k-by-k matrices. There are NDk^2 variational parameters.

Works extremely well for 1d gapped systems. Why?



Complexity classes:

Solve in polynomial time on a classical computer (in the problem size, N).

Examples:

- Sort a list of N numbers
- Find the ground state of a ferromagnetic Ising model of N spins with arbitrary, position-dependent magnetic field
- Simulate quantum dynamics-for a time of order log(N)

Solve in polynomial time on a quantum computer. Example: simulate quantum dynamics

NP: a yes-no decision problem.
If yes, can check proof in polynomial time.

Example:

- Does a frustrated Ising model $H = \sum J_{ij}\sigma_i\sigma_j$ have a state with energy less than or equal to E, for some E? Proof if yes: just give the configuration of spins.

Also NP-complete: if solvable in polynomial time, then every problem in NP is solvable in polynomial time. Widely believed impossible!

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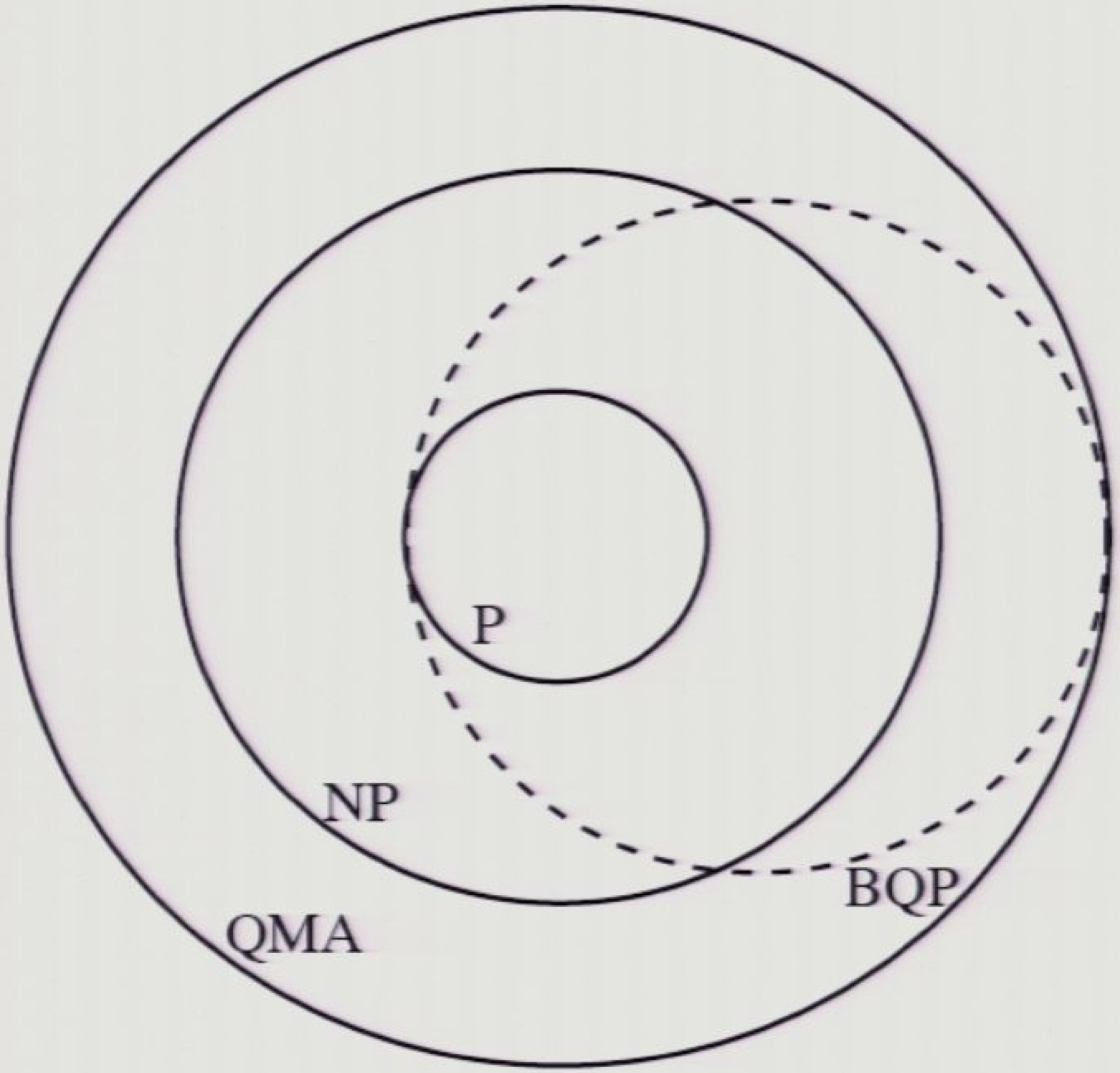
QMA: yes-no decision problem. If yes, can check proof in polynomial time on a quantum computer, with probability at least 2/3 of being right.

- Does a quantum Hamiltonian have a ground state of energy E or less, given a promise that if not, then the energy is at least E+1/N^4. Proof if yes: give the ground state.

Also QMA-complete: if solvable in polynomial time on a quantum computer, then every problem in QMA is solvable in polynomial time. Also believed impossible!

Kitaev 02; Aharonov, Gottesman, Kempe 07; Irani 07.

Relation of complexity classes:



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Perturbation of gapped, decoupled Hamiltonian is in P:

$$H = H_0 + \lambda V \qquad H_0 = \Delta E \sum_i S_i^z$$

$$E_n = E_n^{(0)} + \lambda \langle \Psi_n^{(0)} | V | \Psi_n^{(0)} \rangle + \lambda^2 \sum_{k \neq n} \frac{|\langle \Psi_k^{(0)} | V | \Psi_n^{(0)} \rangle|^2}{E_n^{(0)} - E_k^{(0)}} + \ldots$$

Time to compute m-th coefficient is exponential in m:

Coupled cluster (Bravyi, DiVincenzo, Loss 07)

Rayleigh-Schrodinger (Hastings 07)

Perturbation of gapped, interacting Hamiltonian is exp(polylog(N))

Quasi-adiabatic continuation (Hastings-Wen 05; Osborne 07)

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Entanglement in Matrix Product States:

$$\Psi_{(}s_1, s_2, s_3, ...) = \sum_{\alpha,\beta,\gamma,\delta,...} A^{(1)}_{\alpha\beta}(s_1) A^{(2)}_{\beta\gamma}(s_2) A^{(3)}_{\gamma\delta}(s_3)....$$

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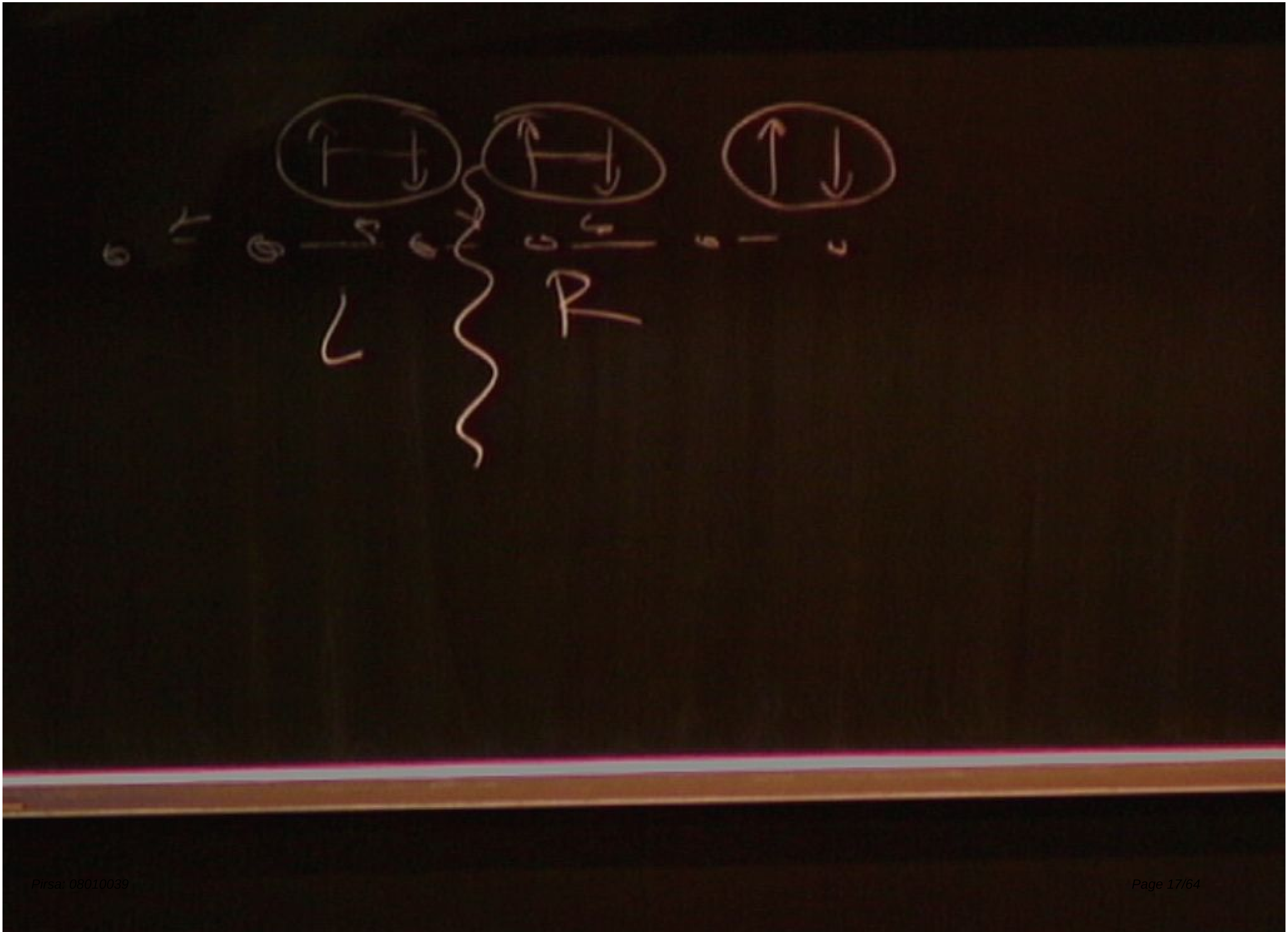
Schmidt rank at most k in matrix product state. Approximately true for ground state?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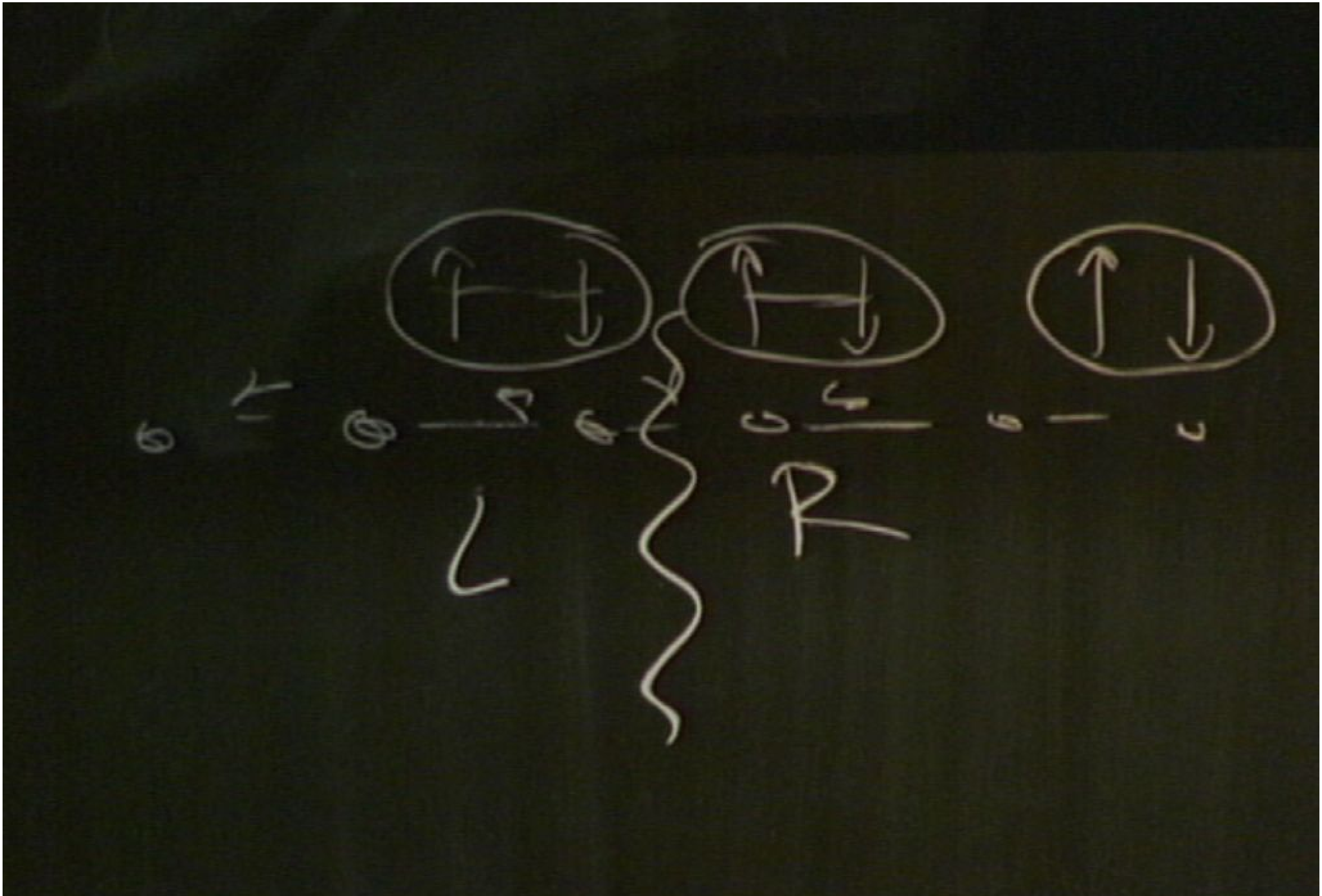
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Handwaving argument for an area law:

Assumptions: short-range Hamiltonian, unique ground state, spectral gap.

- Gap implies short-range correlations.
- Therefore, only the degrees of freedom near the surface of A are entangled with the degrees of freedom in B.
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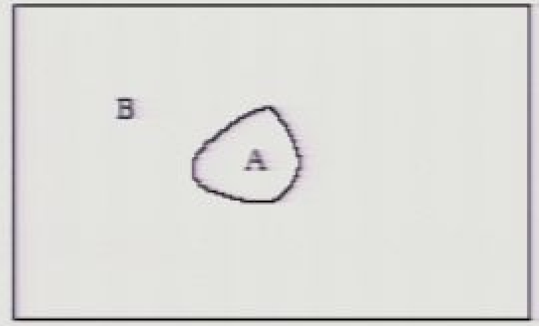
Area laws:

How much entanglement between A and B?
Less entanglement means easier to simulate.



$$\Psi_0 = \sum_\alpha A(\alpha)\Psi_A(\alpha) \otimes \Psi_B(\alpha); \quad S = -\sum_\alpha |A(\alpha)|^2 \ln(|A(\alpha)|^2)$$

Von Neumann and Renyi entropy of a density matrix:

$$S = -\mathrm{tr}(\rho \ln(\rho))$$
$$S_\alpha(\rho) = \frac{1}{1-\alpha} \ln(\mathrm{tr}(\rho^\alpha))$$

Entropy for an arbitrary state is of order the volume of A.
Area law means that entropy is of order the surface area.

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Can we make this rigorous?
(why area laws are tricky)

- Assuming a gap and short-range Hamiltonian, can prove that the correlations are short-range.

M. B. Hastings, PRB 2004;
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- However, even in one-dimension, there exist states with short-range correlations but arbitrarily large entanglement. This is based on quantum expanders.

M. B. Hastings, PRB 2007;
A. Ben-Aroya and A. TaShma, quant-ph/0702129.

Need to consider more than correlations to prove an area law!

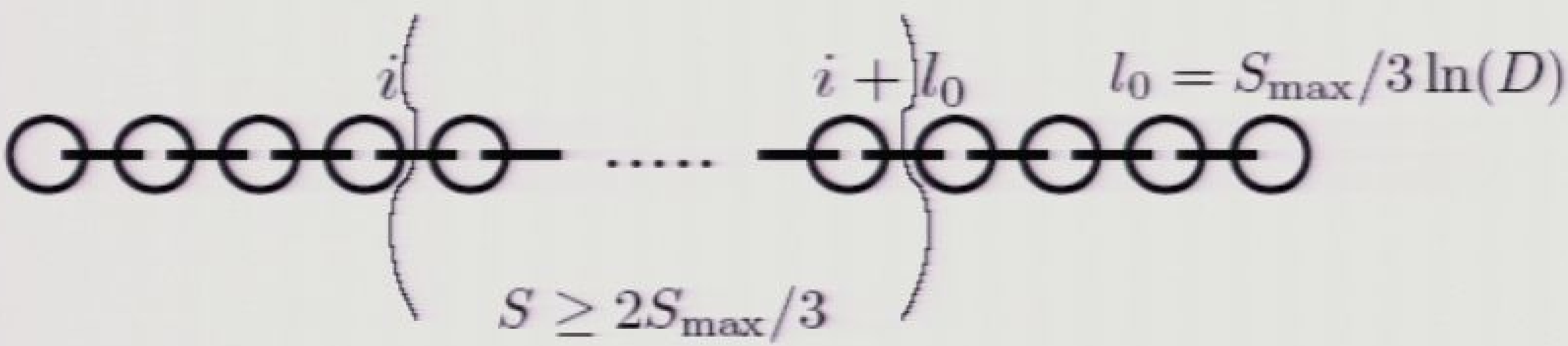
An area law in 1-d

Assumptions: nearest neighbor Hamiltonian with interaction strength bounded by J, finite dimensional Hilbert space D on each site, unique ground state, spectral gap.

$$S \leq S_{\max} = \exp(\mathcal{O}(v/\Delta E))$$ M. B. Hastings, JSTAT 2007.

(Sketched) proof:

Suppose not. Then, the entropy is large over a range of cuts of the chain, not just one.



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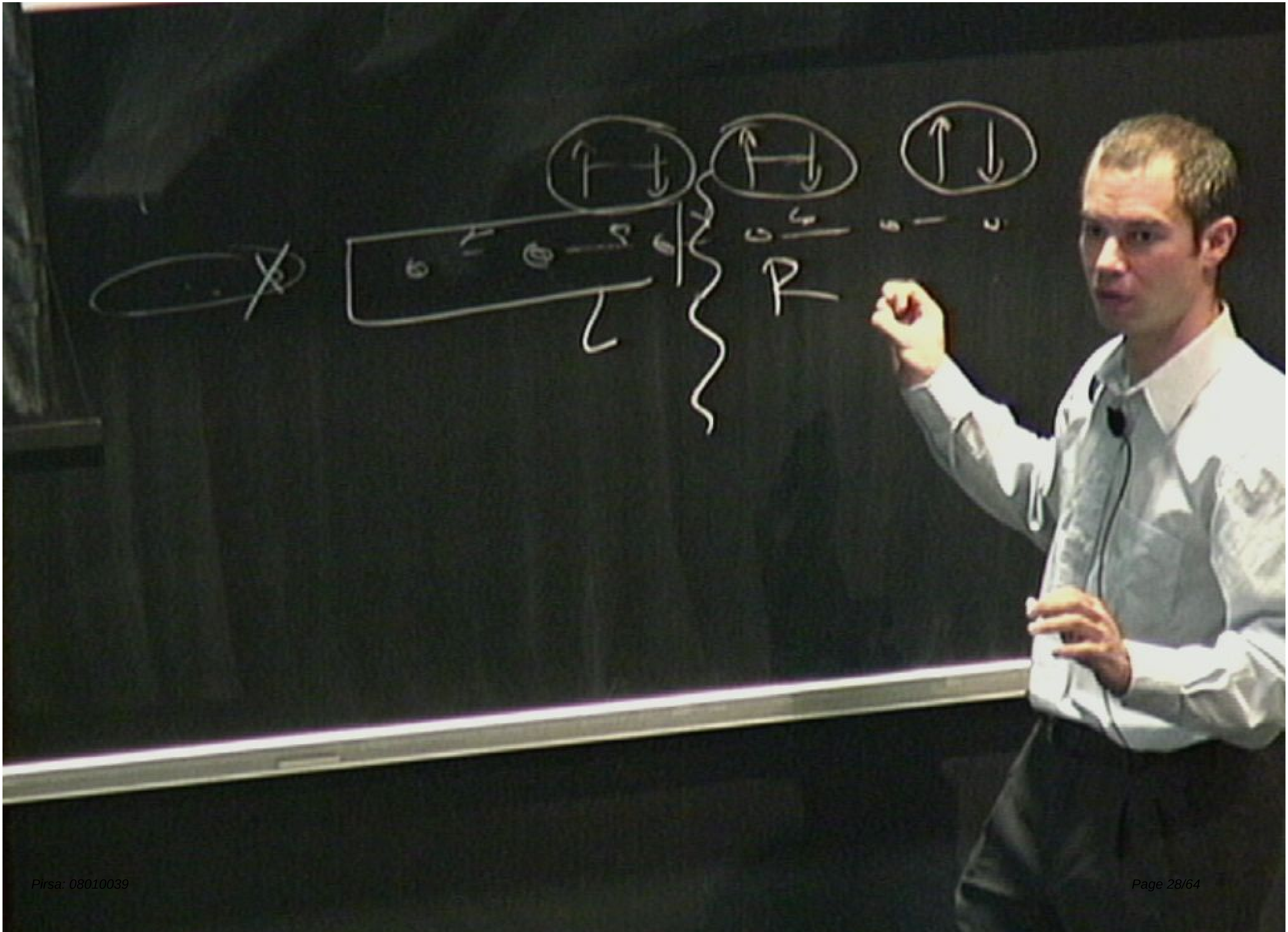
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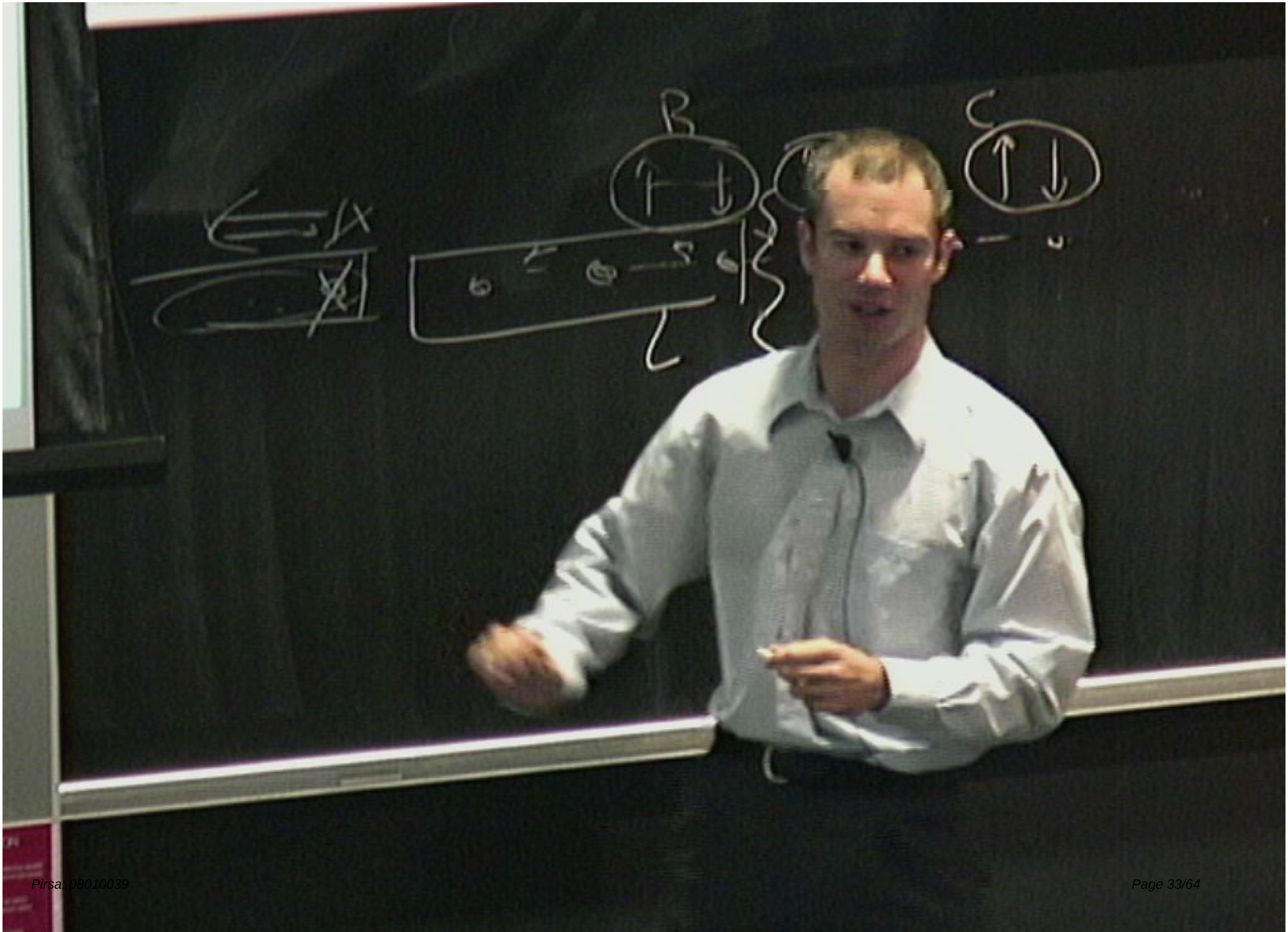
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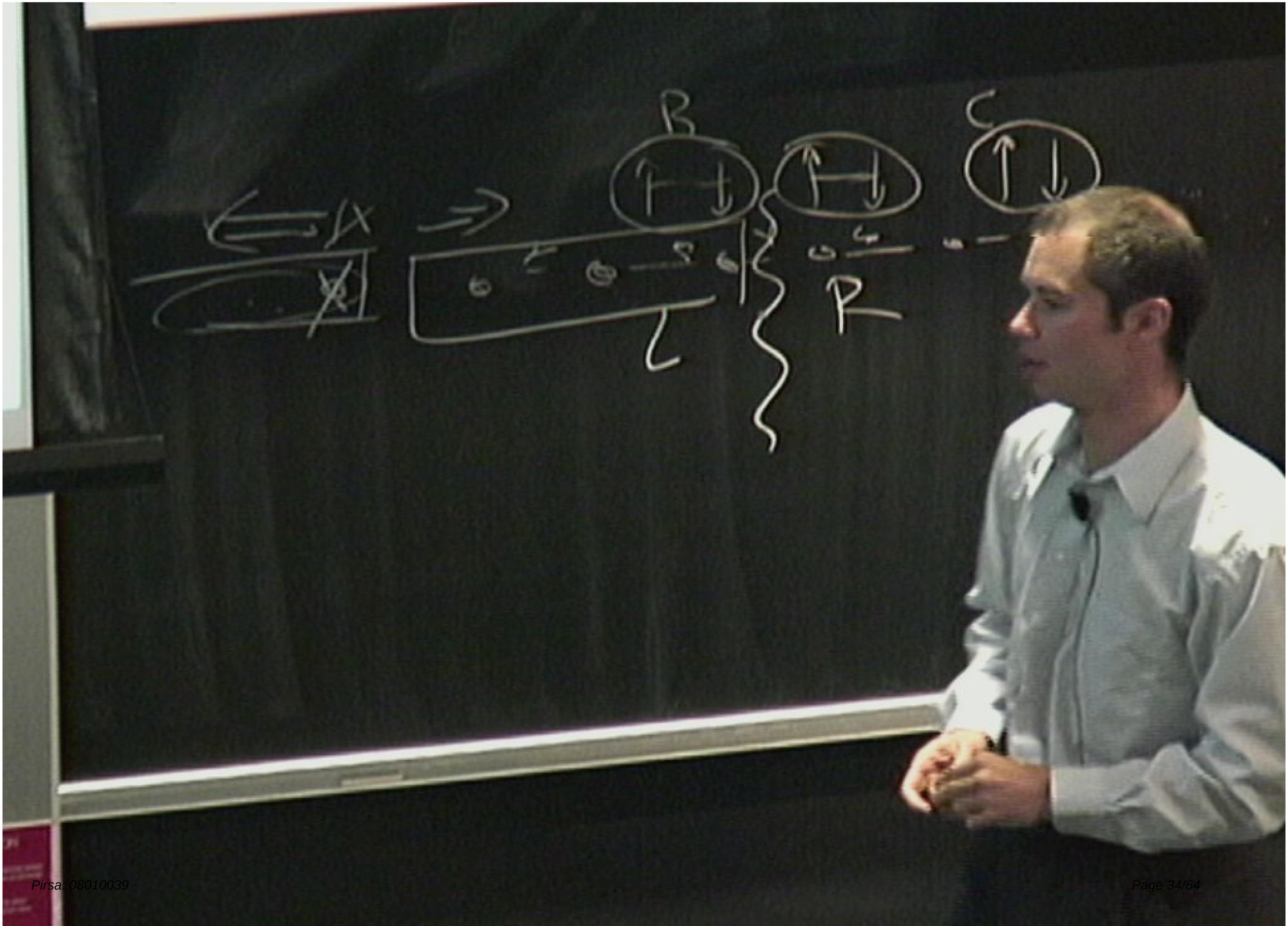
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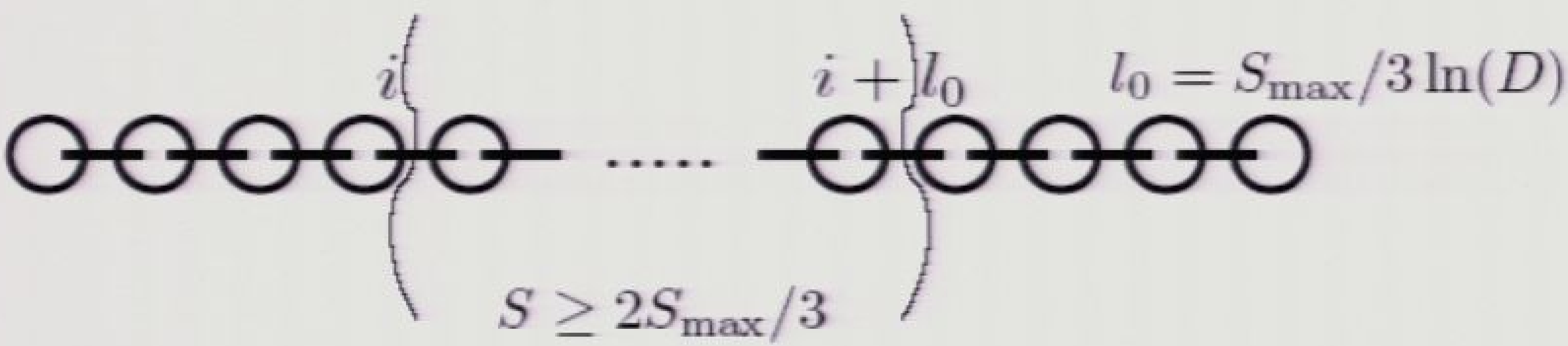

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Define S_l to be the maximum entropy of an interval of length l contained in the interval between $i, i+l$

Some trivial properties:

$$S_1 \leq \ln(D)$$
$$S_{2l} \leq 2S_l$$

Araki, Lieb 1970

If second inequality saturates, $\rho_{i,i+2l} = \rho_{i,i+l} \otimes \rho_{i+l+1,i+2l}$
Then ground state factorizes, contradicting assumption of non-vanishing entanglement entropy.

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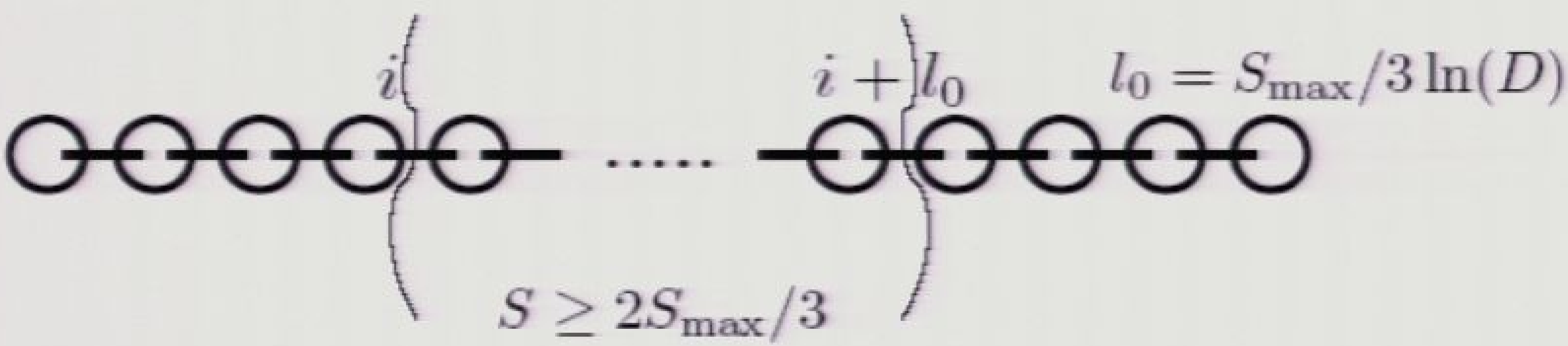

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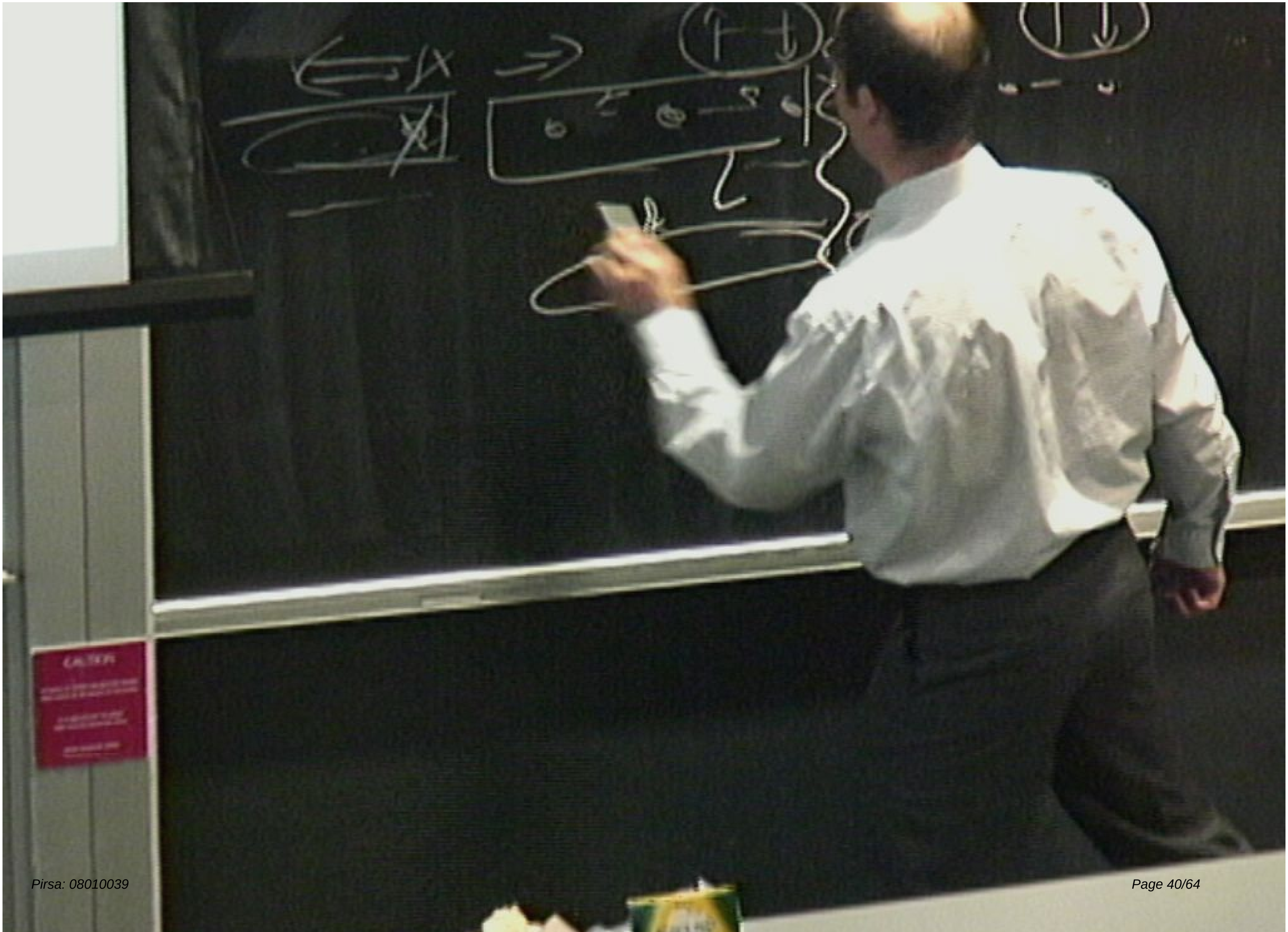

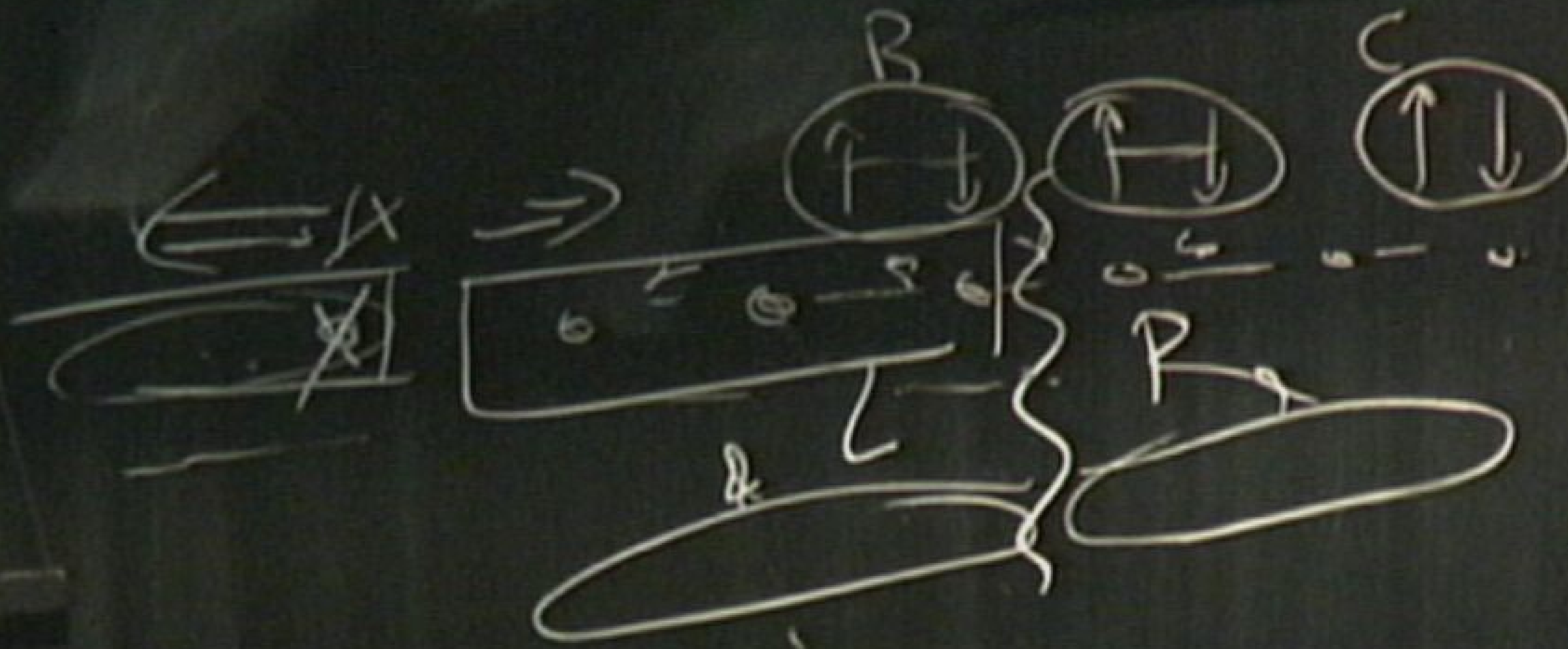
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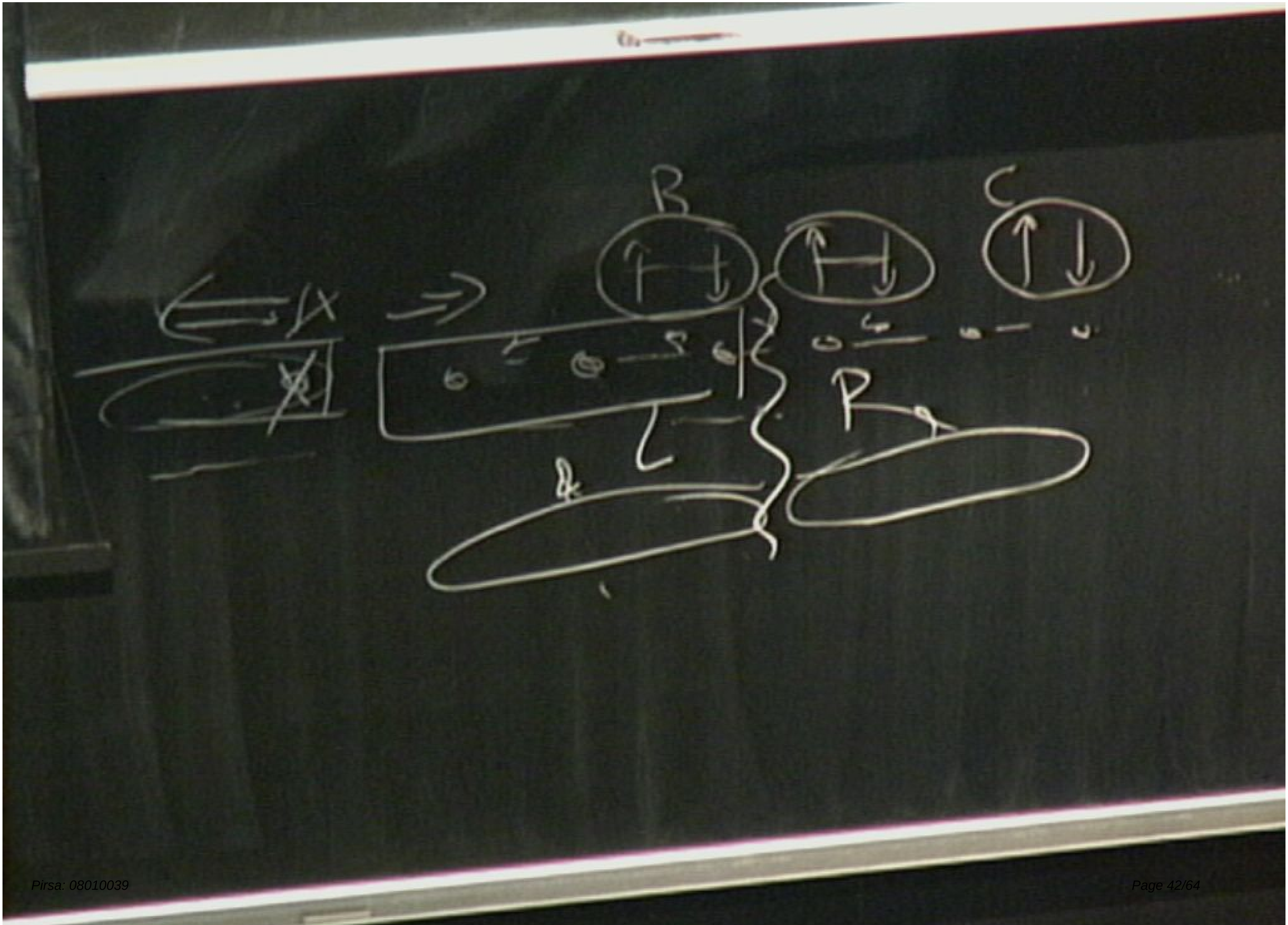
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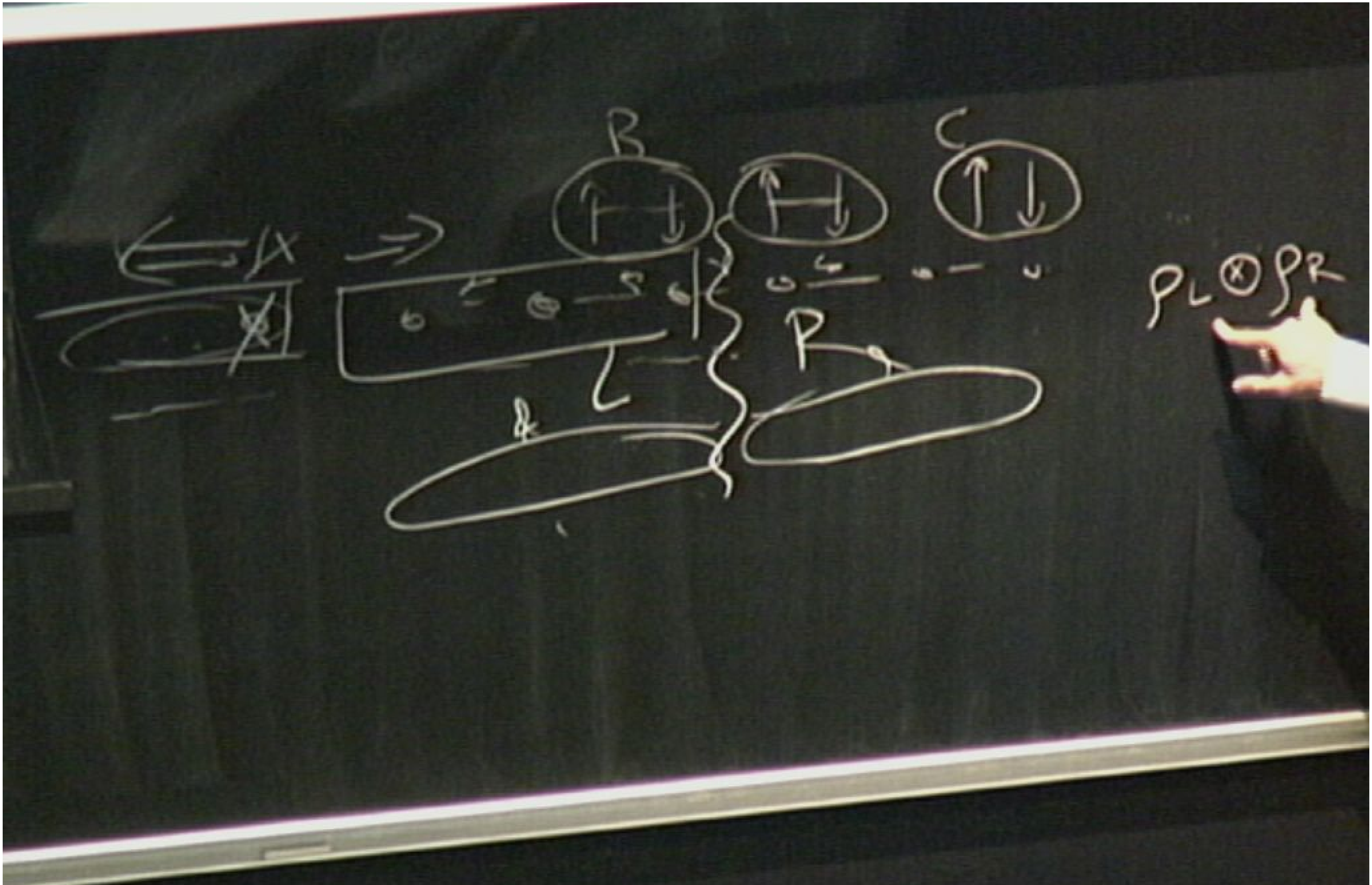
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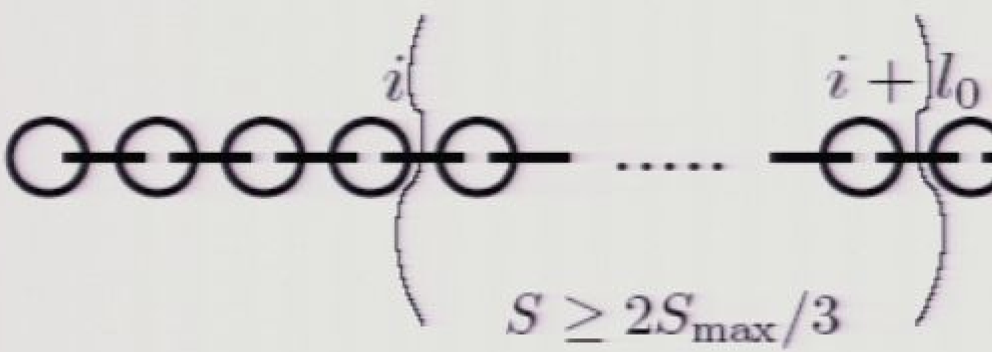

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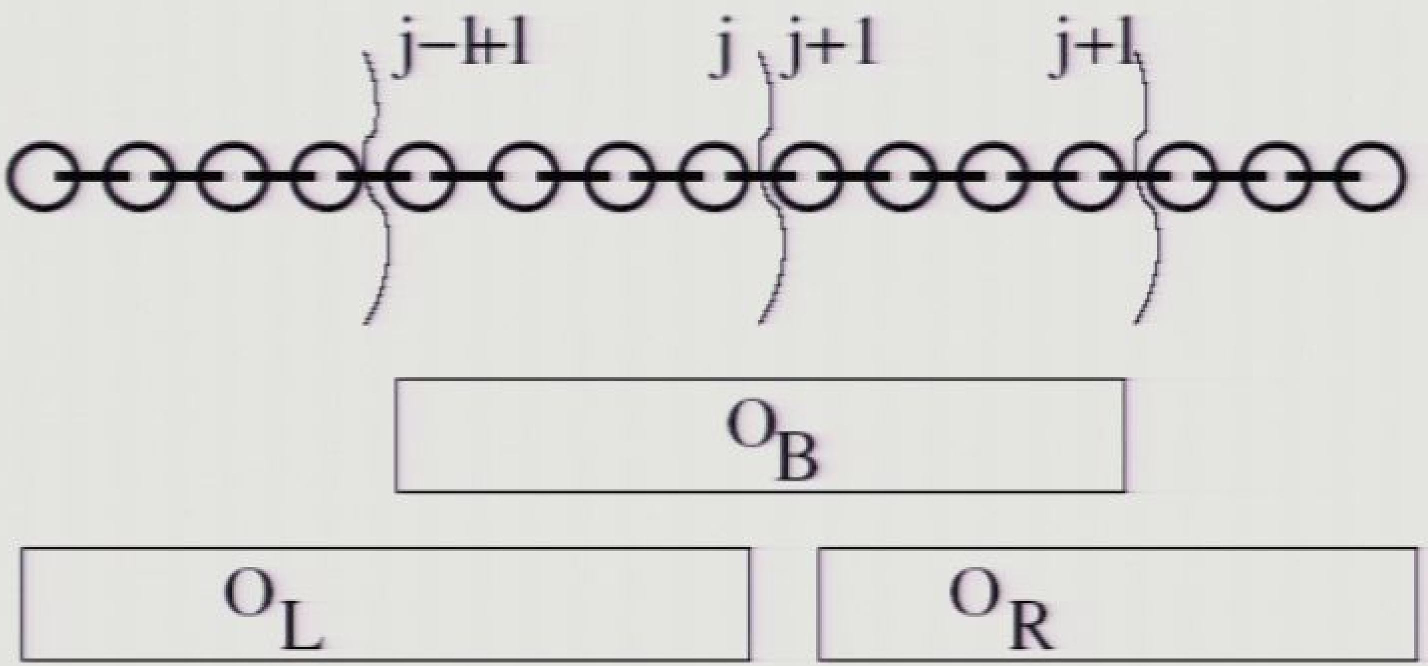
Two lemmas:

1) Given assumptions above, for any j,l we can define Hermitian, positive definite operators, $O_B(j,l), O_L(j,l), O_R(j,l)$, with operator norms bounded by unity such that

$$\|O_B(j,l)O_L(j,l)O_R(j,l) - |\Psi_0\rangle\langle\Psi_0|\| \leq \exp(-\mathcal{O}(l\Delta E/v))$$

and such that the operators are supported like this:



2) Given assumptions above, suppose exists factorized density matrix $\rho = \rho_L \otimes \rho_R$ such that

$$\langle \Psi_0 | \rho | \Psi_0 \rangle = P > 0.$$

Then, the entropy S across the cut is bounded by

$$\begin{aligned} S &\leq \mathcal{O}(v/\Delta E) \ln(D) \ln(1/P) \\ &+ \mathcal{O}(v/\Delta E) \ln(v/\Delta E) \ln(D) \end{aligned}$$

Prove this using lemma 1. Approximate ground state with

$$O_B(j,l) O_L(j,l) O_R(j,l) \rho O_R(j,l) O_L(j,l) O_B(j,l)$$

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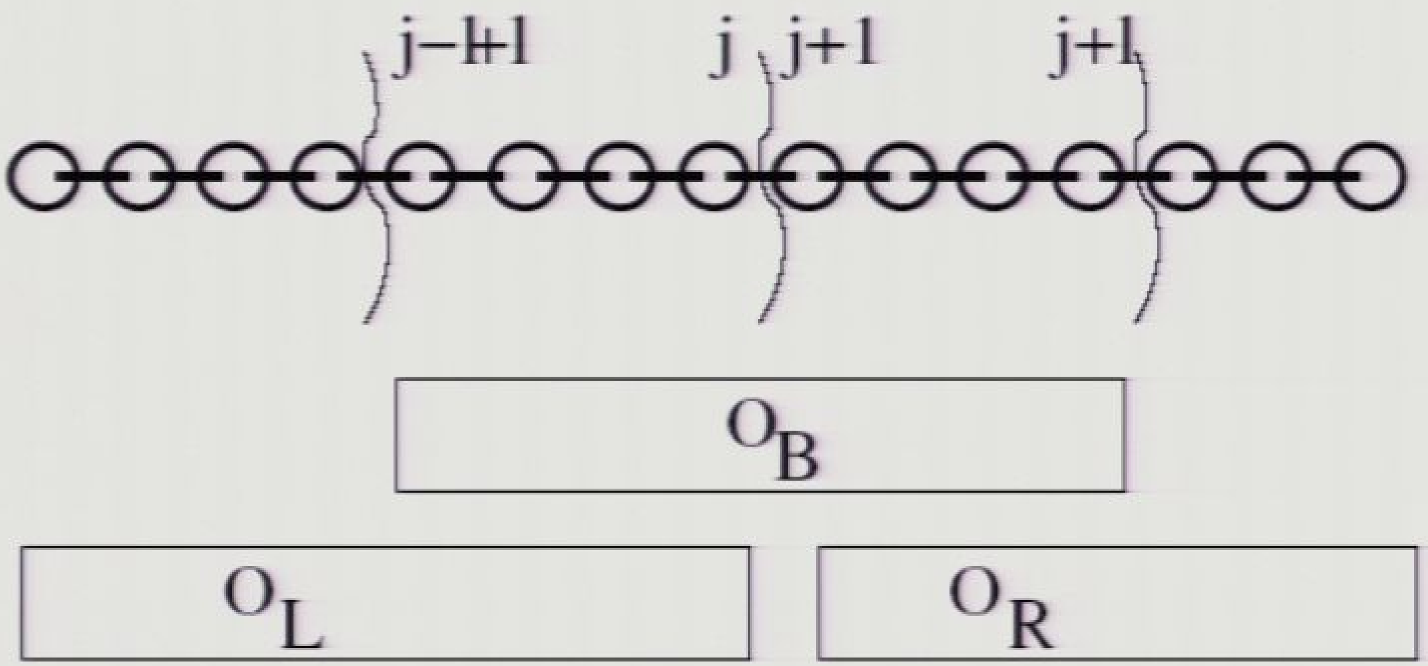

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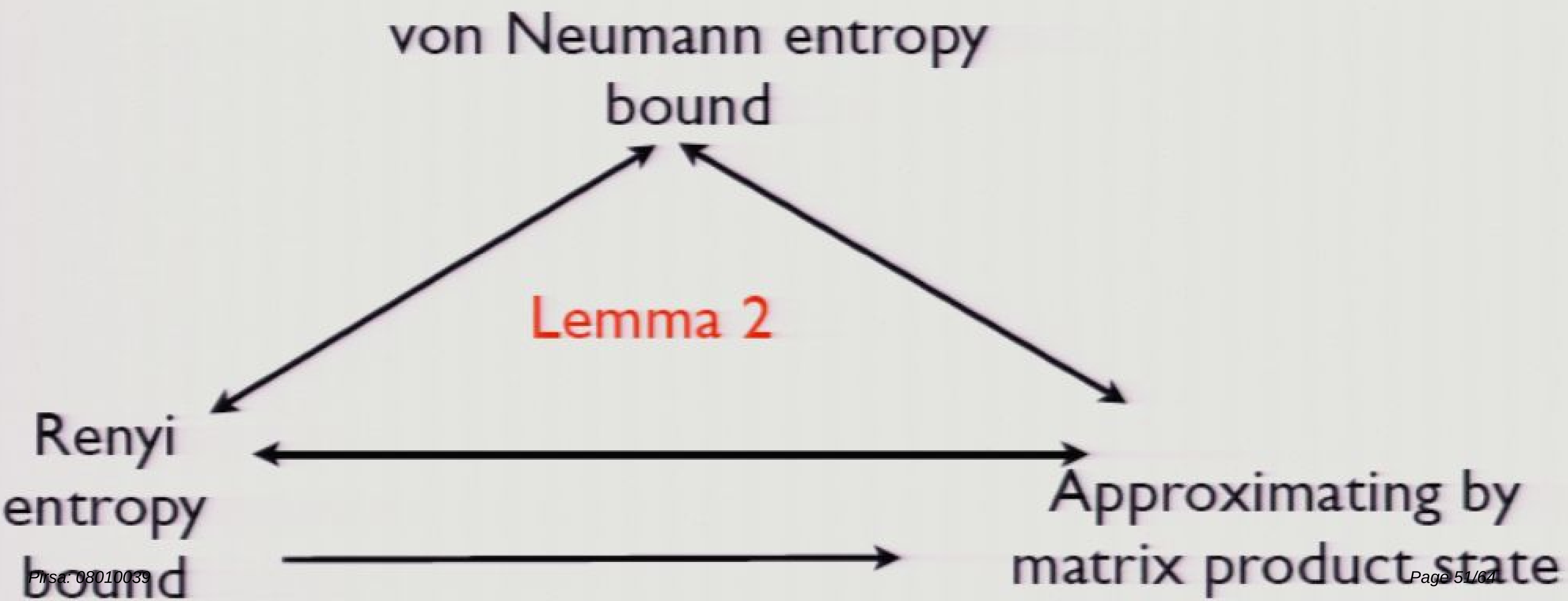
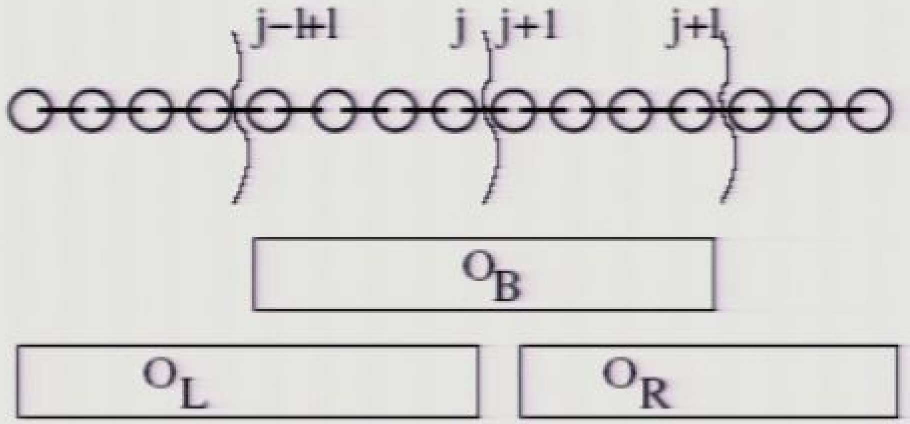
- Lemma 2 works for Renyi entropies also.
- Lemma 2 enables approximating ground state by matrix product state.
- Upper bound on Renyi or von Neumann entropy gives lower bound on the largest Schmidt coefficient across a cut and hence lower bound on P in Lemma 2.



F. Verstraete and J. I. Cirac, PRB 2006.

Back to proving the main theorem:



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But the expectation value $\mathrm{tr}(\rho_{j-l+1,j} \otimes \rho_{j+1,j+l}\, O_B(j,l))$ must be small since the entropy across the cut is large.

So, by Lindblad-Uhlmann theorem, the relative entropy $S(\rho_{j-l+1,j+l}||\rho_{j-l+1,j} \otimes \rho_{j+1,j+l})$ must be large.

But this is bounded by $S_{2l} - 2S_l$.

Putting in the constants gives the desired result.

1d gapped systems are in NP

- Represent ground state as matrix product state $k \gtrsim \exp(S)$
- Hard to find matrix product state in certain cases (NP-complete, Eisert 2006)
- In practice, DMRG or variational matrix product methods work well.

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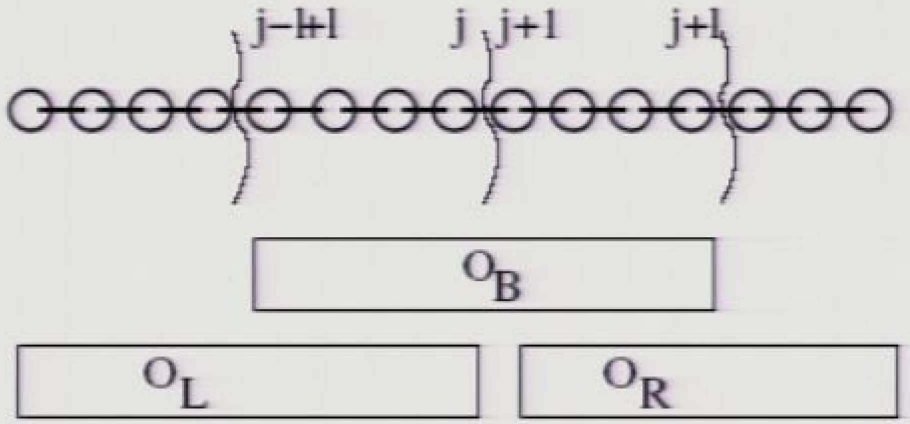

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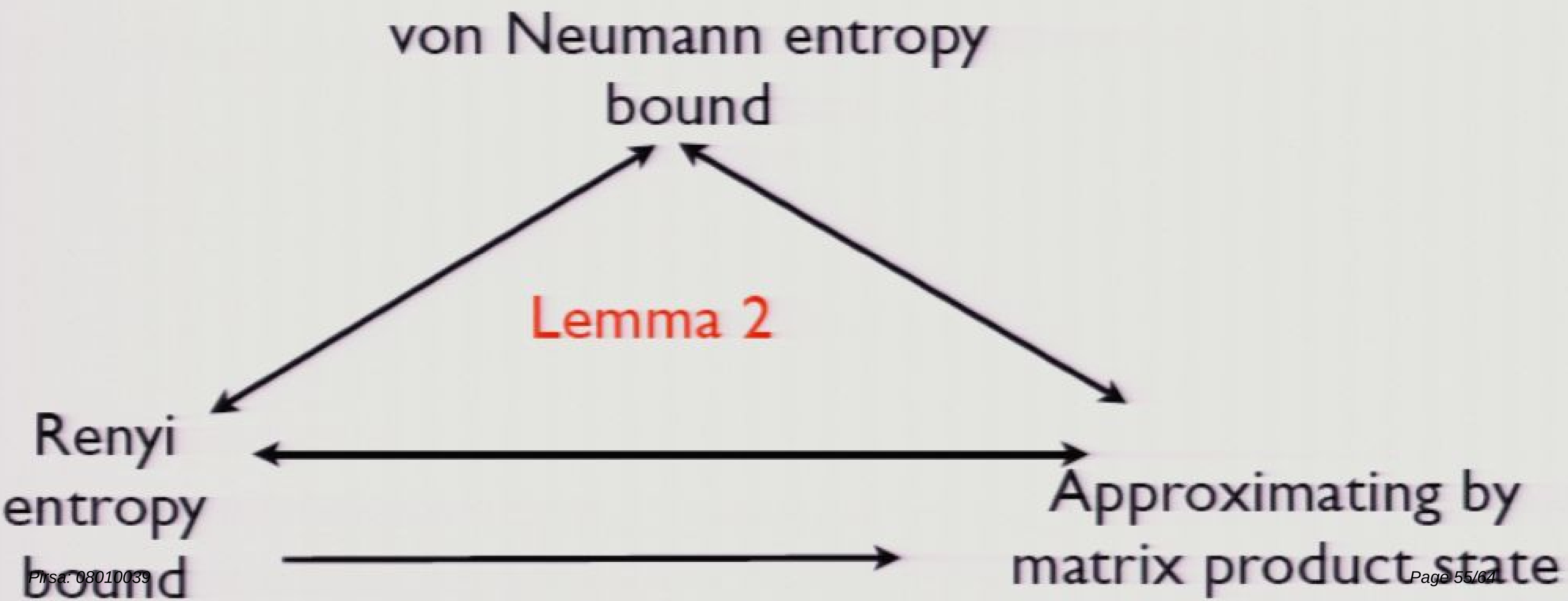
- Lemma 2 enables approximating ground state by matrix product state.
- Upper bound on Renyi or von Neumann entropy gives lower bound on the largest Schmidt coefficient across a cut and hence lower bound on P in Lemma 2.



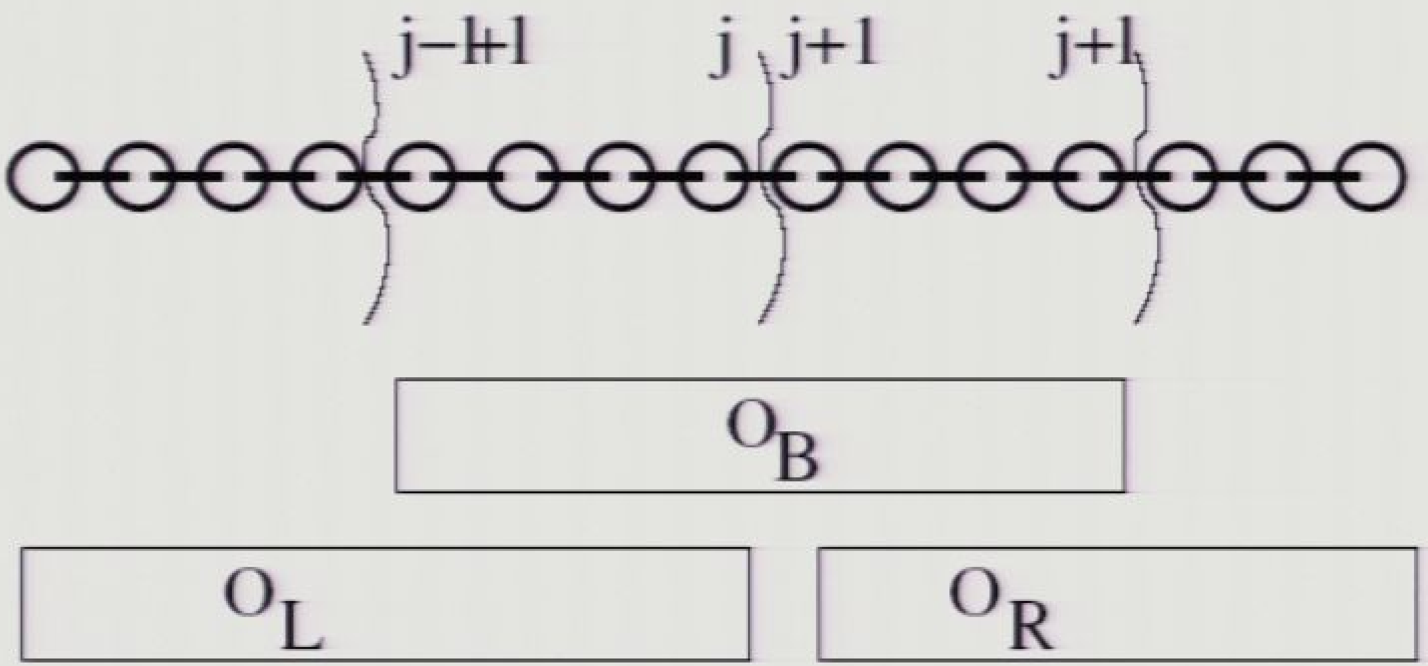
F. Verstraete and J. I. Cirac, PRB 2006.

Two lemmas:

1) Given assumptions above, for any j,l we can define Hermitian, positive definite operators, $O_B(j,l), O_L(j,l), O_R(j,l)$, with operator norms bounded by unity such that

$$||O_B(j,l)O_L(j,l)O_R(j,l) - |\Psi_0\rangle\langle\Psi_0||| \leq \exp(-\mathcal{O}(l\Delta E/v))$$

and such that the operators are supported like this:



1d gapped systems are in NP

- Represent ground state as matrix product state $k \gtrsim \exp(S)$
- Hard to find matrix product state in certain cases (NP-complete, Eisert 2006)
- In practice, DMRG or variational matrix product methods work well.

Outline:

- Overview of different algorithms: perturbation theory, DMRG (matrix product), exact diagonalization.
- Computational complexity classes. Difficulty of the problem depends on entanglement.
- Easy problems (P or almost polynomial): perturbing a system. We can find an efficient representation of the ground state.
- Harder problems: (NP) 1d gapped systems. Area laws for quantum entanglement imply an efficient representation exists.
- Very hard: (QMA-complete) 1d gapless.

What if no gap in1d? How hard is it to compute ground state energy to accuracy 1/N^4?

If gap vanishes at quantum critical point described by conformal field theory, Renyi entropy is log(N). Problem is still in P!

Examples: spin-1/2 Heisenberg chain, 1d transverse field Ising model, etc...

Verstraete, Cirac 05

But with arbitrary interactions the problem is QMA-complete. So, there is probably no hope of an efficient algorithm in general.

Aharonov, Gottesman, Kempe 07; Irani 07.

Other methods:

- Quantum Monte Carlo
- Density functional theory: Hohenberg-Kohn theorem implies exact functional exists. But, unless NP=QMA, exact functional is not tractable.
- Coupled cluster method

Conclusion:

- The difficulty of solving different problems seems to be closely related to the entanglement.
- Can we make the area law bound tight?
- What happens in higher dimensions to the area law?
- Do matrix product states work well in higher dimensions? Are there other better algorithms?

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