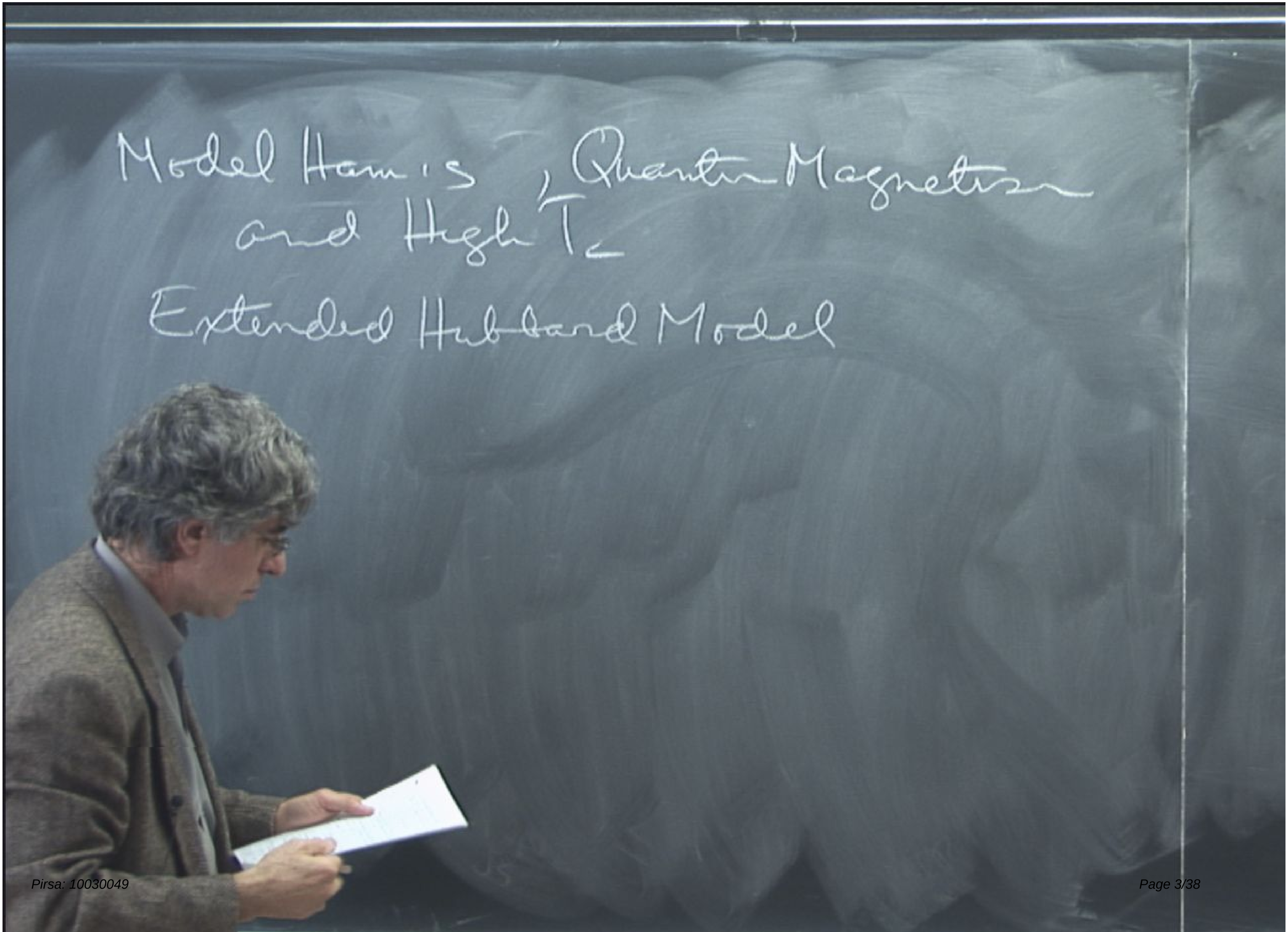
Title: Condensed Matter II - Lecture 11

Date: Mar 02, 2010 10:10 AM

URL: http://pirsa.org/10030049

Abstract:

Model Ham's, Quantum Magnetism
and High $T_c$


Model Ham's, Quantum Magnetism
and High $T_c$
Extended Hubbard Model

Model Ham's, Quantum Magnetism and High $T_c$

Extended Hubbard Model

$$\mathcal{H} = -t \sum_{\substack{i,\delta \\ \alpha}} c^{\dagger}_{i+\delta,\alpha} c_{i\alpha} + U \sum_{i} c^{\dagger}_{i\uparrow} c^{\dagger}_{i\downarrow} c_{i\downarrow} c_{i\uparrow}$$

$$+ \frac{V}{2} \sum_{\substack{i,\delta \\ \alpha,\beta}} c^{\dagger}_{i\alpha} c^{\dagger}_{i+\delta,\beta} c_{i+\delta\beta} c_{i\alpha}$$

Model Ham's, Quantum Magnetism and High $T_c$

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Consider $V=0$ Hubbard Model

Interesting Possibilities

i. $U<0$

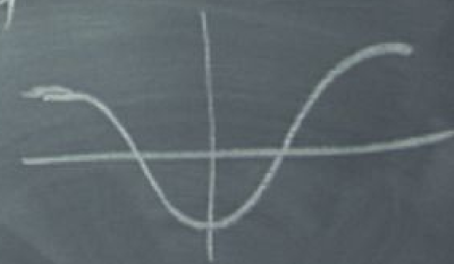
$c_{i\uparrow}$

Consider $V=0$ Hubbard Model

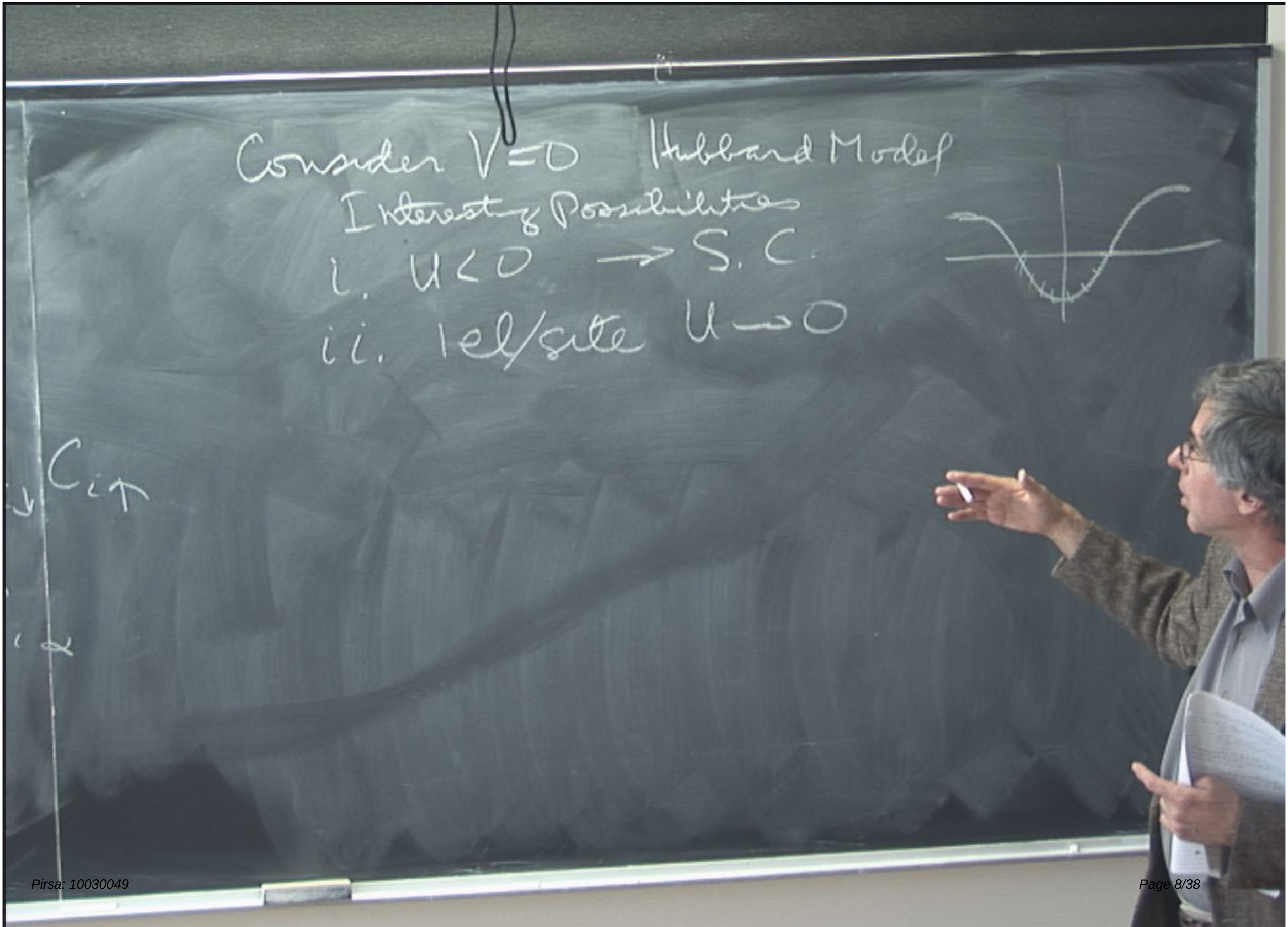
Interesting Possibilities

i. $U<0 \rightarrow$ S.C.

ii. 1el/site $U \rightarrow 0$



$C_{i\uparrow}$


Consider V=0 Hubbard Model
Interesting Possibilities
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ii. 1el/site U→0
Ci↑

Consider $V=0$ Hubbard Model

Interesting Possibilities

i. $U<0 \rightarrow$ S.C.

ii. 1 el/site $U \rightarrow 0^+$

iii. $U \gg t$

$c_{i\uparrow}$

Consider $V=0$ Hubbard Model

Interesting Possibilities

i. $U<0 \longrightarrow$ S.C.

ii. 1el/site $U \to 0^+$

iii. $U \gg t$ 1el/site Mott Insulator

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Consider $V=0$ Hubbard Model

Interesting Possibilities

i. $U<0 \rightarrow$ S.C.

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$2^N$-fold degenerate

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Resolved by virtual processes

$\uparrow \quad \downarrow$

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Resolved by virtual processes

$\uparrow \ \downarrow \longrightarrow 0 \overset{t}{\cdots} \overset{U}{\uparrow\downarrow}$ Lowering of energy by $\Delta E = -\frac{4t^2}{U}$

$\uparrow \ \uparrow$ $\Delta E = 0$

Consider $V=0$ Hubbard Model

Interesting Possibilities

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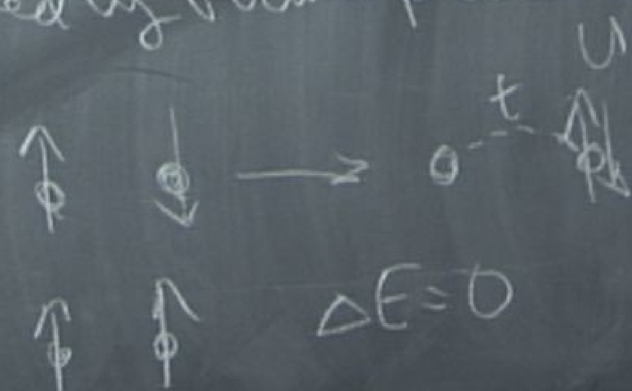
Resolved by virtual processes




Lowering of energy by $\Delta E = -\frac{4t^2}{U}$

Consider $V=0$ Hubbard Model

Interesting Possibilities

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$2^N$-fold degenerate

$C_{i\uparrow}$

Resolved by virtual processes

Relative singlet $\rightarrow \uparrow \quad \downarrow \longrightarrow 0 \overset{t}{\cdots} \overset{U}{\uparrow\downarrow}$ Lowering of energy by $\Delta E = -\frac{4t^2}{U}$

Relative Triplet $\rightarrow \uparrow \quad \uparrow \qquad \Delta E = 0$

Consider $V=0$ Hubbard Model

Interesting Possibilities

i. $U<0 \rightarrow$ S.C.

ii. 1el/site $U \rightarrow 0^+$

iii. $U \gg t$ 1el/site Mott Insulator

$C_{i\uparrow}$

$2^N$-fold degenerate

Resolved by virtual processes

Relative Singlet $\rightarrow \uparrow \; \downarrow \longrightarrow 0 \overset{t}{\cdots} \overset{U}{\uparrow\downarrow}$ Lowering of energy by $\Delta E = -\frac{4t^2}{U}$

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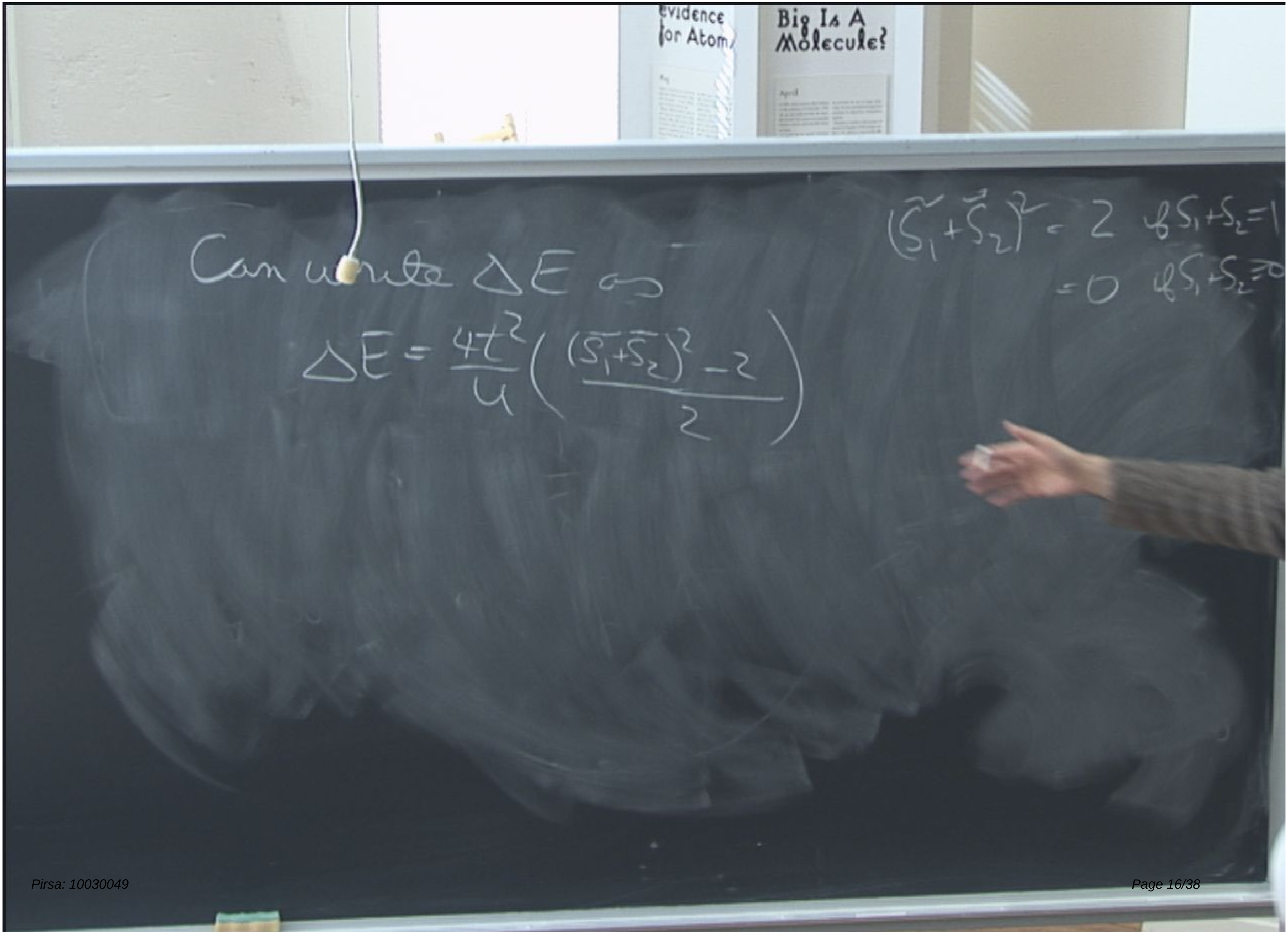
Evidence for Atoms
Big Is A Molecule?
$(\vec{S}_1+\vec{S}_2)^2 = 2$ if $S_1+S_2=1$
$= 0$ if $S_1+S_2=0$
Can write $\Delta E$ as
$\Delta E = \frac{4t^2}{U}\left(\frac{(\vec{S}_1+\vec{S}_2)^2-2}{2}\right)$

$(\vec{S}_1+\vec{S}_2)^2 = 2$ if $S_1+S_2=1$

$= 0$ if $S_1+S_2=0$

Can write $\Delta E$ as

$$\Delta E = \frac{4t^2}{U}\left(\frac{(\vec{S}_1+\vec{S}_2)^2-2}{2}\right)$$

$$= \frac{4t^2}{U}\,\frac{1}{2}\left(\tfrac{3}{4}+\tfrac{3}{4}+2S_1S_2-2\right)$$

$$= \underbrace{\frac{4t^2}{U}}_{J}\vec{S}_1\cdot\vec{S}_2 - \frac{t^2}{U}$$

Exchange Int

Derive Effective Spin Hamiltonian
for solid with $\lesssim 1$ el / site

Derive Effective Spin Hamiltonian
for solid with $\lesssim 1$ el/site

$$\mathcal{H} = \underbrace{-t \sum_{i,\delta,\alpha} c^{\dagger}_{i+\delta,\alpha} c_{i\alpha}}_{\mathcal{H}_t} + \underbrace{U \sum_{i} c^{\dagger}_{i\uparrow} c^{\dagger}_{i\downarrow} c_{i\downarrow} c_{i\uparrow}}_{\mathcal{H}_U}$$

Derive Effective Spin Hamiltonian
for solid with $\leq 1$ el/site

Ref: Web site
of Jonathan Kee
at Cambri

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Derive Effective Spin Hamiltonian for solid with $\lesssim$ 1 el/site

Ref: Web site of Jonathan Keeling at Cambridge

$$\mathcal{H} = \underbrace{-t \sum_{i,\delta,\alpha} C^{+}_{i+\delta,\alpha} C_{i\alpha}}_{\mathcal{H}_t} + \underbrace{U \sum_{i} C^{+}_{i\uparrow} C^{+}_{i\downarrow} C_{i\downarrow} C_{i\uparrow}}_{\mathcal{H}_U}$$

Derive Effective Spin Hamiltonian
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Do unitary transformation

$$\tilde{\mathcal{H}} = e^{iS}(\mathcal{H}_U + \mathcal{H}_{t,D} + \mathcal{H}_{t,OD})e^{-iS}$$

Derive Effective Spin Hamiltonian for solid with $\leq 1$ el/site

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$$\ldots u + \mathcal{H}_{t,D} + \mathcal{H}_{t,OD}) e^{-iS}$$

preserves # of doubly occ'd

Derive Effective Spin Hamiltonian for solid with $\lesssim 1$ el/site

Ref: Web site of Jonathan Keeling at Cambridge

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Preserves # of doubly occ'd site

Changes # of doubly occ'd site

Derive Effective Spin Hamiltonian
for solid with $\lesssim 1$ el/site

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$$\mathcal{H} = \underbrace{-t \sum_{i,\delta,\alpha} C^{+}_{i+\delta,\alpha} C_{i\alpha}}_{\mathcal{H}_t} + \underbrace{U \sum_{i} C^{+}_{i\uparrow} C^{+}_{i\downarrow} C_{i\downarrow} C_{i\uparrow}}_{\mathcal{H}_U}$$

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Lec. Notes
site on Quant. Mag.
on Keeling
ambridge

$\mathcal{H}_{t,D}$ has two parts

1. Hopping of holes $- \uparrow \to \uparrow -$

f
d Site

Lec. Notes
site on Quant. Mag.
on Keeling
Cambridge

$\mathcal{H}_{t,D}$ has two parts

1. Hopping of hole $\underline{\ \ }\ \underline{\uparrow} \rightarrow \underline{\uparrow}\ \underline{\ \ }$

2. Hopping of doublets $\underline{\uparrow\downarrow}\ \underline{\uparrow} \rightarrow \underline{\uparrow}\ \underline{\uparrow\downarrow}$

$\mathcal{H}_{t,OD}$ has two parts

$\underline{\uparrow}\ \underline{\downarrow} \leftrightarrow \underline{\uparrow\downarrow}\ \underline{\ \ }$

or $\underline{\ \ }\ \underline{\uparrow\downarrow}$

d site

site

Lec. Notes on Quant. Mag.

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ambridge

$\mathcal{H}_{t,D}$ has two parts

1. Hopping of holes $\_\ \uparrow \ \rightarrow\ \uparrow\ \_$
2. Hopping of doublets $\uparrow\downarrow\ \uparrow\ \rightarrow\ \uparrow\ \uparrow\downarrow$

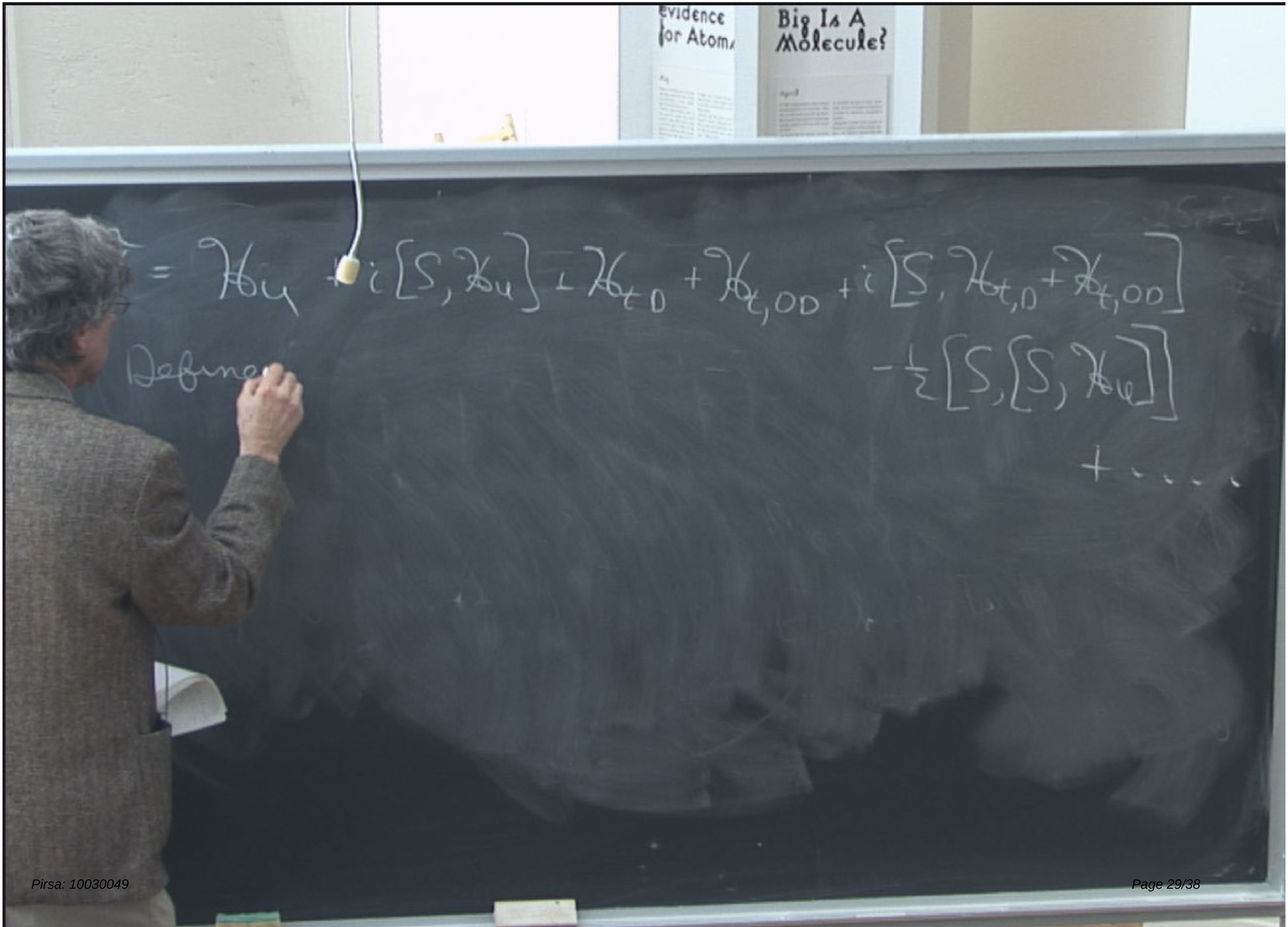
$\mathcal{H}_{t,OD}$ has two parts

$\uparrow\ \downarrow\ \leftrightarrow\ \uparrow\downarrow\ \_$

or $\_\ \uparrow\downarrow$

of

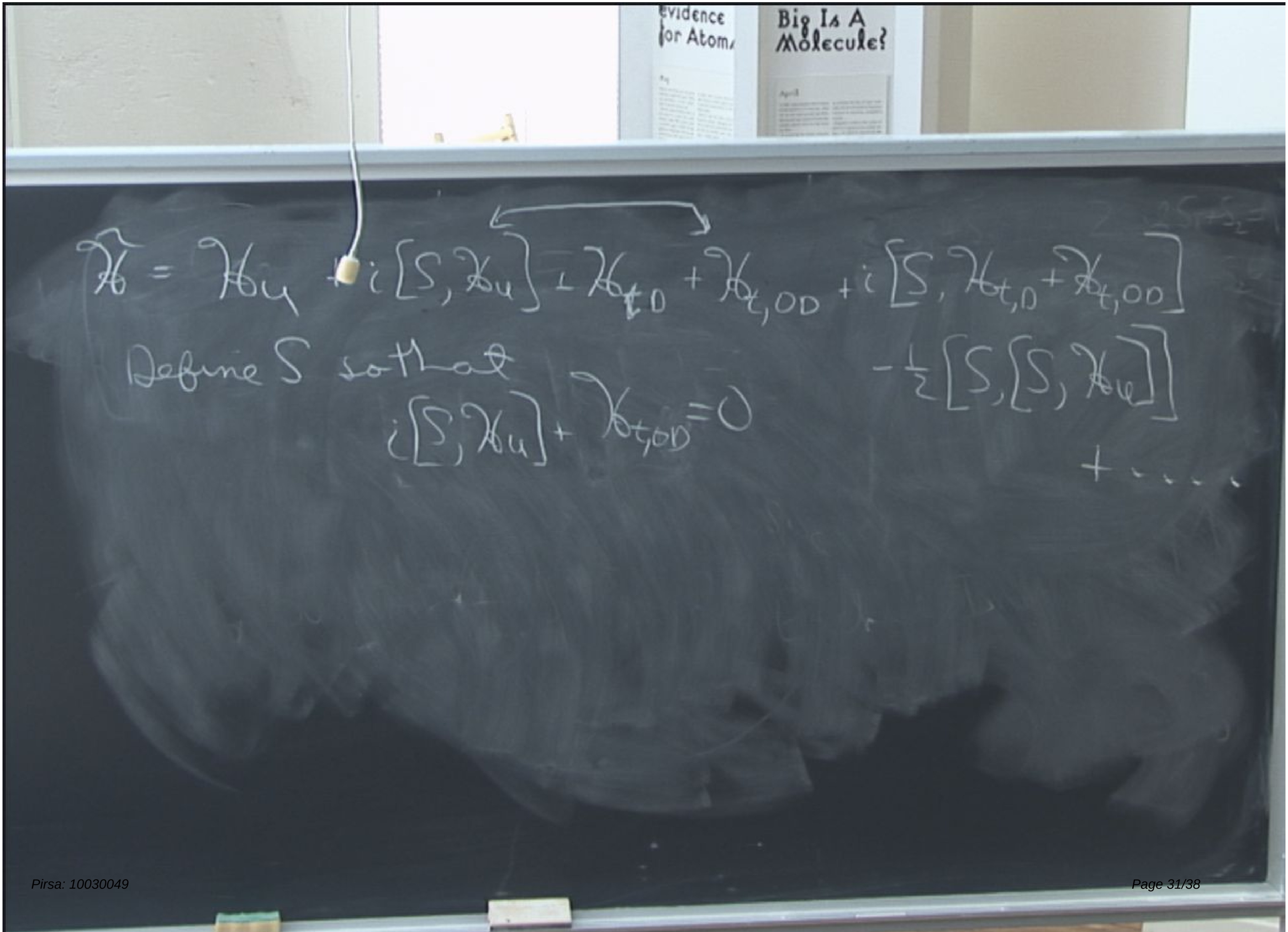
d site


Big Is A Molecule?
$= \mathcal{H}_u + i[S,\mathcal{H}_u] + \mathcal{H}_{t,D} + \mathcal{H}_{t,OD} + i[S, \mathcal{H}_{t,D} + \mathcal{H}_{t,OD}]$
$- \frac{1}{2}[S,[S,\mathcal{H}_u]]$
$+ \dots$
Define

$$\tilde{\mathcal{H}} = \mathcal{H}_u + i[S, \mathcal{H}_u] + \mathcal{H}_{t,D} + \mathcal{H}_{t,OD} + i[S, \mathcal{H}_{t,D} + \mathcal{H}_{t,OD}] - \frac{1}{2}[S,[S,\mathcal{H}_u]] + \dots$$

Define $S$ so that

$$i[S, \mathcal{H}_u] + \mathcal{H}_{t,OD} = 0$$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$+ \dots$
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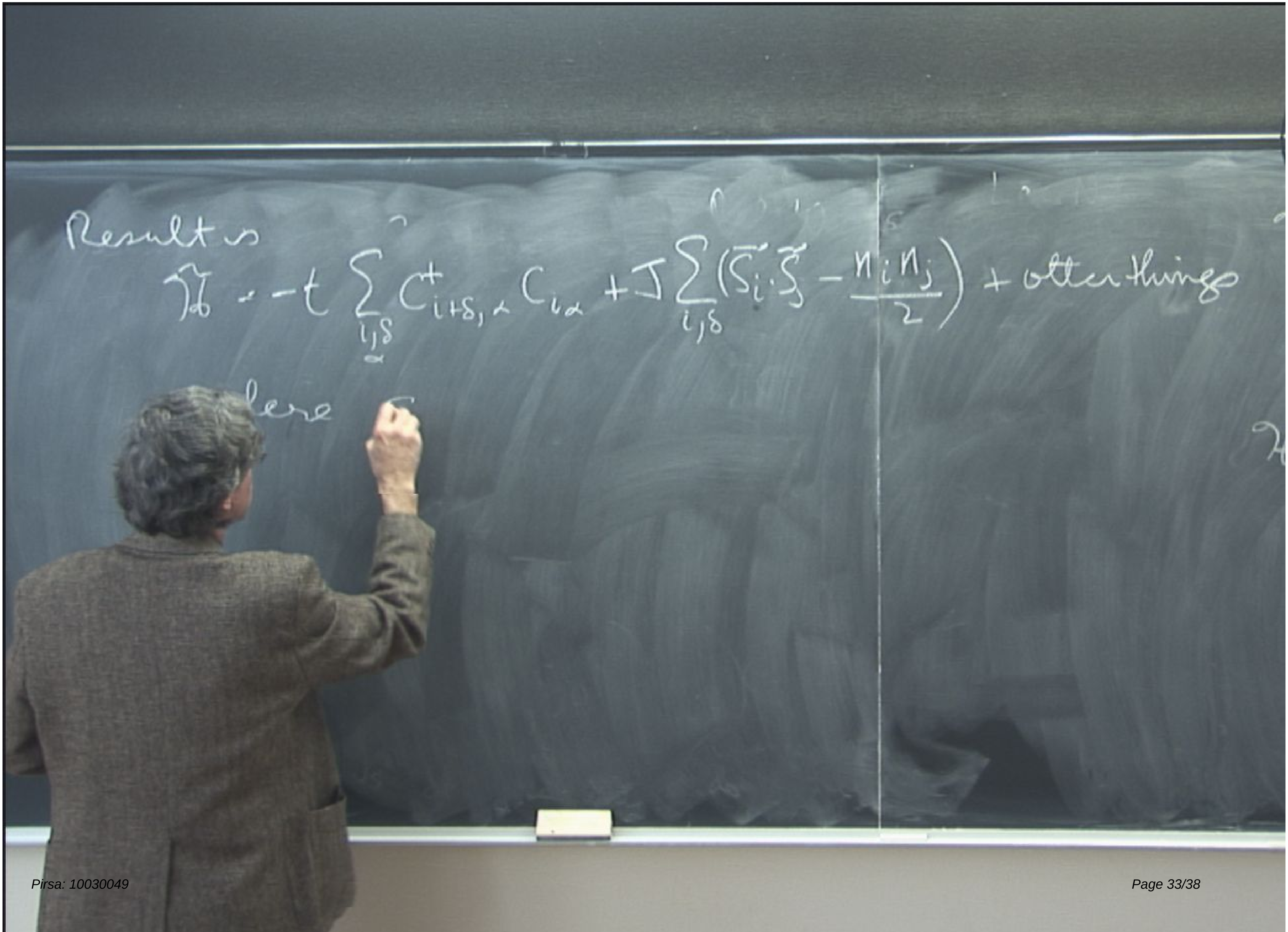
Define $S$ so that

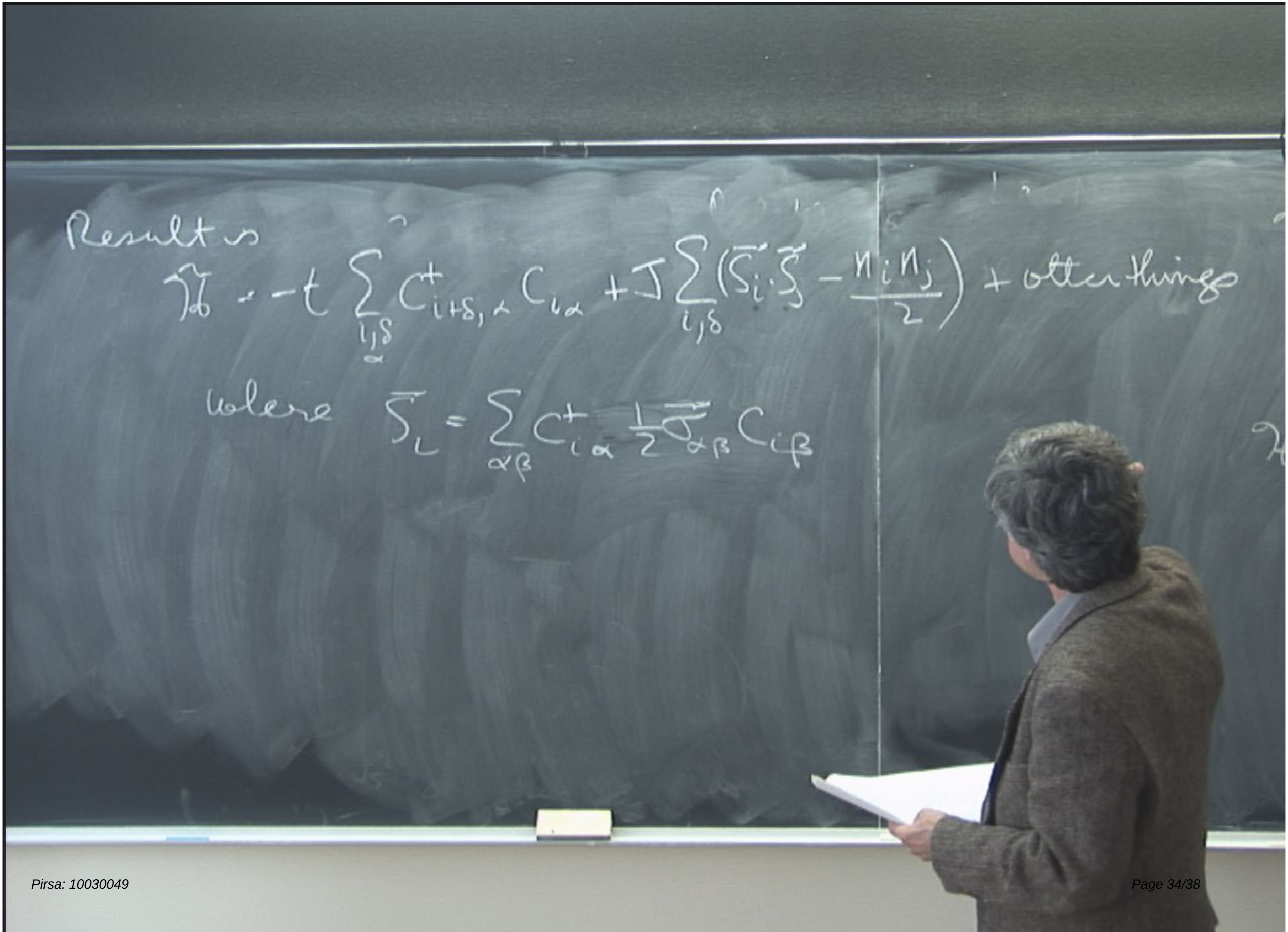
$$i[S,\mathcal{H}_U] + \mathcal{H}_{t,OD} = 0$$

$$S \sim t/U$$

of order $t^2/U$

$t^3/U^2$ or higher


Result is
$\tilde{\mathcal{H}} = -t \sum_{i,\delta,\alpha} c^{\dagger}_{i+\delta,\alpha} c_{i\alpha} + J \sum_{i,\delta} \left( \vec{S}_i \cdot \vec{S}_j - \frac{n_i n_j}{2} \right)$ + other things
where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where $\vec{S}_i = \sum_{\alpha\beta} c^{\dagger}_{i\alpha} \frac{1}{2} \vec{\sigma}_{\alpha\beta} c_{i\beta}$

$$\tilde{\mathcal{H}} = \mathcal{H}_U + i[S,\mathcal{H}_U] + \mathcal{H}_{t,D} + \mathcal{H}_{t,OD} + i[S,\mathcal{H}_{t,D} + \mathcal{H}_{t,OD}] - \frac{1}{2}[S,[S,\mathcal{H}_U]] + \dots$$

Define $S$ so that

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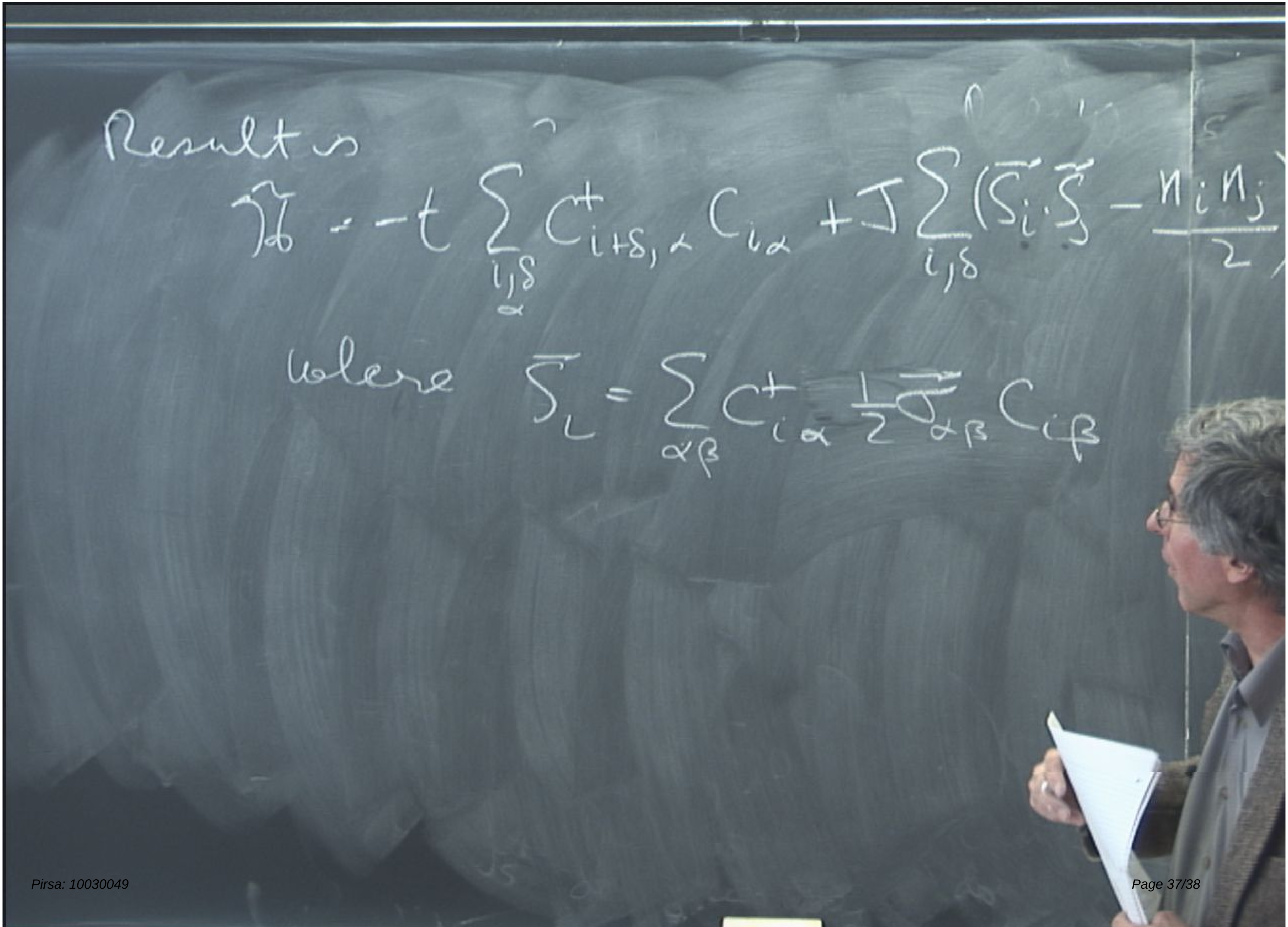
$$\tilde{\mathcal{H}} = -t \sum_{\substack{i,\delta \\ \alpha}} C^{+}_{i+\delta,\alpha} C_{i\alpha} + J \sum_{i,\delta} \left( \vec{S}_i \cdot \vec{S}_j - \frac{n_i n_j}{2} \right)$$

where $\vec{S}_i = \sum_{\alpha\beta} C^{+}_{i\alpha} \frac{1}{2} \vec{\sigma}_{\alpha\beta} C_{i\beta}$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Results

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$J = \frac{4t^2}{U}$

where $\vec{S}_i = \sum_{\alpha\beta} c^{\dagger}_{i\alpha} \frac{1}{2} \vec{\sigma}_{\alpha\beta} c_{i\beta}$

.... → Other terms of order $t^2/U$ contain ops on 3 sites