Title: PSI 2016/2017 Condensed Matter - Lecture 11

Date: Nov 21, 2016 10:45 AM

URL: http://pirsa.org/16110062

Abstract:

"magnetic" interactions

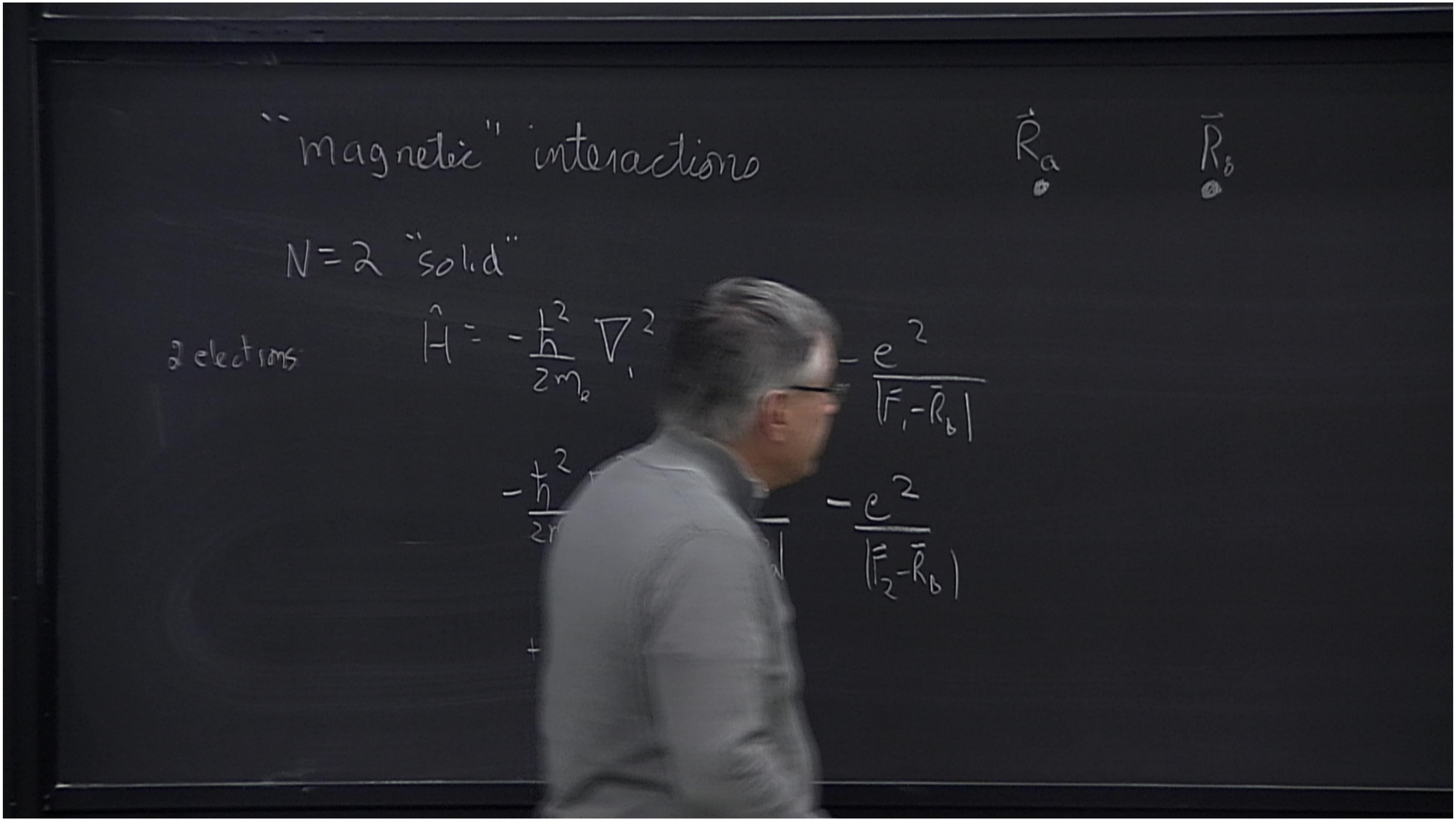
$N = 2$ "solid"

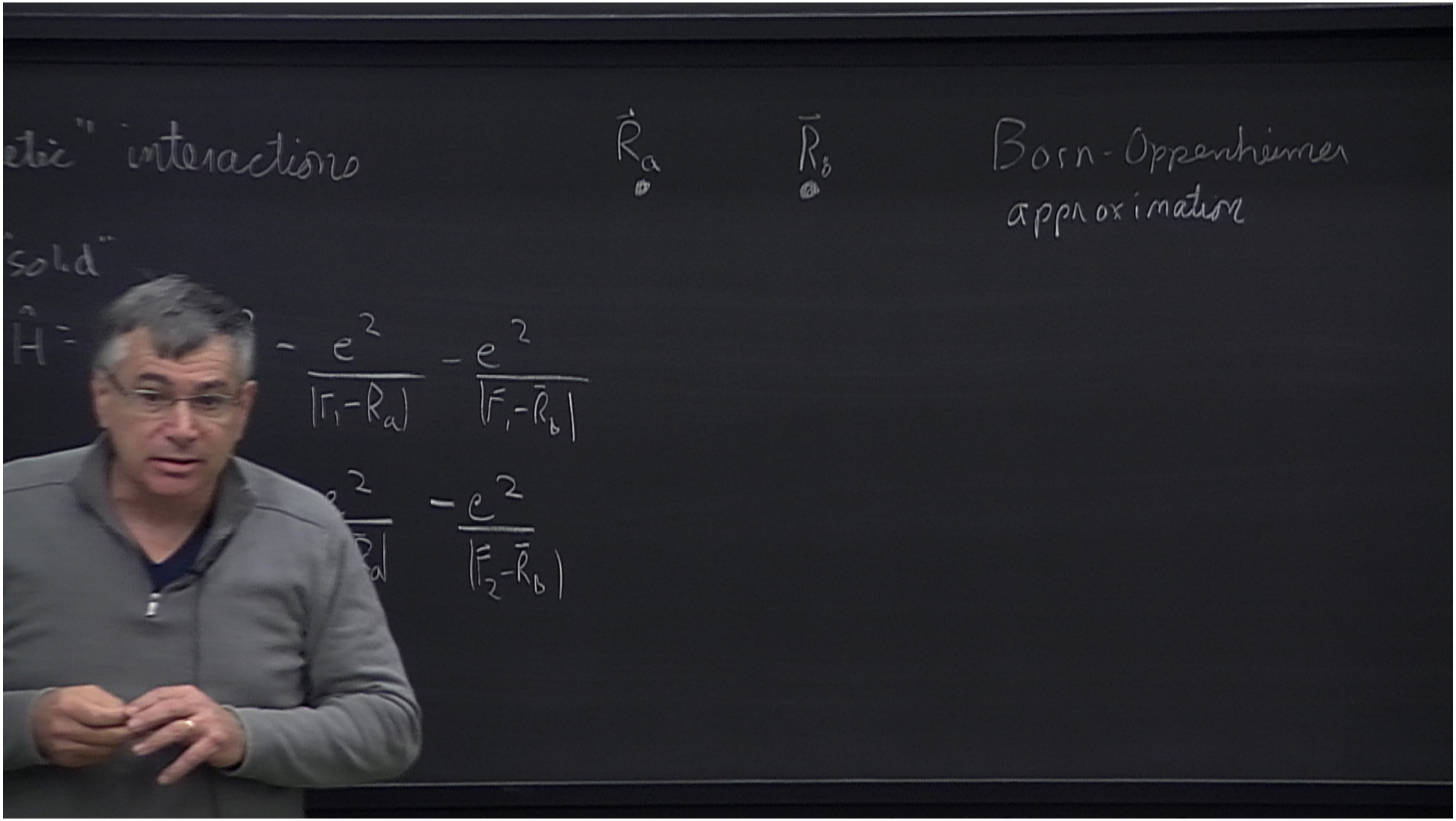
2 electrons:

$$\hat{H} = -\frac{\hbar^2}{2m_e}\nabla_1^2 - \frac{e^2}{|\bar{r}_1 - \bar{R}_a|} - \frac{e^2}{|\bar{r}_1 - \bar{R}_b|}$$

$$-\frac{\hbar^2}{2m_e}\nabla_2^2 - \frac{e^2}{|\bar{r}_2 - \bar{R}_a|} - \frac{e^2}{|\bar{r}_2 - \bar{R}_b|}$$

$$+\frac{e^2}{|\bar{r}_1 - \bar{r}_2|}$$


"magnetic" interactions
$\vec{R}_a$
$\vec{R}_b$
N=2 "solid"
2 electrons
$\hat{H} = -\frac{\hbar^2}{2m_e}\nabla_1^2$
$-\frac{e^2}{|\vec{r}_1-\vec{R}_b|}$
$-\frac{\hbar^2}{2m}$
$-\frac{e^2}{|\vec{r}_2-\vec{R}_b|}$


"etic" interactions
$\vec{R}_a$
$\vec{R}_b$
Born-Oppenheimer approximation
"solid"
$\hat{H} =$
$- \frac{e^2}{|\vec{r}_1 - \vec{R}_a|} - \frac{e^2}{|\vec{r}_1 - \vec{R}_b|}$
$- \frac{e^2}{|\vec{r}_2 - \vec{R}_b|}$

$\vec{R}_a$ $\vec{R}_b$

Born-Oppenheimer approximation

1) spatially symmetric

$\psi_0(\vec{r}_1)\,\psi_0(\vec{r}_2)$

energy: $2\mathcal{E}_0$

spin-part is antisymmetric

$\frac{1}{\sqrt{2}}\left[|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right]$

e_1 e_2 e_1 e_2

|$\vec{R}_b$|

$_b$|

R_a R_b

Born-Oppenheimer approximation

1) spatially symmetric

$$\psi_0(\vec{r}_1)\,\psi_0(\vec{r}_2)$$

energy: $2\varepsilon_0$

spin-part is antisymmetric

$$\frac{1}{\sqrt{2}}\left[\,|\underset{e_1}{\uparrow}\underset{e_2}{\downarrow}\rangle - |\underset{e_1}{\downarrow}\underset{e_2}{\uparrow}\rangle\,\right]$$

2) spatially antisymmetric

$$\frac{1}{\sqrt{2}}\left[\psi_0(\vec{r}_1)\psi_1(\vec{r}_2) - \psi_1(\vec{r}_1)\psi_0(\vec{r}_2)\right]$$

$$\varepsilon_0+\varepsilon_1$$

R_a R_b Born-Oppenheimer approximation

1) spatially symmetric

$\psi_0(\vec{r}_1)\,\psi_0(\vec{r}_2)$

energy: $2\mathcal{E}_0$

spin-part is antisymmetric

$\frac{1}{\sqrt{2}}\Big[|\underset{e_1}{\uparrow}\,\underset{e_2}{\downarrow}\rangle - |\underset{e_1}{\downarrow}\,\underset{e_2}{\uparrow}\rangle\Big]$

2) spatially antisymmetric

$\frac{1}{\sqrt{2}}\Big[\psi_0(\vec{r}_1)\psi_1(\vec{r}_2) - \psi_1(\vec{r}_1)\psi_0(\vec{r}_2)\Big]$

$\mathcal{E}_0 + \mathcal{E}_1$

symmetric

$|\uparrow\uparrow\rangle$

$\frac{1}{\sqrt{2}}\big(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle\big)$

$|\downarrow\downarrow\rangle$

Born-Oppenheimer approximation

1) spatially symmetric

$\psi_0(\vec{r}_1)\,\psi_0(\vec{r}_2)$

energy: $2\varepsilon_0$

spin-part is antisymmetric

$\frac{1}{\sqrt{2}}\left[|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right]$ spin singlet

$e_1 \quad e_2 \quad e_1 \quad e_2$

2) spatially antisymmetric

$\frac{1}{\sqrt{2}}\left[\psi_0(\vec{r}_1)\psi_1(\vec{r}_2) - \psi_1(\vec{r}_1)\psi_0(\vec{r}_2)\right]$

$\varepsilon_0 + \varepsilon_1$

symmetric

$$\left.\begin{array}{l} |\uparrow\uparrow\rangle \\ \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle\right) \\ |\downarrow\downarrow\rangle \end{array}\right\}\text{spin triplet}$$

$S=1$

Born-Oppenheimer approximation

1) spatially symmetric

$\psi_0(\vec{r}_1)\,\psi_0(\vec{r}_2)$

energy: $2\mathcal{E}_0$

spin-part is antisymmetric

$\frac{1}{\sqrt{2}}\left[|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right]$ spin singlet $S=0$, $S_z=0$

e_1 e_2 e_1 e_2

2) spatially antisymmetric

$\frac{1}{\sqrt{2}}\left[\psi_0(\vec{r}_1)\psi_1(\vec{r}_2) - \psi_1(\vec{r}_1)\psi_0(\vec{r}_2)\right]$

$\mathcal{E}_0+\mathcal{E}_1$

symmetric

$$\left.\begin{array}{l} |\uparrow\uparrow\rangle \\ \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle\right) \\ |\downarrow\downarrow\rangle \end{array}\right\} \text{spin triplet} \quad S=1, \; S_z = 1, 0, -1$$

what are ψ_0 + ψ_1 ?

$$\psi_0(\vec{r}_1) = \frac{1}{\sqrt{2}}\left[\phi(\vec{r}_1 - \vec{R}_a) + \phi(\vec{r}_1 - \vec{R}_b)\right]$$

...d is
...ymmetric

$...|\downarrow\uparrow\rangle]$ spin singlet $S=0$, $S_z=0$

$\uparrow$ e_1 $\uparrow$ e_2

...ymmetric

$|\uparrow\uparrow\rangle$

$(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)$

$|\downarrow\downarrow\rangle$

spin triplet $S=1$, $S_z = 1, 0, -1$

…ele interactions

R_a R_b

Born-Oppenheimer approximation

"solid"

$$\hat{H} = -\frac{\hbar^2}{2m_e}\nabla_1^2 - \frac{e^2}{|\vec{r}_1 - \vec{R}_a|} - \frac{e^2}{|\vec{r}_1 - \vec{R}_b|}$$

$$-\frac{\hbar^2}{2m_e}\nabla_2^2 - \frac{e^2}{|\vec{r}_2 - \vec{R}_a|} - \frac{e^2}{|\vec{r}_2 - \vec{R}_b|}$$

$$+\frac{e^2}{|\vec{r}_1 - \vec{r}_2|}$$

1) spatially symmetric

$$\psi_0(\vec{r}_1)\,\psi_0(\vec{r}_2)$$

energy: $2\varepsilon_0$

2) spatially antisymmetric

$$\frac{1}{\sqrt{2}}\left[\psi_0(\vec{r}_1)\psi_1(\vec{r}_2) - \psi_1(\vec{r}_1)\psi_0(\vec{r}_2)\right]$$

$$\varepsilon_0 + \varepsilon_1$$

spin-… ant…

$\frac{1}{\sqrt{2}}[(\uparrow b$ …

e_1 e_2

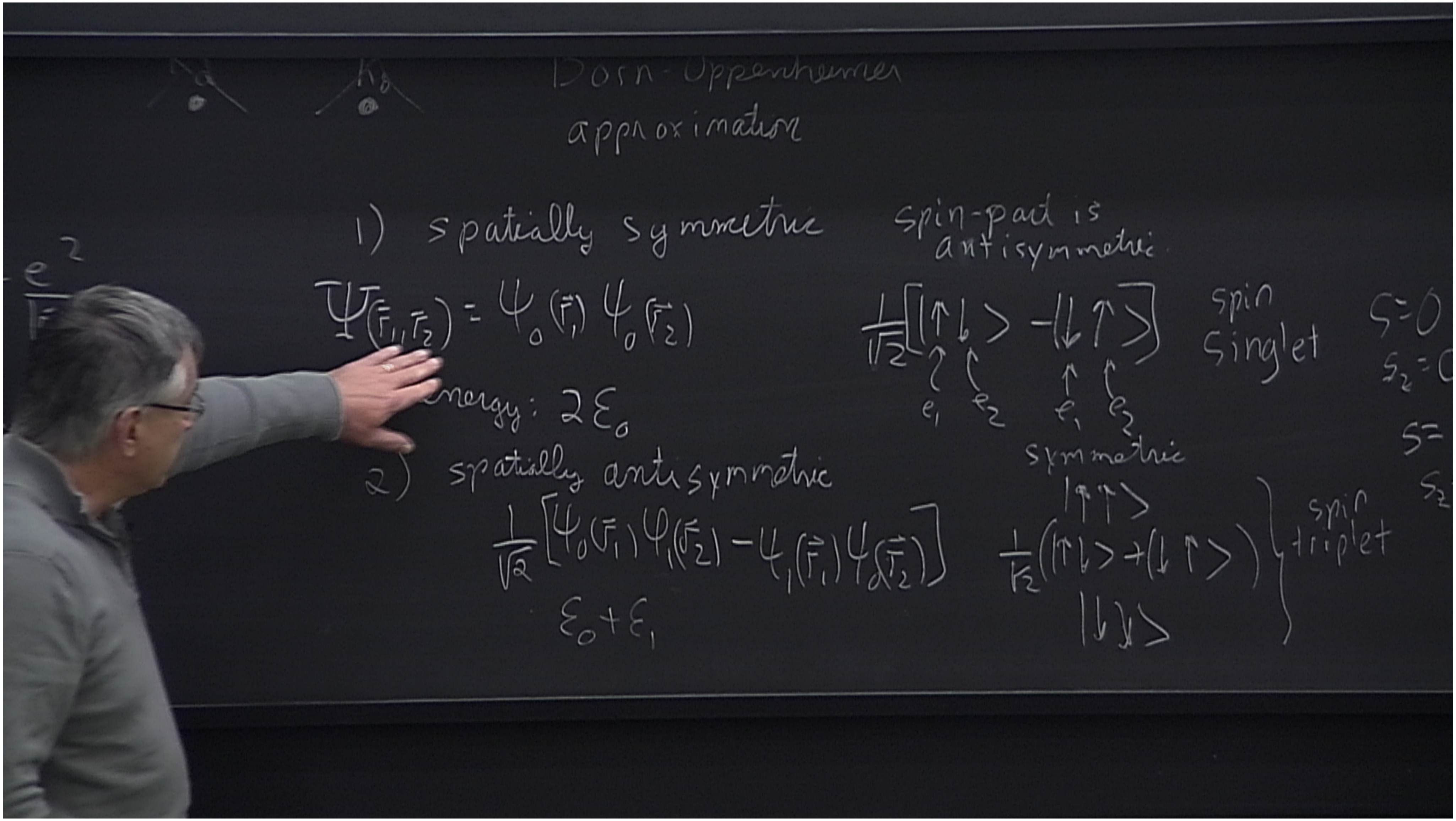
what are ψ_0 + ψ_1 ?

$$\psi_0(\vec{r}_1) = \frac{1}{\sqrt{2}}\left[\phi(\vec{r}_1 - \vec{R}_a) + \phi(\vec{r}_1 - \vec{R}_b)\right]$$

$$\psi_1(\vec{r}_1) = \frac{1}{\sqrt{2}}\left[\phi(\vec{r}_1 - \vec{R}_a) - \phi(\vec{r}_1 - \vec{R}_b)\right]$$

spin singlet $S=0$, $S_z=0$

$S=1$, $S_z = 1, 0, -1$ spin triplet


Born-Oppenheimer
approximation
1) spatially symmetric
spin-part is antisymmetric
$\Psi(\vec{r}_1, \vec{r}_2) = \psi_0(\vec{r}_1)\,\psi_0(\vec{r}_2)$
$\frac{1}{\sqrt{2}}\left[|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right]$
e_1 e_2 e_1 e_2
spin singlet
$S=0$
energy: $2\varepsilon_0$
2) spatially antisymmetric
$\frac{1}{\sqrt{2}}\left[\psi_0(\vec{r}_1)\psi_1(\vec{r}_2) - \psi_1(\vec{r}_1)\psi_0(\vec{r}_2)\right]$
$\varepsilon_0 + \varepsilon_1$
symmetric
$|\uparrow\uparrow\rangle$
$\frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle\right)$
$|\downarrow\downarrow\rangle$
spin triplet

R_a R_b

Born-Oppenheimer approximation

$-\frac{e^2}{|\vec{r}_1 - \vec{R}_b|}$

$-\frac{e^2}{|\vec{r}_2 - \vec{R}_b|}$

1) spatially symmetric

$\Psi(\vec{r}_1, \vec{r}_2) = \psi_0(\vec{r}_1)\,\psi_0(\vec{r}_2)$

energy: $2\varepsilon_0$

spin-part is antisymmetric

$\frac{1}{\sqrt{2}}\left[|\underset{e_1}{\uparrow}\underset{e_2}{\downarrow}\rangle - |\underset{e_1}{\downarrow}\underset{e_2}{\uparrow}\rangle\right]$ spin singlet $S=0$, $S_z=0$

2) spatially antisymmetric

$\frac{1}{\sqrt{2}}\left[\psi_0(\vec{r}_1)\psi_1(\vec{r}_2) - \psi_1(\vec{r}_1)\psi_0(\vec{r}_2)\right]$

$\varepsilon_0 + \varepsilon_1$

symmetric

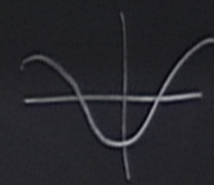
$\left.\begin{array}{l} |\uparrow\uparrow\rangle \\ \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle\right) \\ |\downarrow\downarrow\rangle \end{array}\right\}$ spin triplet

$S=$

S_z

what are ψ_0 & ψ_1 ?

$$\psi_0(\vec{r}_1) = \frac{1}{\sqrt{2}}\left[\phi(\vec{r}_1 - \vec{R}_a) + \phi(\vec{r}_1 - \vec{R}_b)\right]$$



$$\psi_1(\vec{r}_1) = \frac{1}{\sqrt{2}}\left[\phi(\vec{r}_1 - \vec{R}_a) - \phi(\vec{r}_1 - \vec{R}_b)\right]$$

...-part is antisymmetric

$\ldots\downarrow\rangle - |\downarrow\uparrow\rangle]$ spin singlet $S=0$, $S_z=0$

$e_2 \quad e_1 \quad e_2$

symmetric

$|\uparrow\uparrow\rangle$

$\frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle\right)$ spin triplet

$|\downarrow\downarrow\rangle$

$S=1$

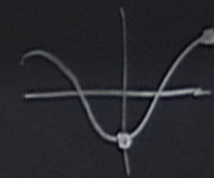
$S_z = 1$

0

-1

what are ψ_0 + ψ_1 ?

$$\psi_0(\vec{r}_1) = \frac{1}{\sqrt{2}}\left[\phi(\vec{r}_1 - \vec{R}_a) + \phi(\vec{r}_1 - \vec{R}_b)\right]$$



$$\psi_1(\vec{r}_1) = \frac{1}{\sqrt{2}}\left[\phi(\vec{r}_1 - \vec{R}_a) - \phi(\vec{r}_1 - \vec{R}_b)\right]$$

-part is

ntisymmetric

$\downarrow\rangle - |\downarrow\uparrow\rangle]$ spin singlet $S=0$

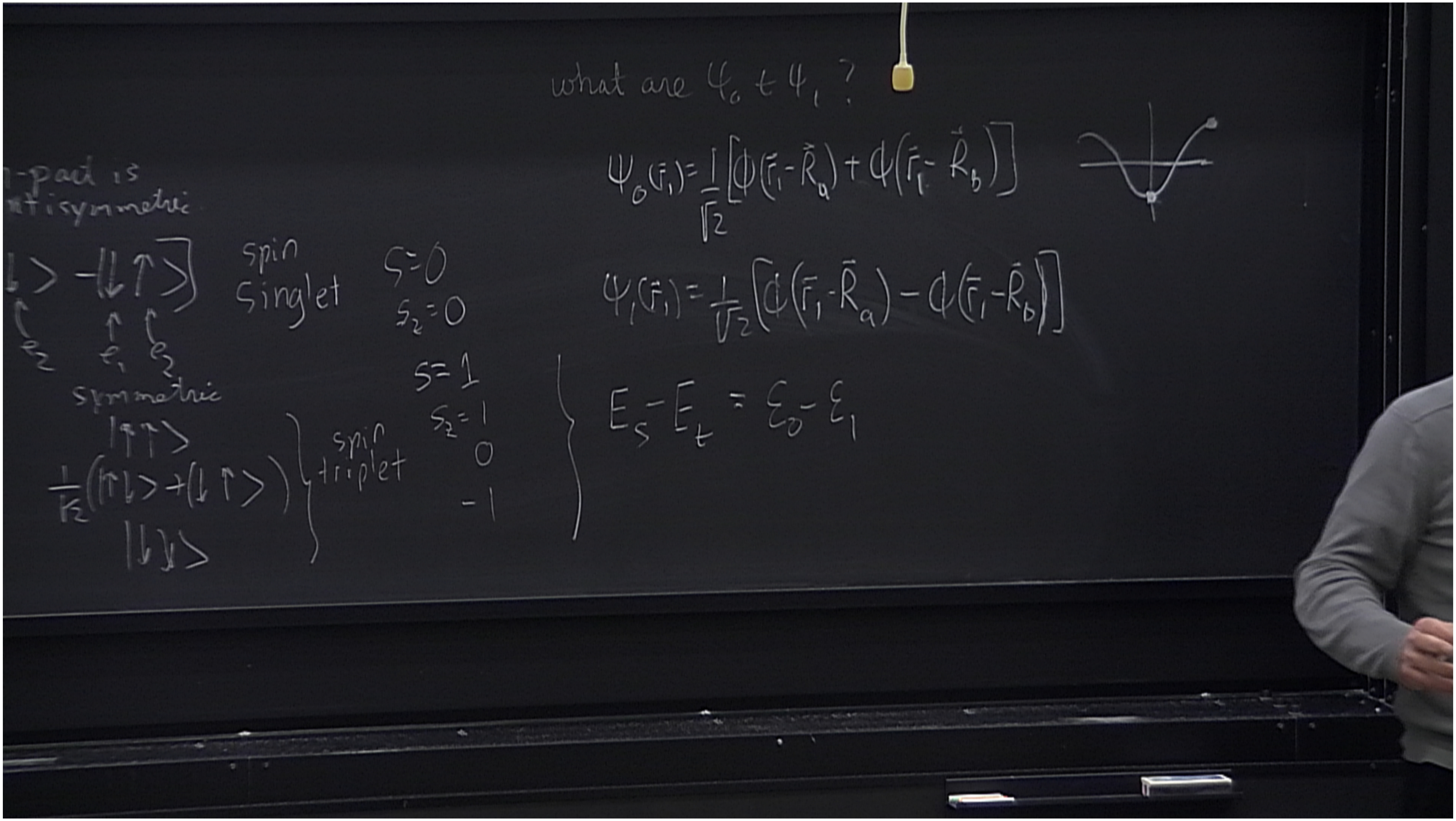
$e_2 \quad e_1 \quad e_2$ $\quad S_z = 0$

symmetric $\quad S = 1$

$|\uparrow\uparrow\rangle$ $\quad S_z = 1$

$\frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle\right)$ spin triplet $\quad 0$

$|\downarrow\downarrow\rangle$ $\quad -1$



what are ψ_0 & ψ_1 ?
$\psi_0(\vec r_1) = \frac{1}{\sqrt2}\left[\phi(\vec r_1 - \vec R_a) + \phi(\vec r_1 - \vec R_b)\right]$
$\psi_1(\vec r_1) = \frac{1}{\sqrt2}\left[\phi(\vec r_1 - \vec R_a) - \phi(\vec r_1 - \vec R_b)\right]$
$E_s - E_t = \varepsilon_0 - \varepsilon_1$
-part is
ntisymmetric
$\downarrow\rangle - |\downarrow\uparrow\rangle]$
e_2 e_1 e_2
spin singlet
$S=0$
$S_z=0$
symmetric
$|\uparrow\uparrow\rangle$
$\frac{1}{\sqrt2}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)$
$|\downarrow\downarrow\rangle$
spin triplet
$S=1$
$S_z=1$
0
-1

-part is
ntisymmetric

$\downarrow\rangle - |\downarrow\uparrow\rangle]$ spin singlet $S=0$, $S_z=0$

$e_2 \quad e_1 \quad e_2$

symmetric

$|\uparrow\uparrow\rangle$

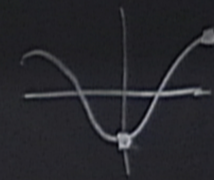
$\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)$

$|\downarrow\downarrow\rangle$

spin triplet $S=1$, $S_z = 1, 0, -1$

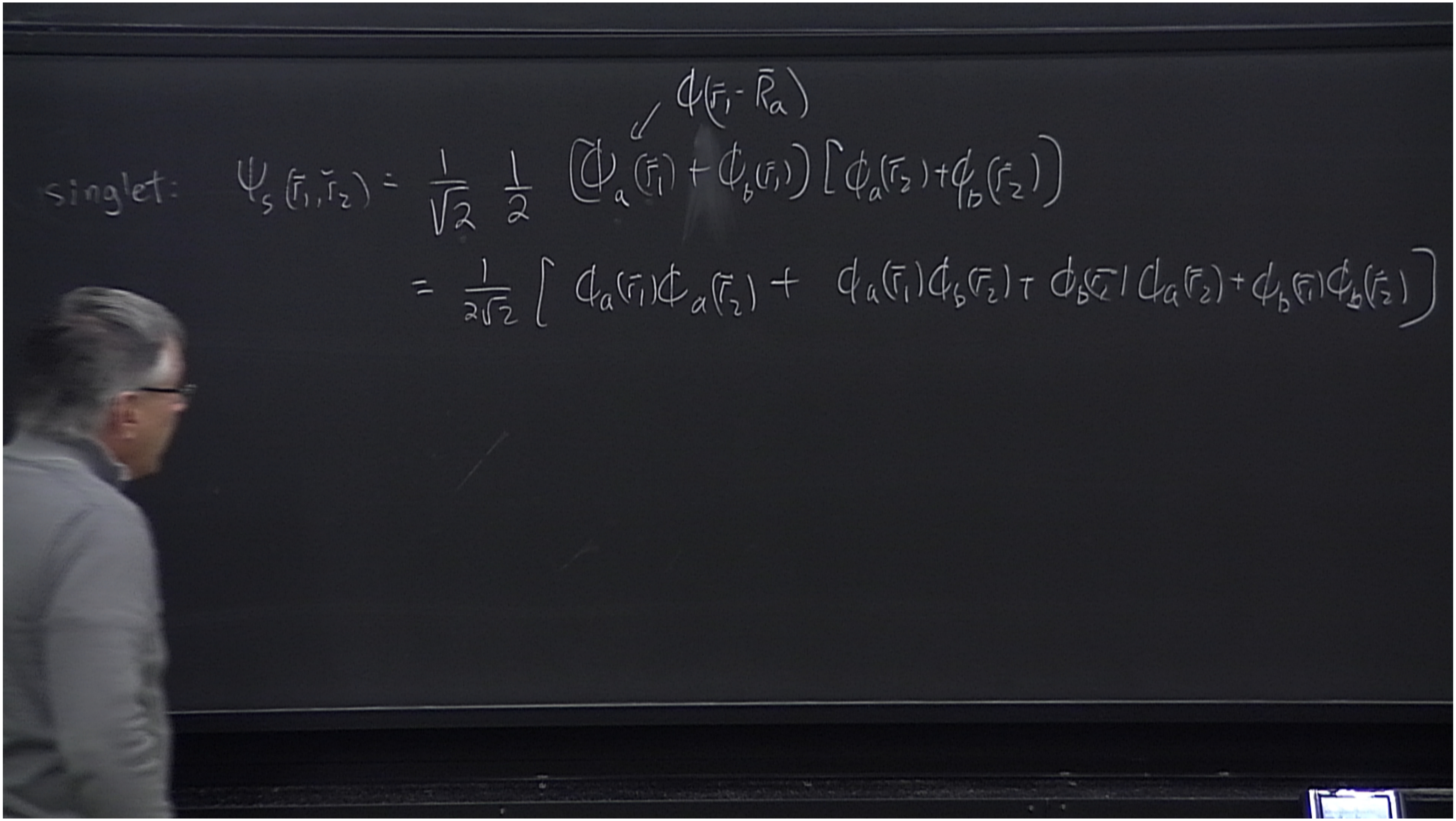
what are ψ_0 & ψ_1?

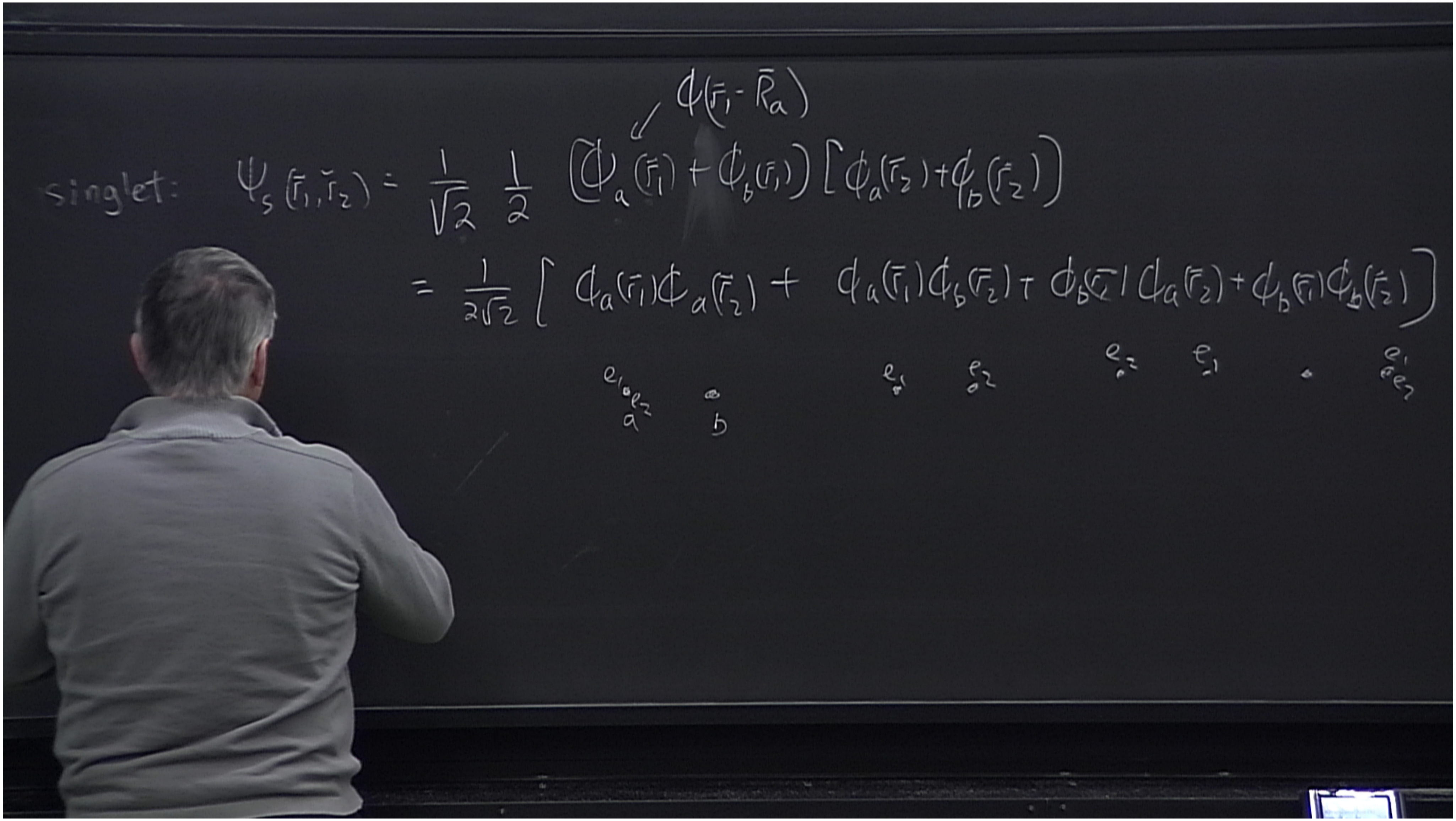
$$\psi_0(\vec r_1) = \frac{1}{\sqrt{2}}\left[\phi(\vec r_1 - \vec R_a) + \phi(\vec r_1 - \vec R_b)\right]$$

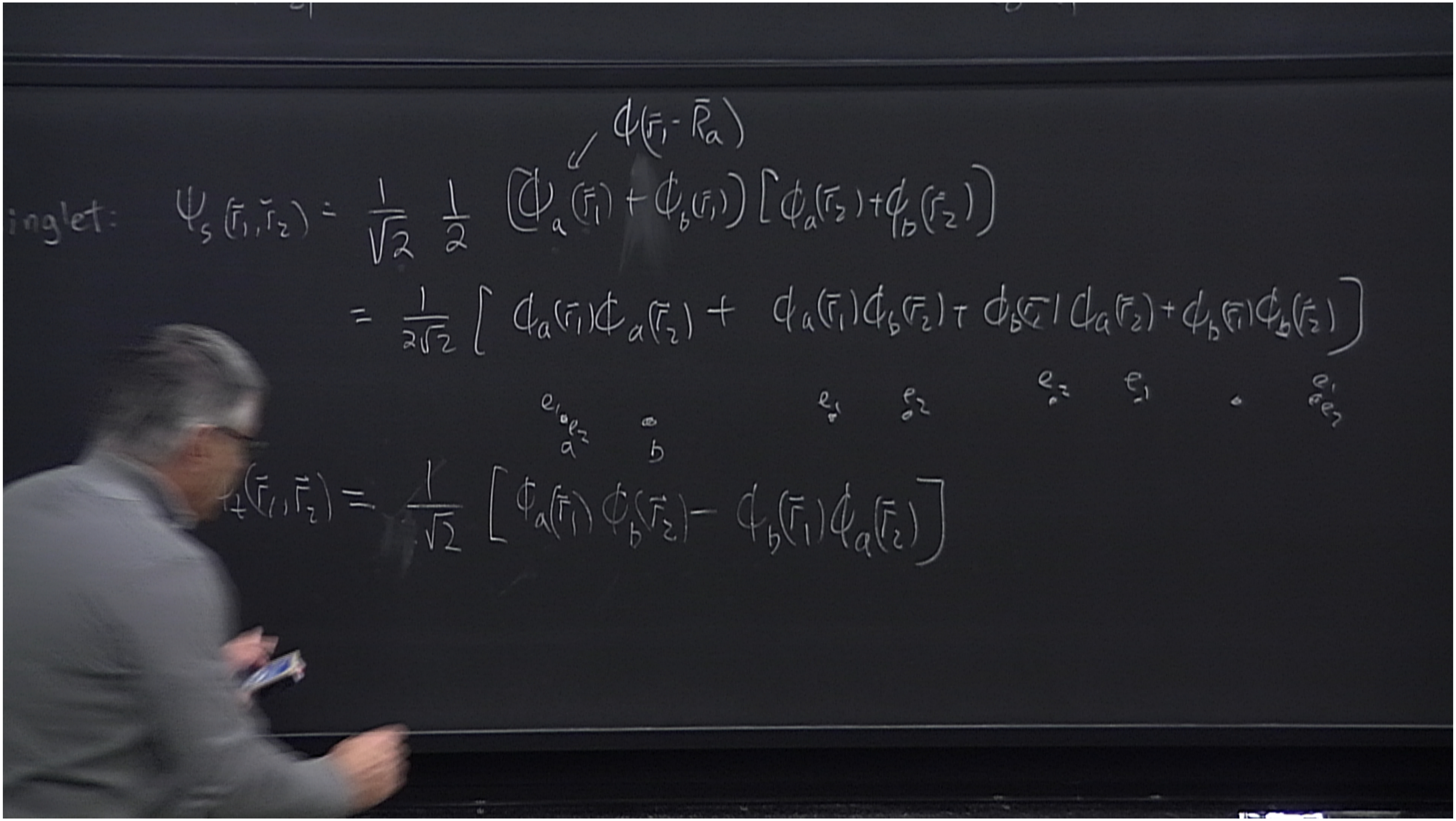


$$\psi_1(\vec r_1) = \frac{1}{\sqrt{2}}\left[\phi(\vec r_1 - \vec R_a) - \phi(\vec r_1 - \vec R_b)\right]$$

$$E_s - E_t = \varepsilon_0 - \varepsilon_1$$ [happens to be the right answer]


$\phi(\bar r_1 - \bar R_a)$
singlet: $\Psi_s(\bar r_1, \bar r_2) = \frac{1}{\sqrt{2}}\frac{1}{2}\left(\phi_a(\bar r_1) + \phi_b(\bar r_1)\right)\left[\phi_a(\bar r_2) + \phi_b(\bar r_2)\right)$
$= \frac{1}{2\sqrt{2}}\left[\phi_a(\bar r_1)\phi_a(\bar r_2) + \phi_a(\bar r_1)\phi_b(\bar r_2) + \phi_b(\bar r_1)\phi_a(\bar r_2) + \phi_b(\bar r_1)\phi_b(\bar r_2)\right]$


$\phi(\bar{r}_1 - \bar{R}_a)$
singlet: $\Psi_s(\bar{r}_1, \bar{r}_2) = \frac{1}{\sqrt{2}} \frac{1}{2} [\phi_a(\bar{r}_1) + \phi_b(\bar{r}_1)][\phi_a(\bar{r}_2) + \phi_b(\bar{r}_2)]$
$= \frac{1}{2\sqrt{2}} [\phi_a(\bar{r}_1)\phi_a(\bar{r}_2) + \phi_a(\bar{r}_1)\phi_b(\bar{r}_2) + \phi_b(\bar{r}_1)\phi_a(\bar{r}_2) + \phi_b(\bar{r}_1)\phi_b(\bar{r}_2)]$
e_1 e_2 a
b


$\phi(\vec{r}_1 - \vec{R}_a)$
inglet: $\Psi_s(\vec{r}_1, \vec{r}_2) = \frac{1}{\sqrt{2}} \frac{1}{2} \left(\phi_a(\vec{r}_1) + \phi_b(\vec{r}_1)\right)\left[\phi_a(\vec{r}_2) + \phi_b(\vec{r}_2)\right)$
$= \frac{1}{2\sqrt{2}} \left[\phi_a(\vec{r}_1)\phi_a(\vec{r}_2) + \phi_a(\vec{r}_1)\phi_b(\vec{r}_2) + \phi_b(\vec{r}_1)\phi_a(\vec{r}_2) + \phi_b(\vec{r}_1)\phi_b(\vec{r}_2) \right]$
$e_1\, e_2$
a
b
e_1
e_2
e_2
e_1
e_1
e_2
$\Psi_t(\vec{r}_1, \vec{r}_2) = \frac{1}{\sqrt{2}} \left[\phi_a(\vec{r}_1)\phi_b(\vec{r}_2) - \phi_b(\vec{r}_1)\phi_a(\vec{r}_2) \right]$

$\phi(\vec{r}_1 - \vec{R}_a)$

Singlet: $$\psi_s(\vec{r}_1, \vec{r}_2) = \frac{1}{\sqrt{2}}\,\frac{1}{2}\left[\phi_a(\vec{r}_1) + \phi_b(\vec{r}_1)\right]\left[\phi_a(\vec{r}_2) + \phi_b(\vec{r}_2)\right]$$

$$= \frac{1}{2\sqrt{2}}\left[\phi_a(\vec{r}_1)\phi_a(\vec{r}_2) + \phi_a(\vec{r}_1)\phi_b(\vec{r}_2) + \phi_b(\vec{r}_1)\phi_a(\vec{r}_2) + \phi_b(\vec{r}_1)\phi_b(\vec{r}_2)\right]$$

$e_1 e_2$ a, b | e_1, e_2 | e_2, e_1 | $e_1 e_2$

$$\psi_t(\vec{r}_1, \vec{r}_2) = \frac{1}{\sqrt{2}}\left[\phi_a(\vec{r}_1)\phi_b(\vec{r}_2) - \phi_b(\vec{r}_1)\phi_a(\vec{r}_2)\right]$$

e_1 a, e_2 b | e_2 a, e_1 b

$$\text{inglet:}\quad \Psi_s(\bar r_1,\bar r_2) = \frac{1}{\sqrt{2}}\,\frac{1}{2}\left(\underset{\phi(\bar r_1-\bar R_a)}{\phi_a(\bar r_1)} + \phi_b(\bar r_1)\right)\left[\phi_a(\bar r_2)+\phi_b(\bar r_2)\right)$$

$$= \frac{1}{2\sqrt{2}}\left[\phi_a(\bar r_1)\phi_a(\bar r_2) + \phi_a(\bar r_1)\phi_b(\bar r_2) + \phi_b(\bar r_1)\phi_a(\bar r_2) + \phi_b(\bar r_1)\phi_b(\bar r_2)\right]$$

$e_1\ e_2$ e_1 e_2 e_2 e_1 $e_1\ e_2$

a b

$$\Psi_t(\vec r_1,\vec r_2) = \frac{1}{\sqrt{2}}\left[\phi_a(\vec r_1)\phi_b(\vec r_2) - \phi_b(\vec r_1)\phi_a(\vec r_2)\right]$$

e_1 e_2 e_2 e_1

a b a b

"good part" version of $\Psi_s(\bar{r}_1, \bar{r}_2)$:

$$\Psi_s^{HL}(\bar{r}_1, \bar{r}_2) = \frac{1}{\sqrt{2}} \left[\phi_a(\bar{r}_1)\phi_b(\bar{r}_2) + \phi_b(\bar{r}_1)\phi_a(\bar{r}_2) \right]$$

Hund-Mulliken

$\phi_b(\bar{r}_2)]$

e_1 e_2

Heitler-London

"good part" version of $\Psi_s(\bar{r}_1, \bar{r}_2)$:

$$\Psi_s^{HL}(\bar{r}_1, \bar{r}_2) = \frac{1}{\sqrt{2}}\left[\phi_a(\bar{r}_1)\phi_b(\bar{r}_2) + \phi_b(\bar{r}_1)\phi_a(\bar{r}_2)\right]$$

Hund-Mulliken

Heitler-London

$\phi_b(\bar{r}_2))$

$$\Psi_t^{HL}(\bar{r}_1, \bar{r}_2) = \frac{1}{\sqrt{2}}\left[\phi_a(\bar{r}_1)\phi_b(\bar{r}_2) - \phi_b(\bar{r}_1)\phi_a(\bar{r}_2)\right]$$

"good part" version of $\Psi_s(\bar{r}_1, \bar{r}_2)$:

$$\Psi_s^{HL}(\bar{r}_1, \bar{r}_2) = \frac{1}{\sqrt{2}}\left[\phi_a(\bar{r}_1)\phi_b(\bar{r}_2) + \phi_b(\bar{r}_1)\phi_a(\bar{r}_2)\right]$$

Heitler-London

$$\Psi_t^{HL}(\bar{r}_1, \bar{r}_2) = \frac{1}{\sqrt{2}}\left[\phi_a(\bar{r}_1)\phi_b(\bar{r}_2) - \phi_b(\bar{r}_1)\phi_a(\bar{r}_2)\right]$$

Hund-Mulliken

$\phi_b(\bar{r}_2)\big)$

e_1 e_2

good when kinetic energy dominates electron-electron interactions

"good part" version of $\Psi_s(\bar{r}_1, \bar{r}_2)$:

$$\Psi_s^{HL}(\bar{r}_1, \bar{r}_2) = \frac{1}{\sqrt{2}} \left[\phi_a(\bar{r}_1)\phi_b(\bar{r}_2) + \phi_b(\bar{r}_1)\phi_a(\bar{r}_2)\right]$$

Heitler-London

$$\Psi_t^{HL}(\bar{r}_1, \bar{r}_2) = \frac{1}{\sqrt{2}} \left[\phi_a(\bar{r}_1)\phi_b(\bar{r}_2) - \phi_b(\bar{r}_1)\phi_a(\bar{r}_2)\right]$$

Use $\Psi^{HL}_{s,t}$ to compute $E_s - E_t$

Hund-Mulliken

good when kinetic energy dominates electron-electron interactions

$\phi_b(\bar{r}_2)]$

e_1 e_2

$$\frac{1}{2}\left(E_s - E_t\right) = \frac{U - V|S_{ab}|^2}{1 - |S_{ab}|^2}$$

$$S_{ab} = \int d^3r \, \phi_a^*(r)\, \phi_b(r)$$

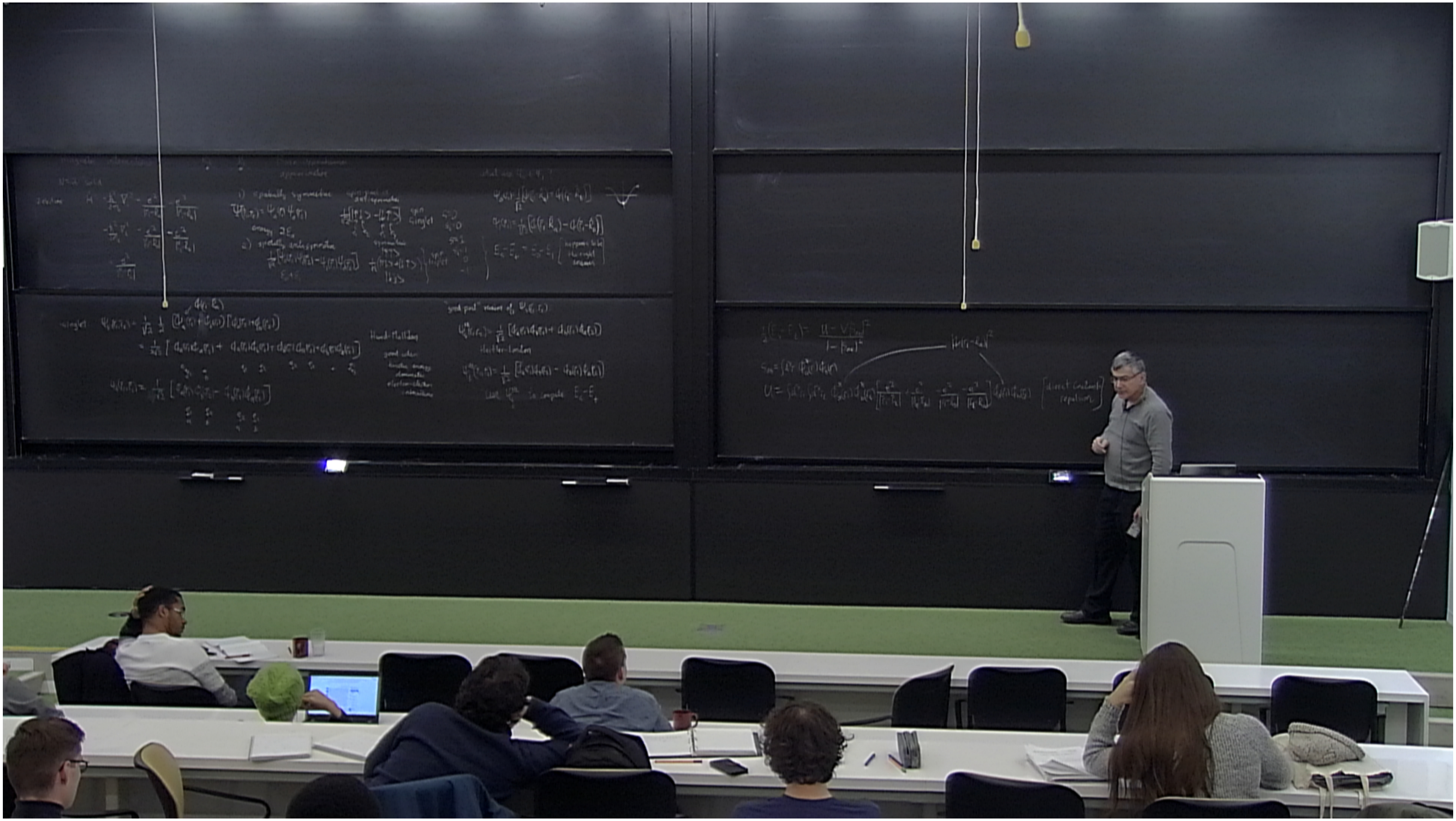
$$U = \int d^3r_1 \int d^3r_2 \, \phi_a^*(r_1)\, \phi_b^*(r_2) \left[\frac{e^2}{|\vec{r}_1 - \vec{r}_2|} + \frac{e^2}{|\vec{R}_1 - \vec{R}_2|} \right] \phi_a(\vec{r}_1)\, \phi_b(\vec{r}_2)$$

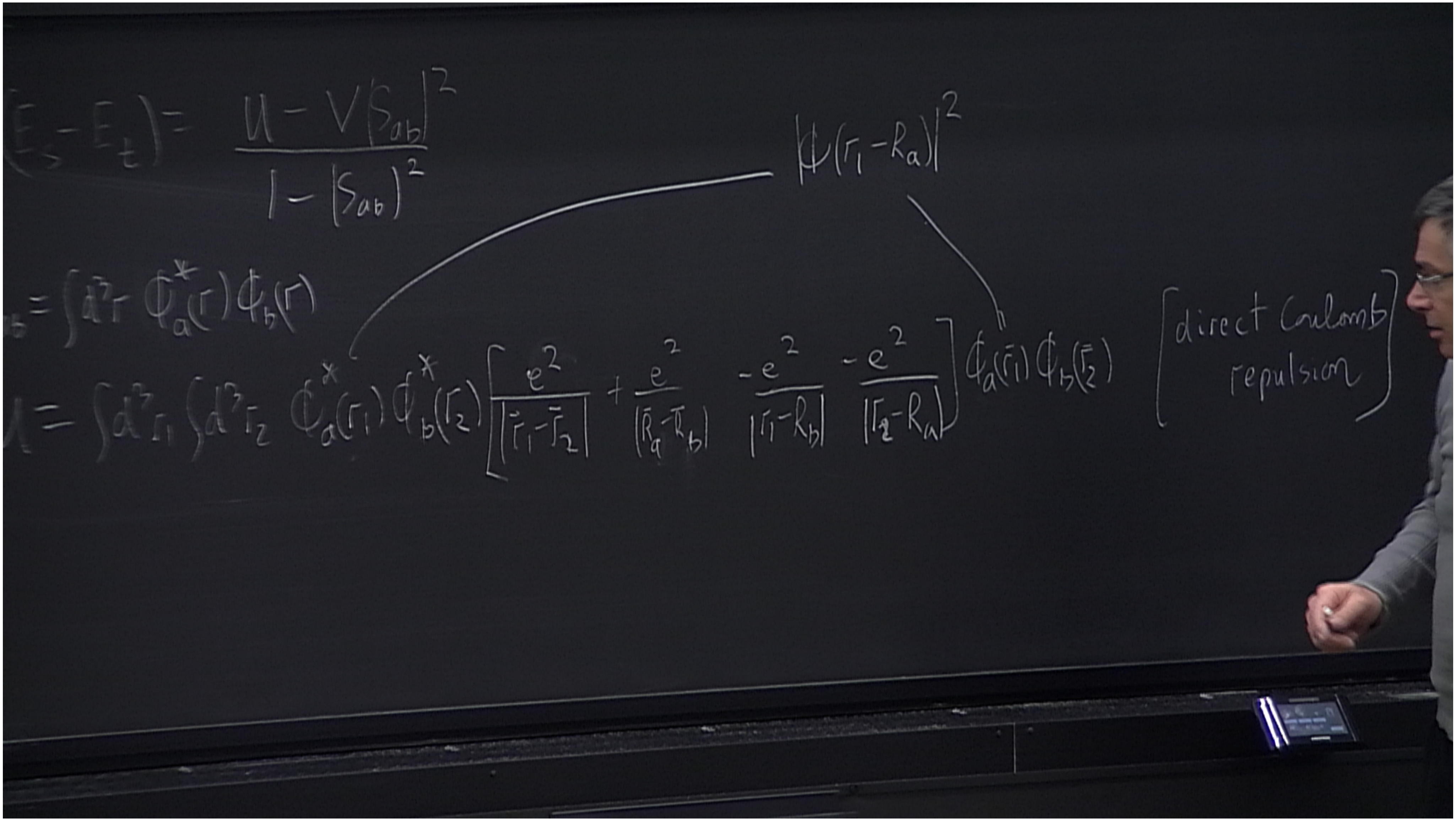
$$\frac{1}{2}(E_s - E_t) = \frac{U - V|S_{ab}|^2}{1 - |S_{ab}|^2}$$

$$S_{ab} = \int d^3r \, \phi_a^*(r)\, \phi_b(r)$$

$$U = \int d^3r_1 \int d^3r_2 \, \phi_a^*(r_1)\, \phi_b^*(r_2) \left[\frac{e^2}{|\bar{r}_1 - \bar{r}_2|} + \frac{e^2}{|\bar{R}_a - \bar{R}_b|} - \frac{e^2}{|\bar{r}_1 - R_b|} - \frac{e^2}{|\bar{r}_2 - R_a|} \right] \phi_a(\bar{r}_1)\, \phi_b(\bar{r}_2)$$

[direct C
rep




$(E_s - E_t) = \frac{U - V|S_{ab}|^2}{1 - |S_{ab}|^2}$
$|\phi(r_1 - R_a)|^2$
$S_{ab} = \int d^3r\, \phi_a^*(r)\, \phi_b(r)$
$U = \int d^3r_1 \int d^3r_2\, \phi_a^*(r_1)\, \phi_b^*(r_2) \left[\frac{e^2}{|\bar{r}_1 - \bar{r}_2|} + \frac{e^2}{|\bar{R}_a - \bar{R}_b|} - \frac{e^2}{|r_1 - R_b|} - \frac{e^2}{|r_2 - R_a|} \right] \phi_a(\bar{r}_1)\, \phi_b(\bar{r}_2)$
[direct Coulomb repulsion]

$$\frac{1}{2}\left(E_s - E_t\right) = \frac{U - V|S_{ab}|^2}{1 - |S_{ab}|^2}$$

$$|\phi(r_1 - R_a)|^2$$

$$S_{ab} = \int d^3r\, \phi_a^*(r)\,\phi_b(r)$$

$$U = \int d^3r_1 \int d^3r_2\, \phi_a^*(r_1)\,\phi_b^*(r_2)\left[\frac{e^2}{|\bar r_1 - \bar r_2|} + \frac{e^2}{|\bar R_a - \bar R_b|} - \frac{e^2}{|\bar r_1 - R_b|} - \frac{e^2}{|\bar r_2 - R_a|}\right]\phi_a(\bar r_1)\,\phi_b(\bar r_2)$$

$$V = \int d^3r_1 \int d^3r_2\, \phi_a^*(r_1)\,\phi_b^*(r_2)\Big[\qquad\Big]\phi_a(\bar r_2)\,\phi_b(\bar r_1)$$

$$\frac{1}{2}(E_s - E_t) = \frac{U - V|S_{ab}|^2}{1 - |S_{ab}|^2}$$

$$|\phi(r_1 - R_a)|^2$$

$$\phi^*(r_1 - R_a)\,\phi(r_1 - R_b)$$

$$S_{ab} = \int d^3r\, \phi_a^*(r)\,\phi_b(r)$$

$$U = \int d^3r_1 \int d^3r_2\, \phi_a^*(r_1)\,\phi_b^*(r_2)\left[\frac{e^2}{|\bar r_1 - \bar r_2|} + \frac{e^2}{|\bar R_a - \bar R_b|} - \frac{e^2}{|r_1 - R_b|} - \frac{e^2}{|r_2 - R_a|}\right]\phi_a(\bar r_1)\,\phi_b(\bar r_2)$$

[direct Coulo
repulsion

$$V = \int d^3r_1 \int d^3r_2\, \phi_a^*(r_1)\,\phi_b^*(r_2)\Big[\qquad\Big]\phi_a(\bar r_2)\,\phi_b(\bar r_1)$$

$$\frac{1}{2}(E_s - E_t) = \frac{U - V|S_{ab}|^2}{1-|S_{ab}|^2}$$

$$|\phi(r_1 - R_a)|^2$$

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[direct C
repuls

$$V = \int d^3r_1 \int d^3r_2\, \phi_a^*(\vec r_1)\,\phi_b^*(\vec r_2)\left[\frac{e^2}{|\vec r_1 - \vec r_2|} + \frac{e^2}{|\vec R_a - \vec R_b|} - \frac{e^2}{|\vec r_1 - \vec R_a|} - \frac{e^2}{|\vec r_2 - \vec R_b|}\right]\phi_a(\vec r_2)\,\phi_b(\vec r_1)$$

$$\frac{1}{2}\left(E_s - E_t\right) = \frac{U - V|S_{ab}|^2}{1 - |S_{ab}|^2}$$

$$|\phi(r_1 - R_a)|^2$$

$$\phi^*(r_1 - R_a)\,\phi(r_1 - R_b)$$

$$S_{ab} = \int d^3r\, \phi_a^*(r)\,\phi_b(r)$$

$$U = \int d^3r_1 \int d^3r_2\, \phi_a^*(r_1)\,\phi_b^*(r_2)\left[\frac{e^2}{|\bar r_1 - \bar r_2|} + \frac{e^2}{|\bar R_a - \bar R_b|} - \frac{e^2}{|r_1 - R_b|} - \frac{e^2}{|r_2 - R_a|}\right]\phi_a(\bar r_1)\,\phi_b(\bar r_2)$$

[direct Coulomb repulsion]

$$V = \int d^3r_1 \int d^3r_2\, \phi_a^*(r_1)\,\phi_b^*(r_2)\left[\frac{e^2}{|\bar r_1 - \bar r_2|} + \frac{e^2}{|\bar R_a - \bar R_b|} - \frac{e^2}{|r_1 - R_a|} - \frac{e^2}{|r_2 - R_b|}\right]\phi_a(\bar r_2)\,\phi_b(\bar r_1)$$

[exchange term]

$$\frac{1}{2}\left(E_s - E_t\right) = \frac{U - V|S_{ab}|^2}{1 - |S_{ab}|^2} \equiv \frac{J}{2}$$

$$|\phi(r_1 - R_a)|^2$$

$$\phi^*(r_1 - R_a)\,\phi(r_1 - R_b)$$

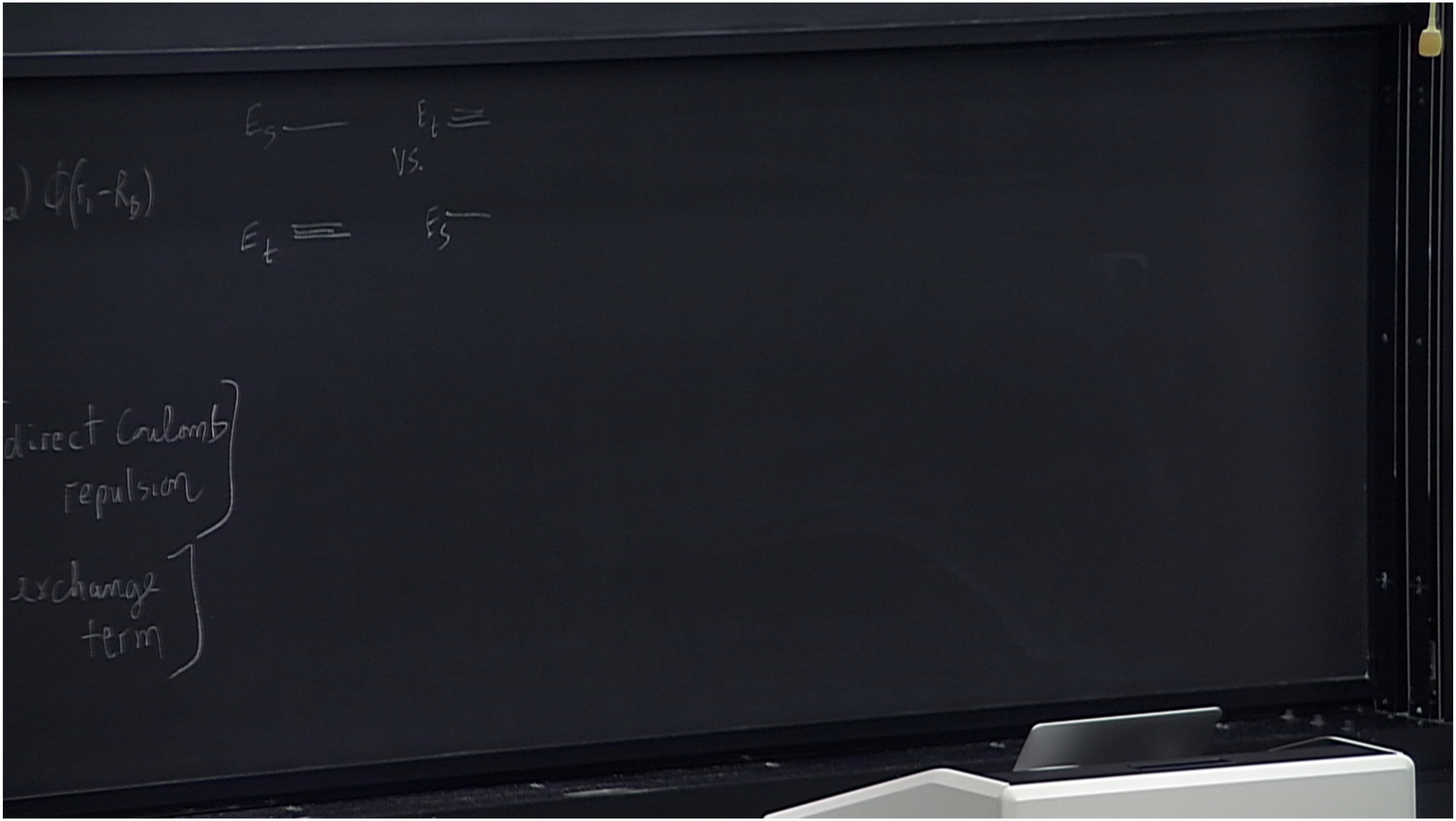
$$S_{ab} = \int d^3r\, \phi_a^*(r)\,\phi_b(r)$$

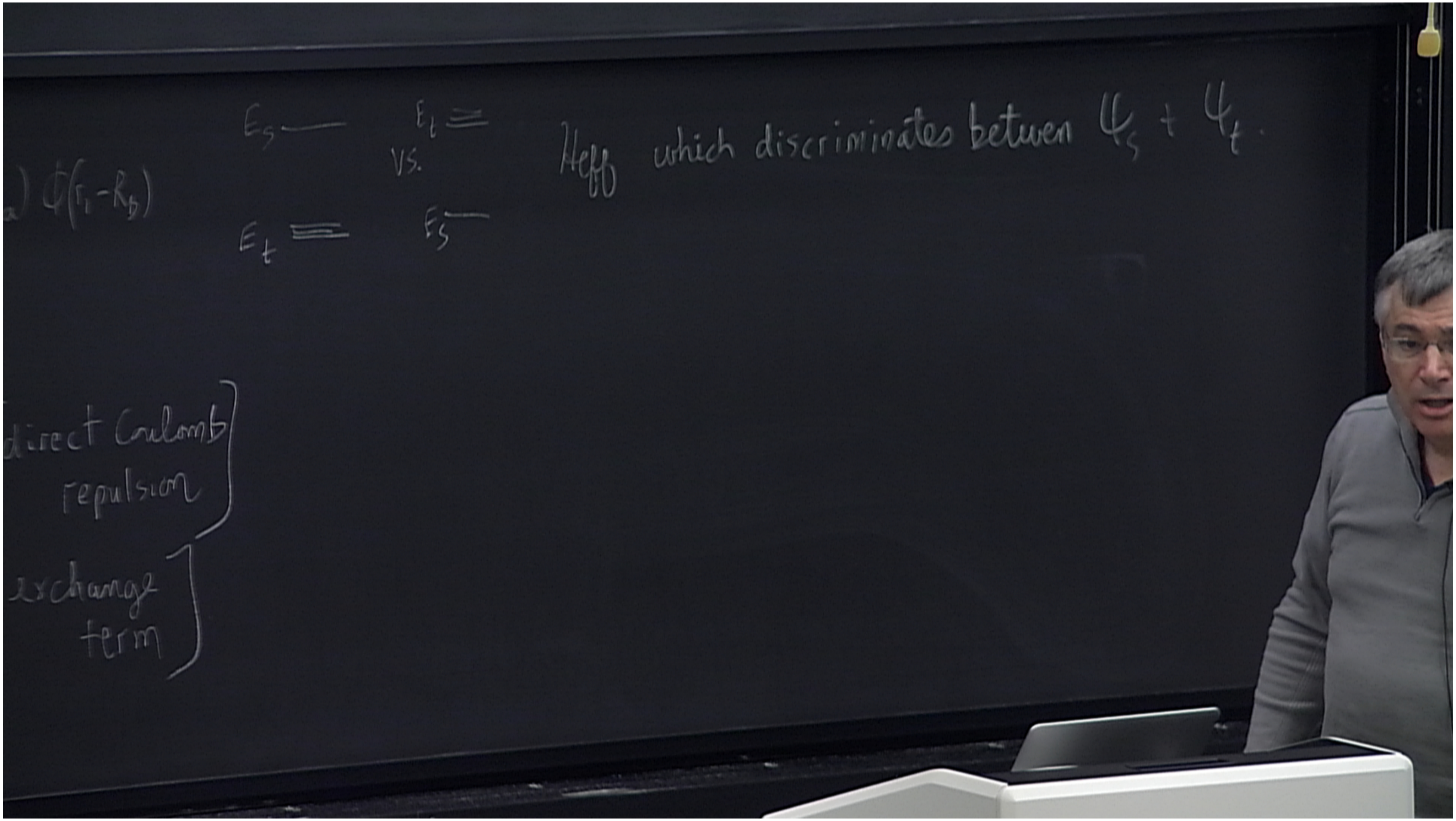
$$U = \int d^3r_1 \int d^3r_2\, \phi_a^*(r_1)\,\phi_b^*(r_2)\left[\frac{e^2}{|\bar{r}_1 - \bar{r}_2|} + \frac{e^2}{|\bar{R}_a - \bar{R}_b|} - \frac{e^2}{|r_1 - R_b|} - \frac{e^2}{|r_2 - R_a|}\right]\phi_a(\bar{r}_1)\,\phi_b(\bar{r}_2)$$

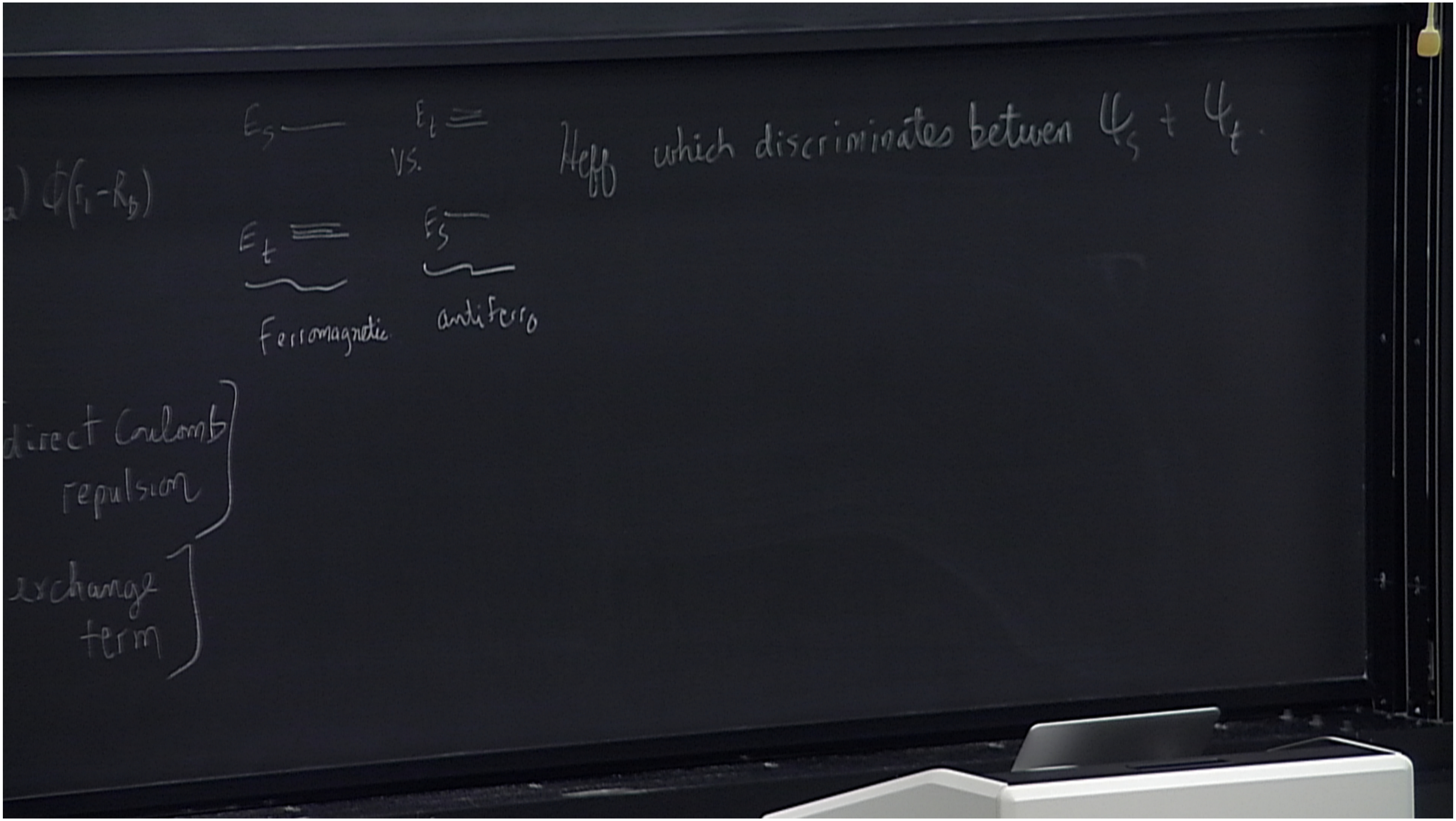
[direct Coulomb repulsion]

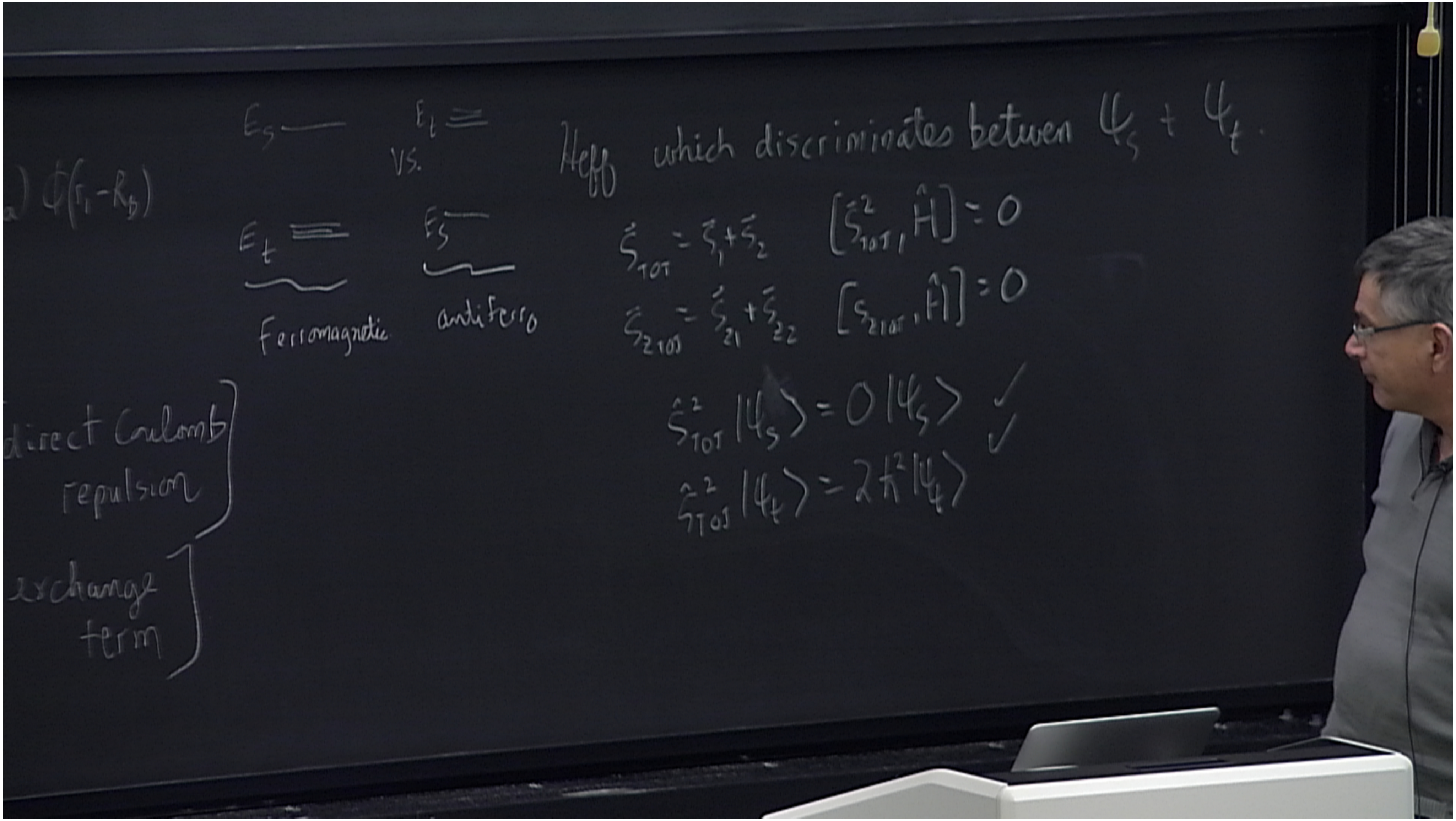
$$V = \int d^3r_1 \int d^3r_2\, \phi_a^*(r_1)\,\phi_b^*(r_2)\left[\frac{e^2}{|r_1 - r_2|} + \frac{e^2}{|R_a - R_b|} - \frac{e^2}{|r_1 - R_a|} - \frac{e^2}{|r_2 - R_b|}\right]\phi_a(\bar{r}_2)\,\phi_b(\bar{r}_1)$$

[exchange term]


E_s —— E_t ==
vs.
E_t == E_s ——
$\phi(r_1 - R_b)$
direct Coulomb repulsion
exchange term


E_s — E_t =
vs.
E_t = E_s —
H_{eff} which discriminates between ψ_s + ψ_t.
$\phi(r_1 - R_b)$
direct Coulomb repulsion
exchange term


E_s — vs. $E_t \equiv$
H_{eff} which discriminates between ψ_s + ψ_t.
$\phi(r_1 - R_b)$
$E_t \equiv$ E_s —
Ferromagnetic antiferro
direct Coulomb repulsion
exchange term



Heff which discriminates between Ψs + Ψt.
vs.
Ferromagnetic
antiferro
S TOT = S1 + S2
[S² TOT, Ĥ] = 0
S 2TOT = S21 + S22
[S 2TOT, Ĥ] = 0
S² TOT |Ψs> = 0 |Ψs>
S² TOT |Ψt> = 2ħ² |Ψt>
direct Coulomb repulsion
exchange term

$$\hat{S}^2_{TOT} = (\hat{S}_1+\hat{S}_2)(\hat{S}_1+\hat{S}_2) = \hat{S}_1^2 + \hat{S}_2^2 + 2\hat{S}_1\cdot\hat{S}_2$$

$$= \frac{3}{4} + \frac{3}{4} + 2\hat{S}_1\cdot\hat{S}_2$$

$$= \frac{3}{2} + 2\hat{S}_1\cdot\hat{S}_2$$

Suggest $\hat{H}_{eff} = a + b\,\hat{S}_1\cdot\hat{S}_2$

$$\hat{S}_{TOT}^2 = (\hat{S}_1+\hat{S}_2)(\hat{S}_1+\hat{S}_2) = \hat{S}_1^2 + \hat{S}_2^2 + 2\hat{S}_1\cdot\hat{S}_2$$

$$= \frac{3}{4} + \frac{3}{4} + 2\hat{S}_1\cdot\hat{S}_2$$

$$= \frac{3}{2} + 2\hat{S}_1\cdot\hat{S}_2$$

Suggest $\hat{H}_{eff} = a + b\,\hat{S}_1\cdot\hat{S}_2$

$$\hat{H}_{eff}|\psi_s\rangle = E_s|\psi_s\rangle = a+b$$

$$\hat{S}^2_{TOT} = (\hat{\vec{S}}_1 + \hat{\vec{S}}_2)(\hat{\vec{S}}_1 + \hat{\vec{S}}_2) = \hat{S}_1^2 + \hat{S}_2^2 + 2\hat{S}_1 \cdot \hat{S}_2$$

$$= \frac{3}{4} + \frac{3}{4} + 2\hat{S}_1 \cdot S_2$$

$$\hat{S}^2_{TOT} = \frac{3}{2} + 2\vec{S}_1 \cdot \vec{S}_2 \Rightarrow \hat{S}_1 \cdot \hat{S}_2 |\psi_s\rangle = -\frac{3}{4}|\psi_s\rangle$$

Suggest $\hat{H}_{eff} = a + b\hat{S}_1 \cdot \hat{S}_2$

$$\hat{H}_{eff}|\psi_s\rangle = E_s|\psi_s\rangle = a + b$$

$$\hat{S}^2_{TOT} = (\hat{S}_1+\hat{S}_2)(\hat{S}_1+\hat{S}_2) = \hat{S}_1^2 + \hat{S}_2^2 + 2\hat{S}_1\cdot\hat{S}_2$$

$$= \frac{3}{4} + \frac{3}{4} + 2\hat{S}_1\cdot S_2$$

$$\hat{S}^2_{TOT} = \frac{3}{2} + 2\hat{S}_1\cdot\hat{S}_2 \Rightarrow \hat{S}_1\cdot\hat{S}_2|\psi_s\rangle = -\frac{3}{4}|\psi_s\rangle$$

$$\Rightarrow S_1\cdot S_2|\psi_t\rangle = \frac{1}{4}|\psi_t\rangle$$

Suggest $\hat{H}_{eff} = a + b\,\hat{S}_1\cdot\hat{S}_2$

$$\left.\begin{aligned} \hat{H}_{eff}|\psi_s\rangle &= E_s|\psi_s\rangle = \left[a+b\left(-\frac{3}{4}\right)\right]\psi_s\rangle \\ H_{eff}|\psi_t\rangle &= E_t|\psi_t\rangle = \left[a+b\left(\frac{1}{4}\right)\right]\psi_t\rangle \end{aligned}\right\}$$

$$\hat{S}^2_{TOT} = (\hat{S}_1+\hat{S}_2)(\hat{S}_1+\hat{S}_2) = \hat{S}_1^2 + \hat{S}_2^2 + 2\hat{S}_1\cdot\hat{S}_2$$

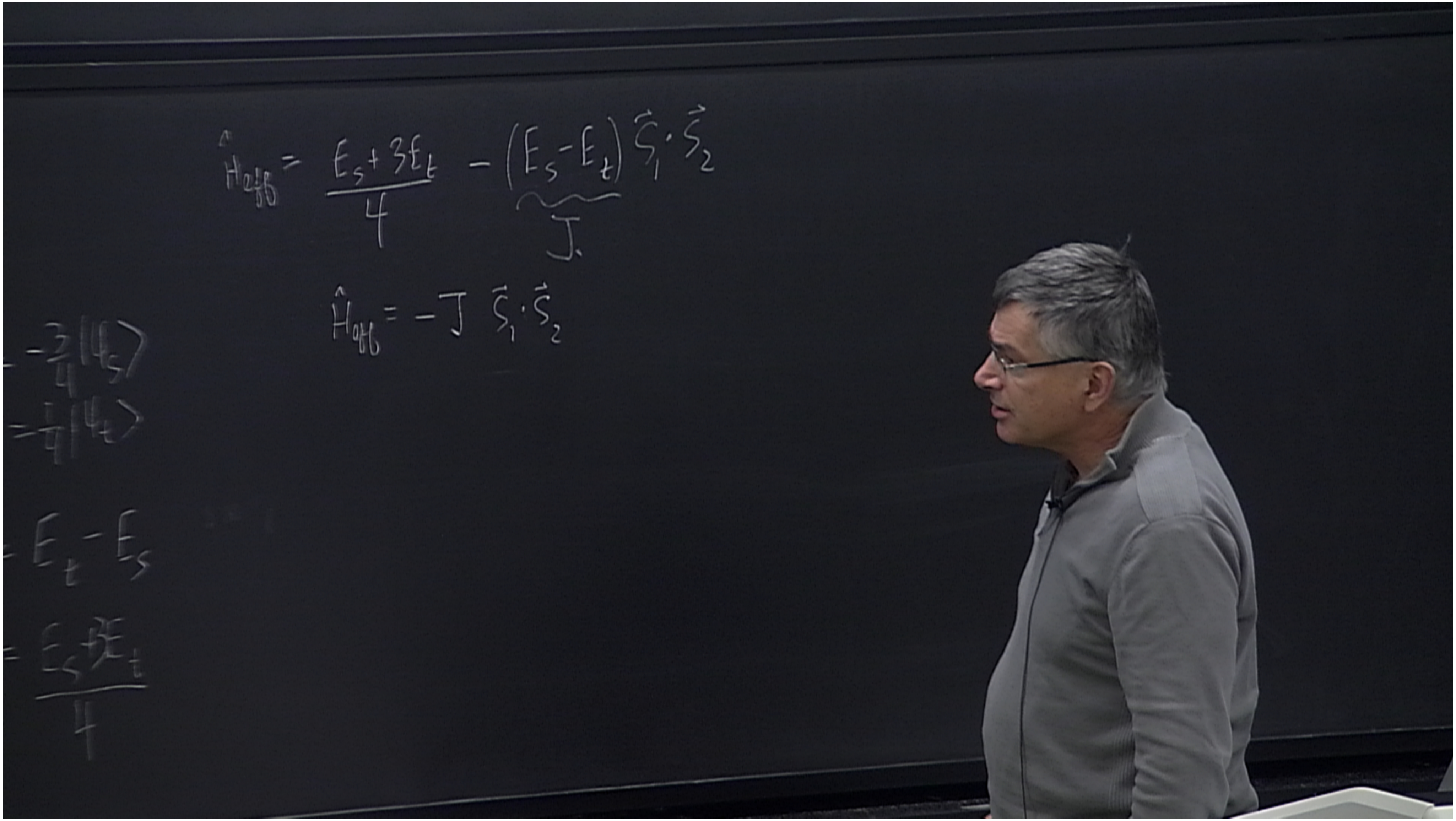
$$= \frac{3}{4} + \frac{3}{4} + 2\hat{S}_1\cdot\hat{S}_2$$

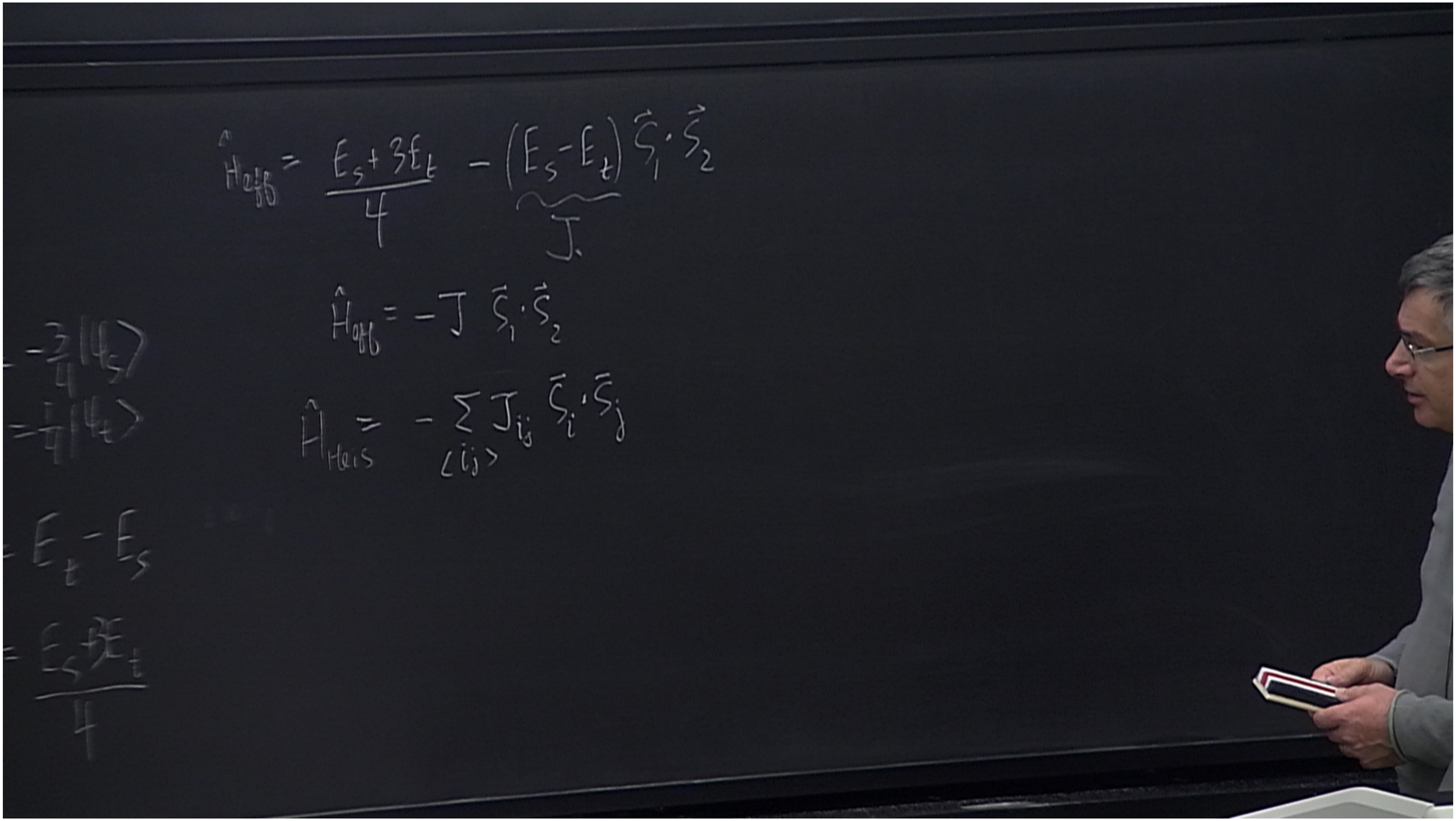
$$\hat{S}^2_{TOT} = \frac{3}{2} + 2\hat{S}_1\cdot\hat{S}_2 \Rightarrow \hat{S}_1\cdot\hat{S}_2|\psi_s\rangle = -\frac{3}{4}|\psi_s\rangle$$

$$\Rightarrow \hat{S}_1\cdot\hat{S}_2|\psi_t\rangle = \frac{1}{4}|\psi_t\rangle$$

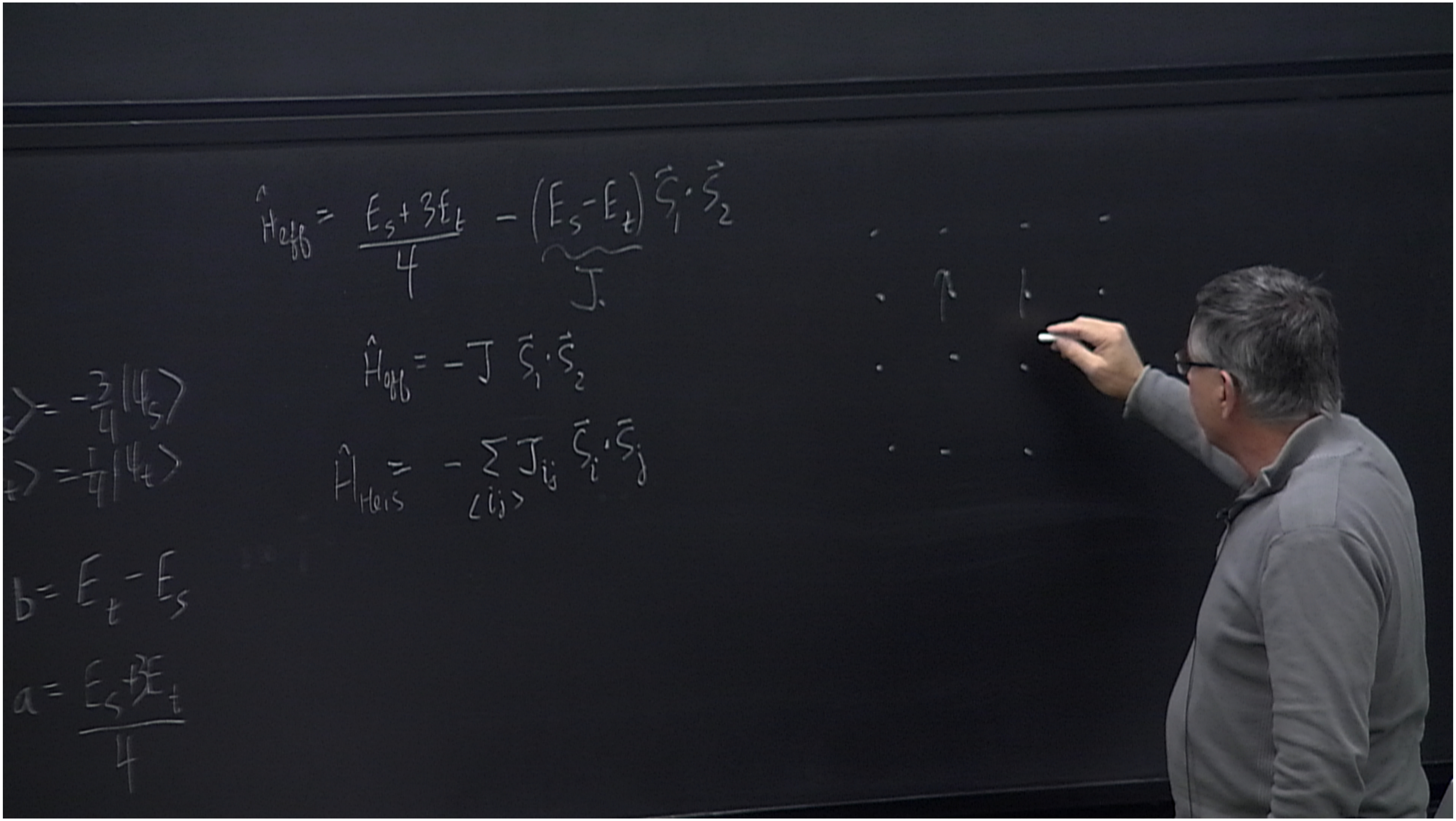
Suggest $\hat{H}_{eff} = a + b\hat{S}_1\cdot\hat{S}_2$

$$\left.\begin{aligned}\hat{H}_{eff}|\psi_s\rangle &= E_s|\psi_s\rangle = \left[a+b\left(-\frac{3}{4}\right)\right]|\psi_s\rangle \\ H_{eff}|\psi_t\rangle &= E_t|\psi_t\rangle = \left[a+b\left(\frac{1}{4}\right)\right]|\psi_t\rangle\end{aligned}\right\} \Rightarrow \begin{aligned} b &= E_t - E_s \\ a &= \frac{E_s+3E_t}{4}\end{aligned}$$


$\hat{H}_{eff} = \frac{E_s + 3E_t}{4} - \underbrace{(E_s - E_t)}_{J} \vec{S}_1 \cdot \vec{S}_2$
$\hat{H}_{eff} = -J \vec{S}_1 \cdot \vec{S}_2$
$-\frac{3}{4}|\psi_s\rangle$
$= \frac{1}{4}|\psi_t\rangle$
$= E_t - E_s$
$= \frac{E_s + 3E_t}{4}$



$\hat{H}_{eff} = \frac{E_s + 3E_t}{4} - \underbrace{(E_s - E_t)}_{J} \vec{S}_1 \cdot \vec{S}_2$
$\hat{H}_{eff} = -J \, \vec{S}_1 \cdot \vec{S}_2$
$\hat{H}_{Heis} = - \sum_{\langle ij \rangle} J_{ij} \, \vec{S}_i \cdot \vec{S}_j$
$-\frac{3}{4} |\psi_s\rangle$
$= \frac{1}{4} |\psi_t\rangle$
$= E_t - E_s$
$= \frac{E_s + 3E_t}{4}$

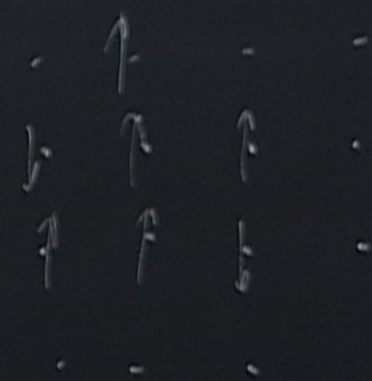


$\hat{H}_{eff} = \frac{E_s + 3E_t}{4} - \underbrace{(E_s - E_t)}_{J} \vec{S}_1 \cdot \vec{S}_2$
$\hat{H}_{eff} = -J \, \vec{S}_1 \cdot \vec{S}_2$
$\hat{H}_{Heis} = -\sum_{\langle ij \rangle} J_{ij} \, \vec{S}_i \cdot \vec{S}_j$
$b = E_t - E_s$
$a = \frac{E_s + 3E_t}{4}$

$$\hat{H}_{eff} = \frac{E_s + 3E_t}{4} - \underbrace{\left(E_s - E_t\right)}_{J} \vec{S}_1 \cdot \vec{S}_2$$

$$\hat{H}_{eff} = -J \, \vec{S}_1 \cdot \vec{S}_2$$

$$\hat{H}_{Heis} = -\sum_{\langle ij \rangle} J_{ij} \, \vec{S}_i \cdot \vec{S}_j$$



$$\rangle = -\frac{3}{4} |\psi_s\rangle$$

$$t\rangle = \frac{1}{4} |\psi_t\rangle$$

$$b = E_t - E_s$$

$$a = \frac{E_s + 3E_t}{4}$$

$$\hat{H}_{eff} = \frac{E_s + 3E_t}{4} - \underbrace{(E_s - E_t)}_{J}\, \vec{S}_1 \cdot \vec{S}_2$$

$$\hat{H}_{eff} = -J\, \vec{S}_1 \cdot \vec{S}_2$$

$$\hat{H}_{Heis} = -\sum_{\langle ij \rangle} J_{ij}\, \vec{S}_i \cdot \vec{S}_j$$

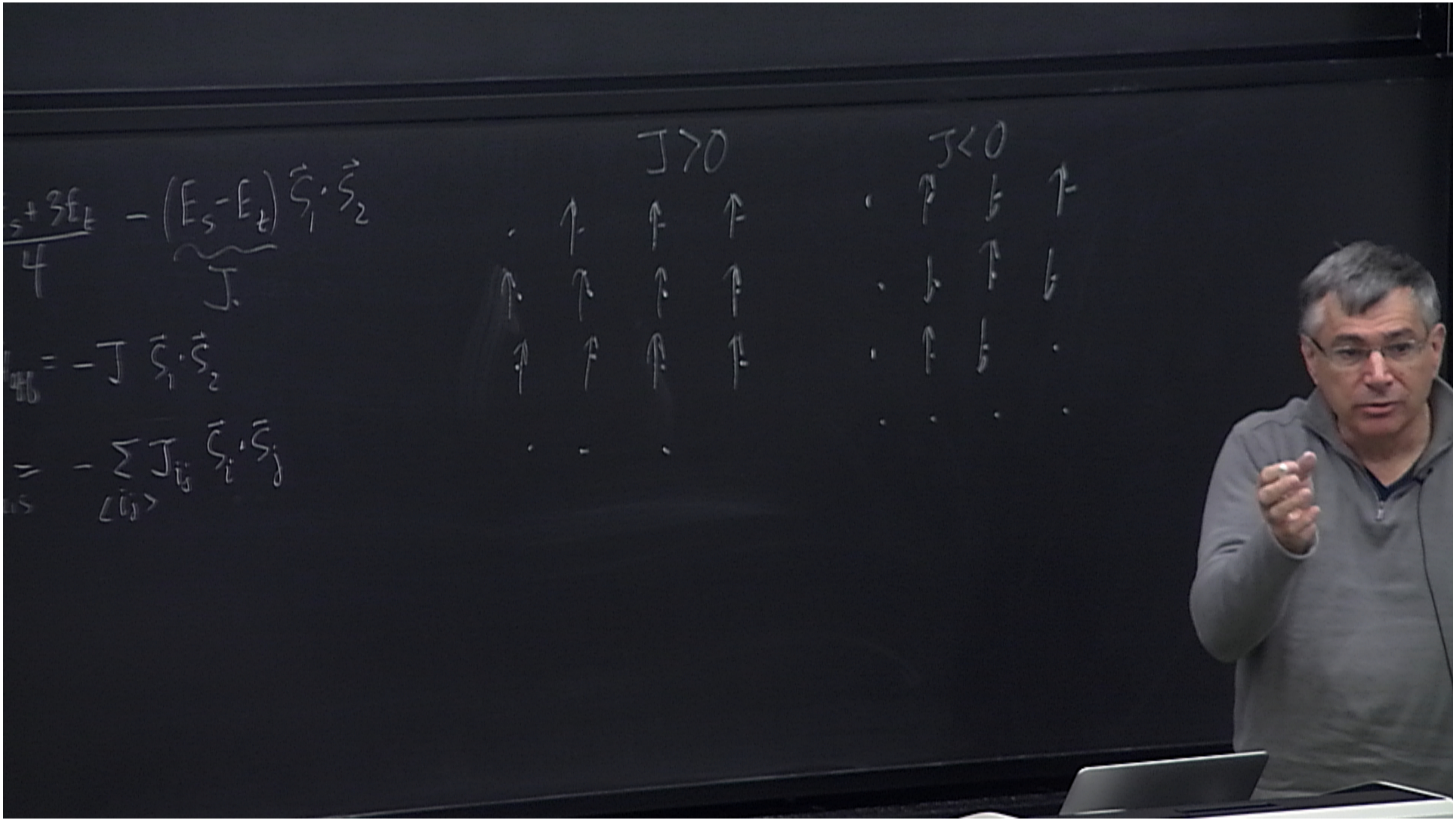
$\rangle = -\frac{3}{4}|\psi_s\rangle$

$t\rangle = \frac{1}{4}|\psi_t\rangle$

$b = E_t - E_s$

$a = \frac{E_s + 3E_t}{4}$

$J > 0$

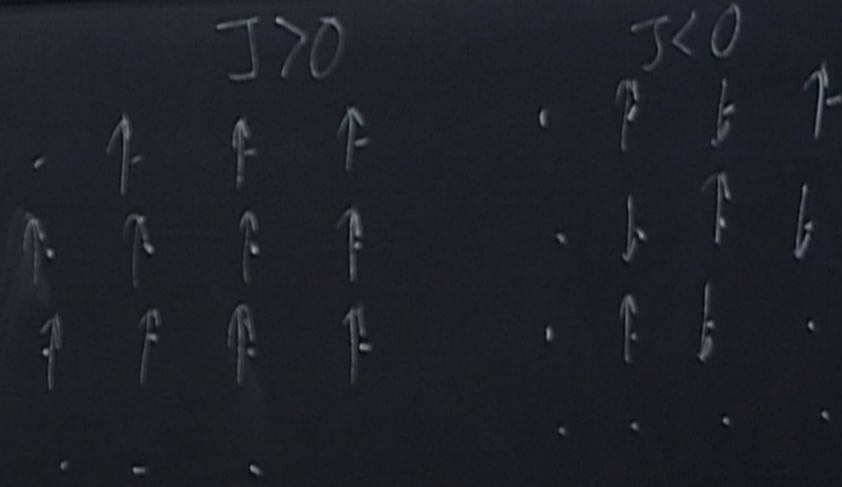

J>0
J<0

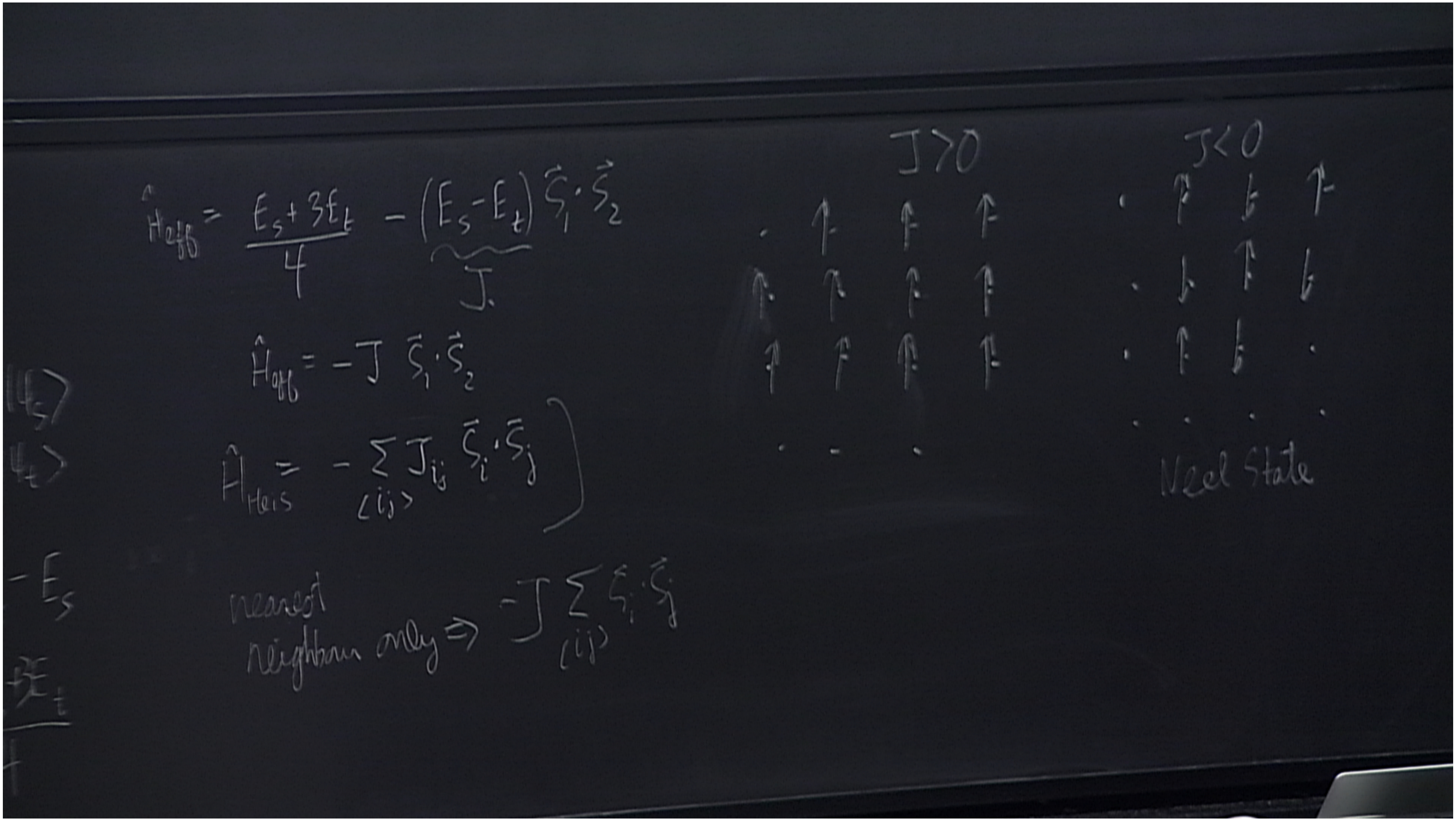
$$\hat{H}_{eff} = \frac{E_s + 3E_t}{4} - \underbrace{(E_s - E_t)}_{J}\, \vec{S}_1 \cdot \vec{S}_2$$

$$\hat{H}_{eff} = -J\, \vec{S}_1 \cdot \vec{S}_2$$

$$\hat{H}_{Heis} = -\sum_{\langle ij \rangle} J_{ij}\, \vec{S}_i \cdot \vec{S}_j$$

nearest neighbour only $\Rightarrow -J \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j$




$\hat{H}_{eff} = \frac{E_s + 3E_t}{4} - \underbrace{(E_s - E_t)}_{J} \vec{S}_1 \cdot \vec{S}_2$
$\hat{H}_{eff} = -J \, \vec{S}_1 \cdot \vec{S}_2$
$\hat{H}_{Heis} = - \sum_{\langle ij \rangle} J_{ij} \, \vec{S}_i \cdot \vec{S}_j$
nearest neighbour only $\Rightarrow -J \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j$
$J > 0$
$J < 0$
Neel State

$|\psi_s\rangle$

$\psi_t\rangle$

$-E_s$

$+3E_t$

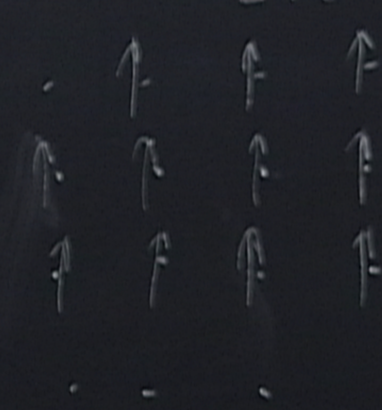
$$\hat H_{eff} = \frac{E_s+3E_t}{4} - \underbrace{\left(E_s-E_t\right)}_{J}\vec S_1\cdot\vec S_2$$

$$\hat H_{eff} = -J\,\vec S_1\cdot\vec S_2$$

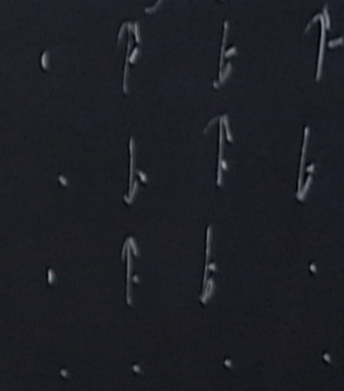
$$\hat H_{Heis} = -\sum_{\langle ij\rangle} J_{ij}\,\vec S_i\cdot\vec S_j$$

nearest neighbour only $\Rightarrow -J\sum_{\langle ij\rangle}\vec S_i\cdot\vec S_j$

$J>0$

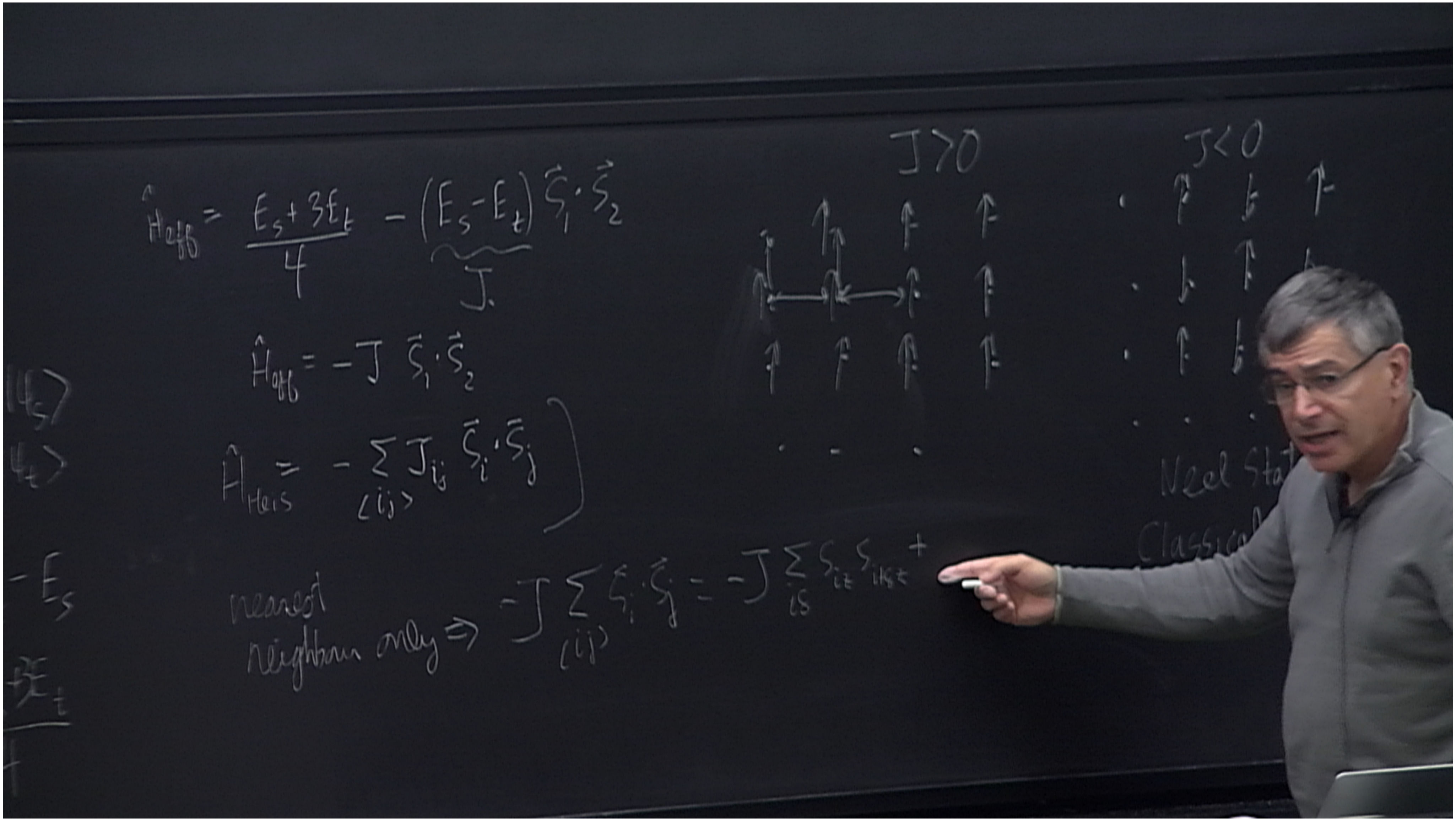


$J<0$



Neel State

Classical.


$\hat{H}_{eff} = \frac{E_s + 3E_t}{4} - \underbrace{(E_s - E_t)}_{J} \vec{S}_1 \cdot \vec{S}_2$
$\hat{H}_{eff} = -J \, \vec{S}_1 \cdot \vec{S}_2$
$\hat{H}_{Heis} = -\sum_{\langle ij \rangle} J_{ij} \, \vec{S}_i \cdot \vec{S}_j$
nearest neighbour only $\Rightarrow$ $-J \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j = -J \sum_{iS} S_{iz} S_{i+\hat{s}z} +$
$J > 0$
$J < 0$
Neel Sta
Classica

$|\psi_s\rangle$

$|\psi_t\rangle$

$-E_s$

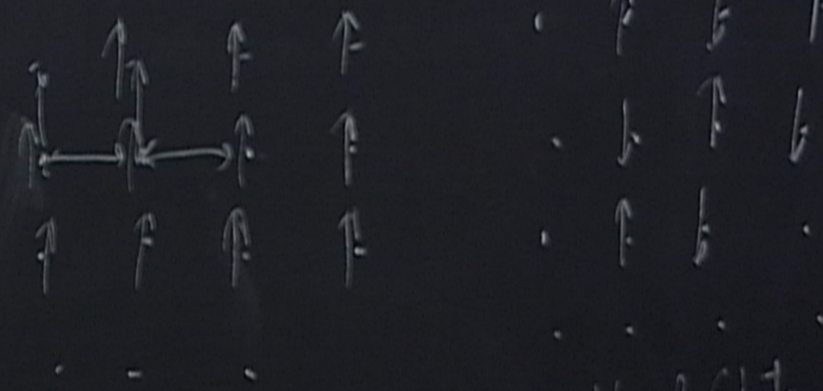
$+3E_t$

$$\hat{H}_{eff} = \frac{E_s + 3E_t}{4} - \underbrace{(E_s - E_t)}_{J} \vec{S}_1 \cdot \vec{S}_2$$

$$\hat{H}_{eff} = -J\, \vec{S}_1 \cdot \vec{S}_2$$

$$\hat{H}_{Heis} = -\sum_{\langle ij \rangle} J_{ij}\, \vec{S}_i \cdot \vec{S}_j$$

J>0 J<0



Neel State

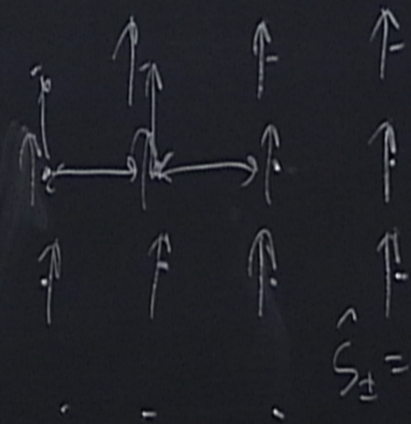
nearest neighbour only $\Rightarrow -J \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j = -J \sum_{i\delta} \left[S_{iz} S_{i+\delta z} + \frac{1}{2}\left(S_{i+} S_{i+\delta -} + S_{i-} S_{i+\delta +} \right) \right]$ Classical.

$$\hat{H}_{eff} = \frac{E_s+3E_t}{4} - \underbrace{(E_s-E_t)}_{J}\, \vec{S}_1\cdot\vec{S}_2$$

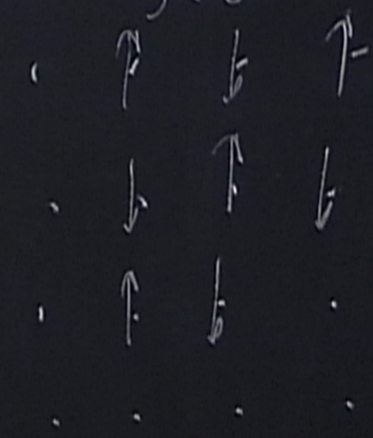
$$\hat{H}_{eff} = -J\, \vec{S}_1\cdot\vec{S}_2$$

$$\hat{H}_{Heis} = -\sum_{\langle ij\rangle} J_{ij}\, \vec{S}_i\cdot\vec{S}_j$$

$J>0$



$J<0$

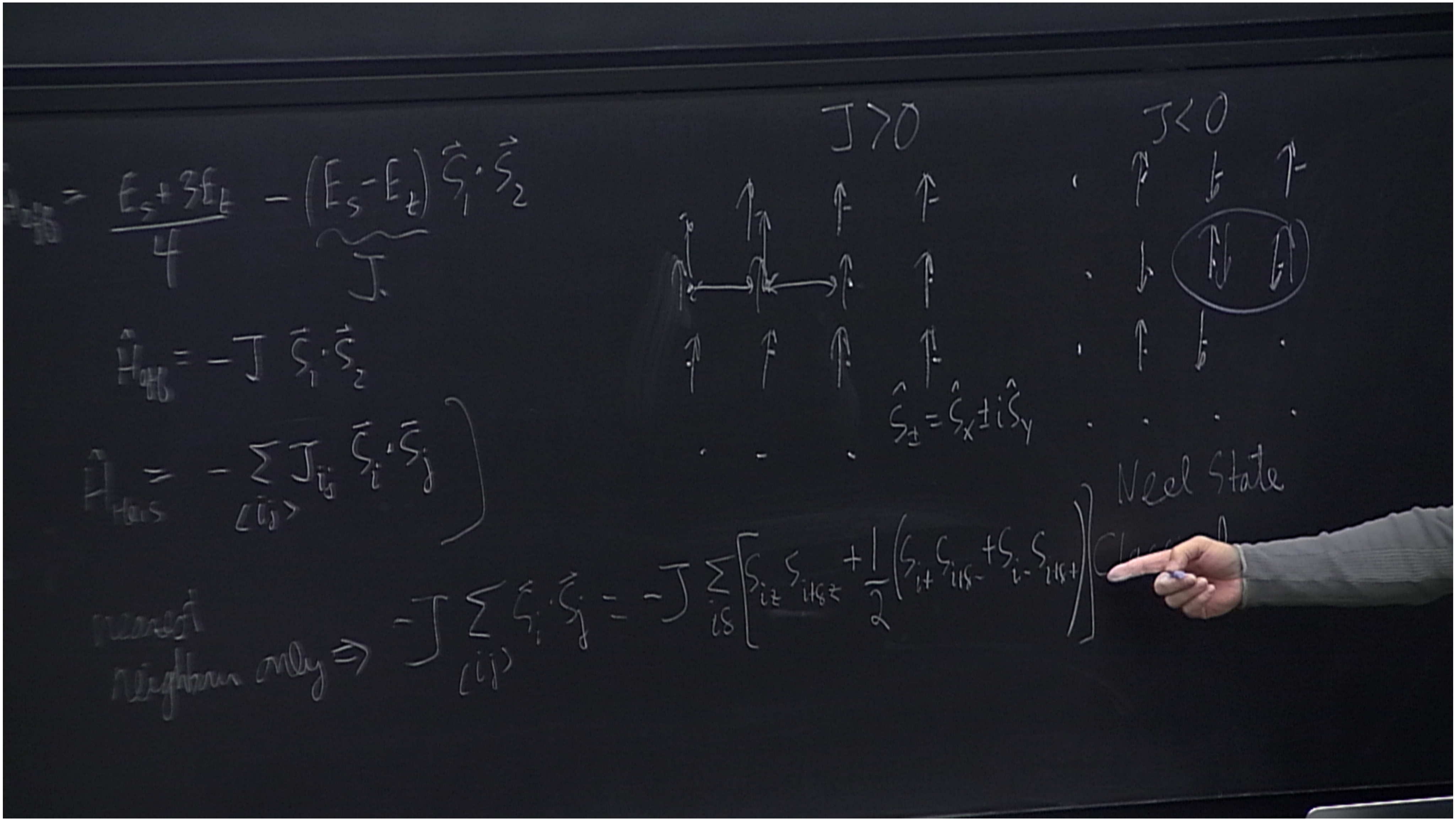


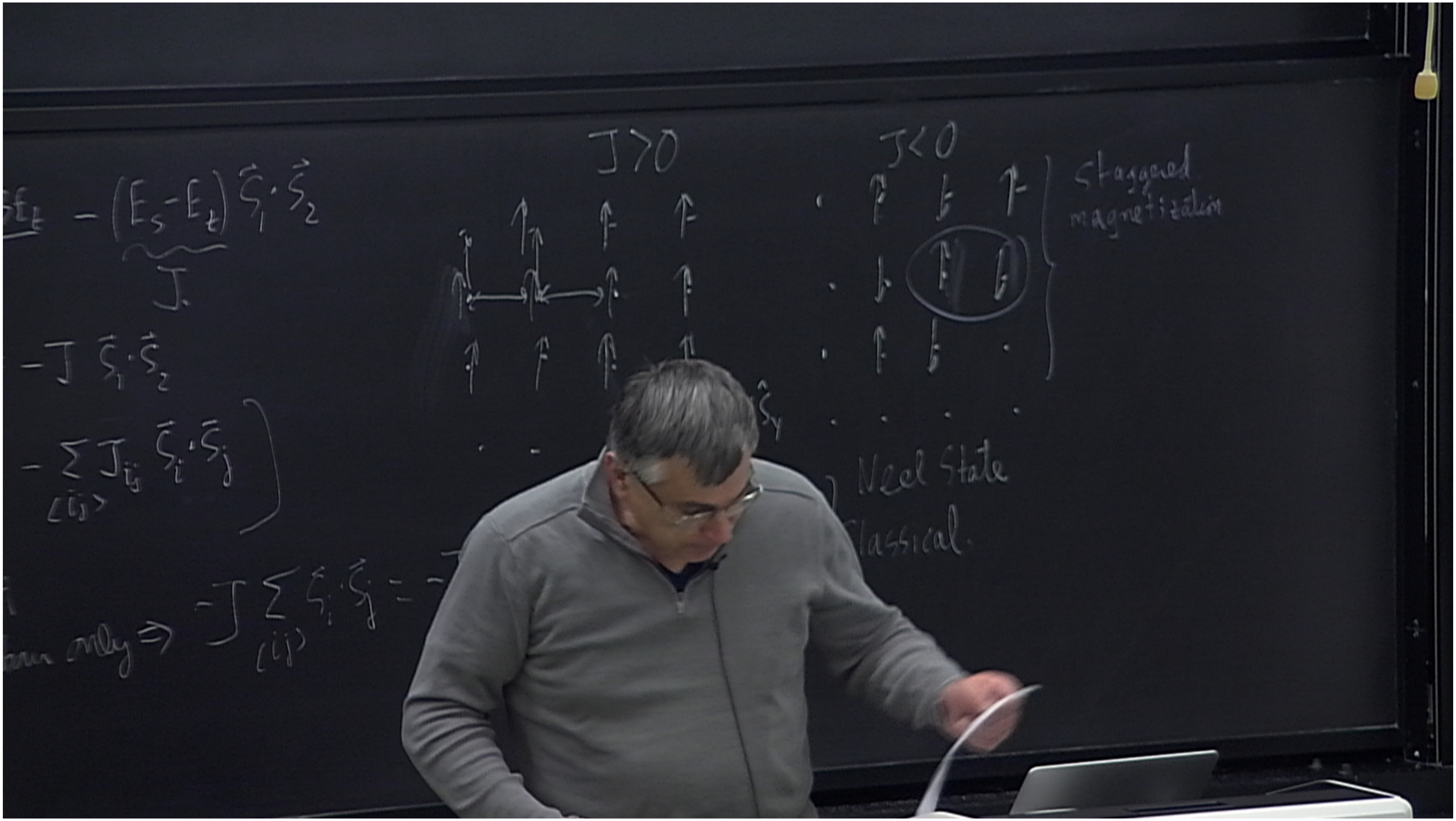
$$\hat{S}_\pm = \hat{S}_x \pm i\hat{S}_y$$

Neel State

Classical.

nearest neighbour only $\Rightarrow$ $$-J\sum_{\langle ij\rangle} \vec{S}_i\cdot\vec{S}_j = -J\sum_{i\delta}\left[S_{iz}S_{i+\delta z} + \frac{1}{2}\left(S_{i+}S_{i+\delta -} + S_{i-}S_{i+\delta +}\right)\right]$$


H = (E_s + 3E_t)/4 − (E_s − E_t) S_1 · S_2
J
H = −J S_1 · S_2
H_Heis = − Σ_⟨ij⟩ J_ij S_i · S_j
J > 0
J < 0
S_± = S_x ± i S_y
Neel State
nearest neighbour only ⇒ −J Σ_⟨ij⟩ S_i · S_j = −J Σ_iδ [S_iz S_i+δz + 1/2 (S_i+ S_i+δ− + S_i− S_i+δ+)]



J>0
J<0
staggered magnetization
Neel State
Classical.

Perimeter: Condensed Matter Fall 2016

PERIMETER INSTITUTE FOR THEORETICAL PHYSICS

…Metals, Insulators, Magnets, and Superconductors…

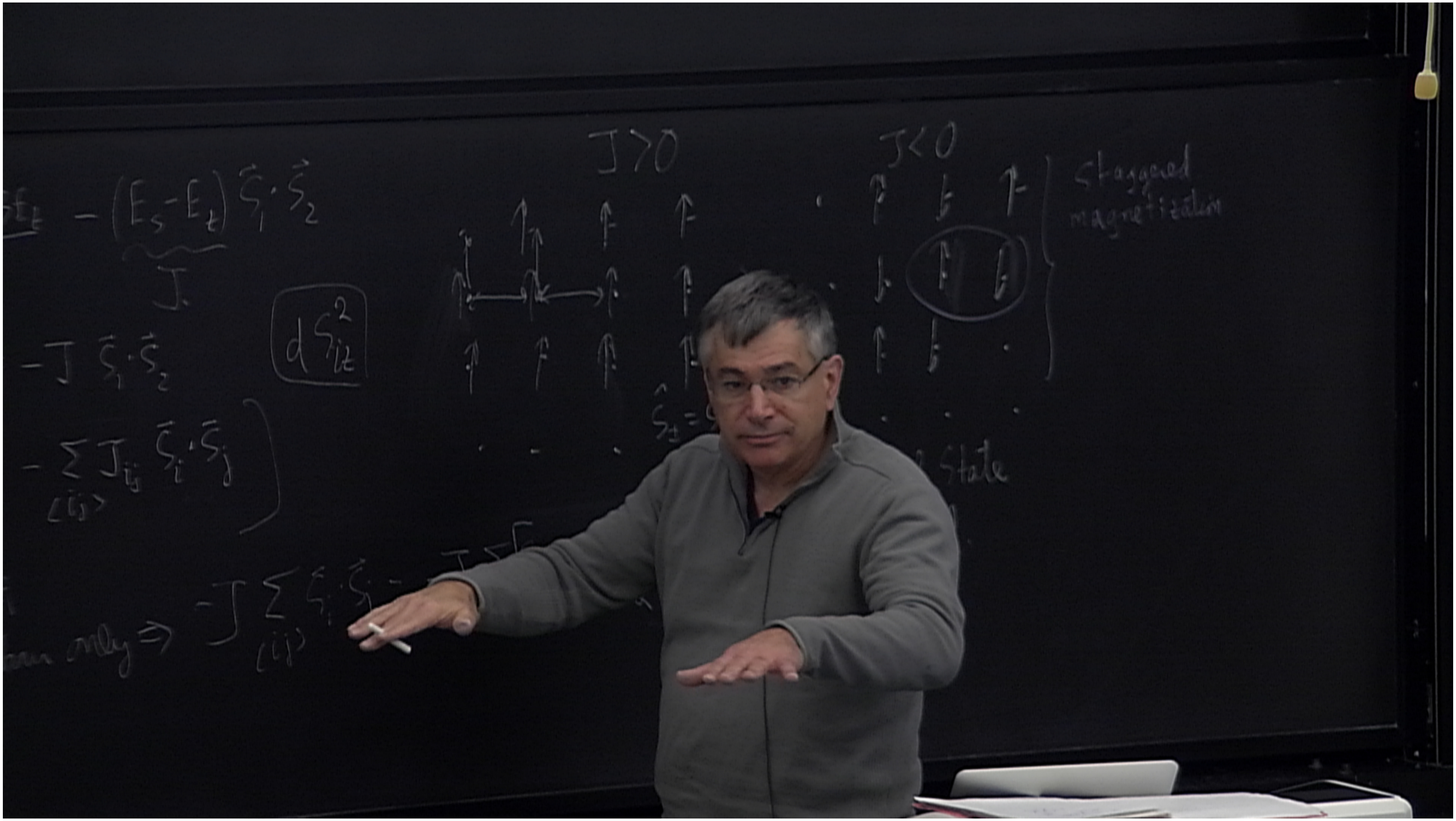
supplementary material to Lecture 10, 11, etc.

F. Marsiglio

fm3@ualberta.ca

UNIVERSITY OF ALBERTA

Theoretical Physics Institute
University of Alberta


$-(E_s - E_t)\,\vec{S}_1 \cdot \vec{S}_2$
J
$-J\,\vec{S}_1 \cdot \vec{S}_2$
$d\,S_{it}^2$
$-\sum_{\langle ij \rangle} J_{ij}\,\vec{S}_i \cdot \vec{S}_j$
J>0
J<0
staggered
magnetization
State
$-J \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j$

History

(1-D Quantum Antiferromagnet)

O. E. Ising (1925)
Ising model (a failure!)

1. H. Bethe, Z. Physik 71, 205 (1931)
   Bethe Ansatz
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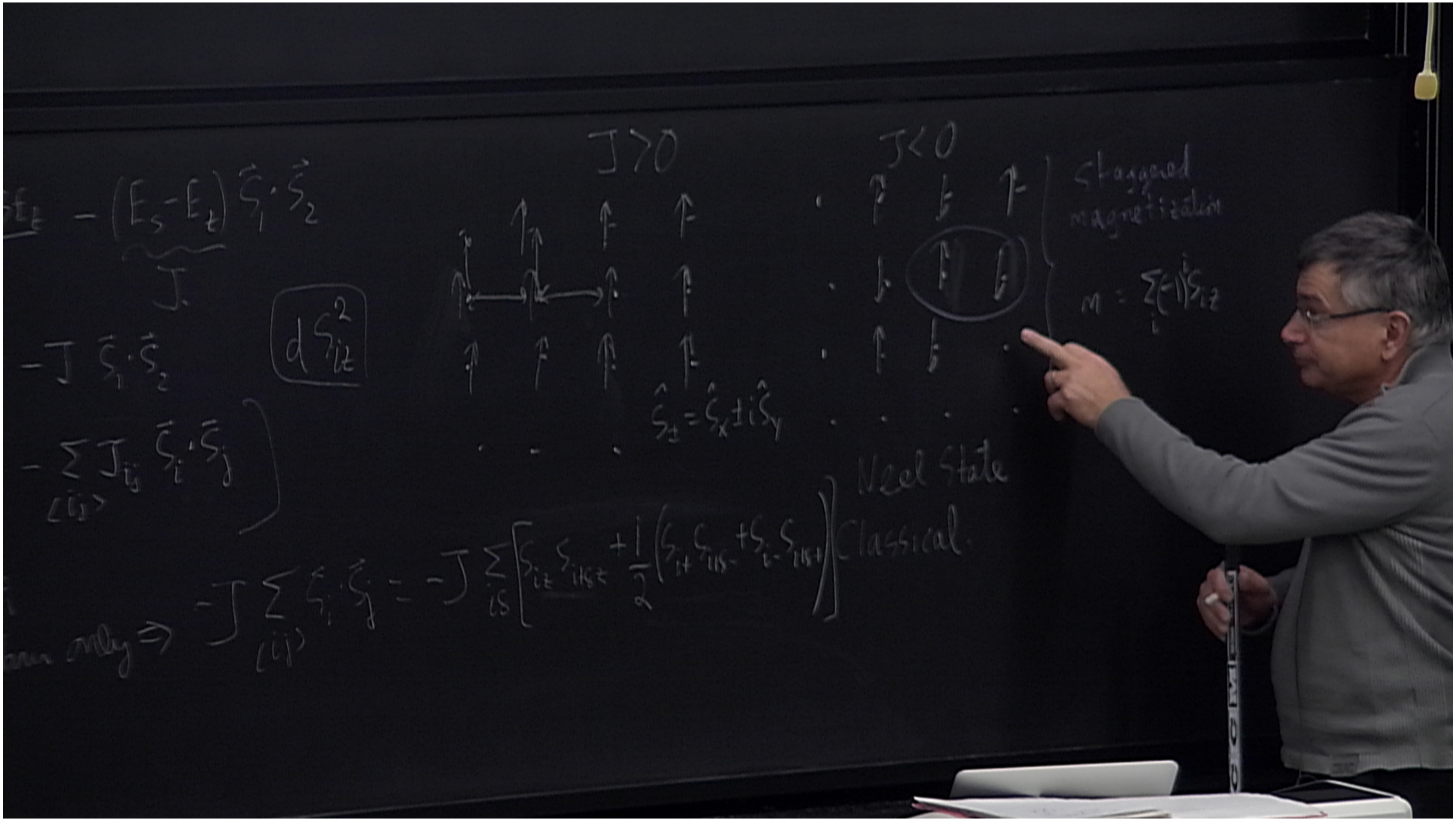
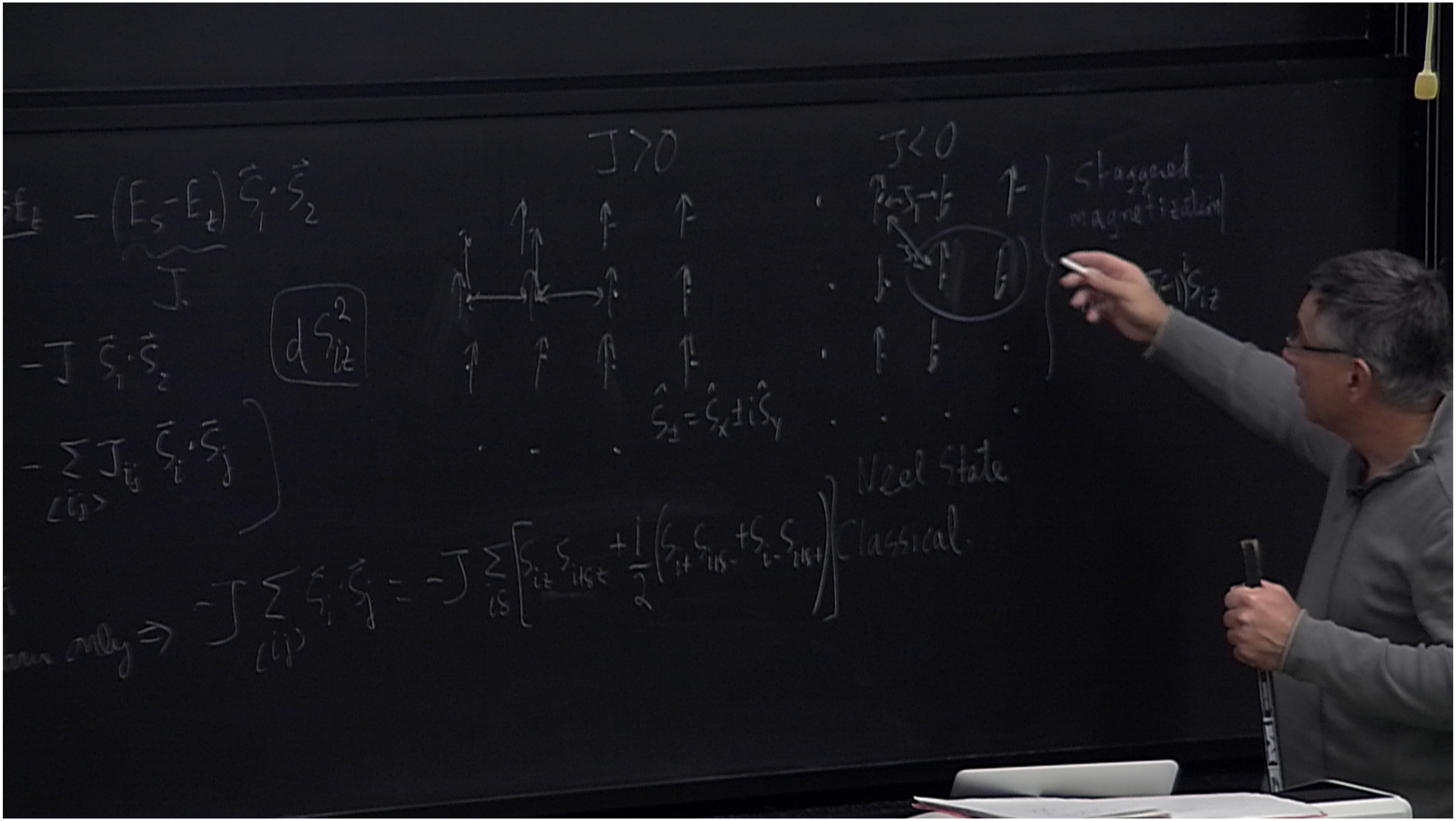
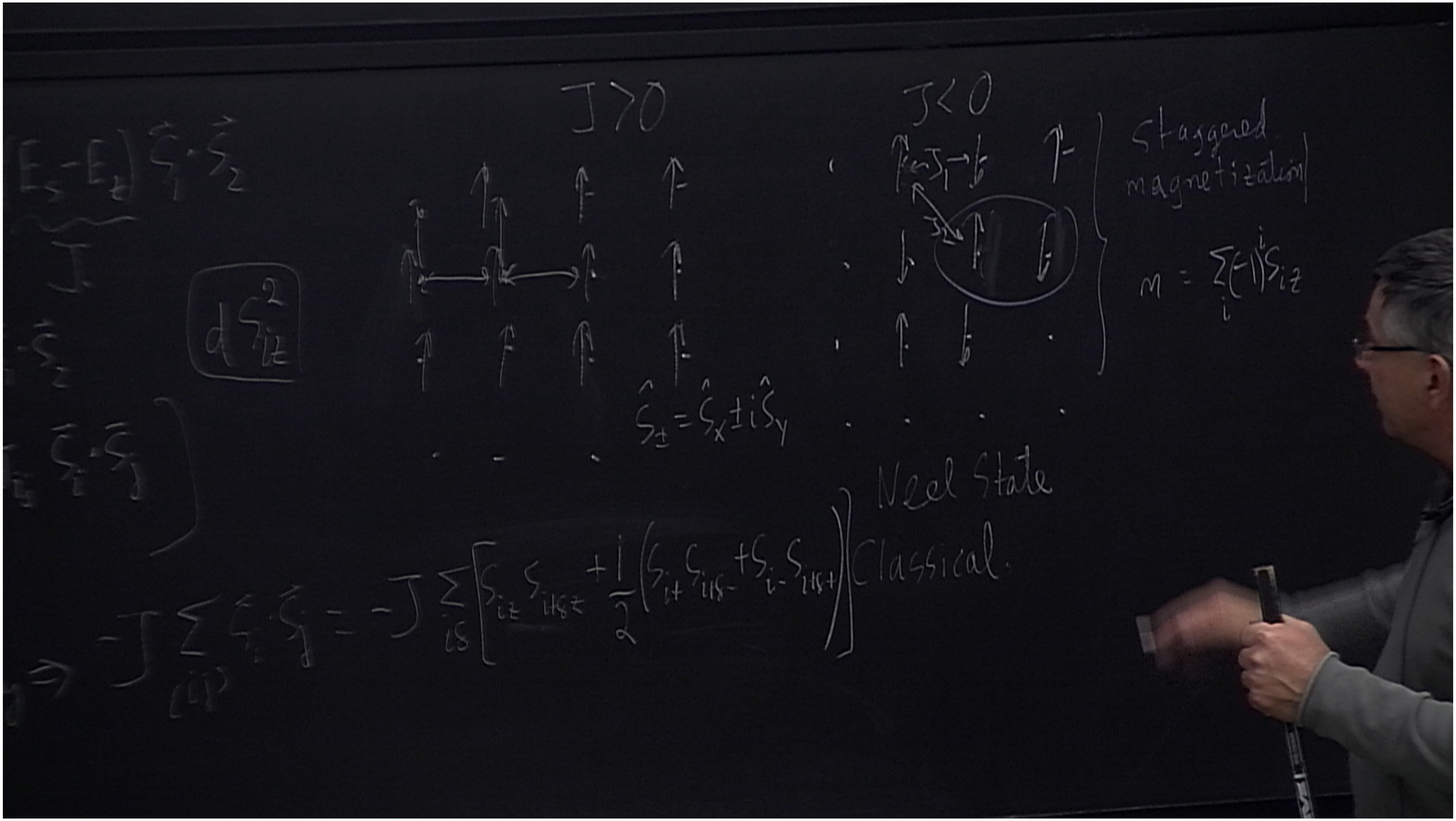
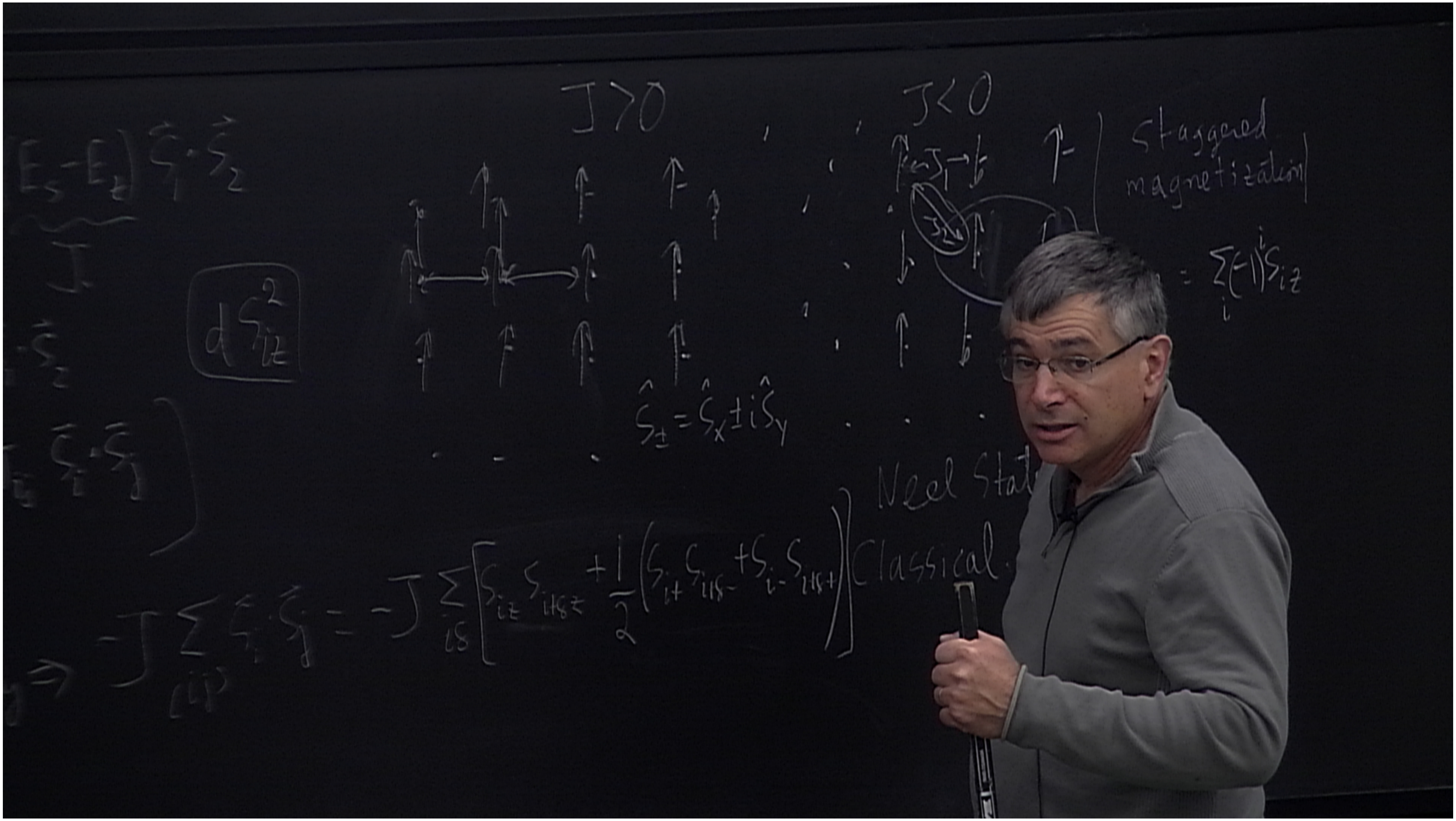
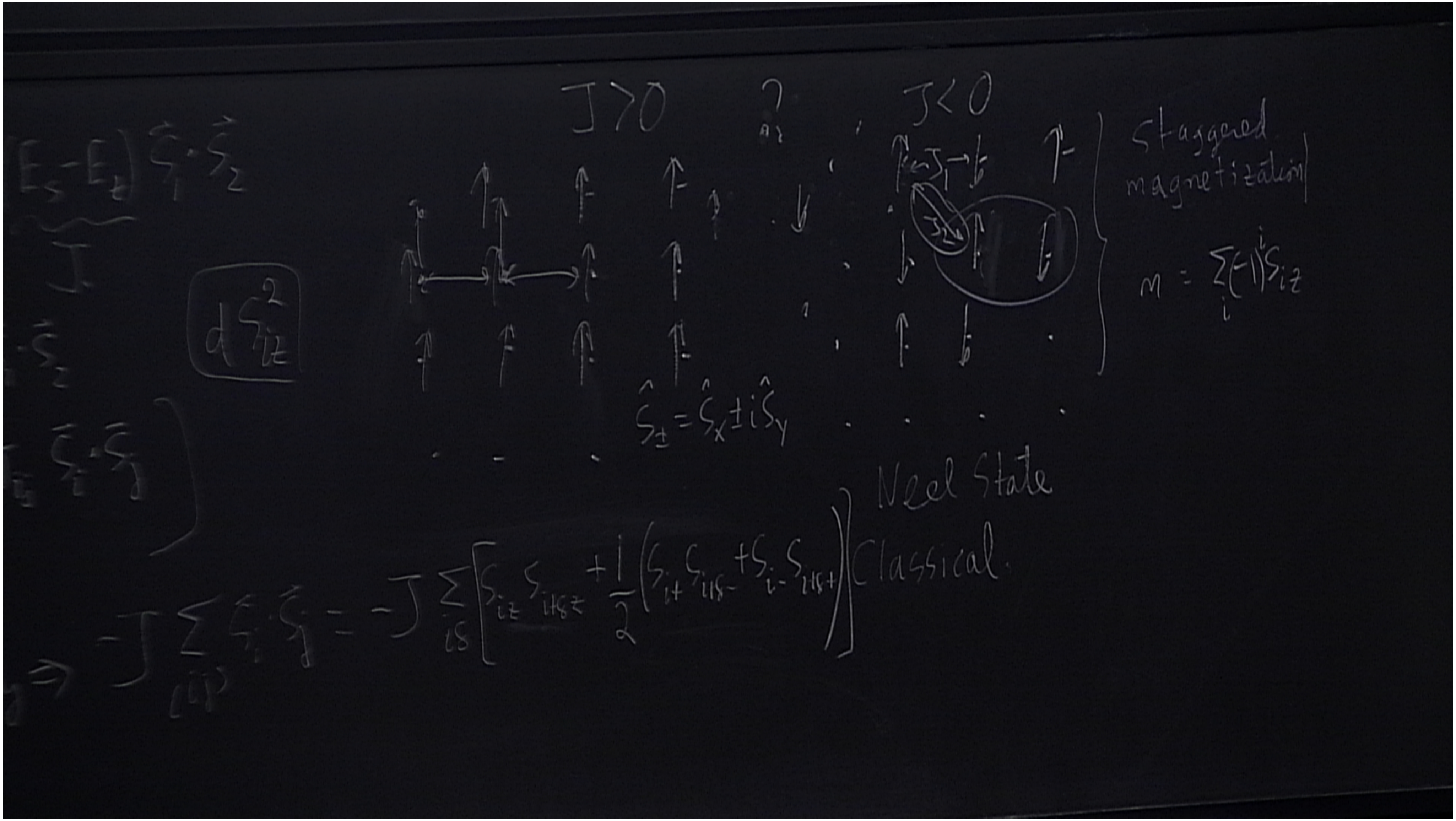
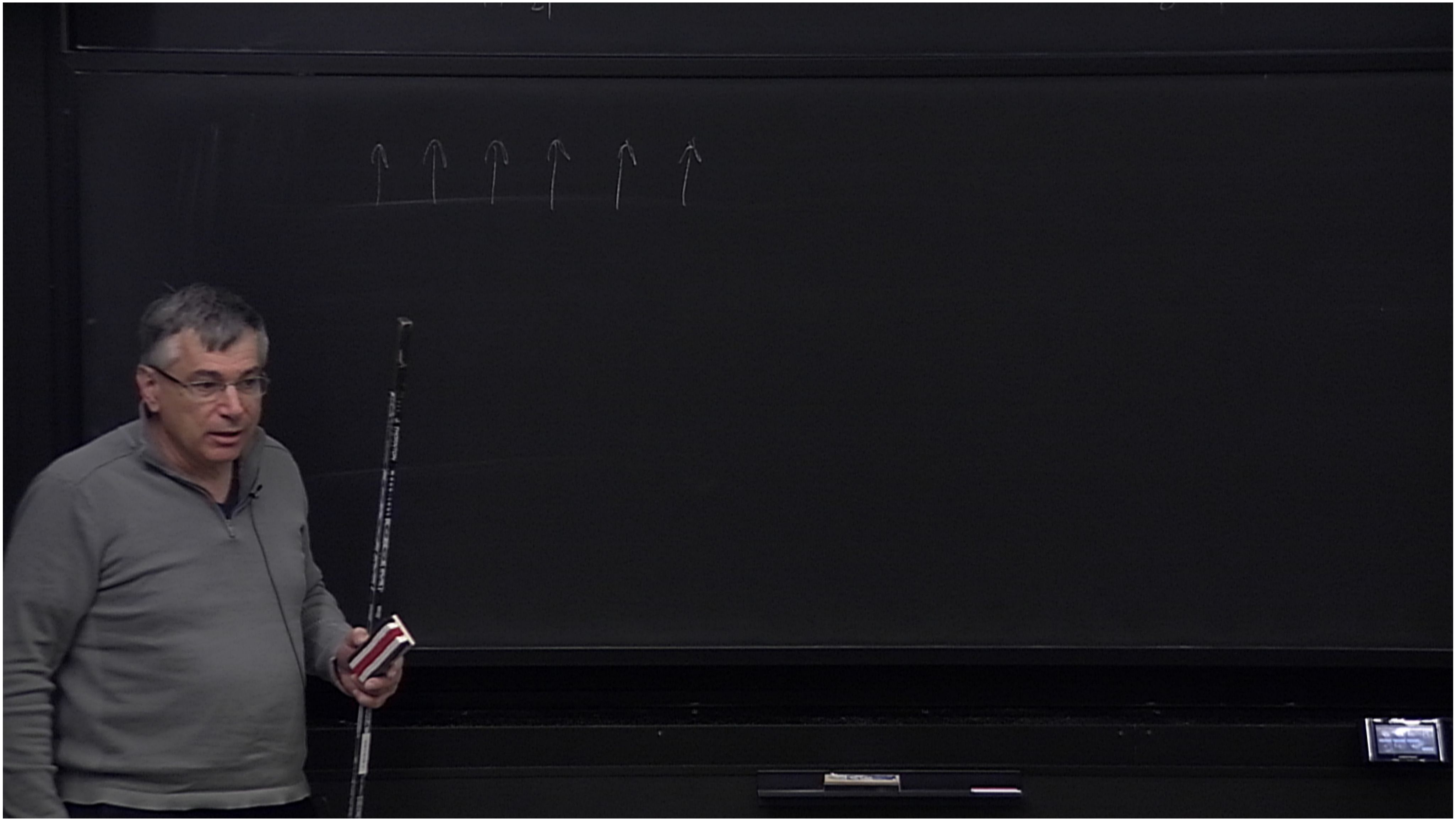

J>0
J<0
Staggered magnetization
Neel State
Classical.

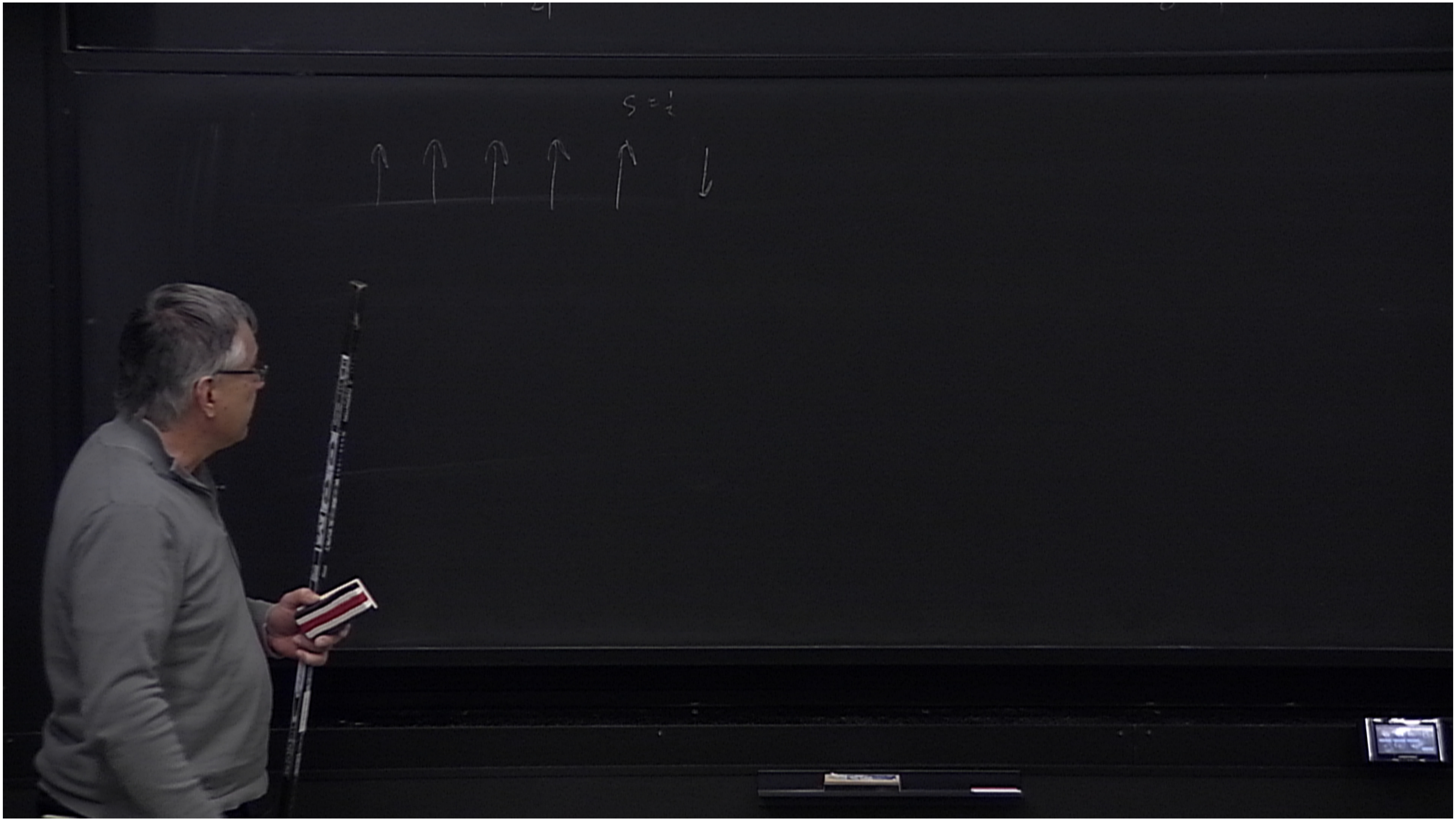

$-(E_s - E_t)\,\vec{S}_1\cdot\vec{S}_2$
$-J\,\vec{S}_1\cdot\vec{S}_2$
$d\,S_{iz}^2$
$-\sum_{\langle ij\rangle} J_{ij}\,\vec{S}_i\cdot\vec{S}_j$
$J>0$
$J<0$
Staggered magnetization
$\hat{S}_\pm = \hat{S}_x \pm i\hat{S}_y$
Neel State
Classical.
$-J\sum_{\langle ij\rangle}\vec{S}_i\cdot\vec{S}_j = -J\sum_{i\delta}\left[S_{iz}S_{i+\delta z} + \frac{1}{2}\left(S_{i+}S_{i+\delta -} + S_{i-}S_{i+\delta +}\right)\right]$

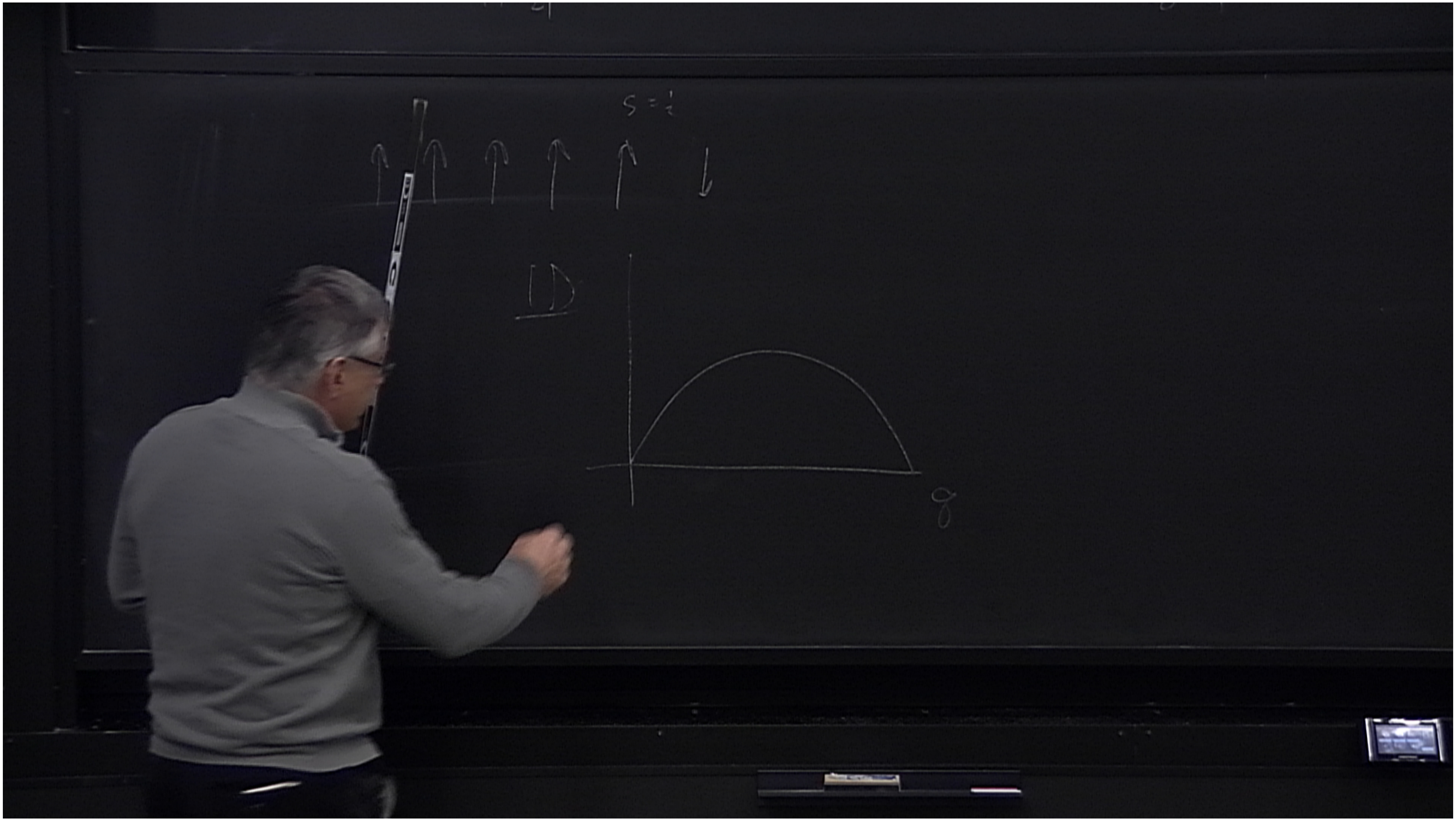

J>0
J<0
Staggered magnetization
Neel State
Classical.


J>0
J<0
Staggered magnetization
Neel State
Classical.


J > 0
J < 0
Staggered magnetization
m = Σ_i (-1)^i S_iz
Ŝ± = Ŝx ± i Ŝy
Neel State
Classical
-J Σ S_i · S_j = -J Σ_iδ [S_iz S_i+δz + 1/2 (S_i+ S_i+δ- + S_i- S_i+δ+)]




S = 1/2

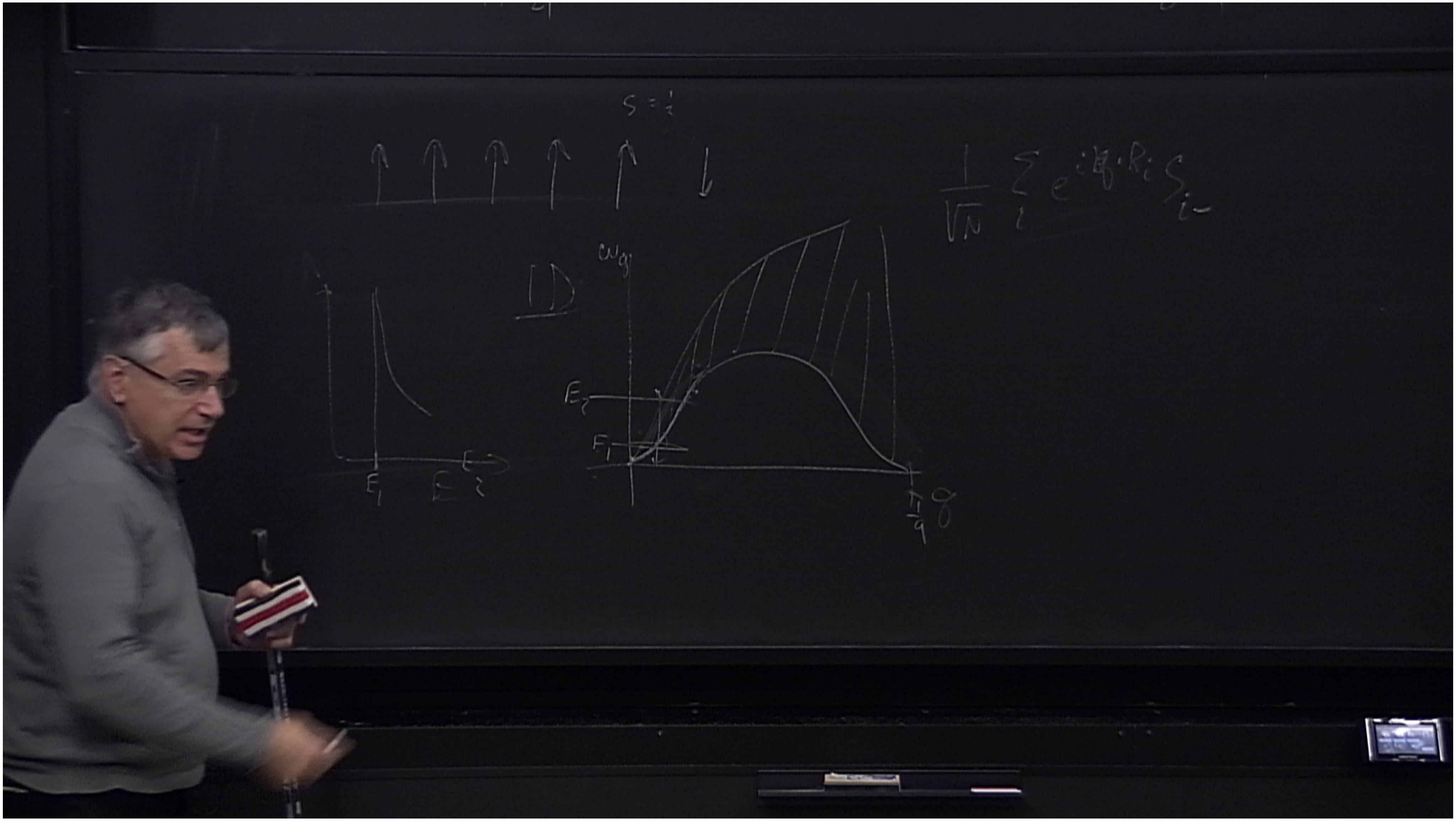


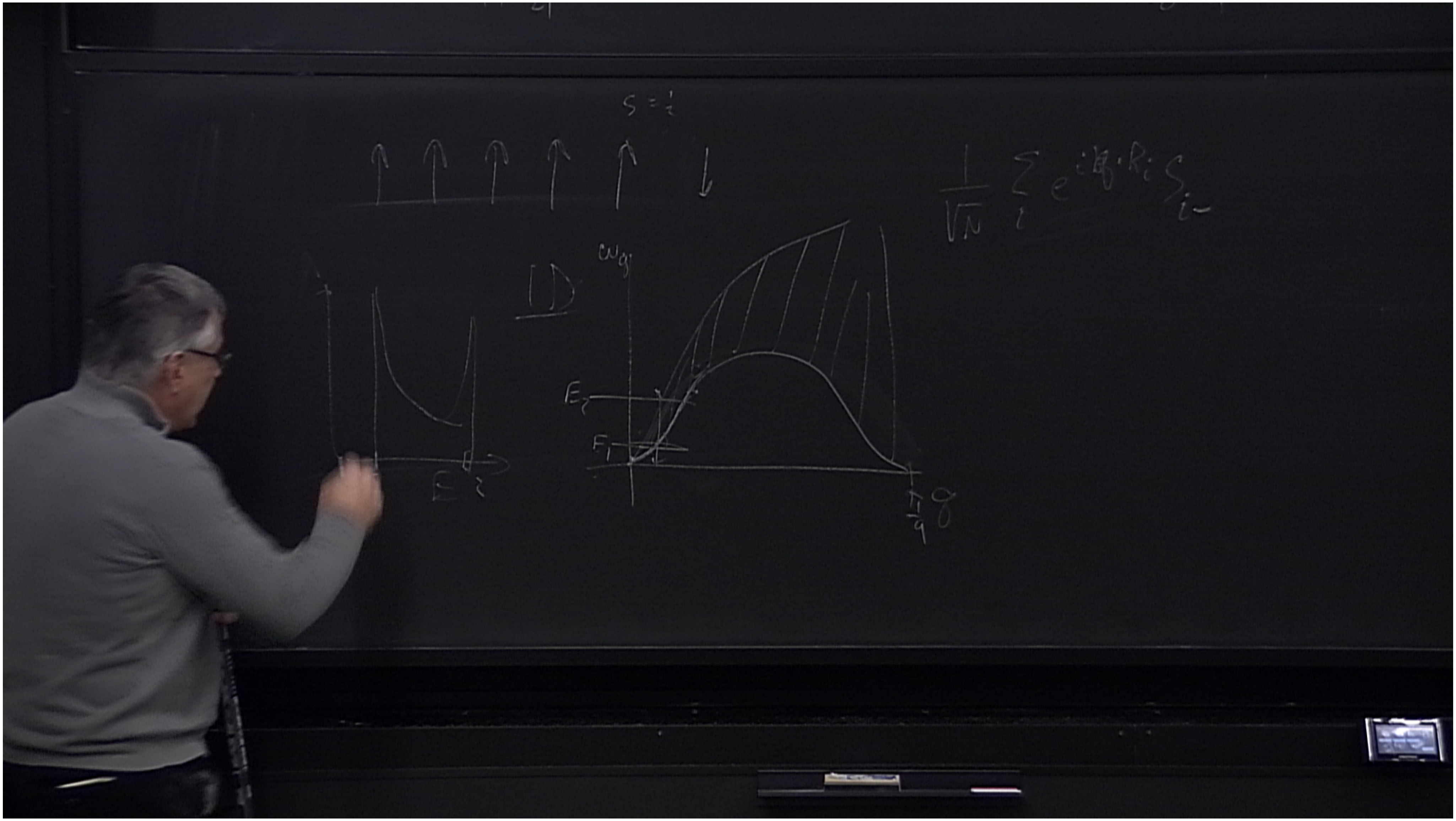
$s = \frac{1}{2}$
1D
q

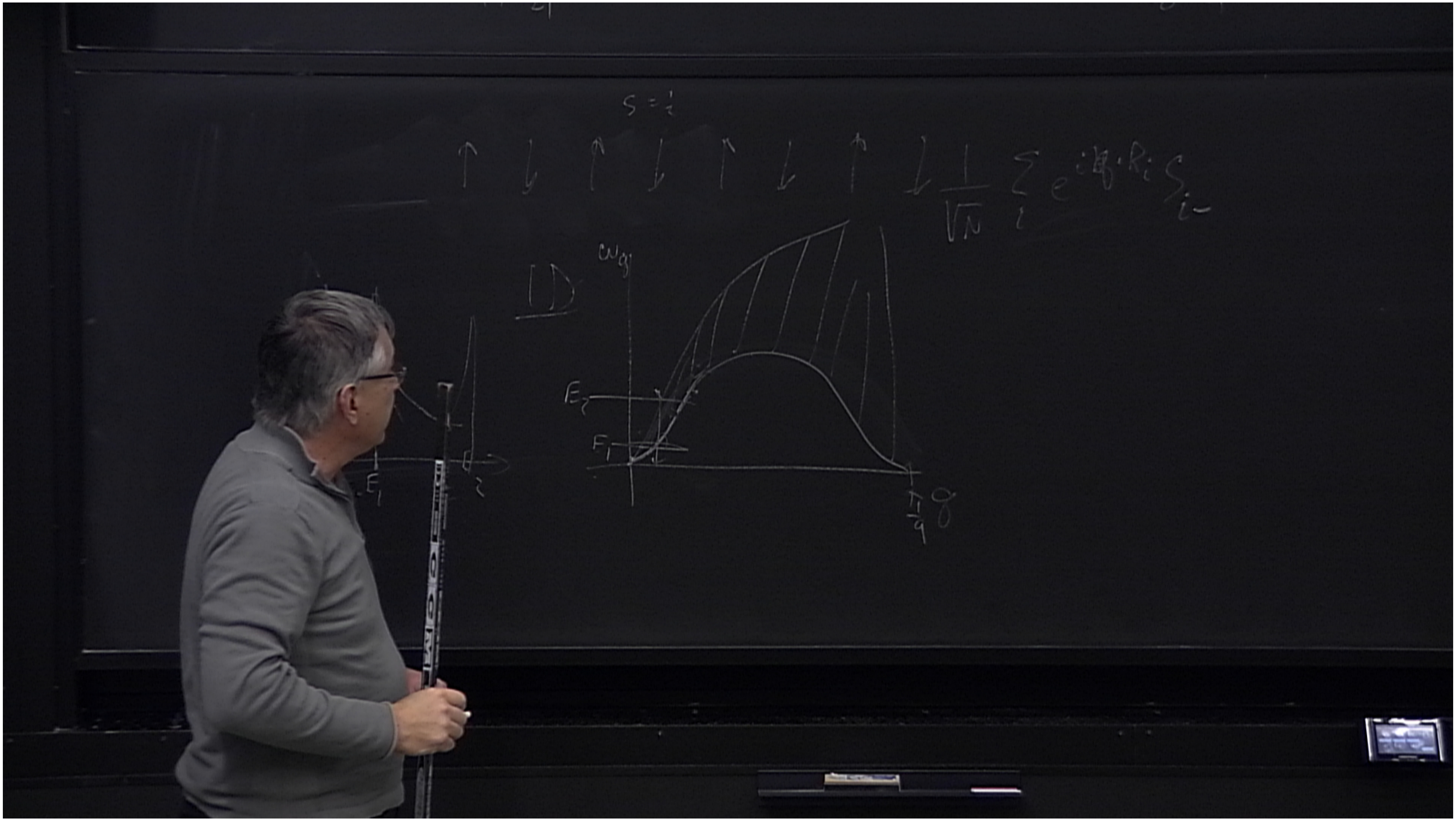
s = ½
1D
ω_q
π/a
q

s = 1/2
1D
ω_q
π/a
q
1/√N Σ_i e^{iq·R_i} S_i^-

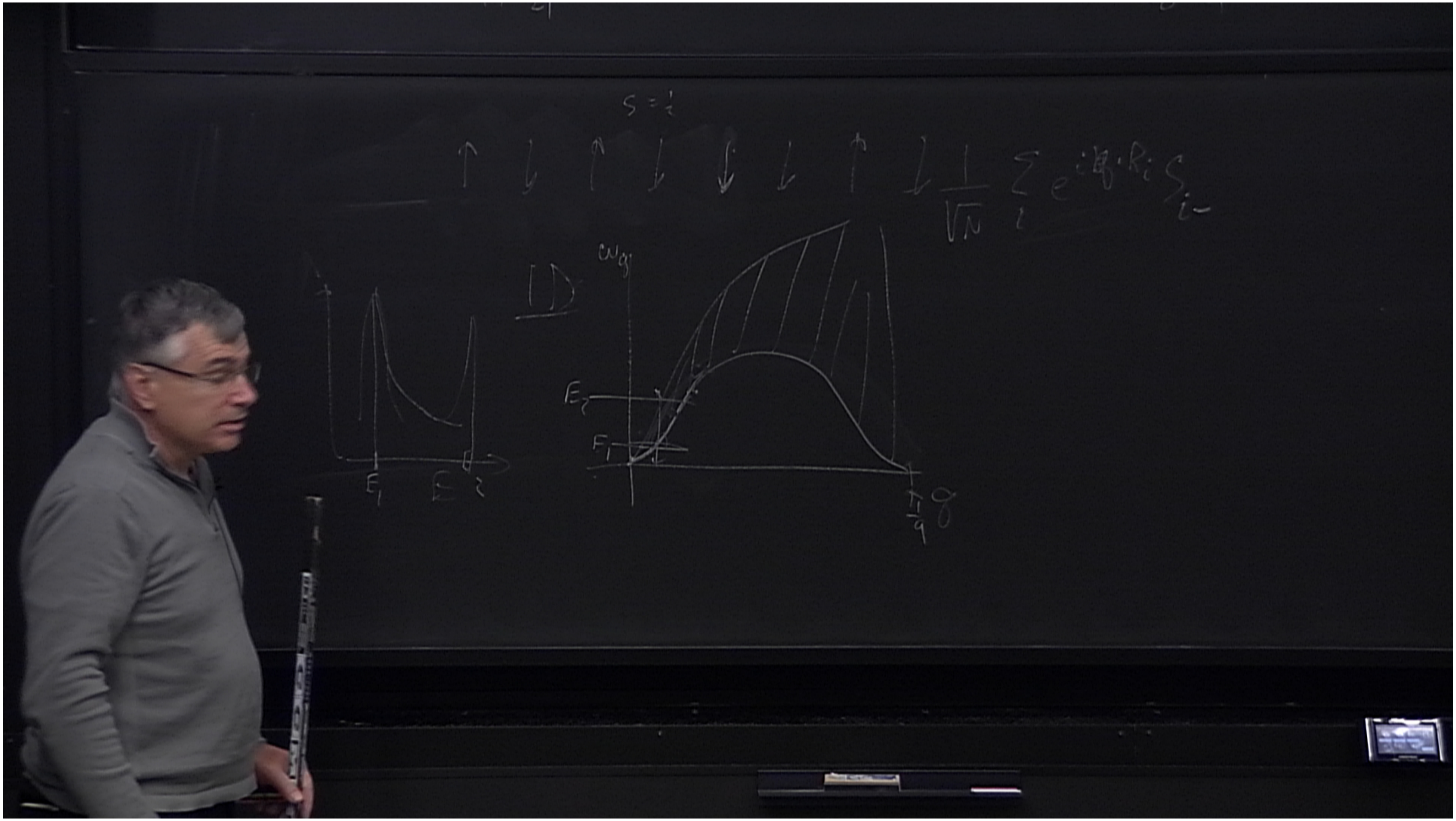

S = 1/2
1D
ω_q
q
π/a
1/√N Σ_i e^{iq·R_i} S_i^-

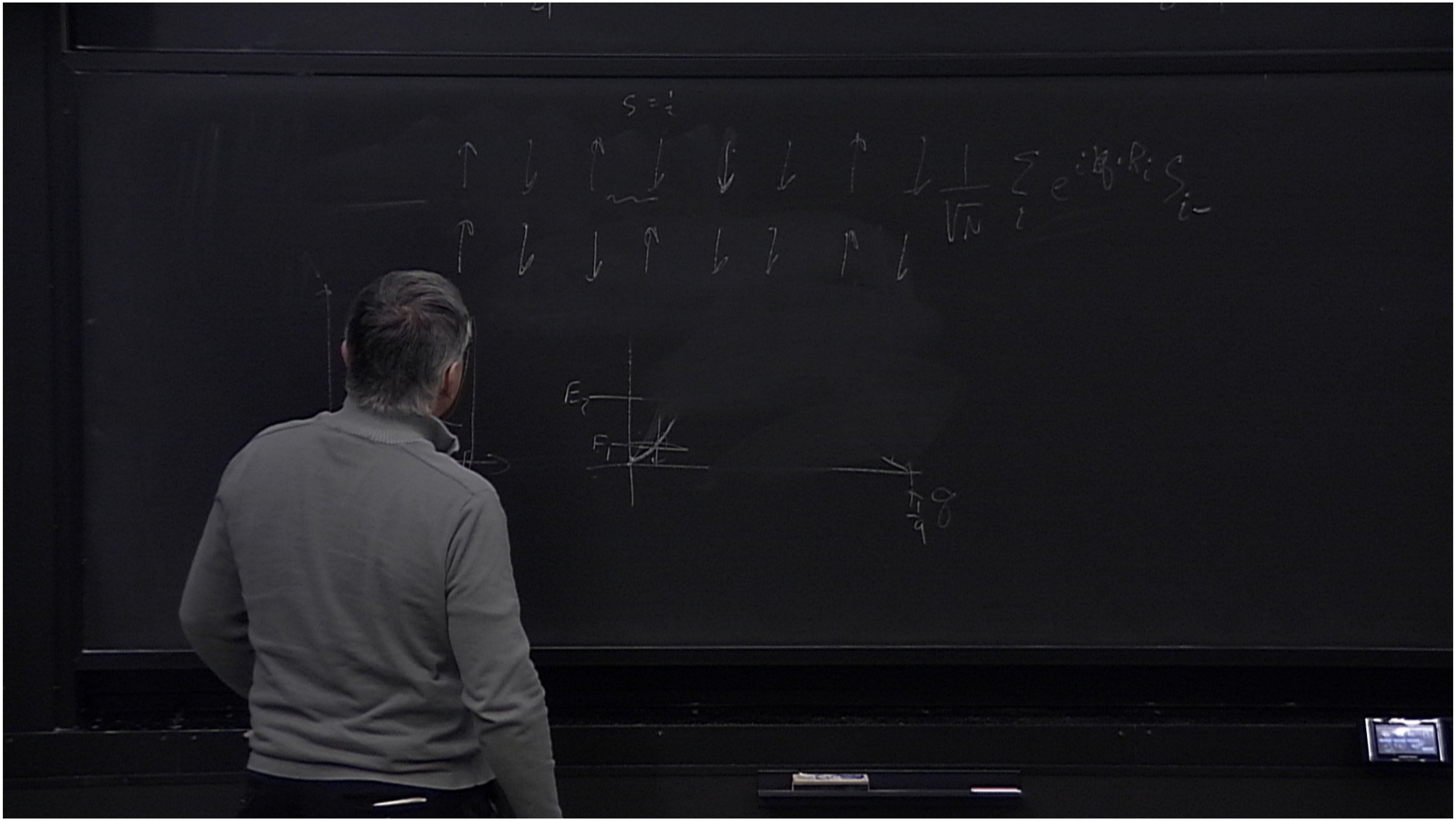


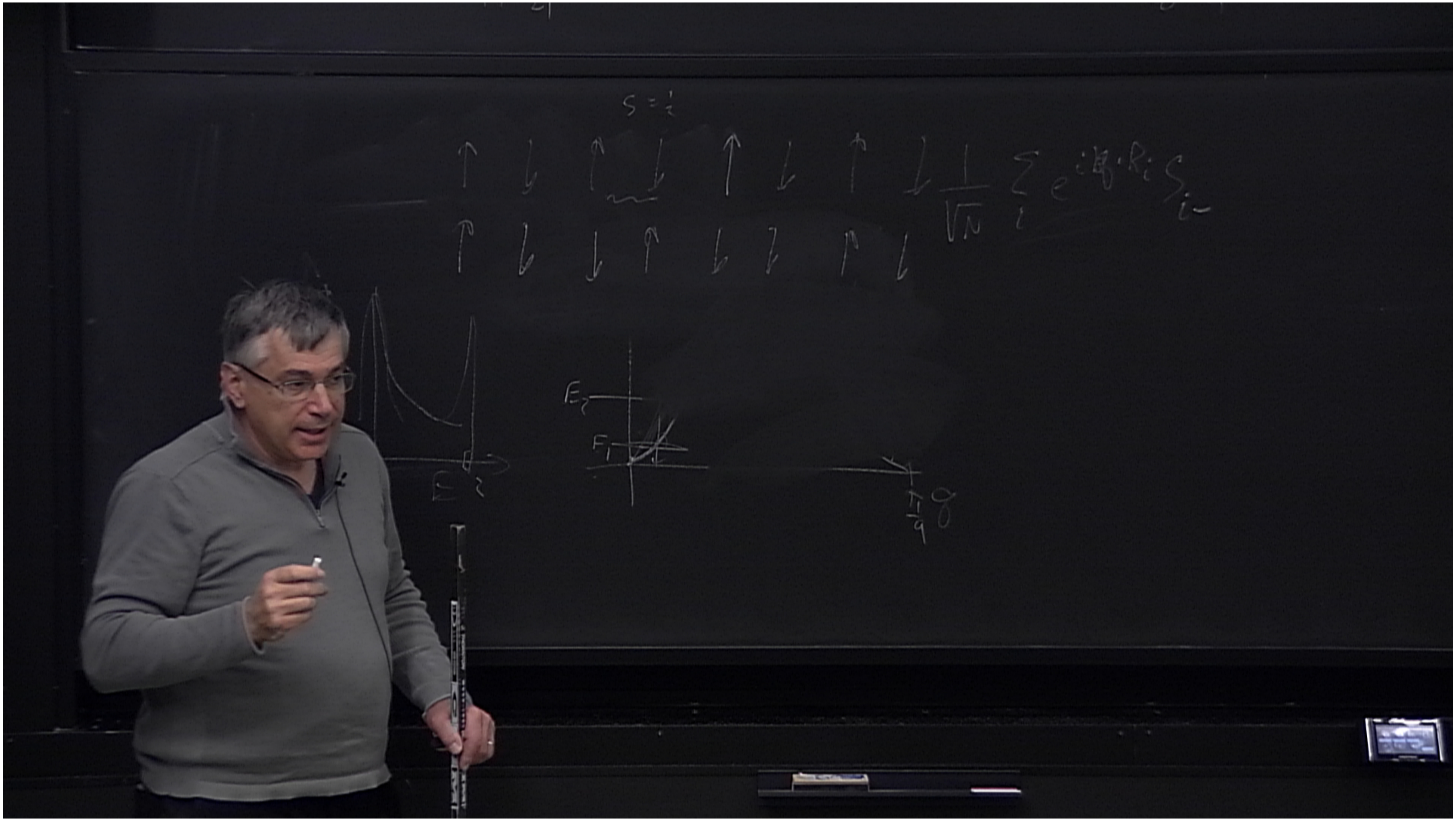

s = 1/2
1D
ω_q
E_2
E_1
q
$\frac{1}{\sqrt{N}} \sum_i e^{i q \cdot R_i} S_{i-}$



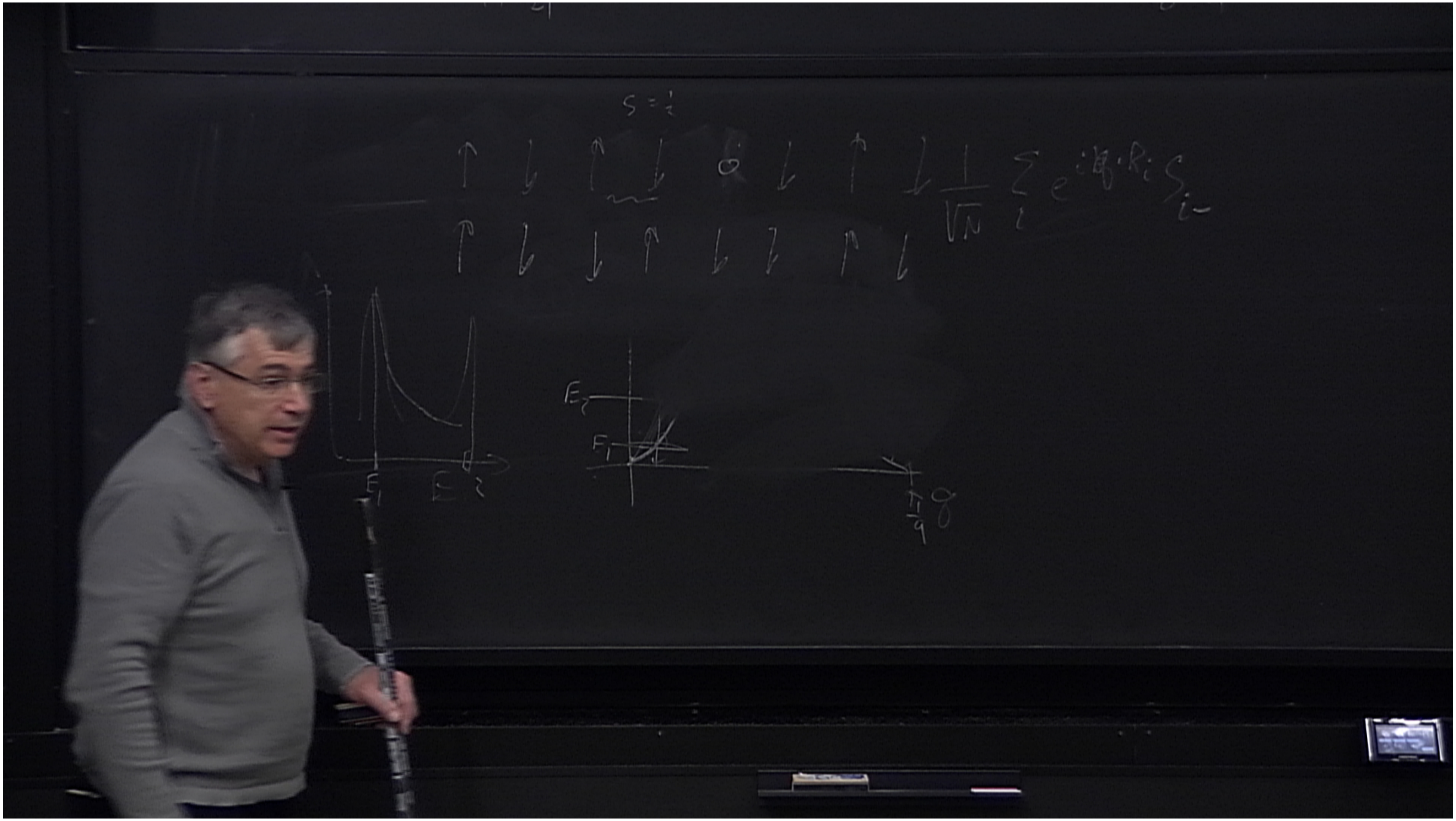
$S = \frac{1}{2}$
$\frac{1}{\sqrt{N}} \sum_i e^{i q \cdot R_i} S_{i-}$
1D
ω_q
E_2
E_1
q

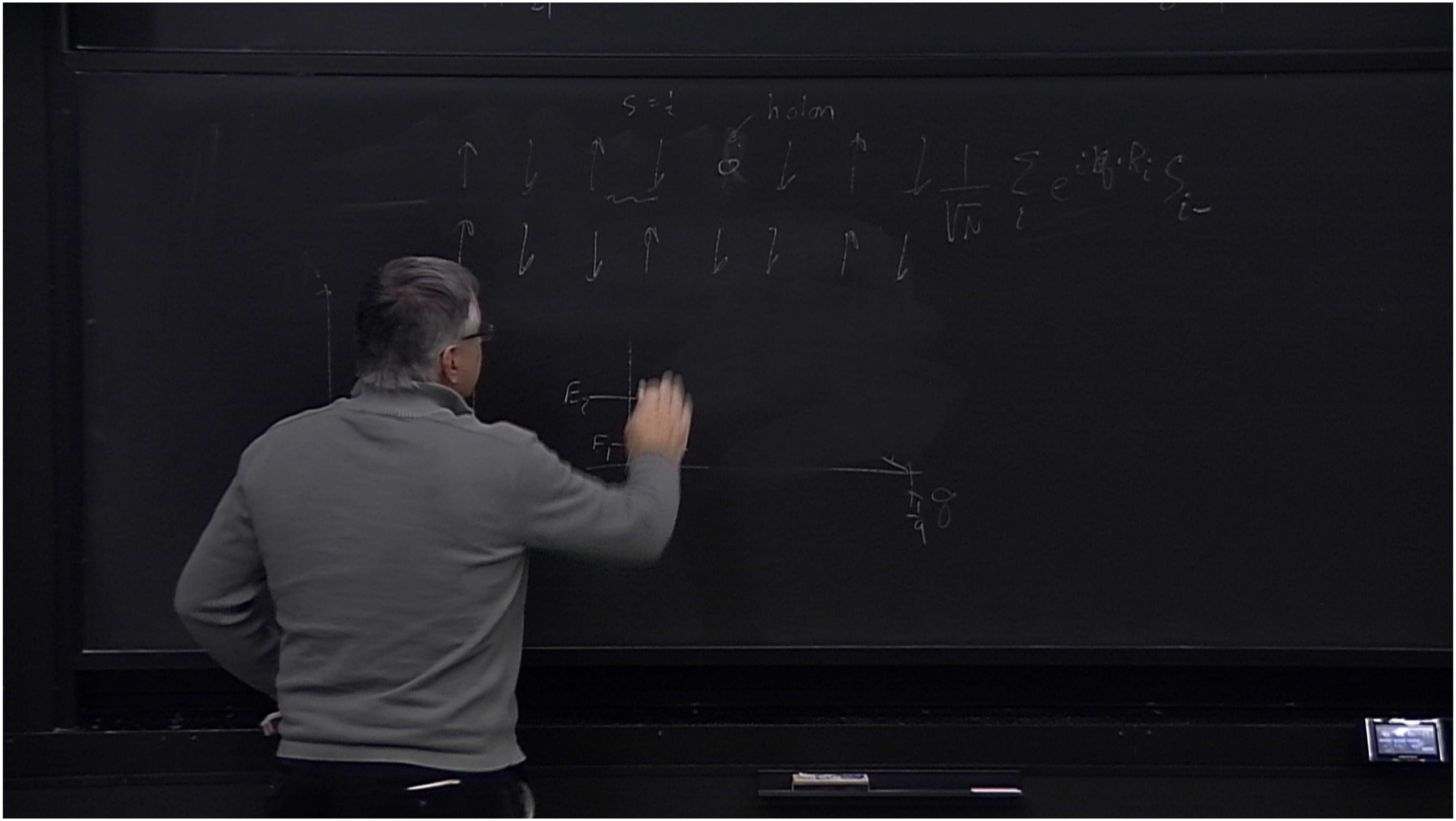

1D
E2
E1
q



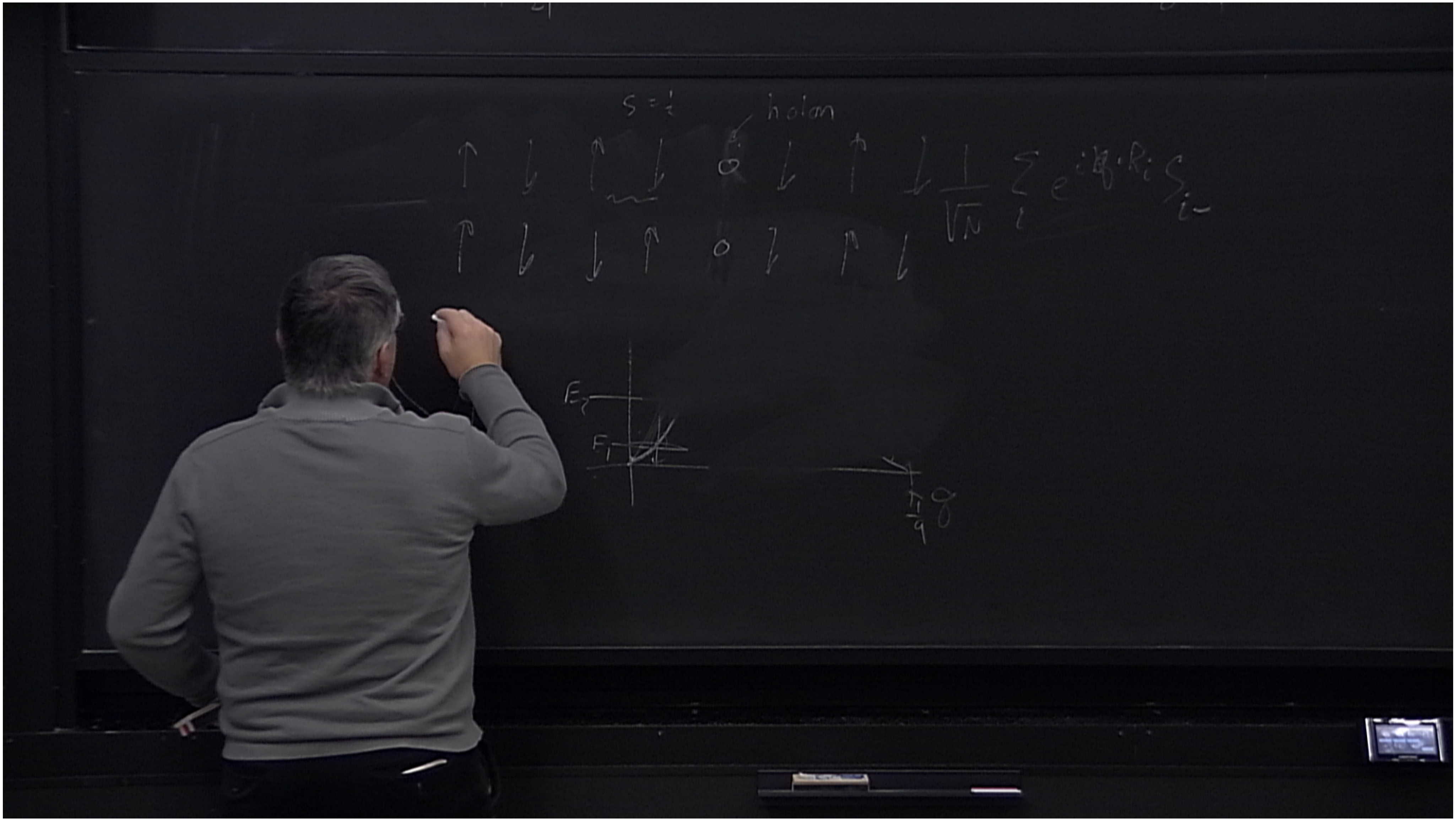


S = ½
E₂
E₁

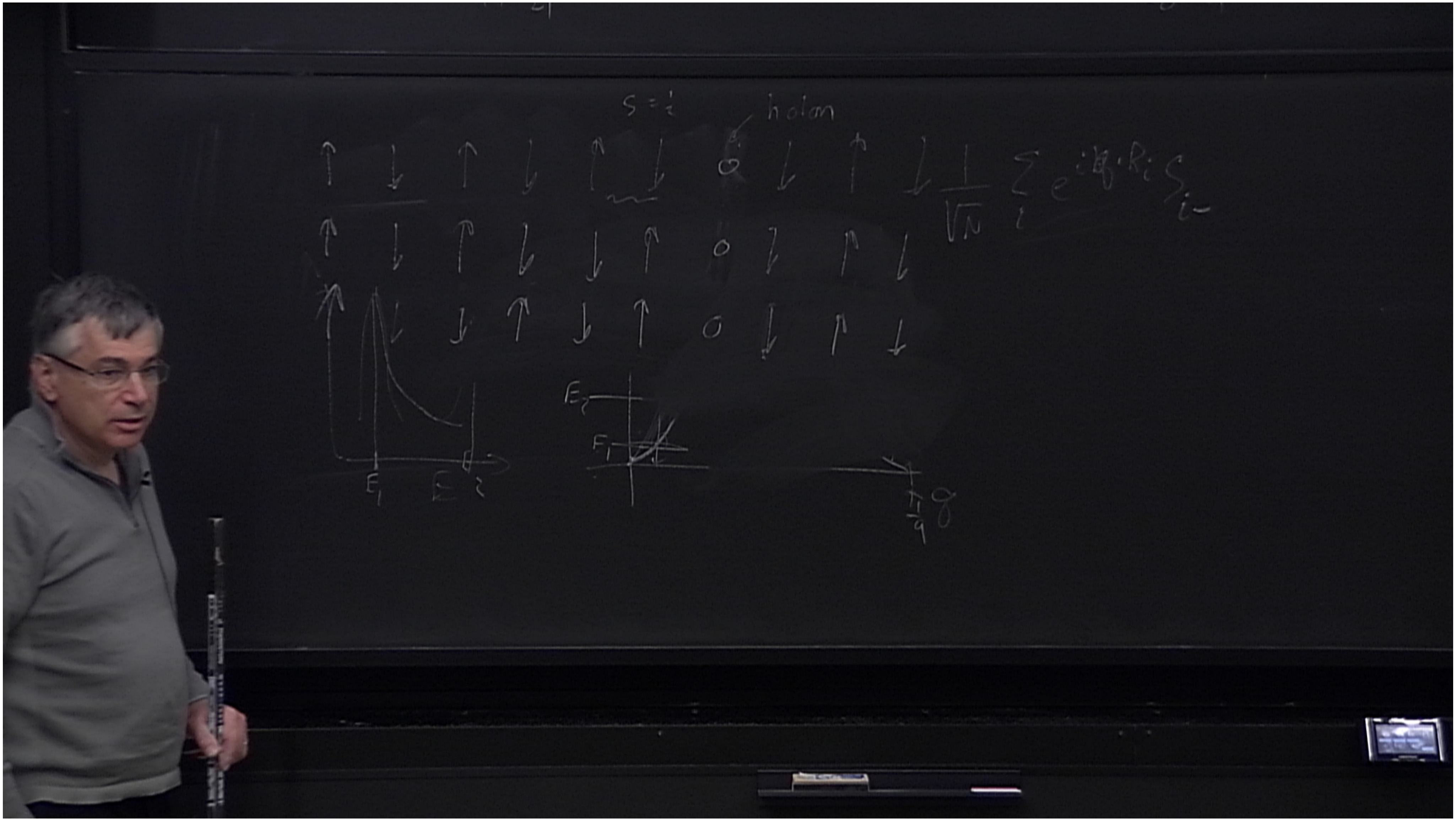


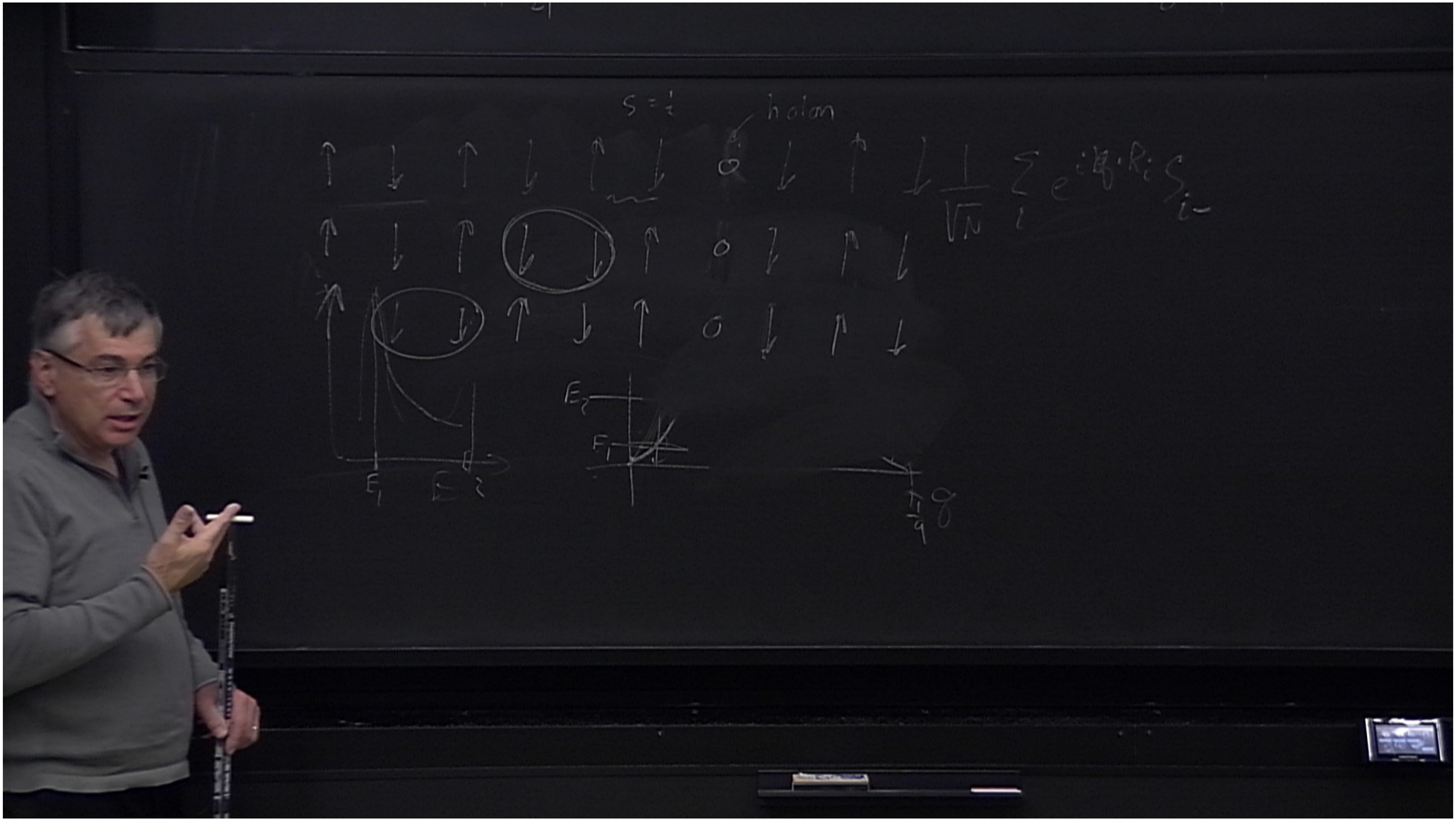


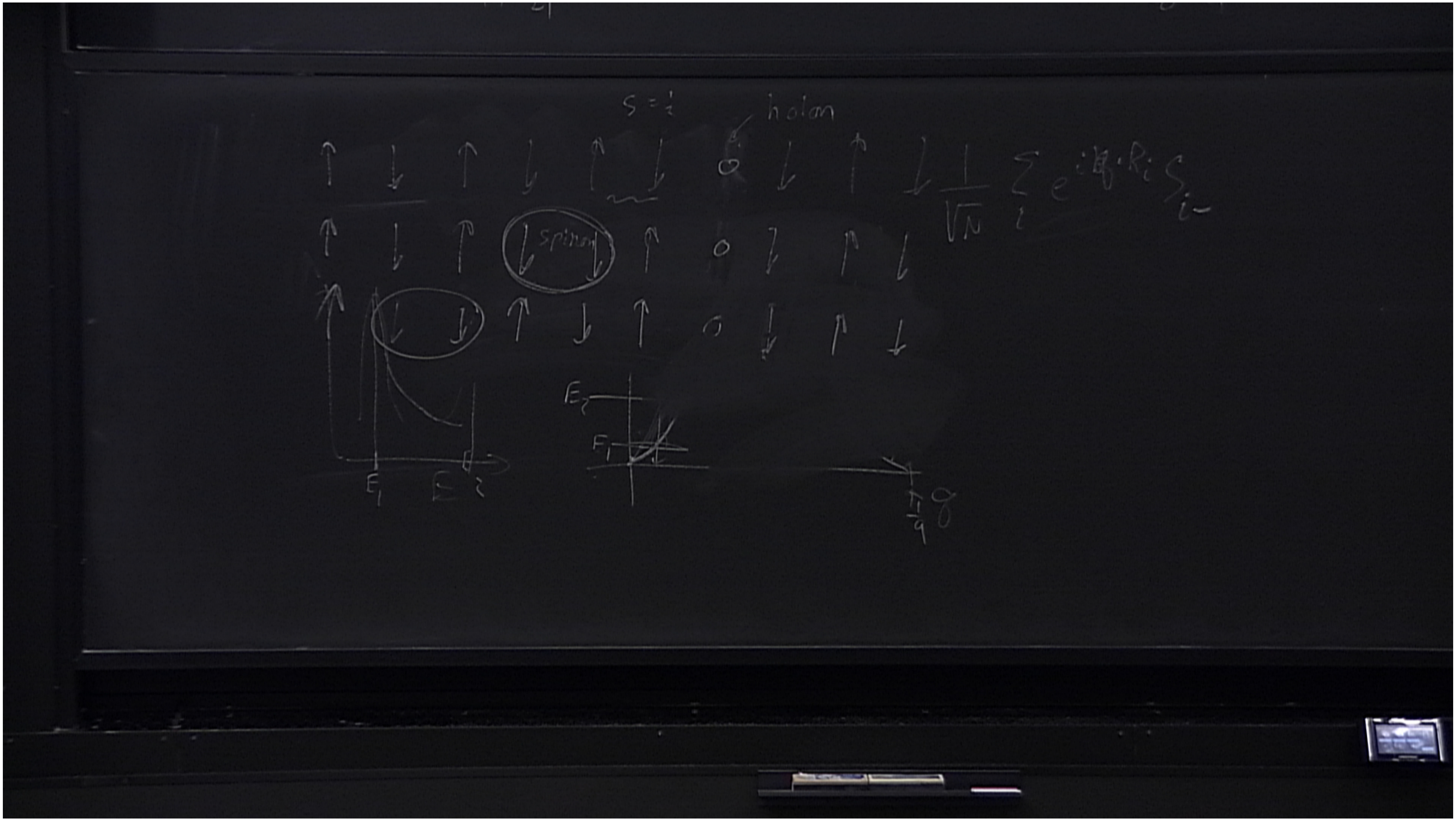
s = ½
holon



s = 1/2
holon
$\frac{1}{\sqrt{N}} \sum_i e^{i q \cdot R_i} S_i^-$
E_2
E_1
q


S = 1/2
holon
$\frac{1}{\sqrt{N}} \sum_i e^{i q \cdot R_i} S_{i-}$
E_2
E_1
q


S = 1/2
holon


S = ½
holon
spinon

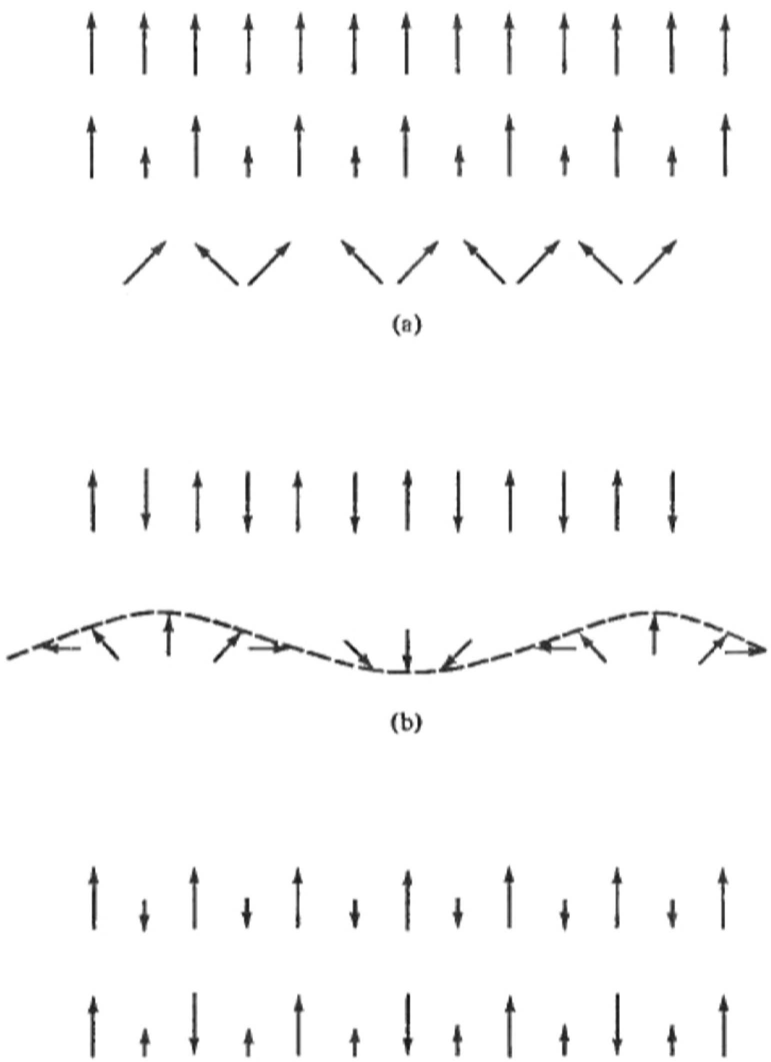


Figure 33.2
Linear arrays of spins illustrating possible (a) ferromagnetic, (b) antiferromagnetic, and (c) ferrimagnetic orderings.

Fig. 33.2 from Ashcroft and Mermin

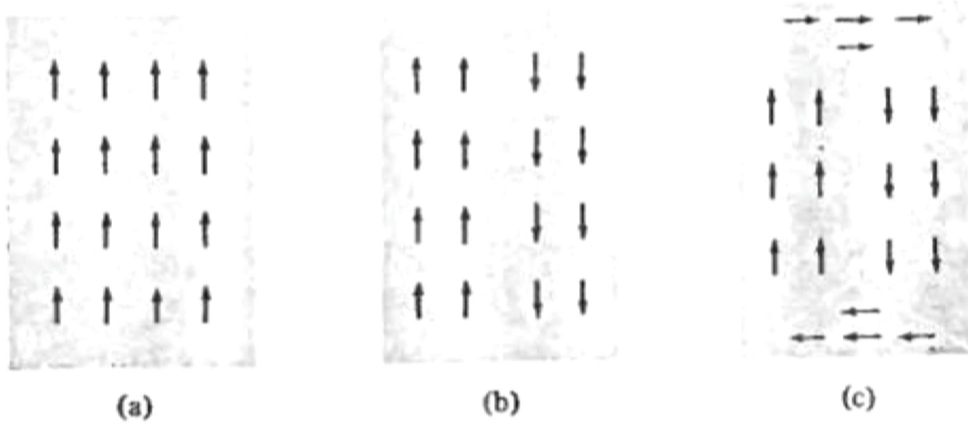
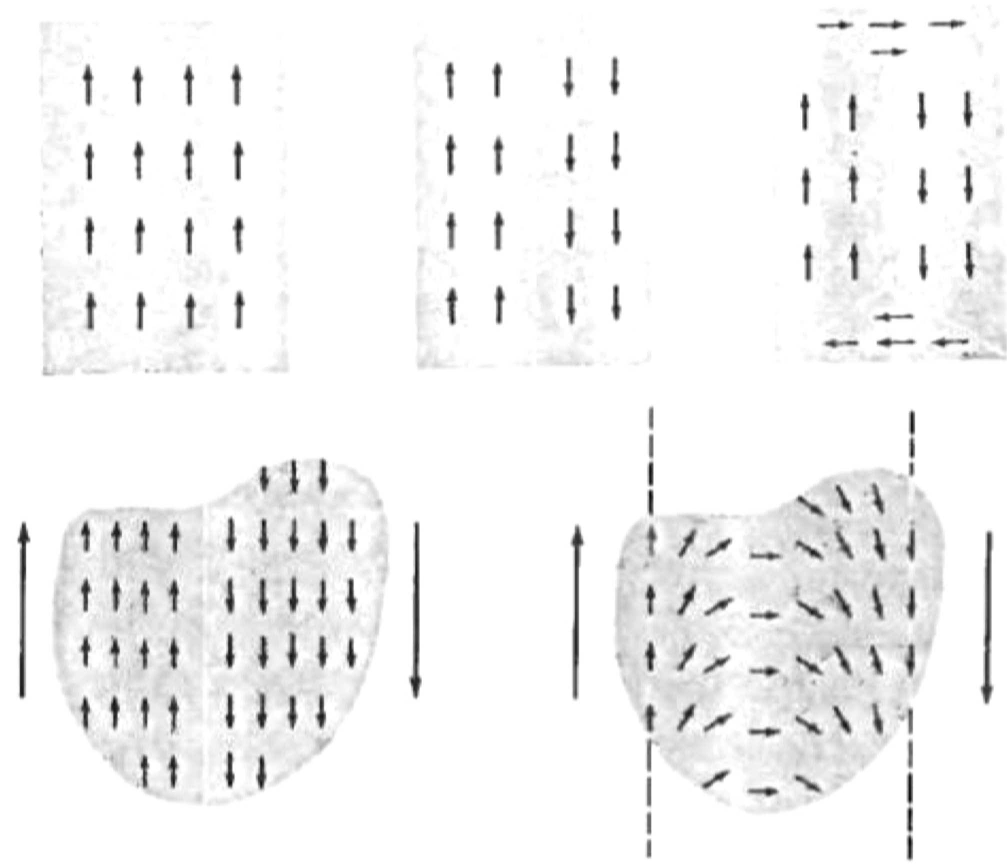


Figure 33.12
A ferromagnetically ordered solid can reduce its magnetic dipolar energy by breaking up into a complex structure of domains. Thus the single-domain structure (a) has a much higher dipolar energy than the structure (b) consisting of two domains. (To see this think of the two halves of (b) as being two bar magnets. To form the single domain (a), one of the magnets in (b) must be reversed, thereby changing a configuration in which opposite poles are near one another to one in which like poles are near one another.) The two-domain structure (b) can lower its dipolar energy still further by producing the additional domains shown in (c).

Figs. 33.12-13 from Ashcroft and Mermin



(a) (b)

Figure 33.13
Detailed view of a portion of domain wall showing (a) an abrupt boundary and (b) a gradual boundary. The latter type is less costly in exchange energy.

Figs. 33.12-13 from Ashcroft and Mermin

Table 33.1
SELECTED FERROMAGNETS, WITH CRITICAL TEMPERATURES T_c AND SATURATION MAGNETIZATION M_0

MATERIAL	T_c (K)	M_0 (gauss)[a]
Fe	1043	1752
Co	1388	1446
Ni	627	510
Gd	293	1980
Dy	85	3000
$CrBr_3$	37	270
Au_2MnAl	200	323
Cu_2MnAl	630	726
Cu_2MnIn	500	613
EuO	77	1910
EuS	16.5	1184
MnAs	318	870
MnBi	670	675
$GdCl_3$	2.2	550

[a] At $T = 0$(K).
Source: F. Keffer, *Handbuch der Physik*, vol. 18, pt. 2, Springer, New York, 1966; P. Heller, *Rep. Progr. Phys.*, **30**, (pt. II), 731 (1967).

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Source: F. Keffer, *Handbuch der Physik*, vol. 18, pt. 2, Springer, New York, 1966; P. Heller, *Rep. Progr. Phys.*, **30**, (pt. II), 731 (1967).

Table 33.2

SELECTED ANTIFERROMAGNETS, WITH CRITICAL TEMPERATURES T_c

MATERIAL	T_c (K)	MATERIAL	T_c (K)
MnO	122	$KCoF_3$	125
FeO	198	MnF_2	67.34
CoO	291	FeF_2	78.4
NiO	600	CoF_2	37.7
$RbMnF_3$	54.5	$MnCl_2$	2
$KFeF_3$	115	VS	1040
$KMnF_3$	88.3	Cr	311

Source: F. Keffer, *Handbuch der Physik*, vol. 18, pt. 2, Springer, New York, 1966.

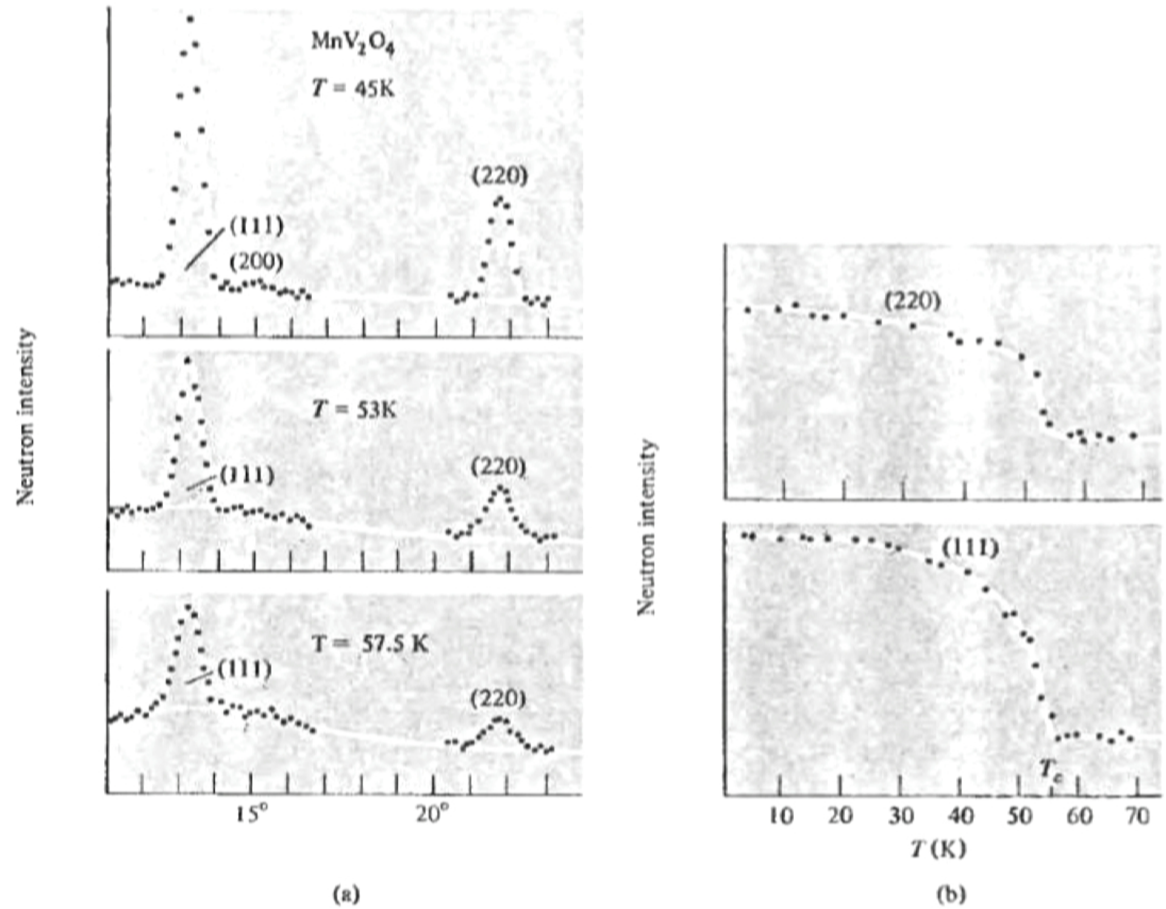

Figure 33.3
(a) Neutron Bragg peaks in manganese vanadite (MnV_2O_4), an antiferromagnet with $T_c = 56$ K. The intensity of the peaks decreases as T rises to T_c. (b) Intensity of the (220) and (111) peaks vs. temperature. Above T_c the temperature dependence is very slight. (From R. Plumier, *Proceedings of the International Conference on Magnetism*, Nottingham, 1964.)

Fig. 33.3 from Ashcroft and Mermin

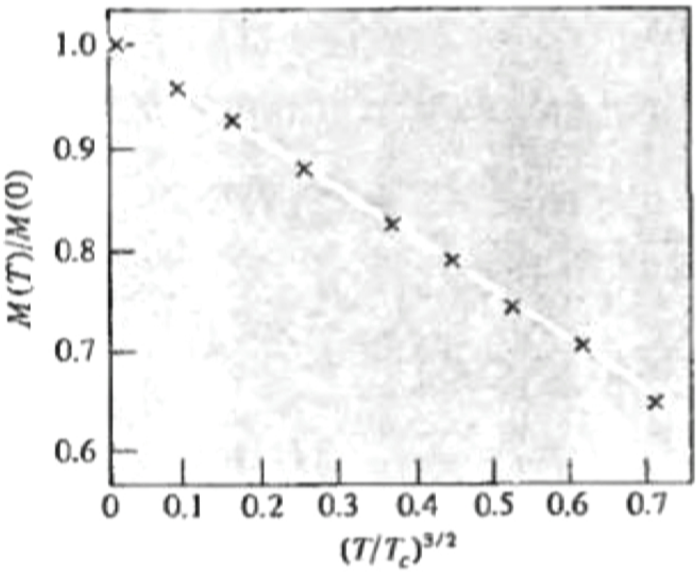

Figure 33.8

The ratio of the spontaneous magnetization at temperature T to its saturation ($T = 0$) value as a function of $(T/T_c)^{3/2}$ for ferromagnetic gadolinium ($T_c = 293$ K). The linearity of the curve accords with the Bloch $T^{3/2}$ law. (After F. Holtzberg et al., *J. Appl. Phys.* **35**, 1033 (1964).)

Fig. 33.8 from Ashcroft and Mermin