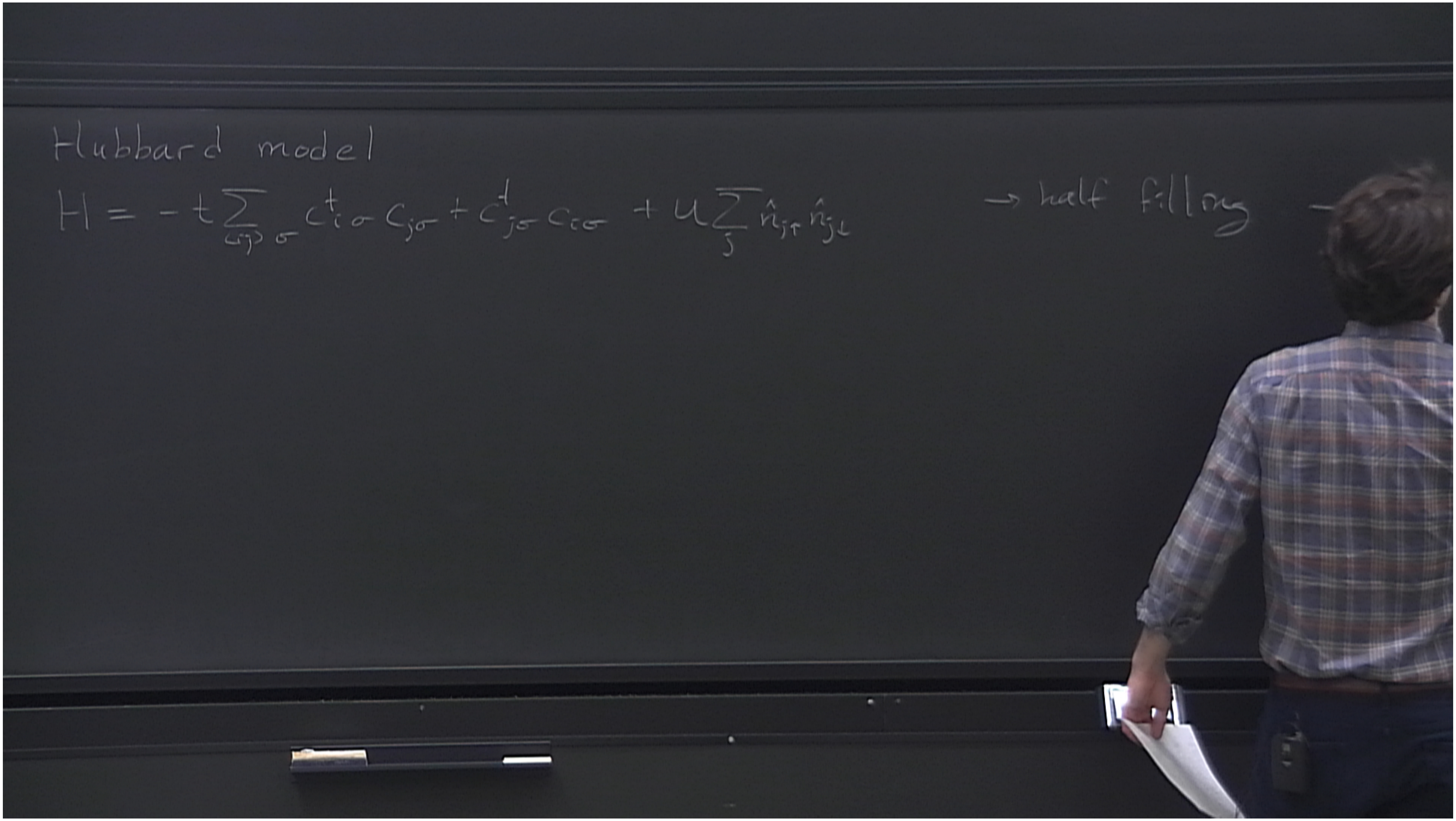
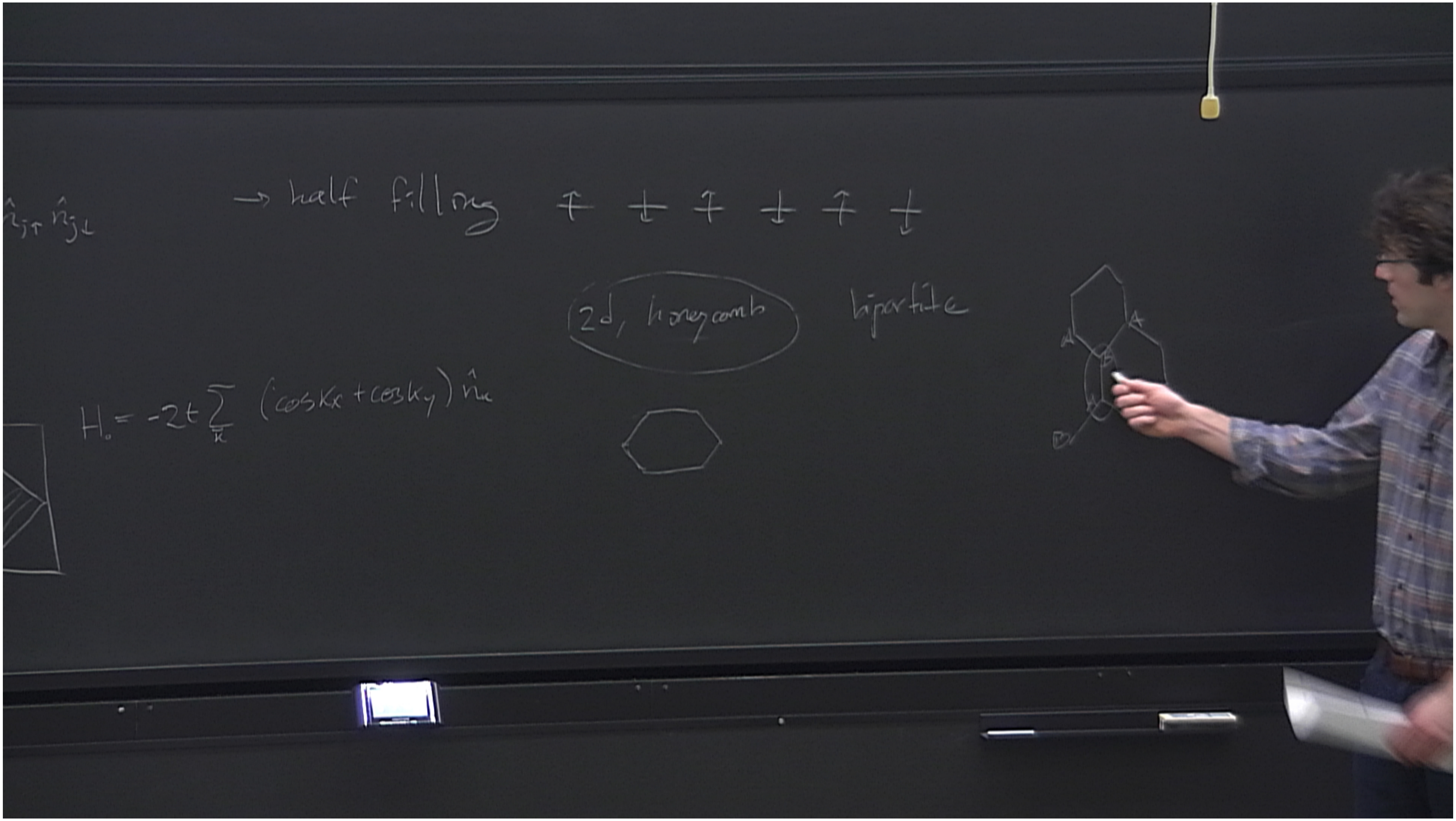
Title: Explorations in Condensed Matter-8

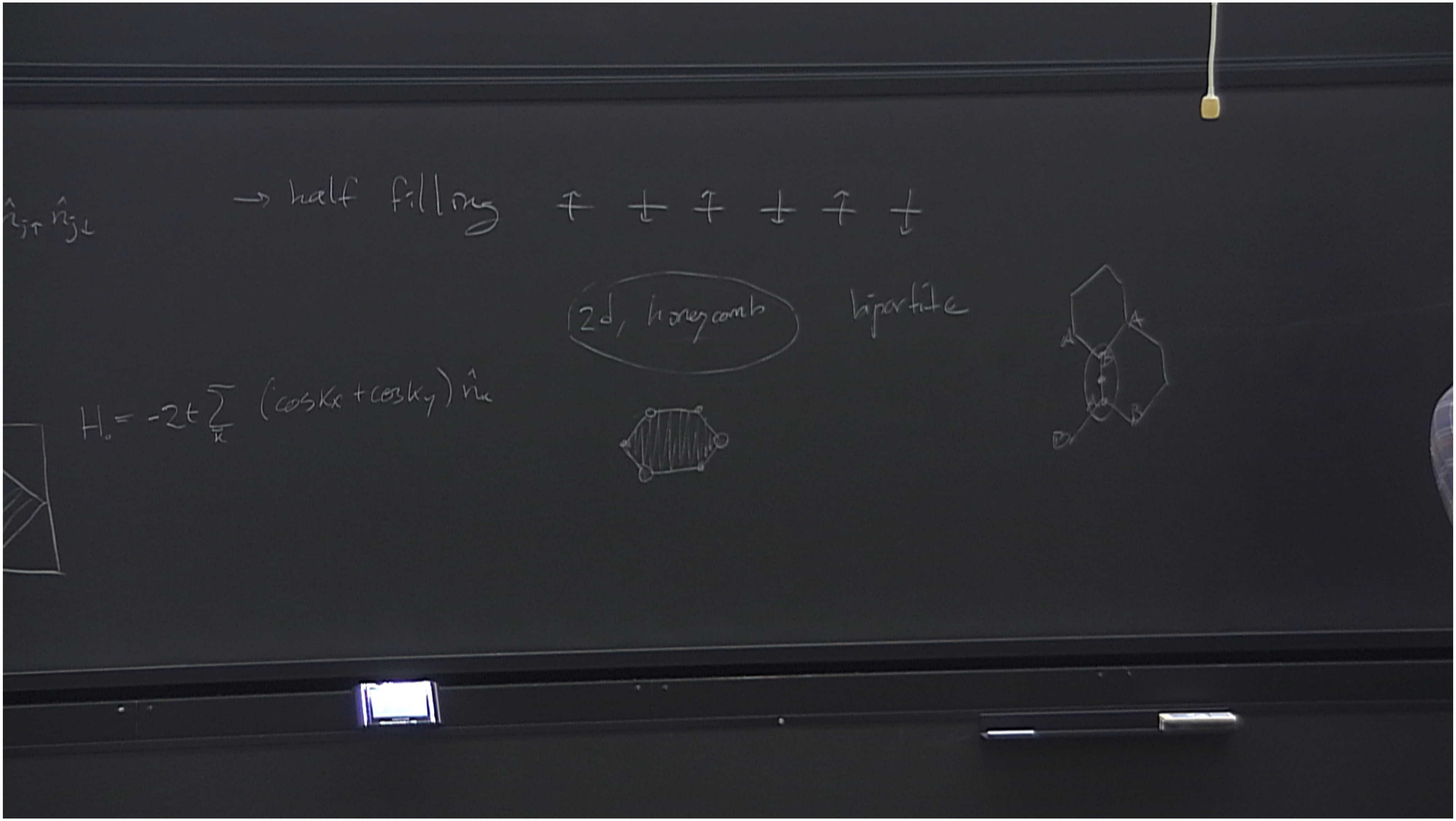
Date: Mar 25, 2015 10:15 AM

URL: http://pirsa.org/15030043

Abstract:


Hubbard model
$H = -t \sum_{\langle ij \rangle \sigma} c^\dagger_{i\sigma} c_{j\sigma} + c^\dagger_{j\sigma} c_{i\sigma} + U \sum_j \hat{n}_{j\uparrow} \hat{n}_{j\downarrow}$
→ half filling


$\hat{n}_{j\uparrow} \hat{n}_{j\downarrow}$
→ half filling
2d, honeycomb
bipartite
A
B
$H_0 = -2t \sum_k (\cos k_x + \cos k_y) \hat{n}_k$


$\hat{n}_{j\uparrow}\hat{n}_{j\downarrow}$
→ half filling
2d, honeycomb
bipartite
$H_0 = -2t\sum_k (\cos k_x + \cos k_y)\hat{n}_k$
A
A
B
B

• $t/U \to 0$ "atomic limit", $U$ only

$$U \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} = \begin{cases} 0 & |0\rangle \\ 0 & |\uparrow\rangle, |\downarrow\rangle \\ U & |\uparrow\downarrow\rangle \end{cases}$$

(1) $\hat{n}_{j\uparrow} \hat{n}_{j\downarrow} = c^\dagger_{j\uparrow} c_{j\uparrow} c^\dagger_{j\downarrow} c_{j\downarrow} = c^\dagger_{j\uparrow} c_{j\uparrow} \left(1 - c_{j\downarrow} c^\dagger_{j\downarrow}\right)$

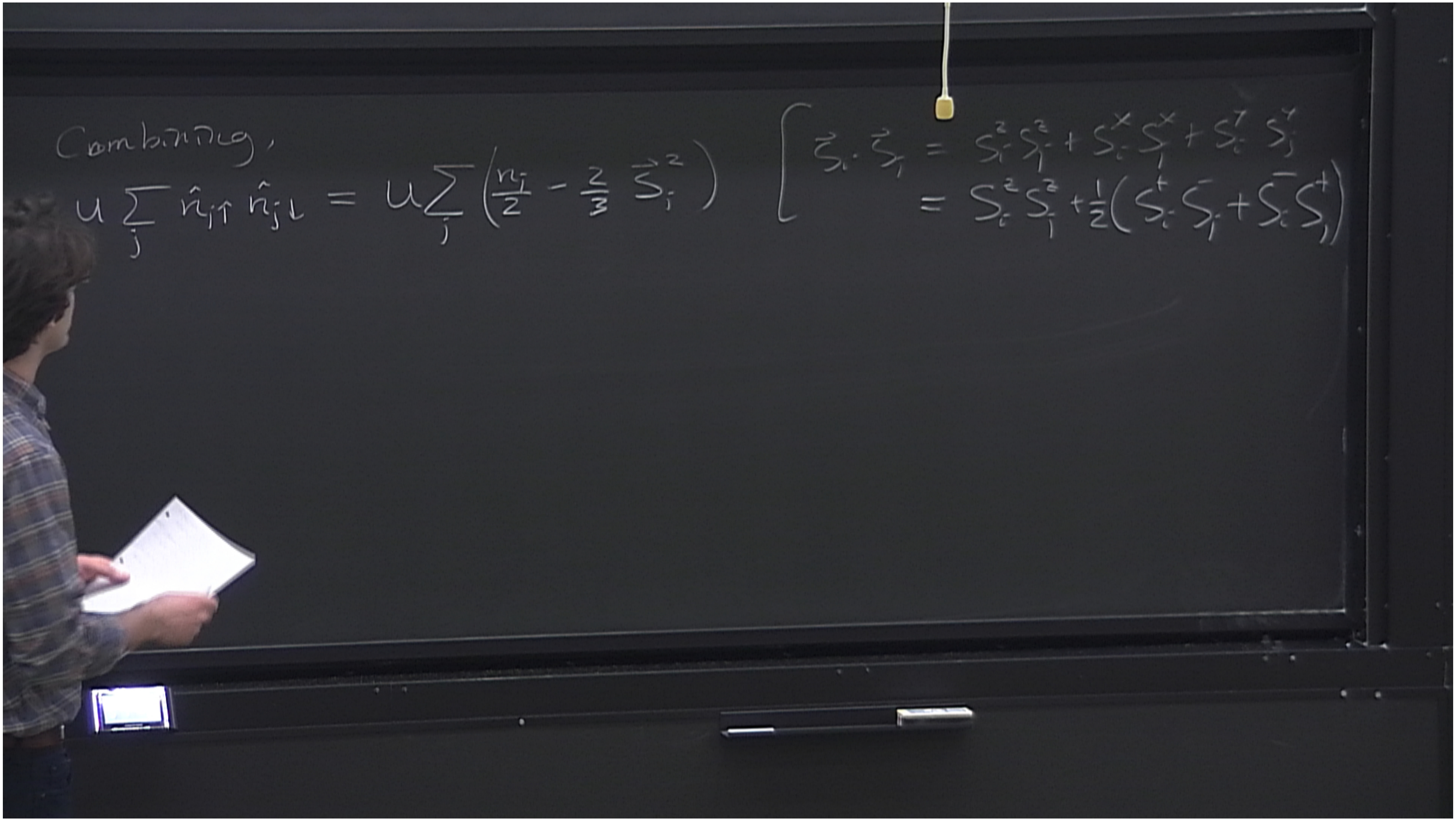
$= \hat{n}_{j\uparrow} - (c^\dagger_{j\uparrow} c_{j\downarrow})(c^\dagger_{j\downarrow} c_{j\uparrow}) = \hat{n}_{j\uparrow} - S^+_j S^-_j$

(2) $n_{j\uparrow} n_{j\downarrow} = \hat{n}_{j\downarrow} - S^-_j S^+$

(3) $n_{j\uparrow} n_{j\downarrow} = \frac{\hat{n}_j}{2} - 2 (S^z_j)^2 \leftarrow$ (use $\hat{n}^2_{j\sigma} = \hat{n}_{j\sigma}$, $S^z = \frac{1}{2}(\hat{n}_{j\uparrow} - \hat{n}_{j\downarrow})$)

Combinin

$U \sum_j$


Combining,
$U \sum_j \hat{n}_{j\uparrow} \hat{n}_{j\downarrow} = U \sum_j \left( \frac{n_j}{2} - \frac{2}{3} \vec{S}_j^{\,2} \right)$
$\vec{S}_i \cdot \vec{S}_j = S_i^z S_j^z + S_i^x S_j^x + S_i^y S_j^y$
$= S_i^z S_j^z + \frac{1}{2}\left( S_i^+ S_j^- + S_i^- S_j^+ \right)$

Combining,

$$U\sum_j \hat{n}_{j\uparrow}\hat{n}_{j\downarrow} = U\sum_j\left(\frac{n_j}{2} - \frac{2}{3}\vec{S}_j^{\,2}\right)$$

$$= U\left(\frac{N}{2} - \frac{2}{3}\sum_j \vec{S}_j^{\,2}\right)$$

$$\vec{S}_i\cdot\vec{S}_j = S_i^z S_j^z + S_i^x S_j^x + S_i^y S_j^y$$
$$= S_i^z S_j^z + \frac{1}{2}\left(S_i^+ S_j^- + S_i^- S_j^+\right)$$

$$\vec{S}_j^{\,2} = \begin{cases} 0 & |0\rangle, |\uparrow\downarrow\rangle \\ 3/4 & |\uparrow\rangle, |\downarrow\rangle \end{cases}$$

$\longrightarrow$ rotation (SU(2)) invariant

$\longrightarrow$ local moment formation

Combining,

$$U\sum_j \hat{n}_{j\uparrow}\hat{n}_{j\downarrow} = U\sum_j\left(\frac{n_j}{2} - \frac{2}{3}\vec{S}_j^{\,2}\right)$$

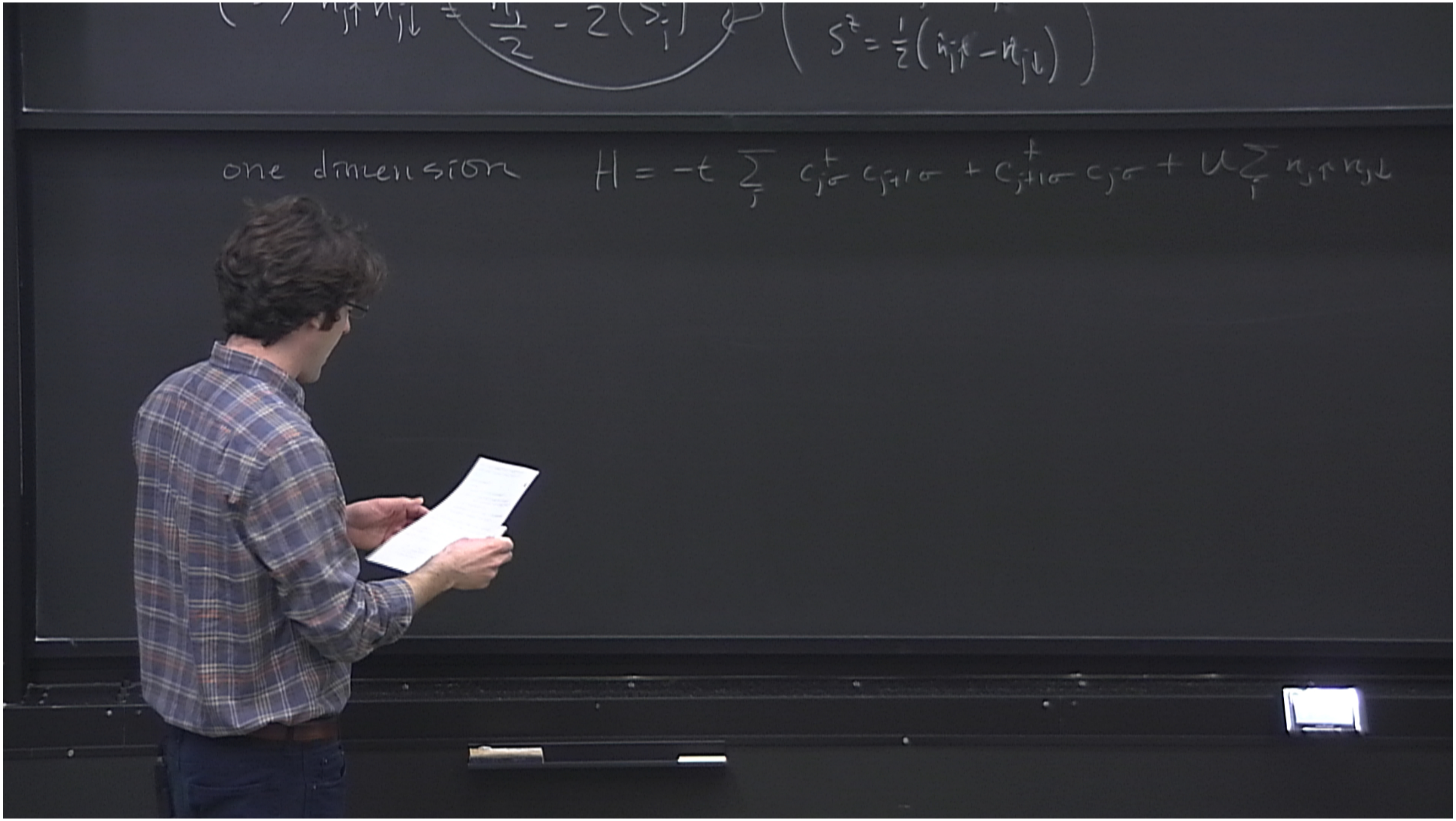
$$= U\left(\frac{N}{2} - \frac{2}{3}\sum_j \vec{S}_j^{\,2}\right)$$

$$\left[\begin{aligned} \vec{S}_i\cdot\vec{S}_j &= S_i^z S_j^z + S_i^x S_j^x + S_i^y S_j^y \\ &= S_i^z S_j^z + \tfrac{1}{2}\left(S_i^+ S_j^- + S_i^- S_j^+\right) \end{aligned}\right.$$

$$\vec{S}_j^{\,2} = \begin{cases} 0 & |0\rangle, |\uparrow\downarrow\rangle \\ 3/4 & |\uparrow\rangle, |\downarrow\rangle \end{cases}$$

$\longrightarrow$ rotation (SU(2)) invariant

$\longrightarrow$ local moment formation


$S^z = \frac{1}{2}(n_{j\uparrow} - n_{j\downarrow})$
one dimension
$H = -t \sum_j c^\dagger_{j\sigma} c_{j+1\sigma} + c^\dagger_{j+1\sigma} c_{j\sigma} + U \sum_j n_{j\uparrow} n_{j\downarrow}$

$$n_{j\uparrow} n_{j\downarrow} = \frac{n_j}{2} - 2(S_j^z)^2 \qquad \left( S^z = \frac{1}{2}(\hat n_{j\uparrow} - \hat n_{j\downarrow}) \right)$$

one dimension $H = -t \sum_j c^\dagger_{j\sigma} c_{j+1\sigma} + c^\dagger_{j+1\sigma} c_{j\sigma} + U \sum_j n_{j\uparrow} n_{j\downarrow}$

$U=0 \longrightarrow$ add small $U/t$, use mean-field theory

$$U \hat n_{j\uparrow} \hat n_{j\downarrow} \simeq U \langle \hat n_{j\uparrow} \rangle \underbrace{\hat n_{j\downarrow}}_{\text{spin down}} + U \langle \hat n_{j\downarrow} \rangle n_{j\uparrow} - U \langle \hat n_{j\uparrow} \rangle \langle \hat n_{j\downarrow} \rangle$$

feels spin up as a external potential

$(\ldots)\, n_{j\uparrow} n_{j\downarrow} = \frac{n_j}{2} - 2(S_j^z)^2$ $\quad \left( S^z = \frac{1}{2}(\hat{n}_{j\uparrow} - \hat{n}_{j\downarrow}) \right)$

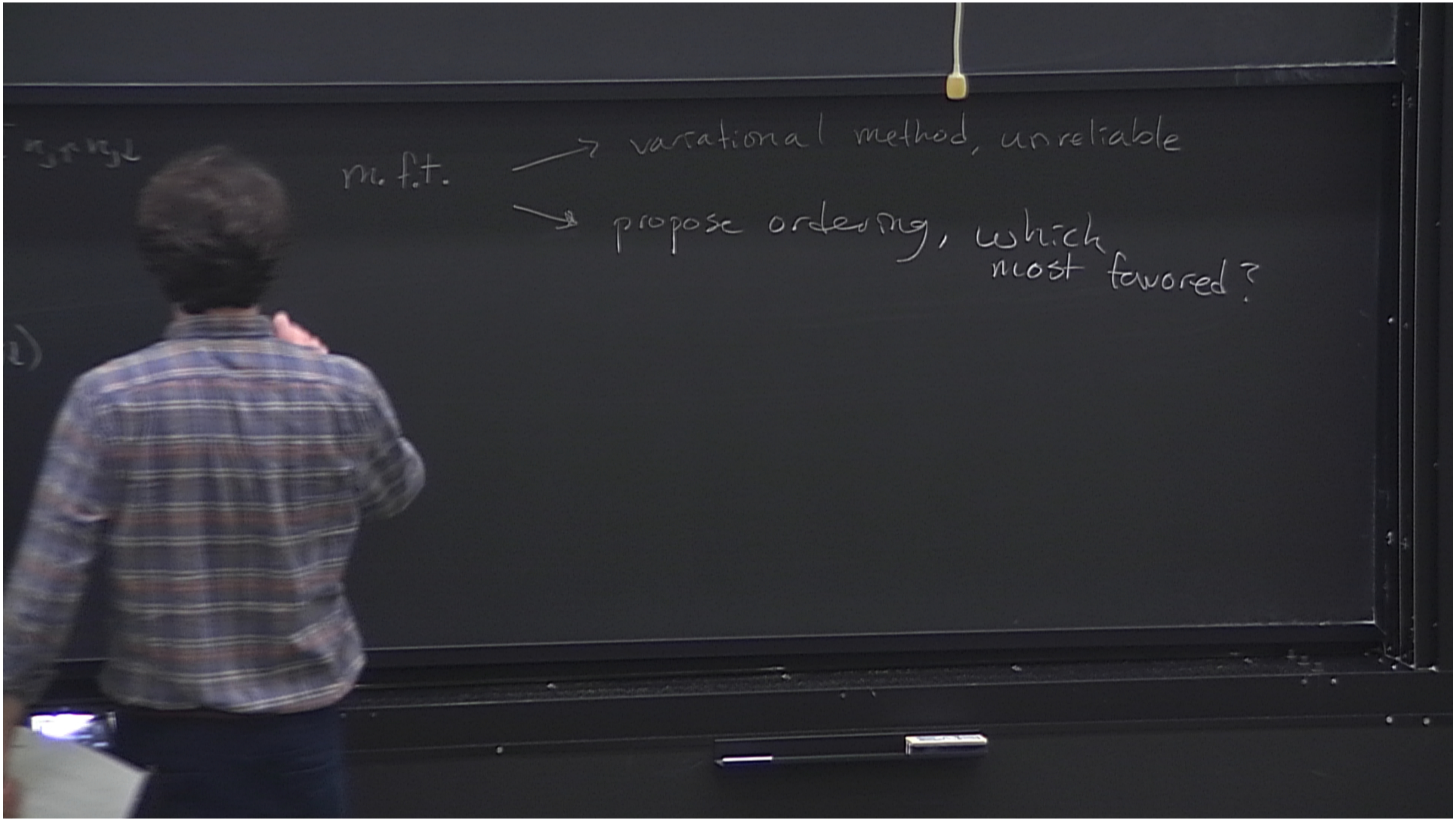
one dimension $\quad H = -t \sum_j c_{j\sigma}^\dagger c_{j+1\sigma} + c_{j+1\sigma}^\dagger c_{j\sigma} + U \sum_j n_{j\uparrow} n_{j\downarrow}$

$U = 0 \longrightarrow$ add small $U/t$, use mean-field theory

$$U \hat{n}_{j\uparrow} \hat{n}_{j\downarrow} \simeq U \langle \hat{n}_{j\uparrow} \rangle \hat{n}_{j\downarrow} + U \langle \hat{n}_{j\downarrow} \rangle n_{j\uparrow} - U \langle \hat{n}_{j\uparrow} \rangle \langle \hat{n}_{j\downarrow} \rangle$$

assumed order

spin down feels spin up as a external potential


m.f.t.
variational method, unreliable
propose ordering, which most favored?

$\ldots c_{j\sigma} + U \sum_j n_{j\uparrow} n_{j\downarrow}$

$\ldots$d theory

m.f.t. → variational method, unreliable

→ propose ordering, which most favore

$- U \langle \hat{n}_{j\uparrow} \rangle \langle \hat{n}_{j\downarrow} \rangle)$

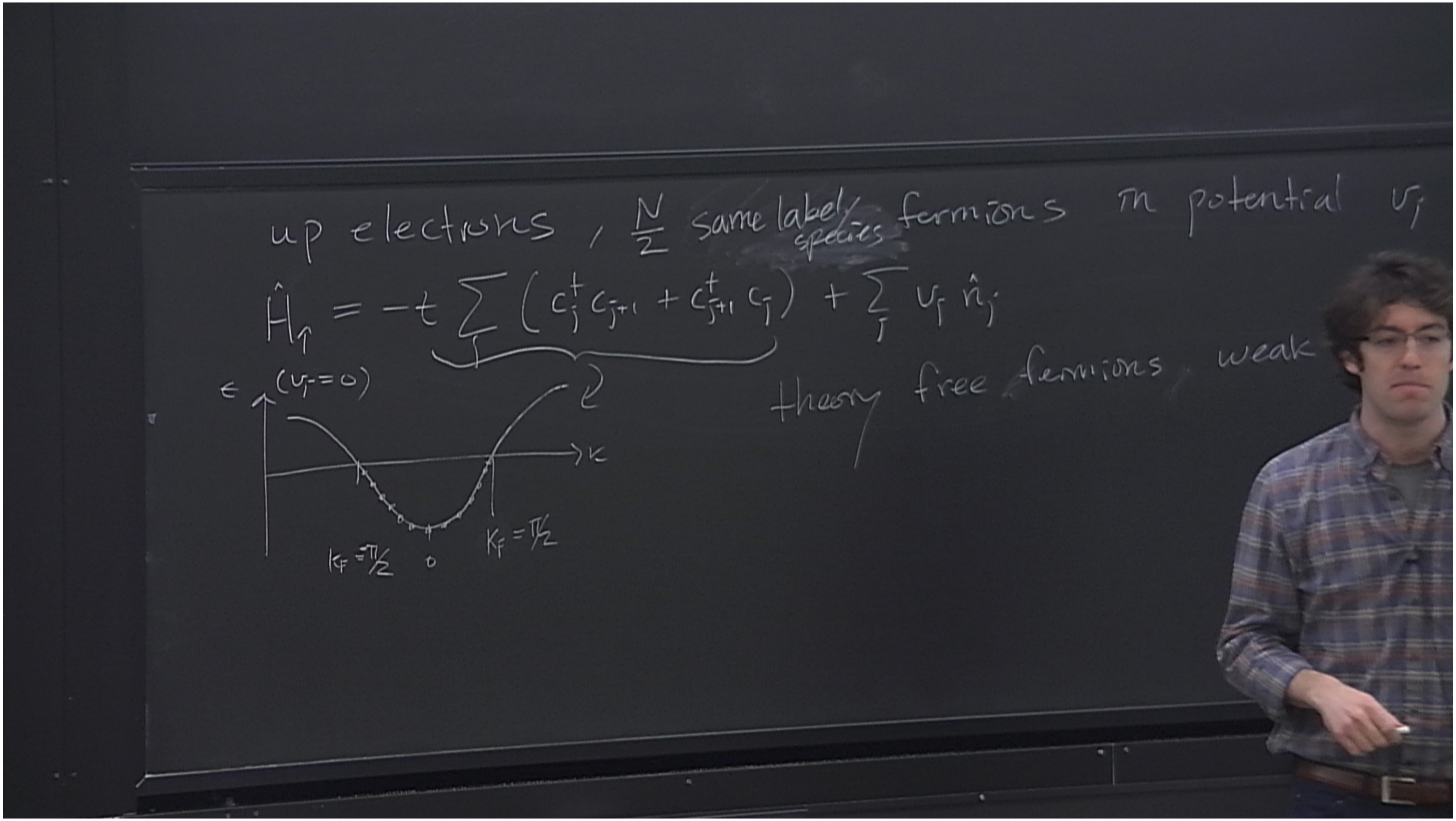
(weak) magnetic ordering

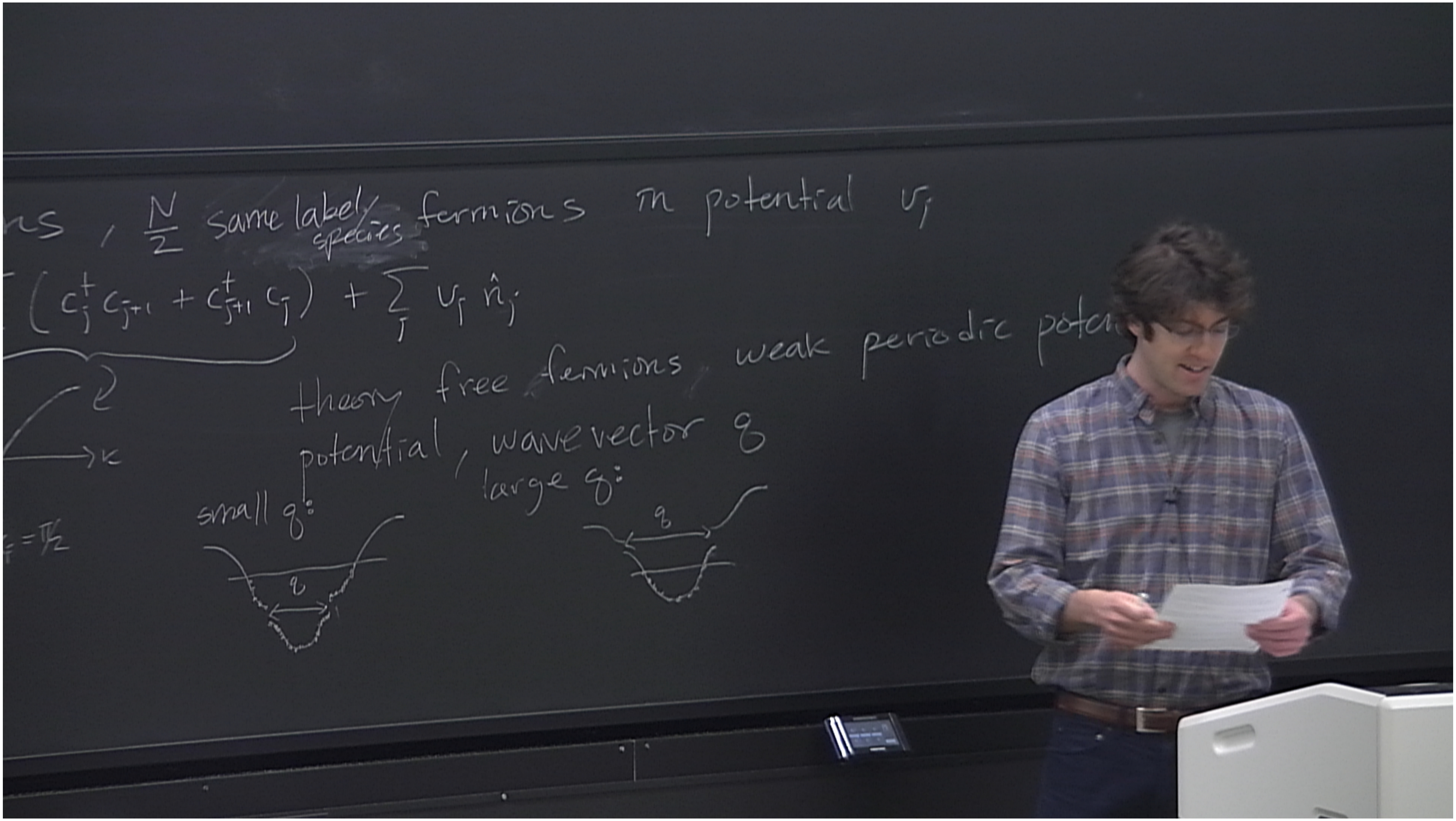
$$\langle \hat{n}_{j\uparrow} \rangle = \frac{n}{2} + m e^{iqj}$$

m small

$$\langle \hat{n}_{j\downarrow} \rangle = \frac{n}{2} - m e^{iqj}$$

q?


up electrons, N/2 same label species fermions in potential $v_j$
$\hat{H}_\uparrow = -t \sum_j (c_j^\dagger c_{j+1} + c_{j+1}^\dagger c_j) + \sum_j v_j \hat{n}_j$
$\epsilon$ $(v_j = 0)$
k
$k_F = -\pi/2$
0
$k_F = \pi/2$
theory free fermions, weak

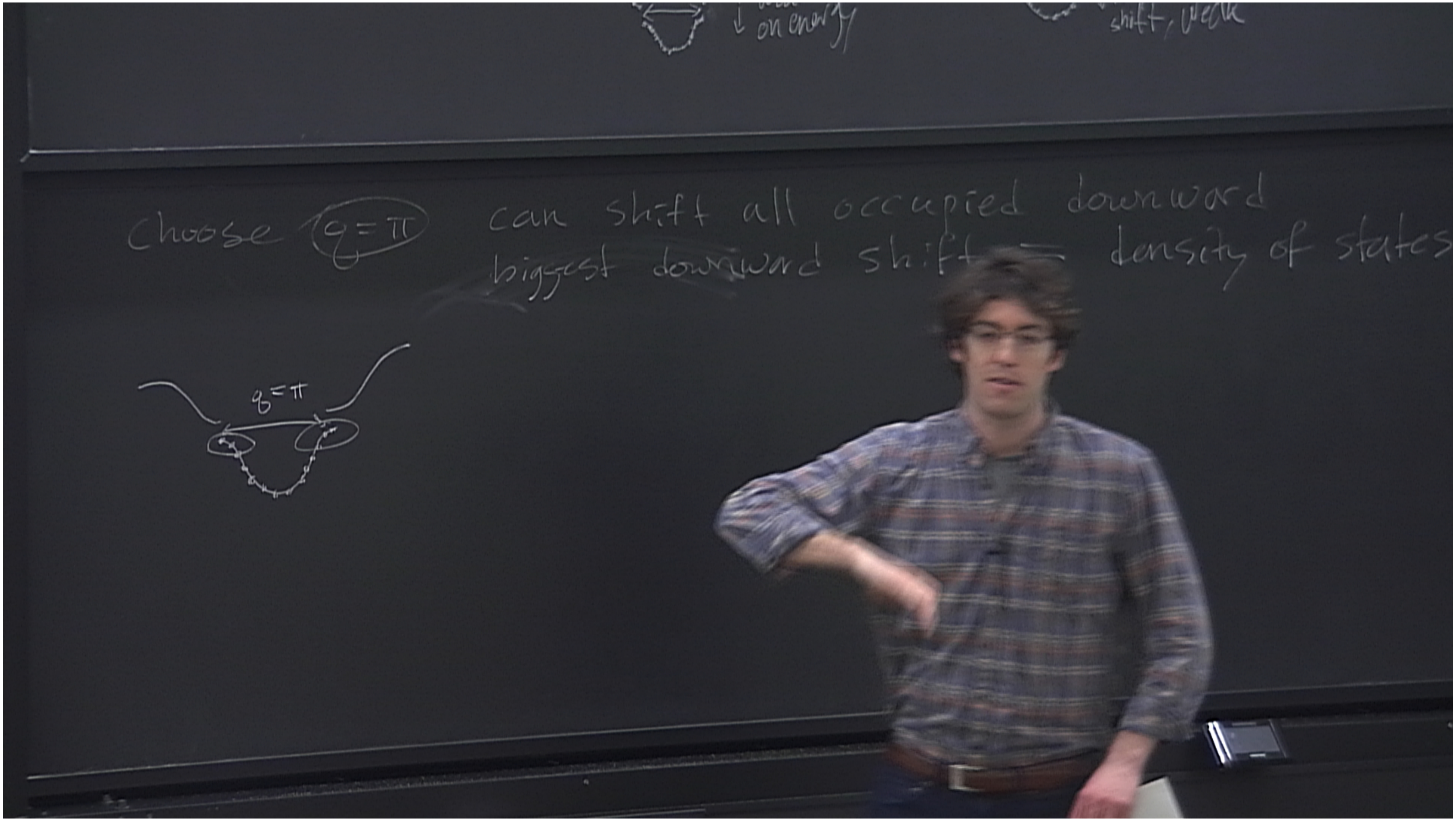

$\frac{N}{2}$ same label/species fermions in potential $v_j$
$(c_j^\dagger c_{j+1} + c_{j+1}^\dagger c_j) + \sum_j v_j \hat{n}_j$
theory free fermions, weak periodic poten
potential, wavevector q
large q:
small q:
q
$=\pi/2$

on energy

shift, weak

Choose $q = \pi$ can shift all occupied downward

biggest downward shift = density of states


on energy
shift, weak
choose q=π
can shift all occupied downward
biggest downward shift ⇒ density of states
q=π

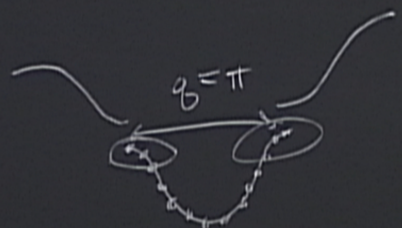
↓ on energy

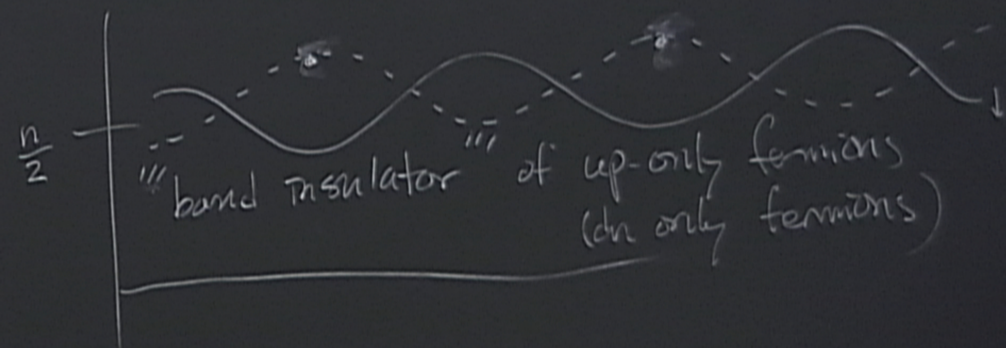
shift, weak

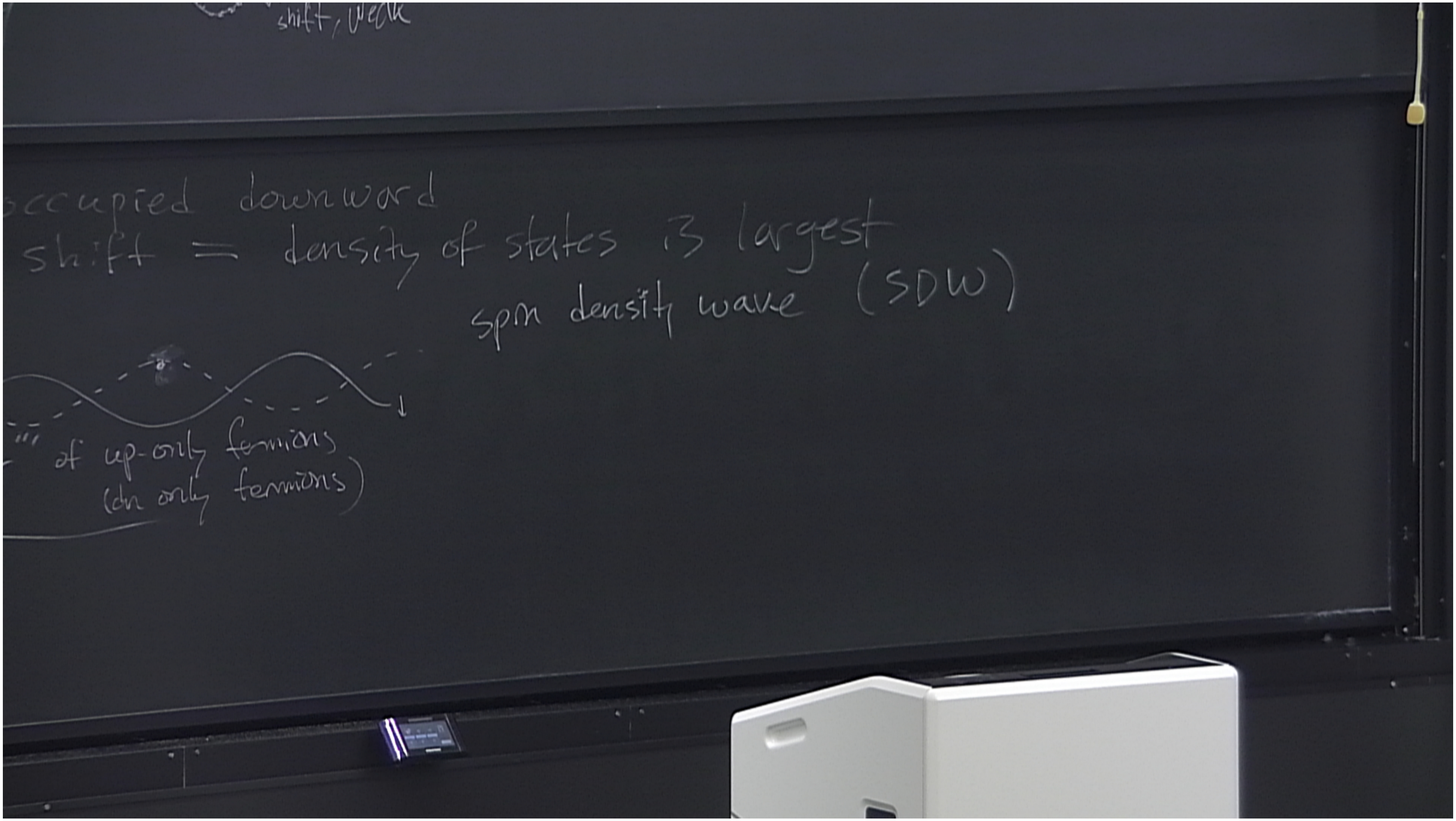
Choose $q=\pi$ can shift all occupied downward

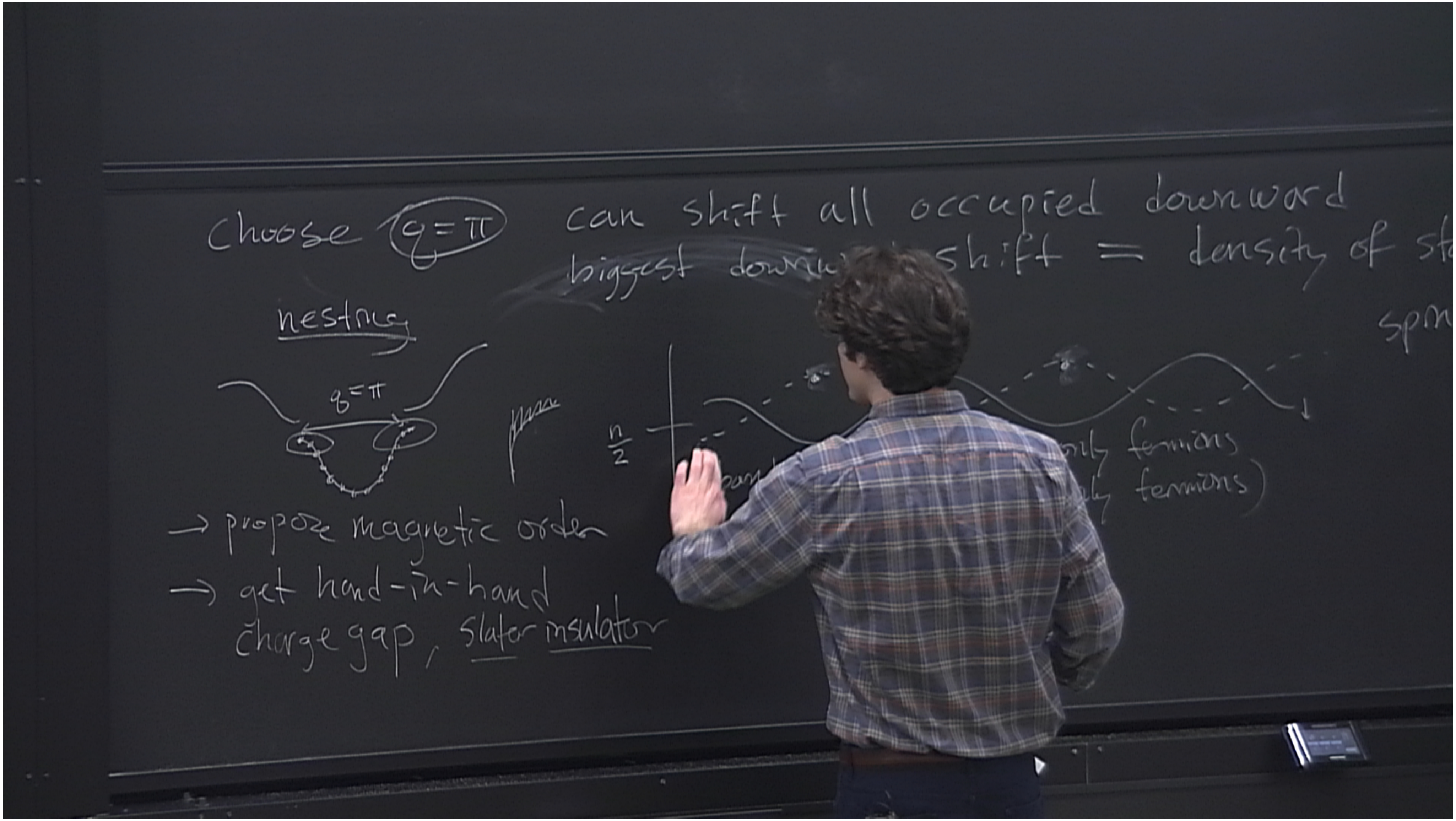
biggest downward shift = density of states

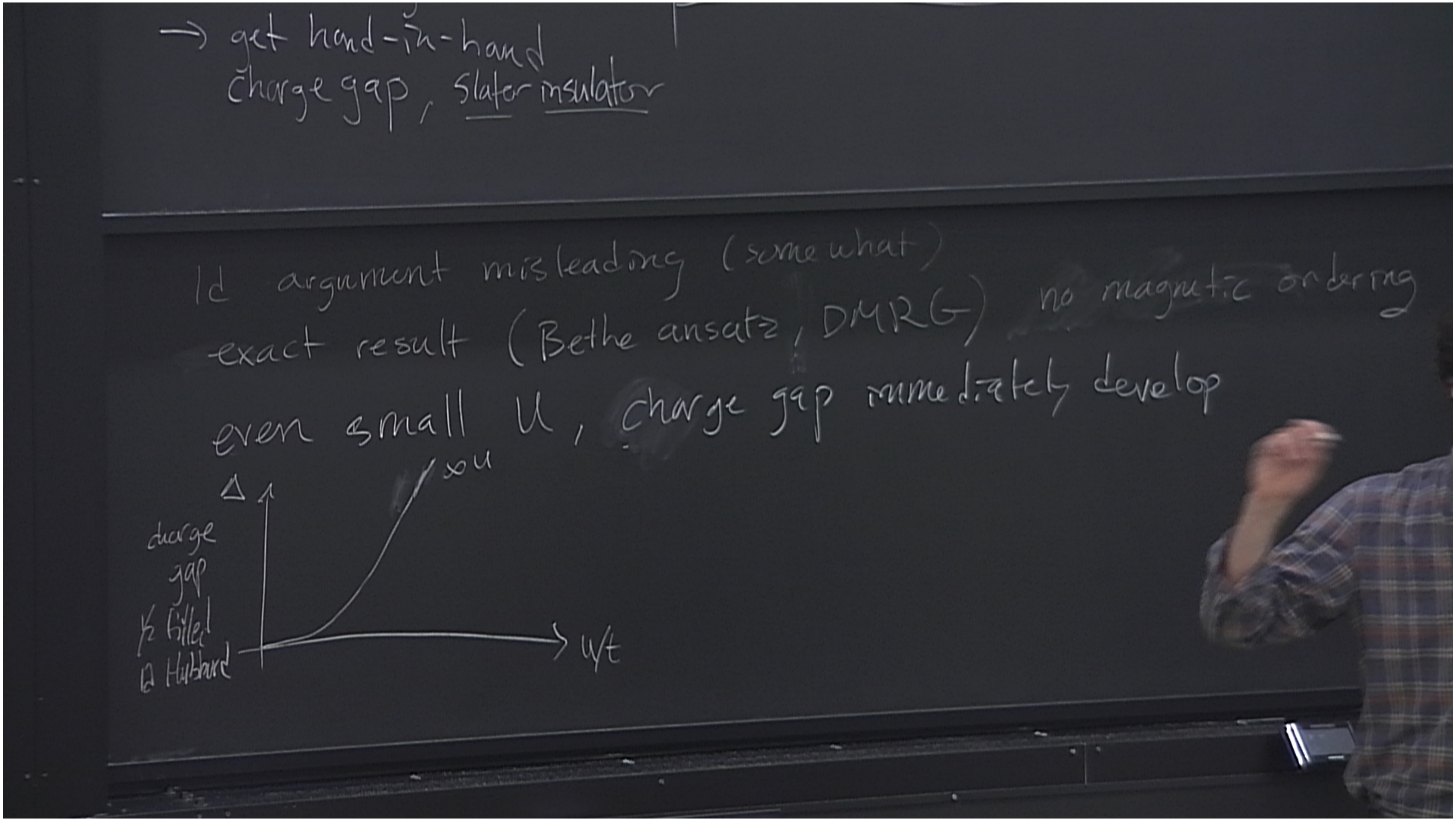
spin den



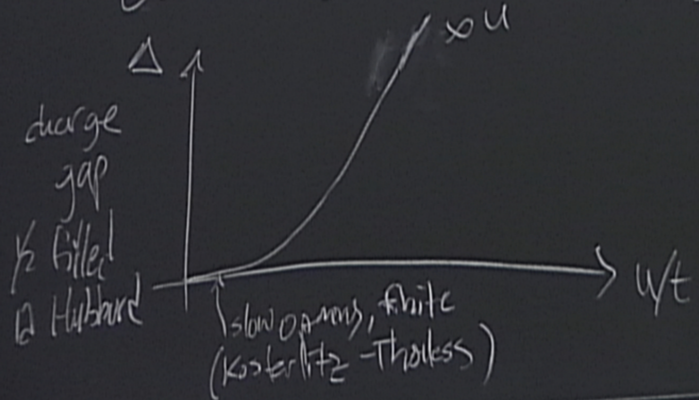

shift, weak
ccupied downward
shift = density of states is largest
spin density wave (SDW)
of up-only fermions
(dn only fermions)

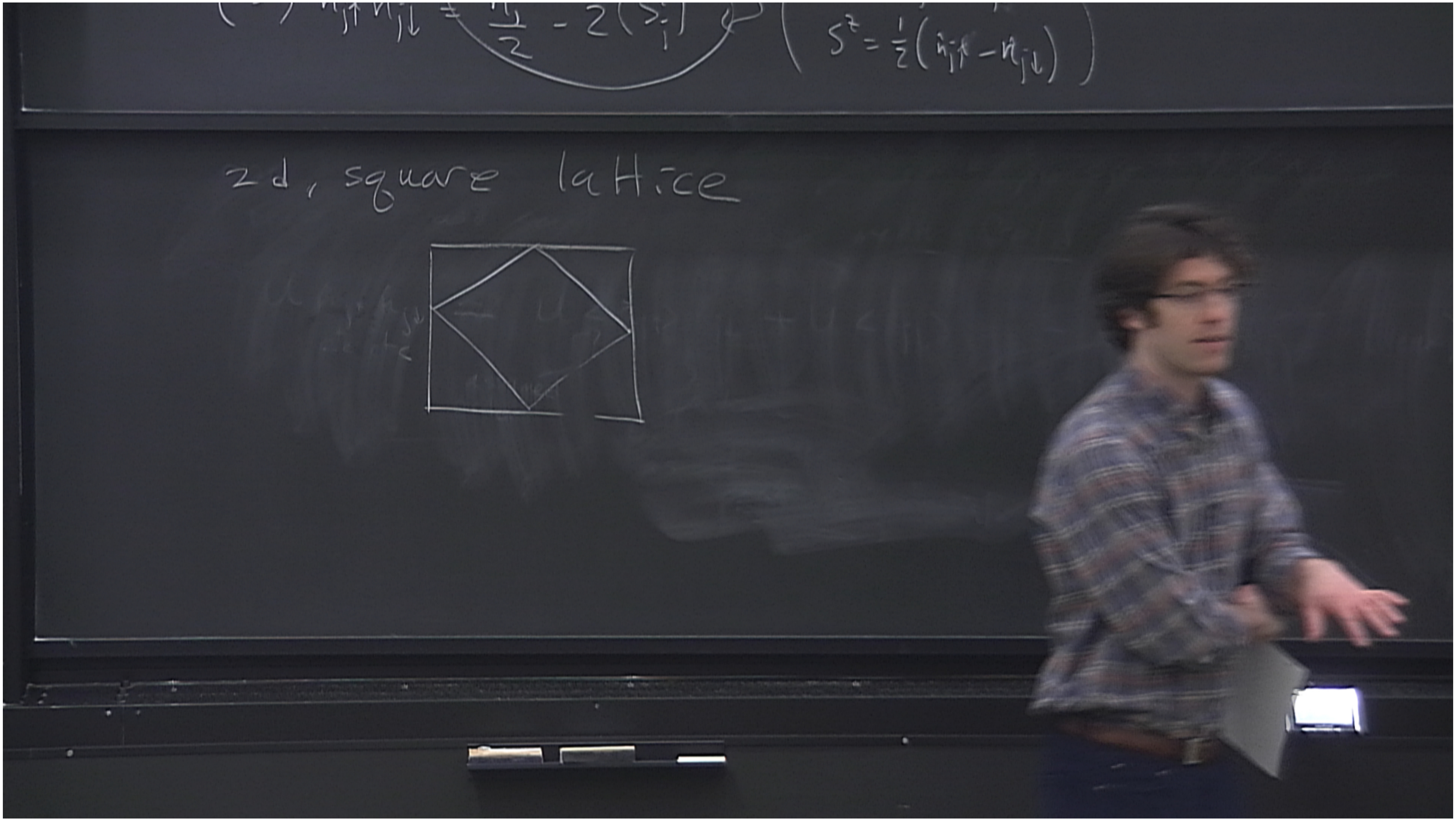

Choose q=π
can shift all occupied downward
shift = density of
nesting
q=π
n/2
fermions
fermions
→ propose magnetic order
→ get hand-in-hand
charge gap, Slater insulator

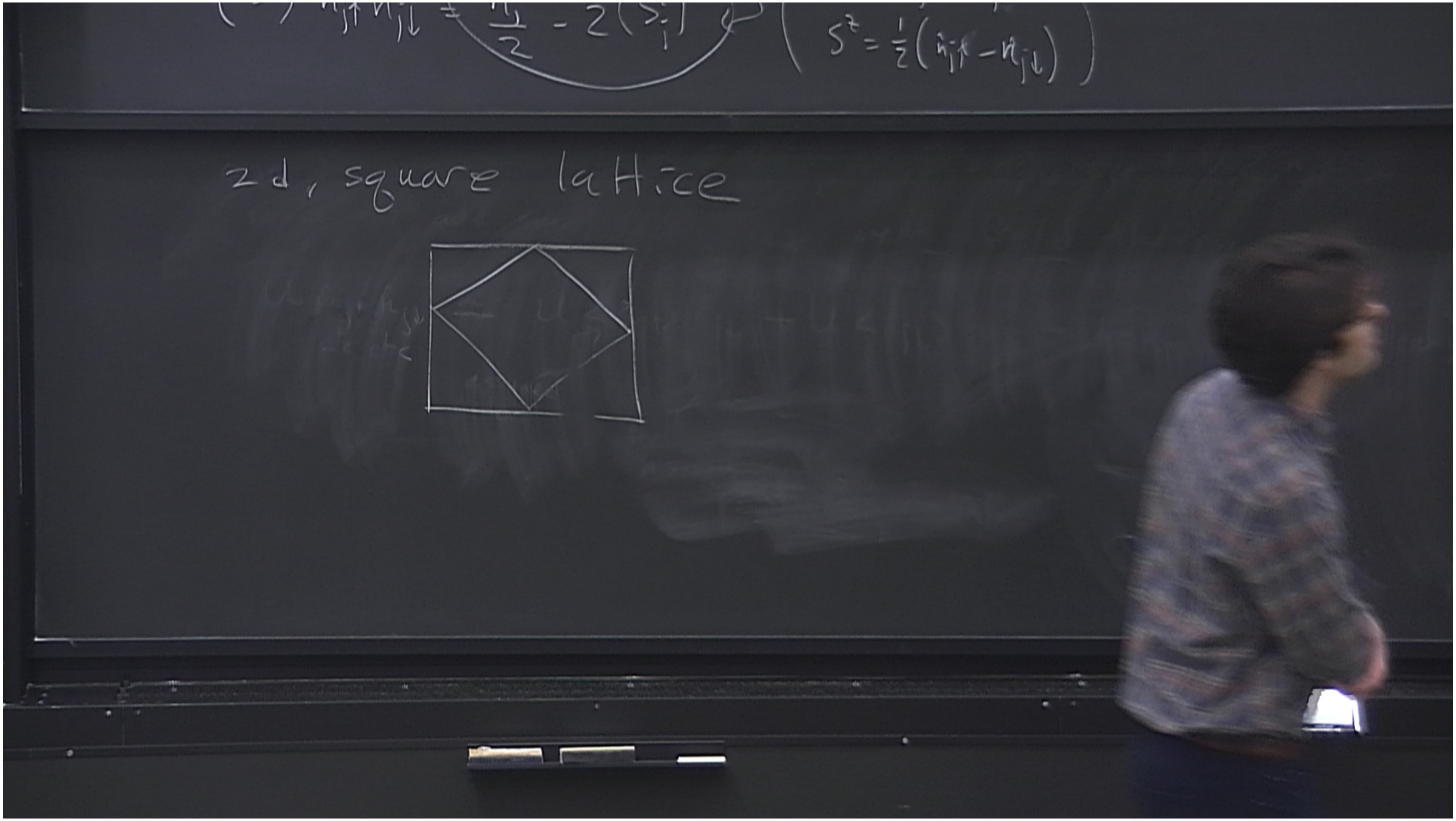

→ get hand-in-hand
charge gap, Slater insulator
1d argument misleading (somewhat)
exact result (Bethe ansatz, DMRG) no magnetic ordering
even small U, charge gap immediately develop
Δ
charge
gap
½ filled
1d Hubbard
U/t

→ get hand-in-hand
charge gap, Slater insulator

1d argument misleading (somewhat)
exact result (Bethe ansatz, DMRG) no magnetic ordering
even small U, charge gap immediately develop




$S^z = \frac{1}{2}(n_{j\uparrow} - n_{j\downarrow})$
2d, square lattice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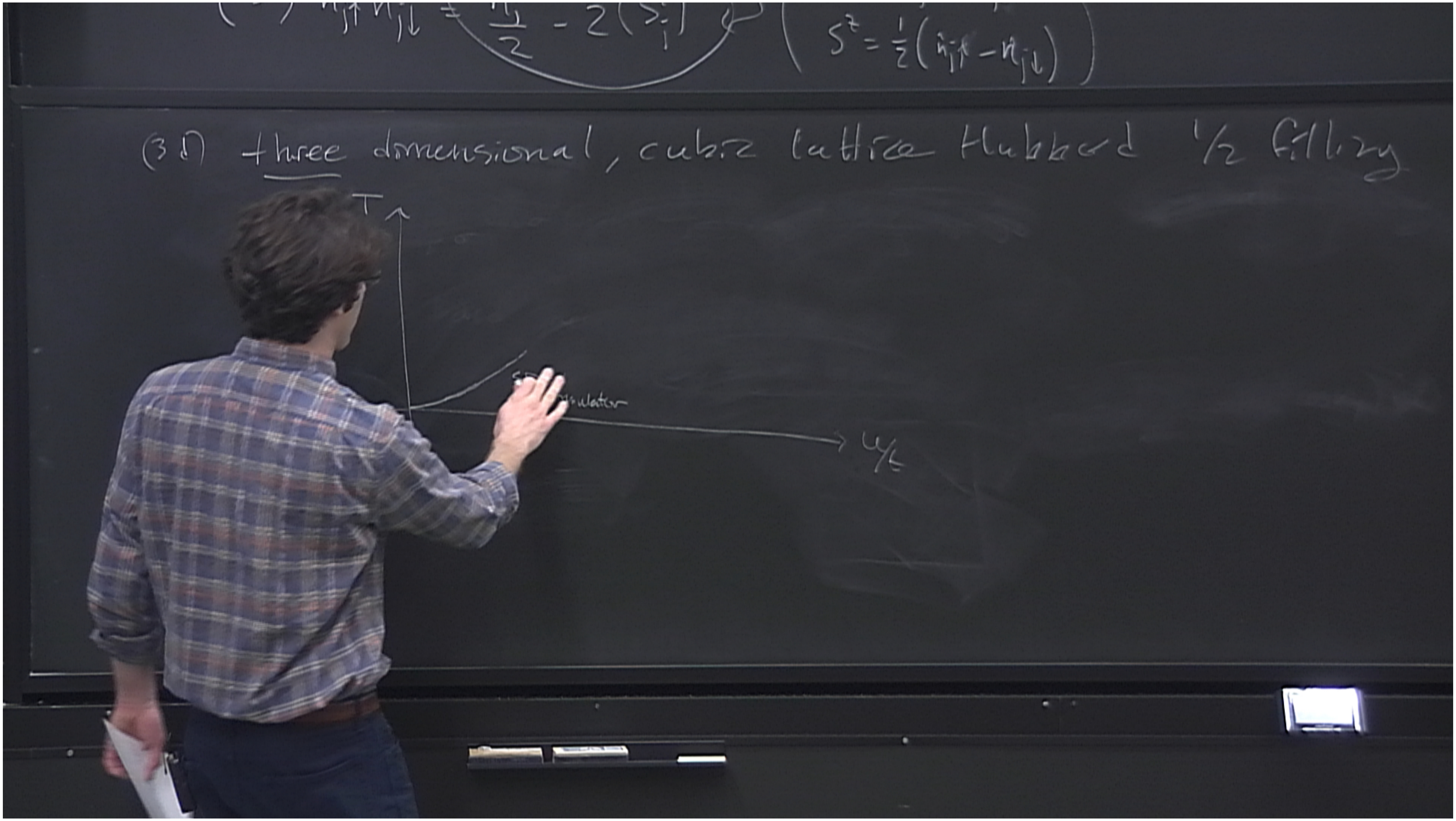
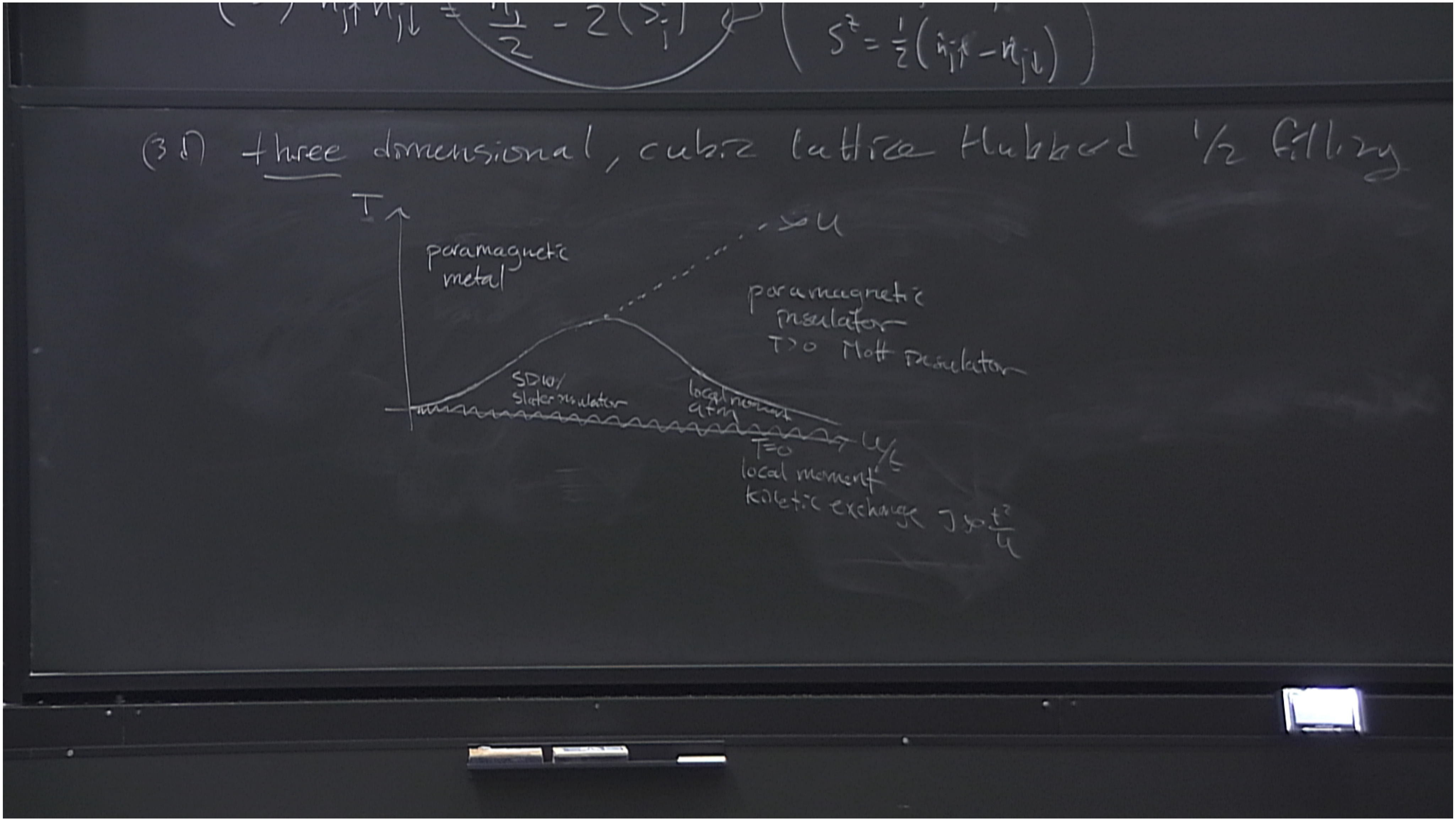
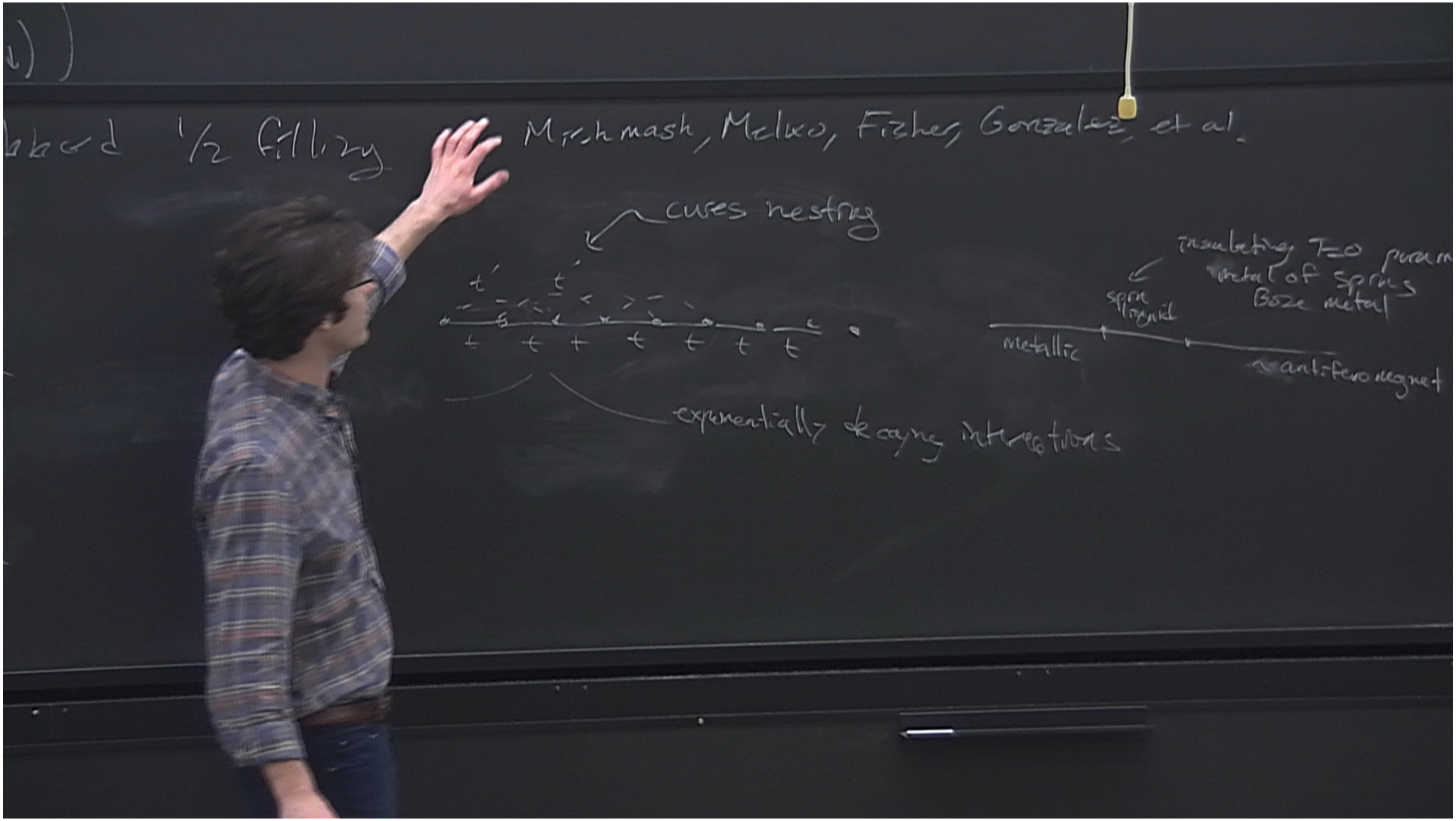


$S^z = \frac{1}{2}(n_{j\uparrow} - n_{j\downarrow})$
(3D) three dimensional, cubic lattice Hubbard 1/2 filling
T
U/t



S^z = 1/2 (n_j↑ − n_j↓)
(3D) three dimensional, cubic lattice Hubbard 1/2 filling
T
U
paramagnetic
metal
paramagnetic
insulator
T>0 Mott insulator
SDW/
Slater insulator
local moment
afm
U/t
T=0
local moment
kinetic exchange J ∝ t²/U


1/2 filling
et al.
cures nesting
t'
t
exponentially decaying interactions
insulating T=0
metal of spins
Bose metal
spin liquid
metallic
antiferromagnet