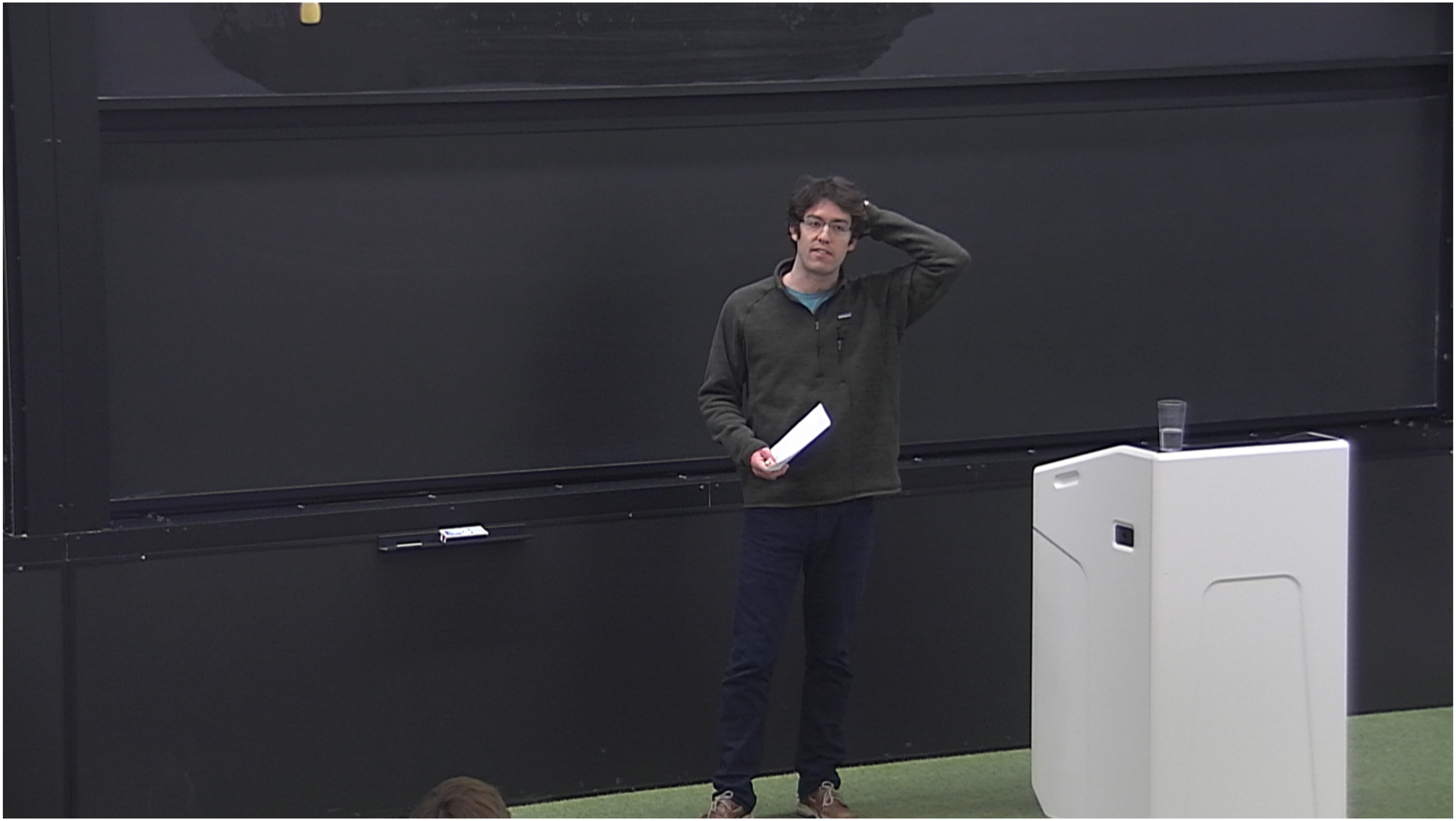
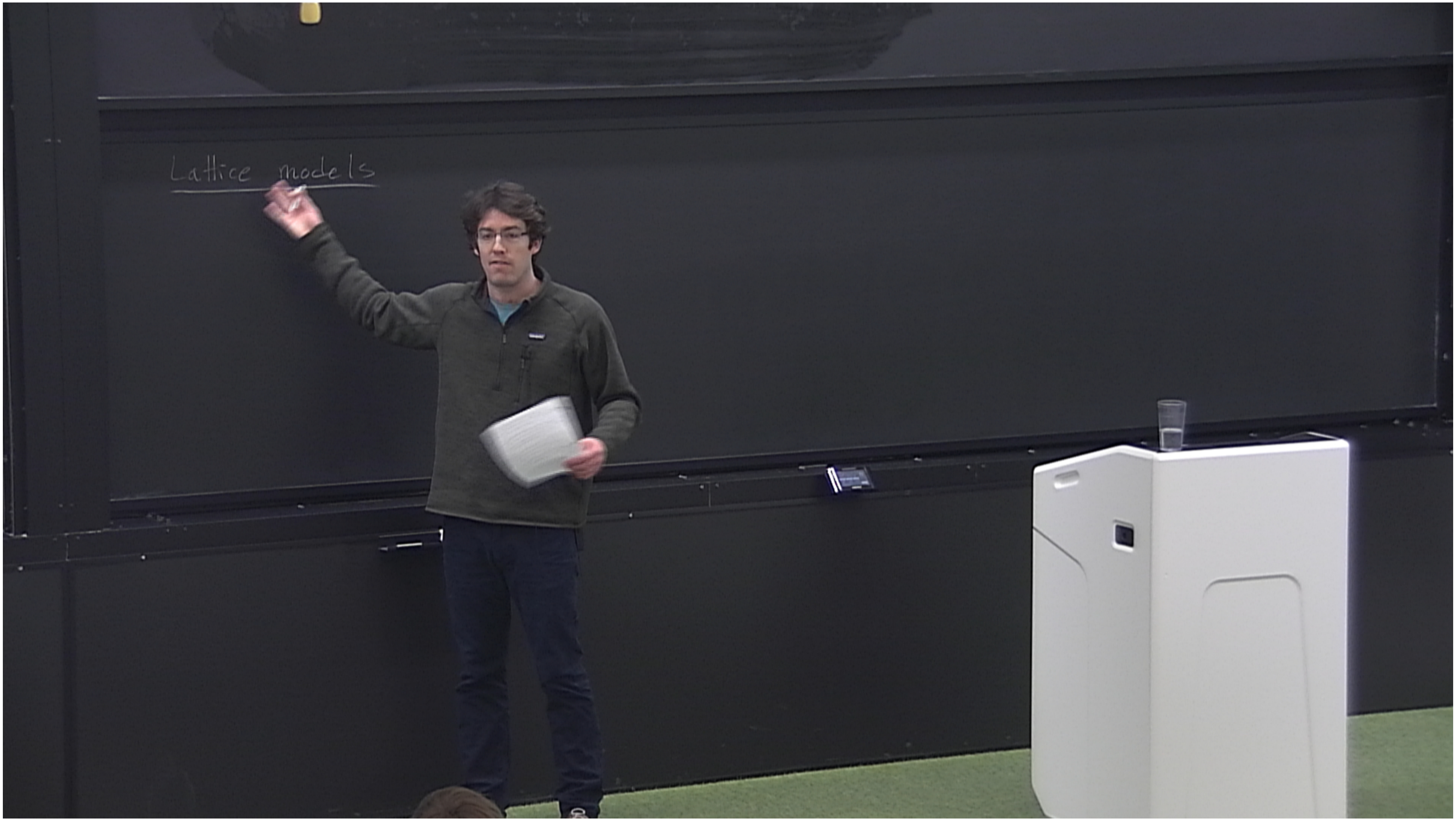
Title: Explorations in Condensed Matter-6

Date: Mar 23, 2015 10:15 AM

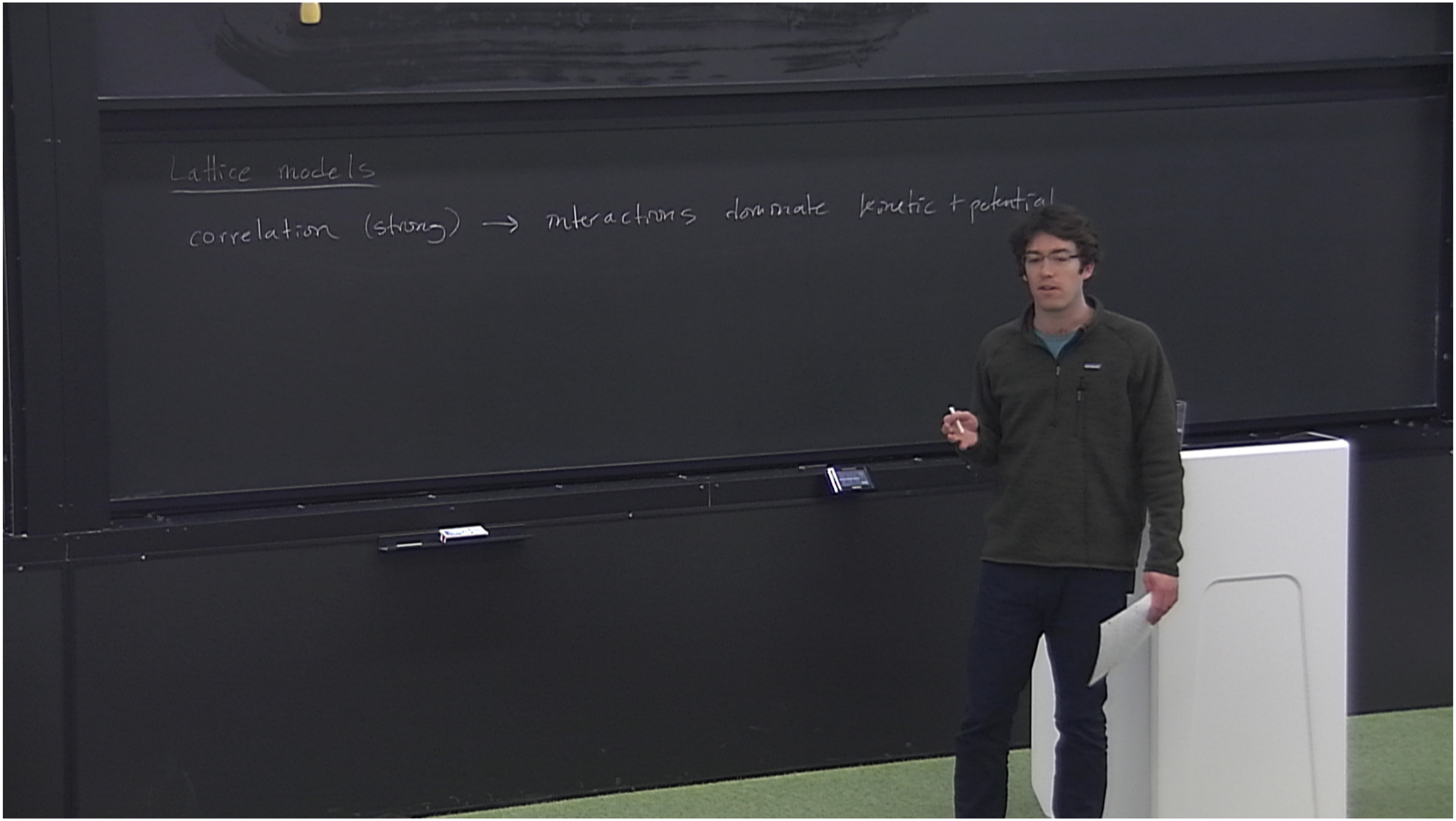
URL: http://pirsa.org/15030041

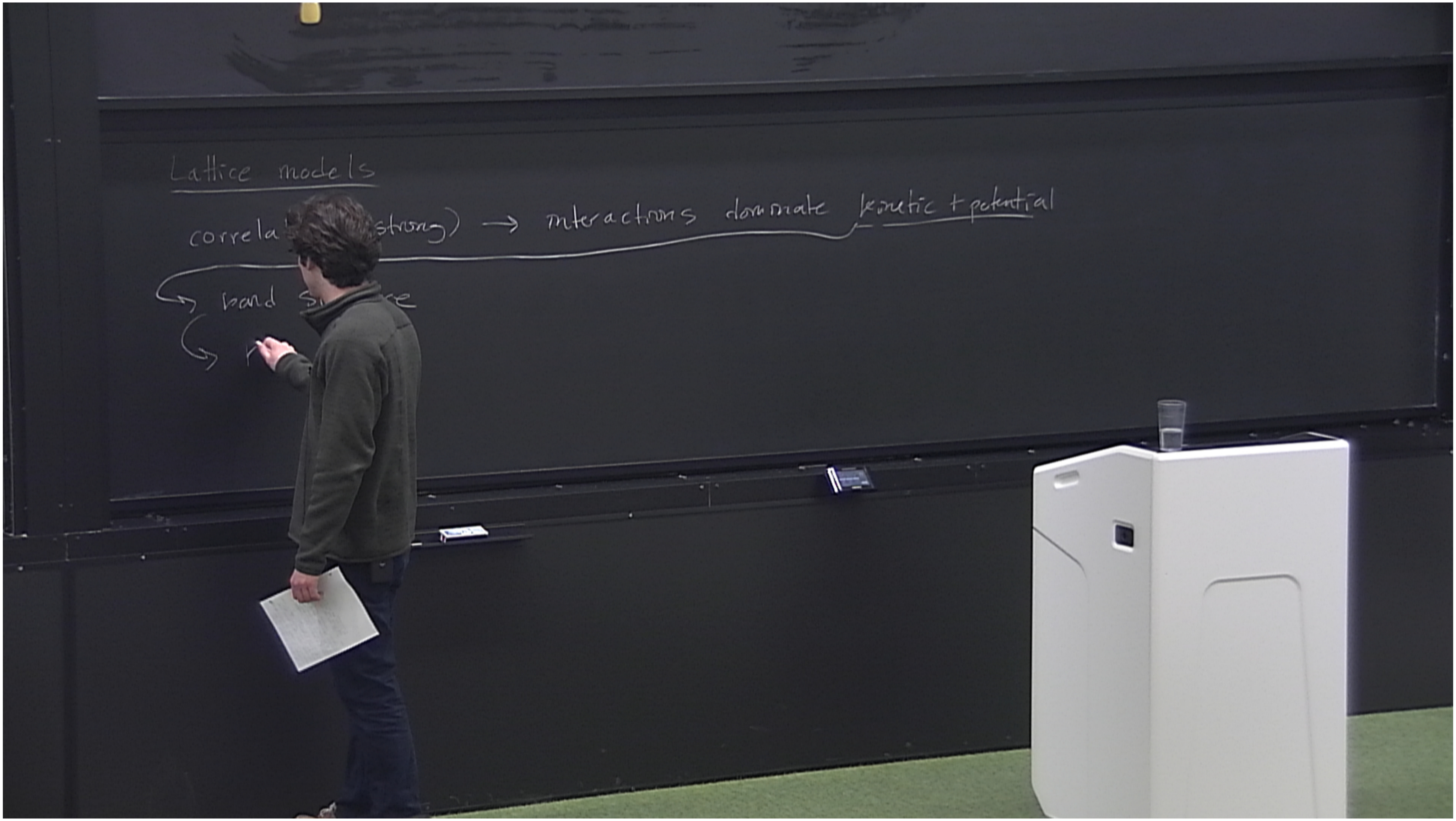
Abstract:

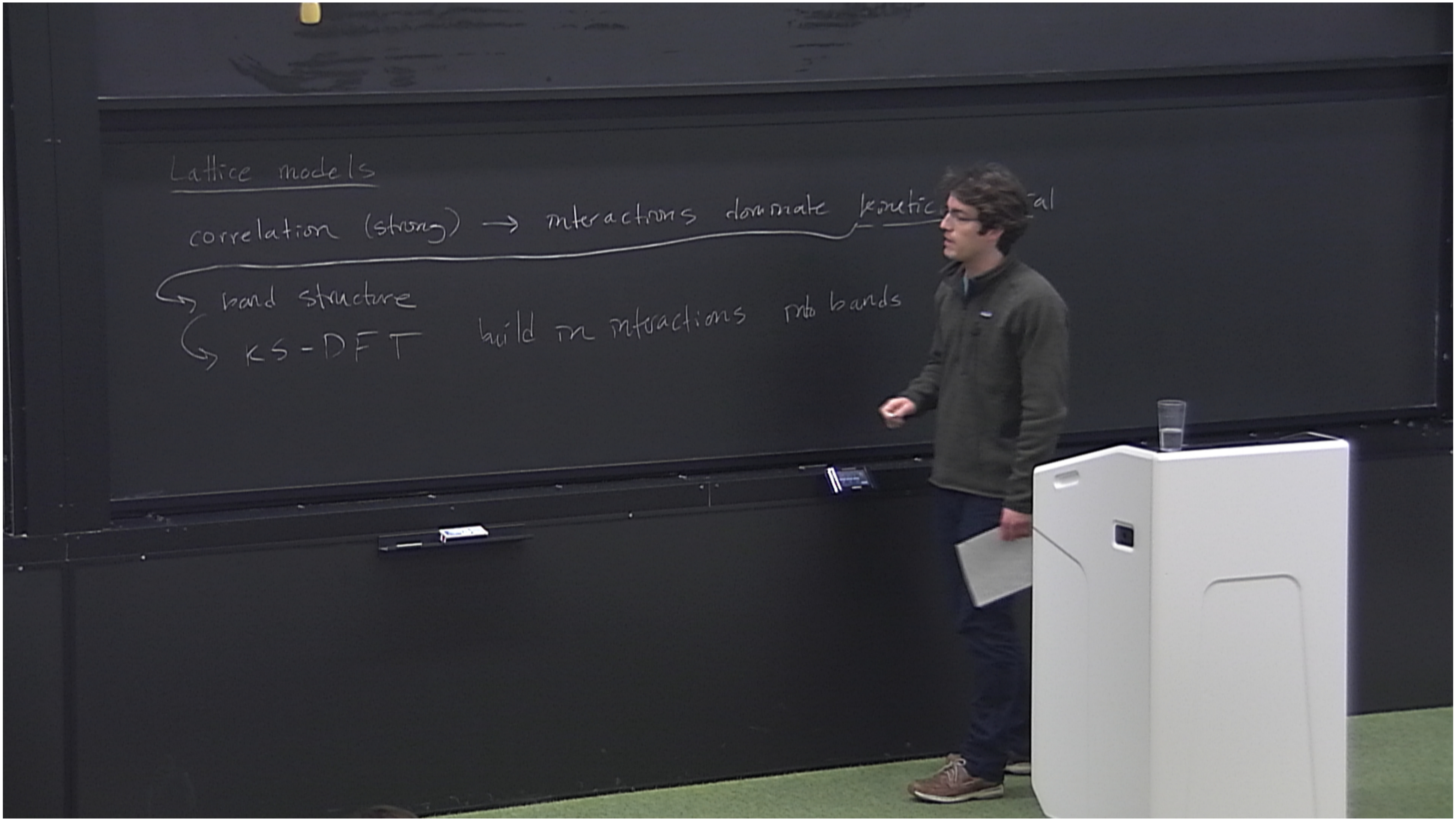


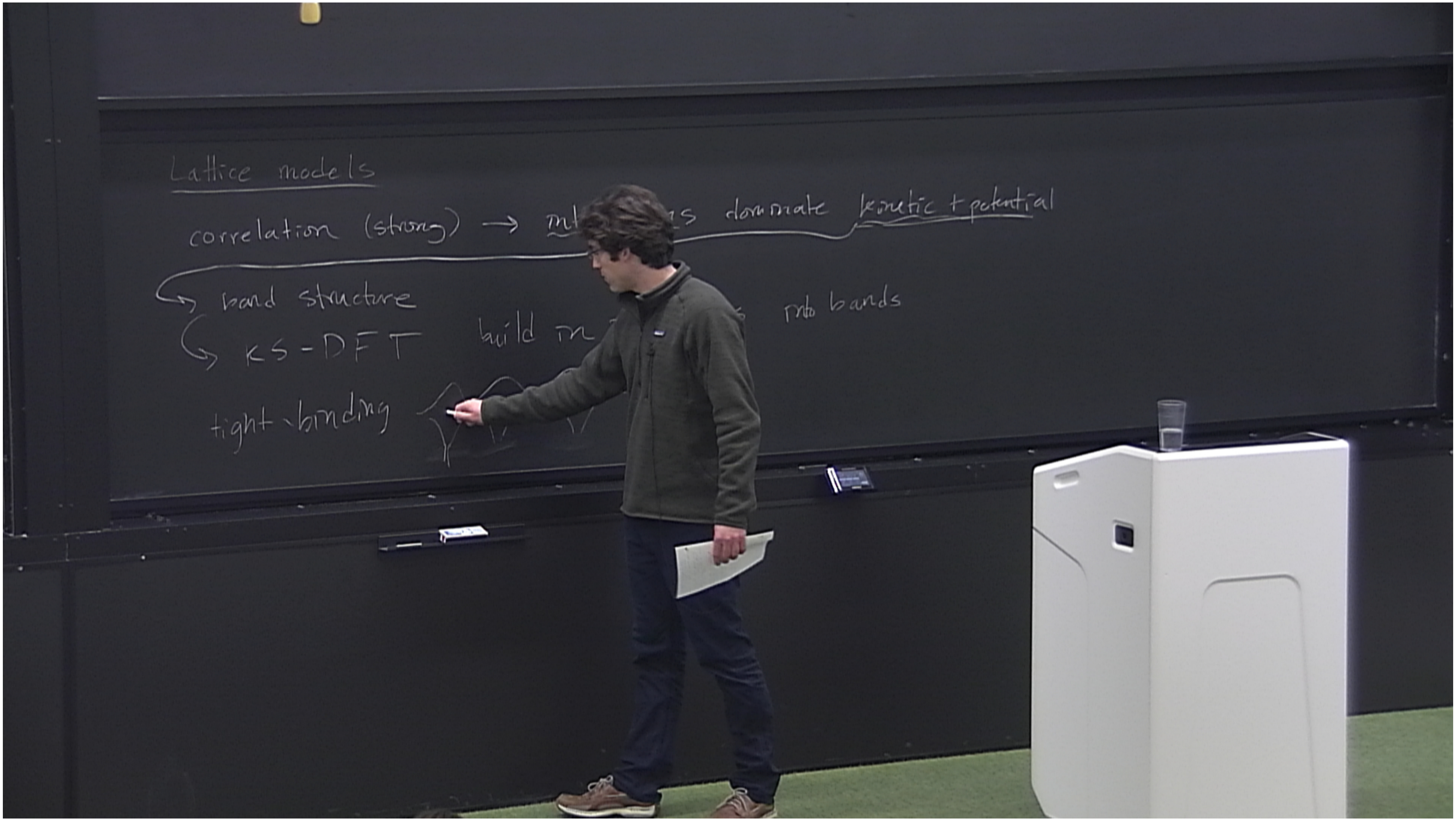

Lattice models

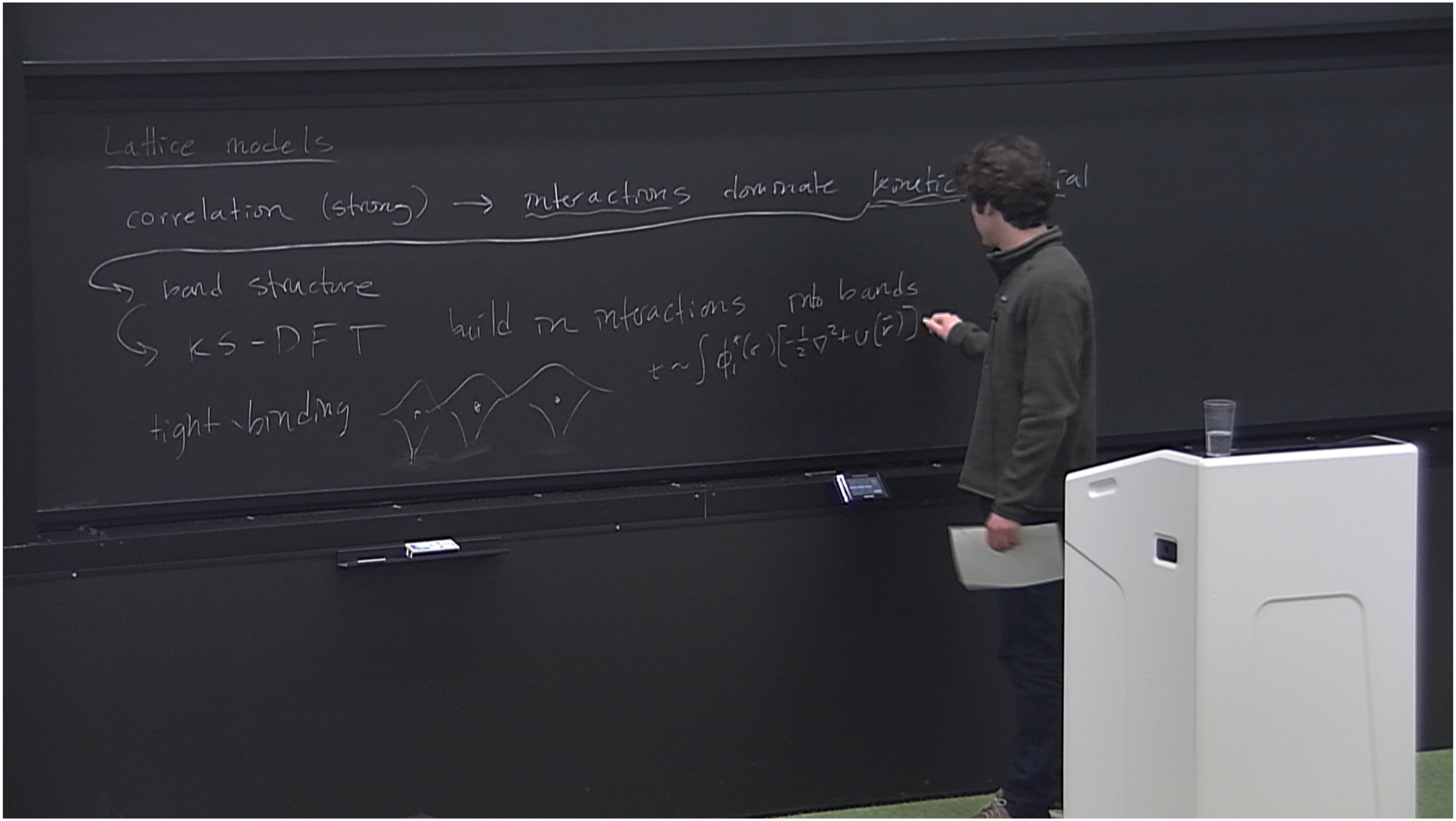

Lattice models

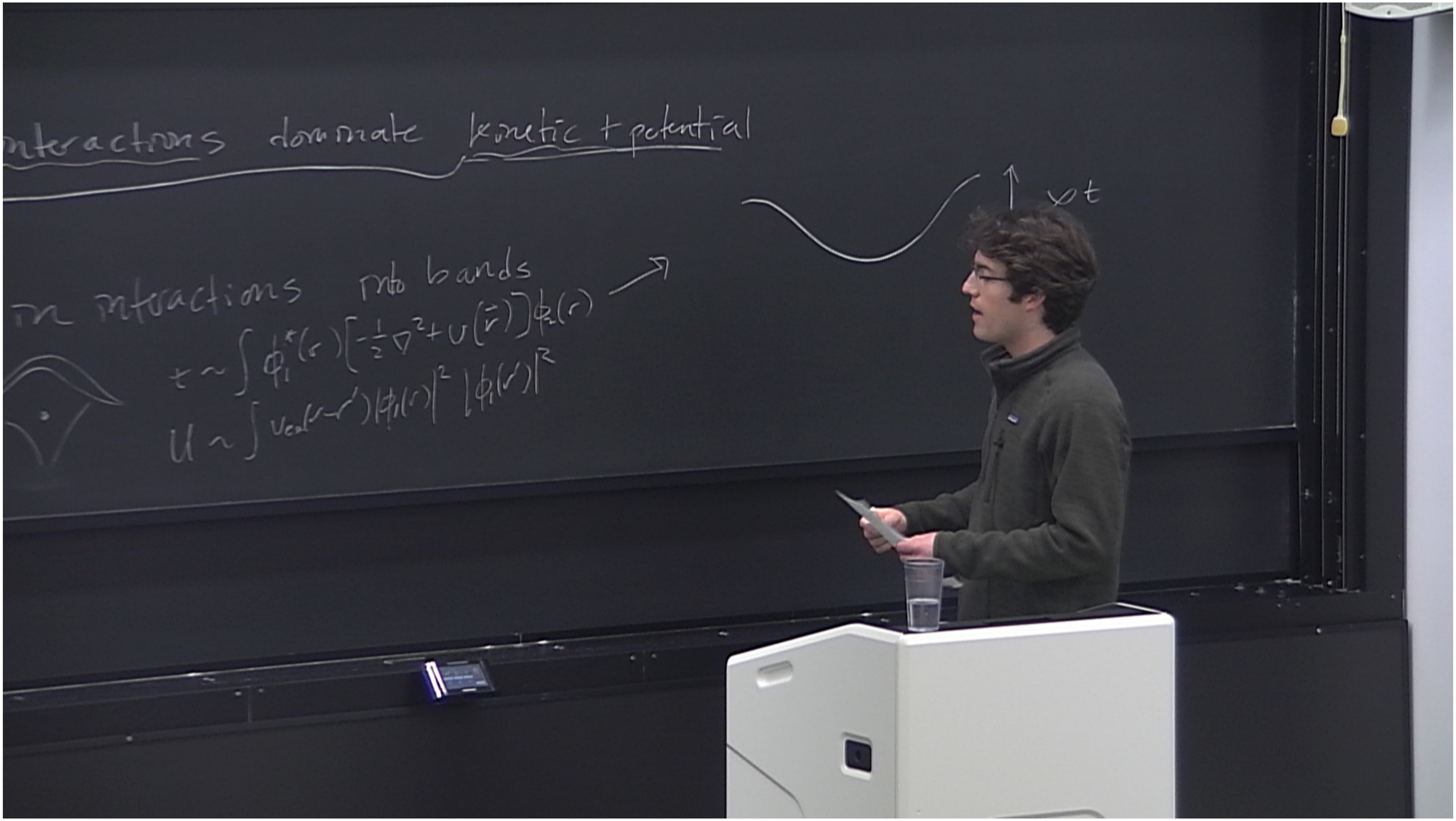

Lattice models
correlation (strong) → interactions dominate kinetic + potential

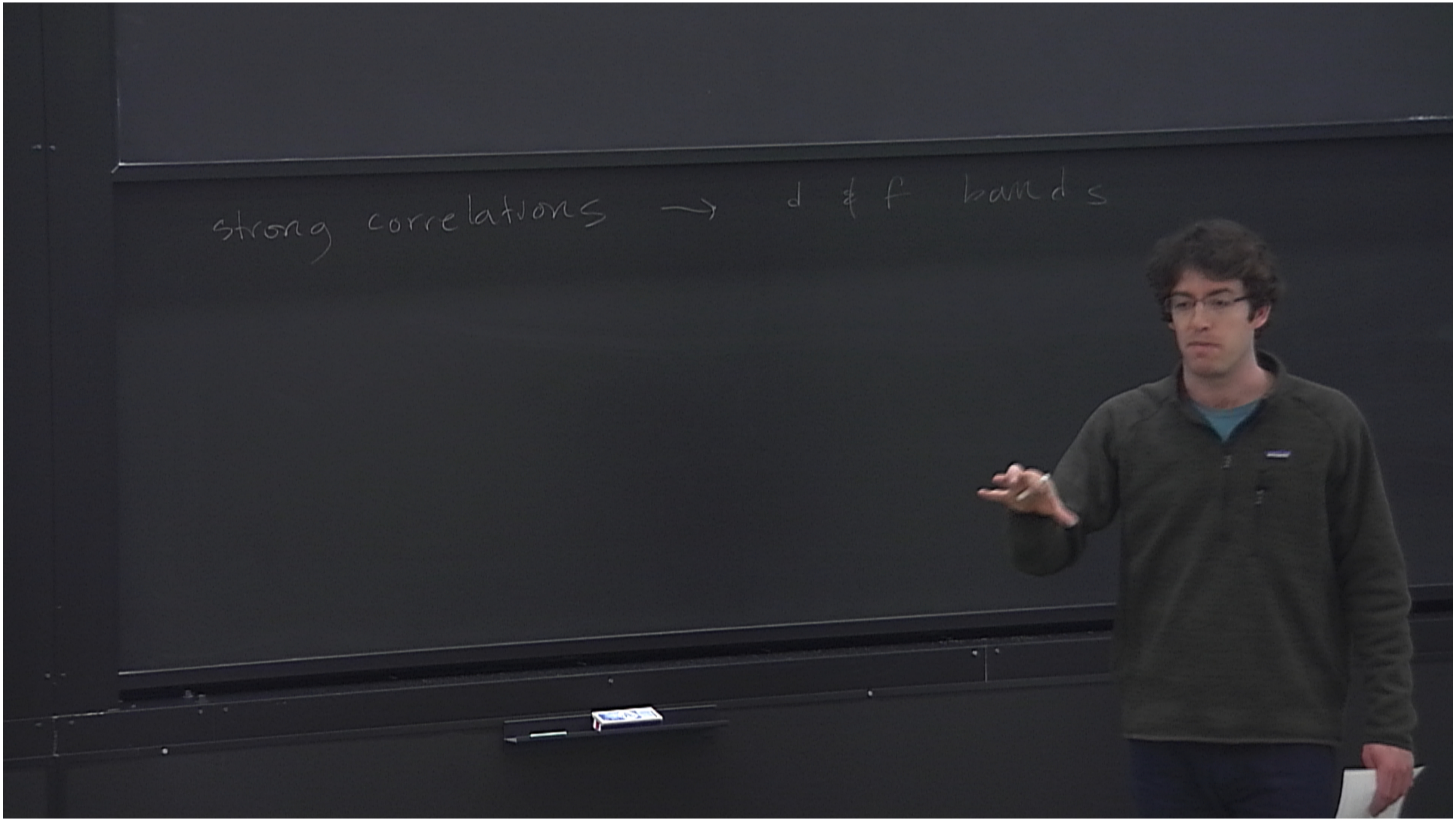

Lattice models
interactions dominate kinetic + potential

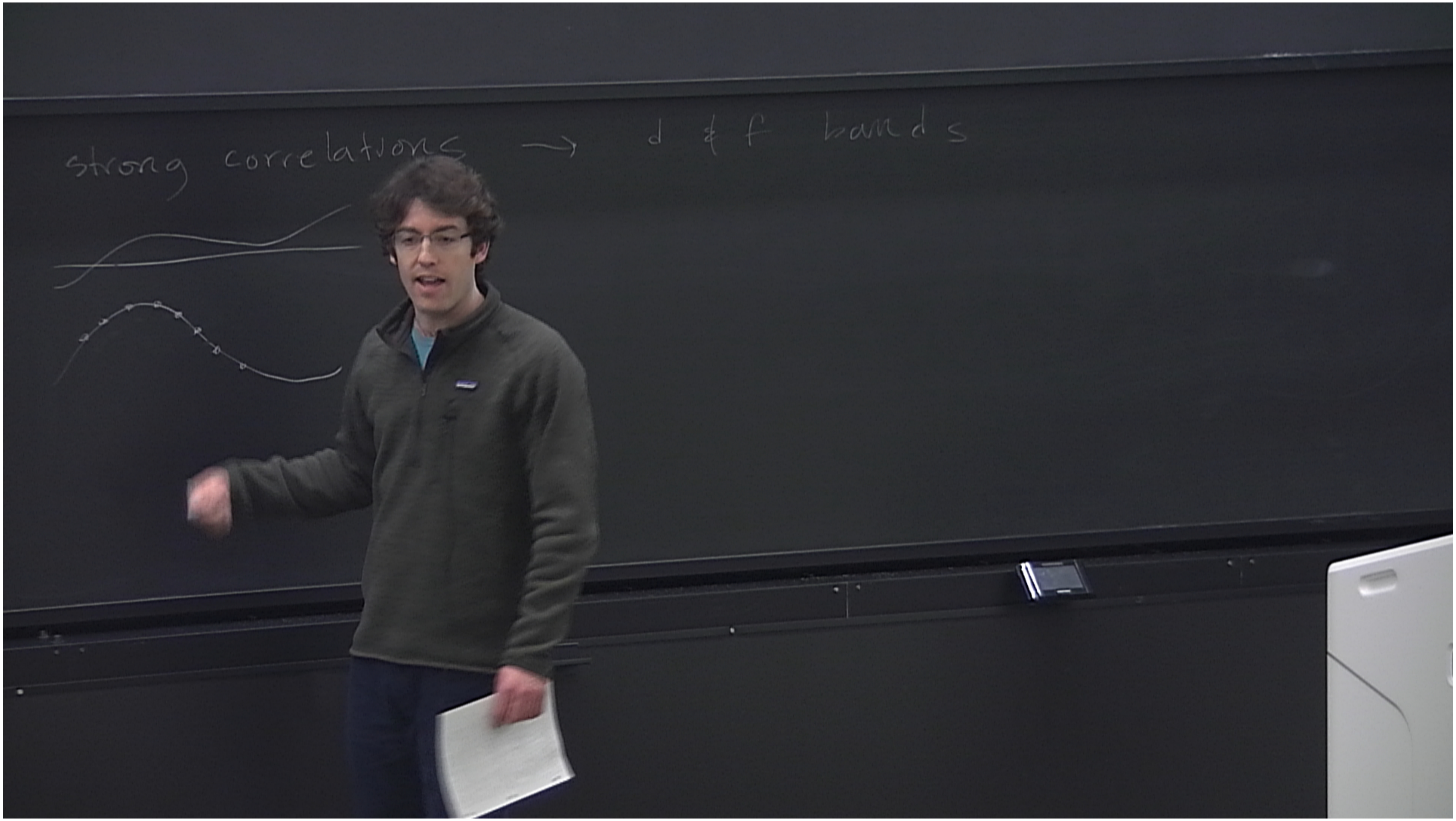

Lattice models
correlation (strong) → interactions dominate kinetic
band structure
KS-DFT
build in interactions into bands

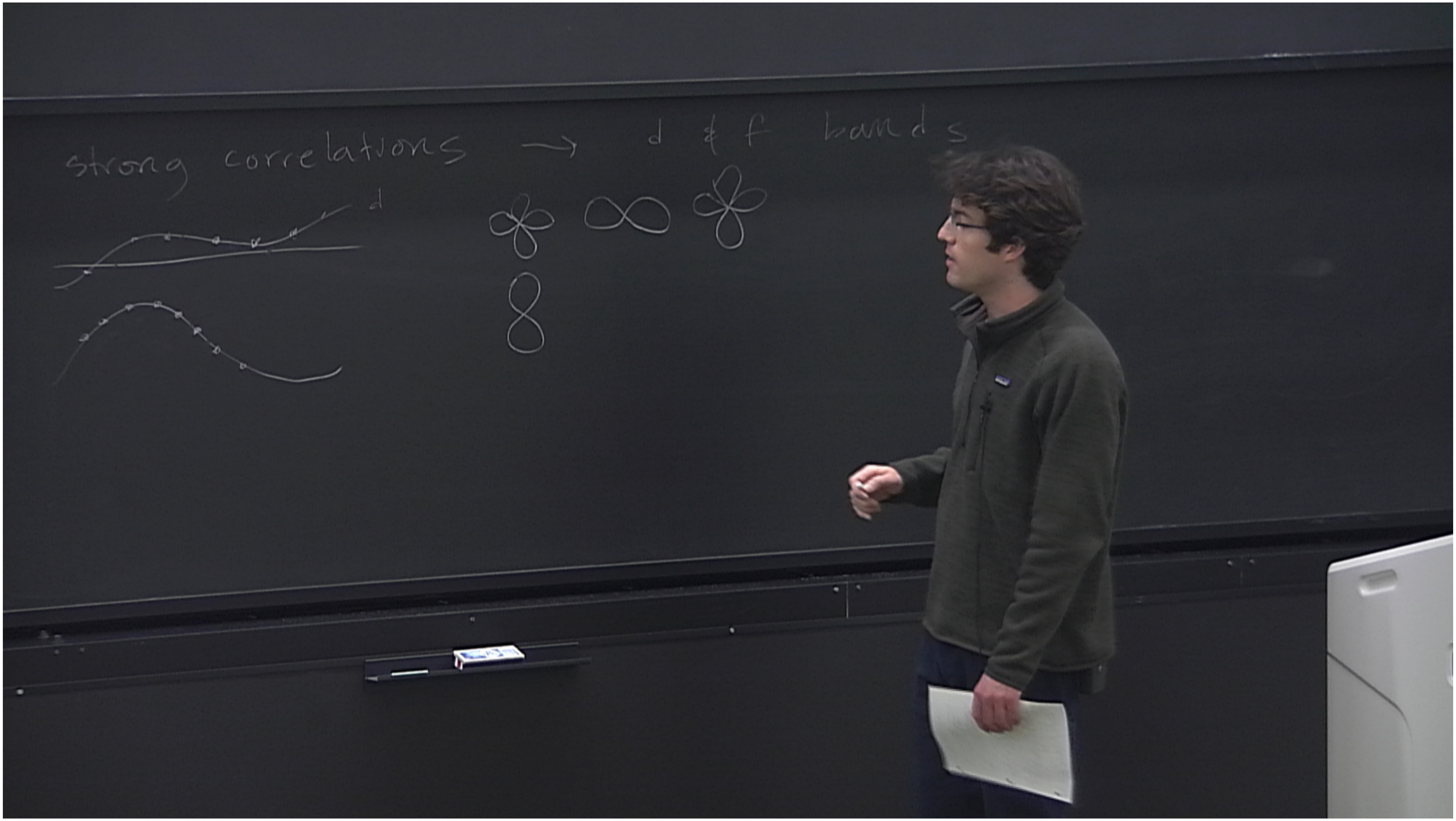

Lattice models
correlation (strong) →
dominate kinetic + potential
band structure
into bands
KS-DFT
build in
tight-binding

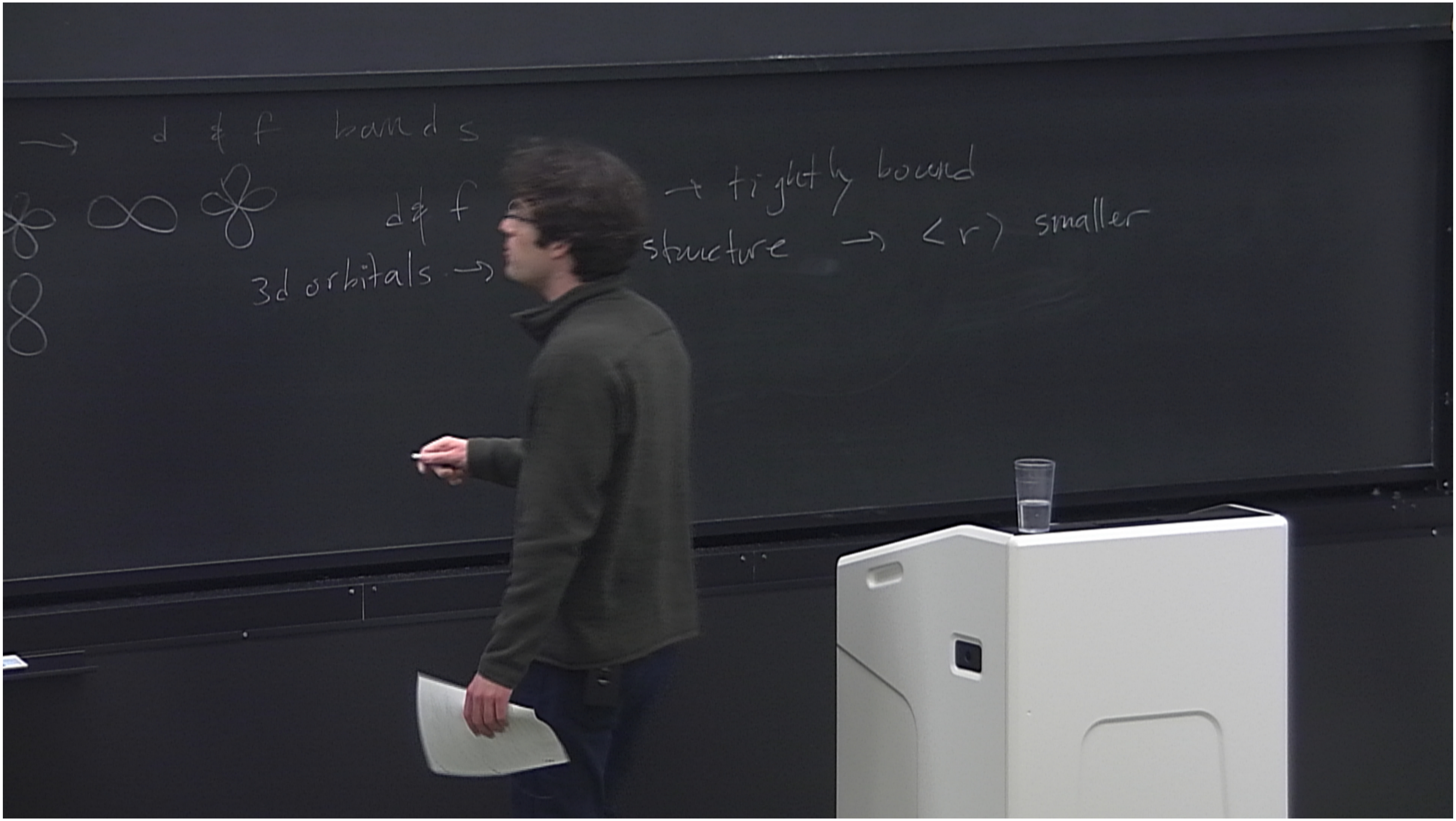

Lattice models
correlation (strong) → interactions dominate kinetic
band structure
KS-DFT
build in interactions into bands
t ~ ∫ φ*(r)[-½∇²+v(r)]
tight-binding

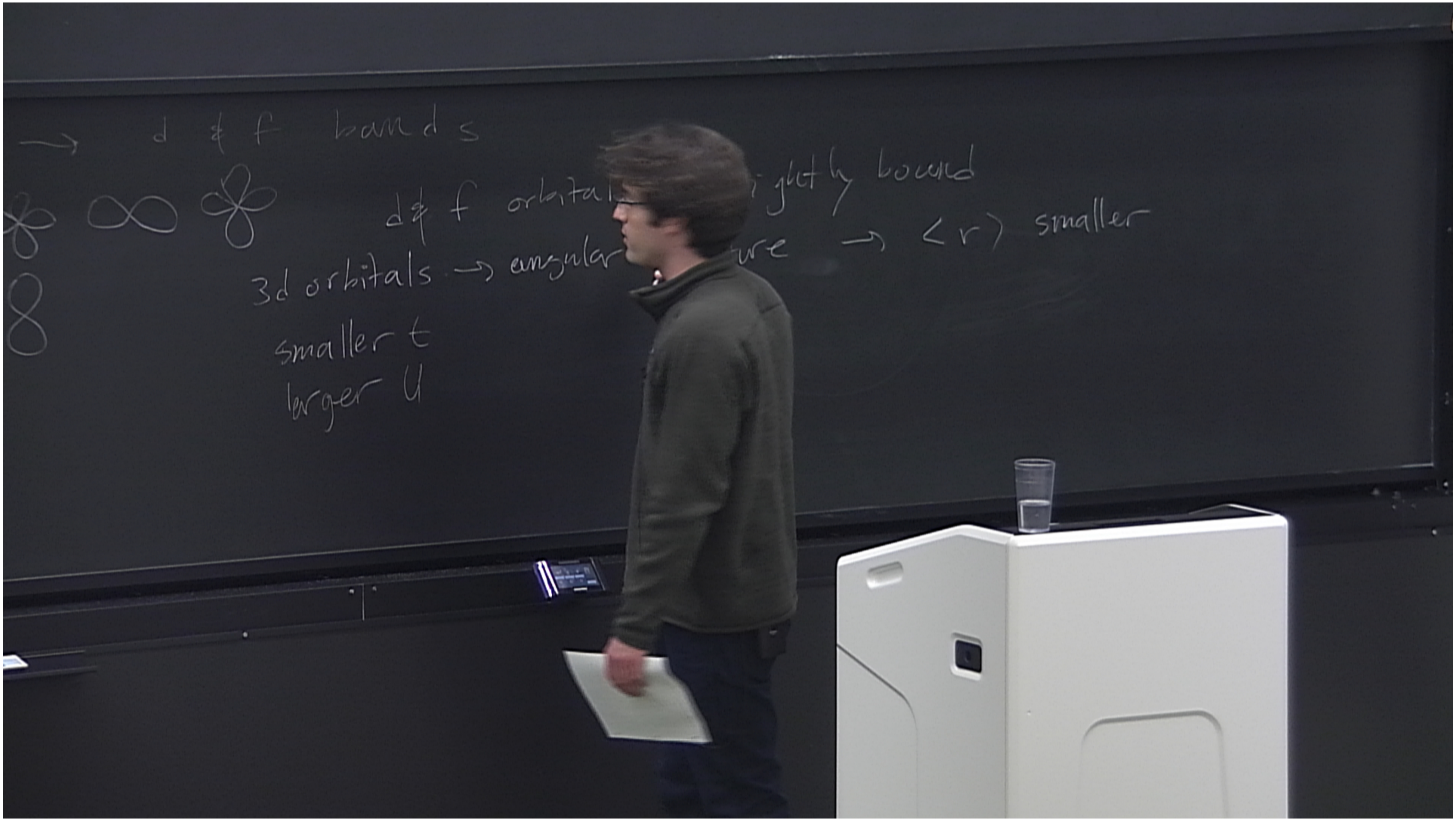

nteractions dominate kinetic + potential
interactions into bands
$t \sim \int \phi_1^*(r)\left[-\frac{1}{2}\nabla^2 + U(\vec{r})\right]\phi_2(r)$
$U \sim \int V_{col}(r-r')|\phi_1(r)|^2 |\phi_1(r')|^2$

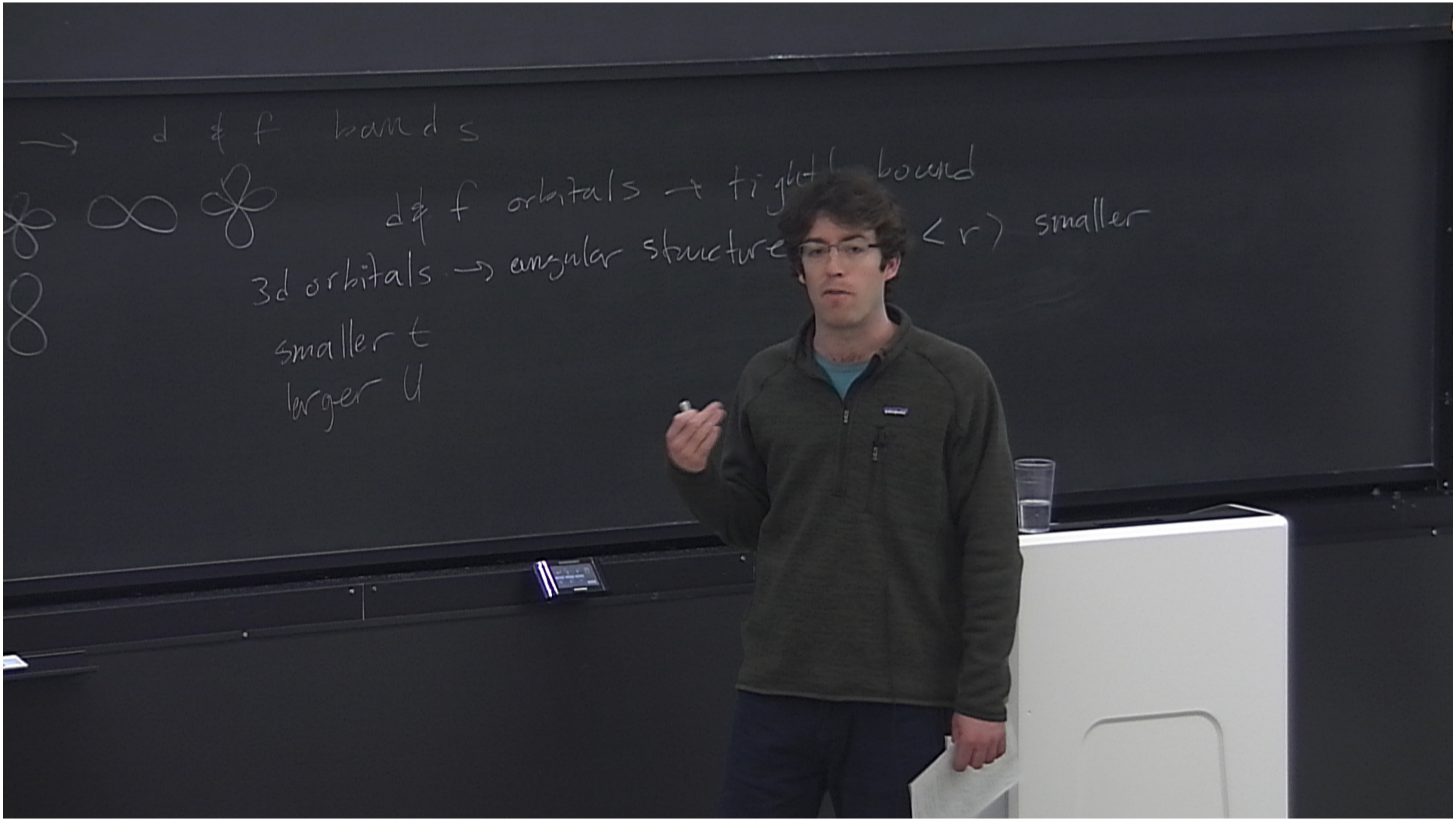

strong correlations → d & f bands

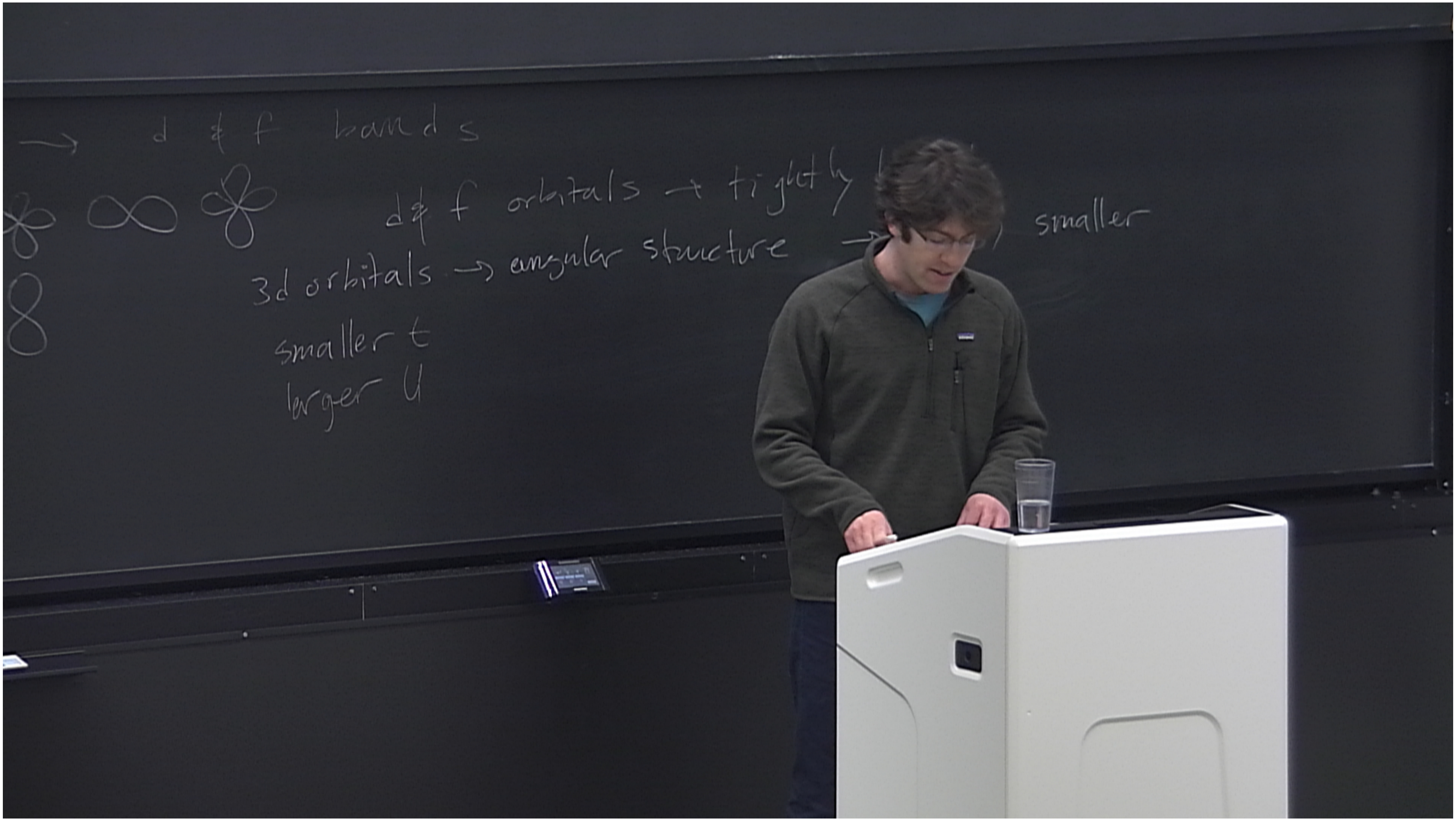

strong correlations → d & f bands

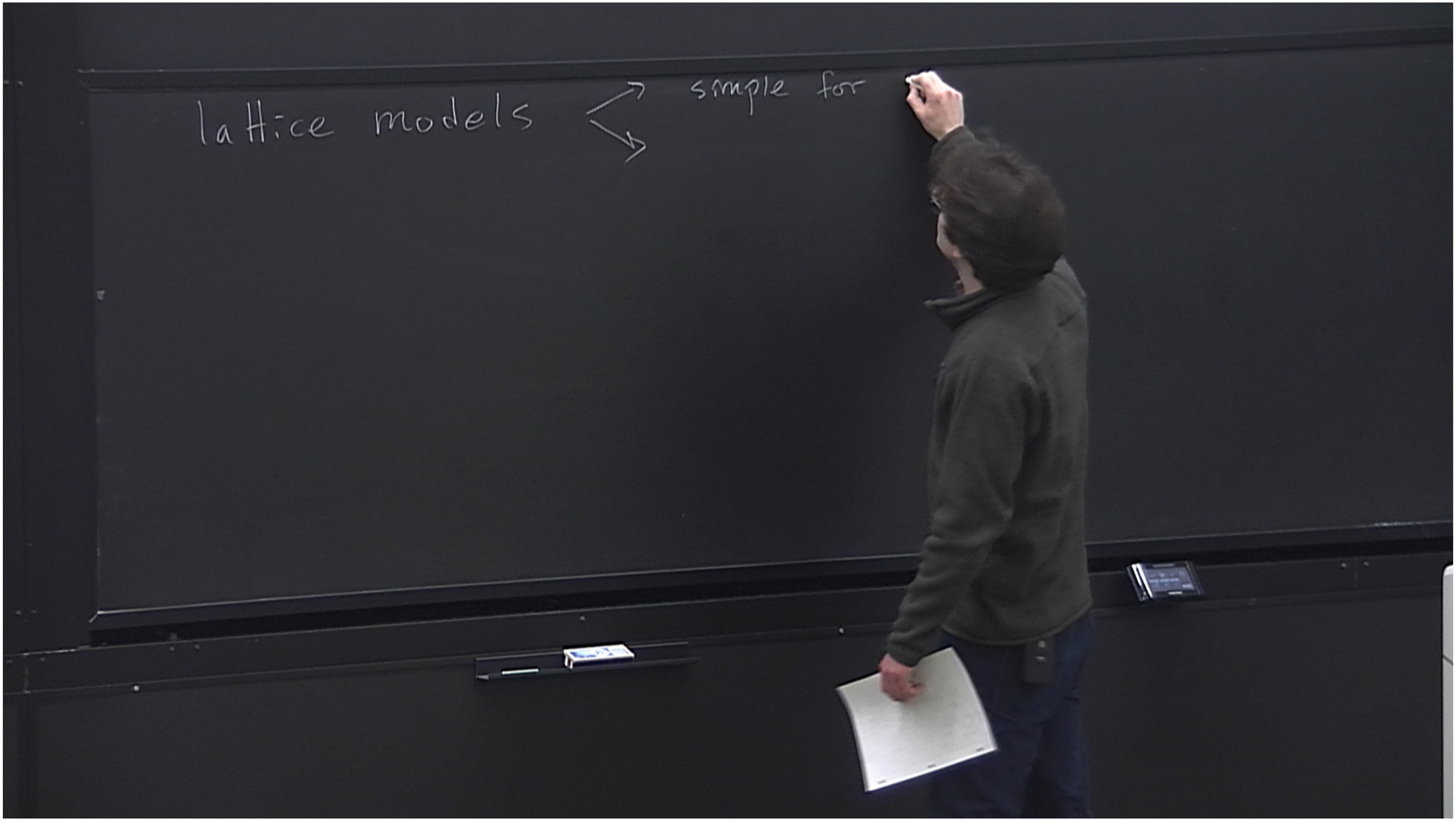

strong correlations → d & f bands
d

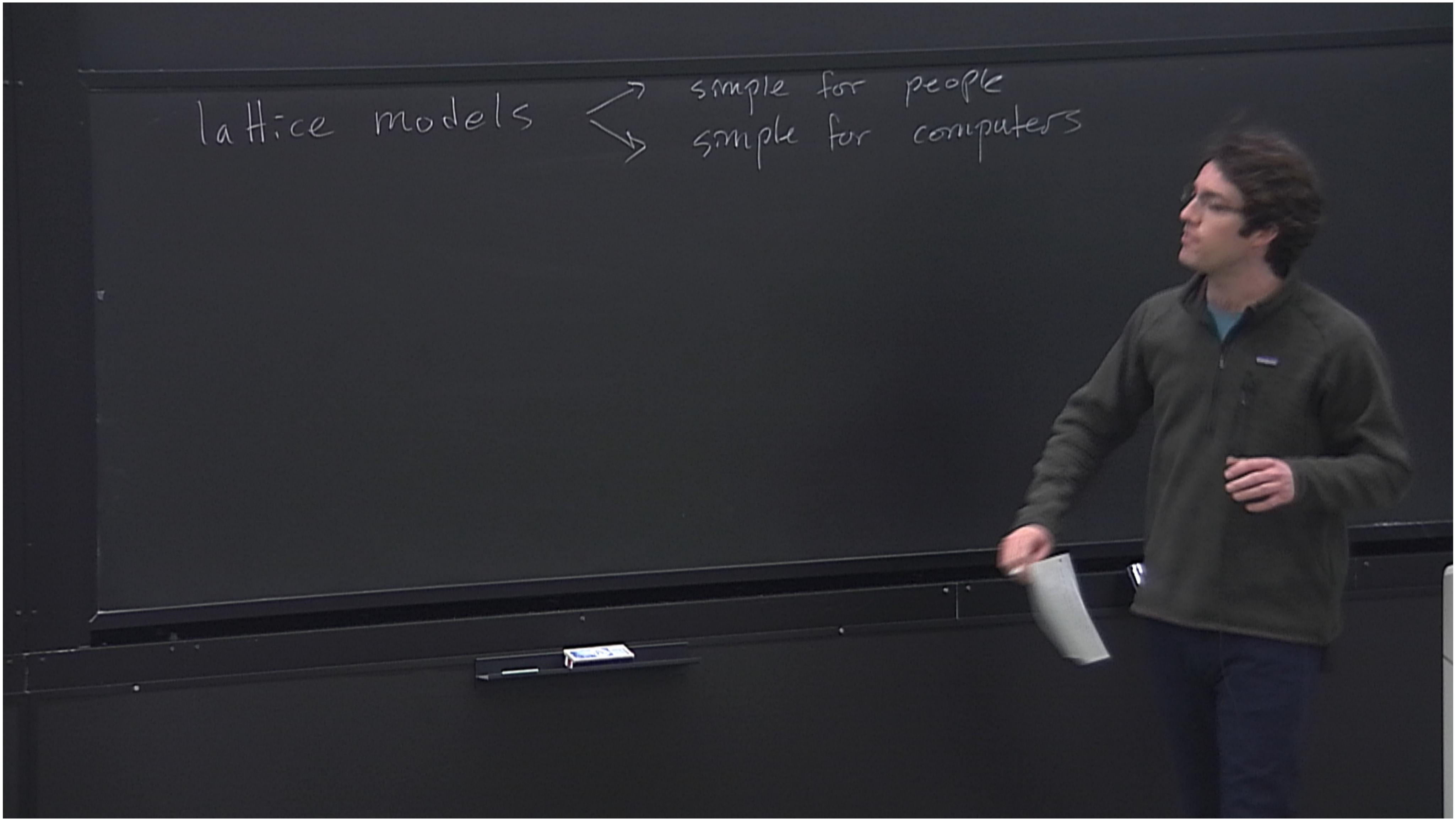

d & f bands
tightly bound
d & f
structure
<r> smaller
3d orbitals

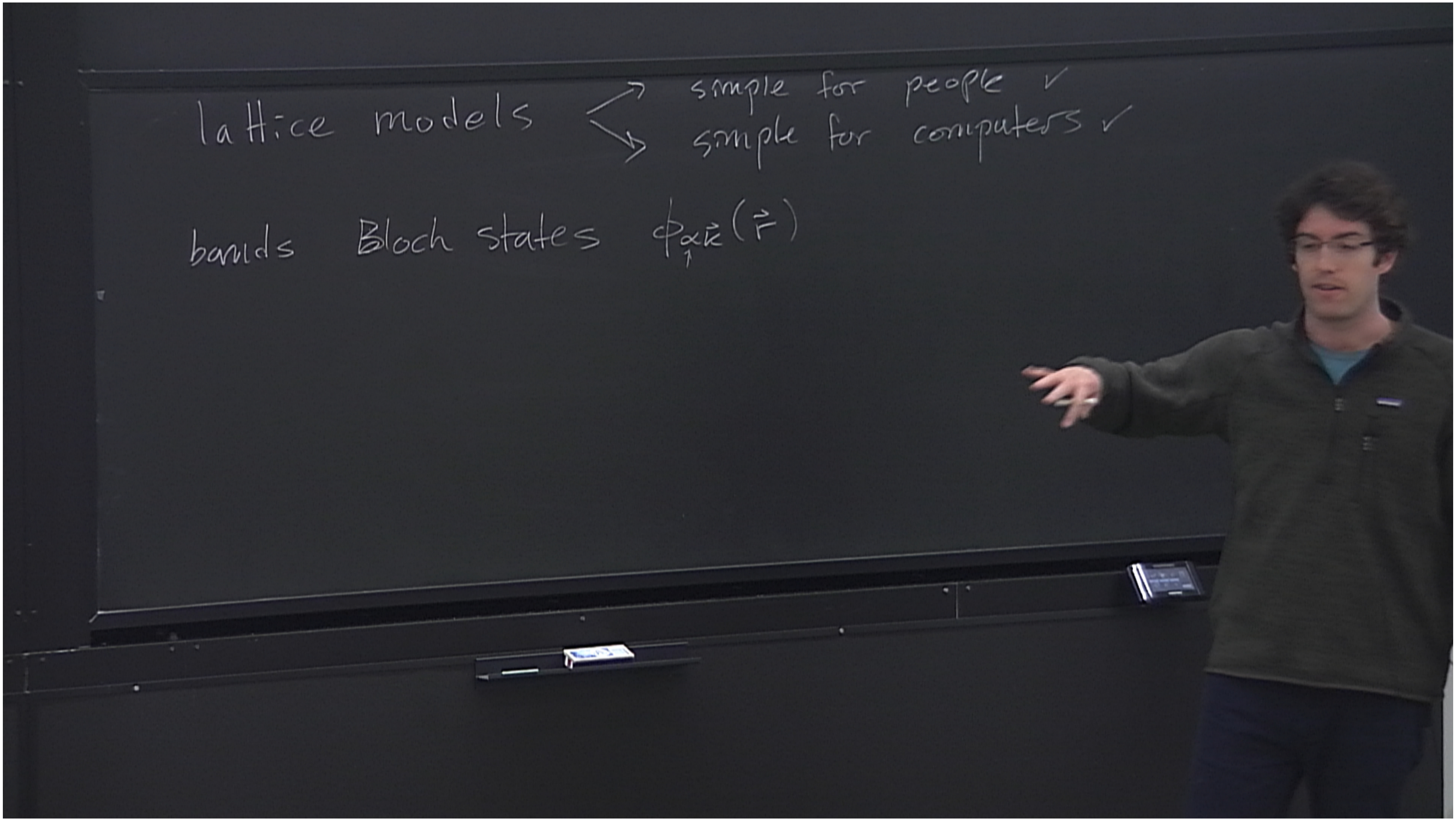

→ d & f bands
d & f
bound
3d orbitals → angular
→ $\langle r \rangle$ smaller
smaller t
larger U

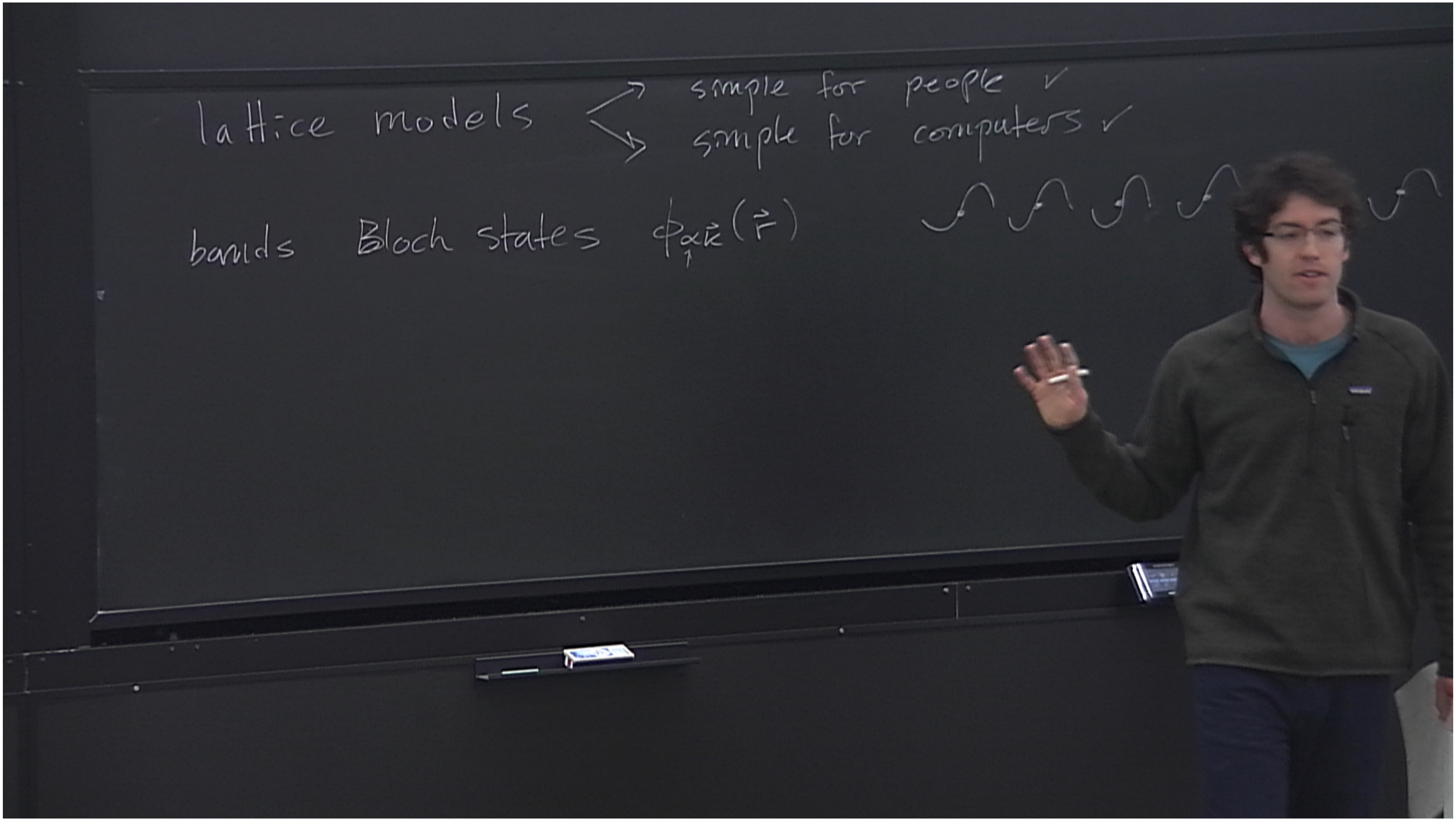

→ d & f bands
d & f orbitals →
bound
$\langle r \rangle$ smaller
3d orbitals → angular structure
smaller t
larger U

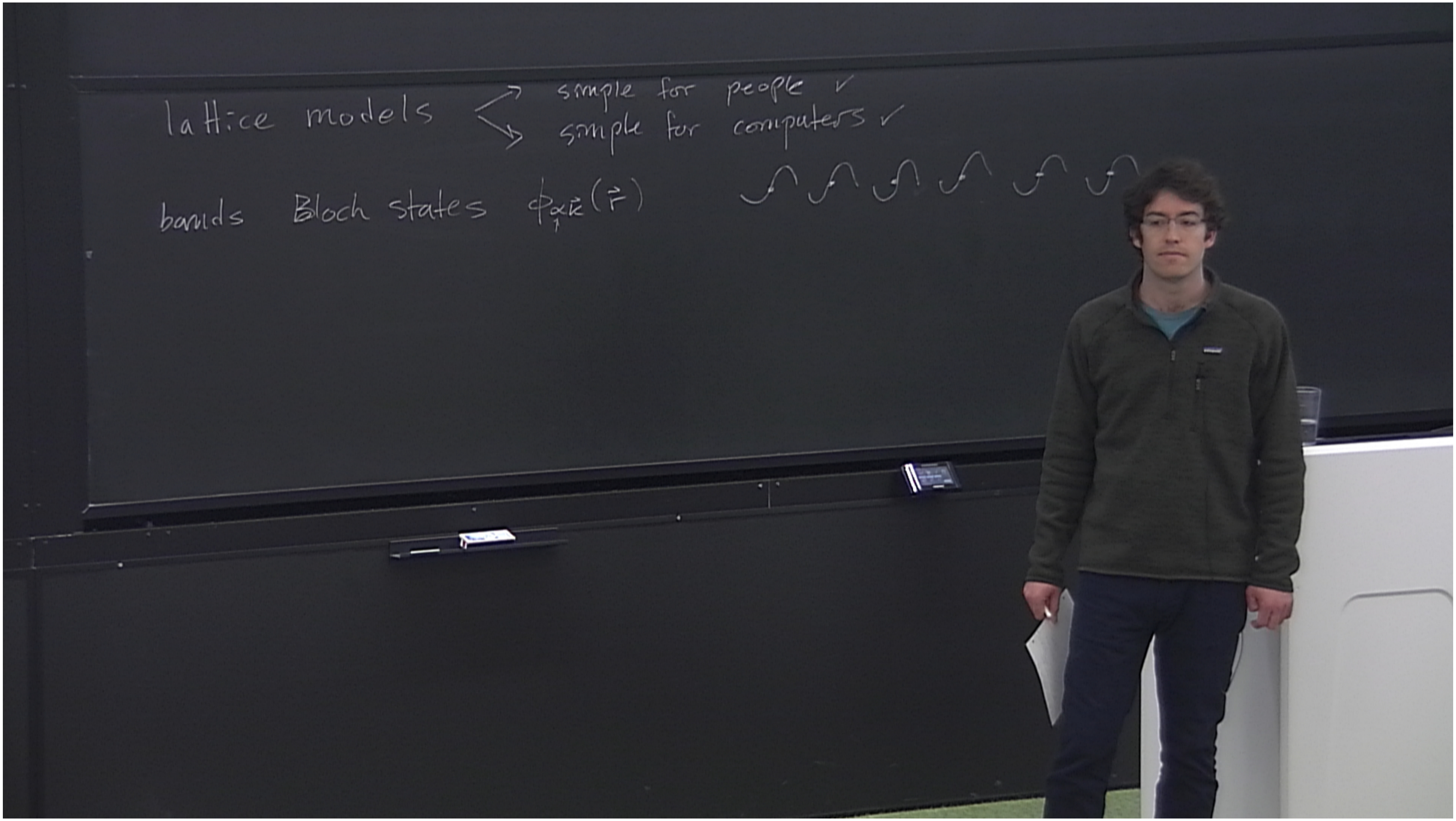

→ d & f bands
d & f orbitals → tightly
smaller
3d orbitals → angular structure →
smaller t
larger U

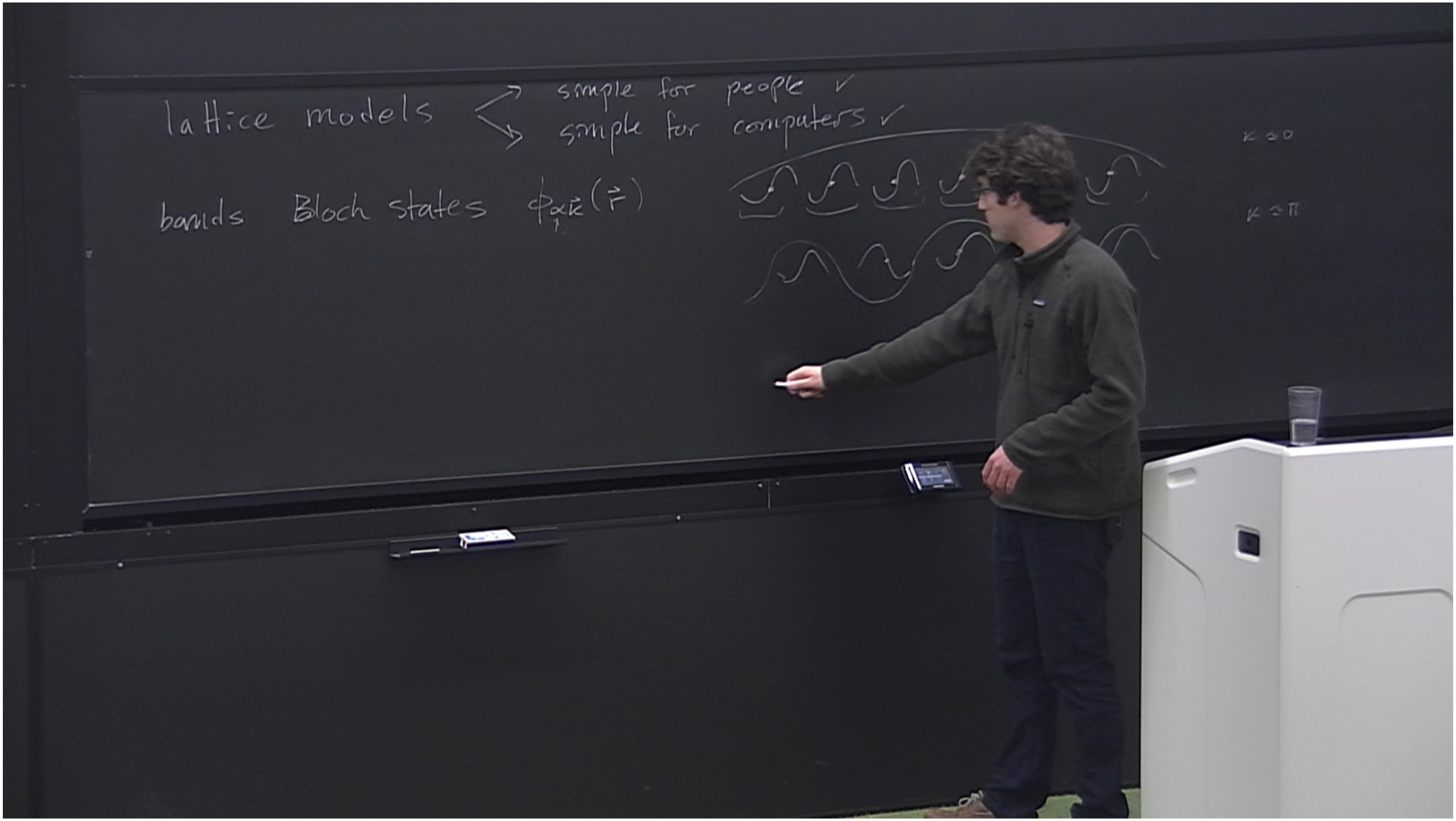

lattice models
simple for

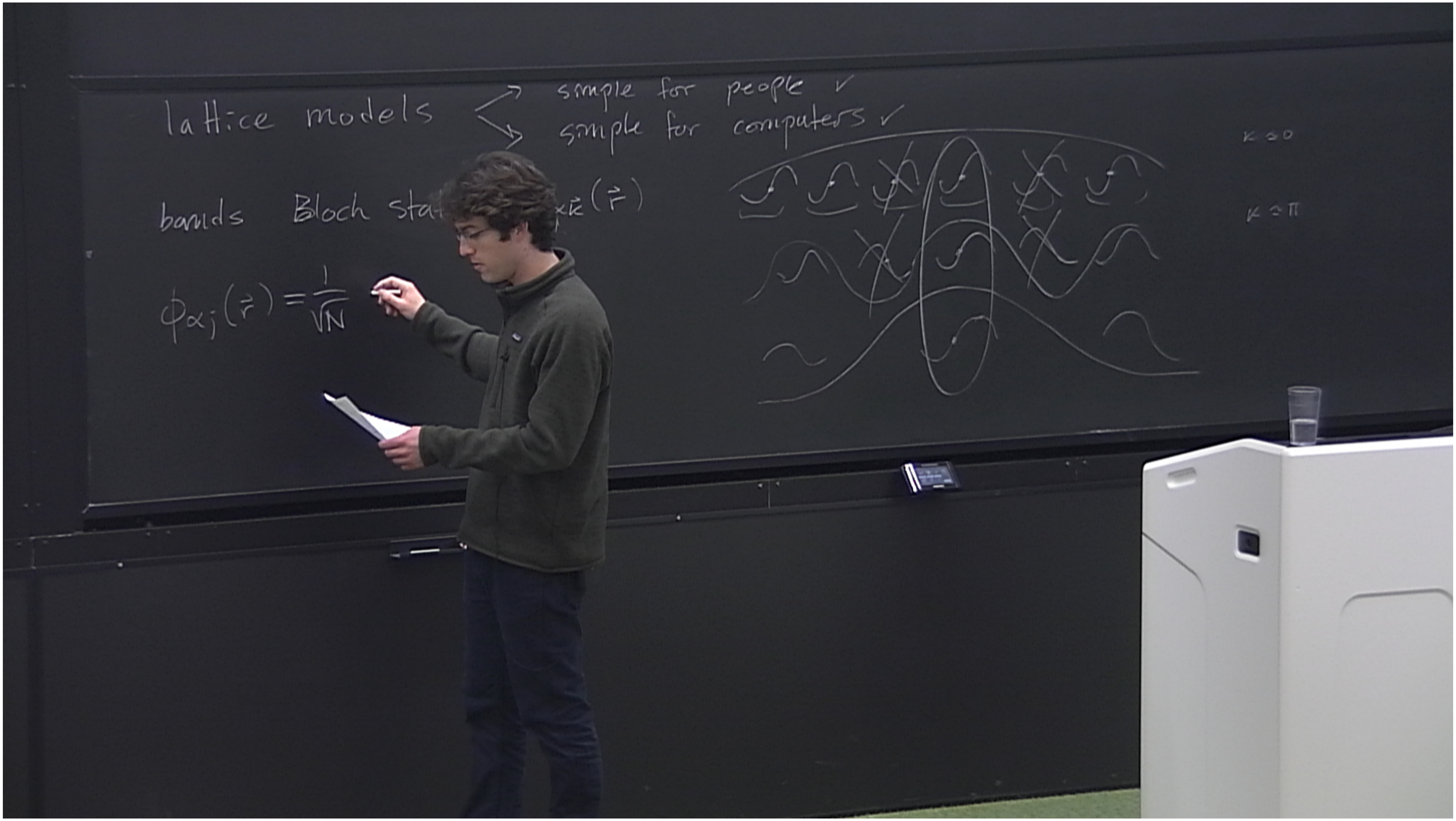

lattice models
simple for people
simple for computers

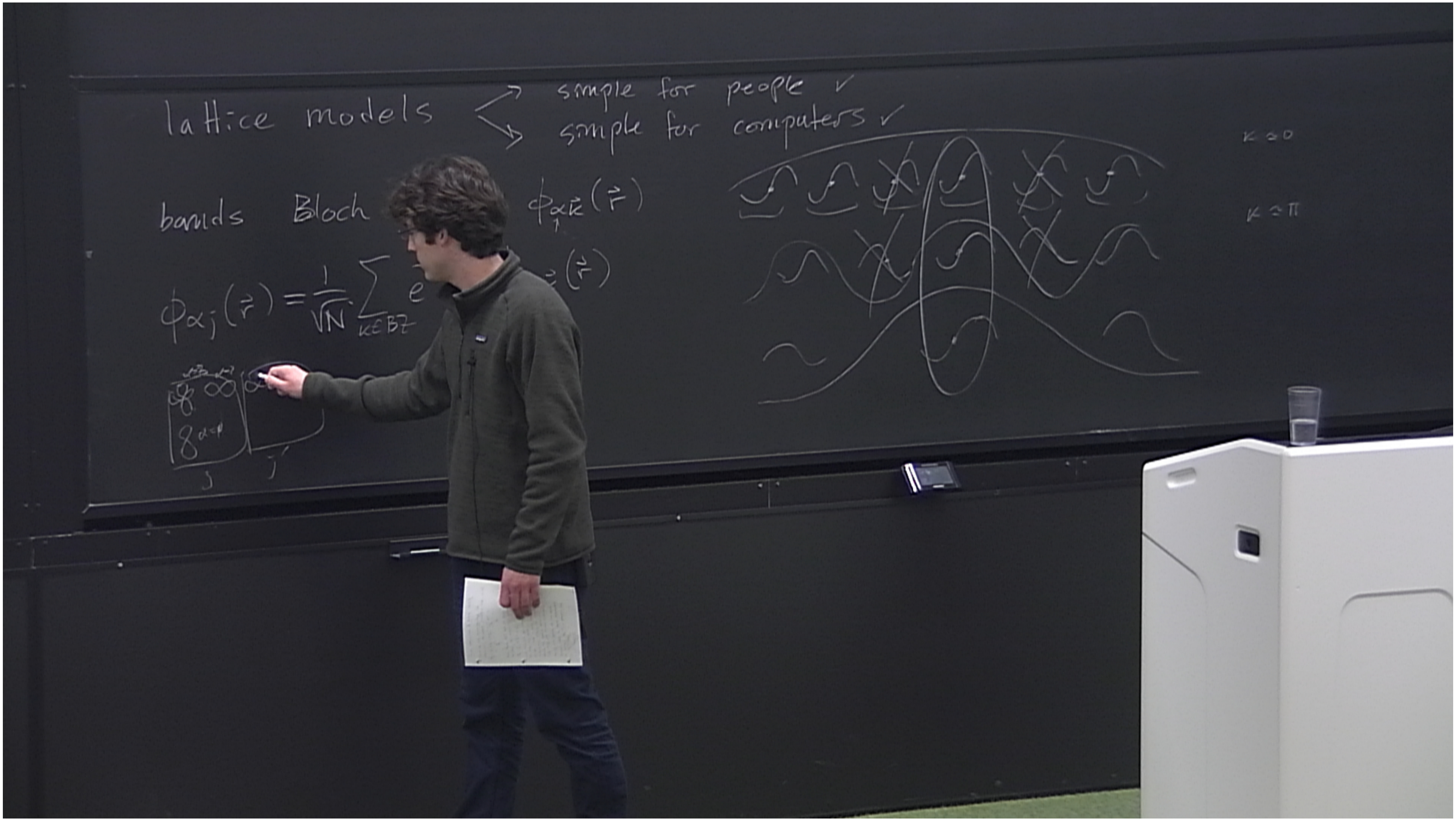

lattice models
simple for people ✓
simple for computers ✓
bands Bloch states $\phi_{\alpha\vec{k}}(\vec{r})$


lattice models
simple for people ✓
simple for computers ✓
bands Bloch states $\phi_{\alpha\vec{k}}(\vec{r})$


lattice models
simple for people ✓
simple for computers ✓
bands Bloch states $\phi_{\alpha\vec{k}}(\vec{r})$

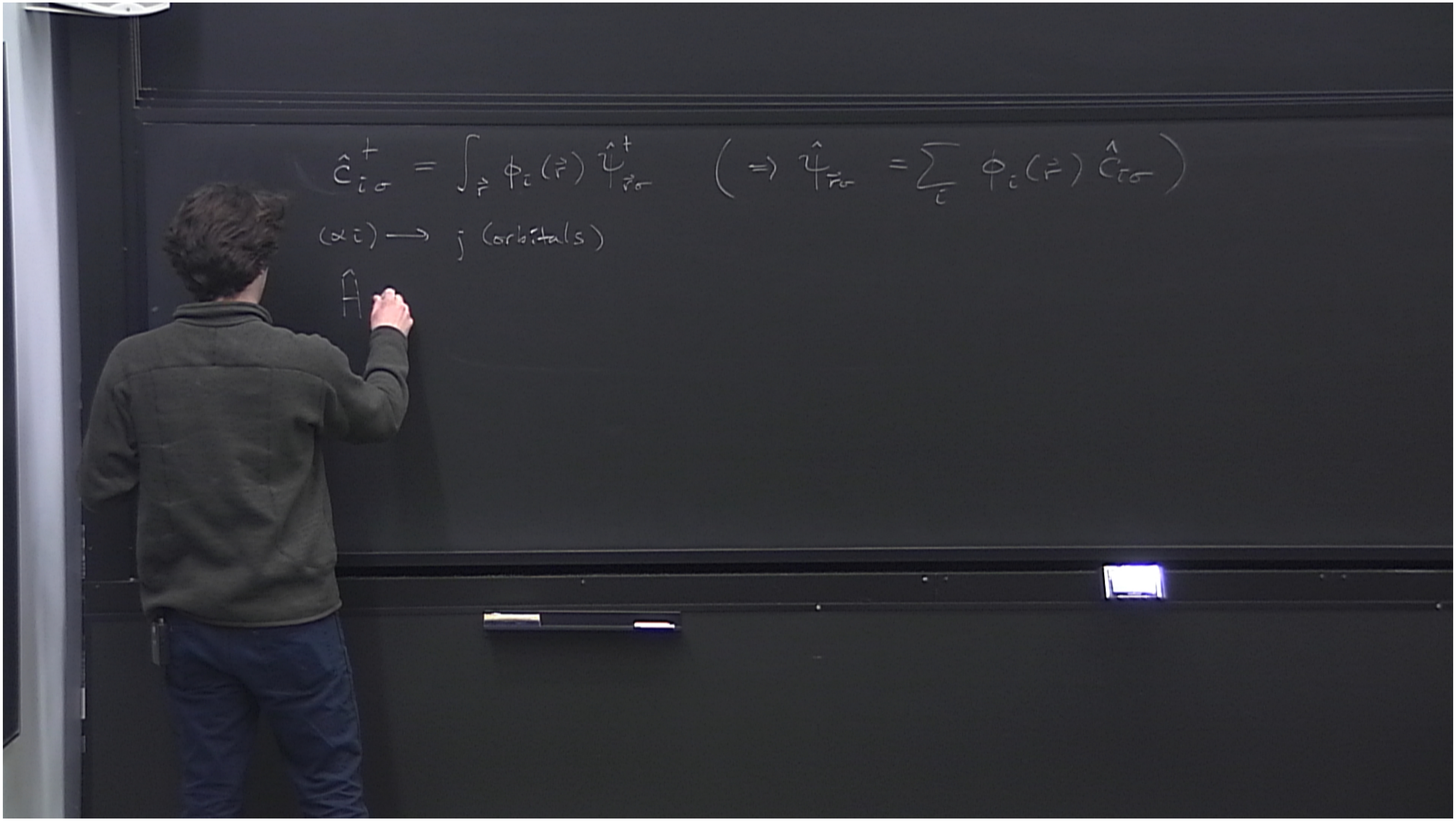

lattice models
simple for people ✓
simple for computers ✓
bands
Bloch states
$\phi_{\alpha \vec{k}}(\vec{r})$
k ≈ 0
k ≈ π

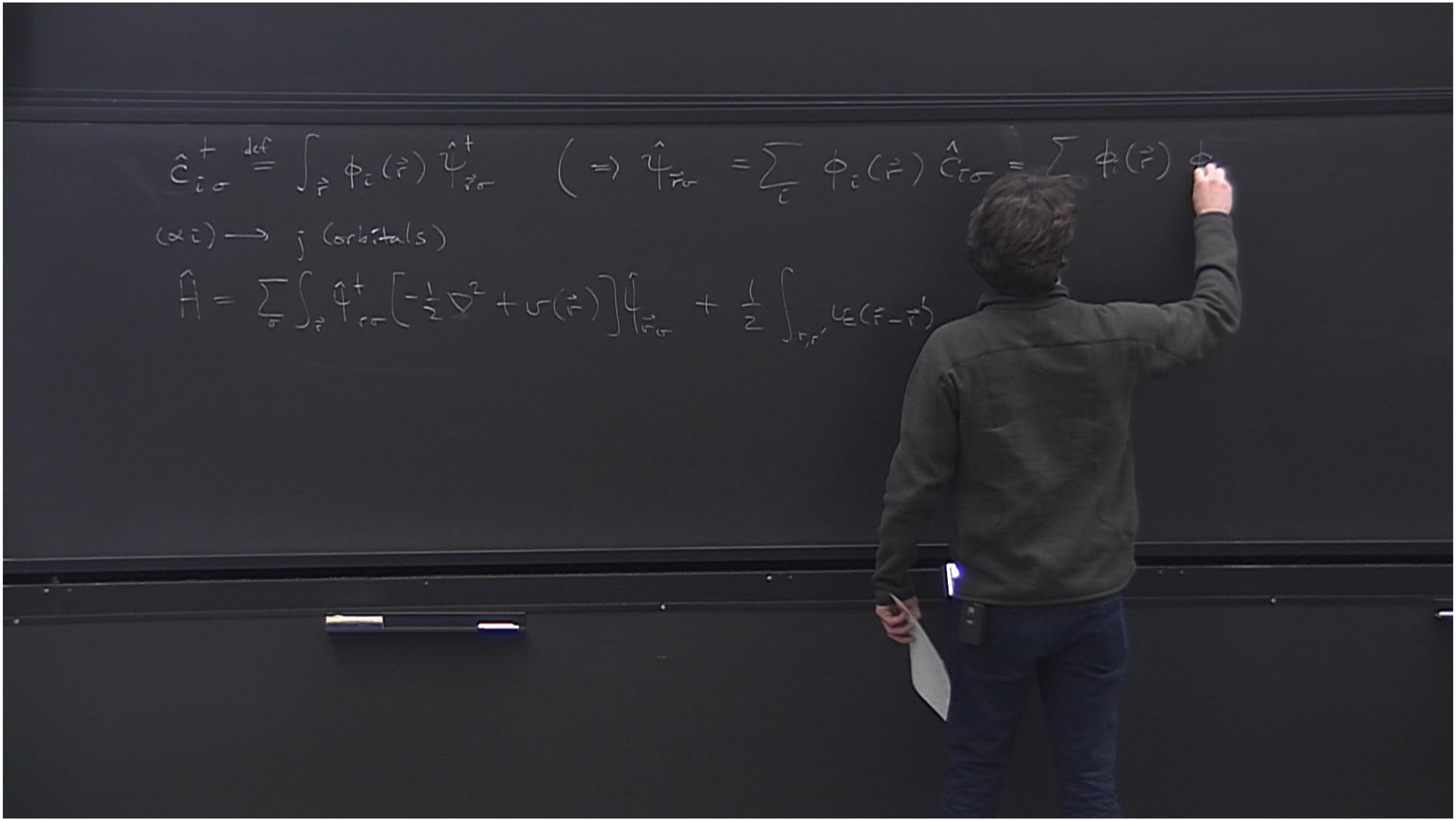

lattice models
simple for people
simple for computers
bands
Bloch sta

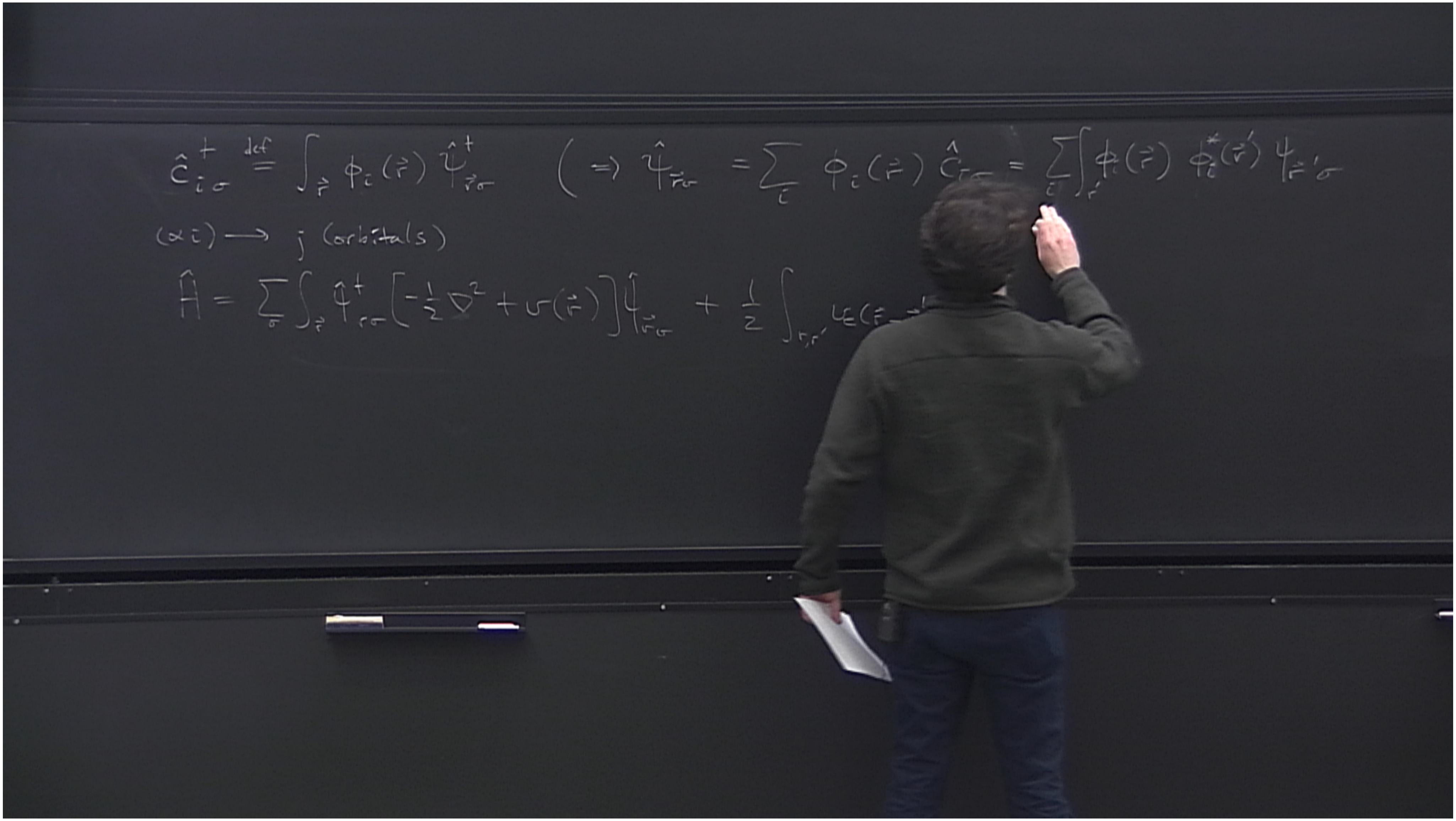

lattice models
simple for people ✓
simple for computers ✓
bands
Bloch
κ = 0
κ = π
κ ∈ BZ

$$\hat{c}^{\dagger}_{i\sigma} = \int_{\vec{r}} \phi_i(\vec{r})\, \hat{\psi}^{\dagger}_{\vec{r}\sigma}$$

$$(\alpha i) \longrightarrow j$$


$\hat{c}^{\dagger}_{i\sigma} = \int_{\vec{r}} \phi_i(\vec{r})\, \hat{\psi}^{\dagger}_{\vec{r}\sigma}$ $\left(\Rightarrow \hat{\psi}_{\vec{r}\sigma} = \sum_i \phi_i(\vec{r})\, \hat{c}_{i\sigma} \right)$
$(\alpha i) \longrightarrow j$ (orbitals)
$\hat{A}$

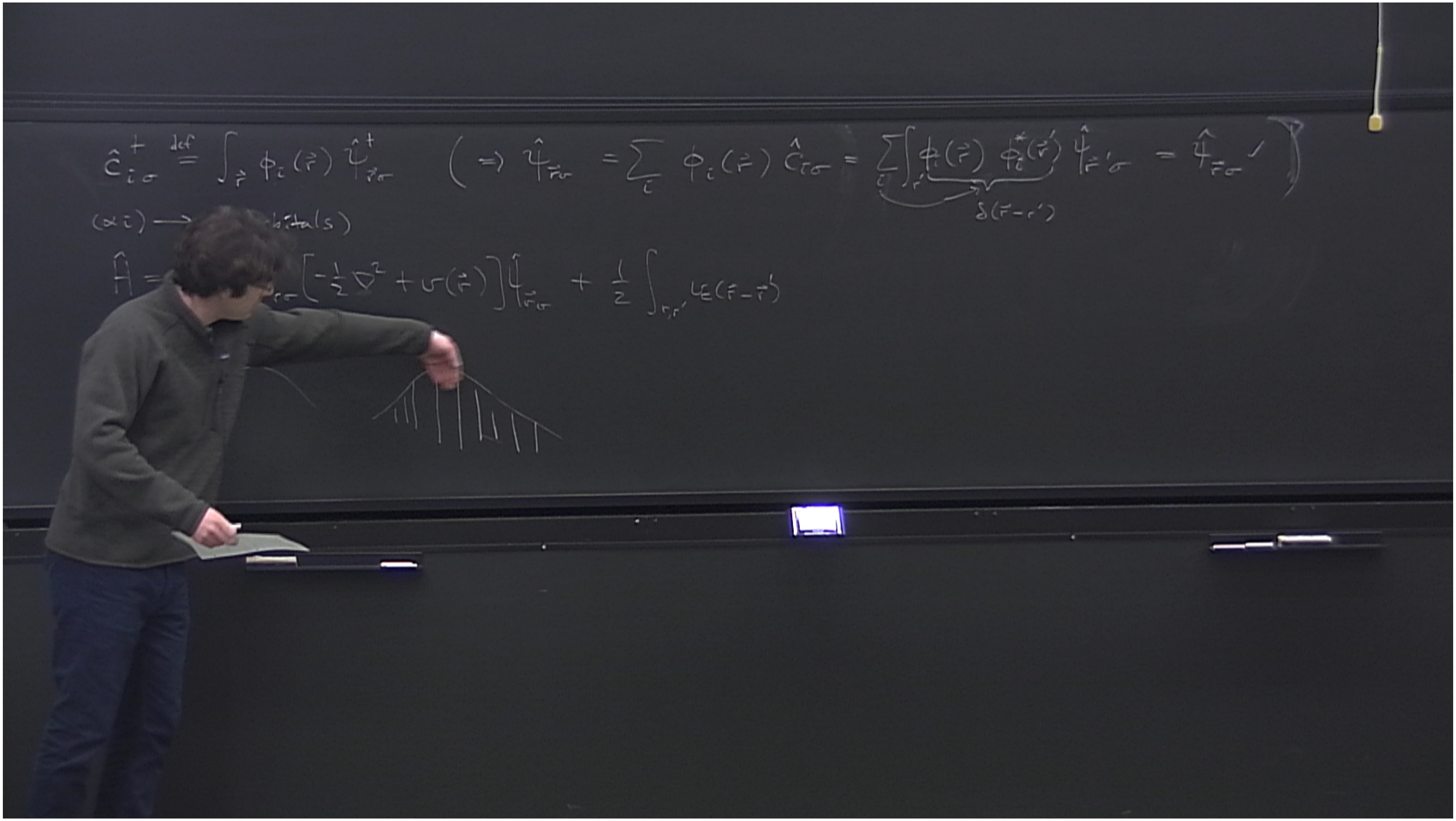

$\hat{c}^{\dagger}_{i\sigma} \overset{\text{def}}{=} \int_{\vec{r}} \phi_i(\vec{r})\, \hat{\psi}^{\dagger}_{\vec{r}\sigma}$ $\Big(\Rightarrow \hat{\psi}_{\vec{r}\sigma} = \sum_i \phi_i(\vec{r})\, \hat{c}_{i\sigma} = \sum \phi_i(\vec{r})\, \phi$
$(\alpha i) \longrightarrow j$ (orbitals)
$\hat{H} = \sum_\sigma \int_{\vec{r}} \hat{\psi}^{\dagger}_{\vec{r}\sigma} \left[-\frac{1}{2}\nabla^2 + v(\vec{r}) \right] \hat{\psi}_{\vec{r}\sigma} + \frac{1}{2} \int_{r,r'} w(\vec{r}-\vec{r}')$

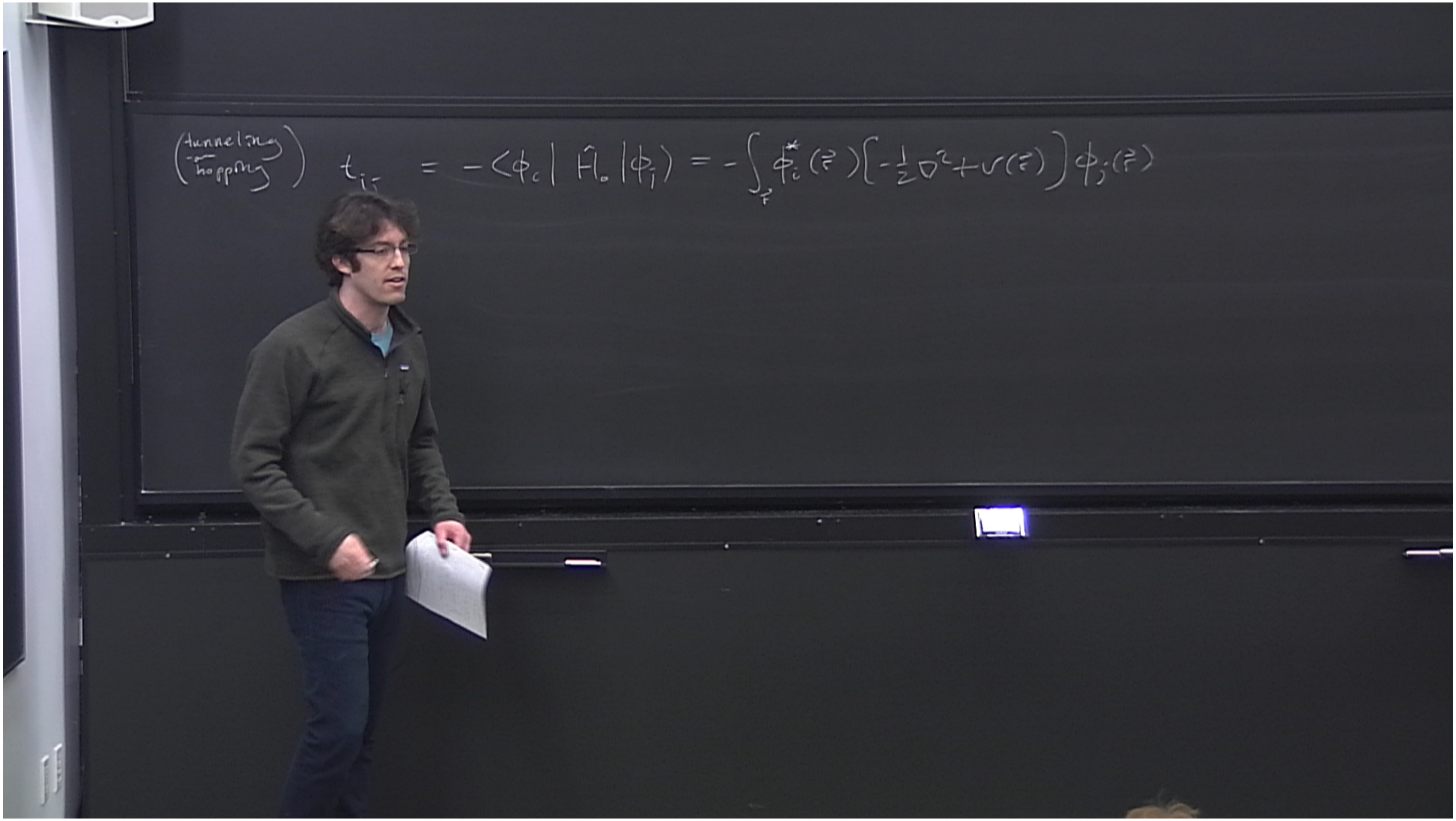

$\hat{c}^{\dagger}_{i\sigma} \stackrel{def}{=} \int_{\vec r} \phi_i(\vec r)\, \hat\psi^{\dagger}_{\vec r\sigma}$ $\Big(\Rightarrow \hat\psi_{\vec r\sigma} = \sum_i \phi_i(\vec r)\, \hat c_{i\sigma} = \sum_i \int_{r'} \phi_i(\vec r)\, \phi_i^*(\vec r')\, \psi_{\vec r'\sigma}$
$(\alpha i) \longrightarrow j$ (orbitals)
$\hat H = \sum_\sigma \int_{\vec r} \hat\psi^{\dagger}_{r\sigma} \left[-\frac{1}{2}\nabla^2 + v(\vec r)\right] \hat\psi_{\vec r\sigma} + \frac{1}{2}\int_{r,r'}$

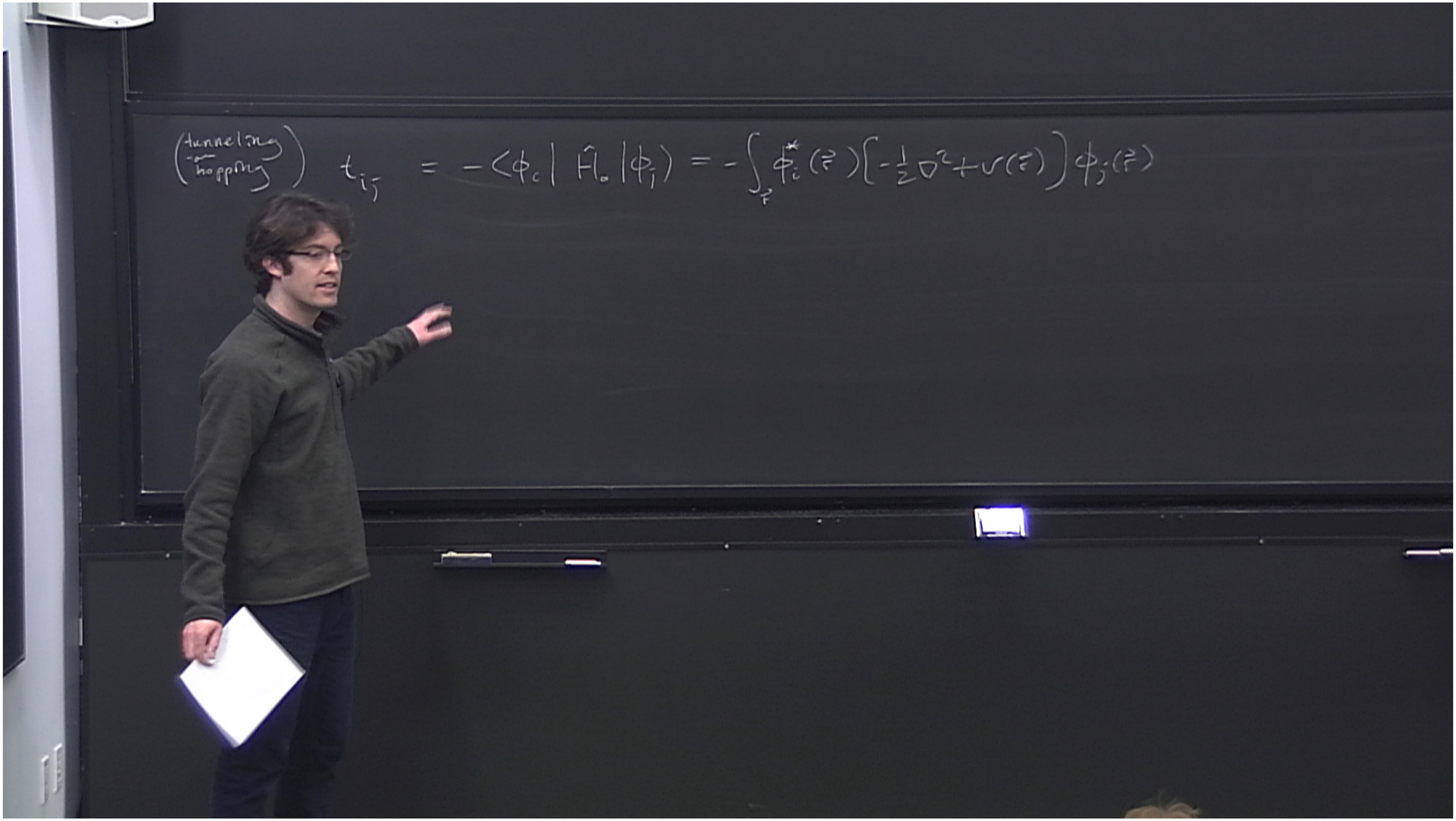
$$\hat{c}^{\dagger}_{i\sigma} \stackrel{\text{def}}{=} \int_{\vec{r}} \phi_i(\vec{r})\, \hat{\psi}^{\dagger}_{\vec{r}\sigma} \qquad \left(\Rightarrow \hat{\psi}_{\vec{r}\sigma} = \sum_i \phi_i(\vec{r})\, \hat{c}_{i\sigma} = \sum_i \int_{r'} \underbrace{\phi_i(\vec{r})\, \phi_i^*(\vec{r}')}_{\delta(\vec{r}-\vec{r}')} \hat{\psi}_{\vec{r}'\sigma} = \hat{\psi}_{\vec{r}\sigma} \checkmark \right)$$

$(\alpha i) \longrightarrow j$ (orbitals)

$$\hat{H} = \sum_\sigma \int_{\vec{r}} \hat{\psi}^{\dagger}_{\vec{r}\sigma} \left[-\frac{1}{2}\nabla^2 + v(\vec{r}) \right] \hat{\psi}_{\vec{r}\sigma} + \frac{1}{2} \int_{r,r'} u(\vec{r}-\vec{r}')$$


$\hat{c}^\dagger_{i\sigma} \overset{\text{def}}{=} \int_{\vec{r}} \phi_i(\vec{r})\, \hat{\psi}^\dagger_{\vec{r}\sigma}$ $\left(\Rightarrow \hat{\psi}_{\vec{r}\sigma} = \sum_i \phi_i(\vec{r})\, \hat{c}_{i\sigma} = \sum_i \int_{\vec{r}'} \underbrace{\phi_i(\vec{r})\, \phi_i^*(\vec{r}')}_{\delta(\vec{r}-\vec{r}')} \hat{\psi}_{\vec{r}'\sigma} = \hat{\psi}_{\vec{r}\sigma} \checkmark \right)$
$(\alpha i) \longrightarrow$
$\hat{H} =$
$\left[-\frac{1}{2}\nabla^2 + v(\vec{r})\right]\hat{\psi}_{\vec{r}\sigma} + \frac{1}{2}\int_{r,r'}$


(tunneling or hopping)
$t_{ij} = -\langle \phi_i | \hat{H}_0 | \phi_j \rangle = -\int_{\vec{r}} \phi_i^*(\vec{r}) \left[-\frac{1}{2}\nabla^2 + v(\vec{r}) \right] \phi_j(\vec{r})$


(tunneling or hopping)
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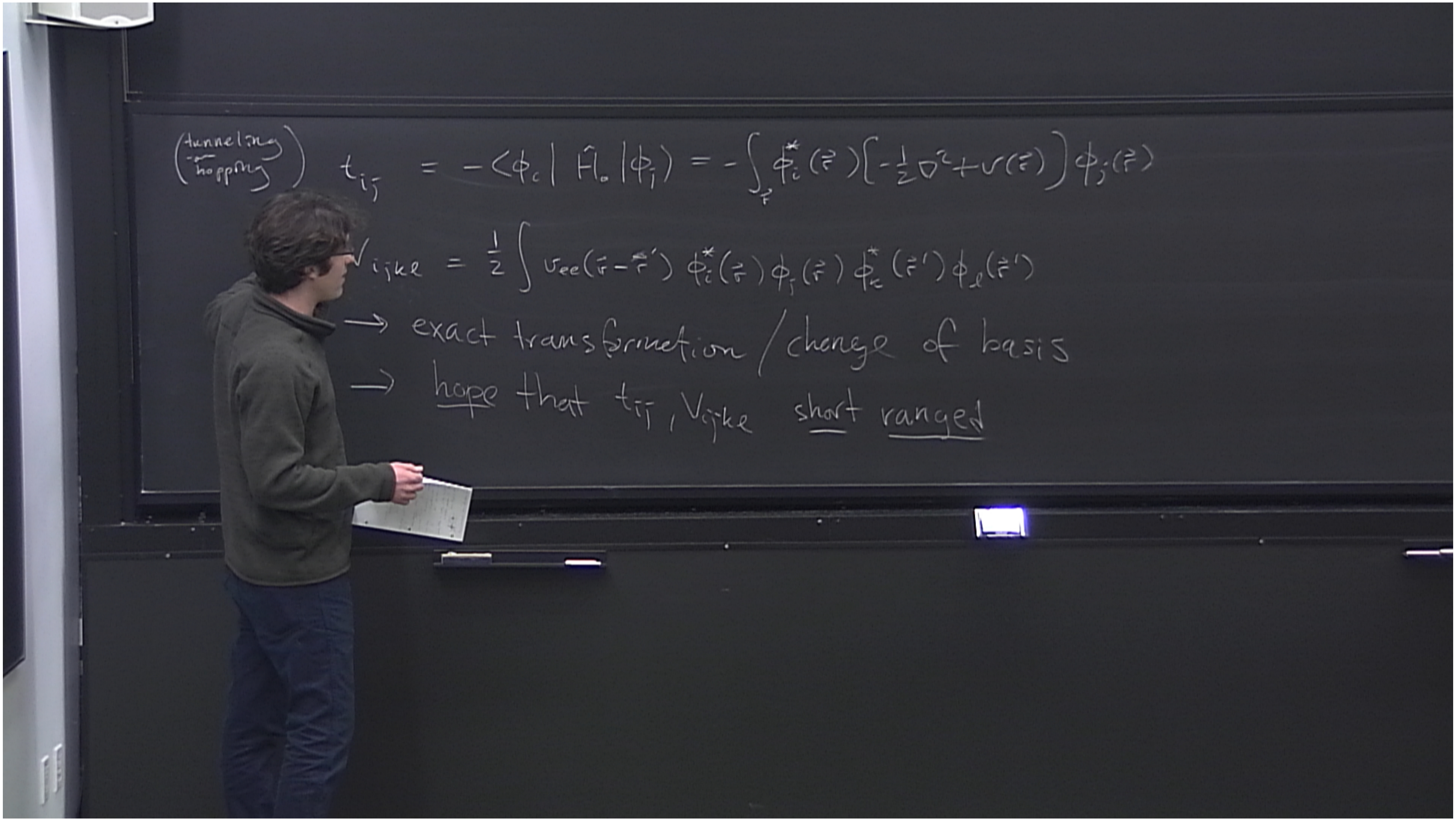
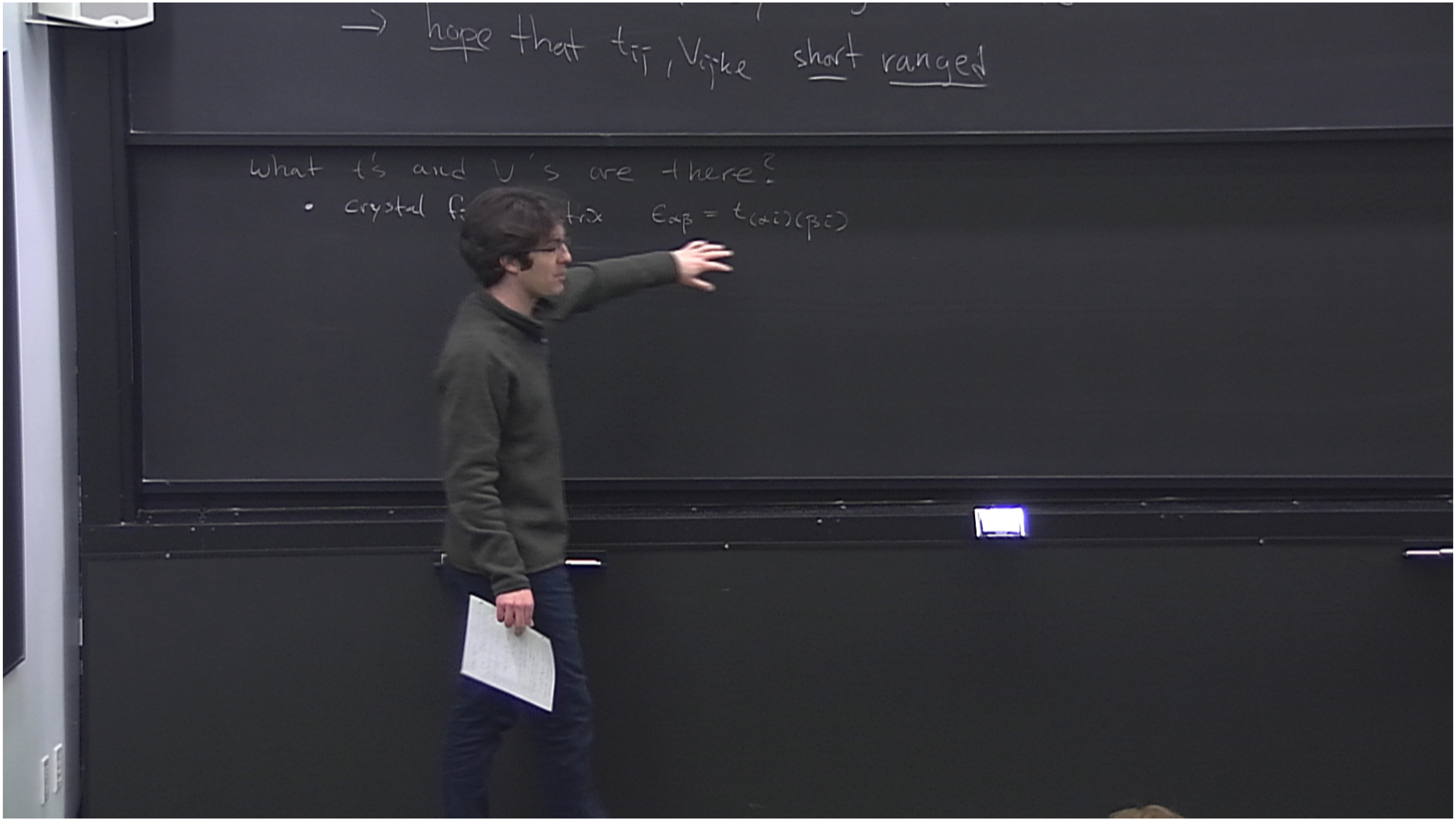
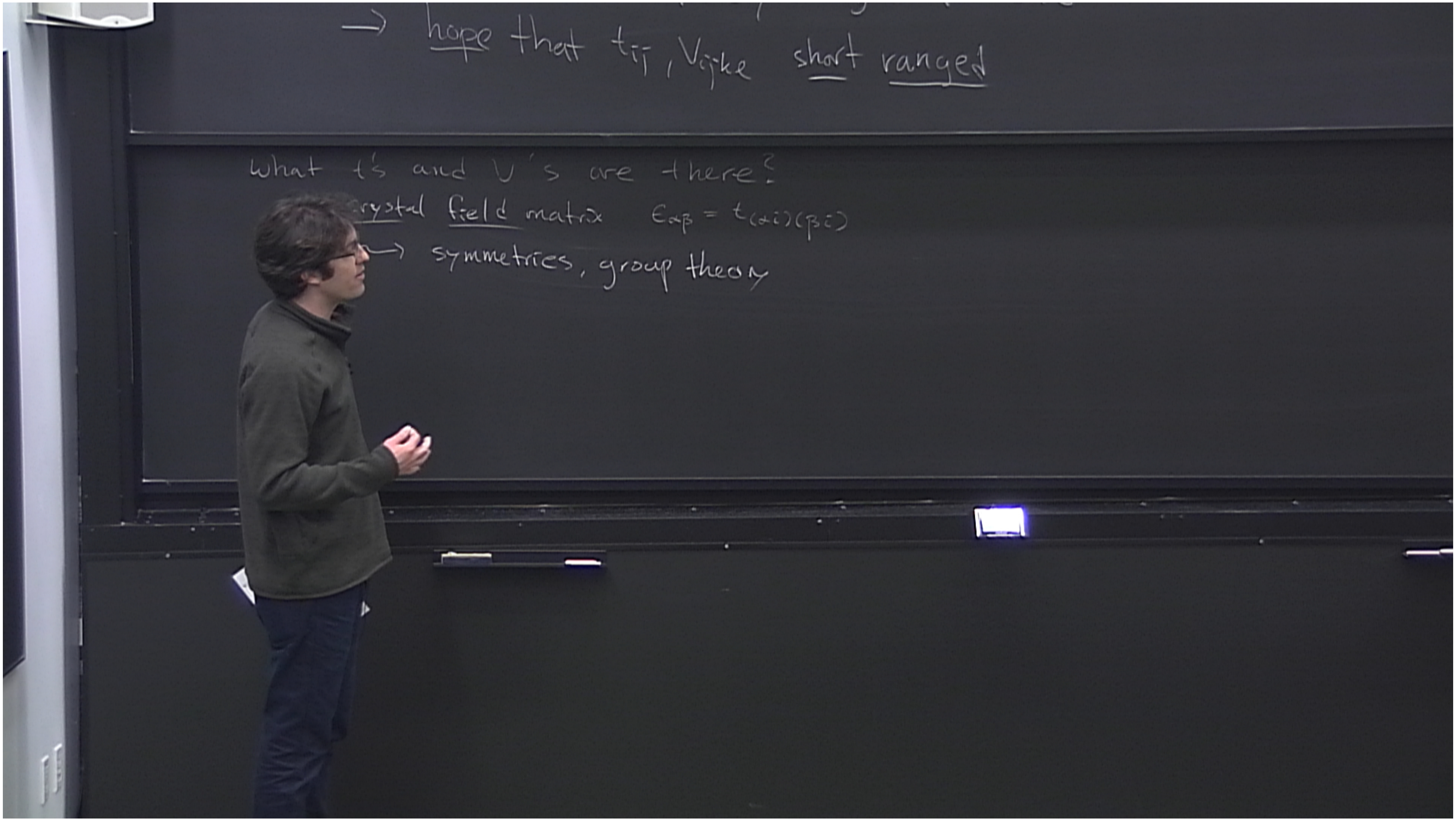
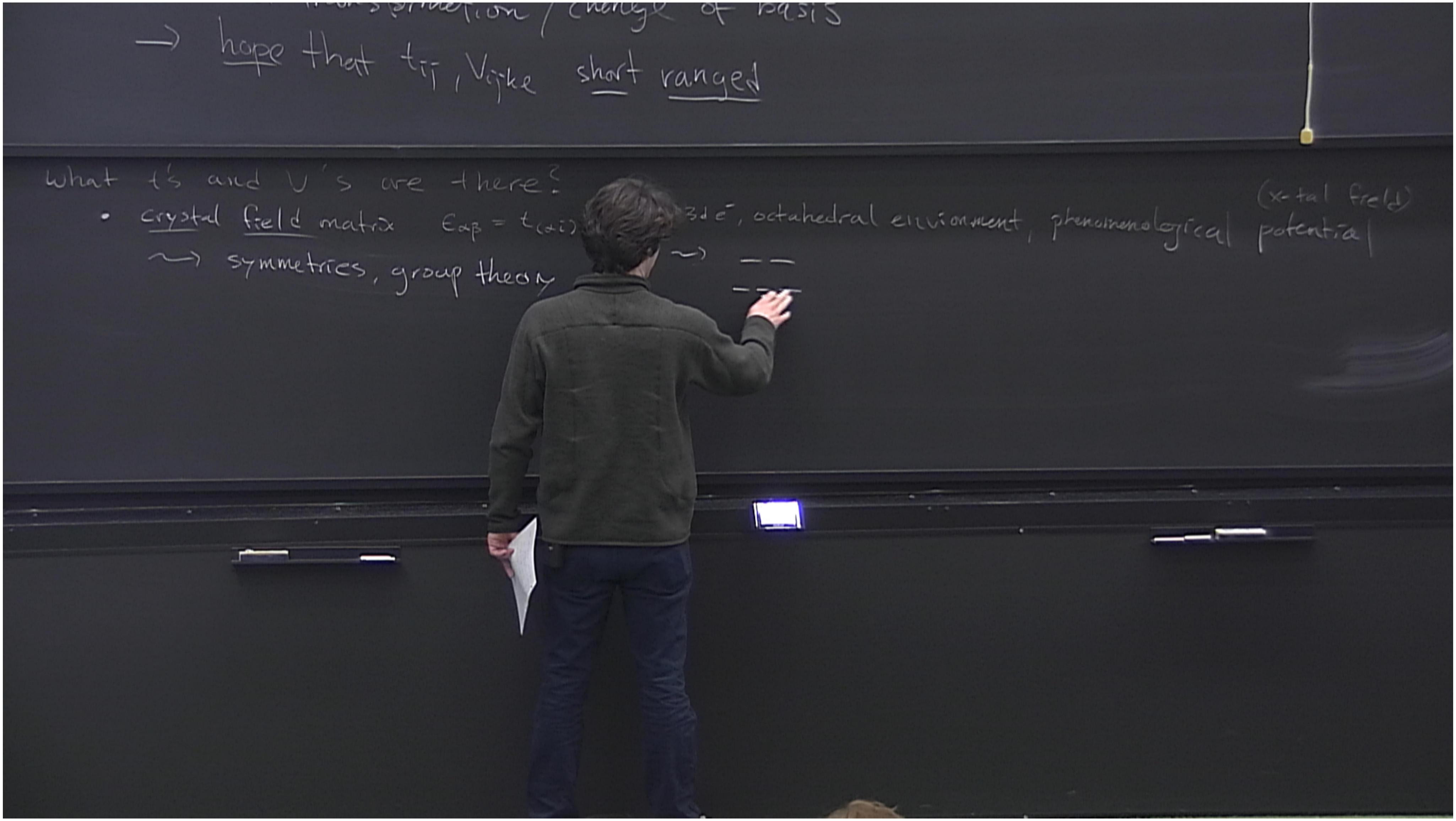
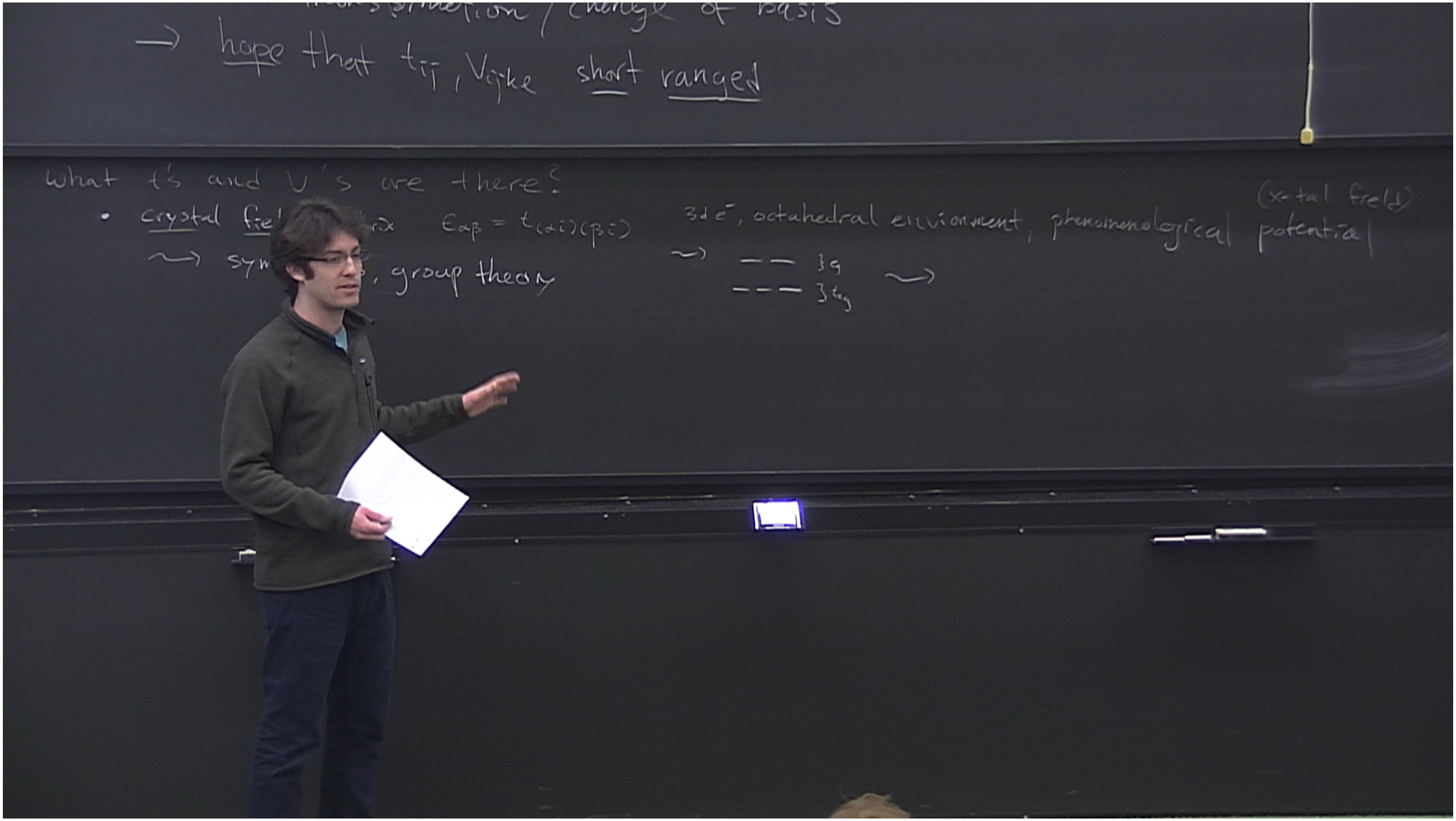
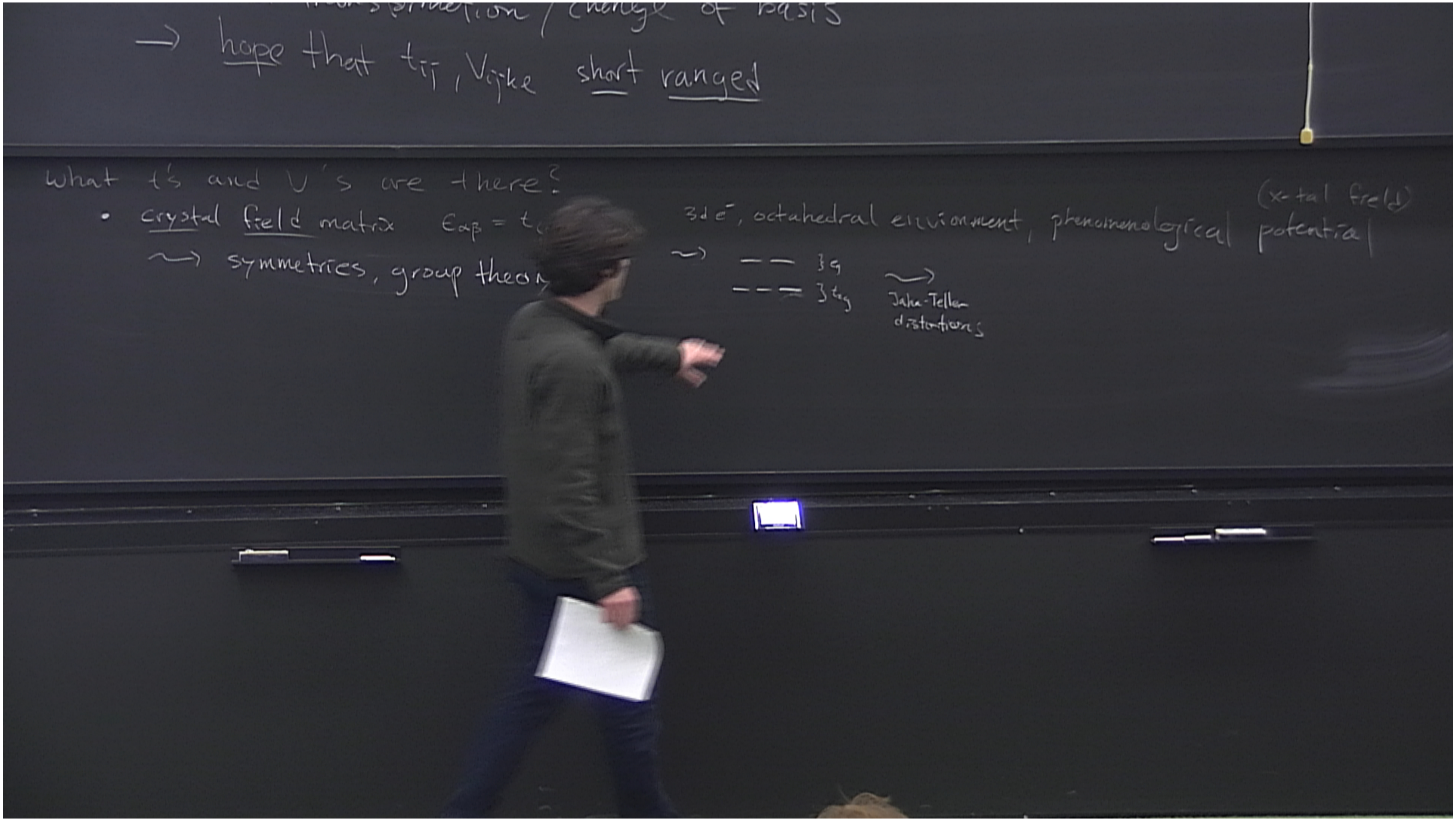

(tunneling or hopping) $t_{ij} = -\langle \phi_i | \hat{H}_0 | \phi_j \rangle = -\int_{\vec r} \phi_i^*(\vec r)\left[-\frac{1}{2}\nabla^2 + v(\vec r)\right]\phi_j(\vec r)$
$V_{ijkl} = \frac{1}{2}\int v_{ee}(\vec r - \vec r')\, \phi_i^*(\vec r)\,\phi_j(\vec r)\,\phi_k^*(\vec r')\,\phi_l(\vec r')$
→ exact transformation / change of basis
→ hope that t_{ij}, V_{ijkl} short ranged


→ hope that t_{ij}, V_{ijkl} short ranged
what t's and V's are there?
• crystal
$\epsilon_{\alpha\beta} = t_{(\alpha i)(\beta i)}$

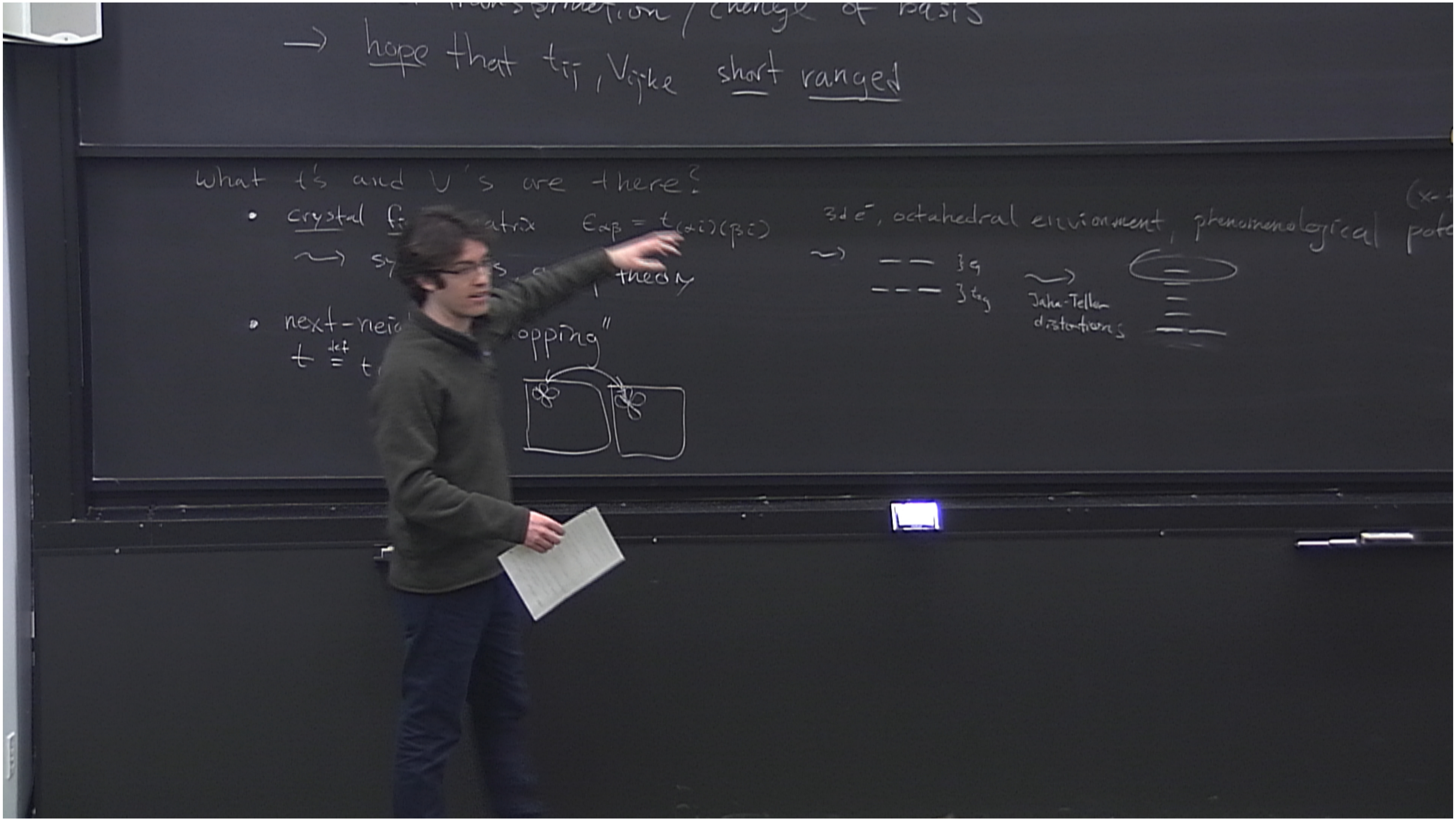

→ hope that tij, Vijkl short ranged
what t's and V's are there?
rystal field matrix ϵαβ = t(αi)(βi)
→ symmetries, group theory

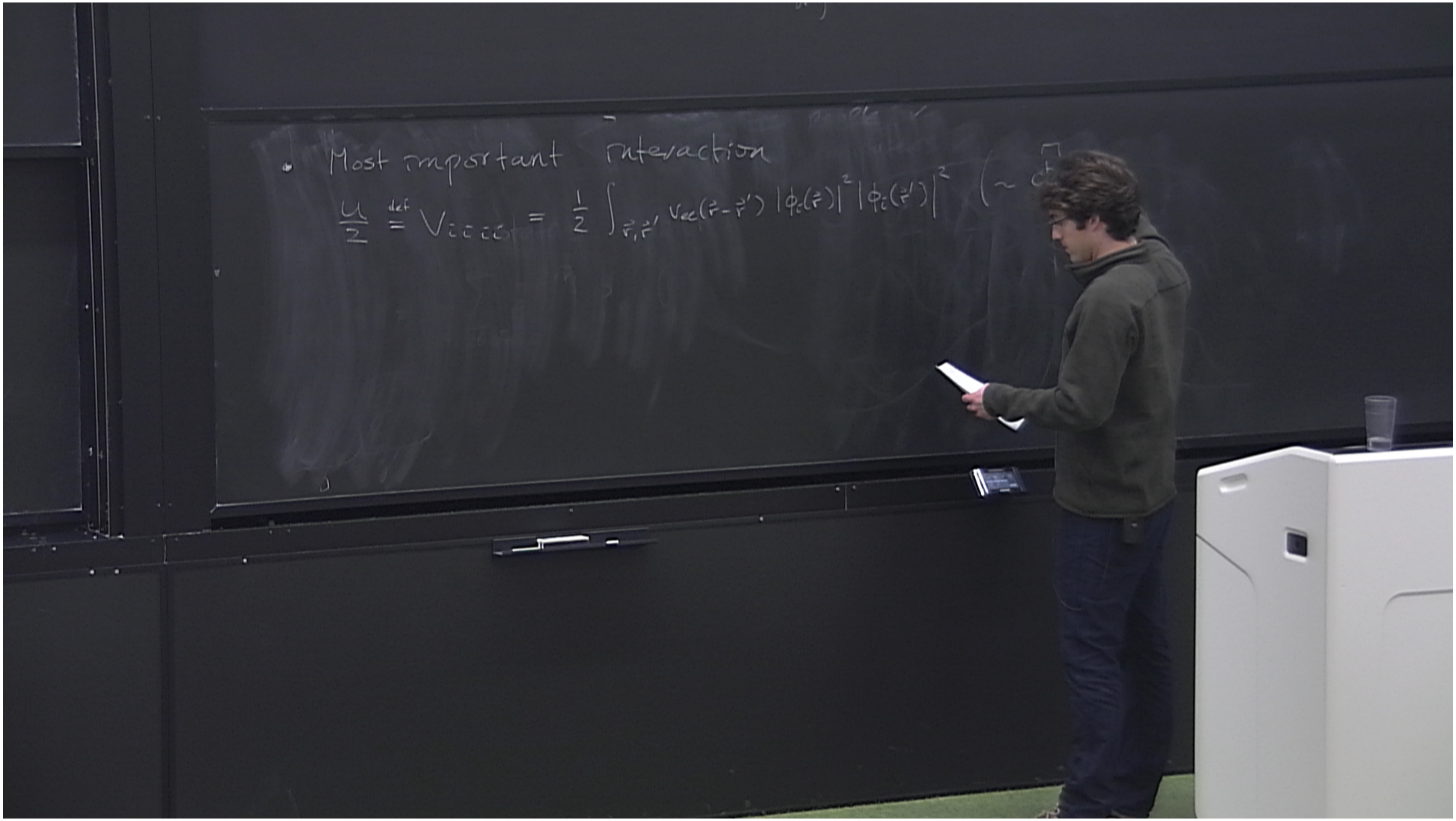

→ hope that t_ij, V_ijkl short ranged
what t's and V's are there?
• crystal field matrix ε_αβ = t_(αi)
3d e⁻, octahedral environment, phenomenological potential
(x-tal field)
symmetries, group theory

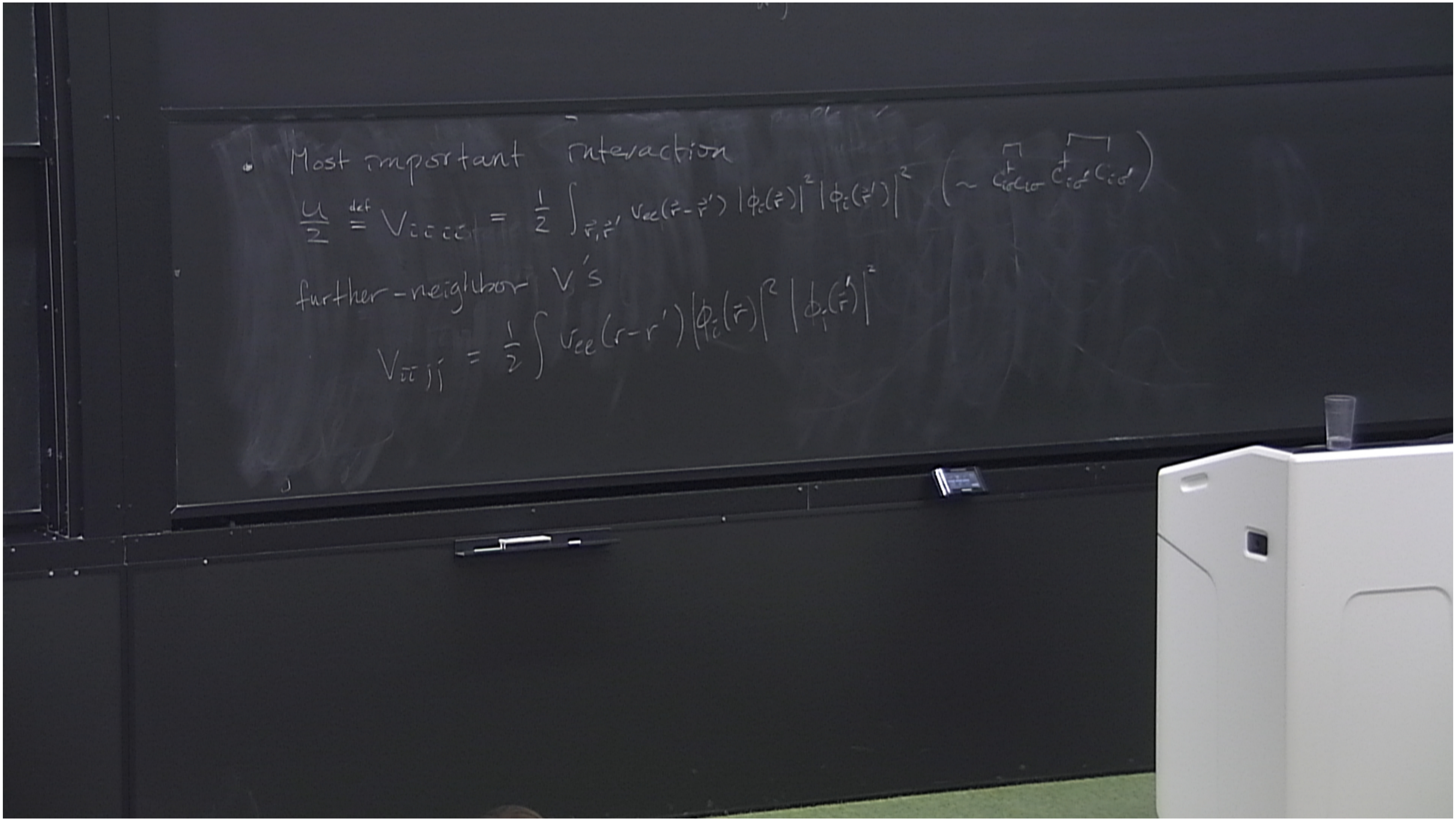

→ hope that t_ij, V_ijkl short ranged
what t's and U's are there?
• crystal fie... ε_αβ = t_(αi)(βi)
group theory
(x-tal field)
3d e⁻, octahedral environment, phenomenological potential
e_g
t_2g



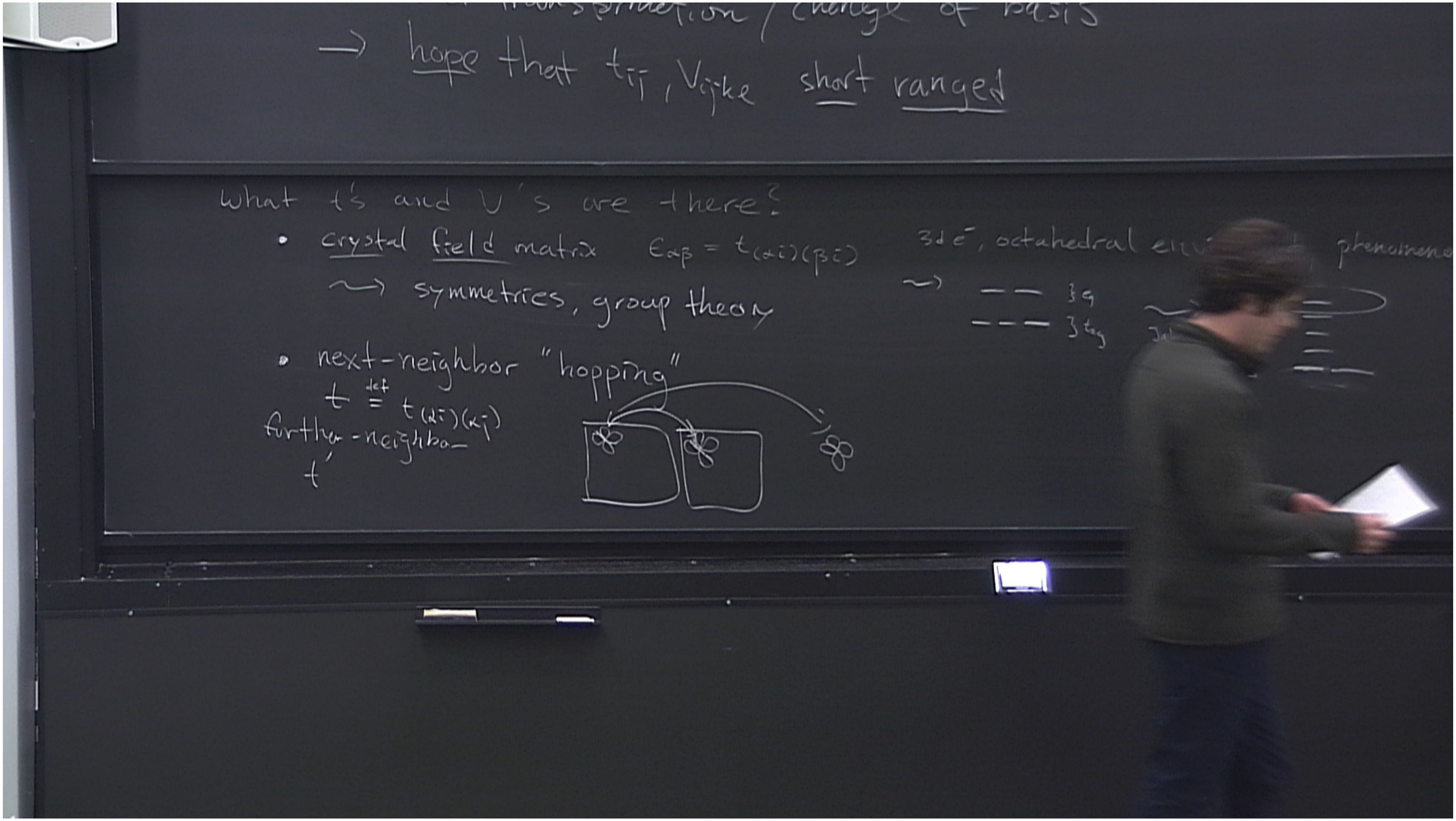
hope that short ranged
what t's and V's are there?
crystal field matrix
symmetries, group
(x-tal field)
octahedral environment, phenomenological potential
Jahn-Teller
distortions


hope that t_ij , V_ijkl short ranged
what t's and V's are there?
crystal
matrix ε_αβ = t_(αi)(βi)
theory
next-
hopping"
3d e⁻, octahedral environment, phenomenological
e_g
t_2g
Jahn-Teller
distortions

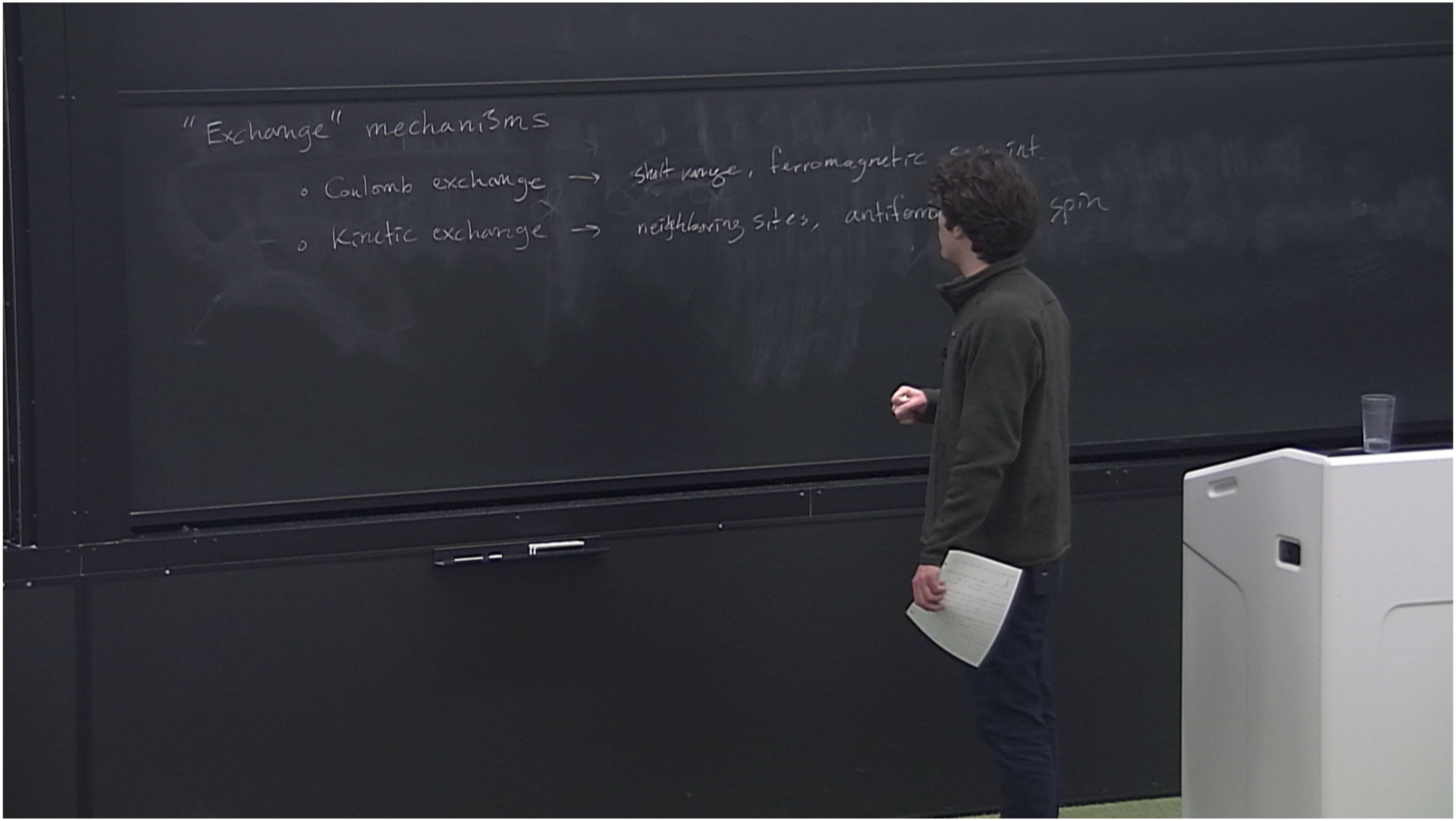

• Most important interaction
$\frac{U}{2} \overset{\text{def}}{=} V_{iiii} = \frac{1}{2} \int_{\vec{r},\vec{r}'} V_{ee}(\vec{r}-\vec{r}') \, |\phi_i(\vec{r})|^2 \, |\phi_i(\vec{r}')|^2$

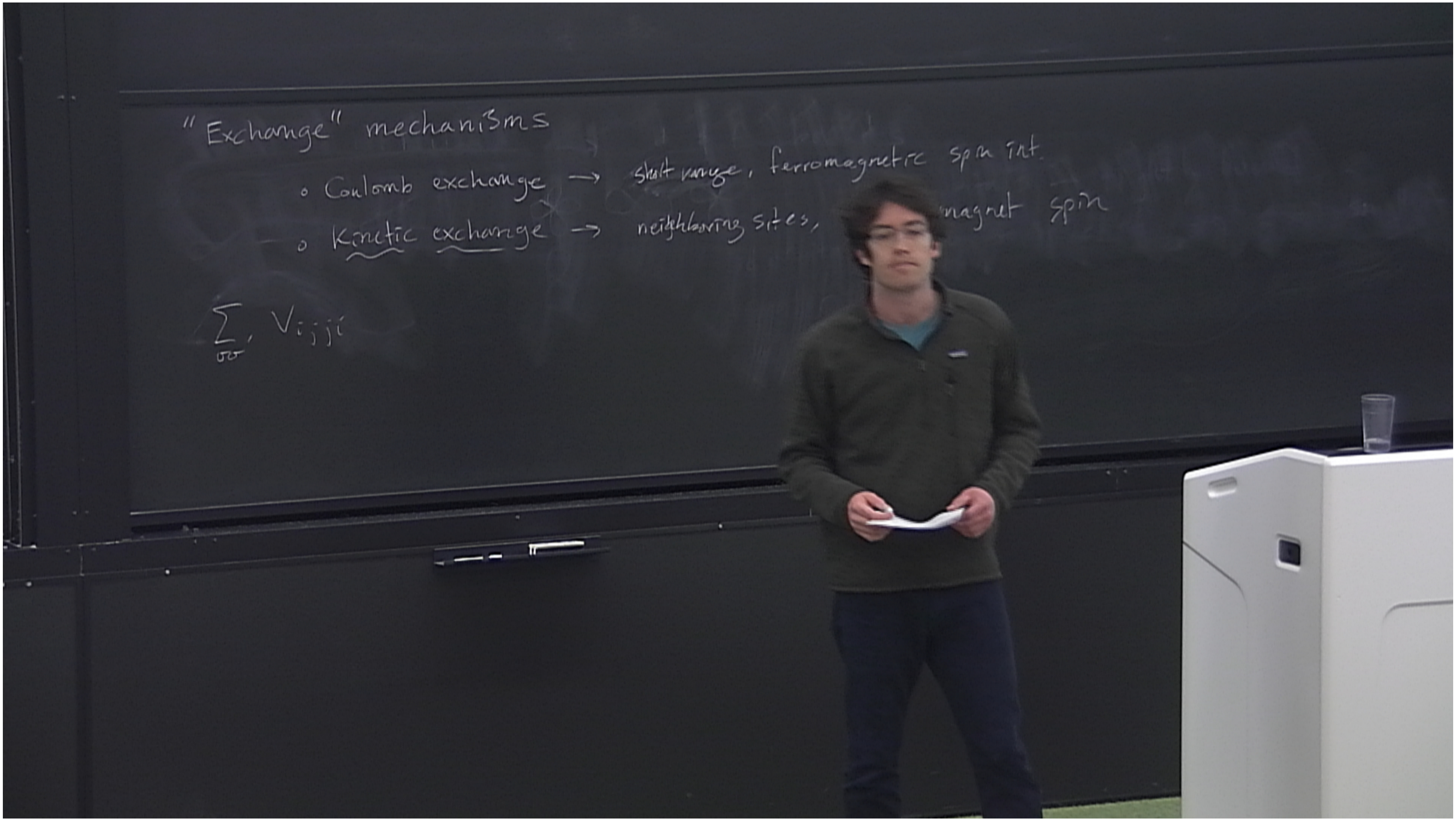


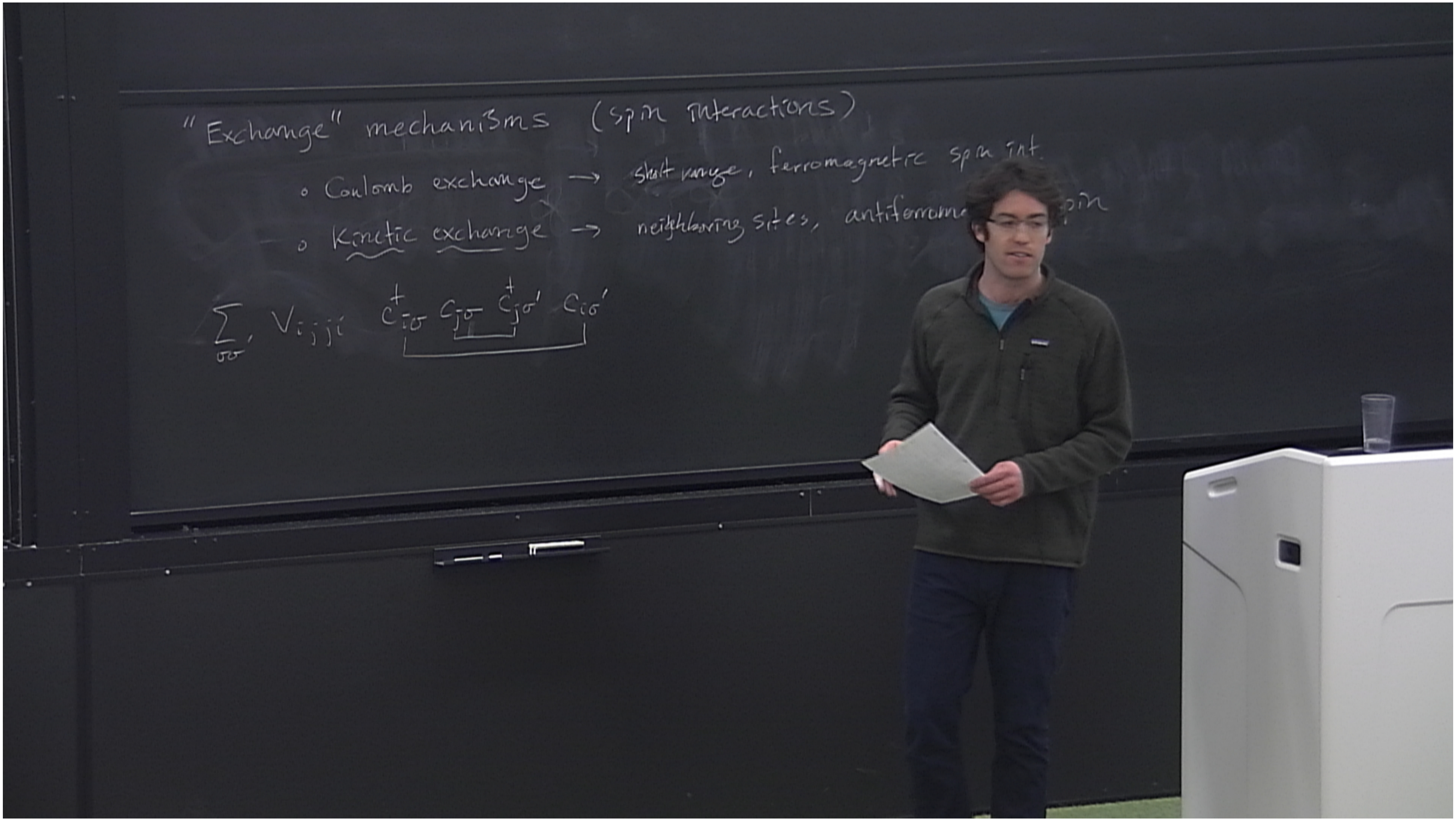
• Most important interaction
$\frac{U}{2} \overset{\text{def}}{=} V_{iiii} = \frac{1}{2} \int_{\vec{r},\vec{r}'} v_{ee}(\vec{r}-\vec{r}') |\phi_i(\vec{r})|^2 |\phi_i(\vec{r}')|^2 \quad (\sim c^\dagger_{i\sigma} c_{i\sigma} c^\dagger_{i\sigma'} c_{i\sigma'})$
further-neighbor V's
$V_{iijj} = \frac{1}{2} \int v_{ee}(r-r') |\phi_i(\vec{r})|^2 |\phi_j(\vec{r}')|^2$

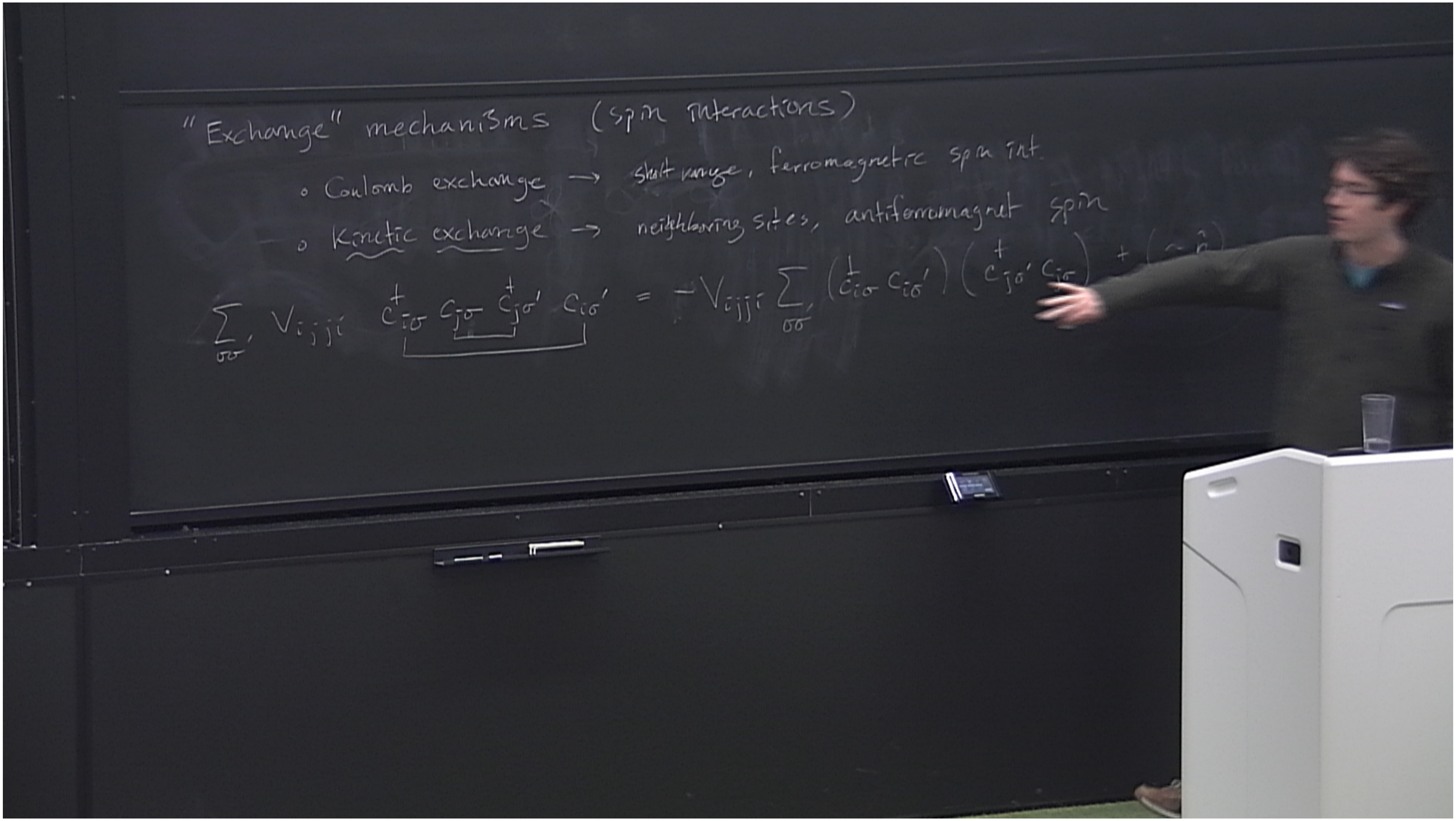


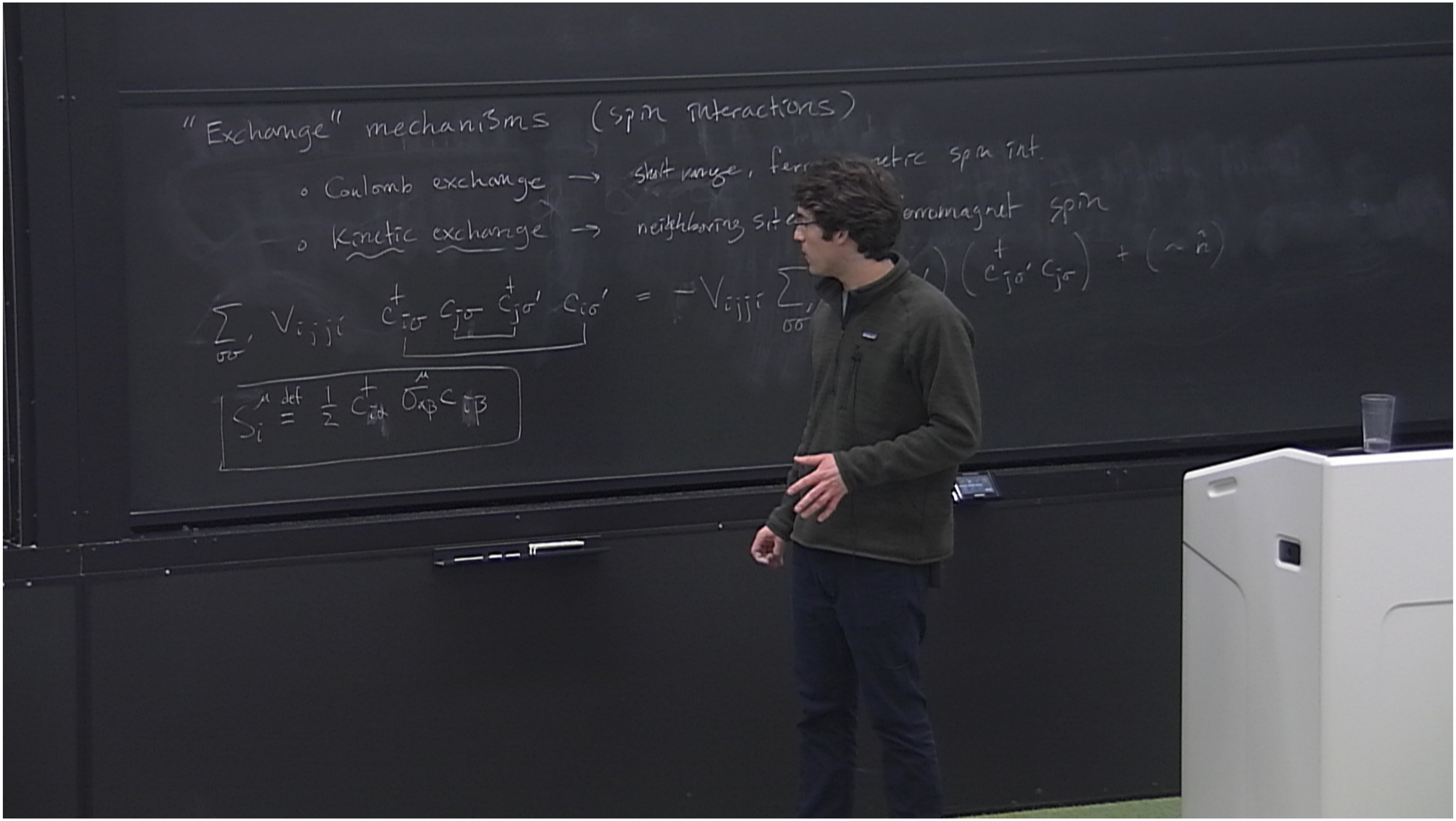
→ hope that t_ij, V_ijkl short ranged
What t's and V's are there?
• crystal field matrix ε_αβ = t_(αi)(βi)
~→ symmetries, group theory
3d e⁻, octahedral env
phenomena
e_g
t_2g
• next-neighbor "hopping"
t def= t_(αi)(αj)
further-neighbor
t'


"Exchange" mechanisms
Coulomb exchange → short range, ferromagnetic
int.
Kinetic exchange → neighboring sites,
spin


"Exchange" mechanisms
∘ Coulomb exchange → short range, ferromagnetic spin int.
∘ Kinetic exchange → neighboring sites,
magnet spin


"Exchange" mechanisms (spin interactions)
◦ Coulomb exchange → short range, ferromagnetic spin int.
◦ Kinetic exchange → neighboring sites, antiferroma spin
$\sum_{\sigma\sigma'} V_{ijji} \, c^\dagger_{i\sigma} c_{j\sigma} c^\dagger_{j\sigma'} c_{i\sigma'}$


"Exchange" mechanisms (spin interactions)
∘ Coulomb exchange → short range, ferromagnetic spin int.
∘ Kinetic exchange → neighboring sites, antiferromagnet spin
$\sum_{\sigma\sigma'} V_{ijji} \, c^\dagger_{i\sigma} c_{j\sigma} c^\dagger_{j\sigma'} c_{i\sigma'} = -V_{ijji} \sum_{\sigma\sigma'} (c^\dagger_{i\sigma} c_{i\sigma'})(c^\dagger_{j\sigma'} c_{j\sigma}) +$


"Exchange" mechanisms (spin interactions)
∘ Coulomb exchange → short range, fer
etic spin int.
∘ Kinetic exchange → neighboring site
ferromagnet spin
$\sum_{\sigma\sigma'} V_{ijji} \, c^\dagger_{i\sigma} c_{j\sigma} c^\dagger_{j\sigma'} c_{i\sigma'} = -V_{ijji} \sum_{\sigma\sigma'}$
$\left(c^\dagger_{j\sigma'} c_{j\sigma}\right) + (\sim \hat{n})$
$S_i^\mu \overset{\text{def}}{=} \frac{1}{2} c^\dagger_{i\alpha} \sigma^\mu_{\alpha\beta} c_{i\beta}$