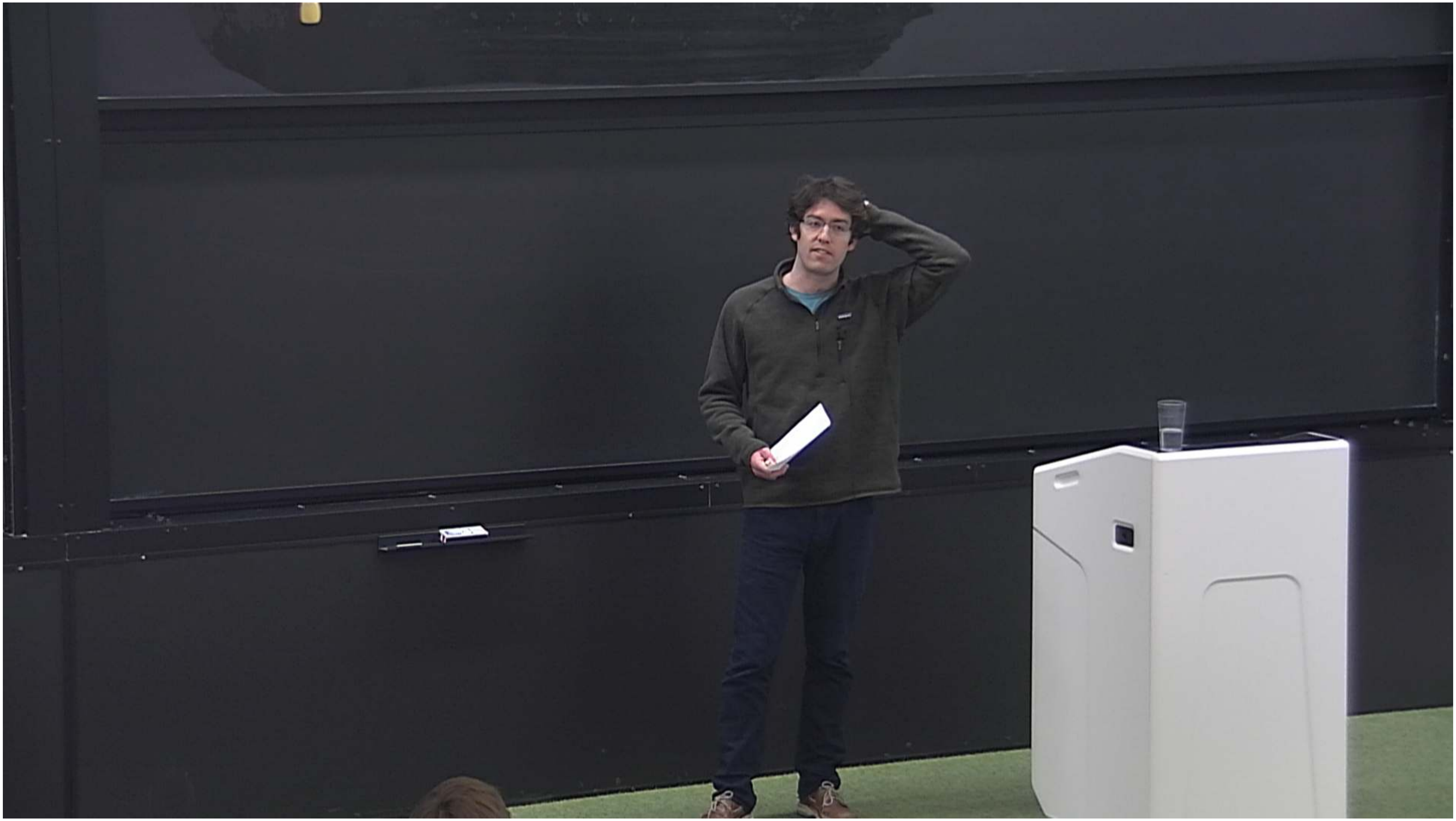
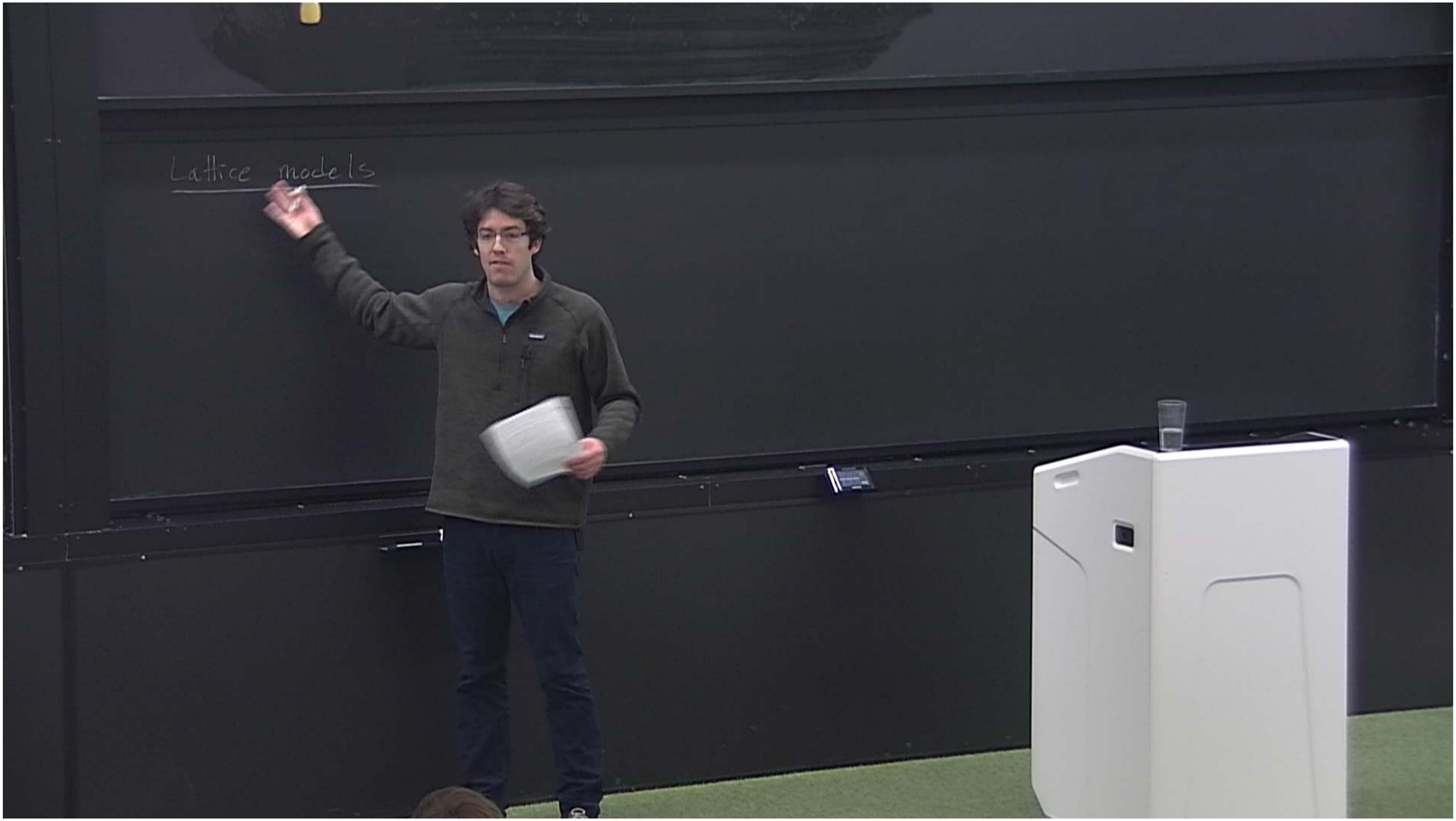
Title: Explorations in Condensed Matter-6

Date: Mar 23, 2015 10:15 AM

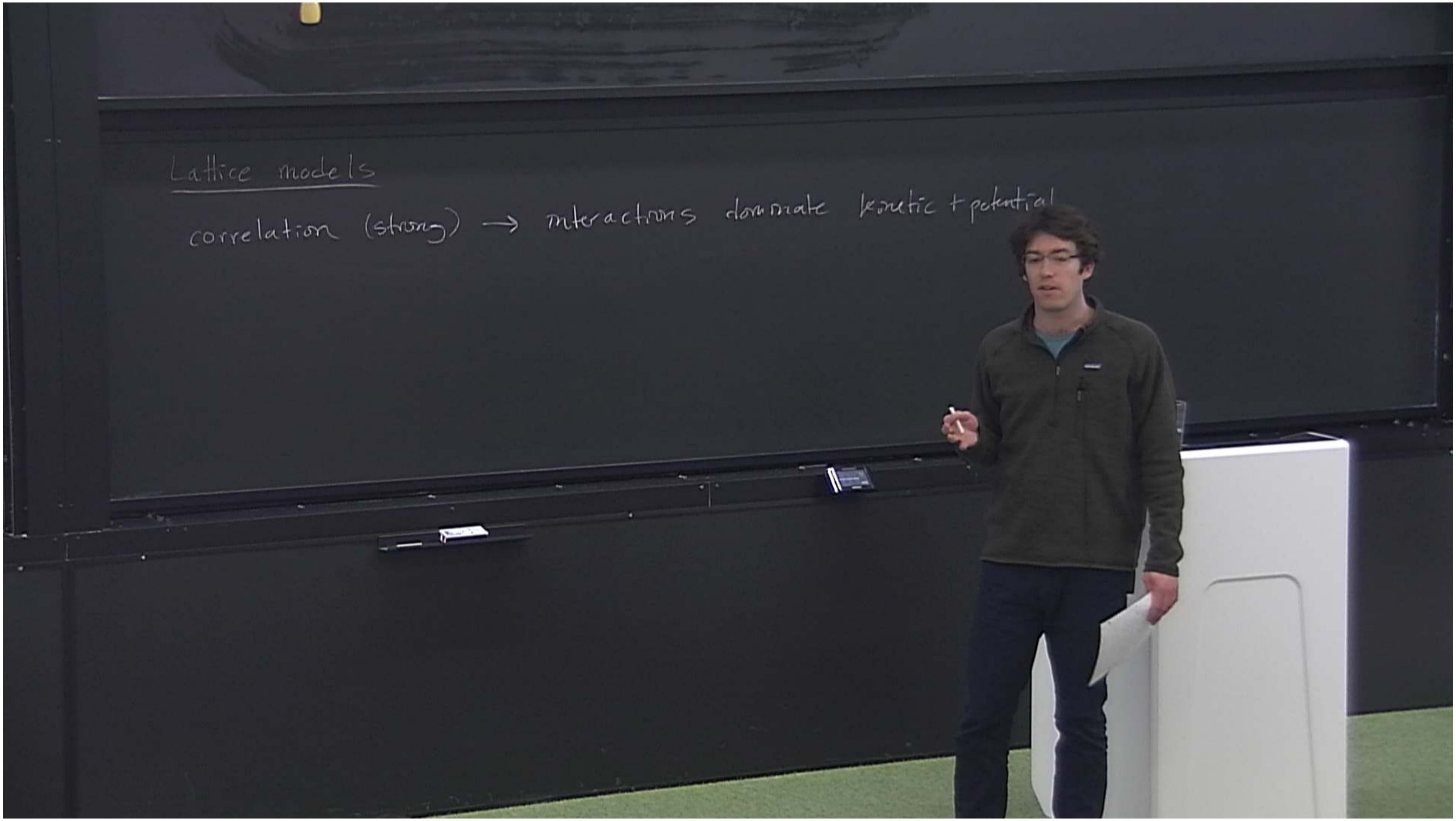
URL: http://pirsa.org/15030041

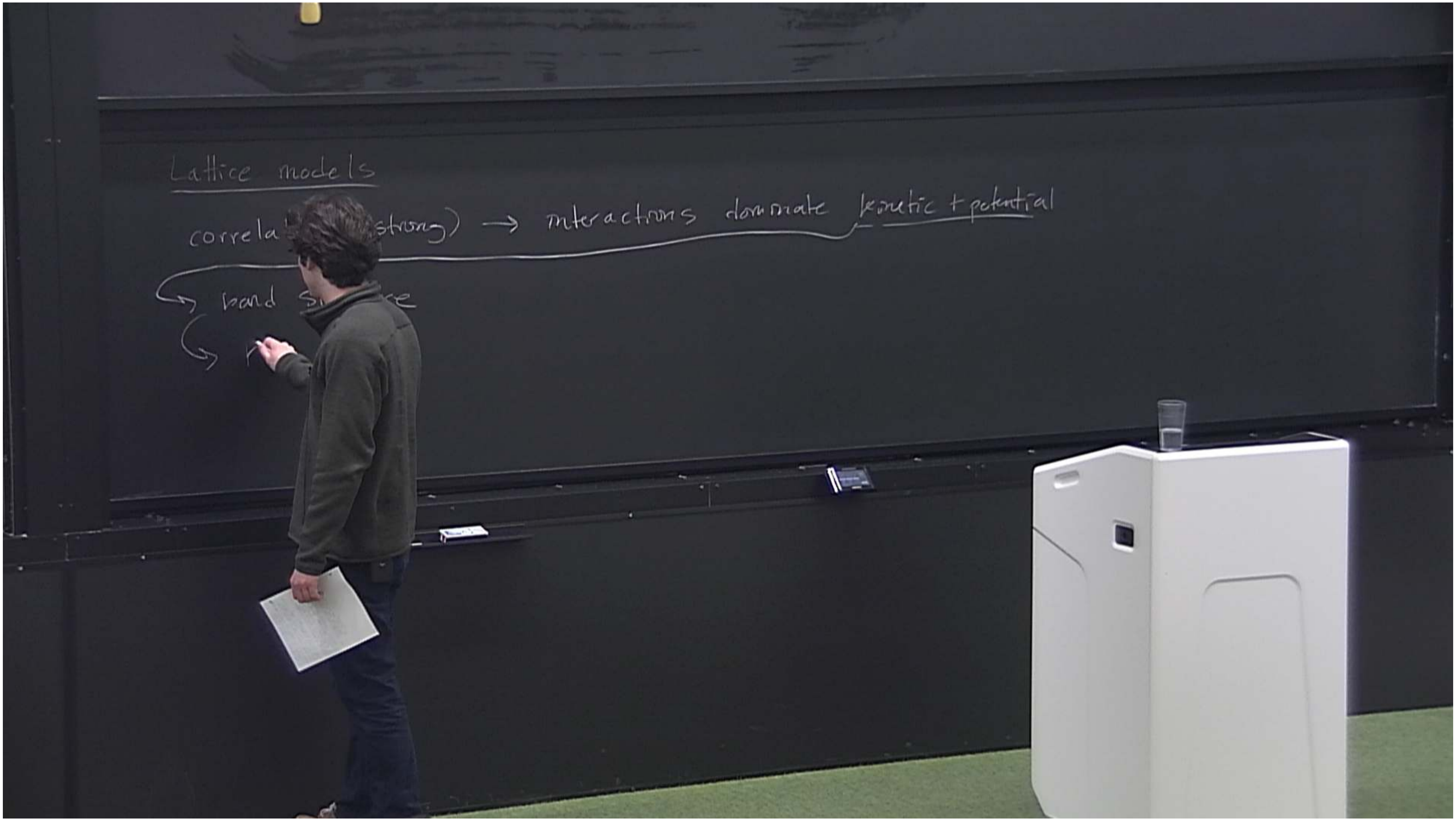
Abstract:

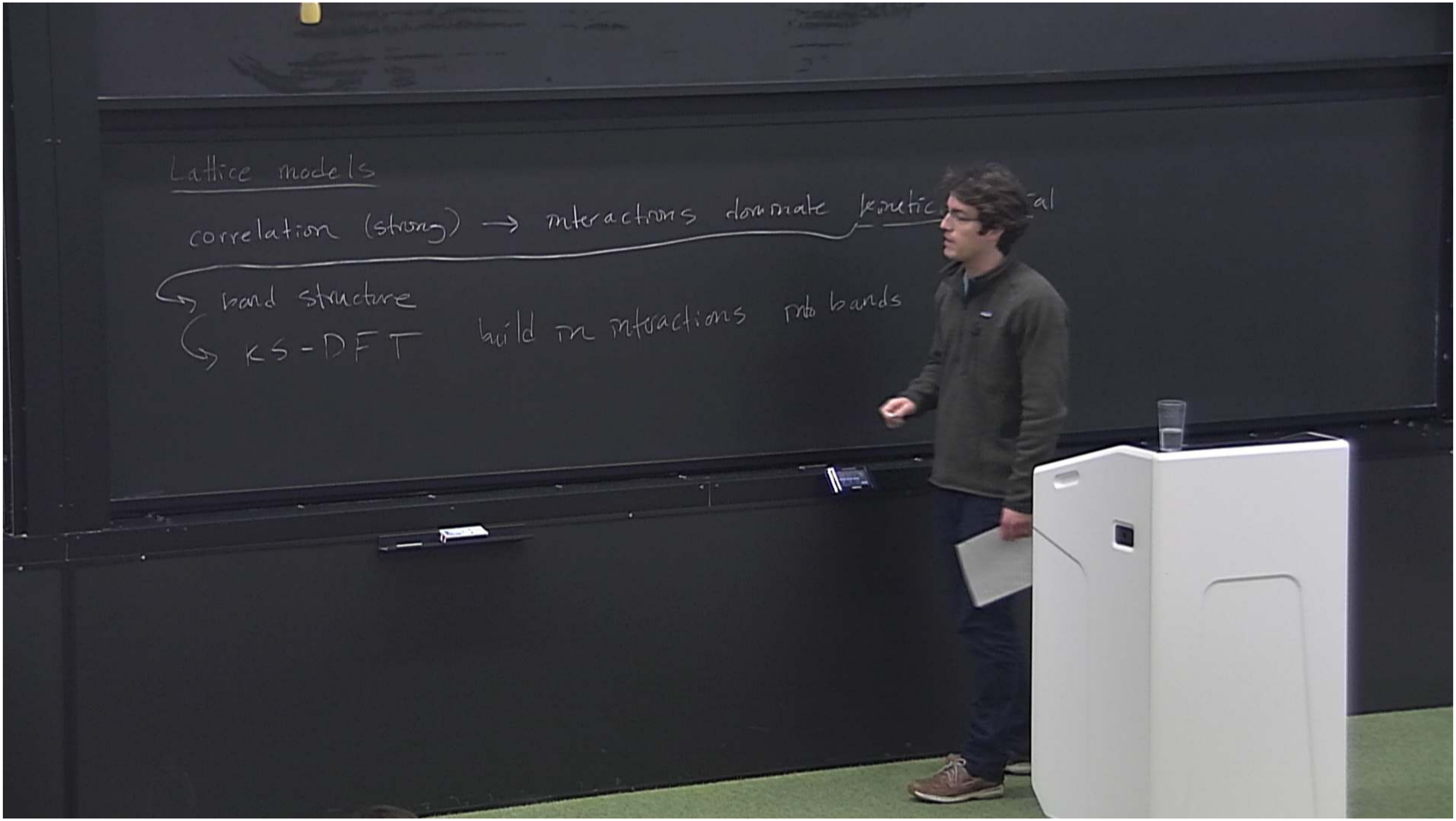


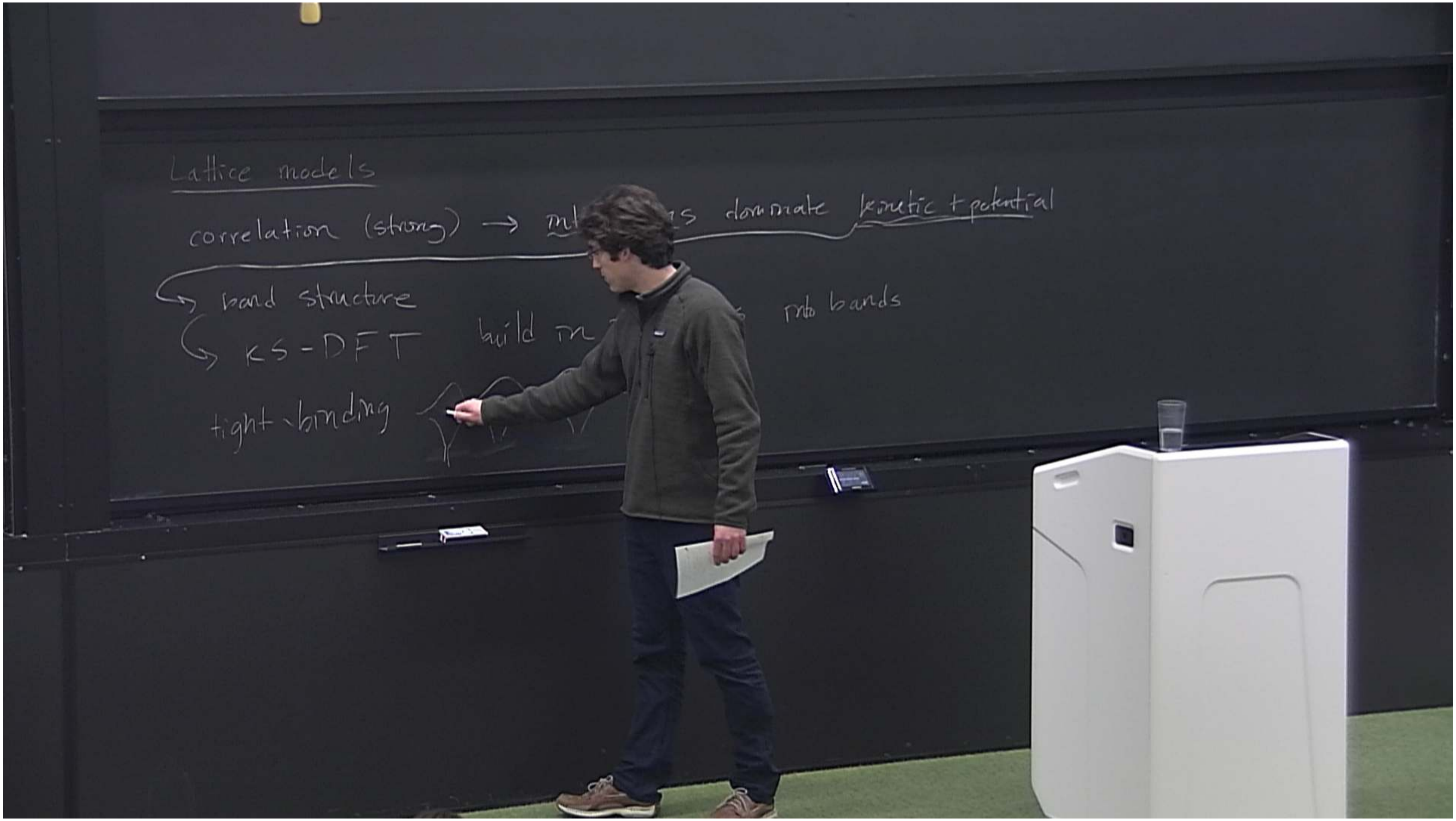

Lattice models

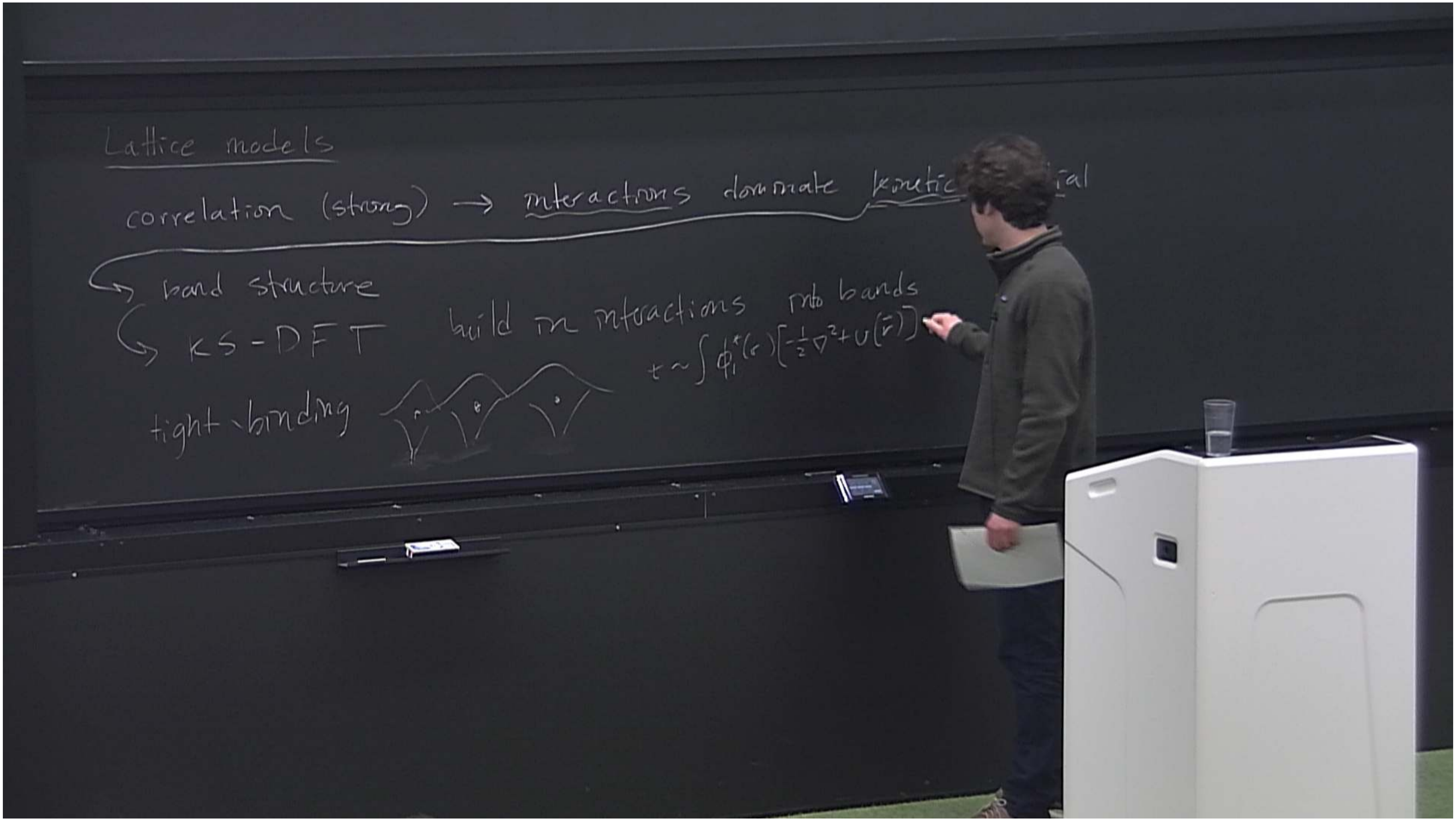

Lattice models


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

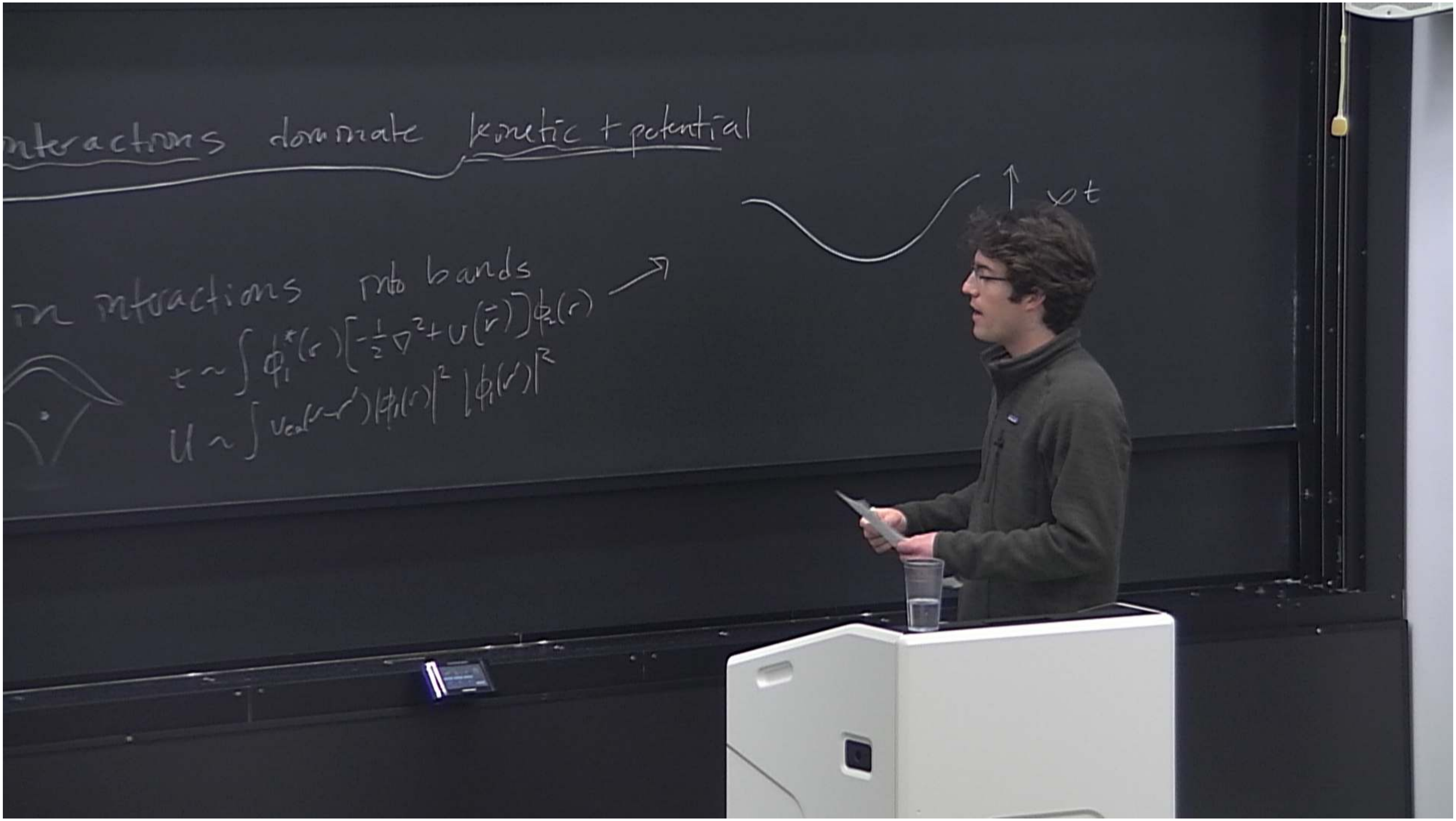

Lattice models
interactions dominate kinetic + potential
band

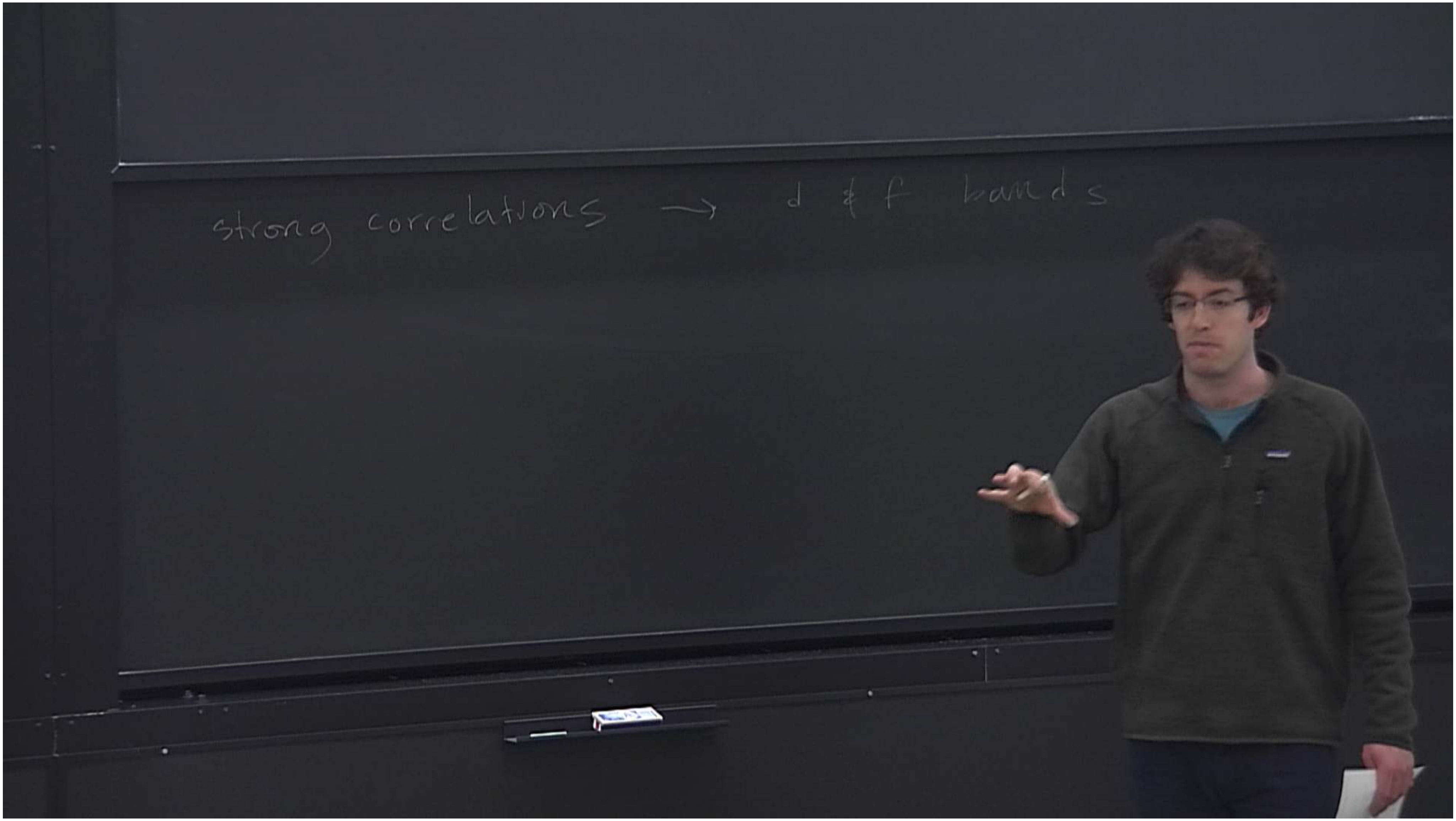

Lattice models
correlation (strong) → interactions dominate kinetic
band structure
KS-DFT
build in interactions into bands

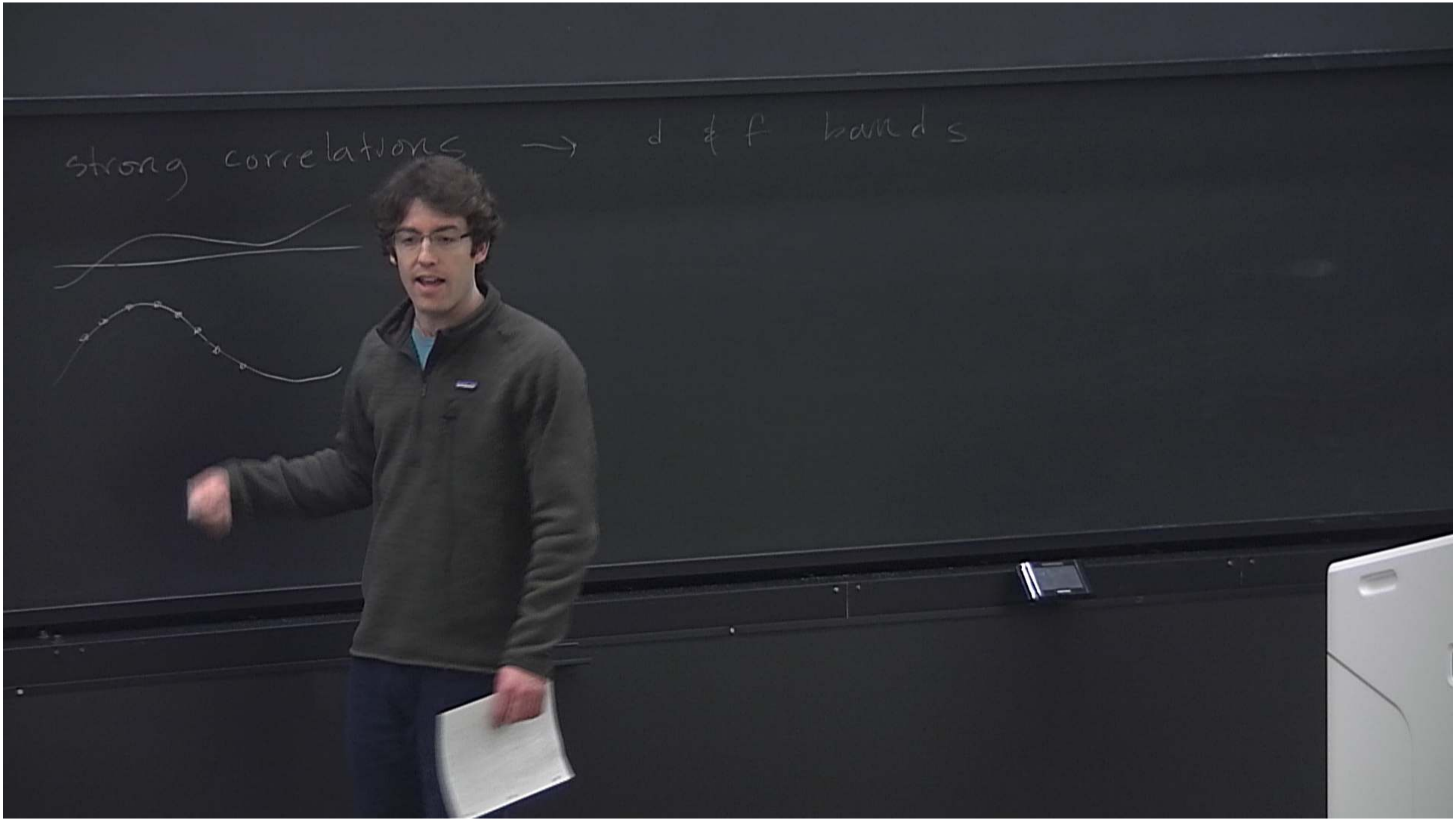

Lattice models
correlation (strong) →
dominate kinetic + potential
band structure
KS-DFT
build in
bands
tight-binding

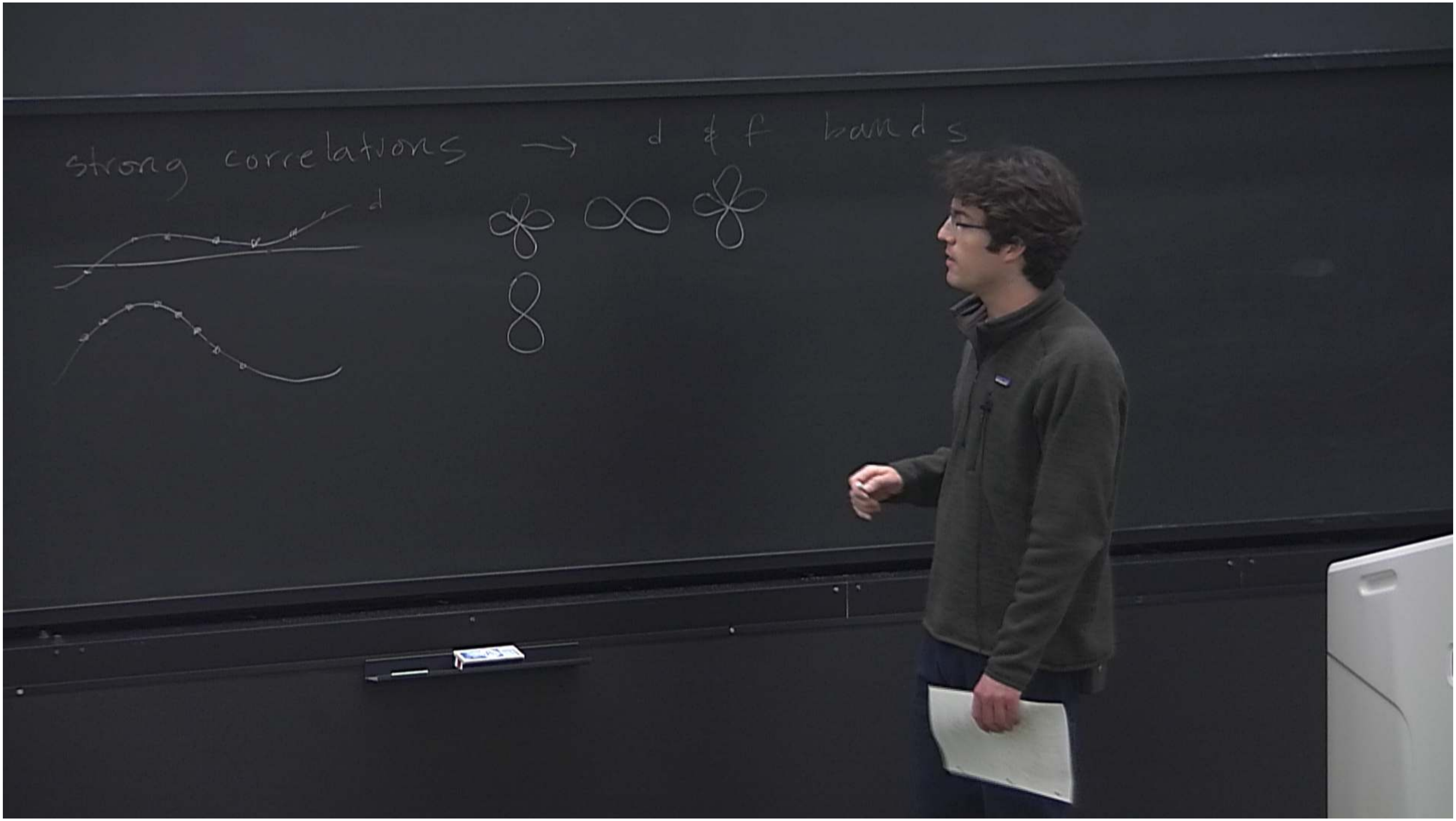


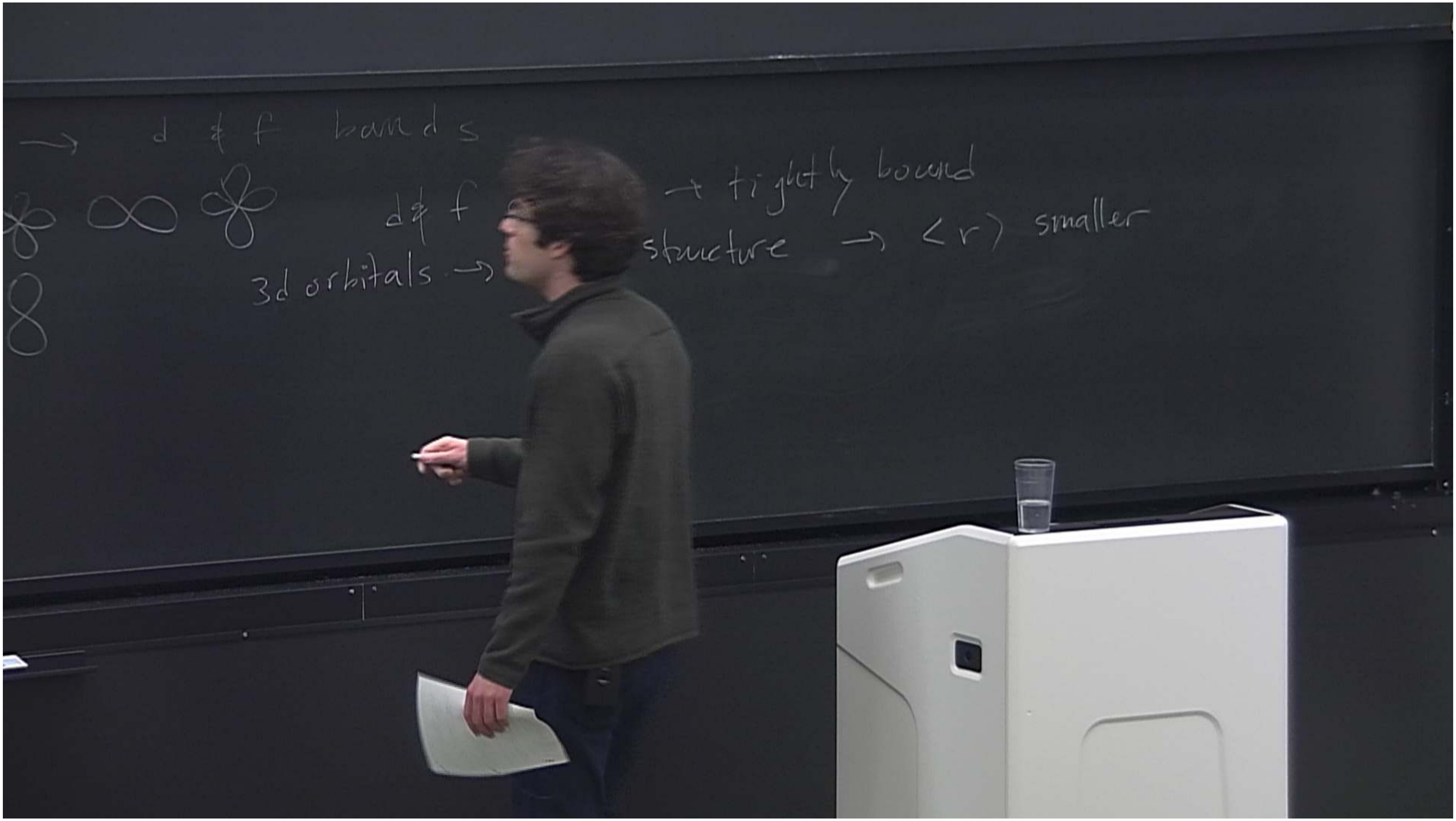
Lattice models
correlation (strong) → interactions dominate kinetic
band structure
KS-DFT
build in interactions into bands
$t \sim \int \phi_i^*(r)\left[-\frac{1}{2}\nabla^2 + v(\vec{r})\right]$
tight-binding


nteractions dominate kinetic + potential
n interactions into bands
t ~ ∫ φ₁*(r) [−½∇² + U(r)] φ₂(r)
U ~ ∫ V_coul(r−r') |φ₁(r)|² |φ₁(r')|²
∝ t

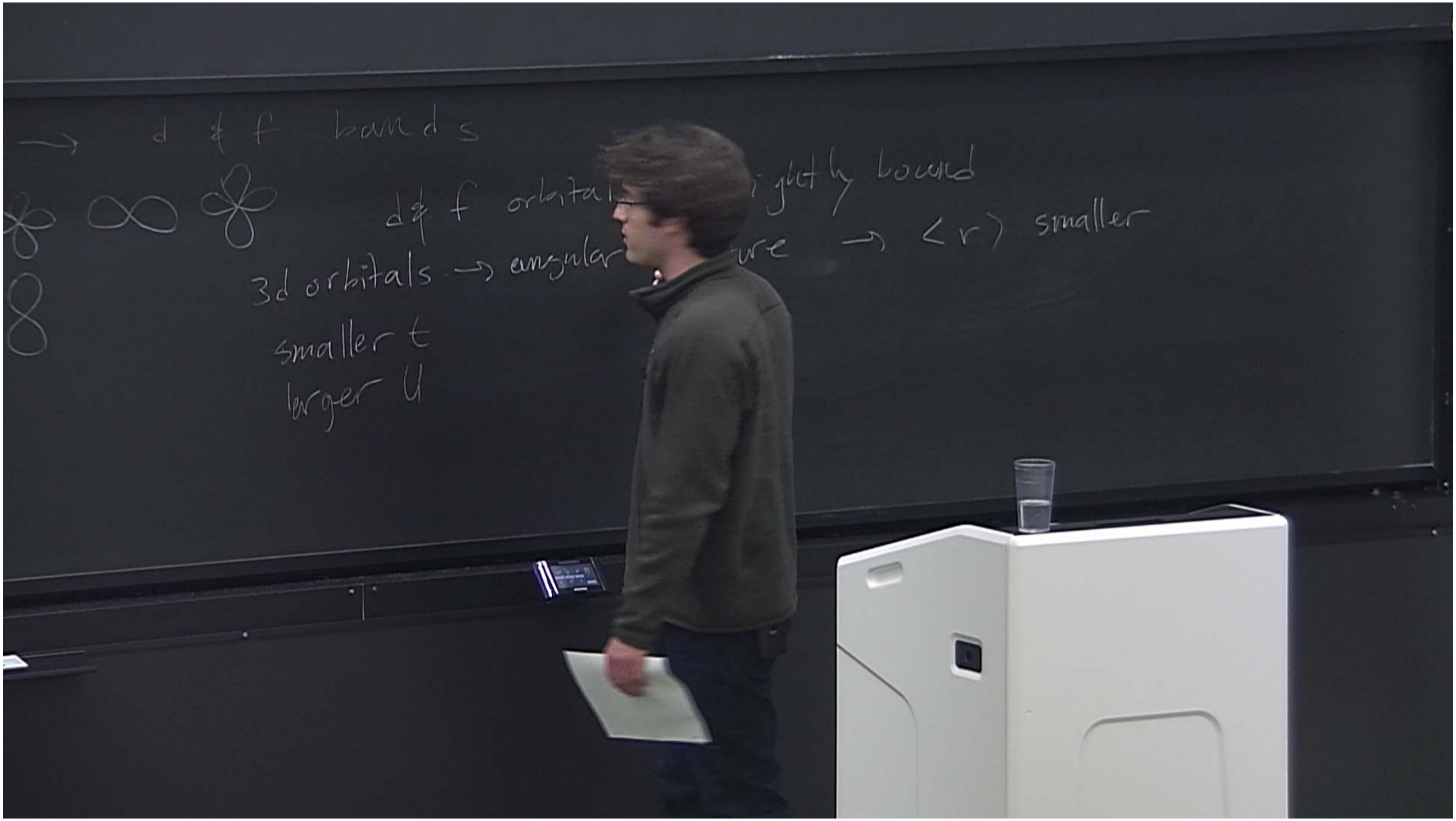

strong correlations → d & f bands

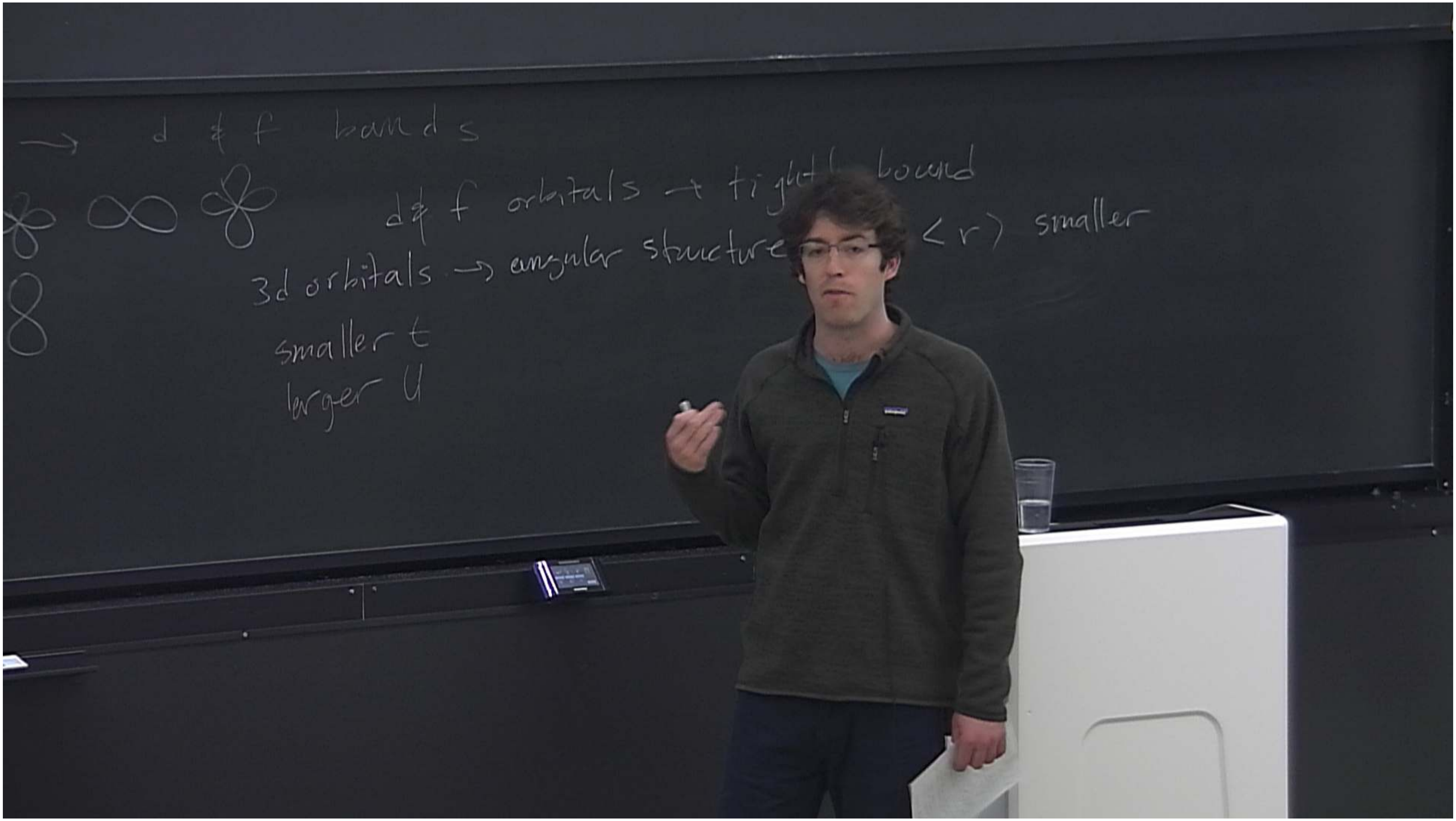

strong correlations → d & f bands

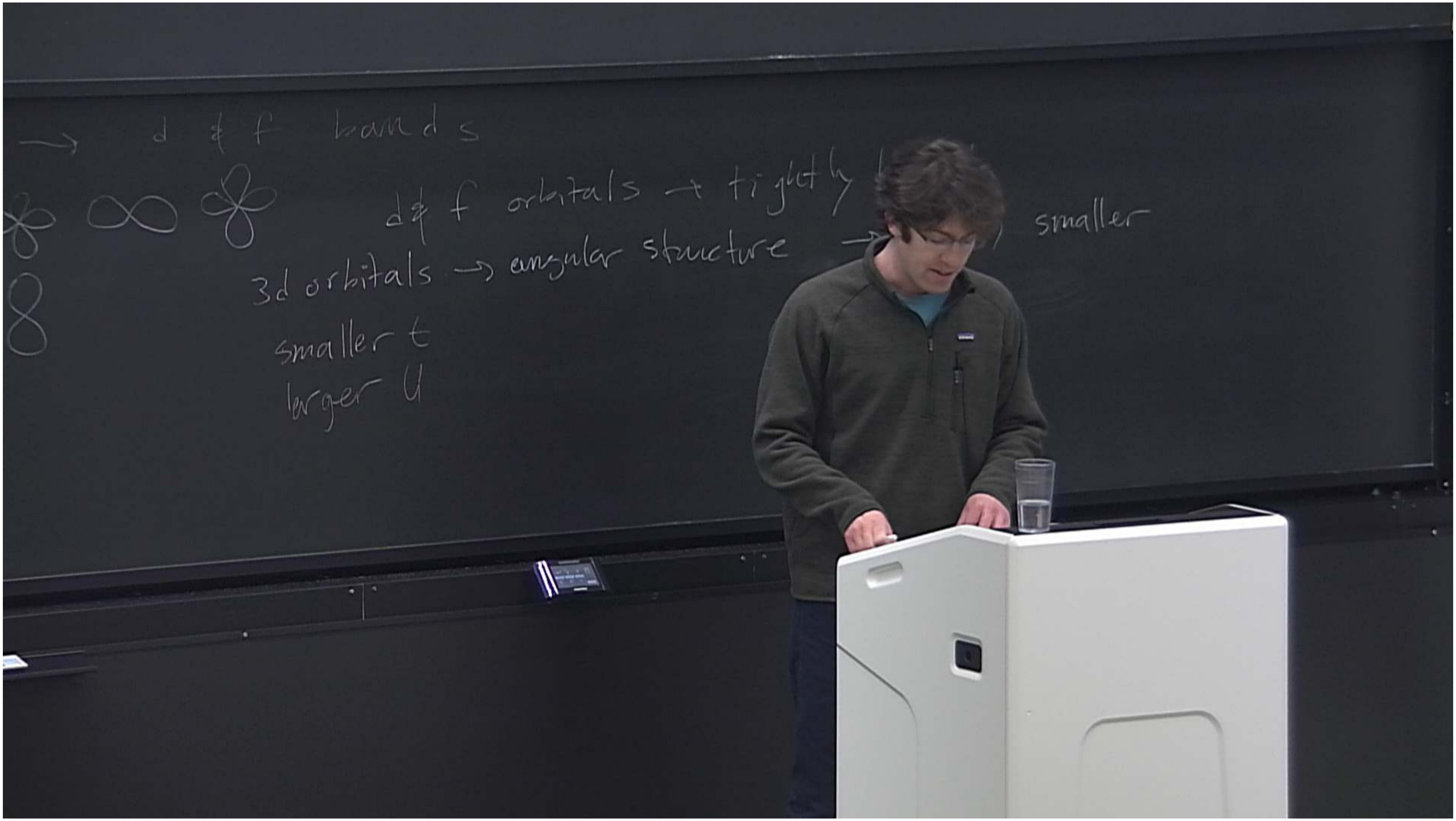

strong correlations → d & f bands
d

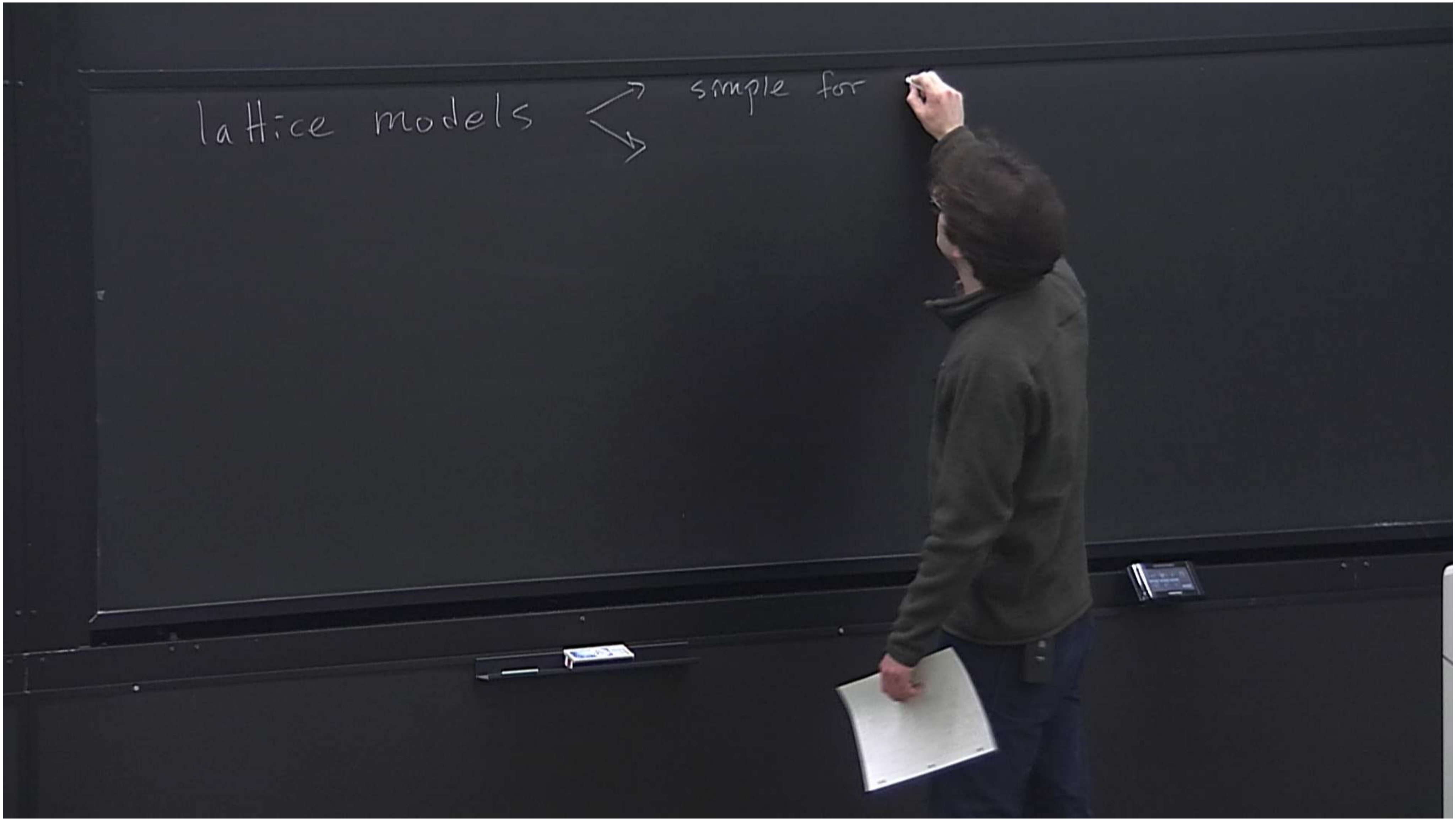


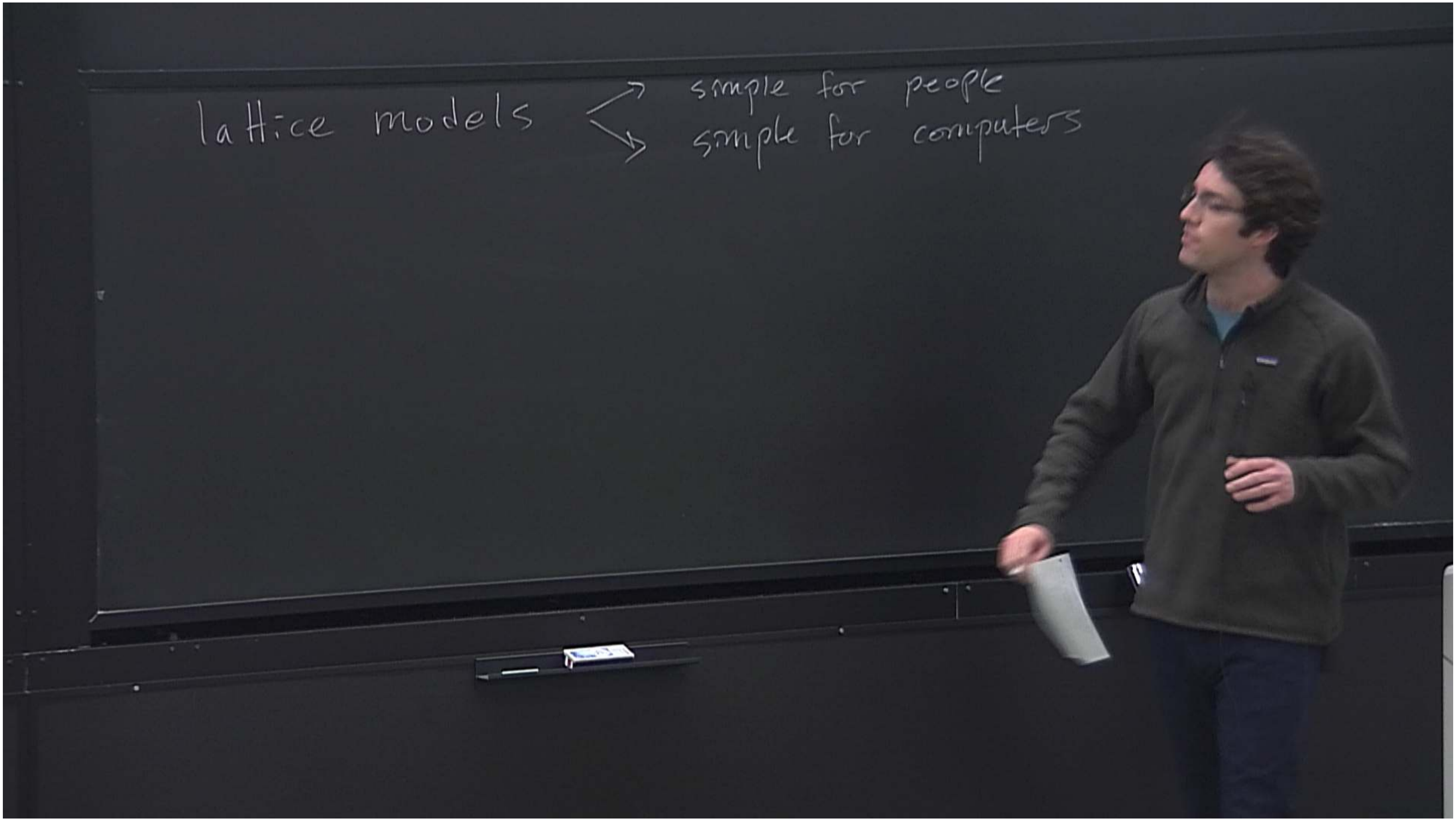
d & f bands
d & f
→ tightly bound
structure → ⟨r⟩ smaller
3d orbitals →

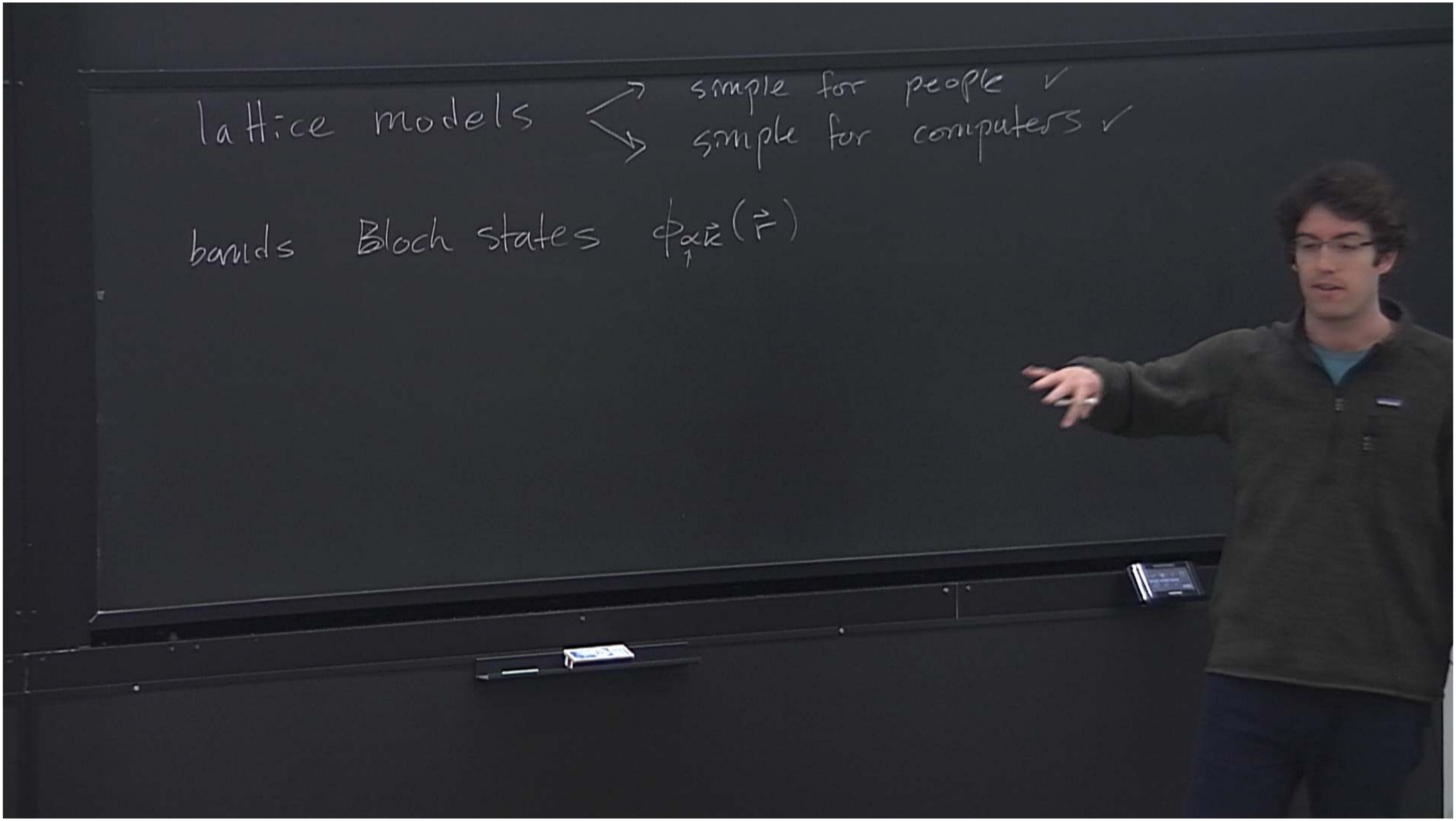

→ d & f bands
d & f
bound
3d orbitals → angular
→ <r> smaller
smaller t
larger U

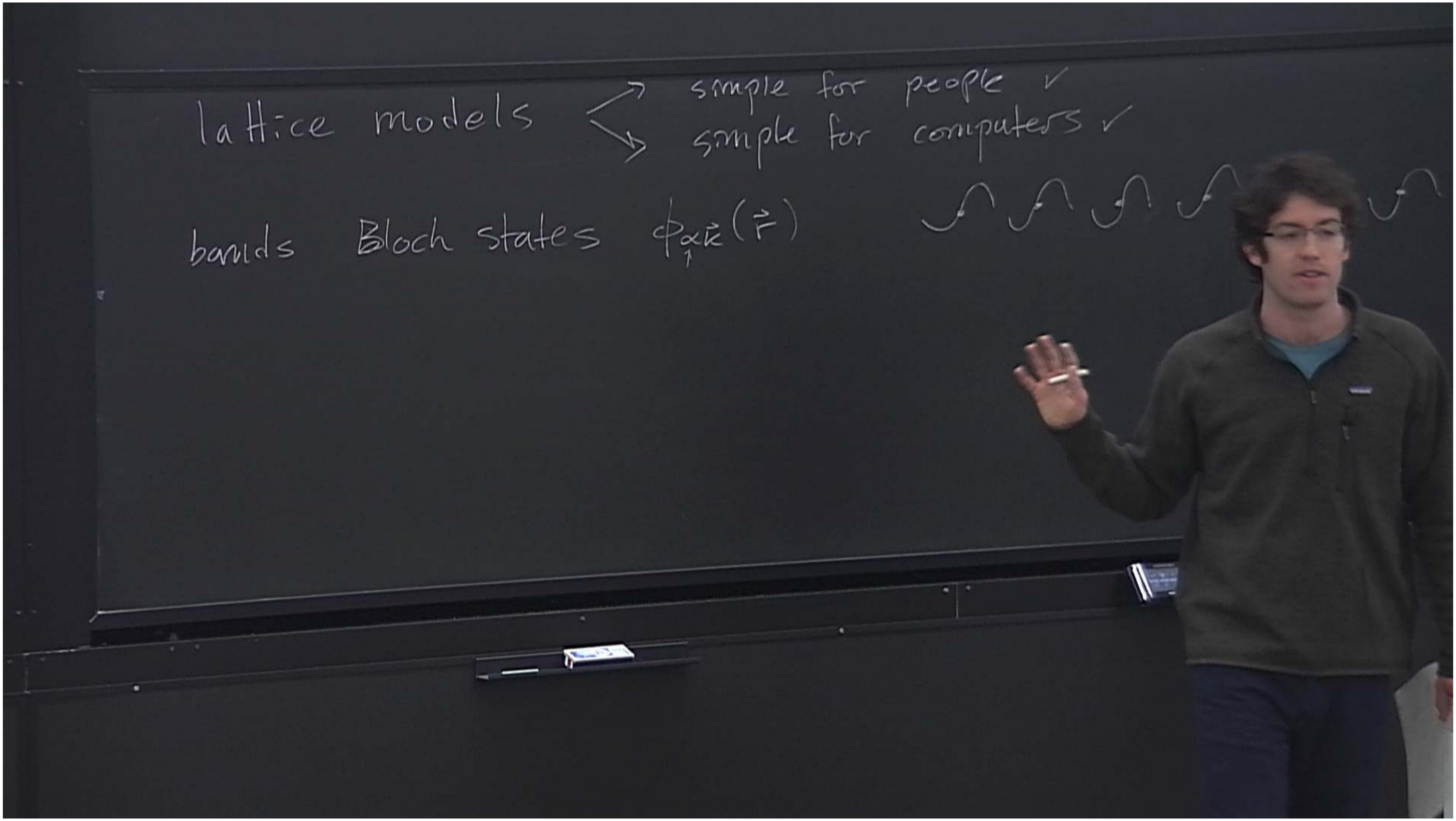

d & f bands
d & f orbitals
bound
$\langle r \rangle$ smaller
3d orbitals → angular structure
smaller t
larger U

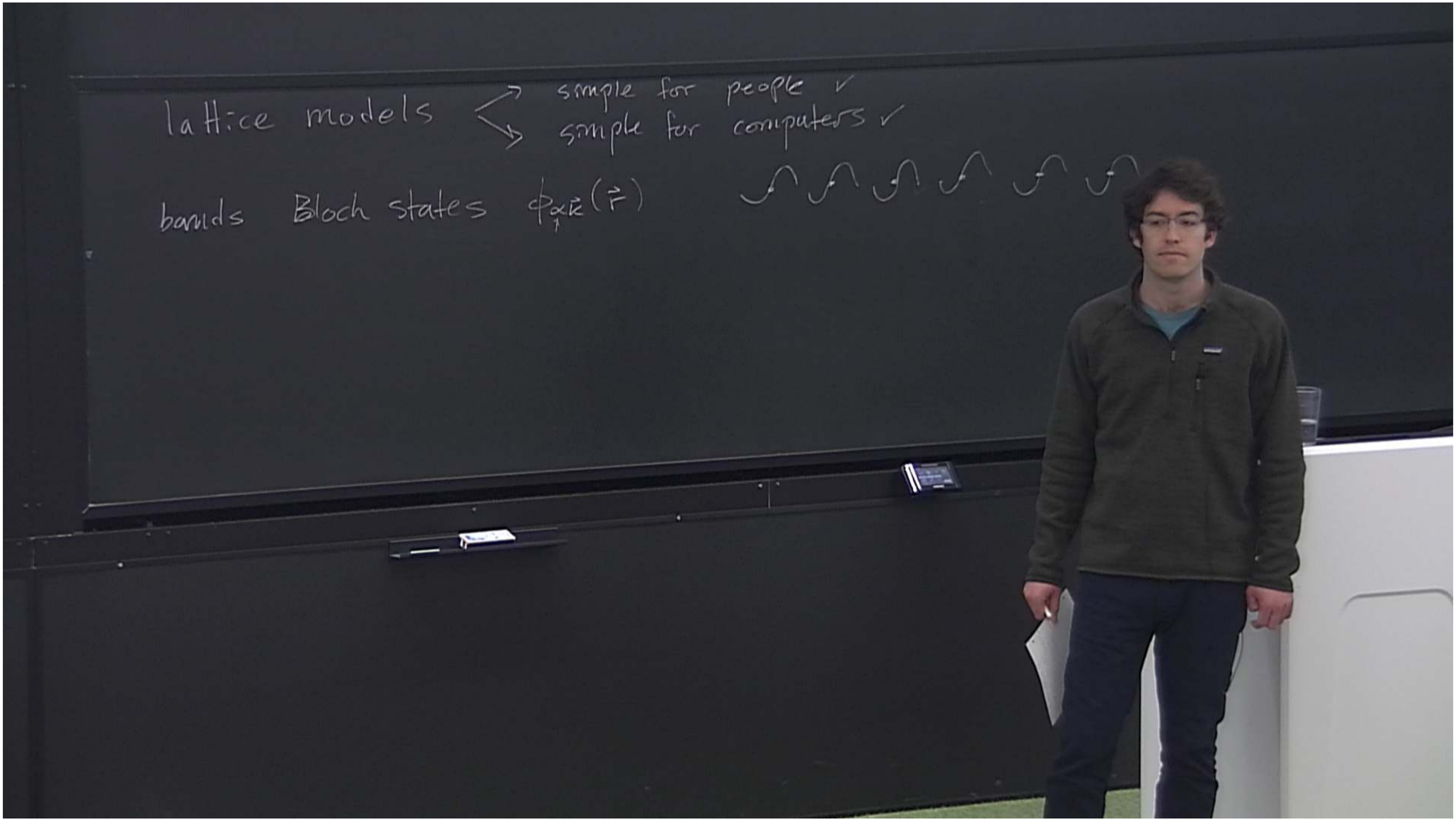

d & f bands
d & f orbitals → tightly
smaller
3d orbitals → angular structure →
smaller t
larger U

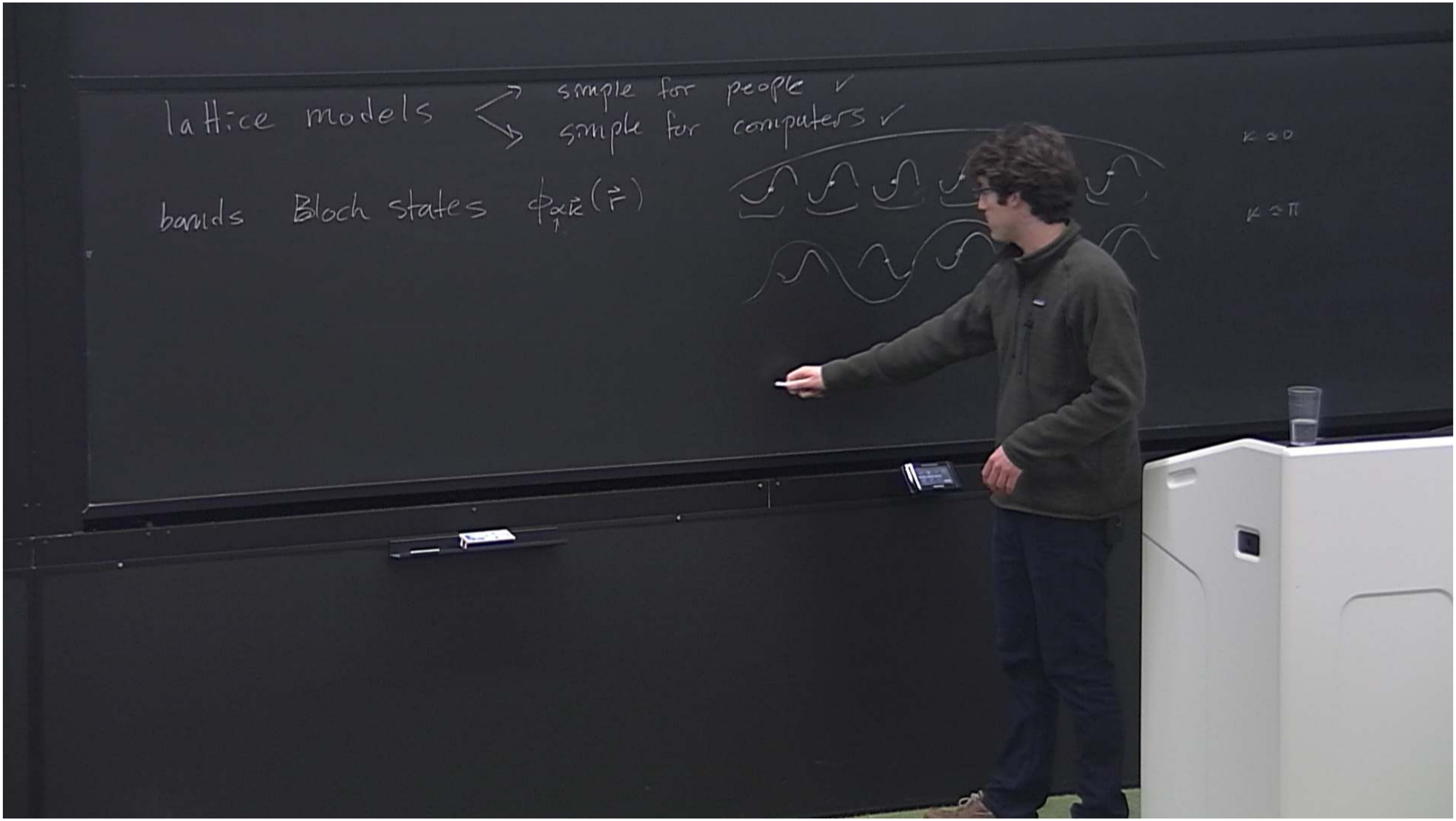

lattice models
simple for

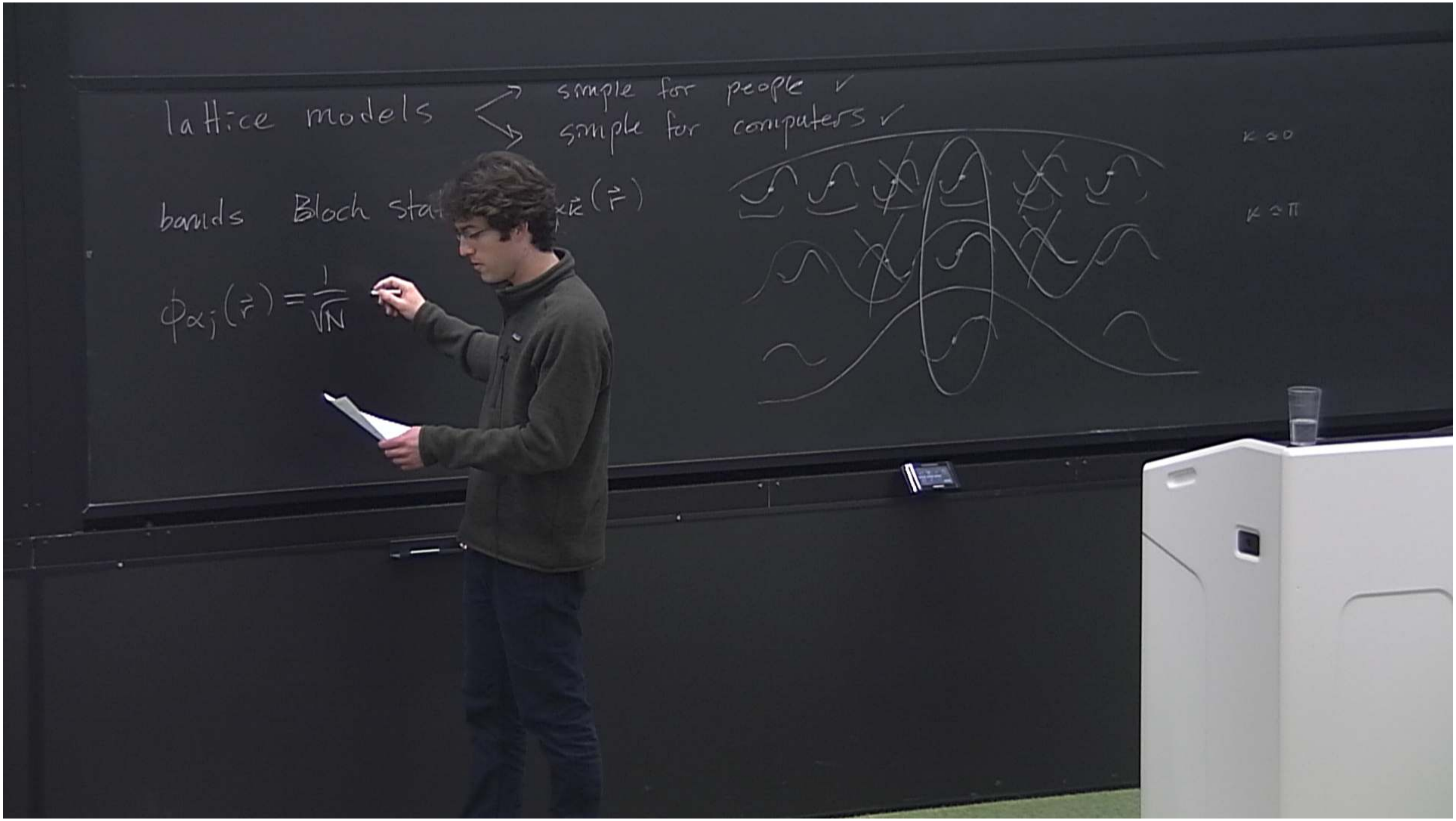

lattice models
simple for people
simple for computers

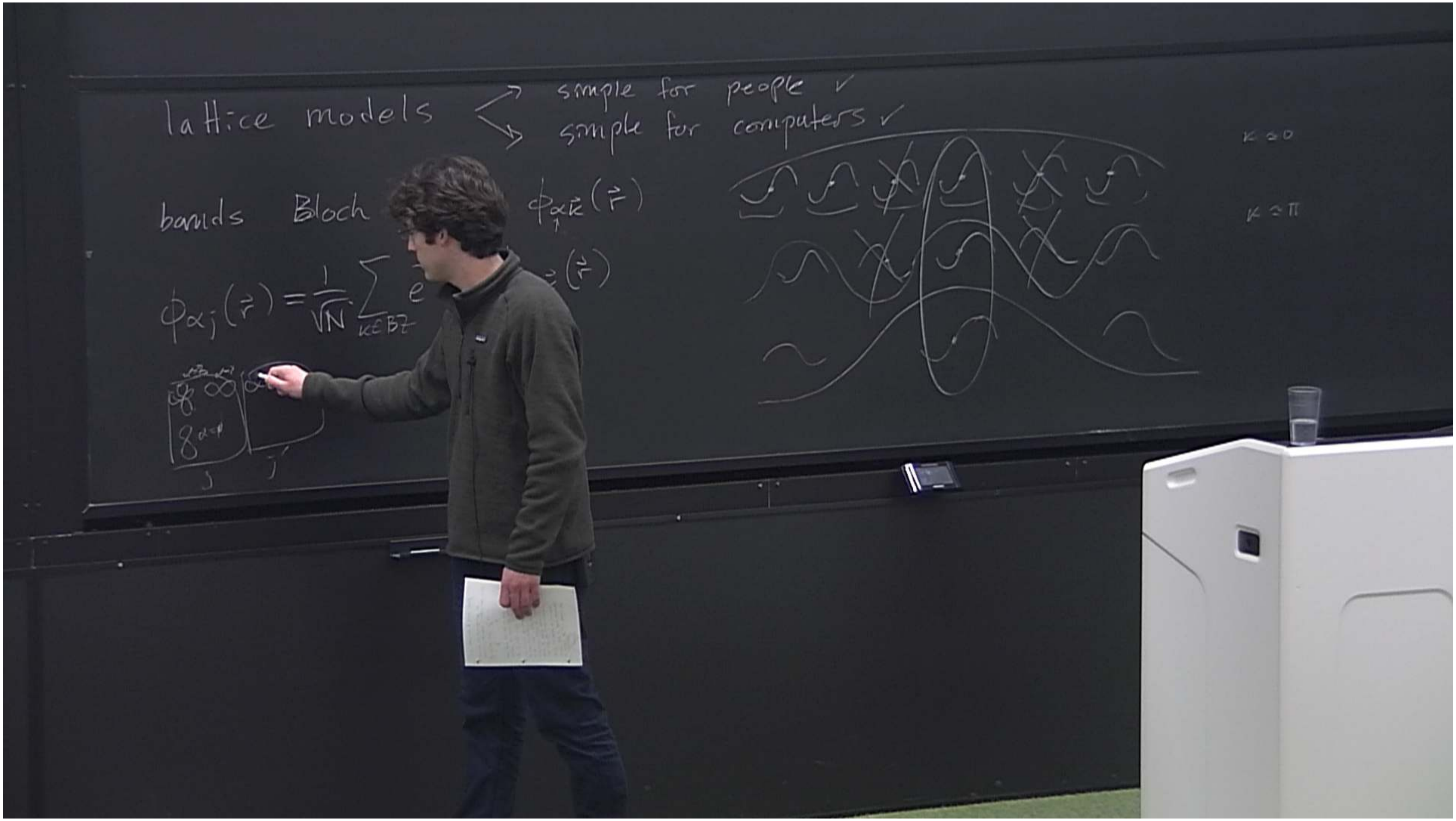

lattice models
simple for people ✓
simple for computers ✓
bands Bloch states $\phi_{\alpha \vec{k}}(\vec{r})$


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 $\phi_{\alpha \vec{k}}(\vec{r})$

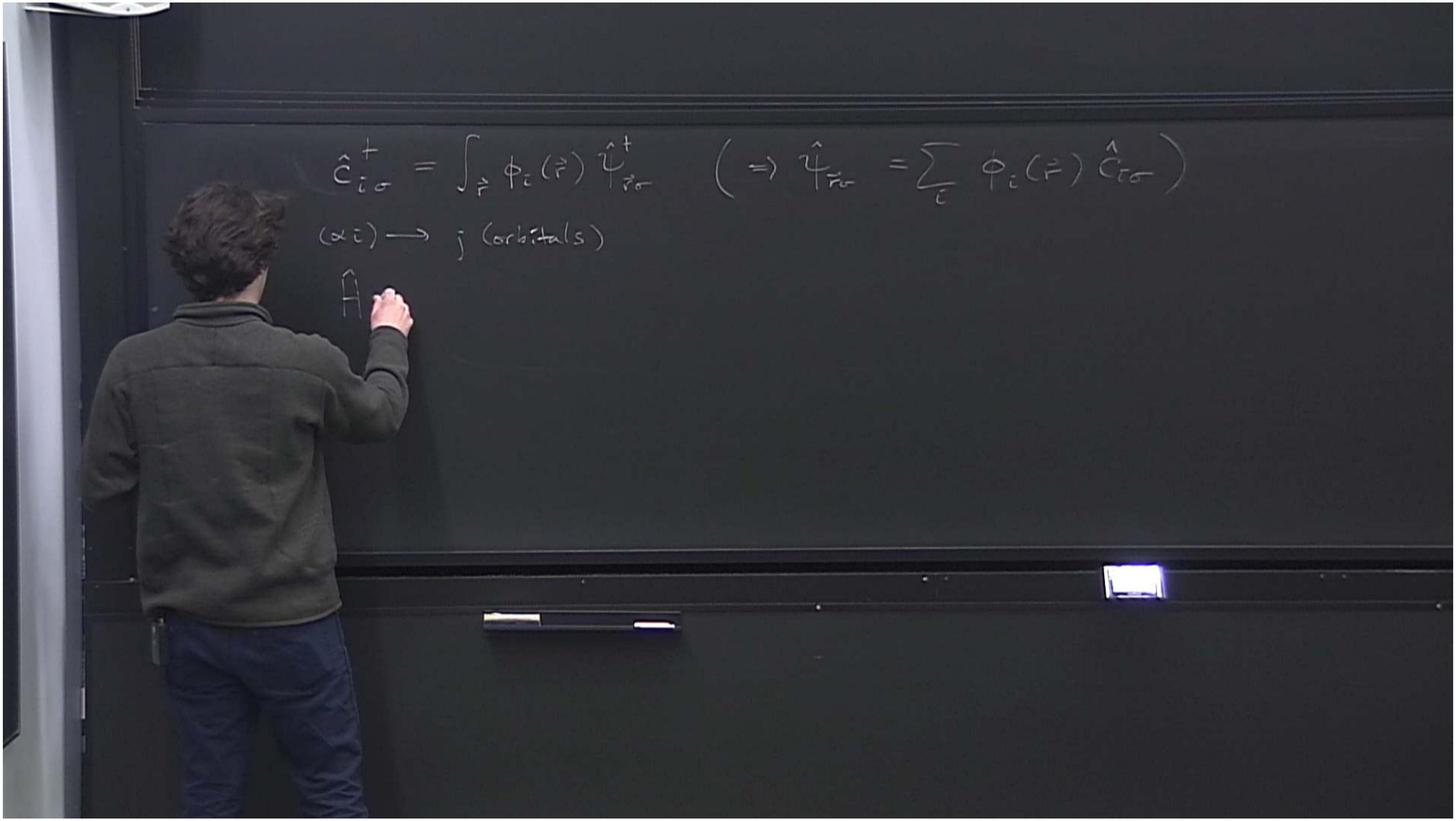

lattice models
simple for people ✓
simple for computers ✓
bands Bloch states $\phi_{\alpha \vec{k}}(\vec{r})$
k = 0
k = π

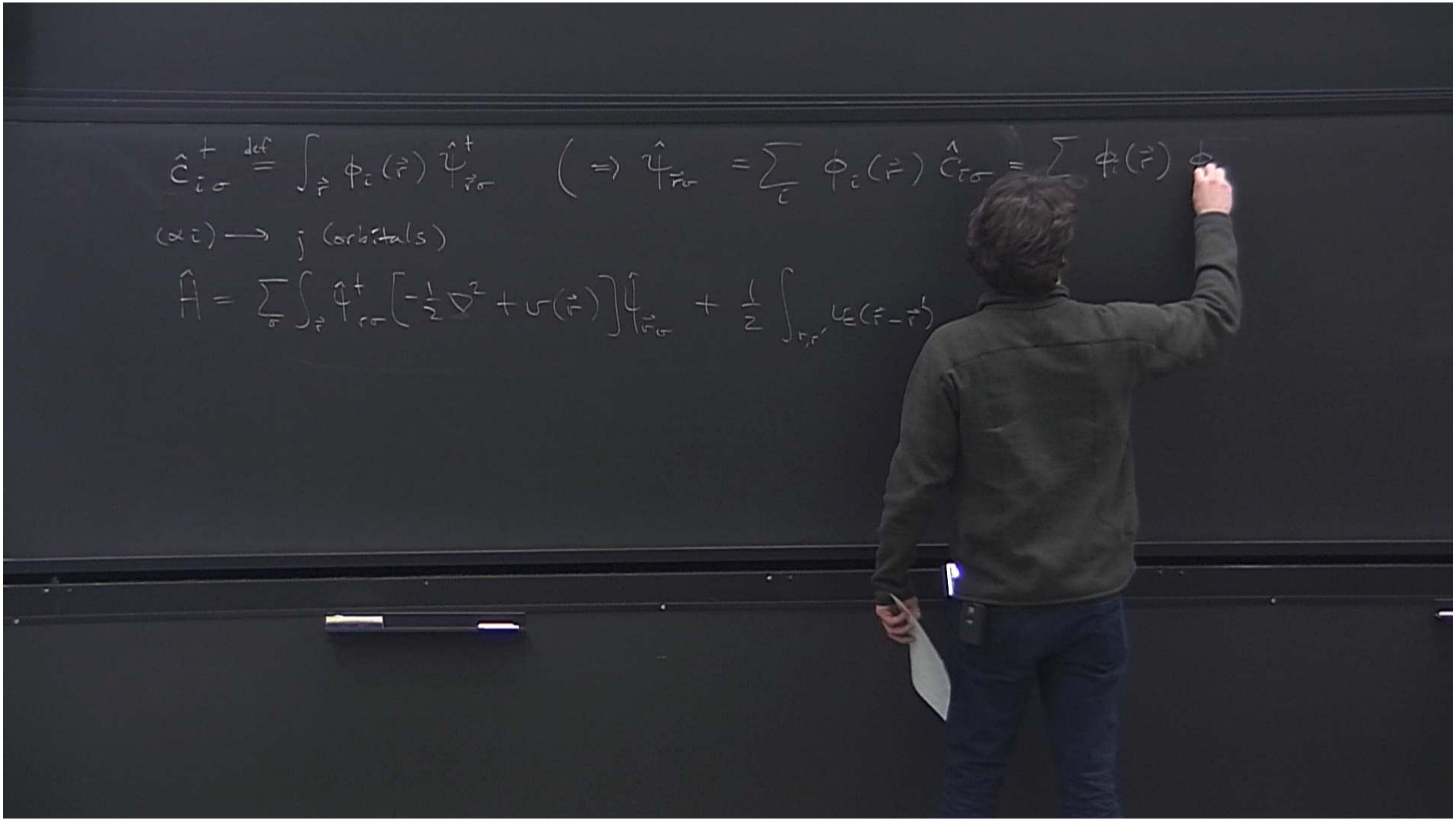

lattice models
simple for people ✓
simple for computers ✓
bands Bloch stat
$\kappa = 0$
$\kappa = \pi$
$\phi_{\alpha j}(\vec{r}) = \frac{1}{\sqrt{N}}$

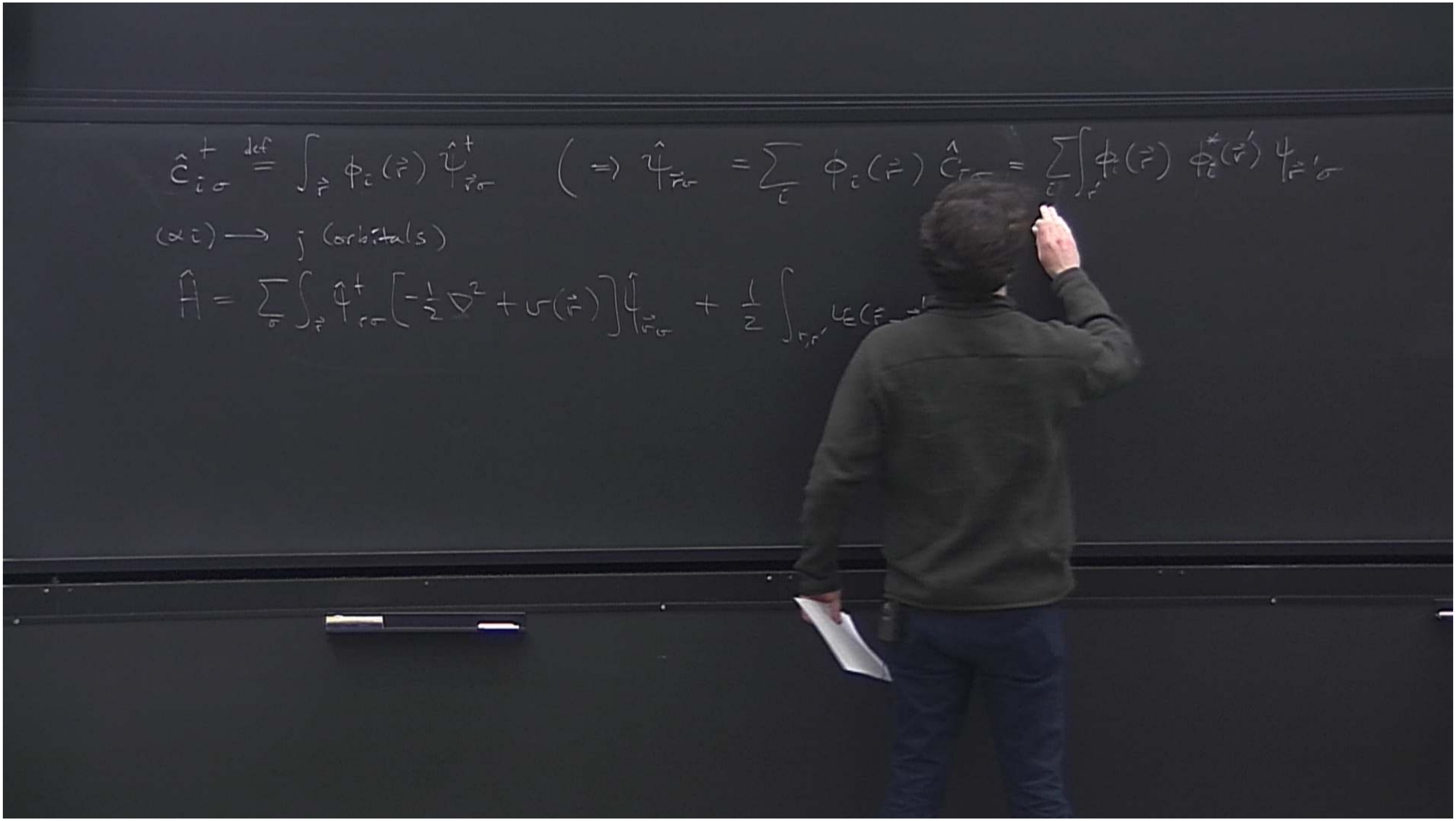

lattice models
simple for people ✓
simple for computers ✓
bands Bloch
$\phi_{\alpha \vec{k}}(\vec{r})$
$\phi_{\alpha j}(\vec{r}) = \frac{1}{\sqrt{N}} \sum_{k \in BZ} e$
$\kappa \approx 0$
$\kappa \approx \pi$

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

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


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

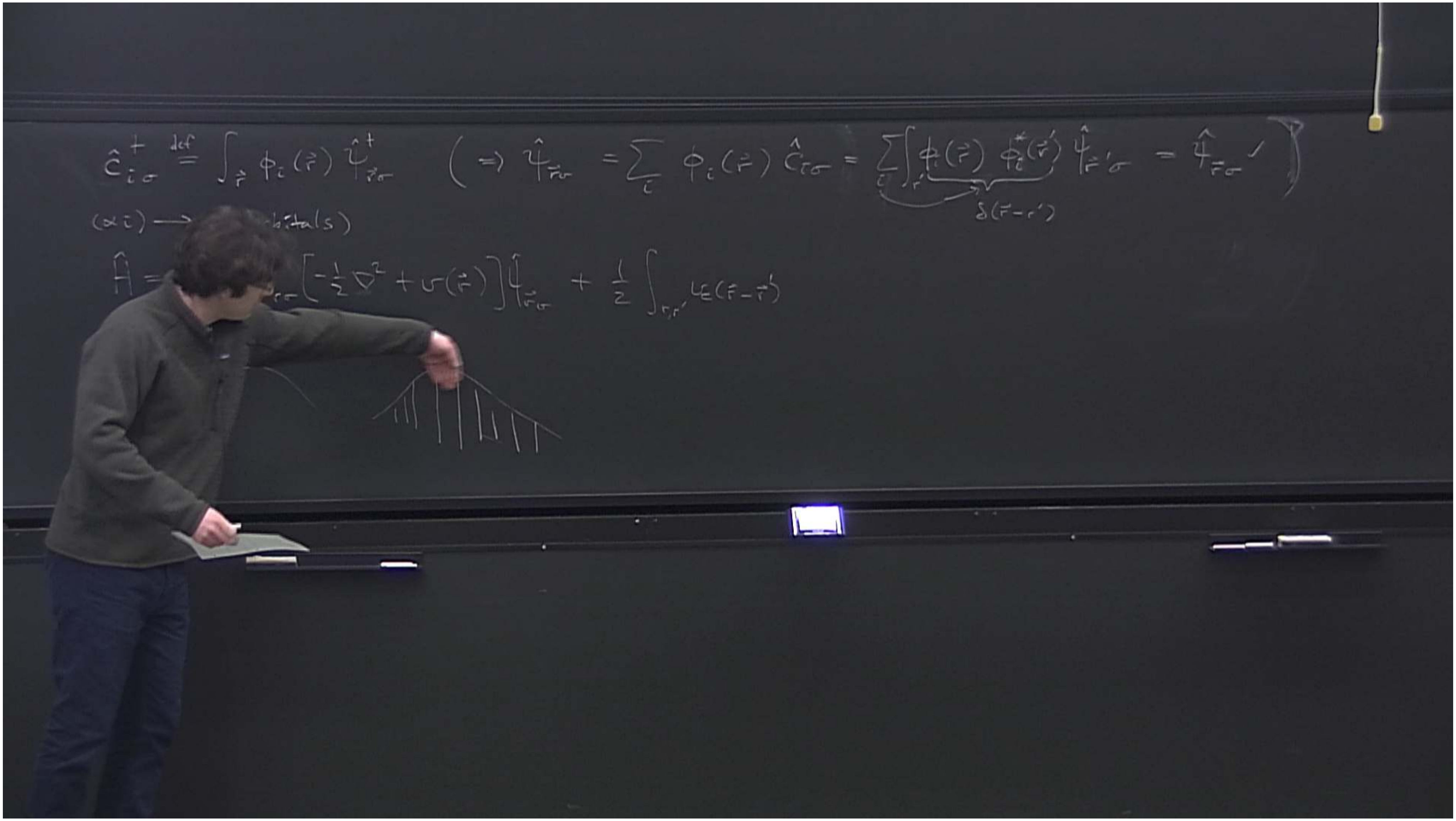

$\hat{c}^{\dagger}_{i\sigma} \overset{def}{=} \int_{\vec{r}} \phi_i(\vec{r})\, \hat{\psi}^{\dagger}_{\vec{r}\sigma} \quad (\Rightarrow \hat{\psi}_{\vec{r}\sigma} = \sum_i \phi_i(\vec{r})\, \hat{c}_{i\sigma} = \sum \phi_i(\vec{r})\, \phi$
$(\alpha i) \longrightarrow j$ (orbitals)
$\hat{H} = \sum_{\sigma}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

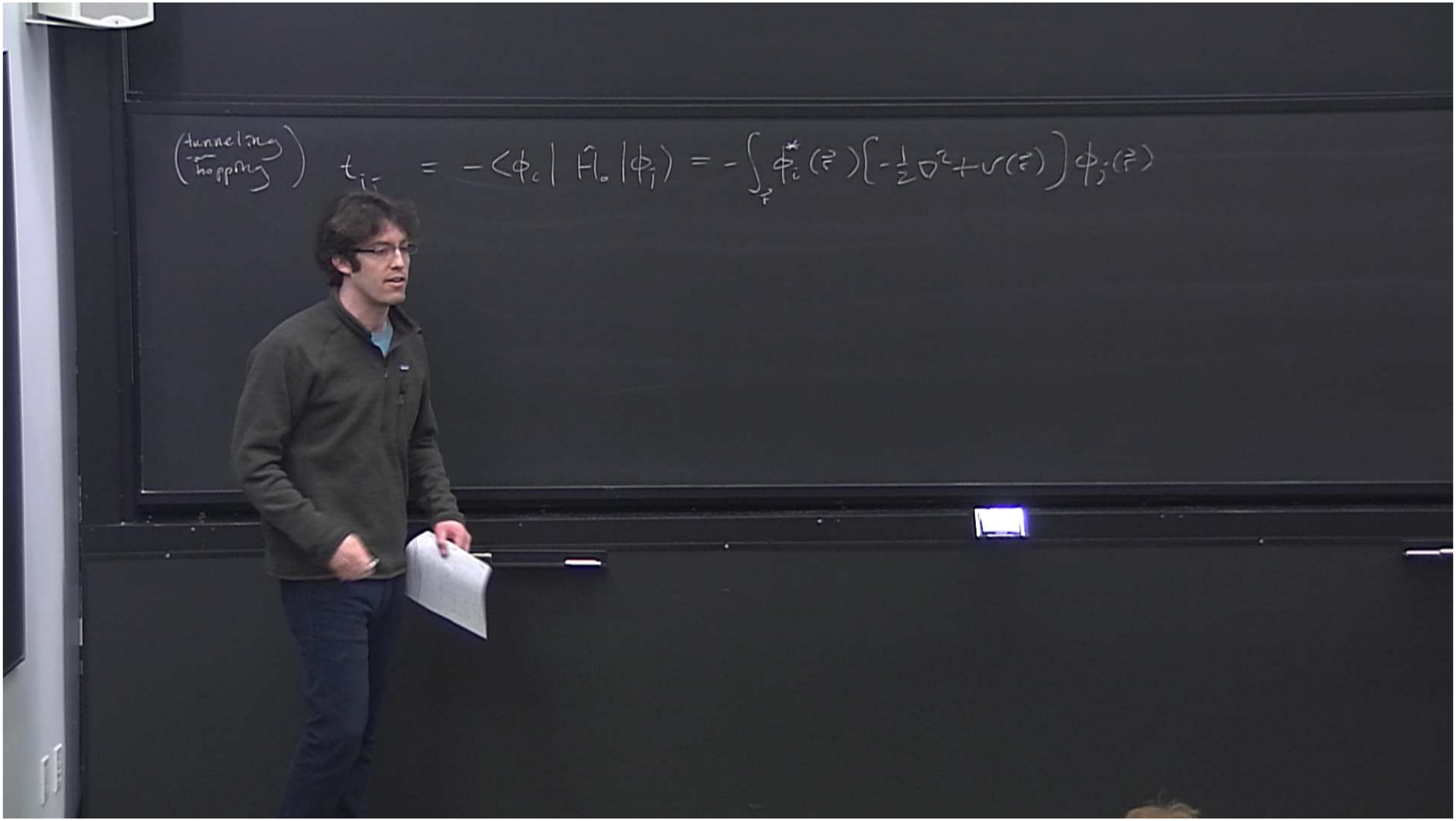

$\hat{c}^{\dagger}_{i\sigma} \overset{\text{def}}{=} \int_{\vec{r}} \phi_i(\vec{r})\, \hat{\psi}^{\dagger}_{\vec{r}\sigma}$ $\Big(\Rightarrow \hat{\psi}_{\vec{r}\sigma} = \sum_i \phi_i(\vec{r})\, \hat{c}_{i\sigma} = \sum_i \int_{\vec{r}'} \phi_i(\vec{r})\, \phi_i^*(\vec{r}')\, \psi_{\vec{r}'\sigma}$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

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

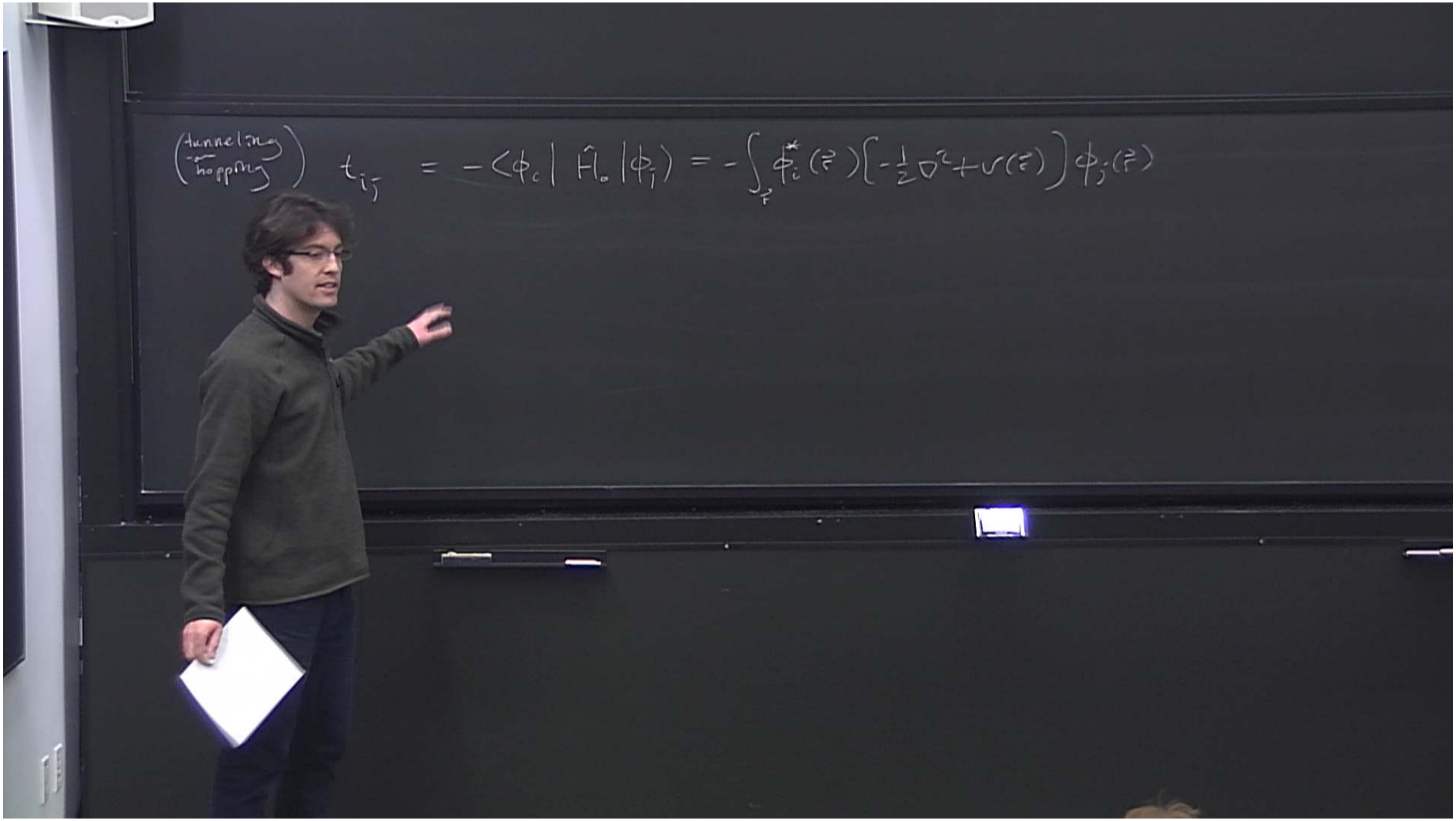
$(\alpha i) \longrightarrow j$ (orbitals)

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





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

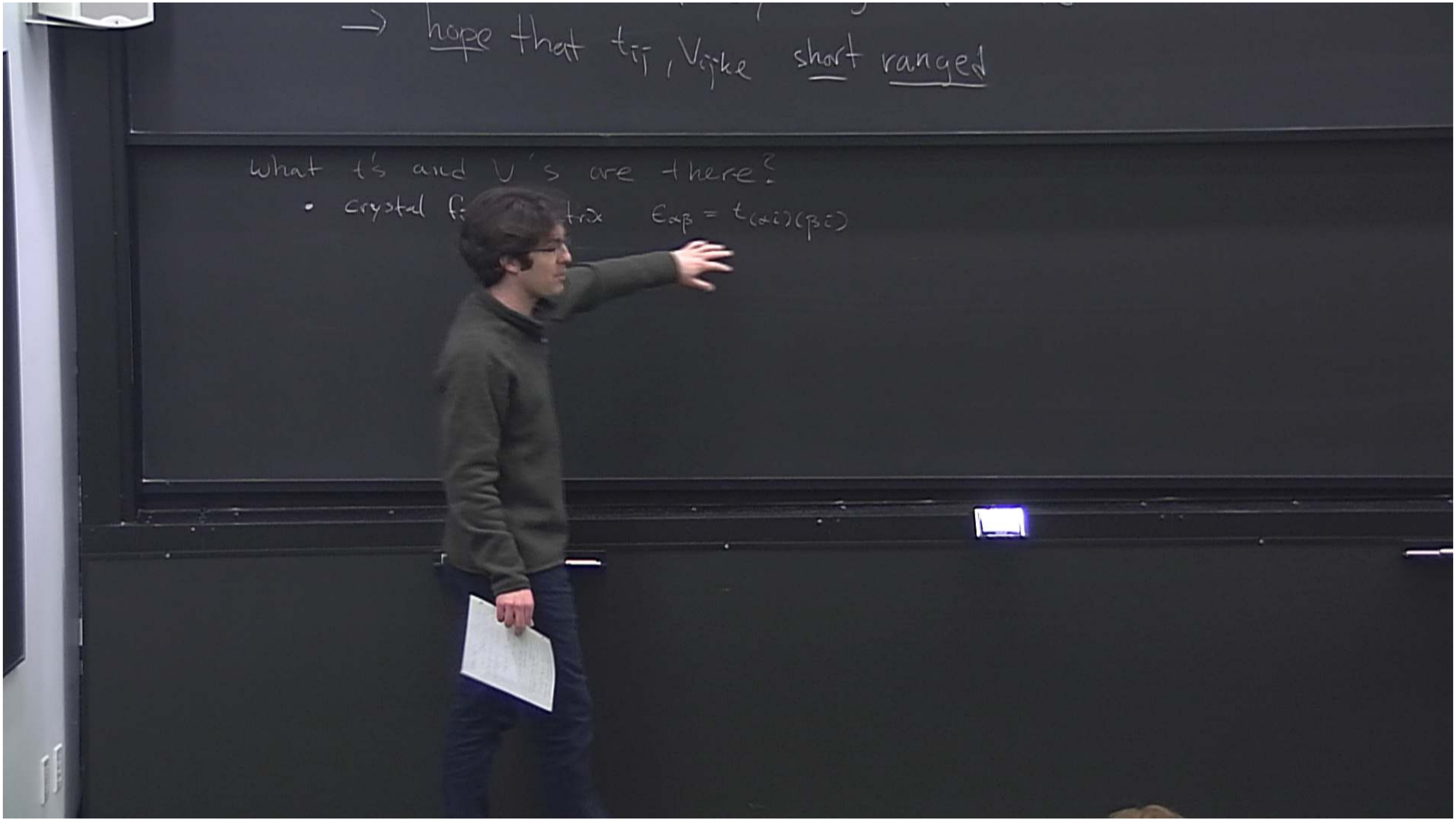

(tunneling or hopping)
$t_{ij} = -\langle \phi_i | \hat{H}_0 | \phi_j \rangle = -\int_{\vec{r}} \phi_i^*(\vec{r}) \left[-\frac{1}{2}\nabla^2 + v(\vec{r}) \right] \phi_j(\vec{r})$

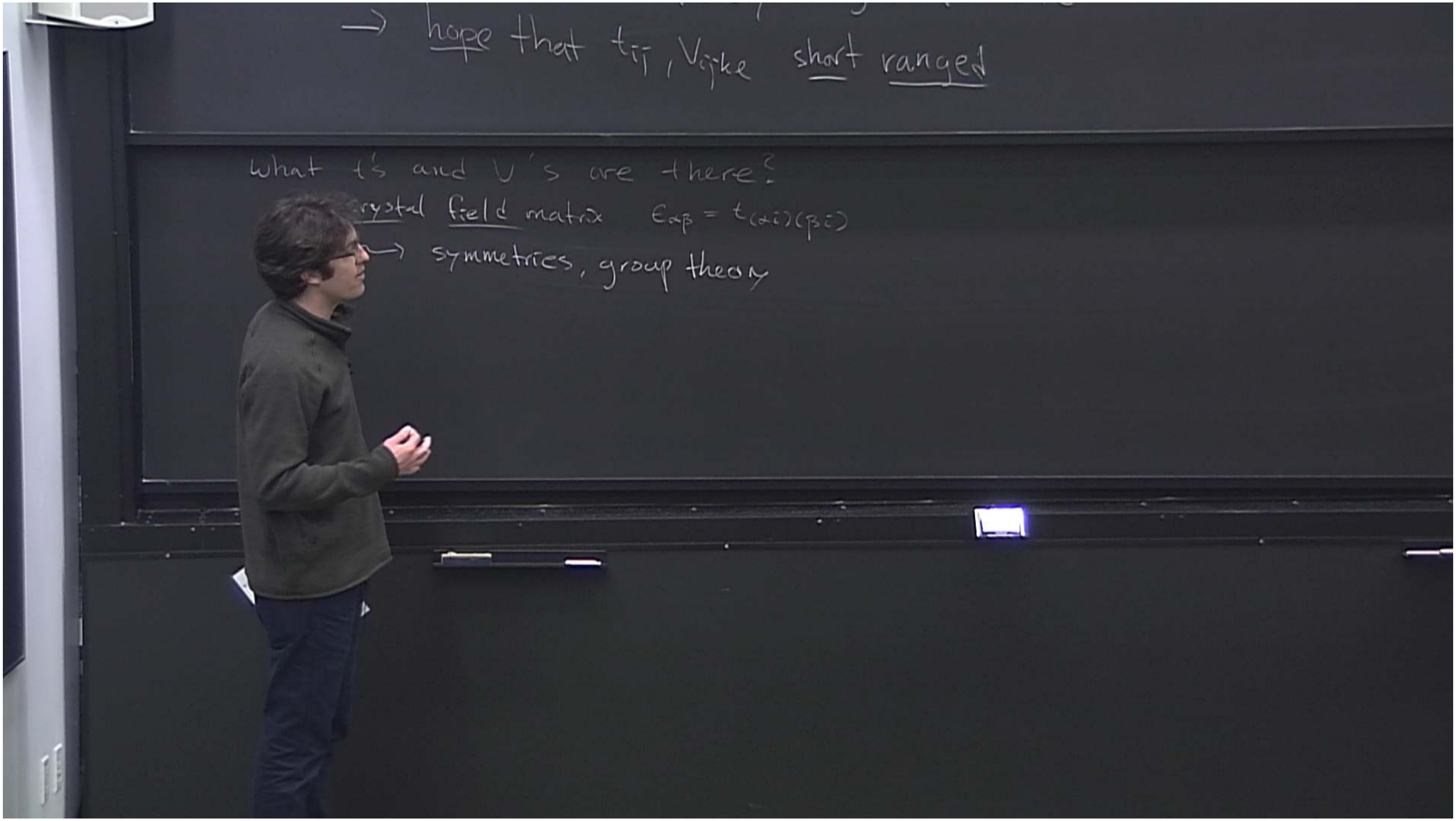
(tunneling / hopping) $t_{ij} = -\langle \phi_i | \hat{H}_0 | \phi_j \rangle = -\int_{\vec{r}} \phi_i^*(\vec{r}) \left[-\frac{1}{2}\nabla^2 + v(\vec{r}) \right] \phi_j(\vec{r})$

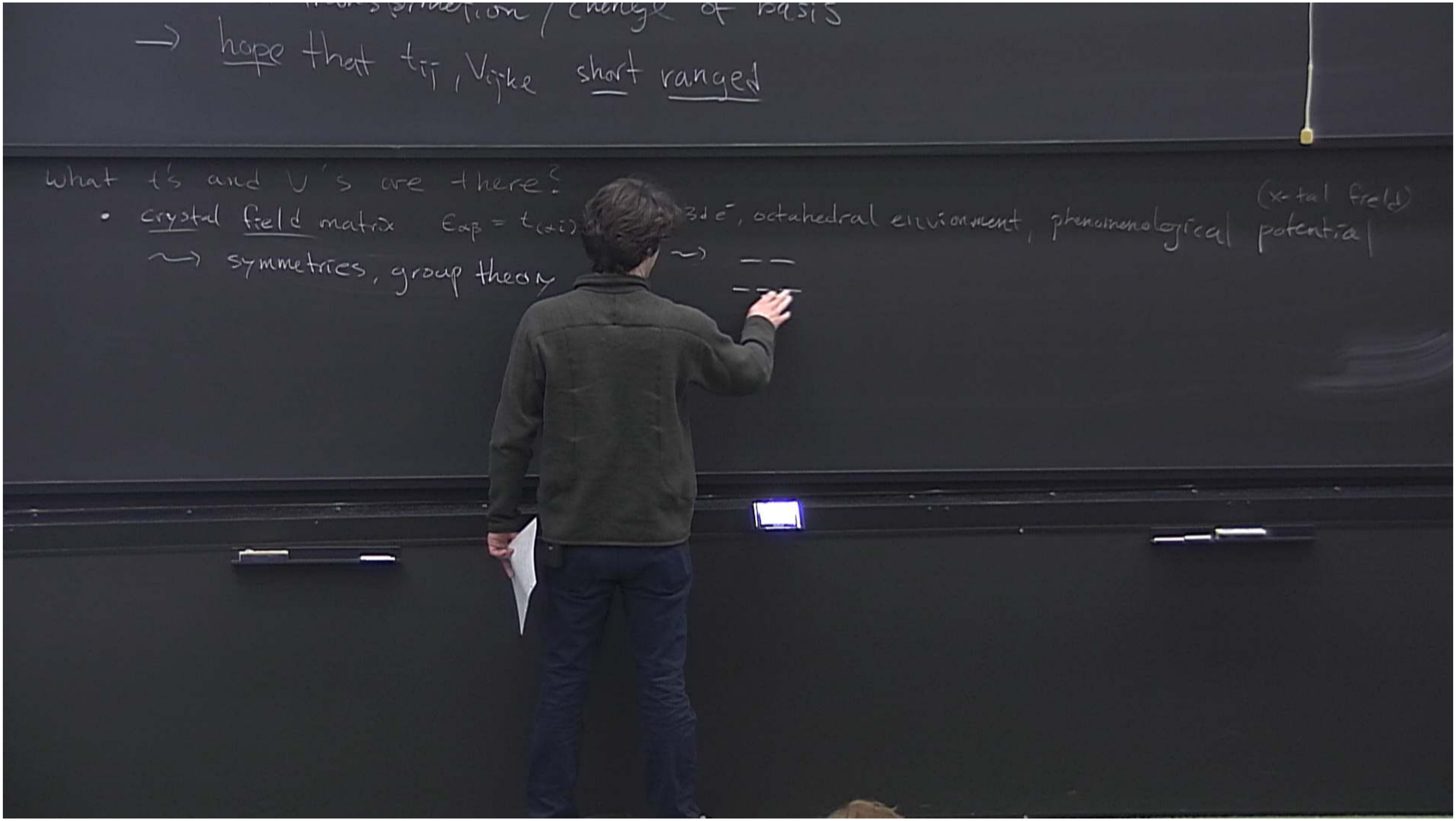
$V_{ijkl} = \frac{1}{2} \int v_{ee}(\vec{r} - \vec{r}') \, \phi_i^*(\vec{r}) \phi_j(\vec{r}) \phi_k^*(\vec{r}') \phi_l(\vec{r}')$

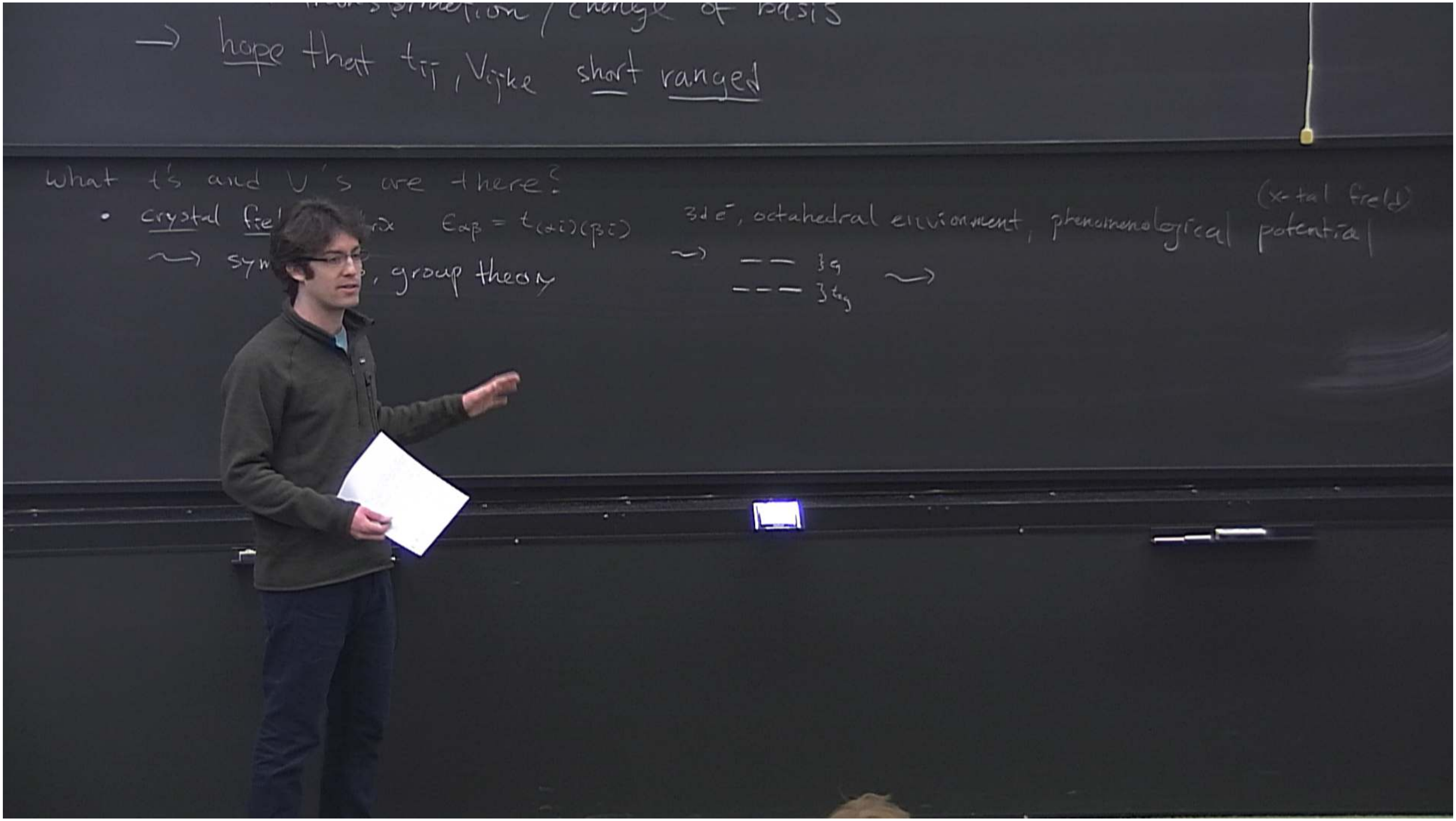
→ exact transformation / change of basis

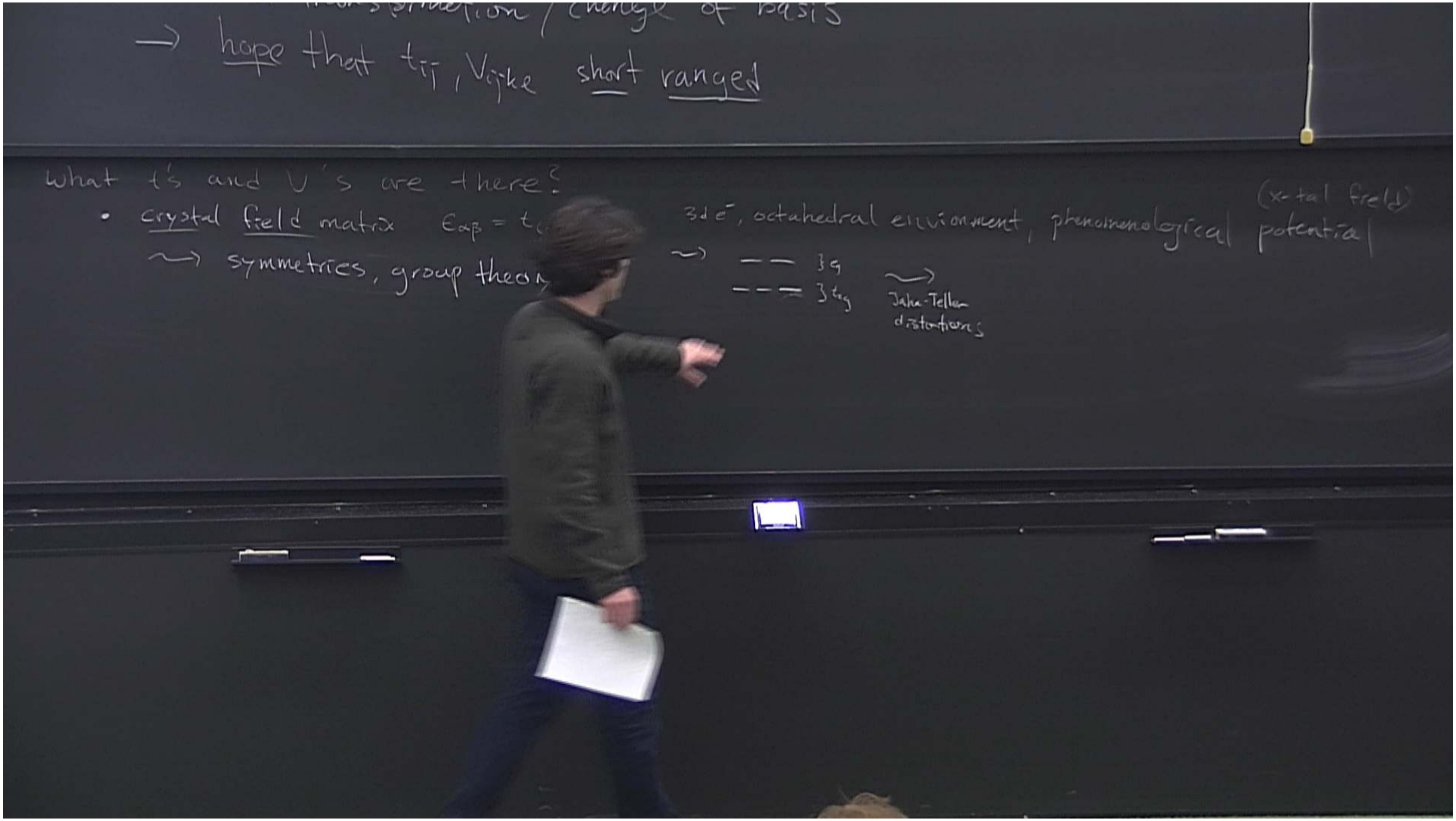
→ <u>hope</u> that t_{ij}, V_{ijkl} <u>short</u> <u>ranged</u>

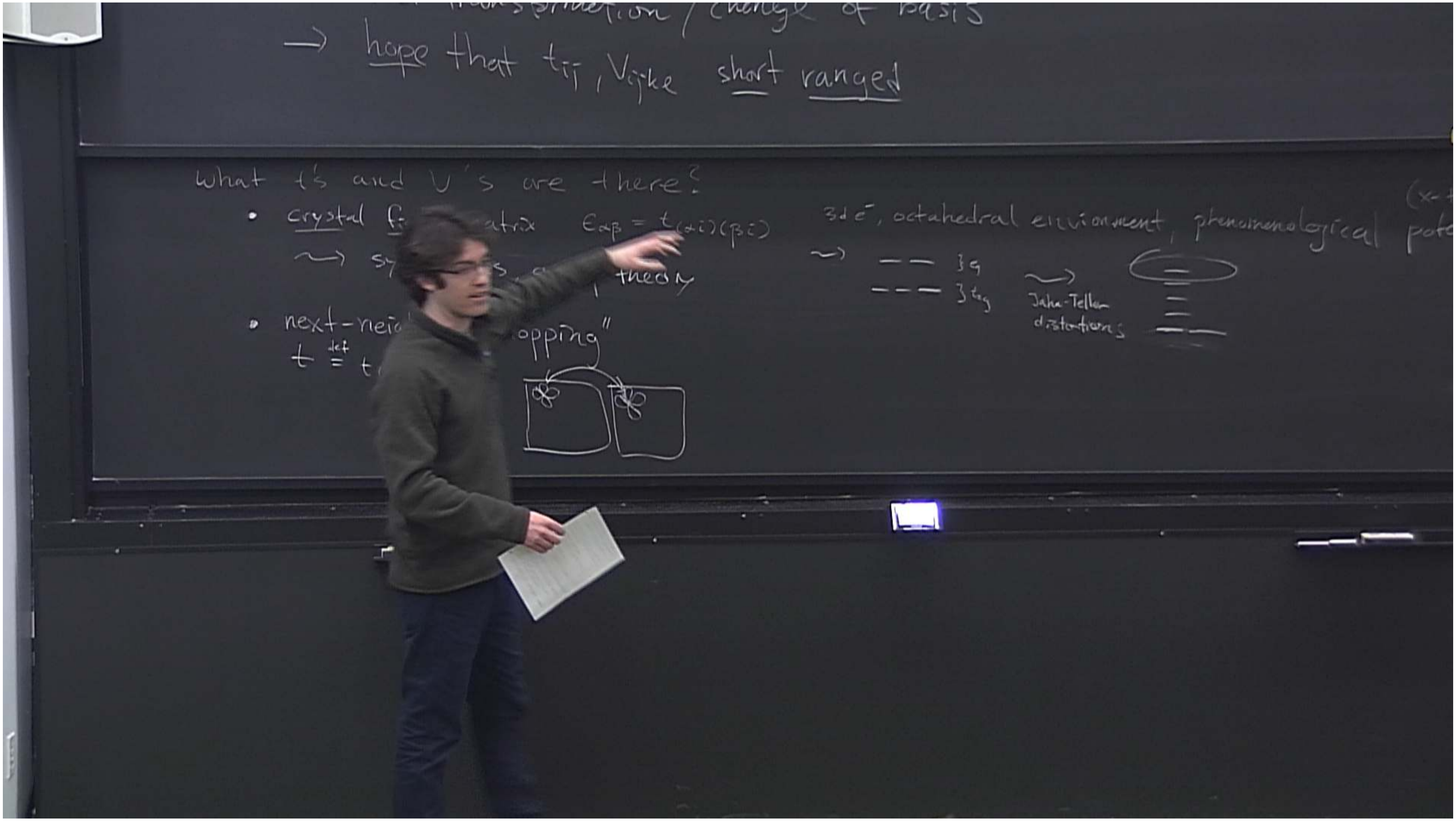

→ hope that t_ij, V_ijkl short ranged
what t's and V's are there?
• crystal fi trix ε_αβ = t_(αi)(βi)


→ hope that t_{ij}, V_{ijkl} short ranged
what t's and V's are there?
rystal field matrix $\epsilon_{\alpha\beta} = t_{(\alpha i)(\beta i)}$
→ symmetries, group theory


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


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


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


→ hope that tij, Vijkl short ranged
what t's and V's are there?
crystal
atrix
3d e⁻, octahedral environment, phenomenological
theory
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Jahn-Teller distortions
next-nei
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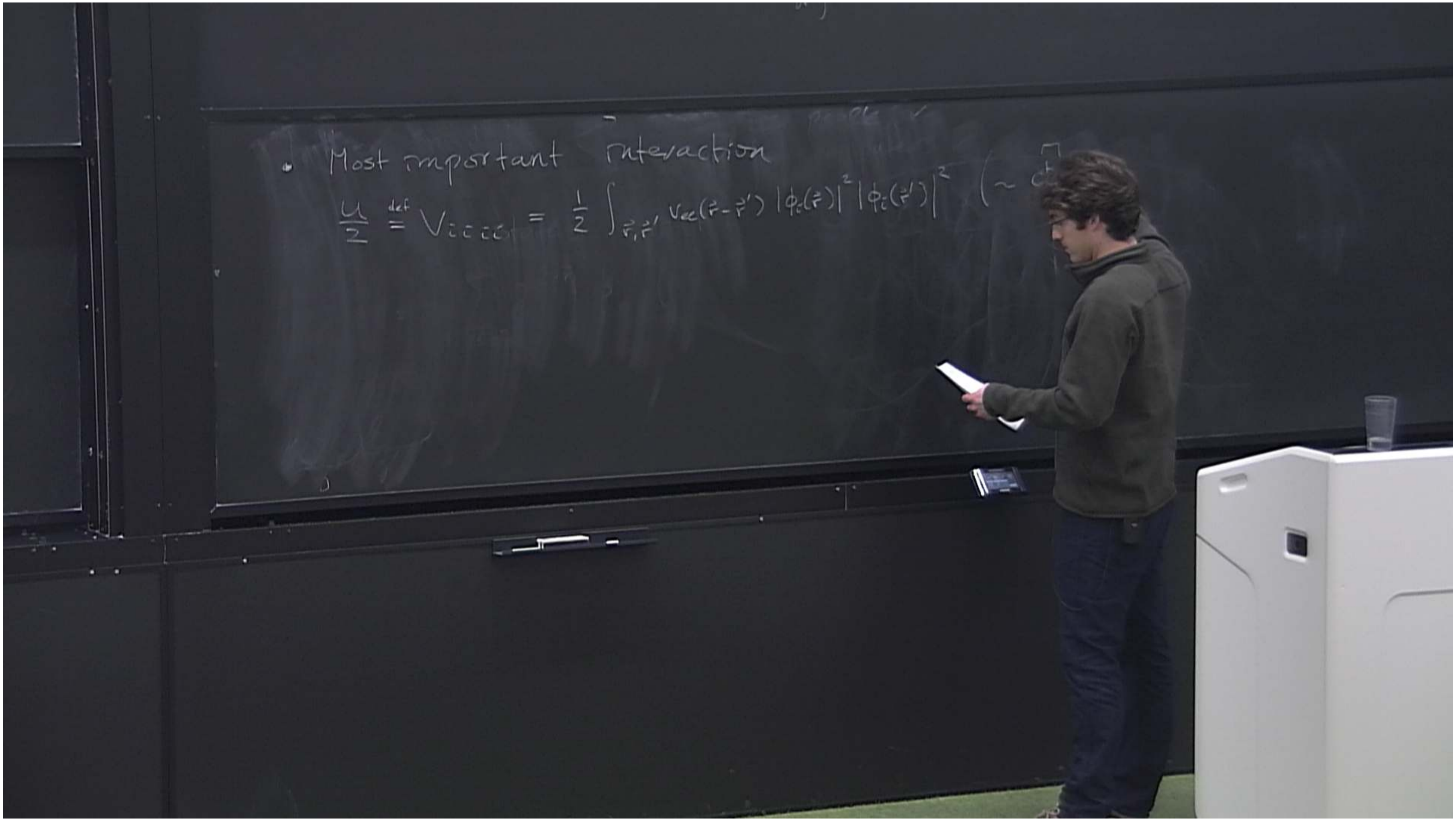
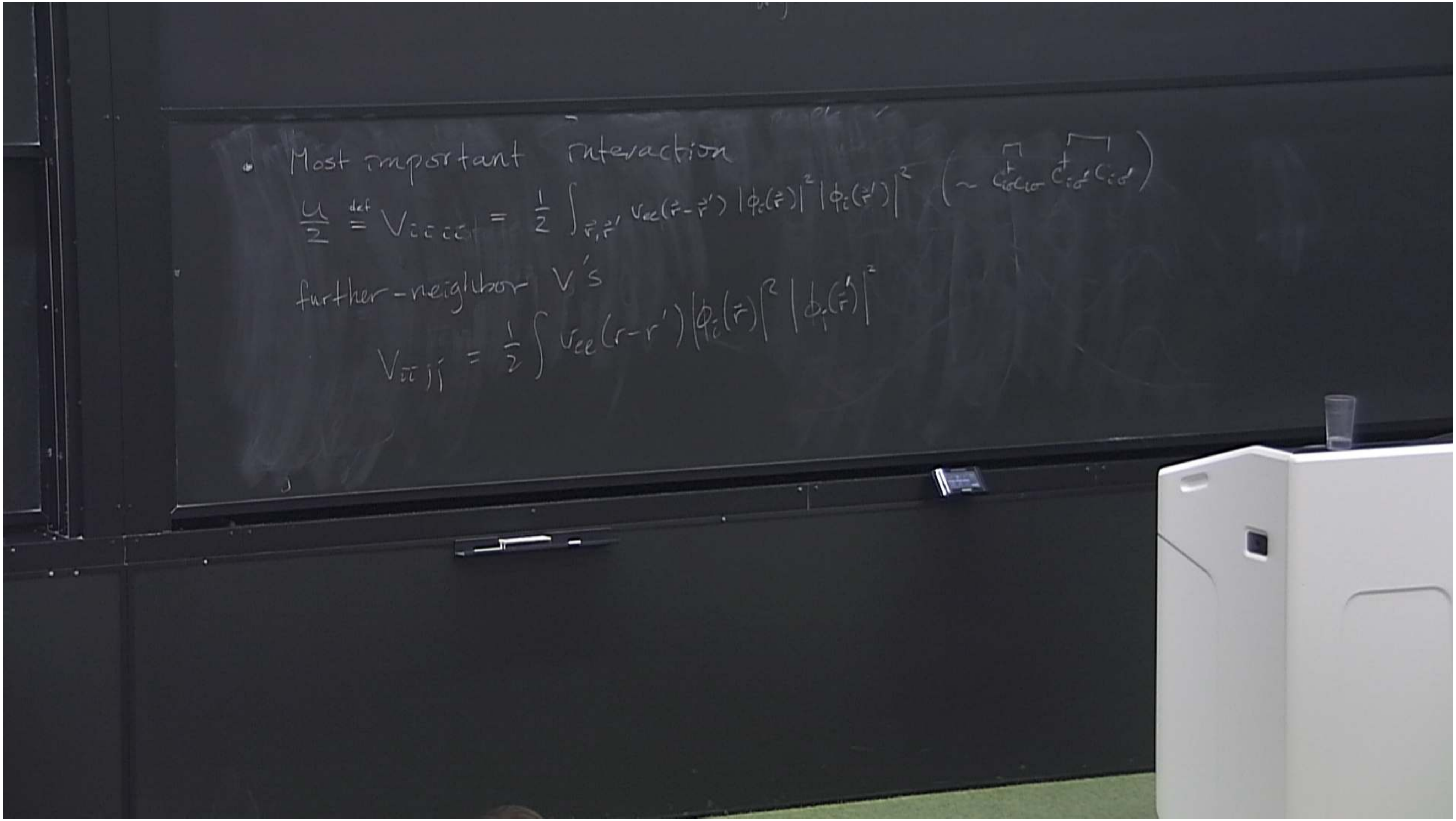
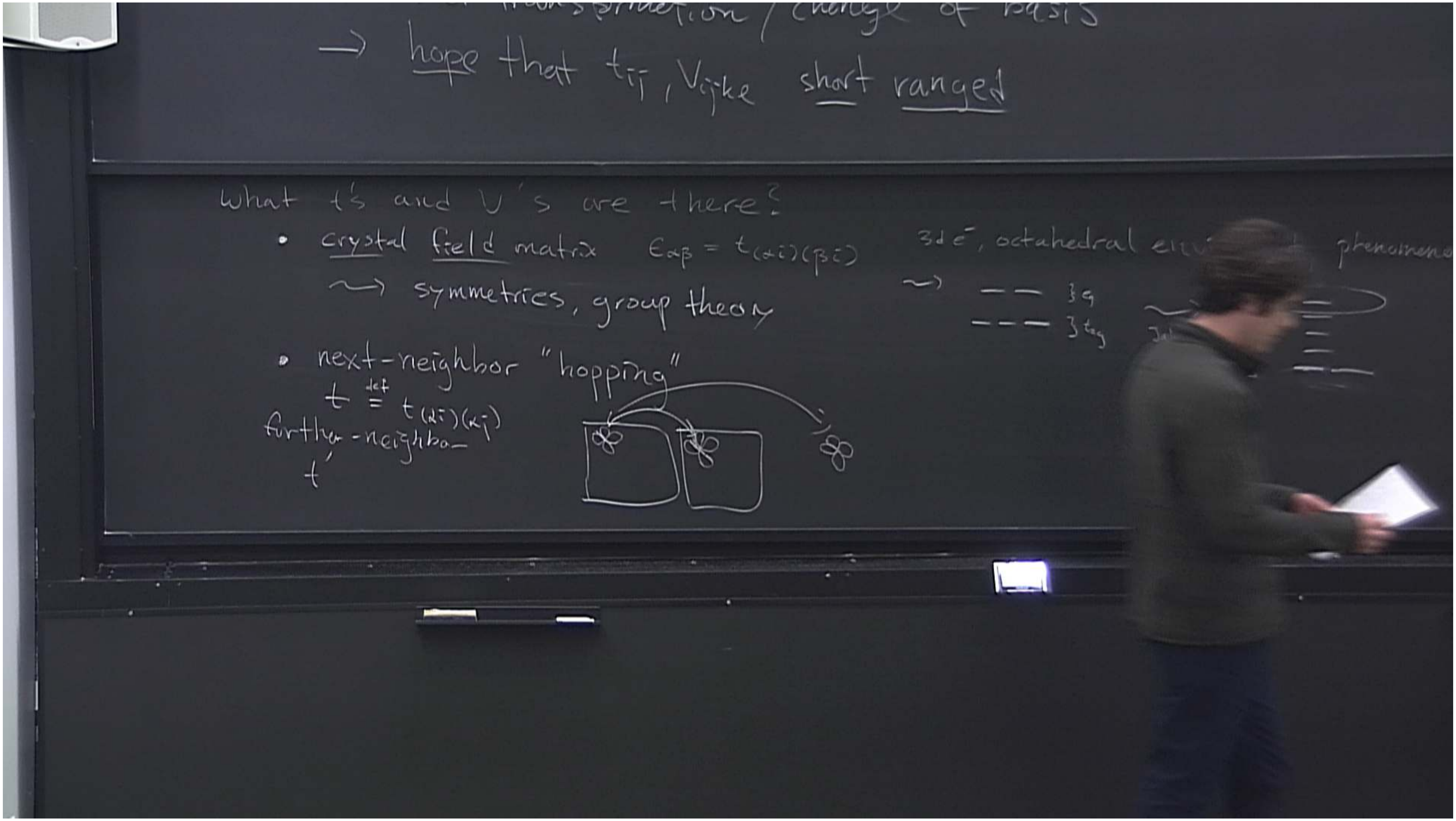
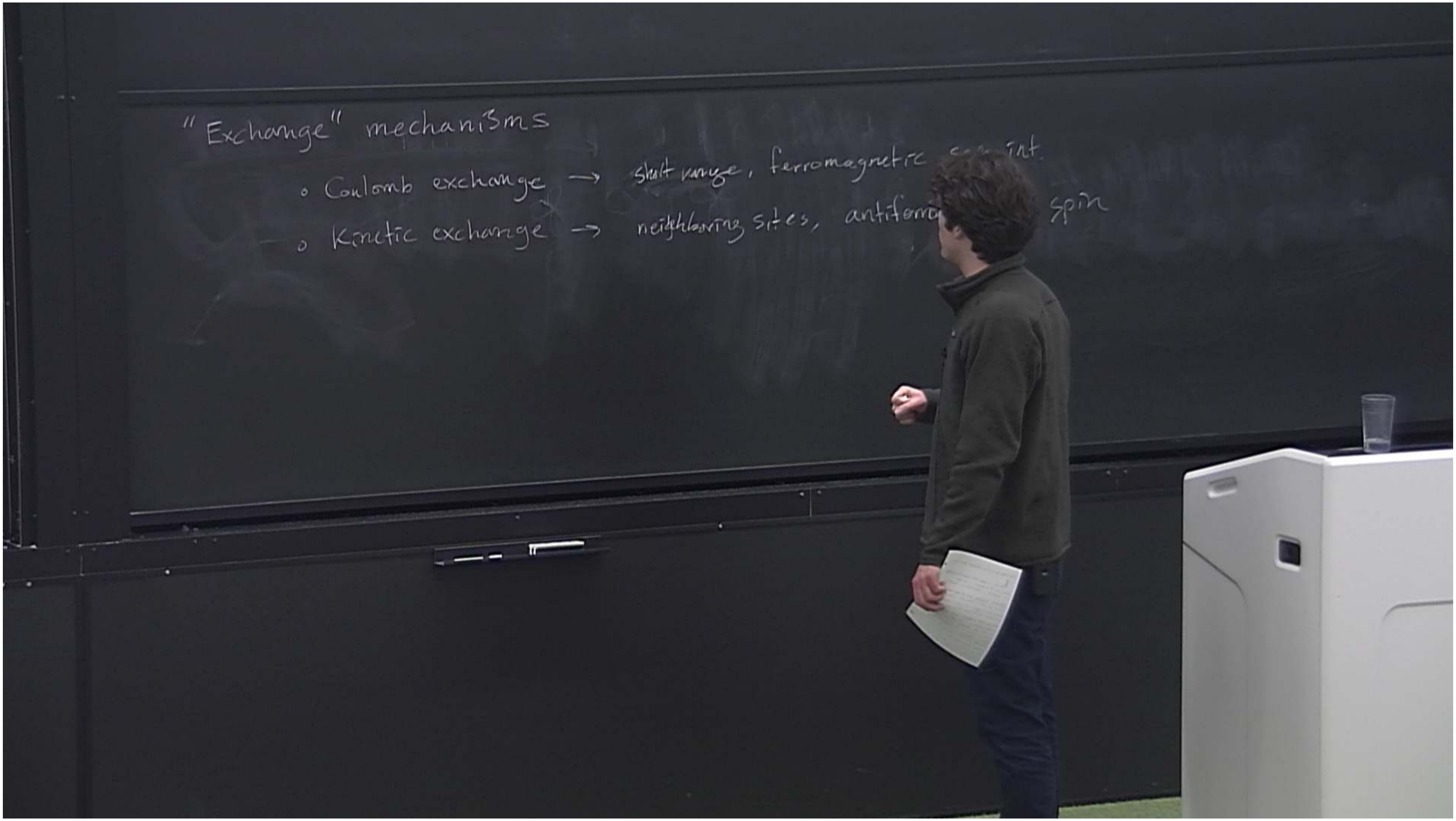
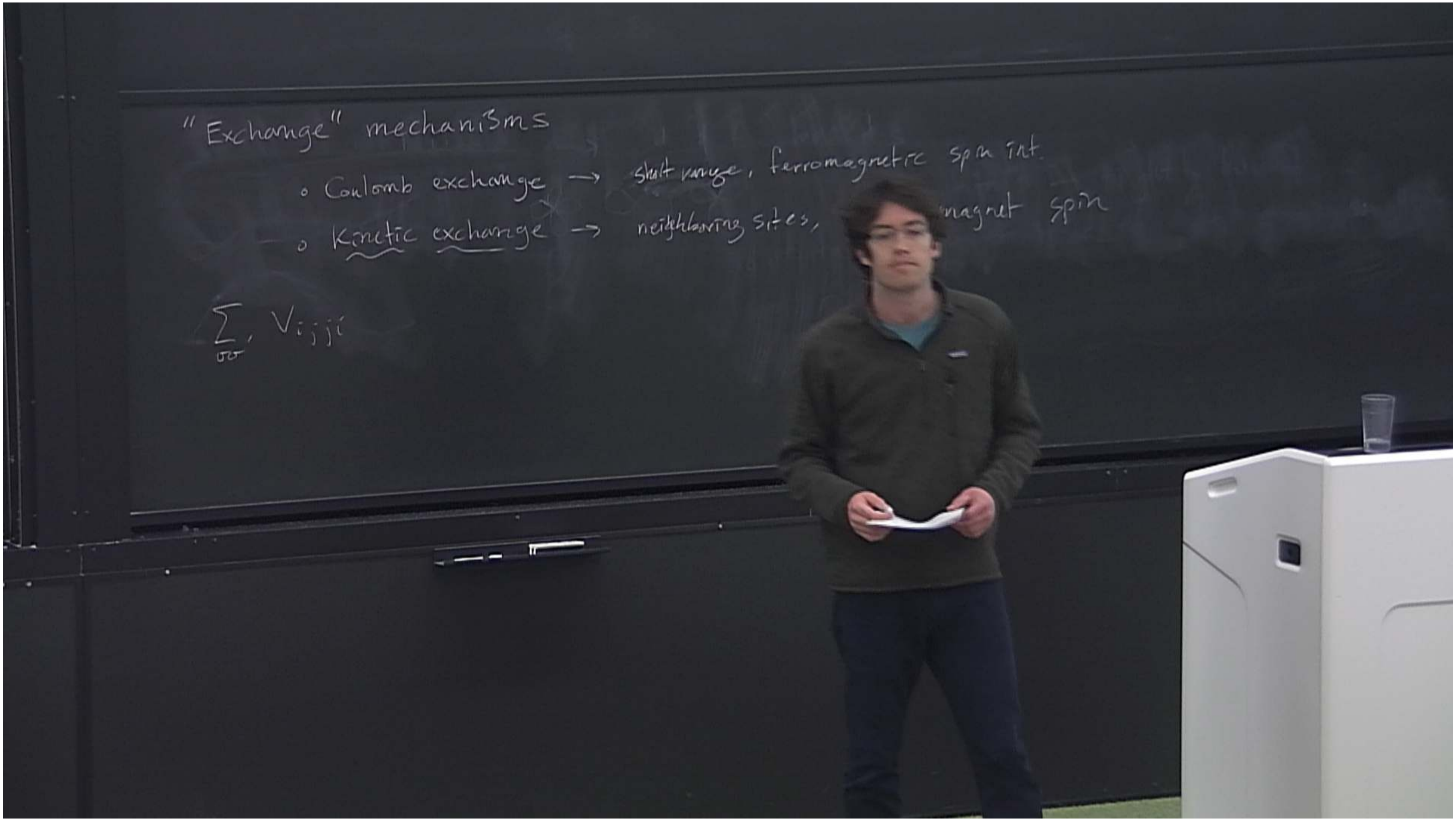

Most important interaction
$\frac{U}{2} \overset{\text{def}}{=} V_{iiii} = \frac{1}{2} \int_{\vec{r},\vec{r}'} V_{ee}(\vec{r}-\vec{r}') \, |\phi_i(\vec{r})|^2 |\phi_i(\vec{r}')|^2$ (~



• Most important interaction
$\frac{U}{2} \stackrel{\text{def}}{=} V_{iiii} = \frac{1}{2}\int_{\vec{r},\vec{r}'} v_{ee}(\vec{r}-\vec{r}')\,|\phi_i(\vec{r})|^2\,|\phi_i(\vec{r}')|^2 \quad (\sim c^\dagger_{i\sigma} c_{i\sigma}\, c^\dagger_{i\sigma'} c_{i\sigma'})$
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 $\epsilon_{\alpha\beta} = t_{(\alpha i)(\beta i)}$
⇝ symmetries, group theory
3d e^-, octahedral env
phenomena
e_g
t_{2g}
• next-neighbor "hopping"
$t \overset{def}{=} t_{(\alpha i)(\alpha j)}$
further-neighbor
t'


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


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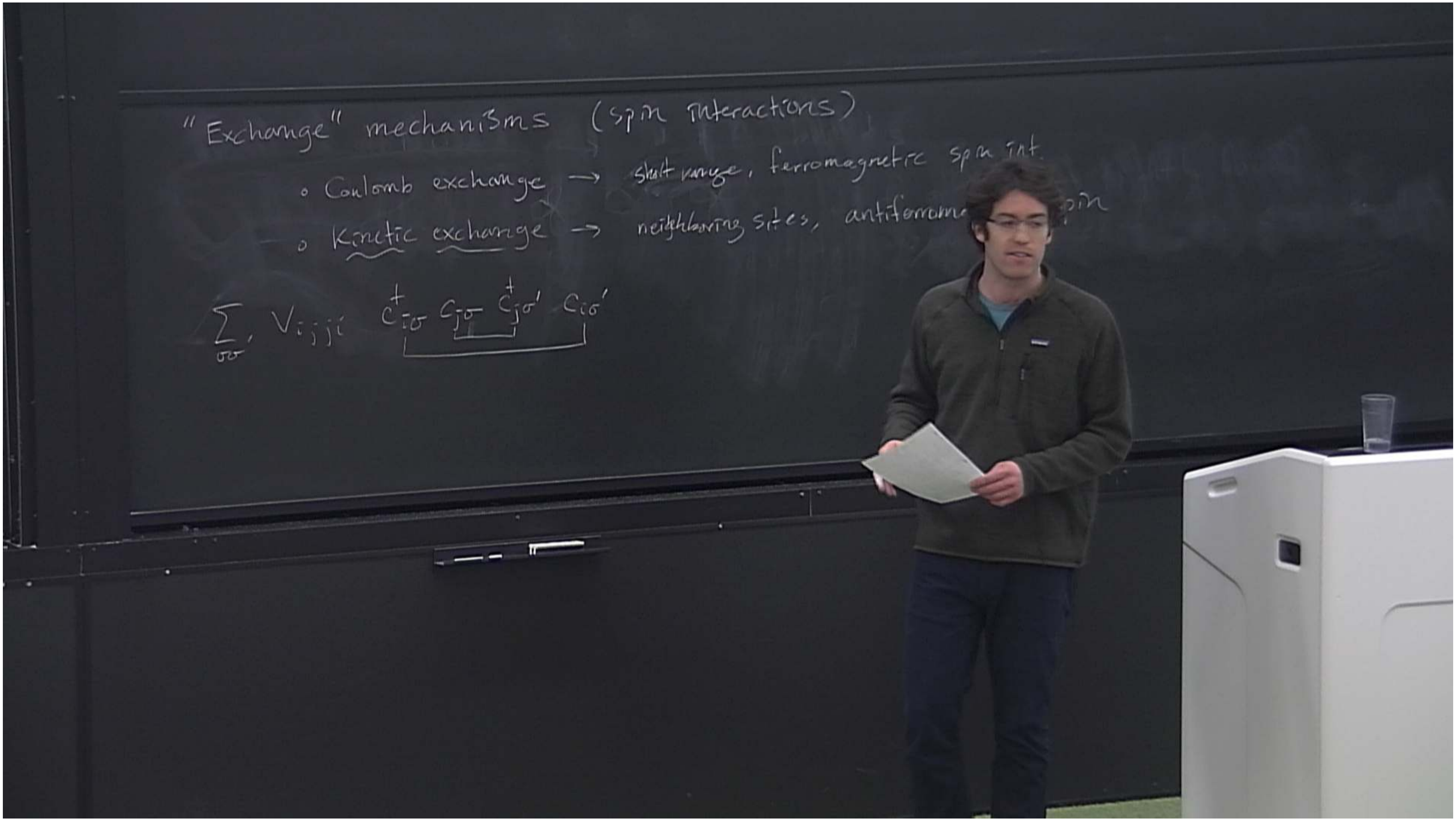
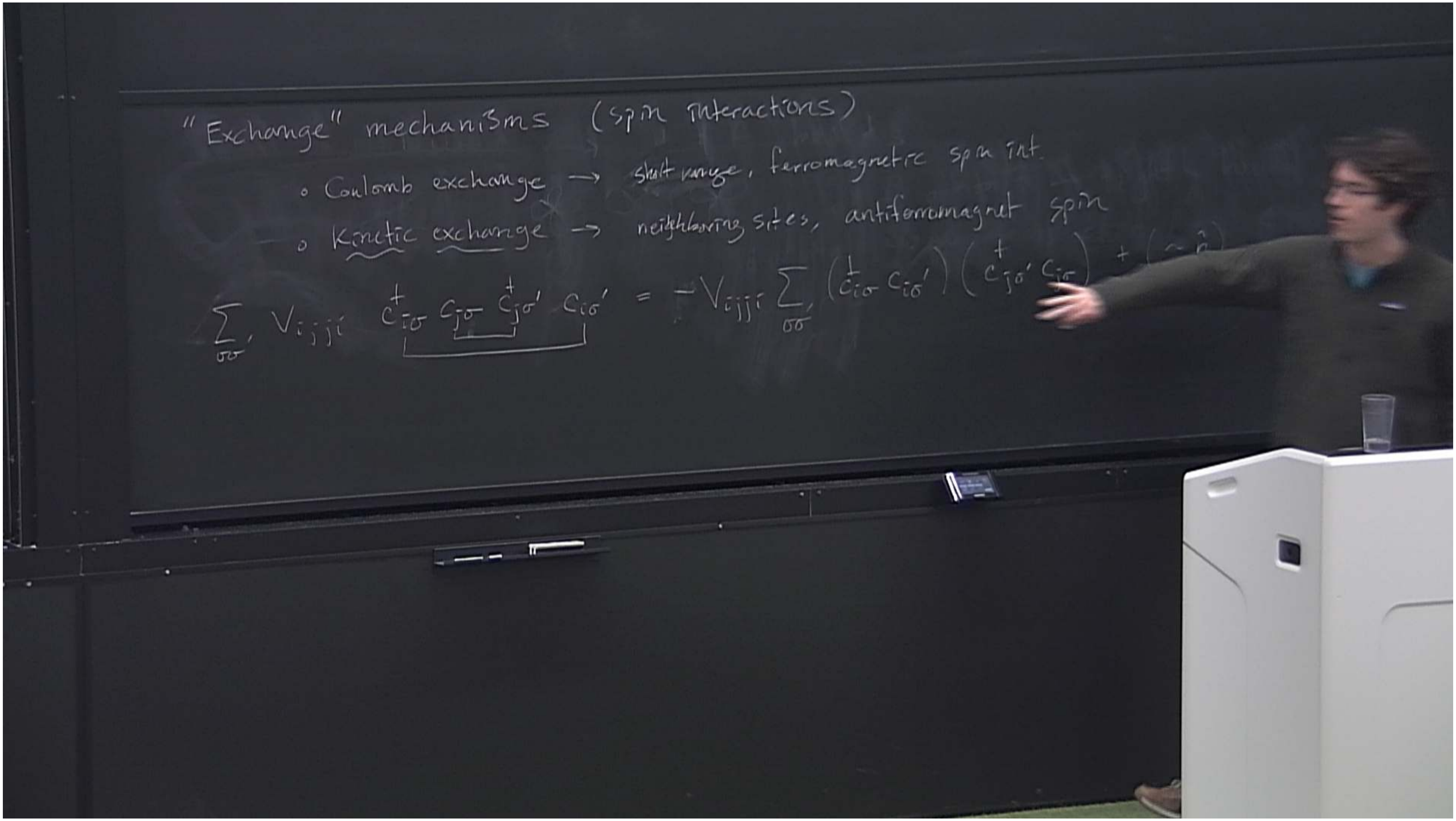
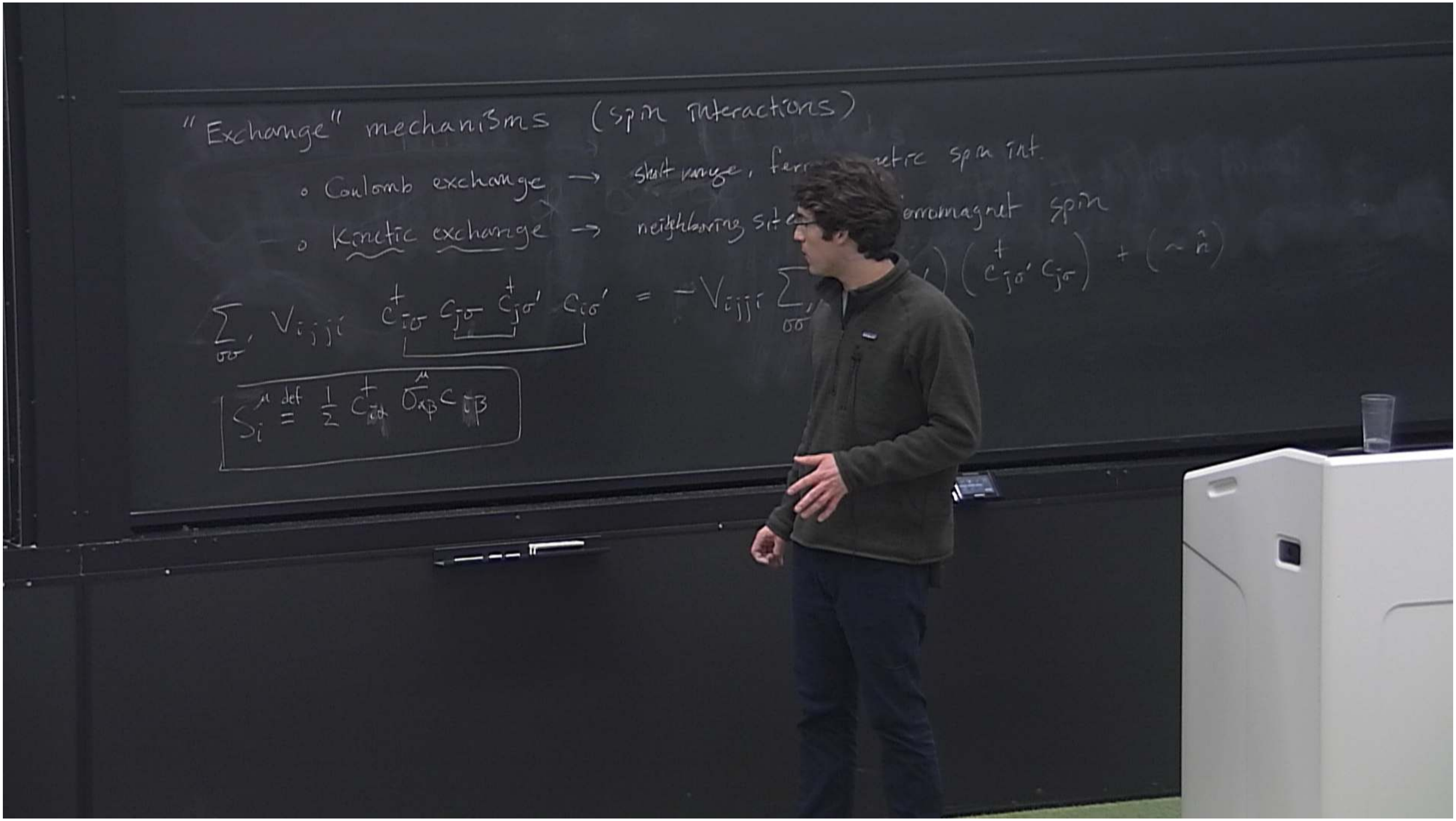
magnet spin


"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
$\sum_{\sigma\sigma'} V_{ijji}\, c^\dagger_{i\sigma} c_{j\sigma} c^\dagger_{j\sigma'} c_{i\sigma'} = -V_{ijji} \sum_{\sigma\sigma'} \left(c^\dagger_{i\sigma} c_{i\sigma'}\right)\left(c^\dagger_{j\sigma'} c_{j\sigma}\right) +$


"Exchange" mechanisms (spin interactions)
∘ Coulomb exchange →
∘ Kinetic exchange →
spin
$S_i^\mu \stackrel{def}{=} \frac{1}{2} c^\dagger_{i\alpha} \sigma^\mu_{\alpha\beta} c_{i\beta}$