Title: Explorations in Condensed Matter-1

Date: Mar 16, 2015 10:15 AM

URL: http://pirsa.org/15030034

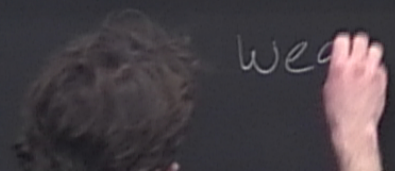
Abstract:

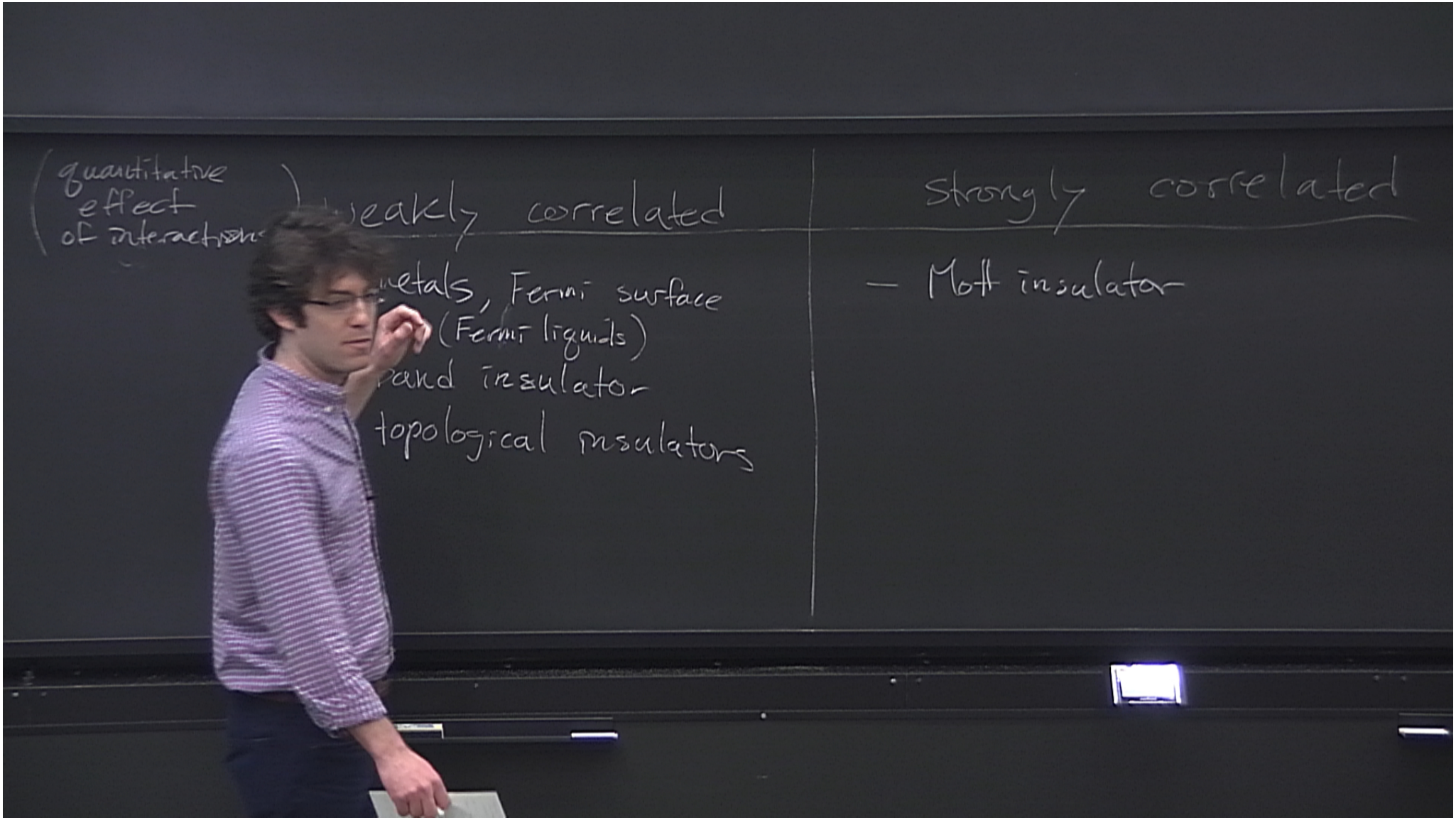
Miles Stoudenmire

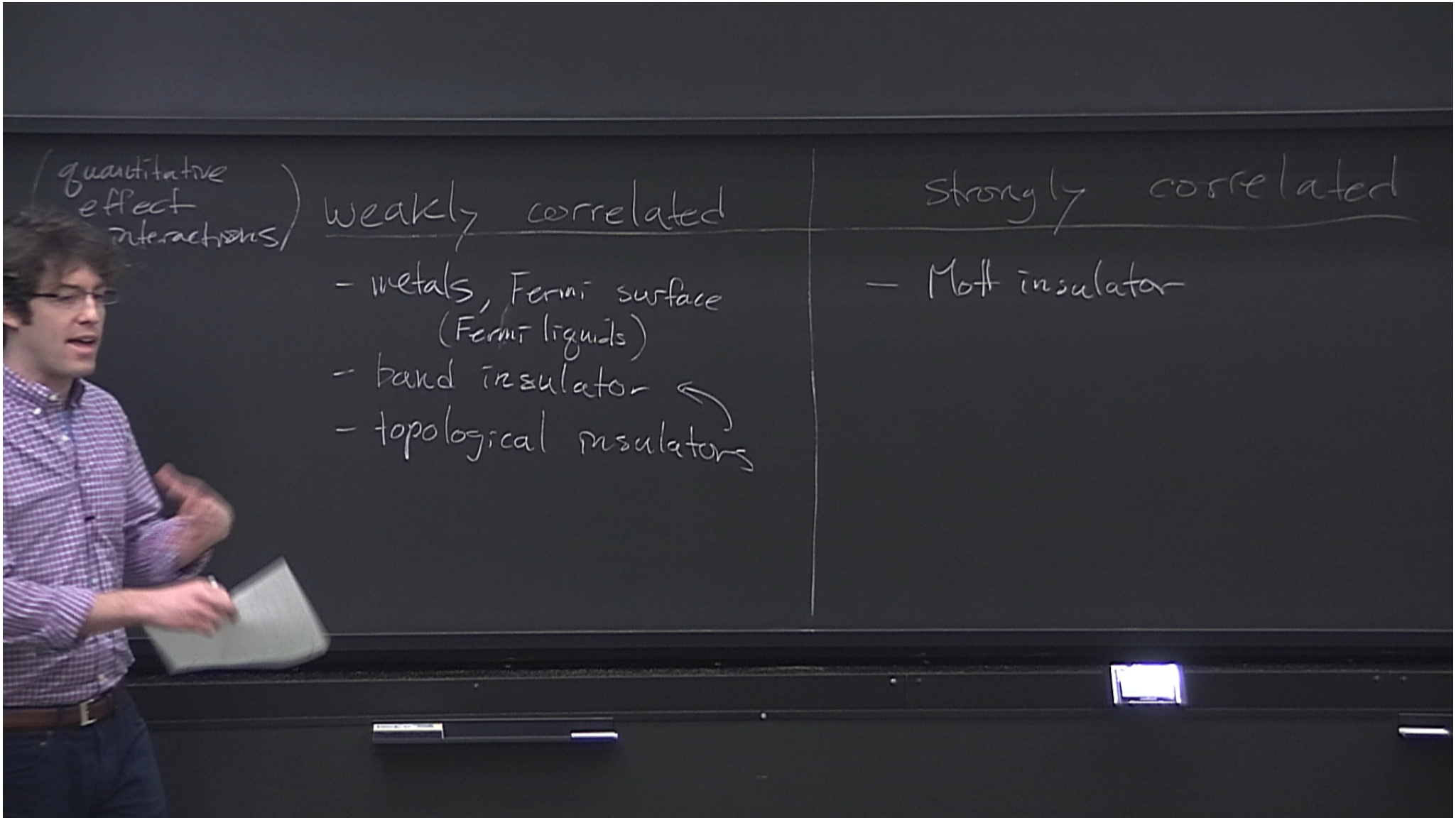
Theme: weakly and strongly correlated electrons

condensed matter physics $\subseteq$ quantum many-body physics

"more is different" collective behavior




(quantitative effect of interactions)
weakly correlated
metals, Fermi surface
(Fermi liquids)
band insulator
topological insulators
strongly correlated
– Mott insulator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weakly correlated
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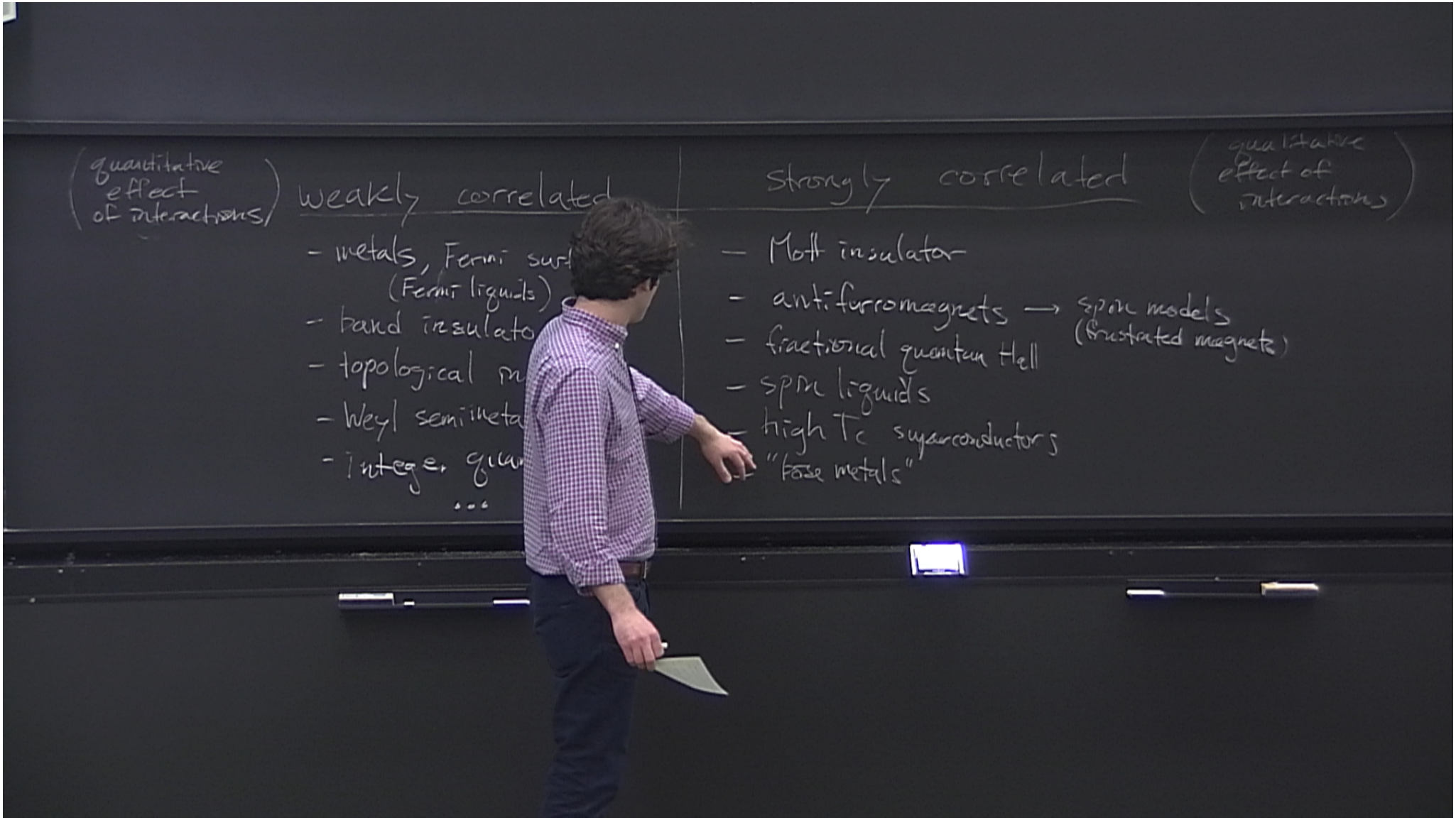
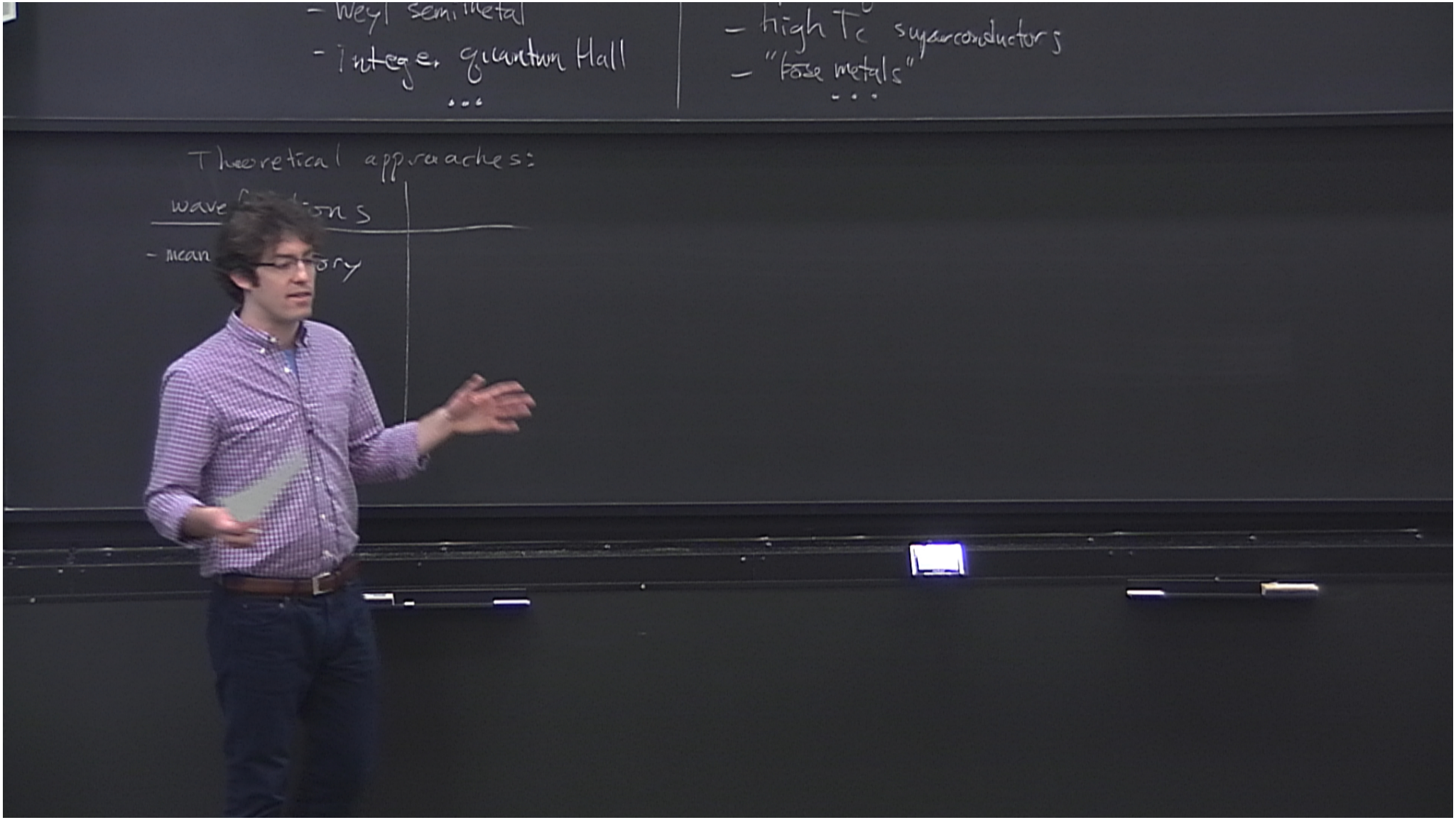

(quantitative effect of interactions)
weakly correlated
- metals, Fermi surf
(Fermi liquids)
- band insulato
- topological m
- Weyl semimeta
- integer qua
...
strongly correlated
(qualitative effect of interactions)
- Mott insulator
- antiferromagnets → spin models (frustrated magnets)
- fractional quantum Hall
- spin liquids
- high Tc superconductors
- "bose metals"


- Weyl semimetal
- Integer quantum Hall
...
- high T_c superconductors
- "bose metals"
...
Theoretical approaches:
wave
ions
- mean
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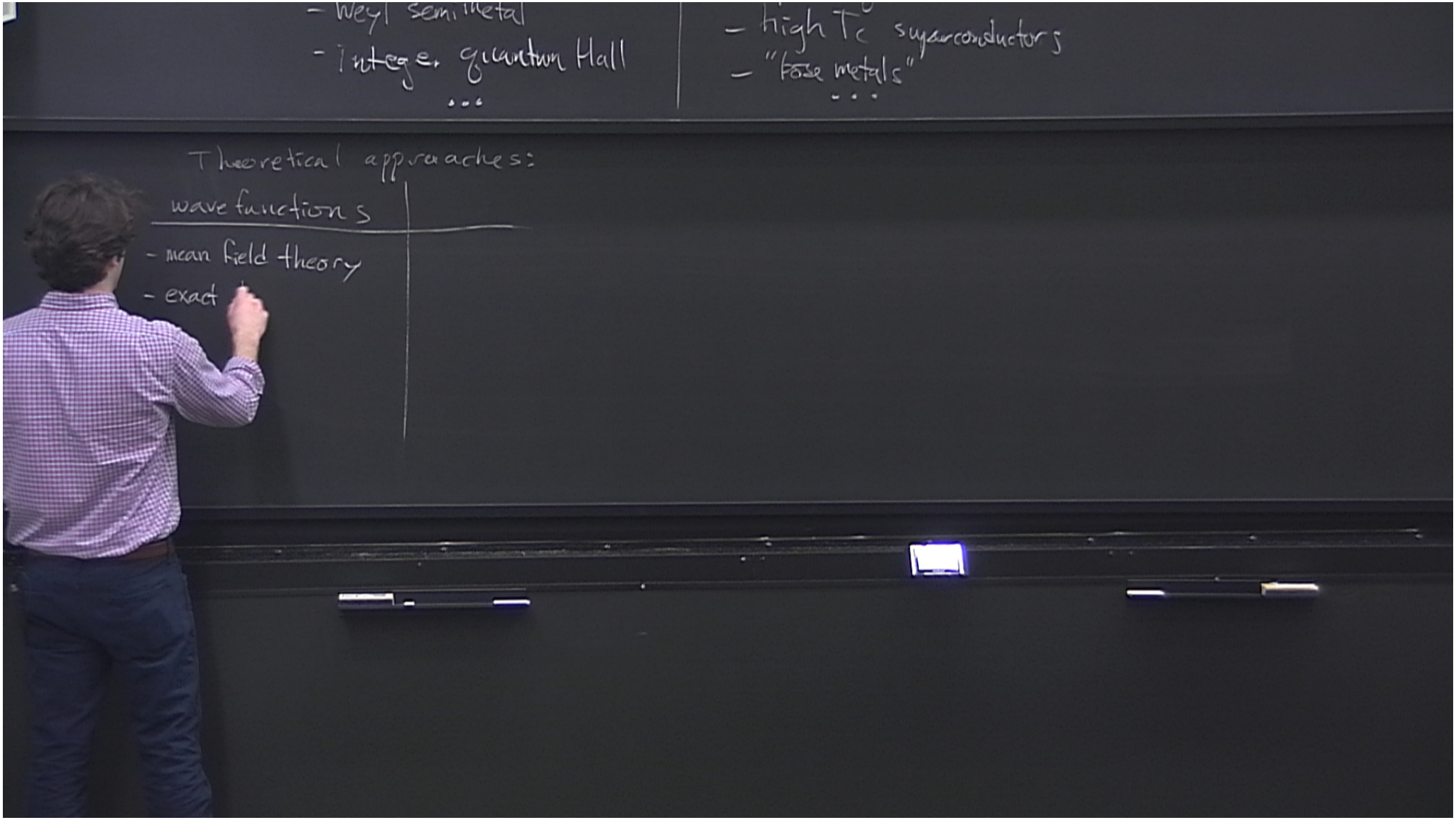
- Weyl semimetal
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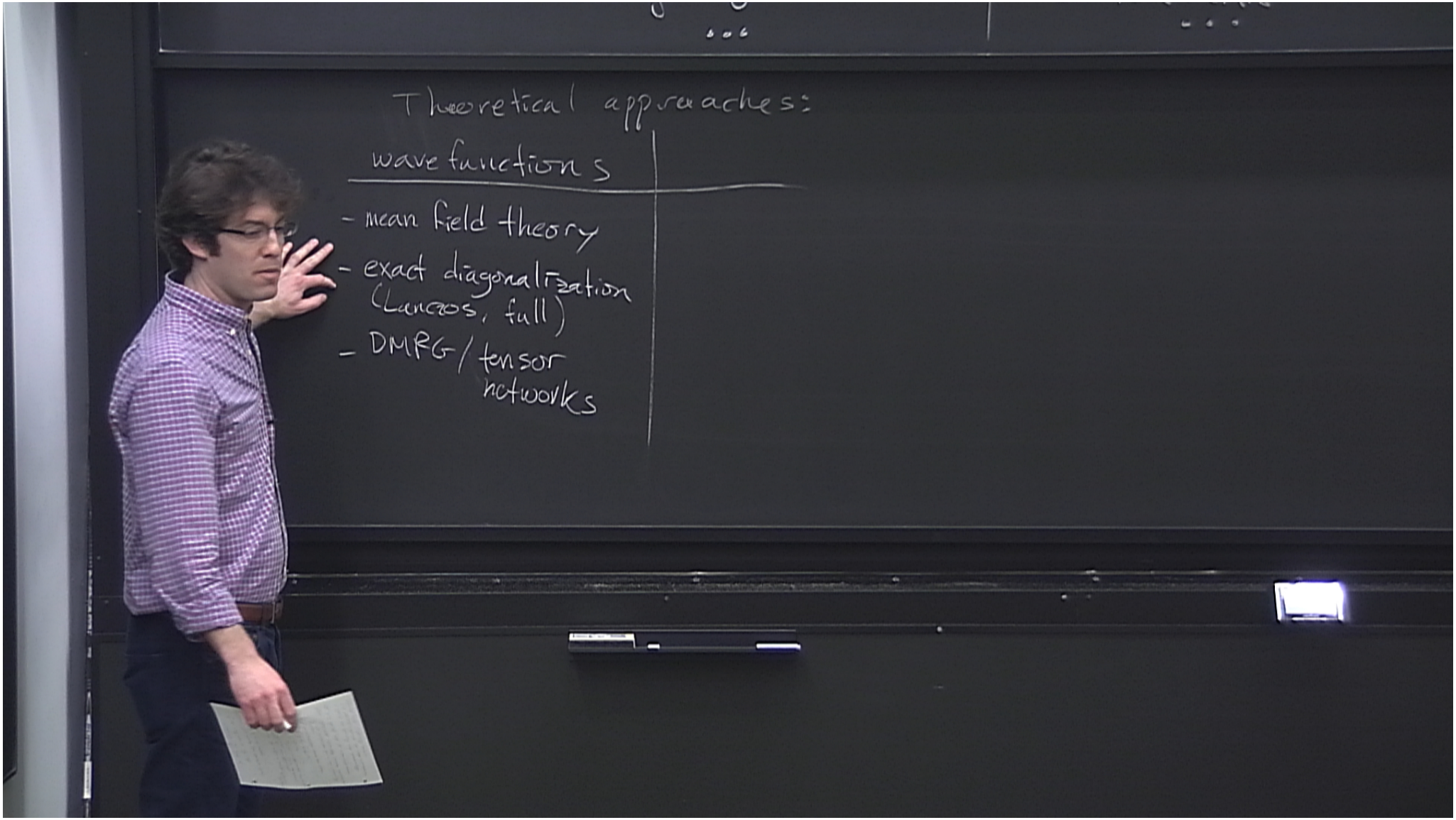
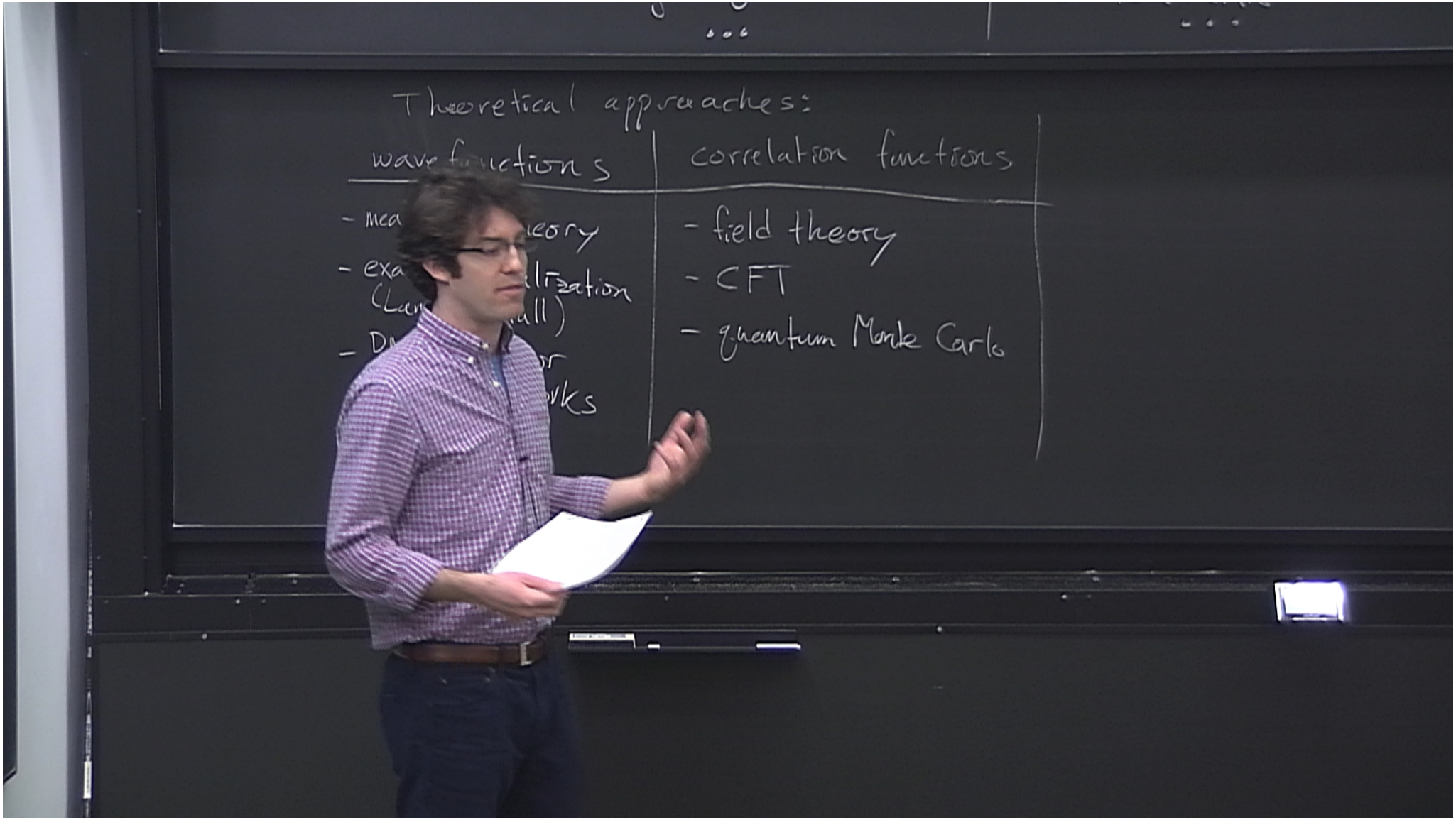
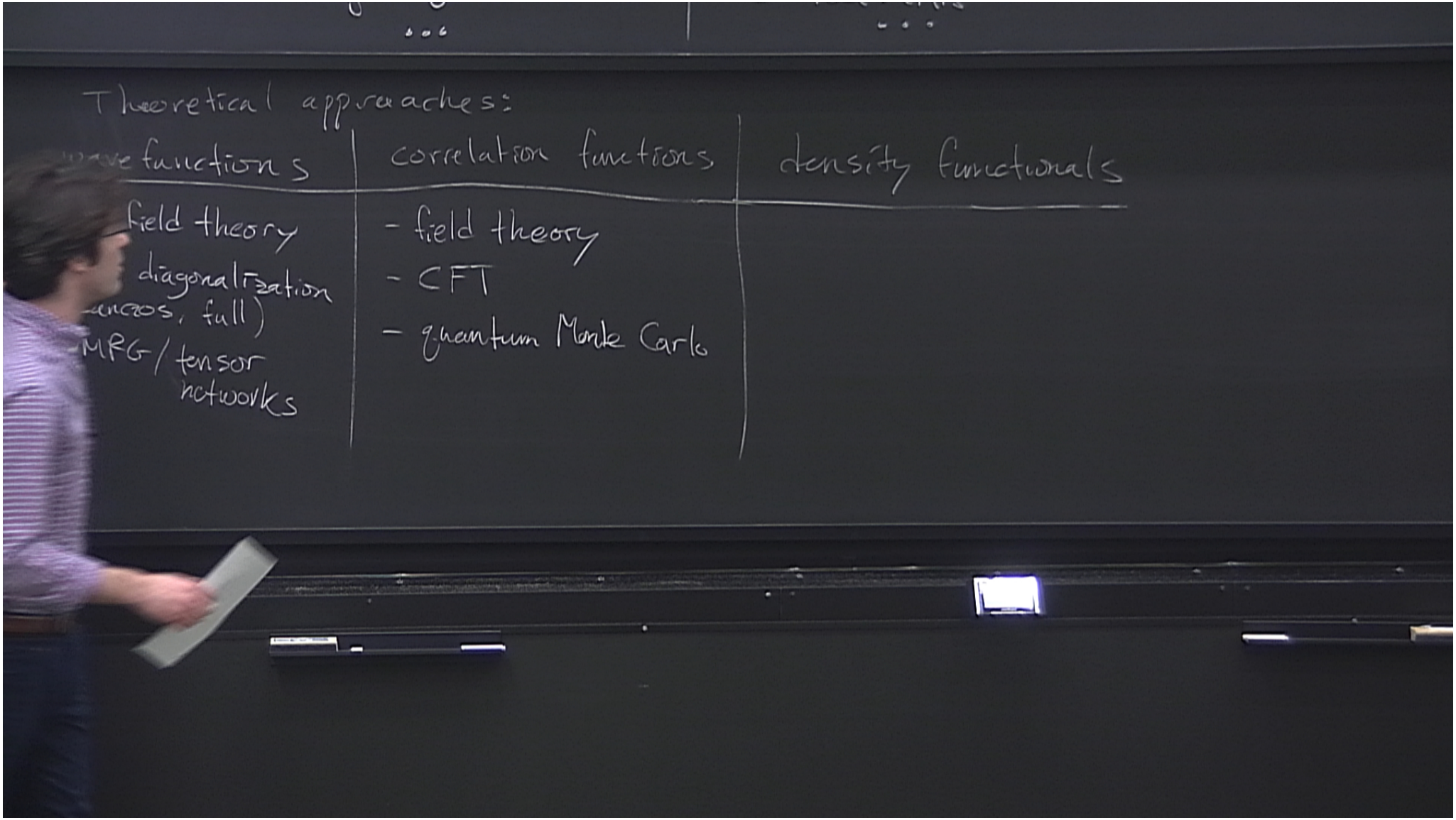
Theoretical approaches:
wave functions
- mean field theory
- exact


Theoretical approaches:
wavefunctions
- mean field theory
- exact diagonalization (Lanczos, full)
- DMRG / tensor networks


Theoretical approaches:
wave functions
correlation functions
- field theory
- CFT
- quantum Monte Carlo


Theoretical approaches:
wavefunctions
correlation functions
density functionals
- field theory
- diagonalization (-ncaos, full)
- MRG / tensor networks
- field theory
- CFT
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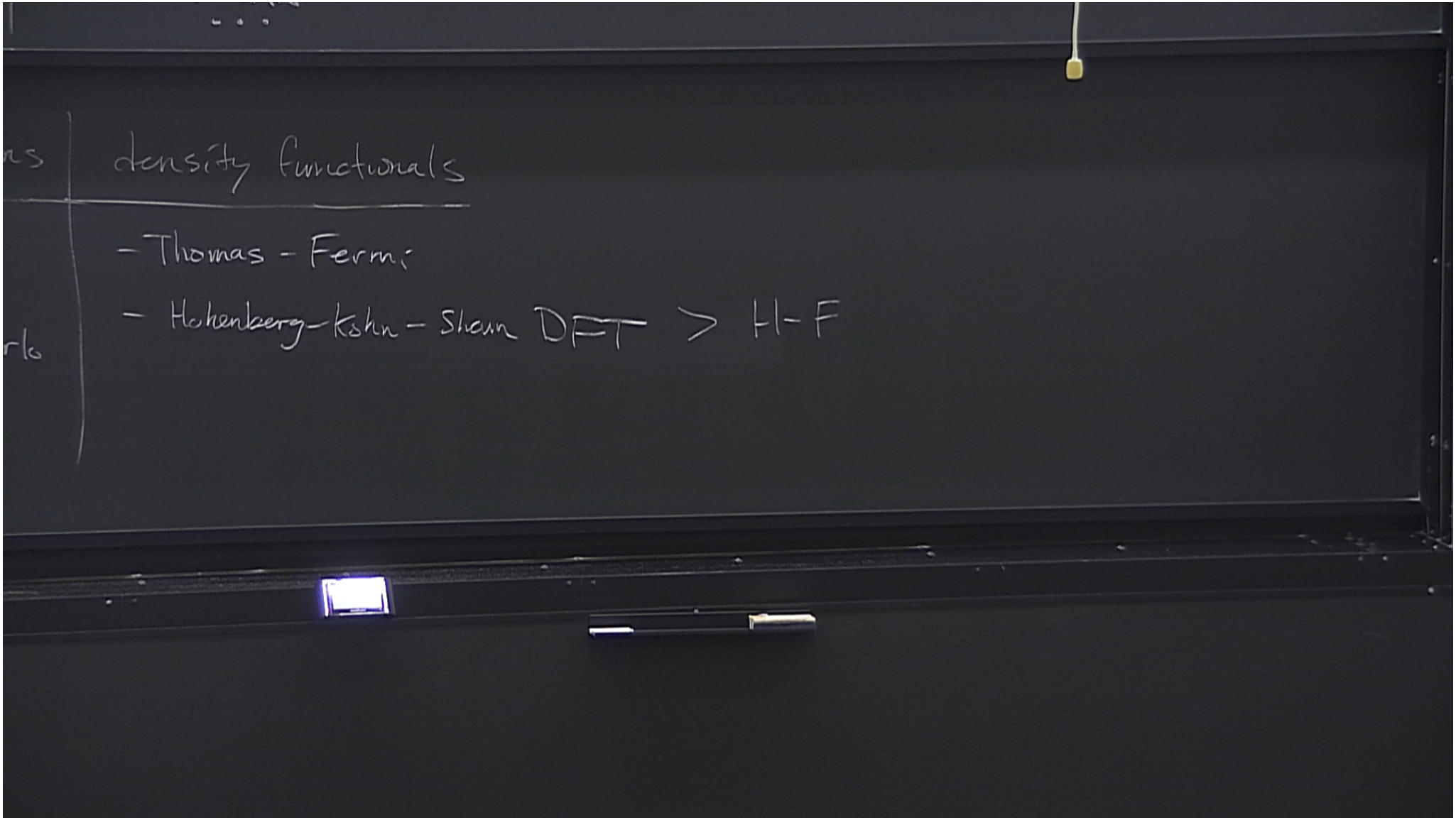
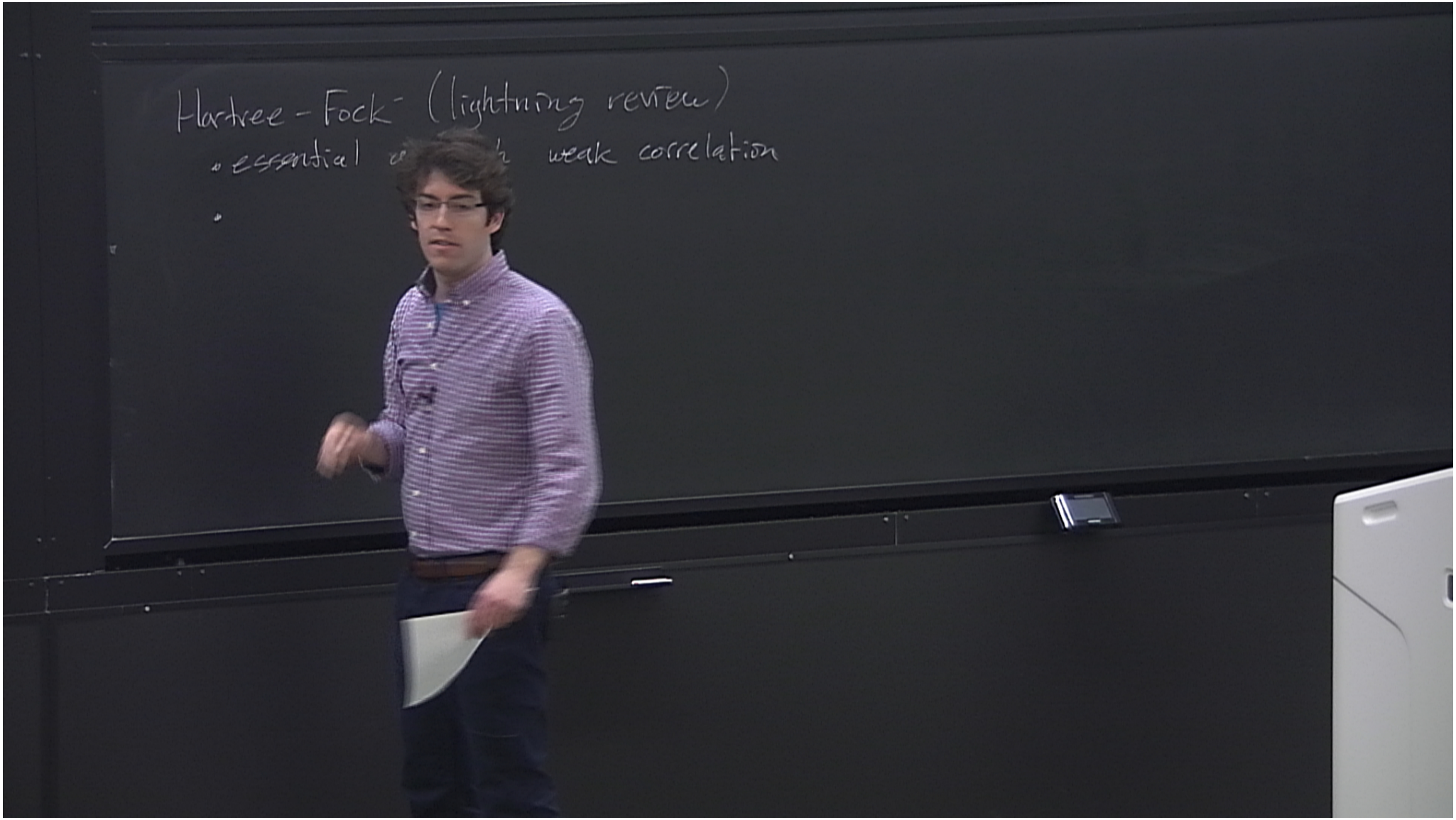
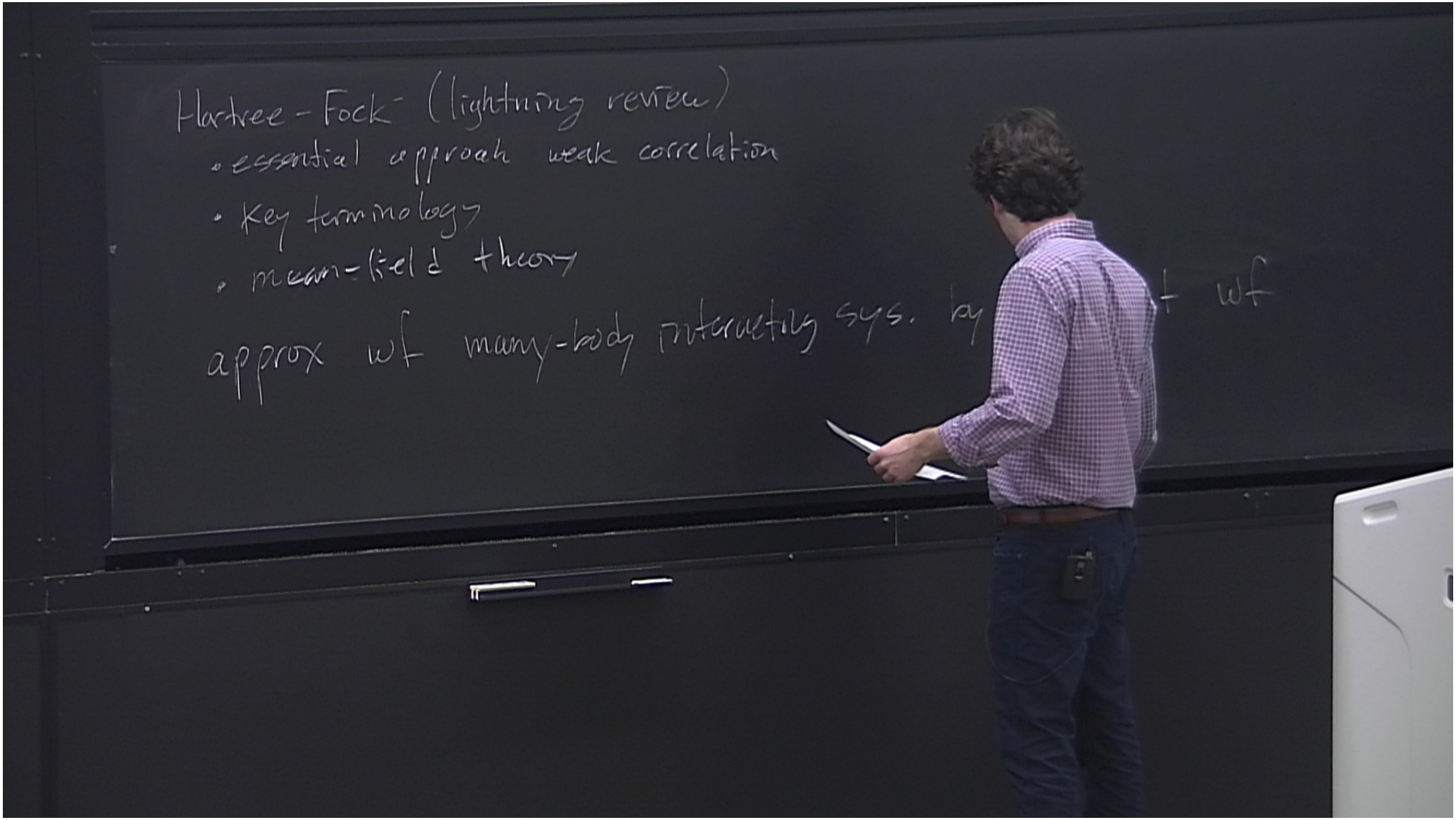
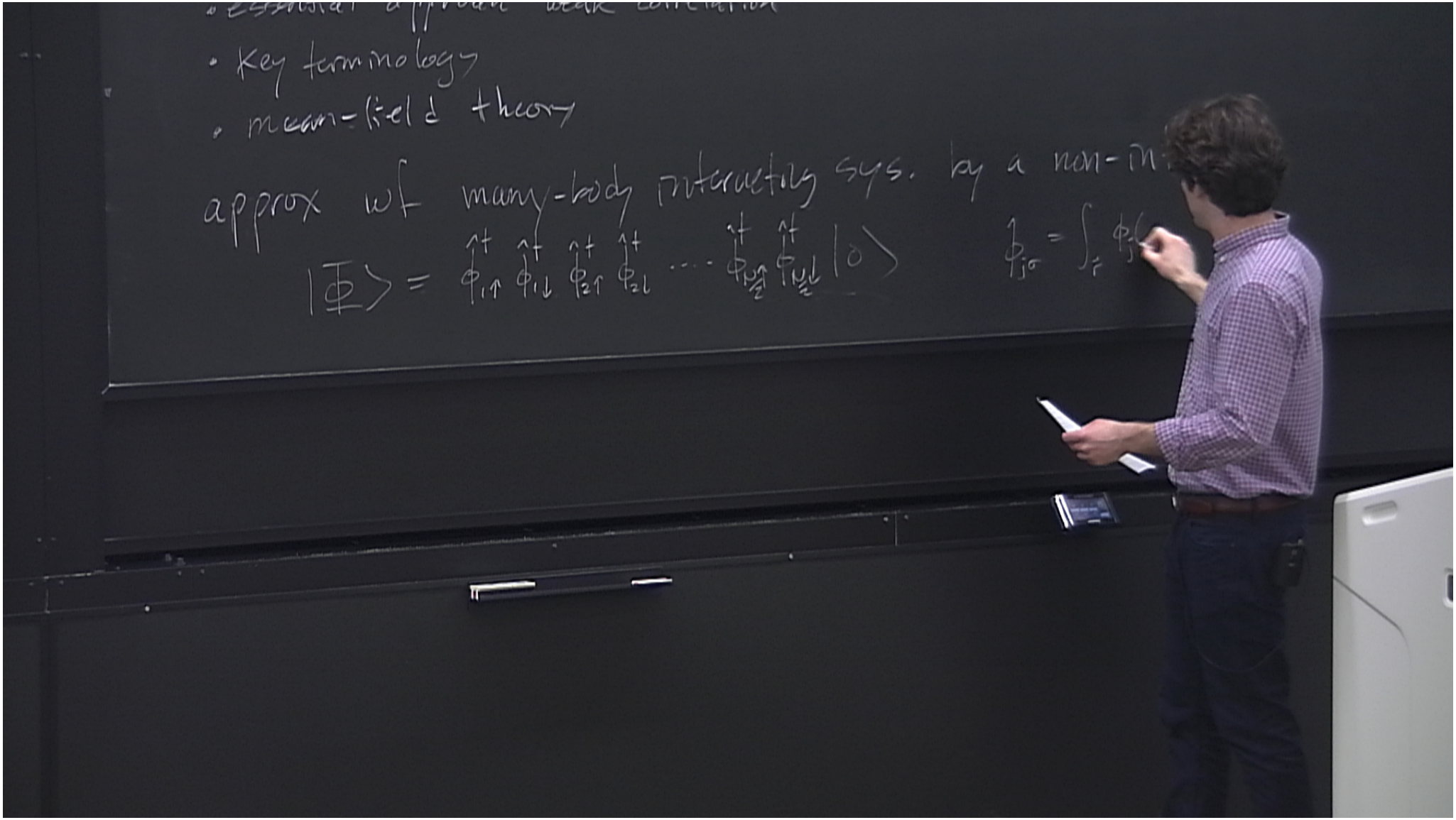

density functionals
- Thomas - Fermi
- Hohenberg-Kohn-Sham DFT > H-F


Hartree-Fock (lightning review)
• essential
weak correlation


Hartree-Fock (lightning review)
• essential approach weak correlation
• key terminology
• mean-field theory
approx wf many-body interacting sys. by
wf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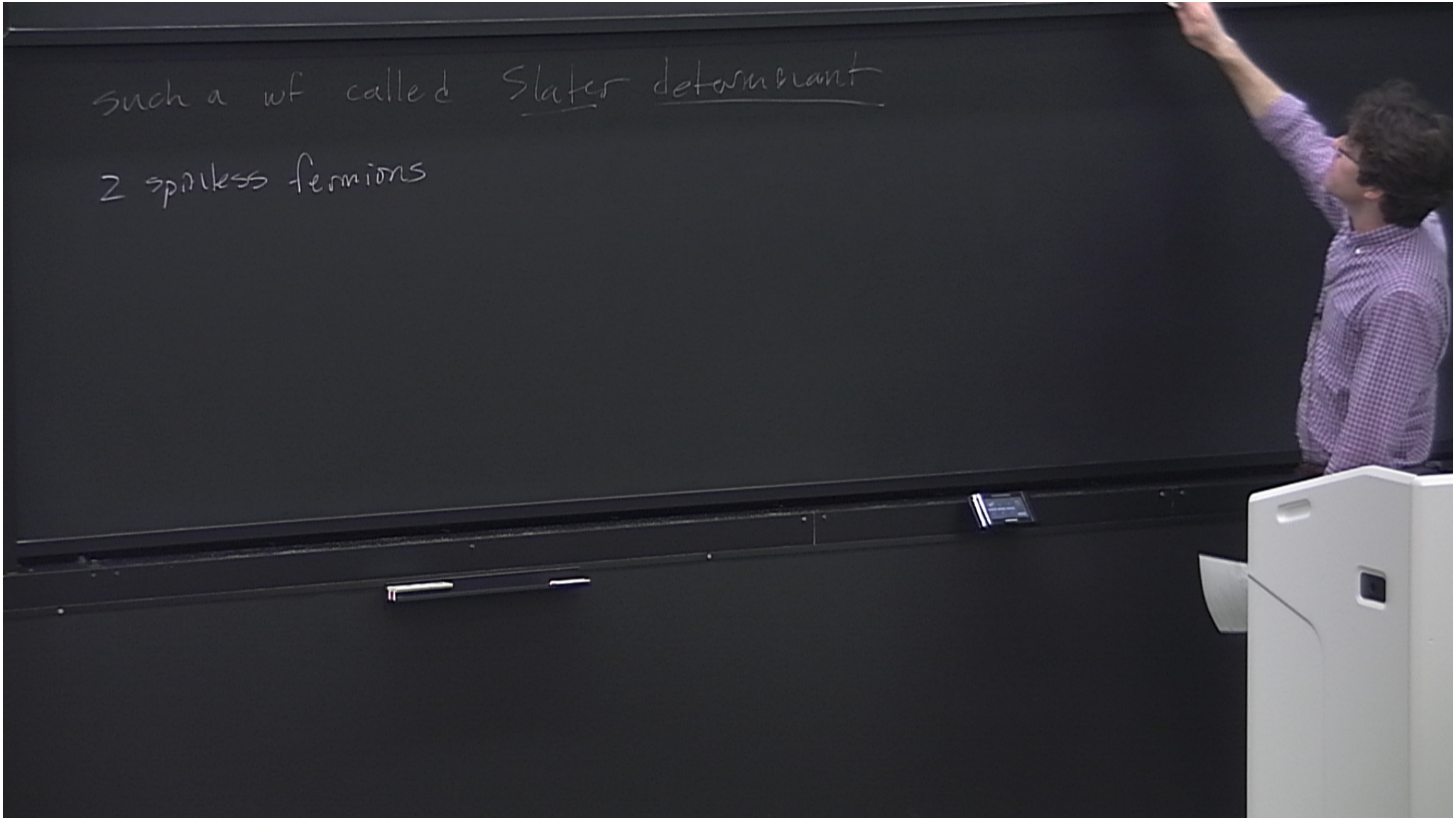
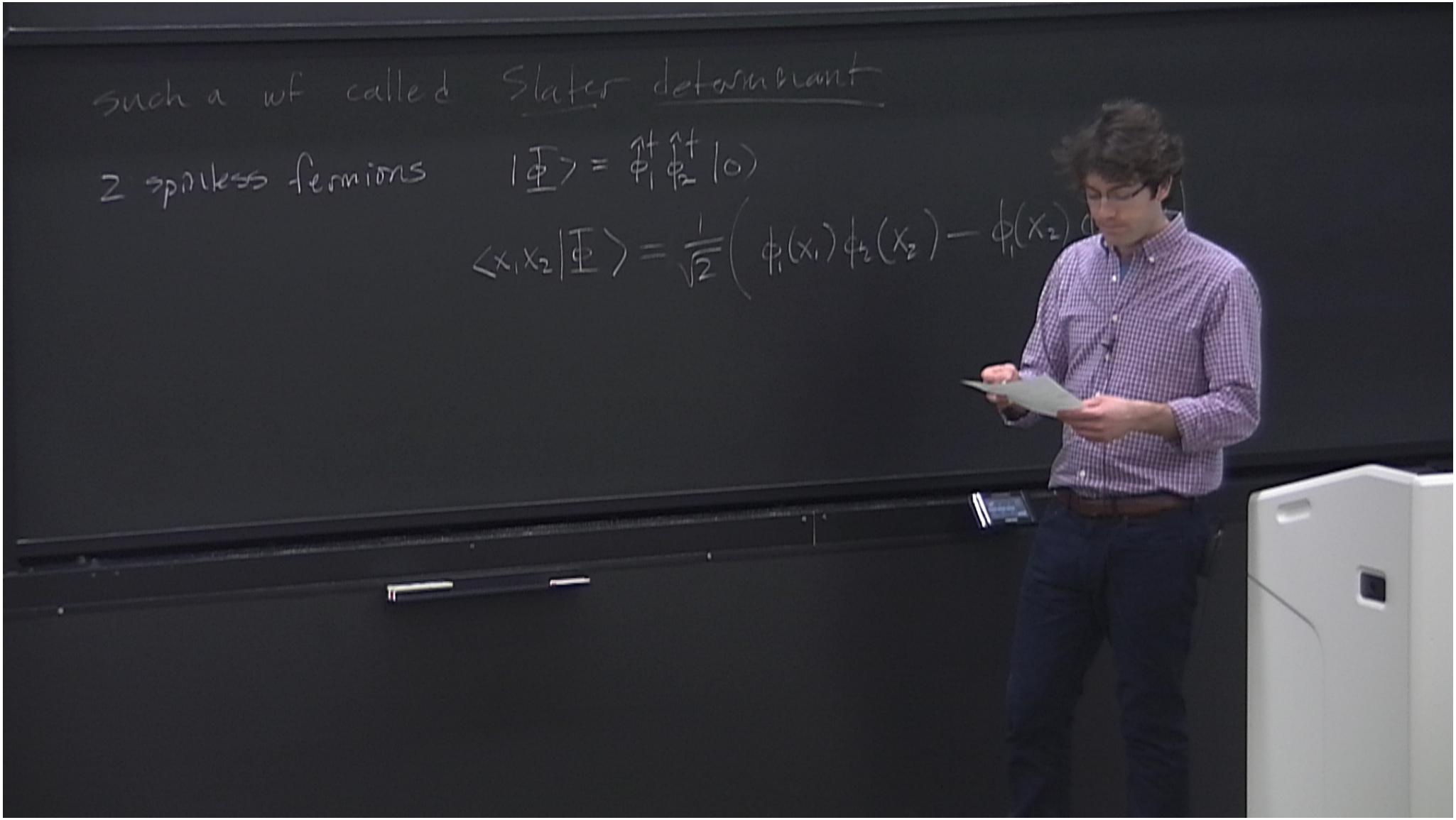

such a wf called Slater determinant
2 spinless fermions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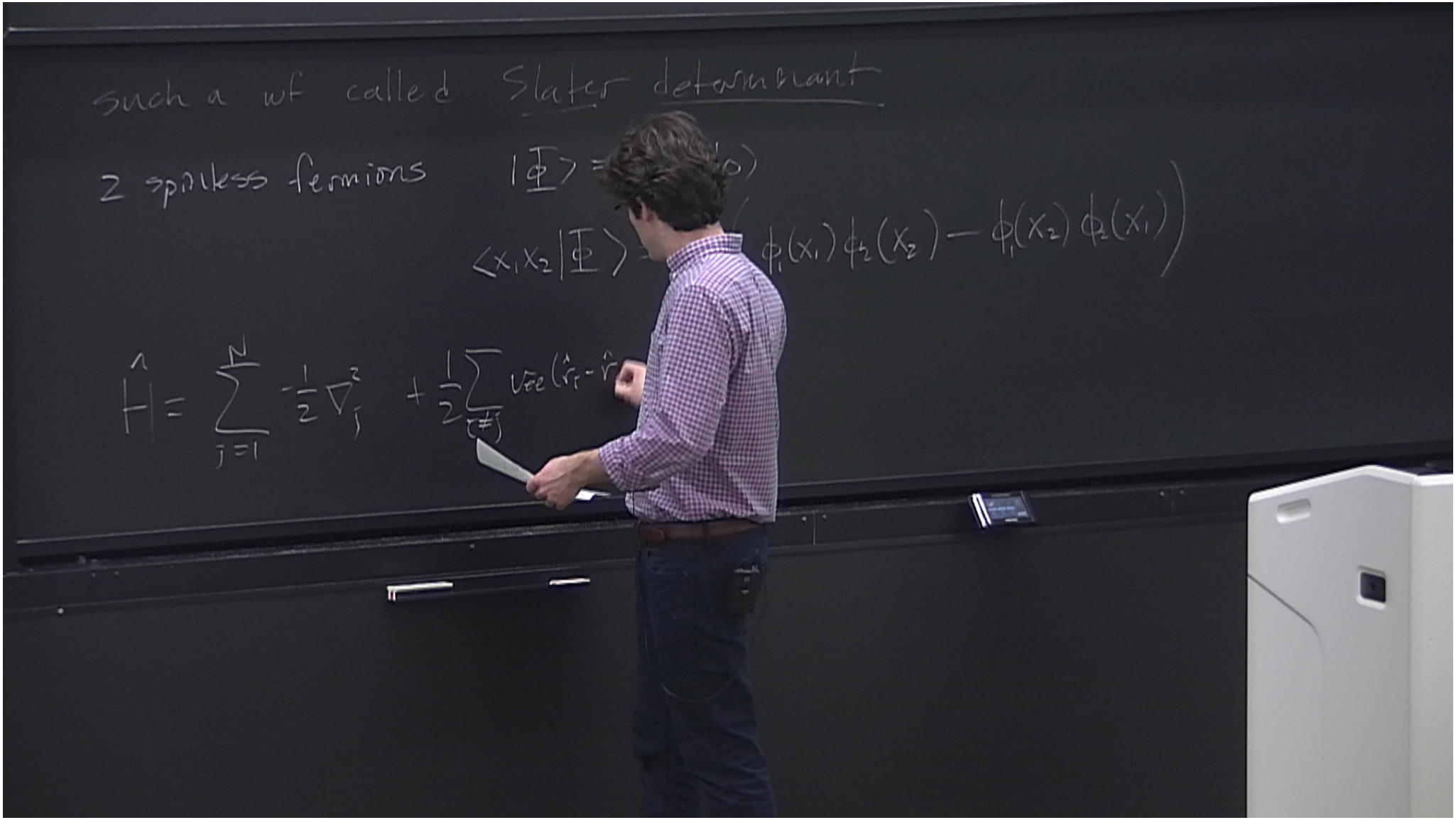
$|\Phi\rangle = \hat{\phi}_1^\dagger \hat{\phi}_2^\dagger |0\rangle$
$\langle x_1 x_2 | \Phi \rangle = \frac{1}{\sqrt{2}} \left(\phi_1(x_1) \phi_2(x_2) - \phi_1(x_2)$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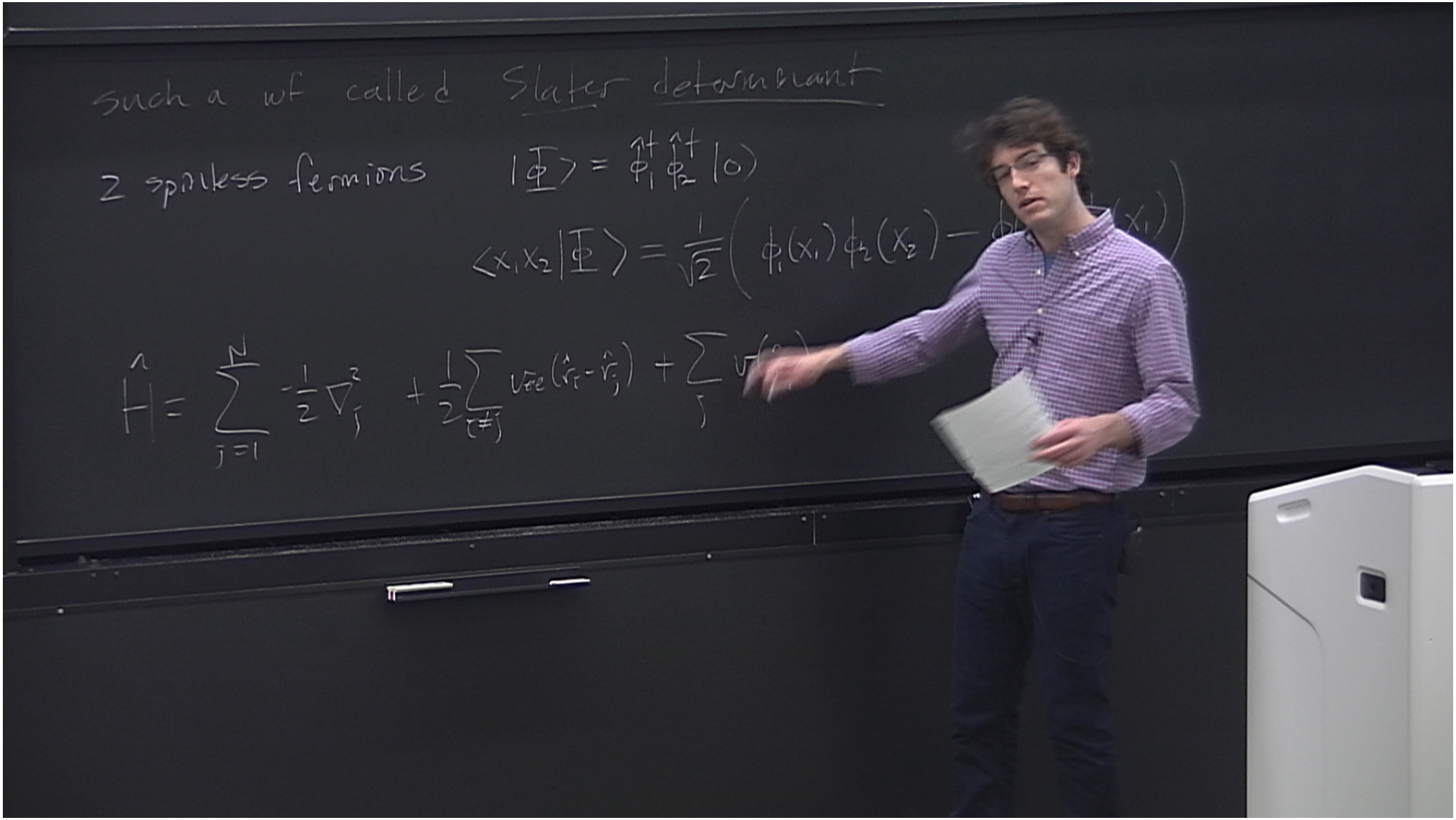
$\phi_1(x_1)\phi_2(x_2) - \phi_1(x_2)\phi_2(x_1)$
$\hat{H} = \sum_{i=1}^{N} -\frac{1}{2}\nabla_i^2 + \frac{1}{2}\sum_{i \neq j} v_{ee}(\hat{r}_i - \hat{r}$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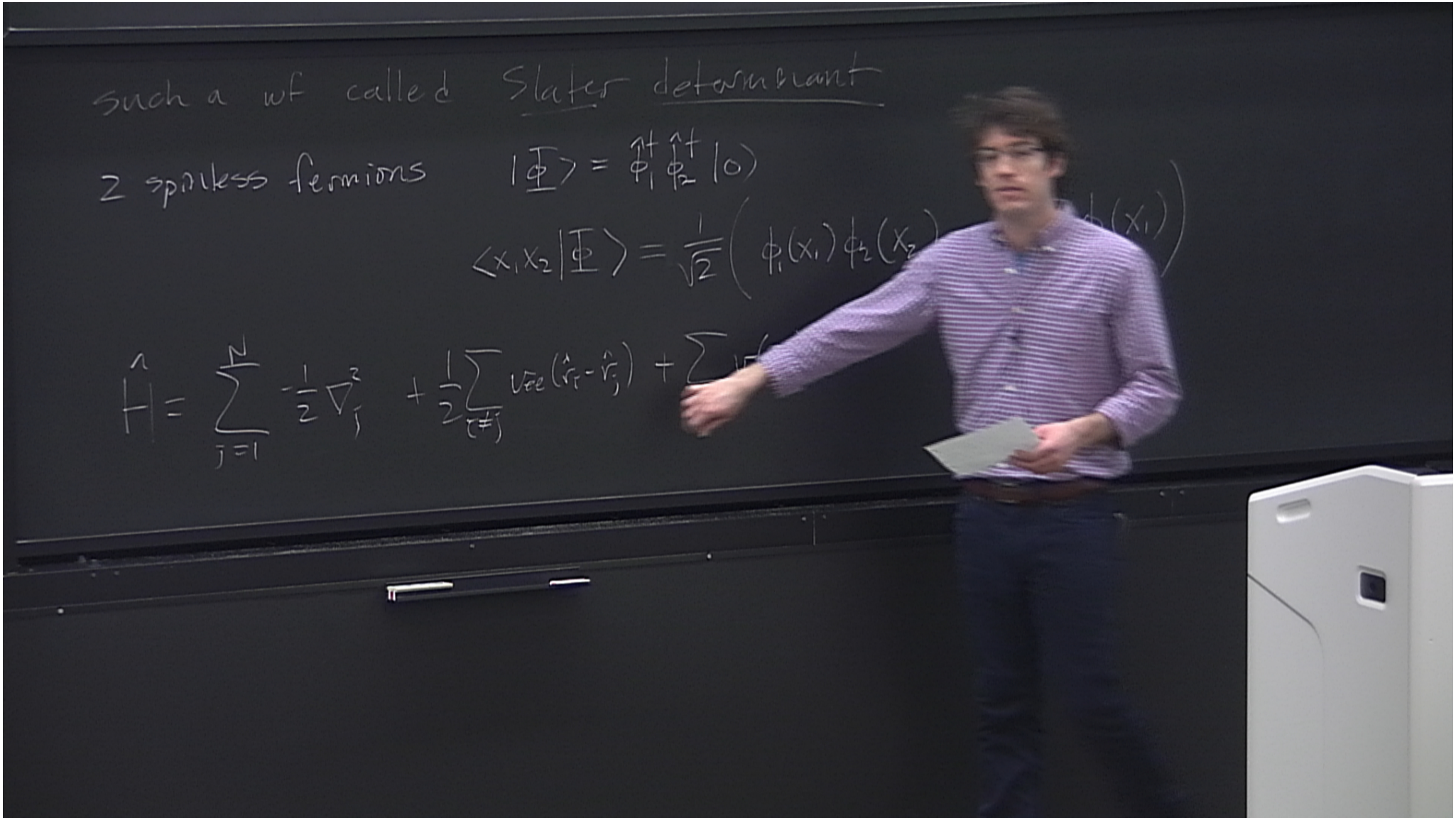
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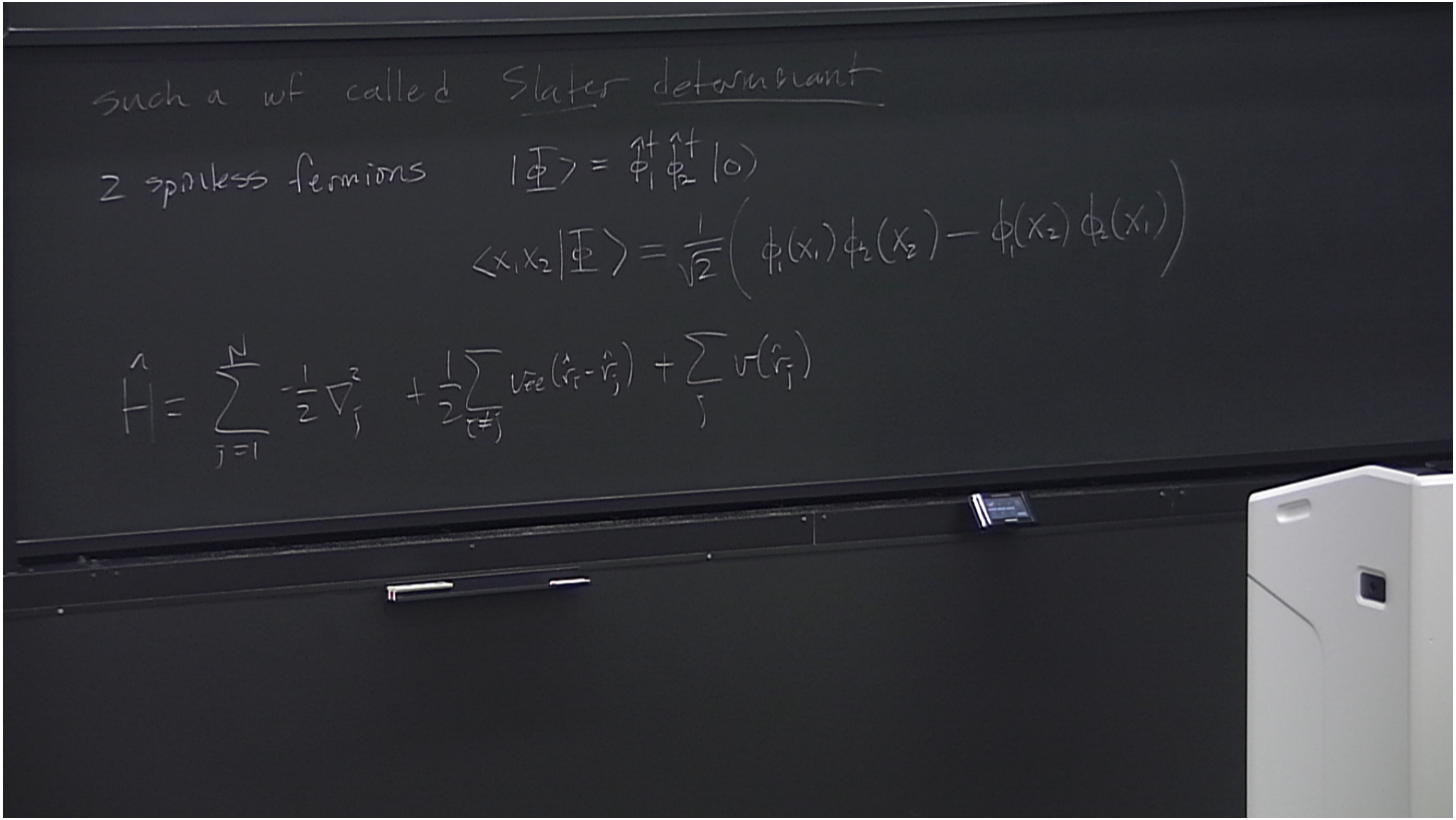
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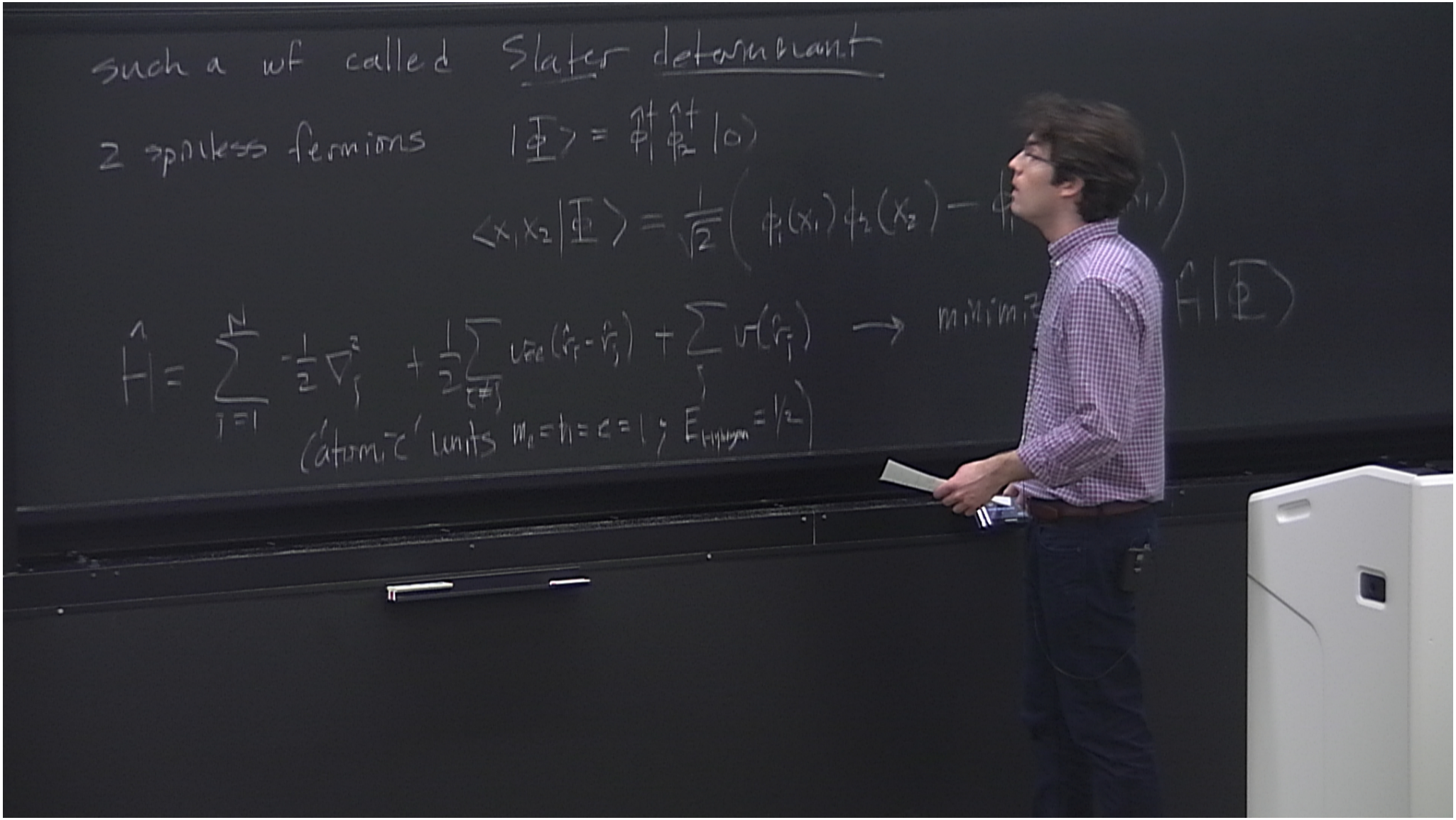
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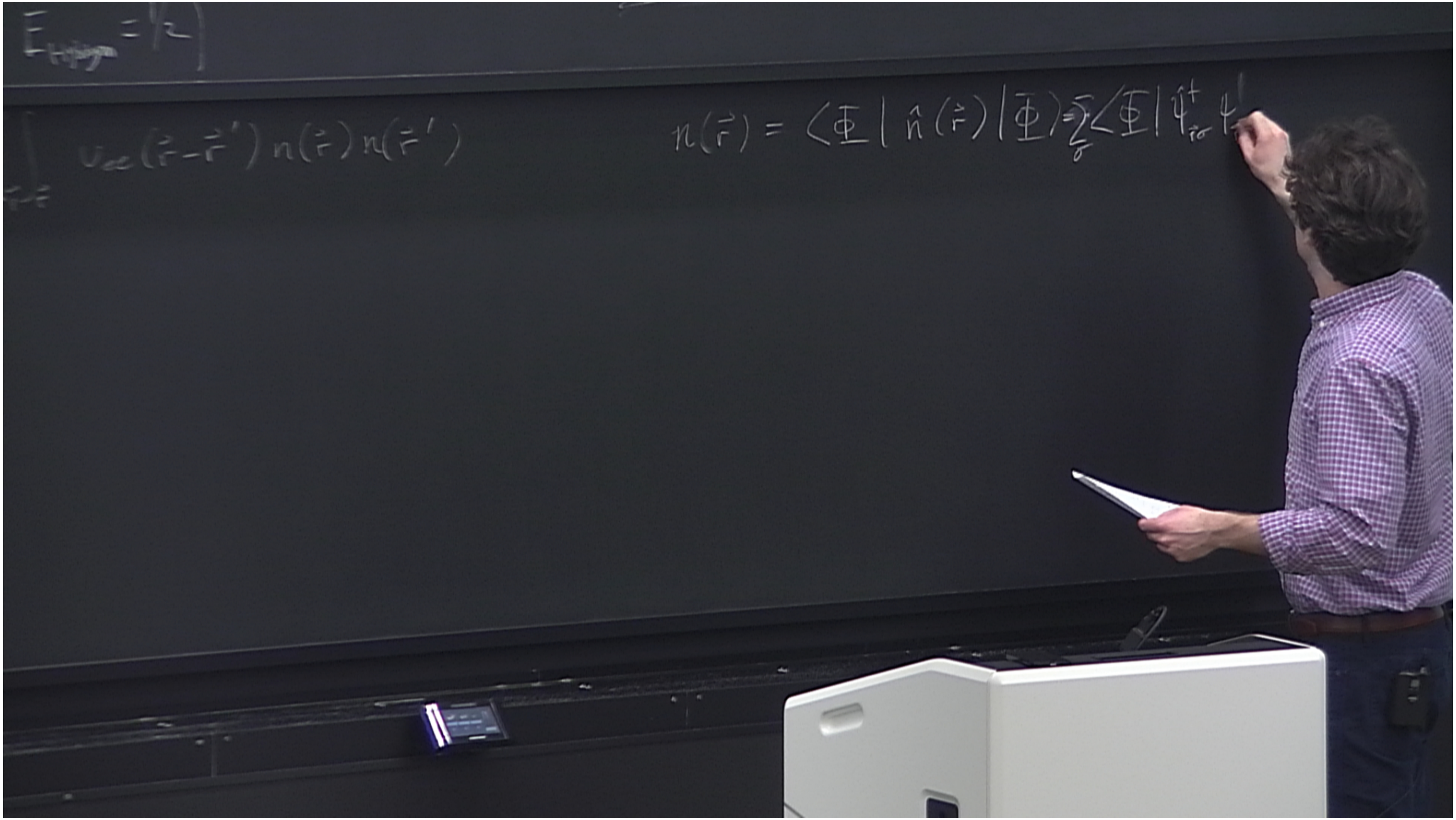
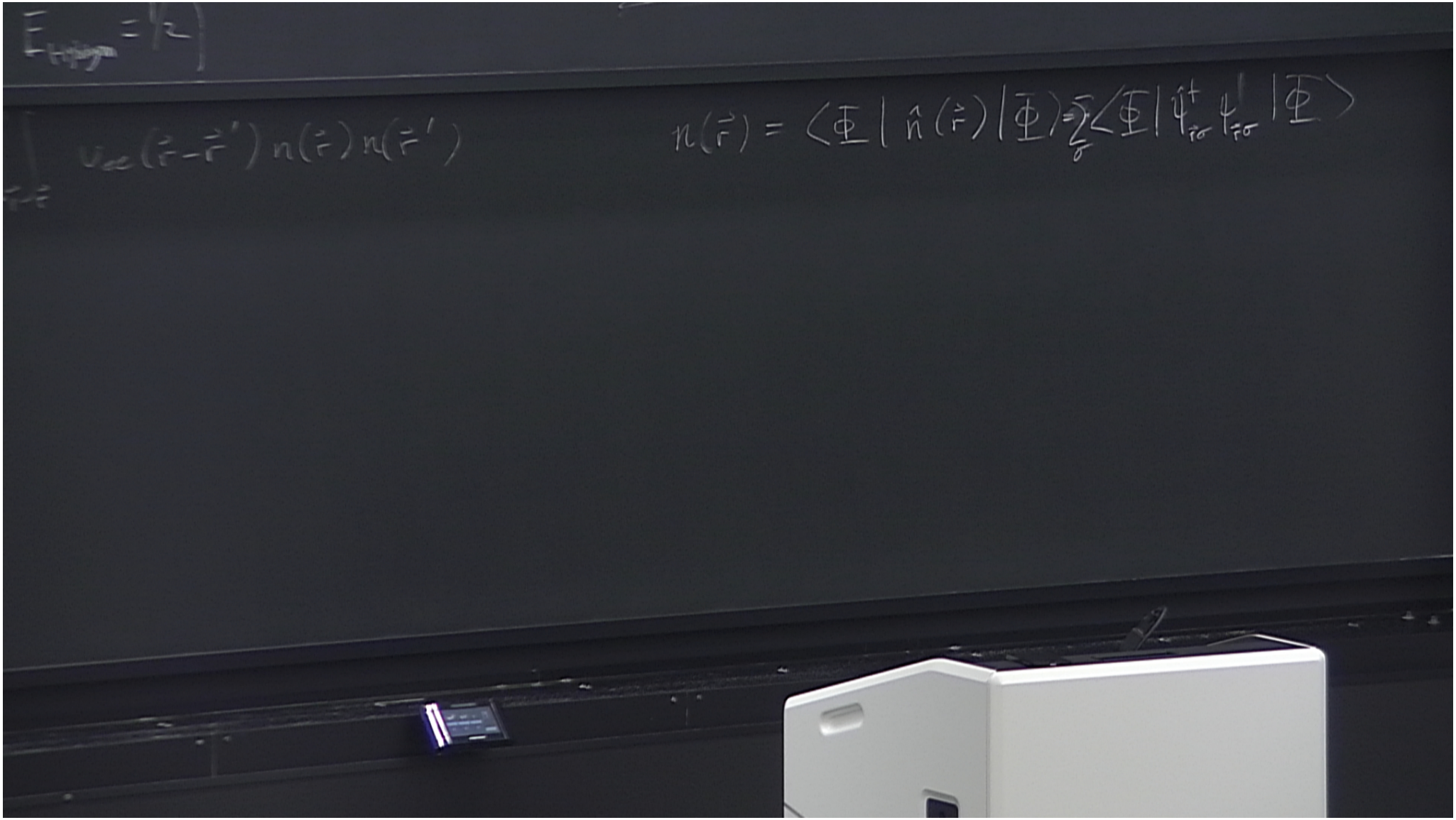
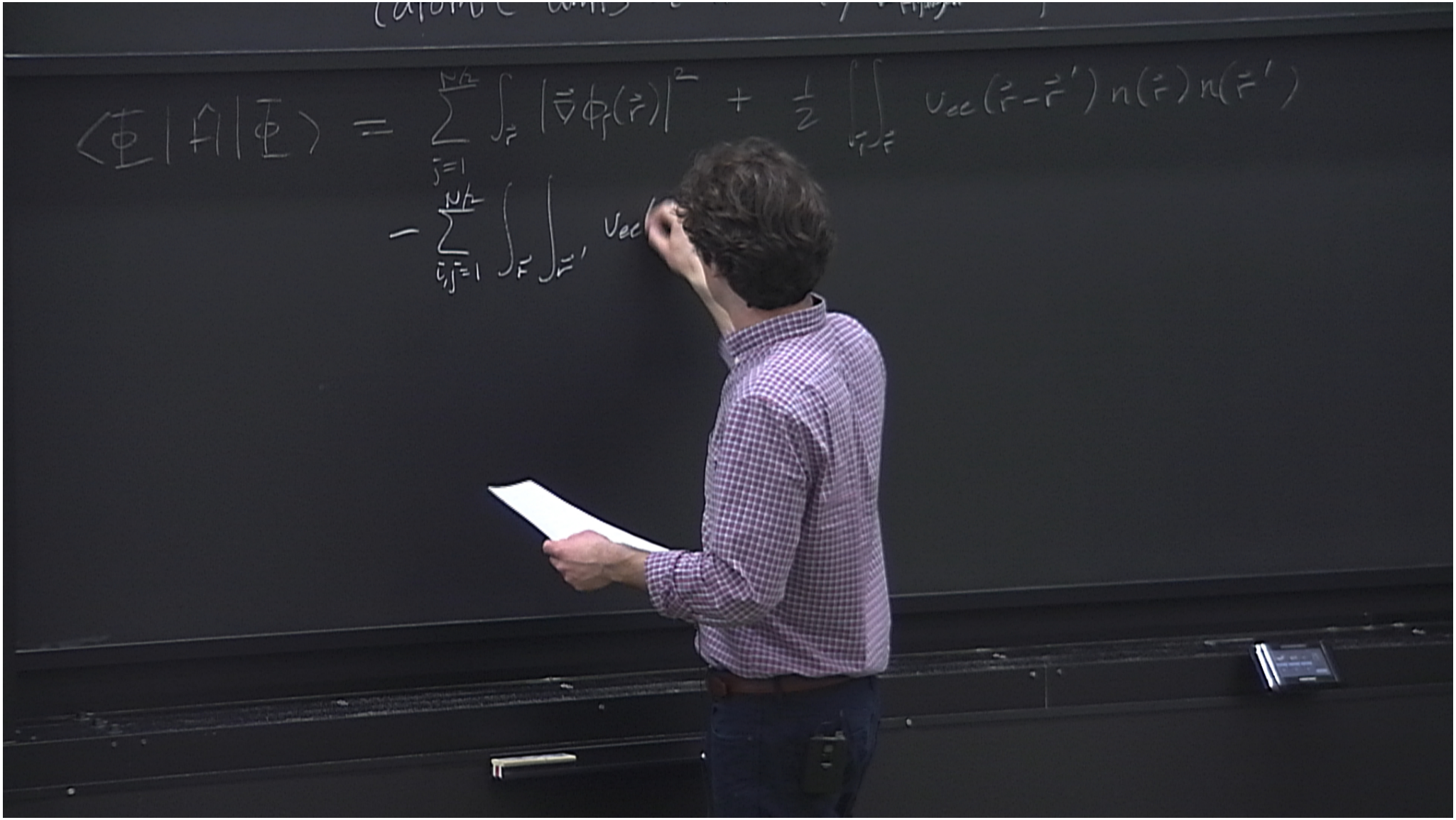
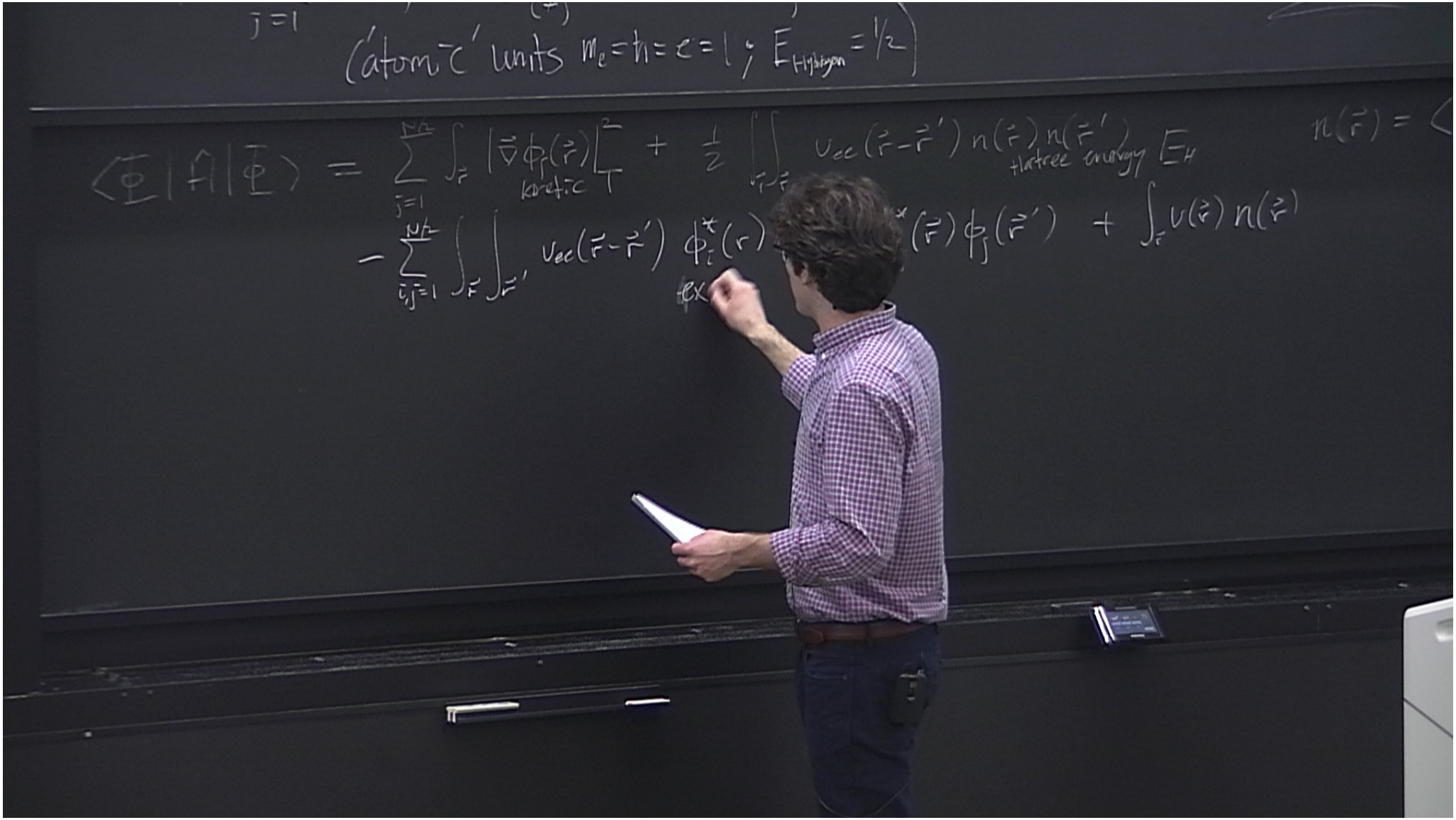
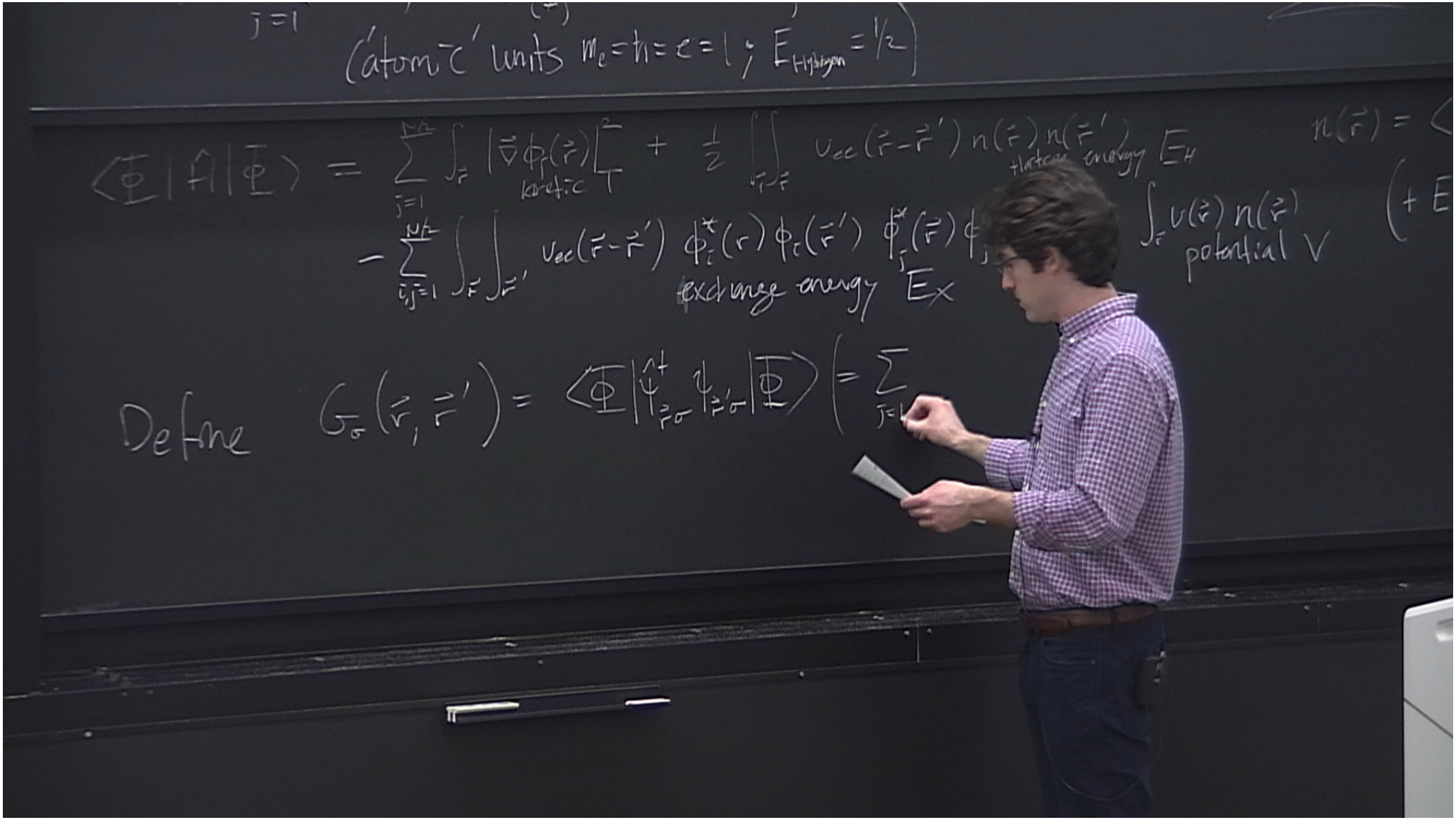
$\rightarrow$ minim
$\hat{H}|\Phi\rangle$
('atomic' units $m_e = \hbar = e = 1$; $E_{Hydrogen} = 1/2$)


$E_{Hubbard} =$
$\int U_{ee}(\vec{r}-\vec{r}')\, n(\vec{r})\, n(\vec{r}')$
$n(\vec{r}) = \langle \Psi | \hat{n}(\vec{r}) | \Psi \rangle = \sum_\sigma \langle \Psi | \psi^\dagger_{i\sigma} \psi$


$E_{Hartree} = \frac{1}{2}$
$\int U_{ee}(\vec{r}-\vec{r}')\, n(\vec{r})\, n(\vec{r}')$
$n(\vec{r}) = \langle \Phi | \hat{n}(\vec{r}) | \Phi \rangle = \sum_\sigma \langle \Phi | \psi^+_{r\sigma} \psi_{r\sigma} | \Phi \rangle$


$\langle \Phi | \hat{H} | \Phi \rangle = \sum_{j=1}^{N/2} \int_r |\vec{\nabla} \phi_j(\vec{r})|^2 + \frac{1}{2} \iint_{r,r'} U_{ee}(\vec{r}-\vec{r}') n(\vec{r}) n(\vec{r}')$
$- \sum_{i,j=1}^{N/2} \int_r \int_{r'} , U_{ee}$


'atomic' units $m_e = \hbar = e = 1$; $E_{H\,\text{Hydrogen}} = 1/2$
$\langle \Phi | \hat{H} | \Phi \rangle = \sum_{j=1}^{N_e} \int_{\vec{r}} |\vec{\nabla} \phi_j(\vec{r})|^2$
kinetic
$+ \frac{1}{2} \iint_{\vec{r},\vec{r}'} v_{ee}(\vec{r}-\vec{r}')\, n(\vec{r})\, n(\vec{r}')$
Hartree energy E_H
$n(\vec{r}) =$
$- \sum_{i,j=1}^{N_e} \int_{\vec{r}} \int_{\vec{r}'} v_{ee}(\vec{r}-\vec{r}')\, \phi_i^*(\vec{r})$
$(\vec{r})\, \phi_j(\vec{r}')$
$+ \int_{\vec{r}} v(\vec{r})\, n(\vec{r})$
ex


'atomic' units $m_e = \hbar = e = 1$; $E_{H\,Hydrogen} = 1/2$
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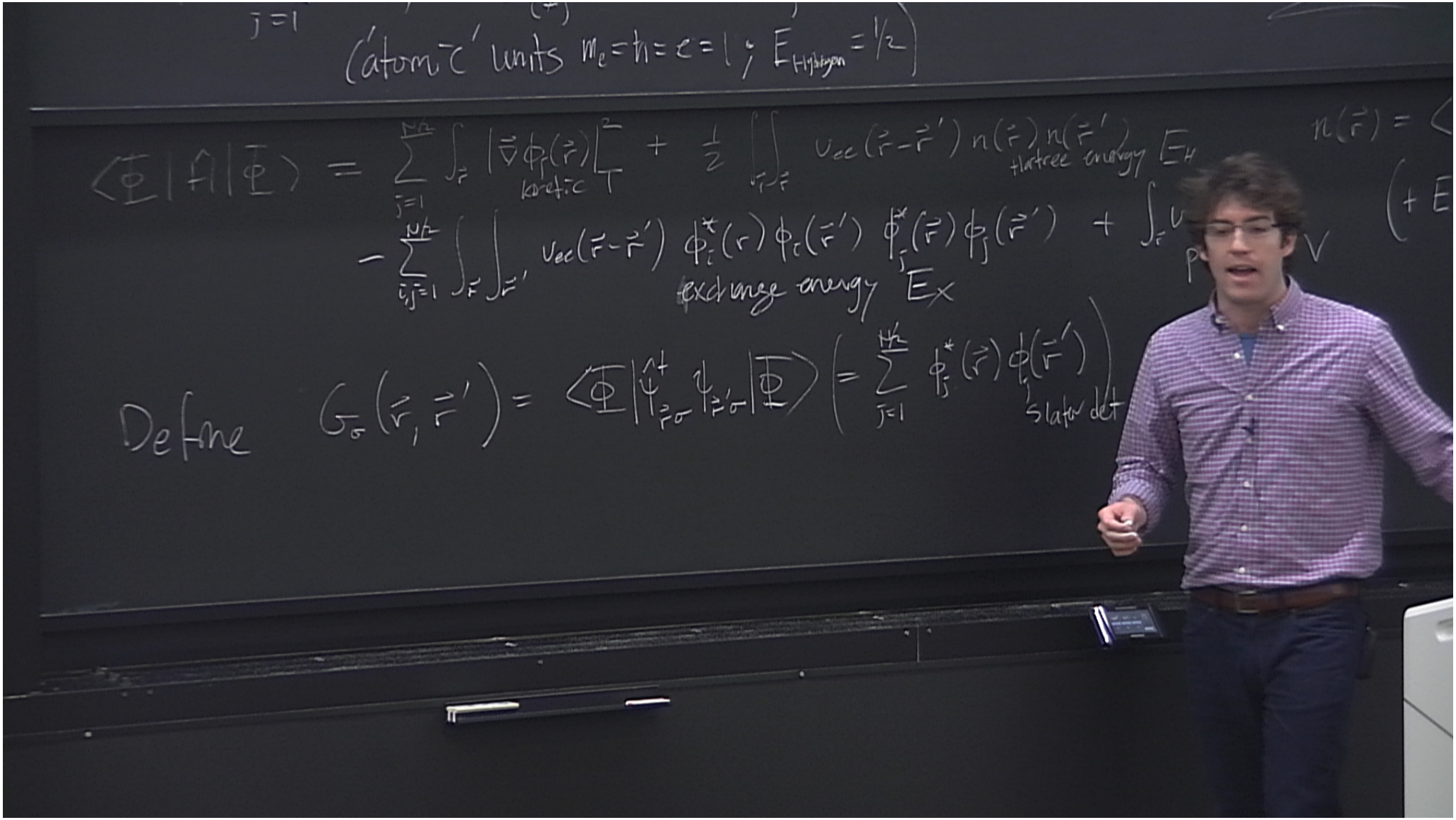
kinetic
$+ \frac{1}{2} \iint_{r\,r'} v_{ee}(\vec{r}-\vec{r}')\, n(\vec{r})\, n(\vec{r}')$
Hartree energy E_H
$- \sum_{i,j=1}^{N_e} \int_r \int_{r'} v_{ee}(\vec{r}-\vec{r}')\, \phi_i^*(\vec{r})\, \phi_i(\vec{r}')\, \phi_j^*(\vec{r}')\, \phi_j$
exchange energy E_x
$\int_r v(\vec{r})\, n(\vec{r})$
potential V
$n(\vec{r}) =$
Define $G_\sigma(\vec{r}, \vec{r}') = \langle \Phi | \hat{\psi}^\dagger_{\vec{r}\sigma} \psi_{\vec{r}'\sigma} | \Phi \rangle$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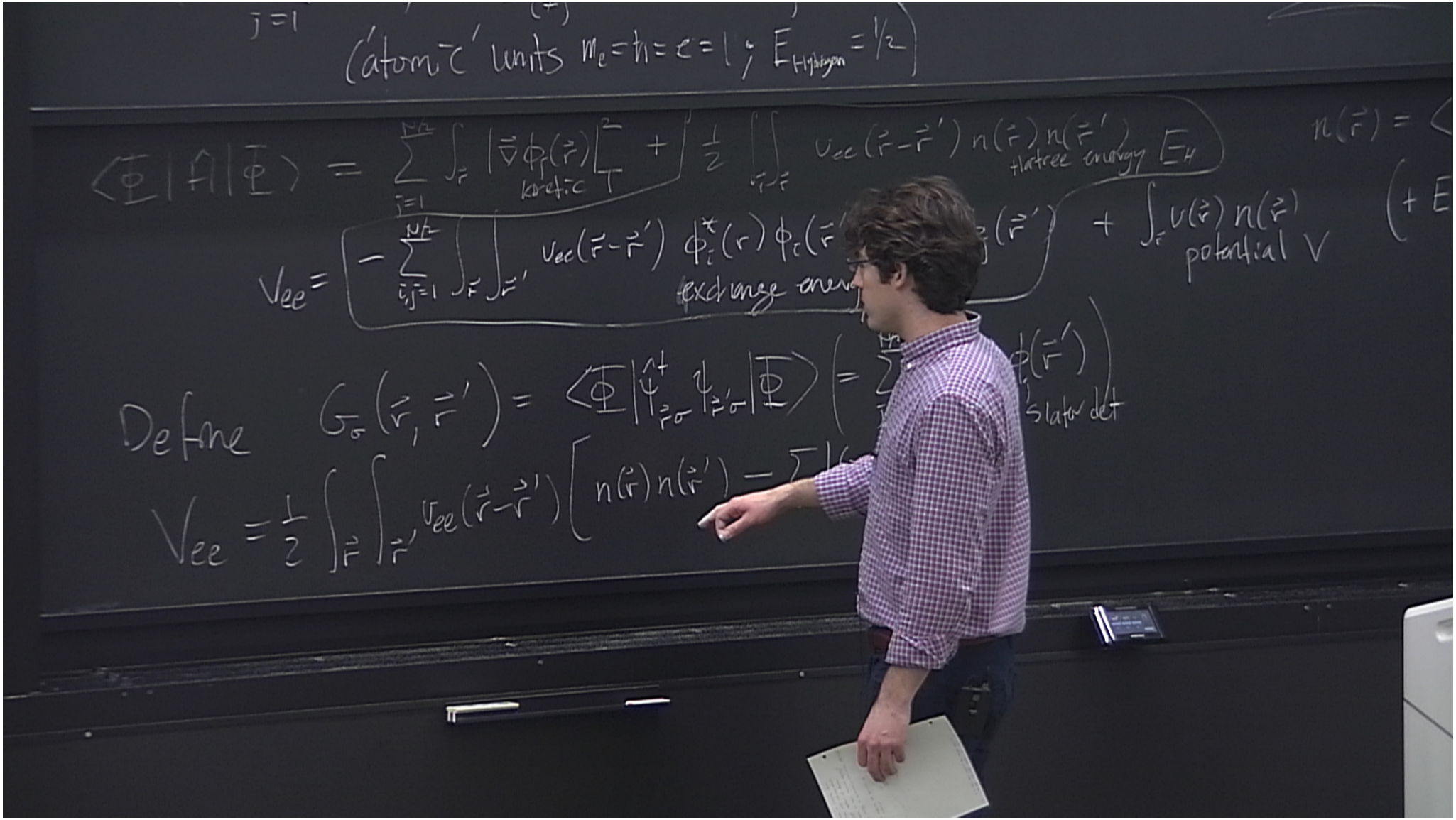
$- \sum_{i,j=1}^{N_e} \int_{\vec{r}} \int_{\vec{r}'} V_{ee}(\vec{r}-\vec{r}')\, \phi_i^*(\vec{r})\, \phi_i(\vec{r}')\, \phi_j^*(\vec{r})\, \phi_j(\vec{r}')$ exchange energy E_X $+ \int_{\vec{r}} V$
Define $G_\sigma(\vec{r},\vec{r}') = \langle \Phi | \hat{\psi}^\dagger_{\vec{r}\sigma} \psi_{\vec{r}'\sigma} | \Phi \rangle$ $\left(= \sum_{j=1}^{N_e} \phi_j^*(\vec{r})\, \phi_j(\vec{r}') \right)$ Slater det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$\frac{1}{2} \iint_{\vec{r}, \vec{r}'} v_{ee}(\vec{r} - \vec{r}')\, n(\vec{r})\, n(\vec{r}')$ hartree energy E_H
$n(\vec{r}) =$
$V_{ee} =$ $-\sum_{i,j=1}^{N_e} \int_{\vec{r}} \int_{\vec{r}'} v_{ee}(\vec{r} - \vec{r}')\, \phi_i^*(\vec{r})\, \phi_i(\vec{r}$
exchange ener
$\int_{\vec{r}} v(\vec{r})\, n(\vec{r})$ potential V
$(+ E$
Define $G_\sigma(\vec{r}, \vec{r}') = \langle \Phi | \hat{\psi}^\dagger_{\vec{r}\sigma} \psi_{\vec{r}'\sigma} | \Phi \rangle$ $\left(= \sum_i^{N_e} \phi_i^*(\vec{r}) \phi_i(\vec{r}') \right)$
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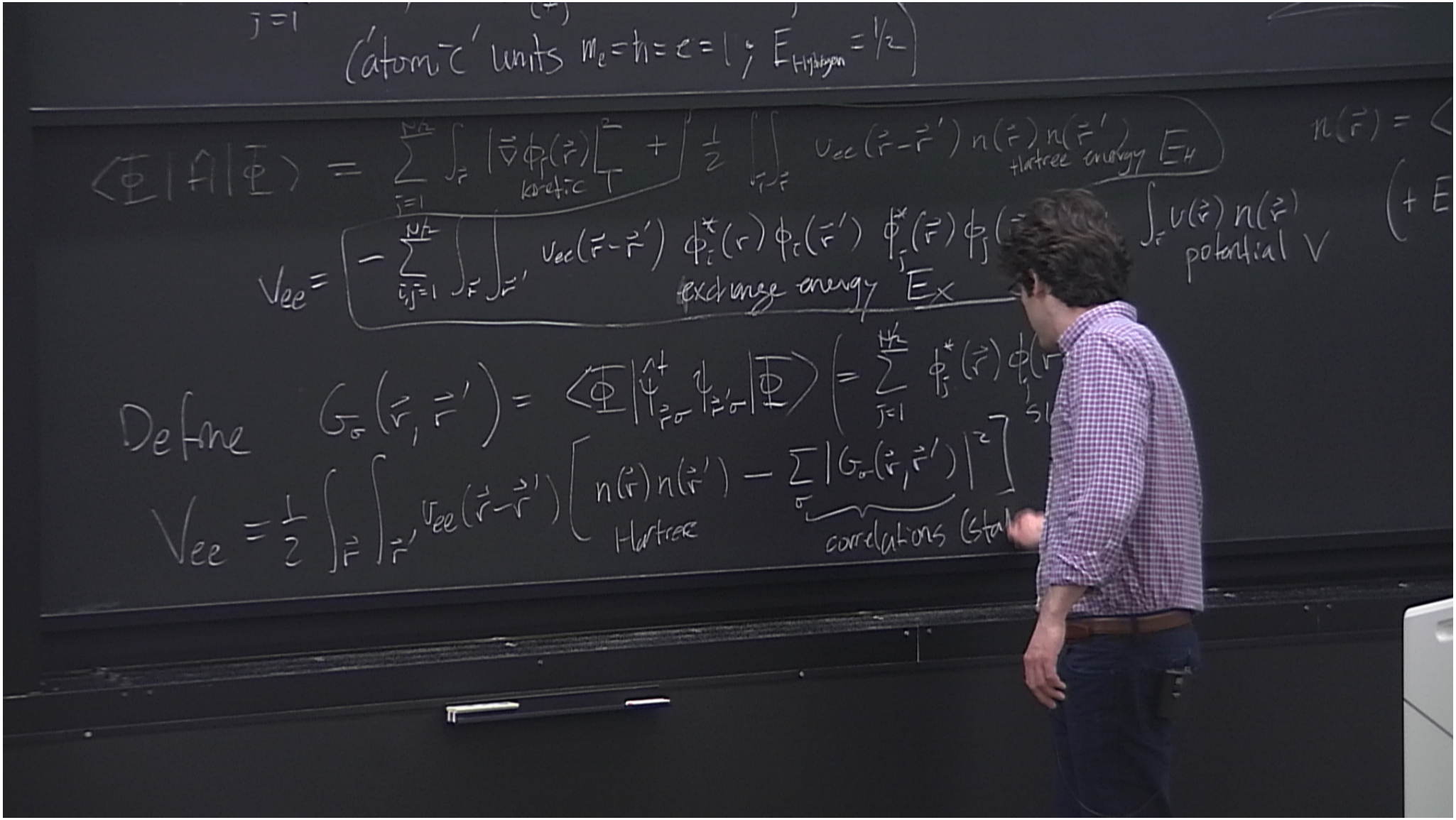
$V_{ee} = \frac{1}{2} \int_{\vec{r}} \int_{\vec{r}'} v_{ee}(\vec{r} - \vec{r}') \left[n(\vec{r})\, n(\vec{r}') - \right.$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$V_{ee} = -\sum_{i,j=1}^{N_e} \int_{\vec{r}} \int_{\vec{r}'} V_{ee}(\vec{r}-\vec{r}')\, \phi_i^*(\vec{r})\, \phi_i(\vec{r}')\, \phi_j^*(\vec{r}')\, \phi_j(\vec{r})$ exchange energy E_X
$\int_{\vec{r}} V(\vec{r})\, n(\vec{r})$ potential V
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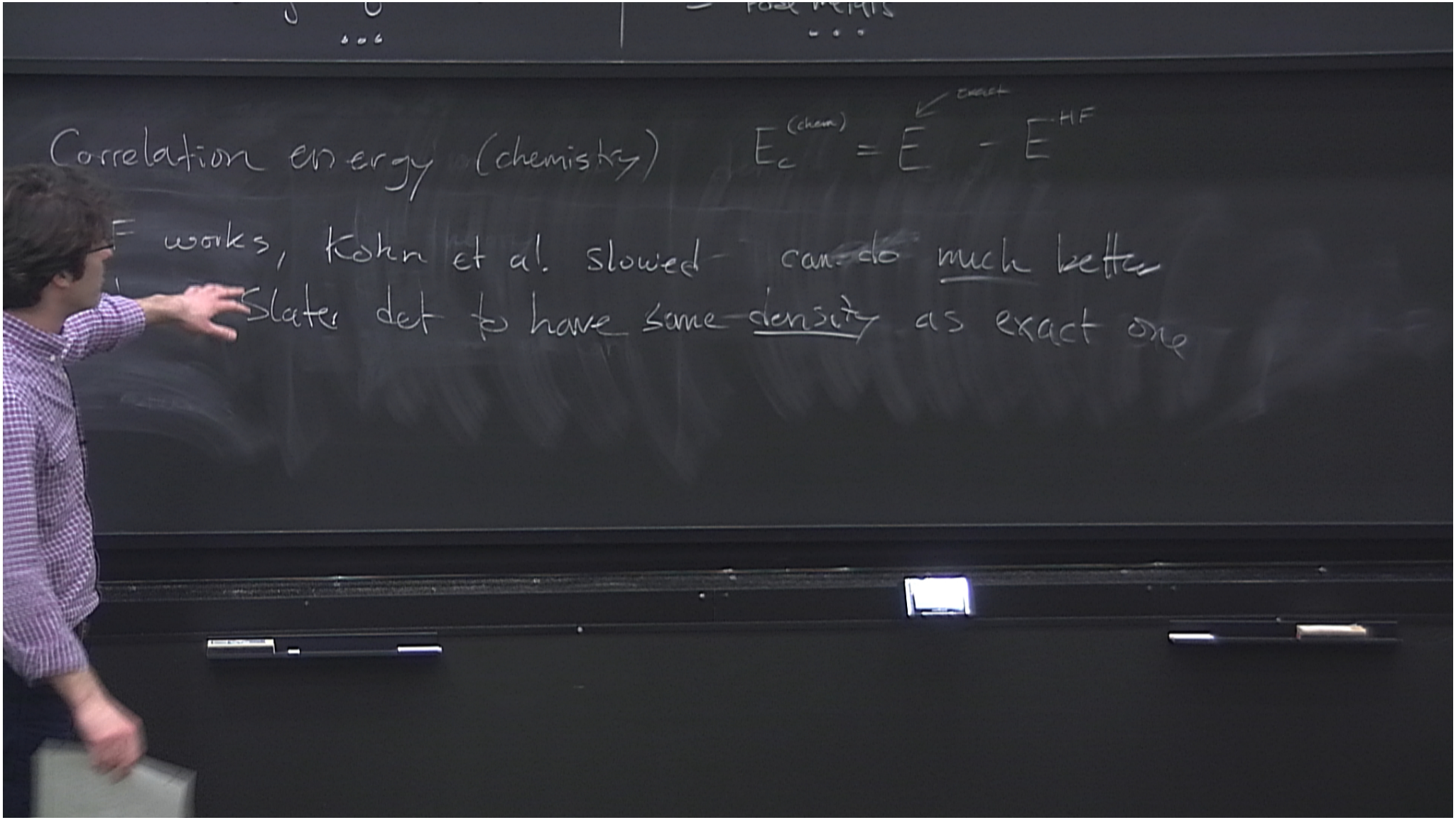
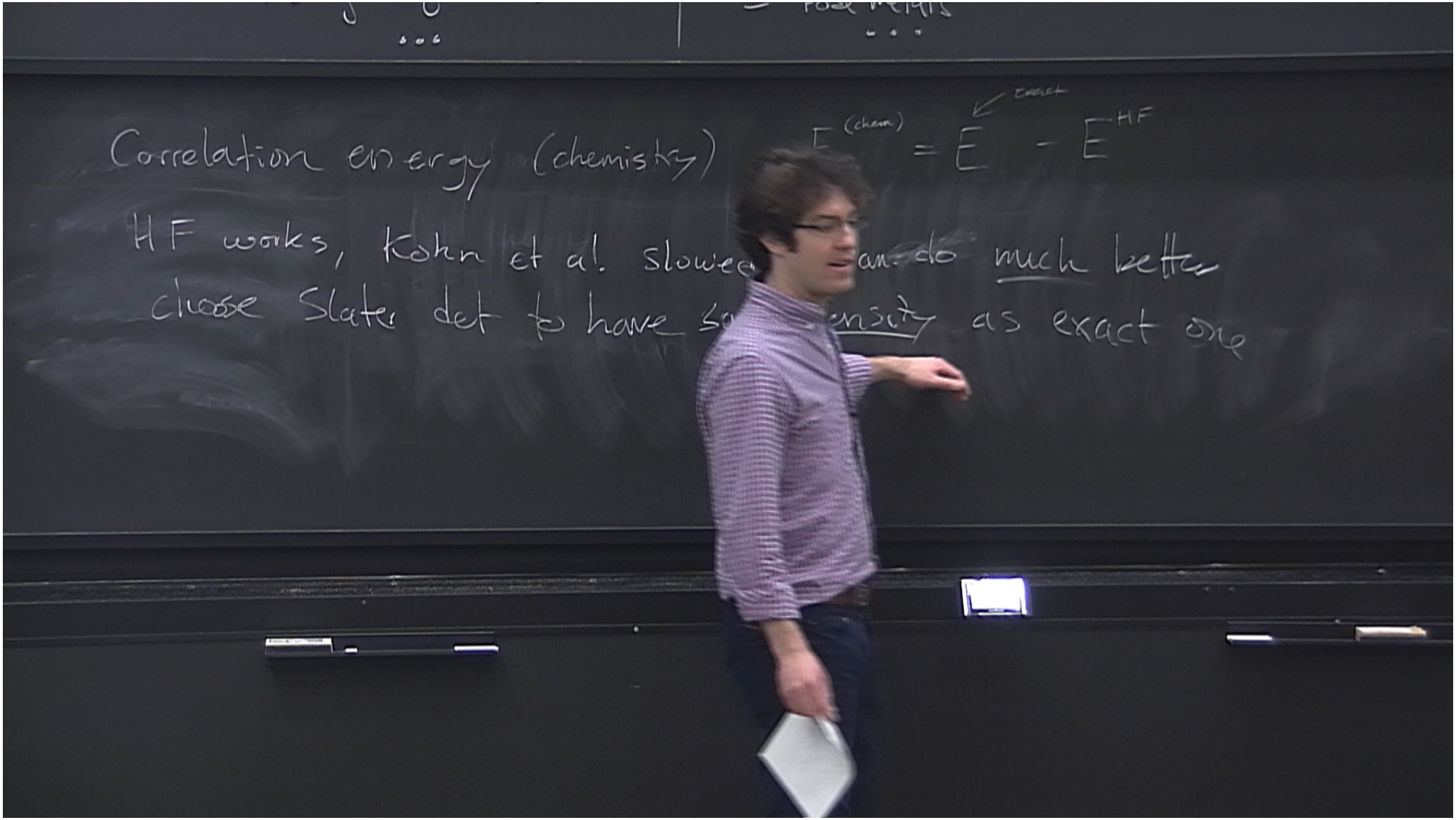
Hartree
correlations (Sta


Correlation energy (chemistry) $E_c^{(chem)} = E^{exact} - E^{HF}$
F works, Kohn et al. showed can do much better
Slater det to have same density as exact one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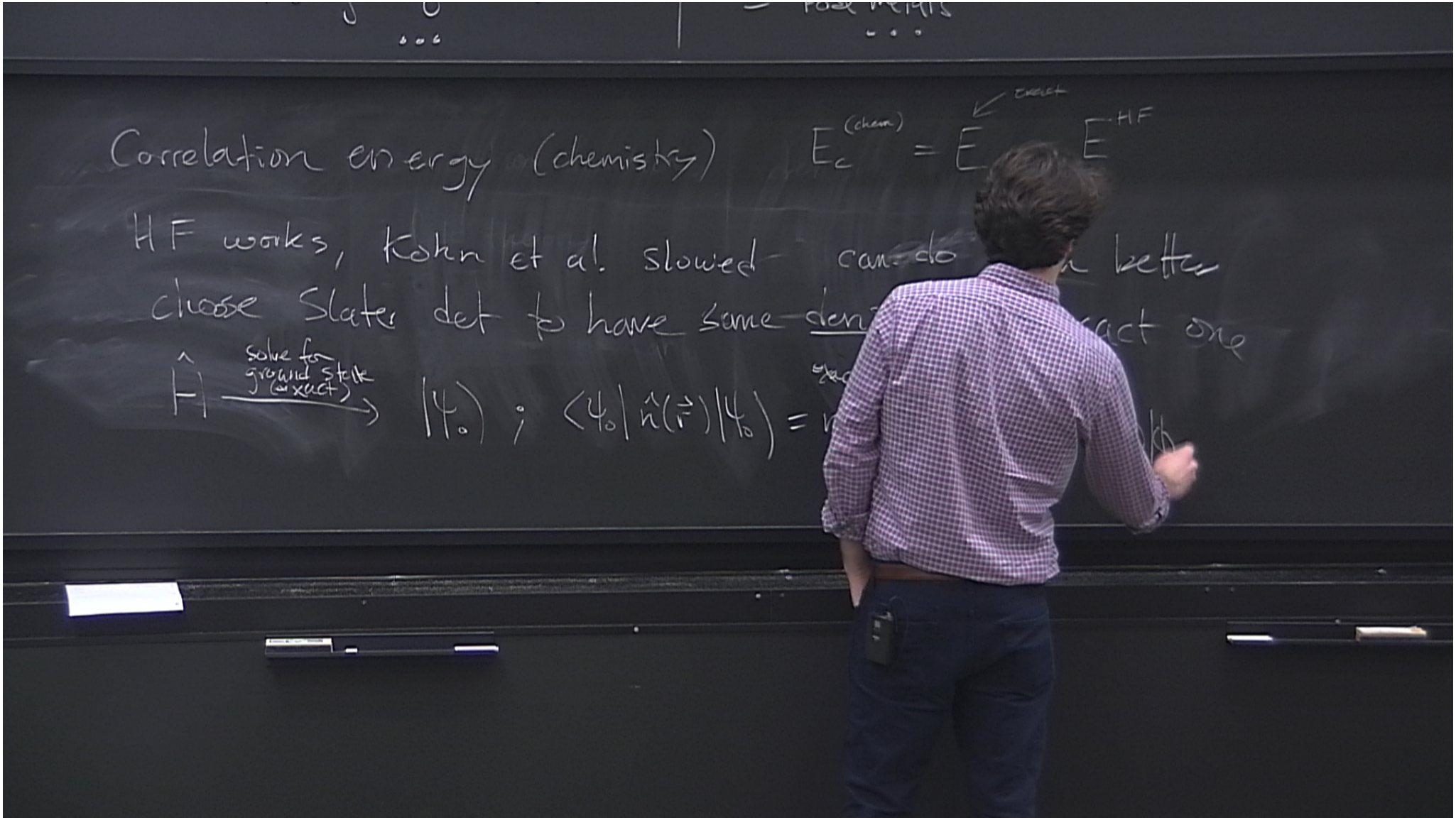
$\hat{H} \xrightarrow{\text{solve for ground state (exact)}} |\psi_0\rangle \; ; \; \langle\psi_0|\hat{n}(\vec{r})|\psi_0\rangle$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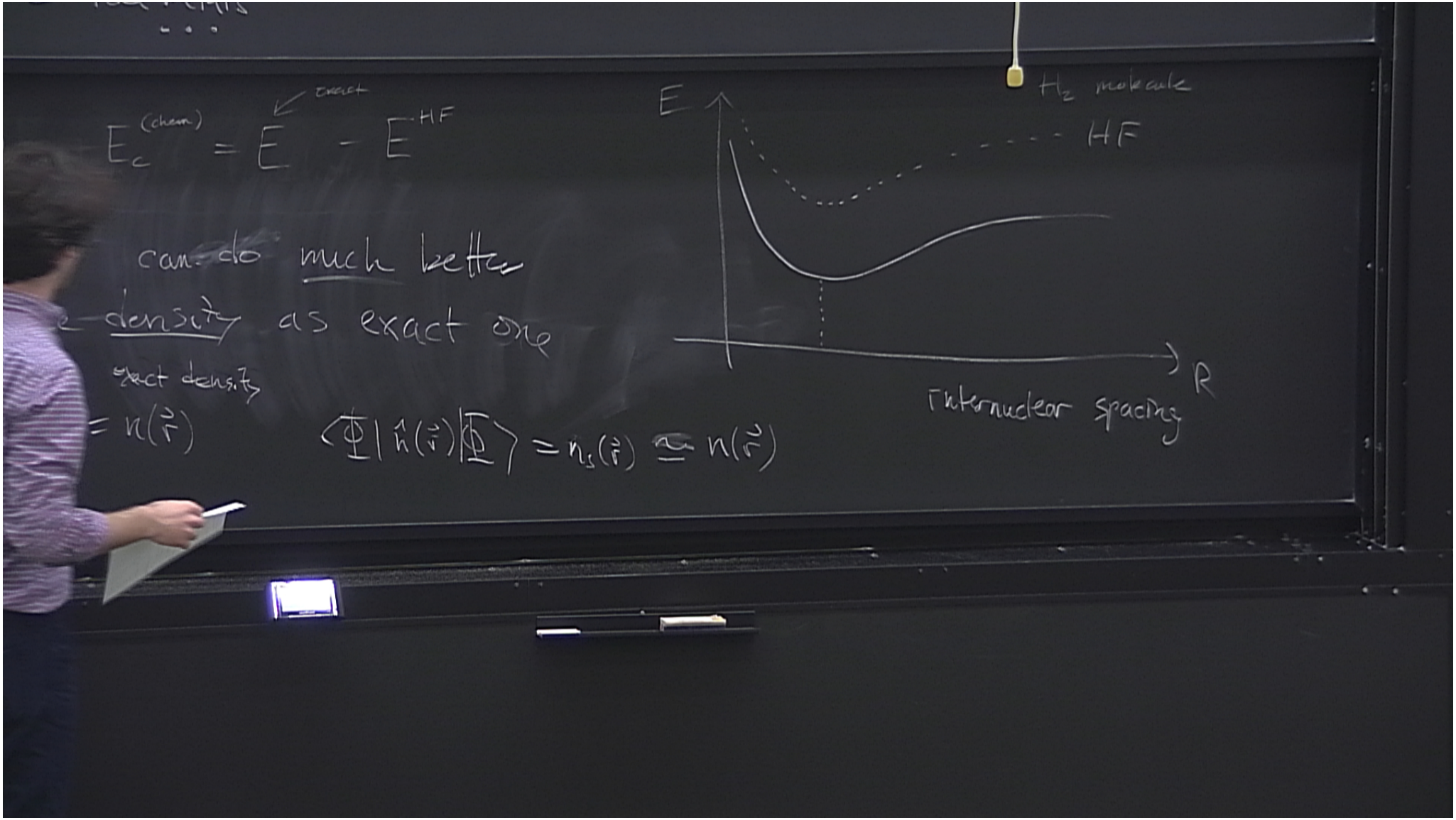
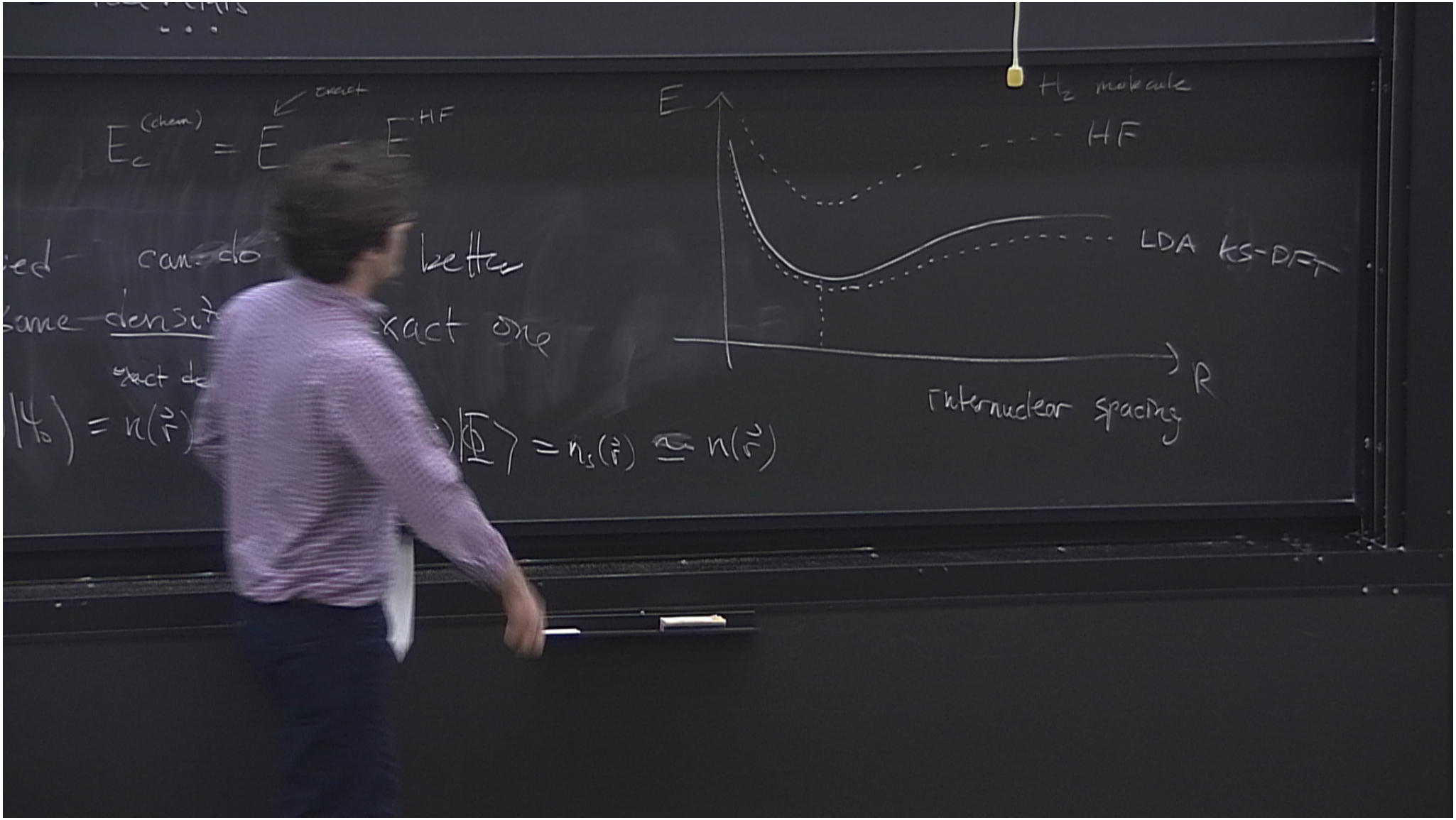
choose Slater det to have same
$\hat{H} \xrightarrow{\text{solve for ground state (exact)}} |\psi_0\rangle$; $\langle\psi_0|\hat{n}(\vec{r})|\psi_0\rangle$


$E_c^{(chem)} = E^{exact} - E^{HF}$
can do much better
density as exact one
exact density
$= n(\vec{r})$
$\langle \Phi | \hat{n}(\vec{r}) | \Phi \rangle = n_s(\vec{r}) \approx n(\vec{r})$
E
H_2 molecule
HF
R
Internuclear spacing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same density
exact one
$|\Psi_0\rangle = n(\vec{r})$
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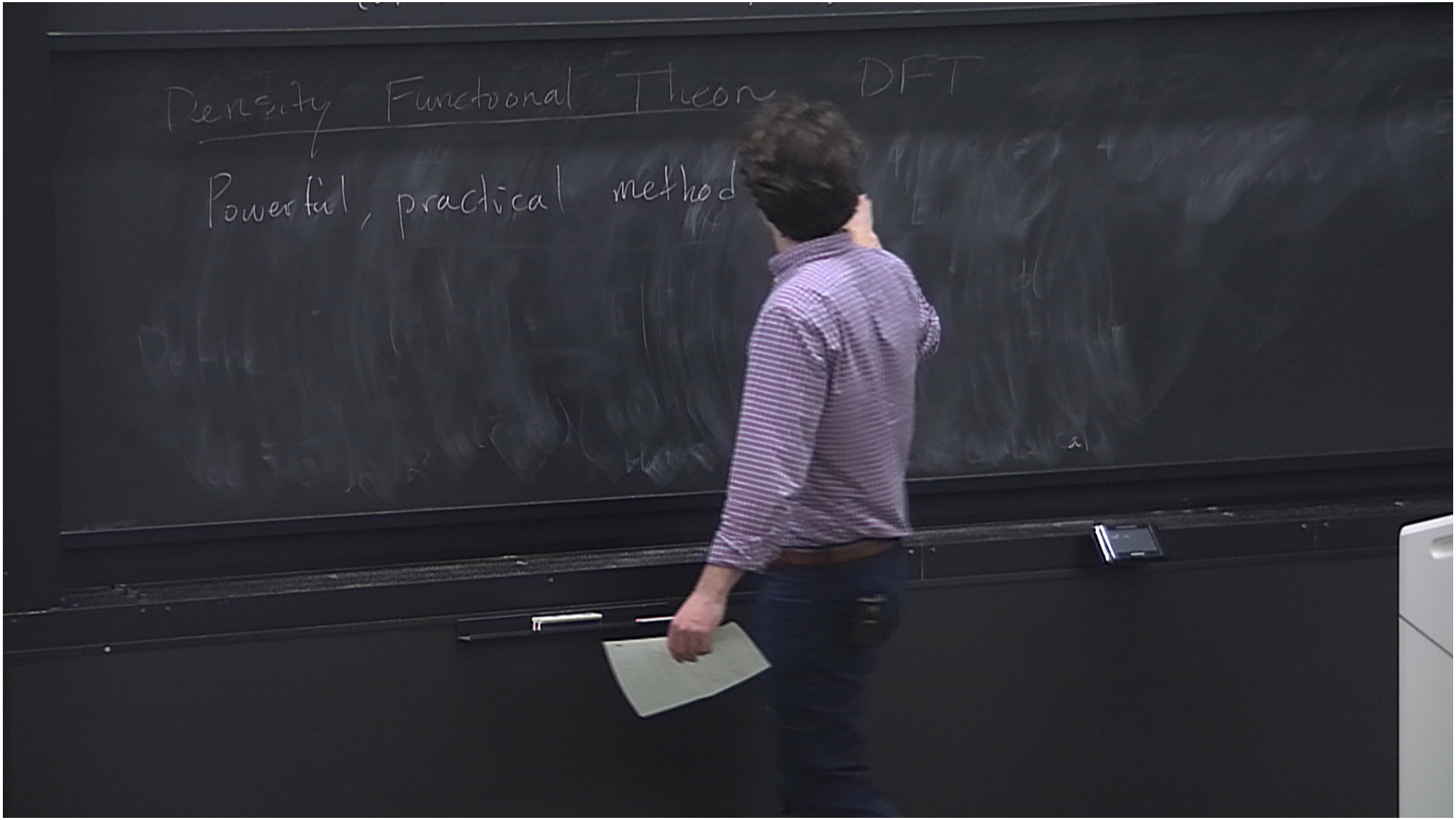
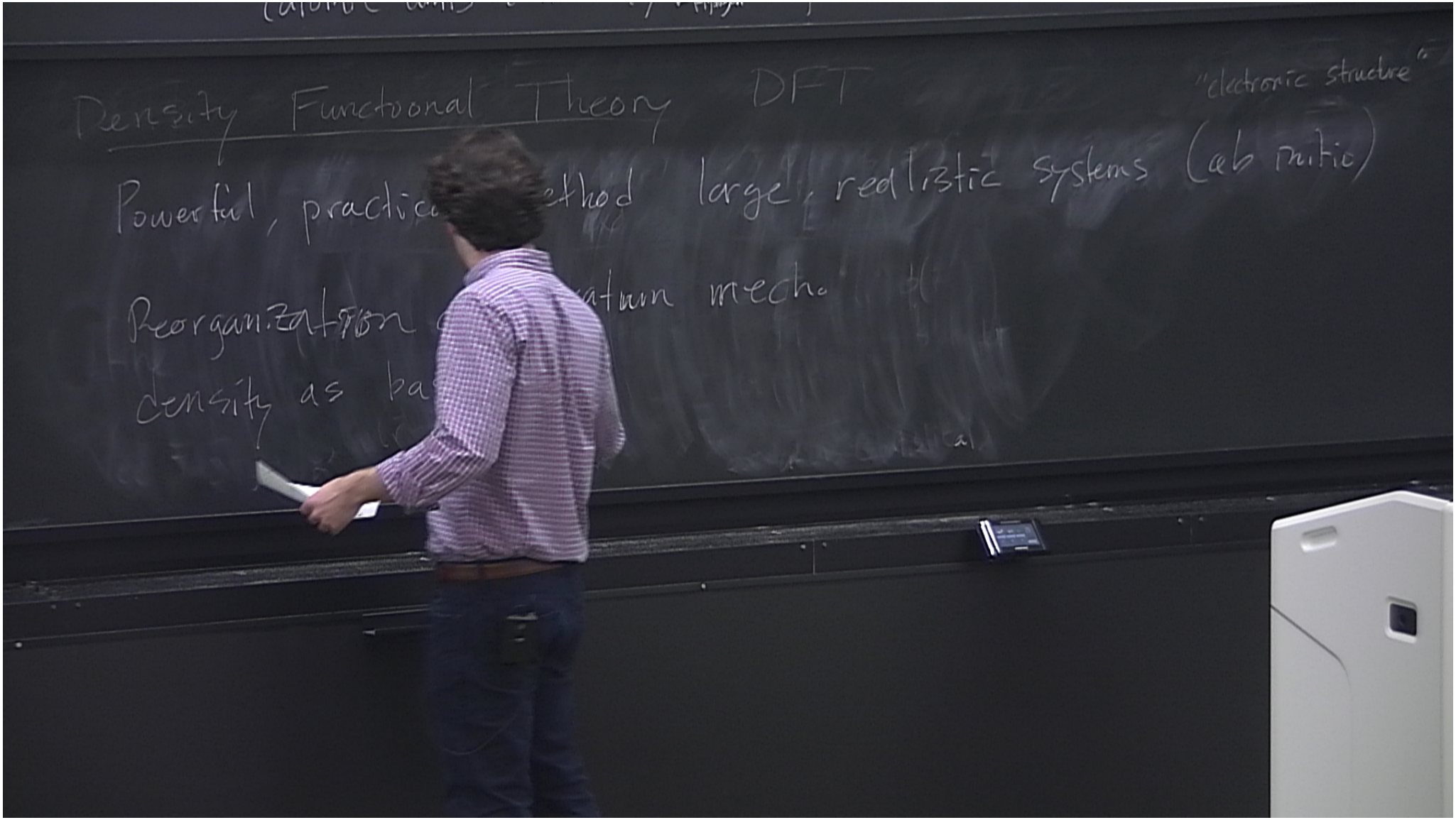
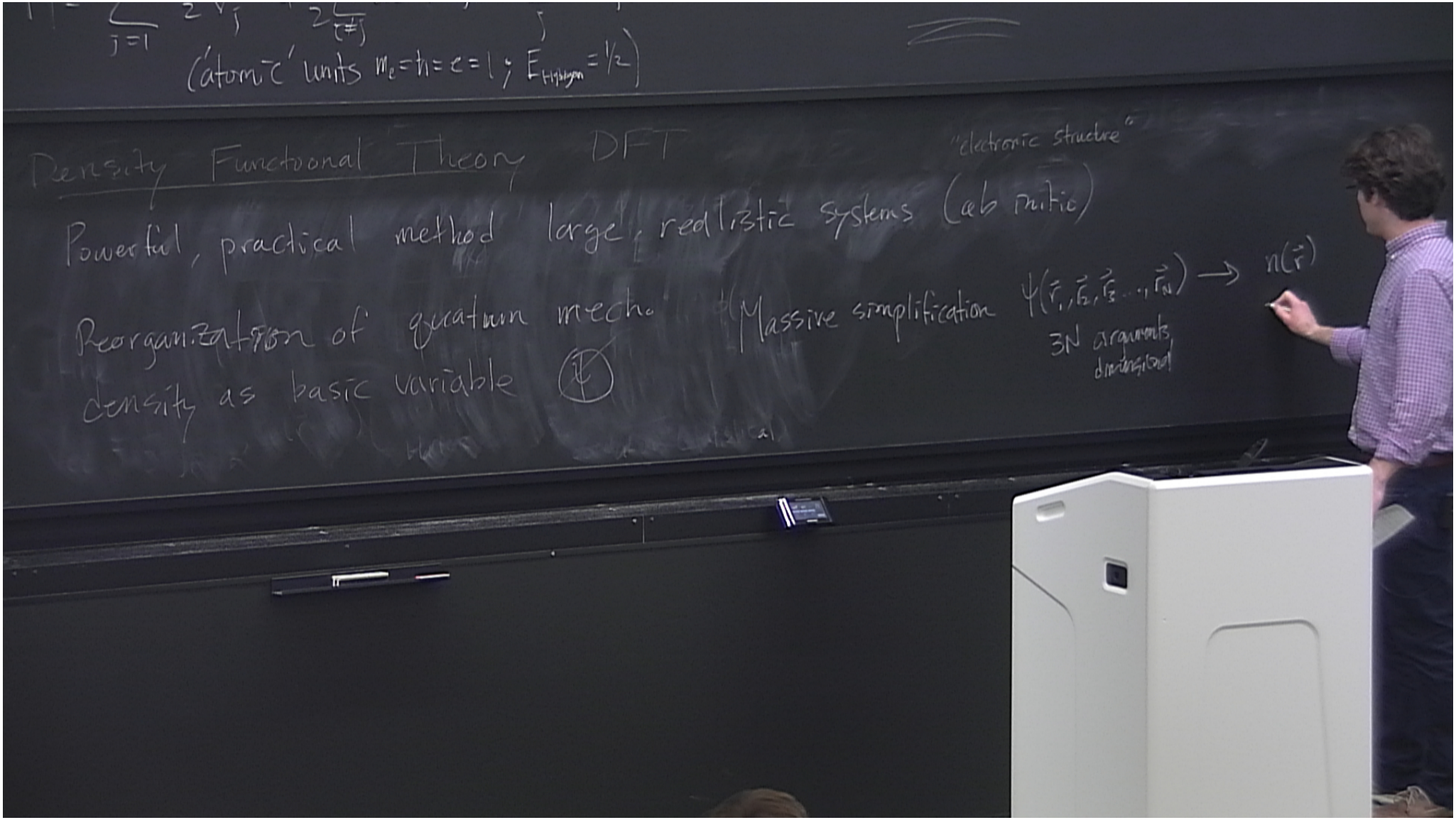
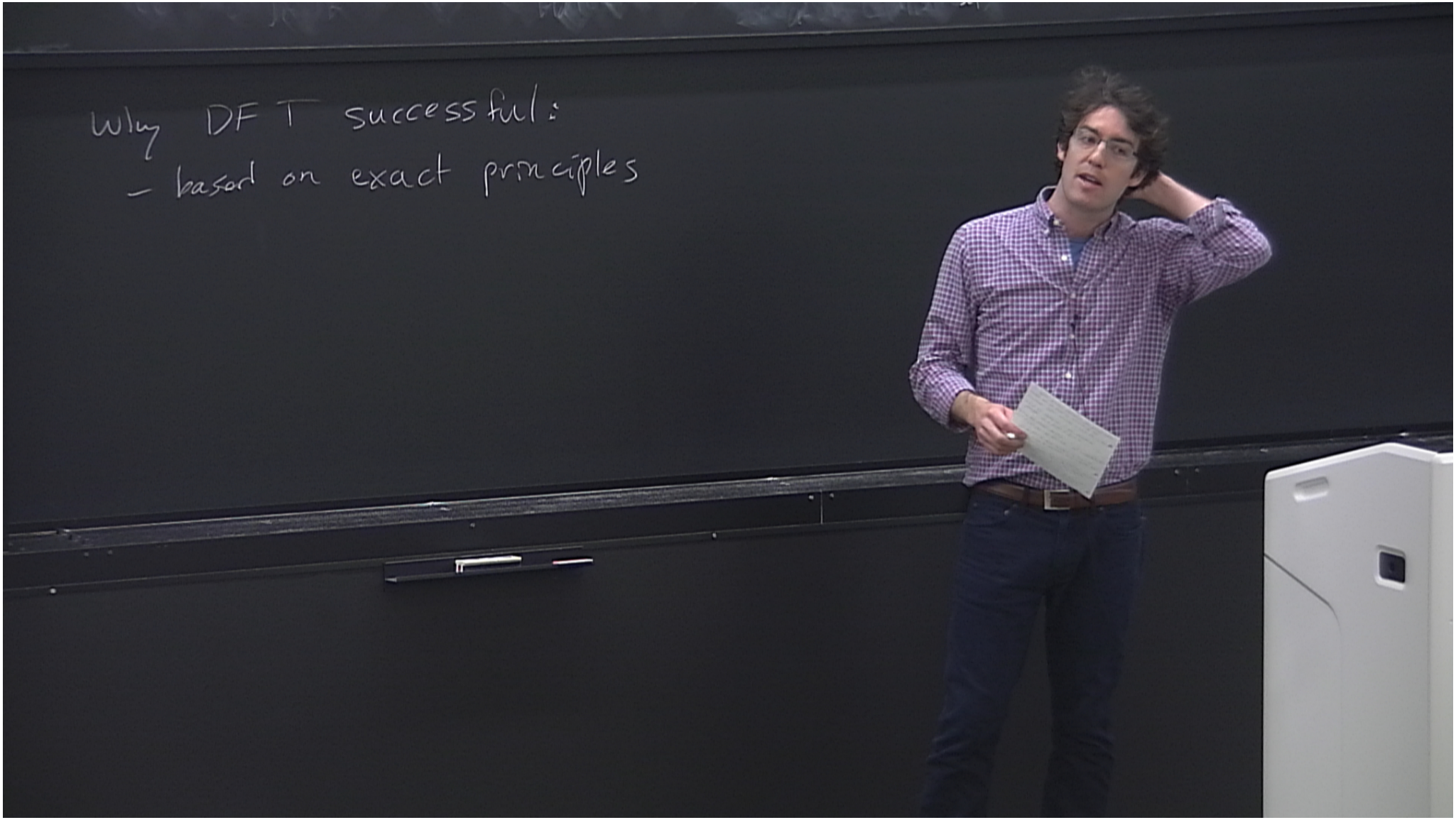
E
H_2 molecule
HF
LDA KS-DFT
R
Internuclear spacing


Density Functional Theory DFT
Powerful, practical method


Density Functional Theory DFT
"electronic structure"
Powerful, practical method large, realistic systems (ab initio)
Reorganization
density as ba
atum mech.


("atomic" units $m_e = \hbar = e = 1$; $E_{Hydrogen} = 1/2$)
Density Functional Theory DFT
"electronic structure"
Powerful, practical method large, realistic systems (ab initio)
Reorganization of quantum mech. (Massive simplification $\psi(\vec{r}_1, \vec{r}_2, \vec{r}_3 \ldots, \vec{r}_N) \rightarrow n(\vec{r})$
3N arguments, dramatically
density as basic variable


Why DFT successful:
- based on exact principles


Why DFT successful:
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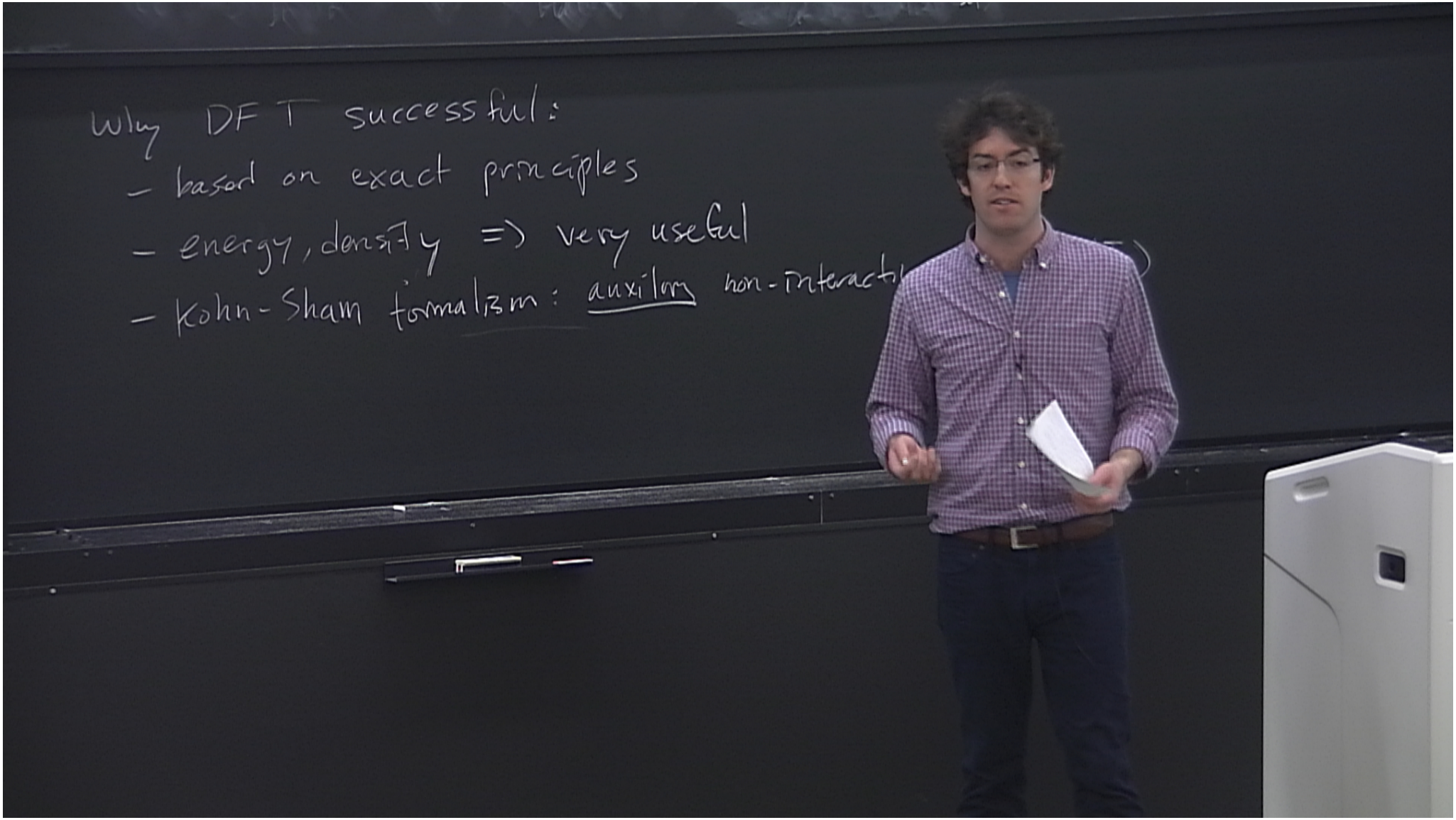
- Kohn-Sham formalism: auxiliary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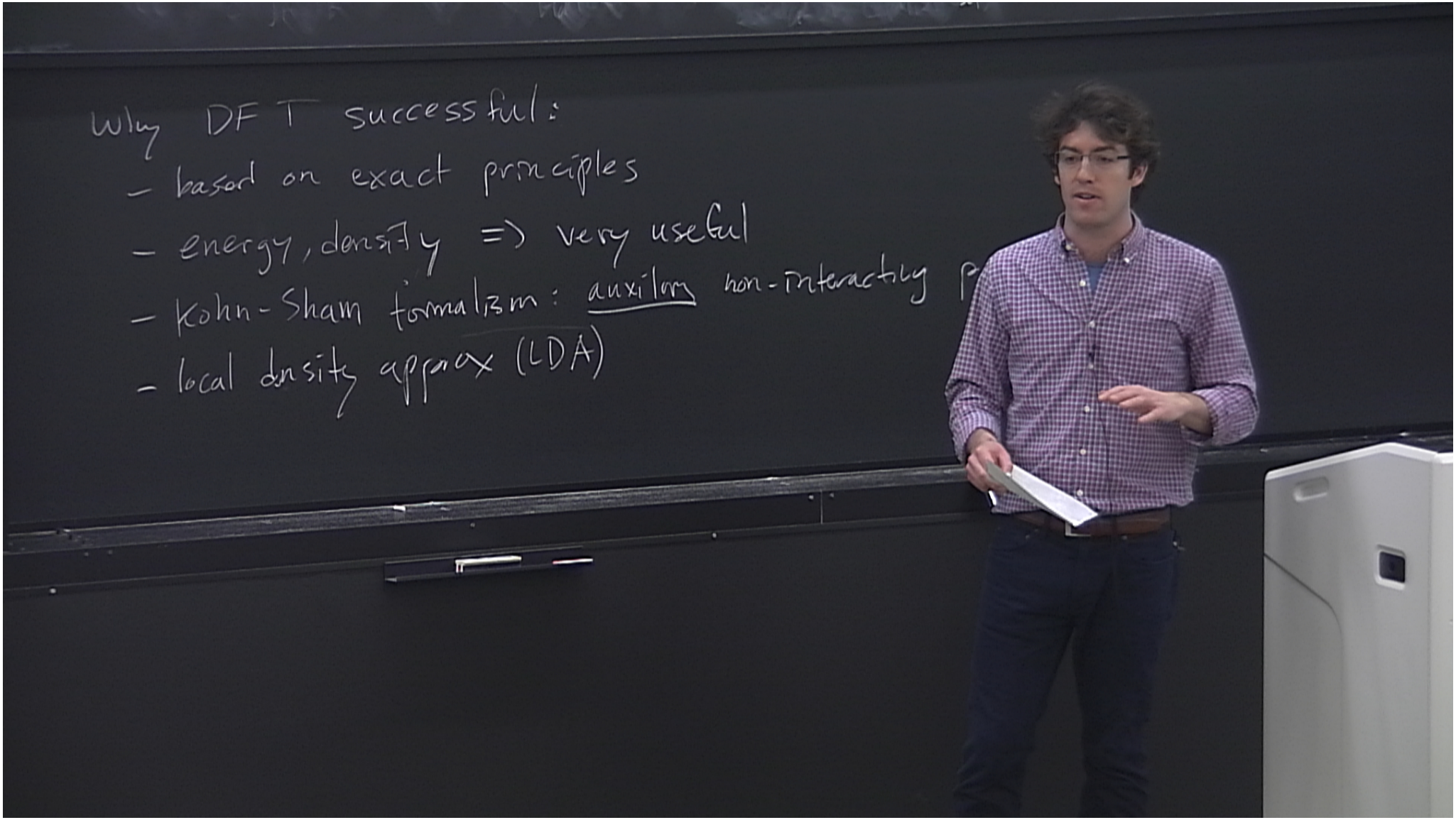
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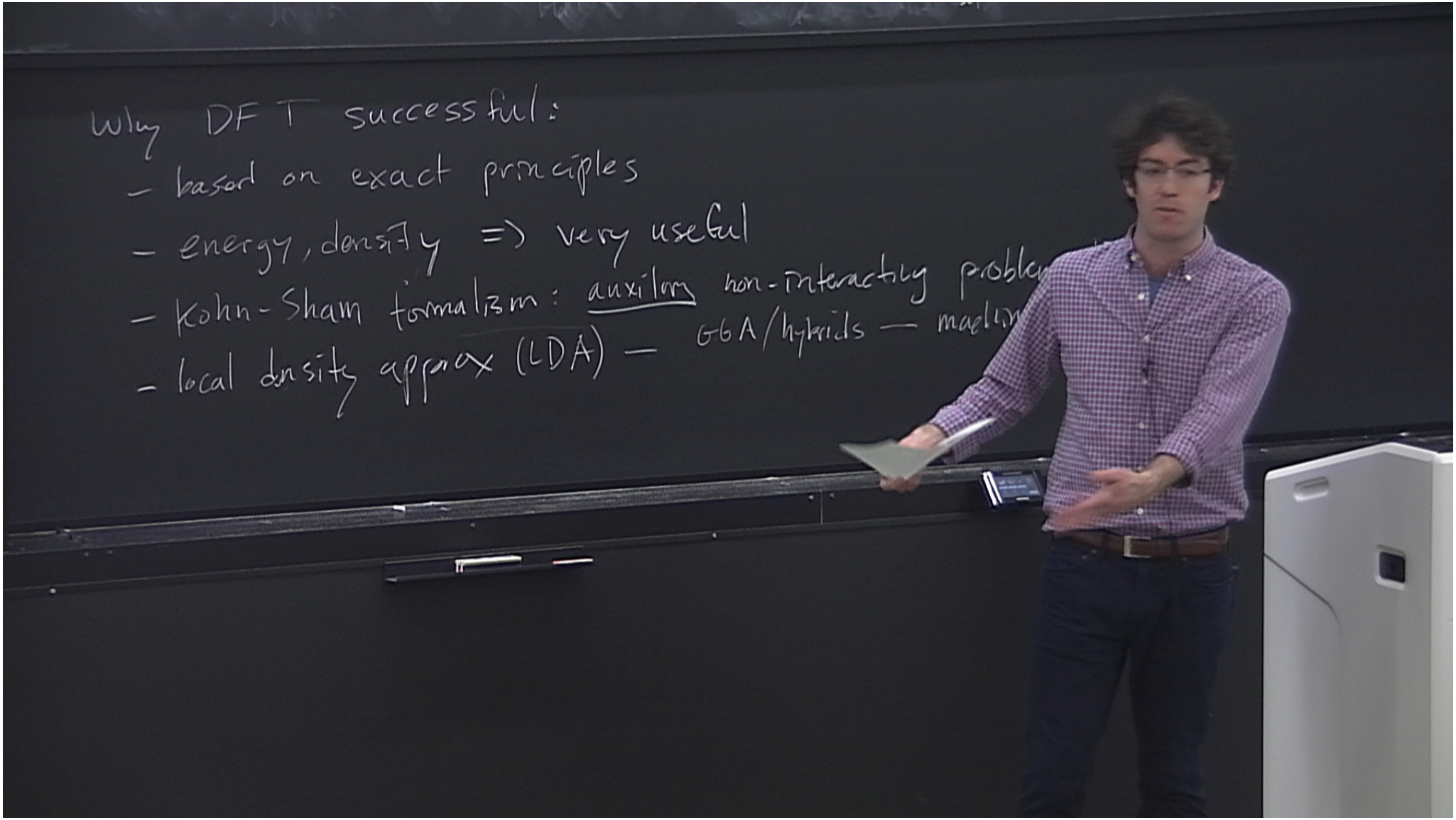
- local density approx (LDA)


Why DFT successful:
- based on exact principles
- energy, density => very useful
- Kohn-Sham formalism: auxiliary non-interacting
- local density approx (LDA) — GGA/hybrids —