Title: Explorations in Condensed Matter-2

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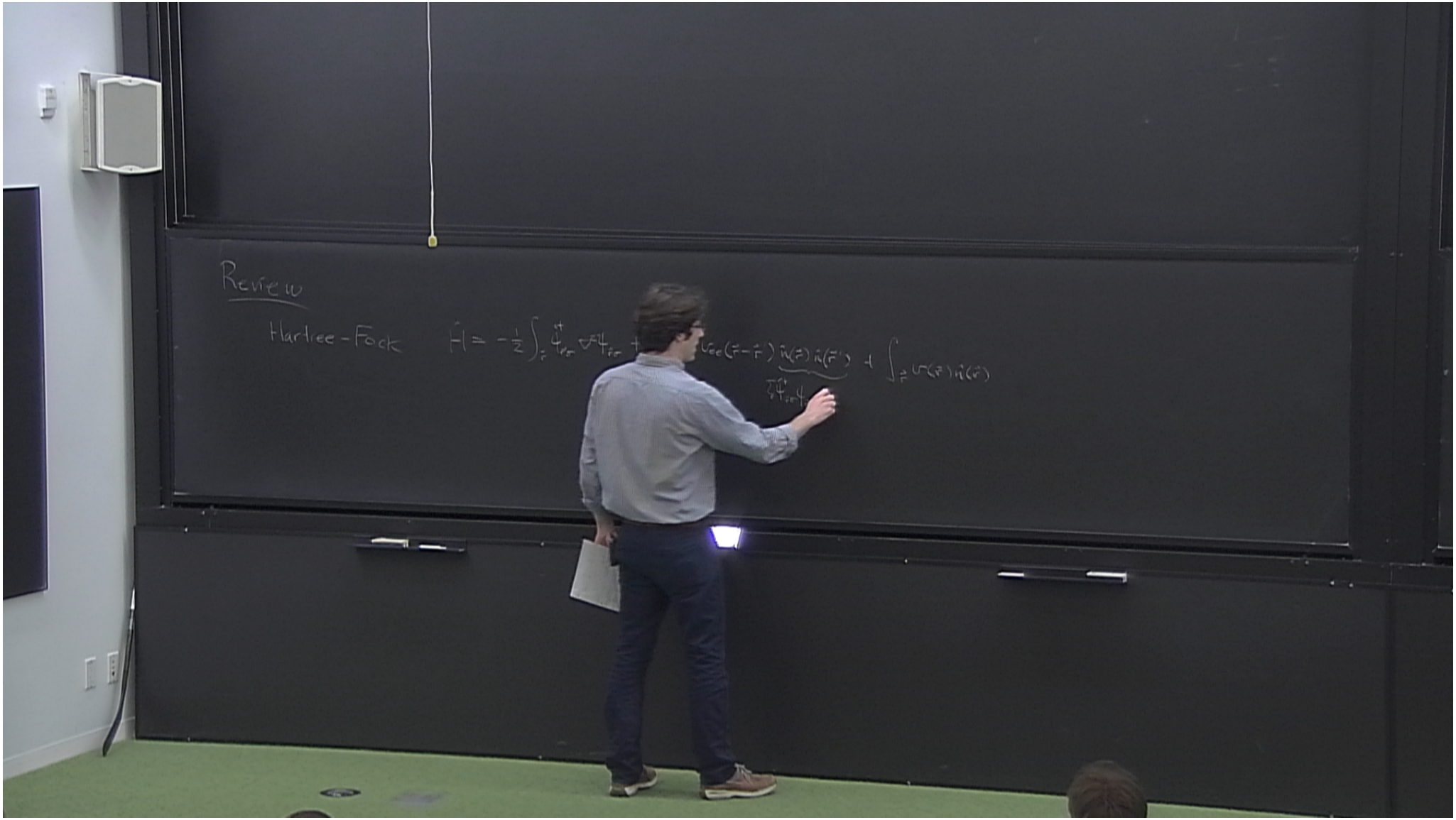
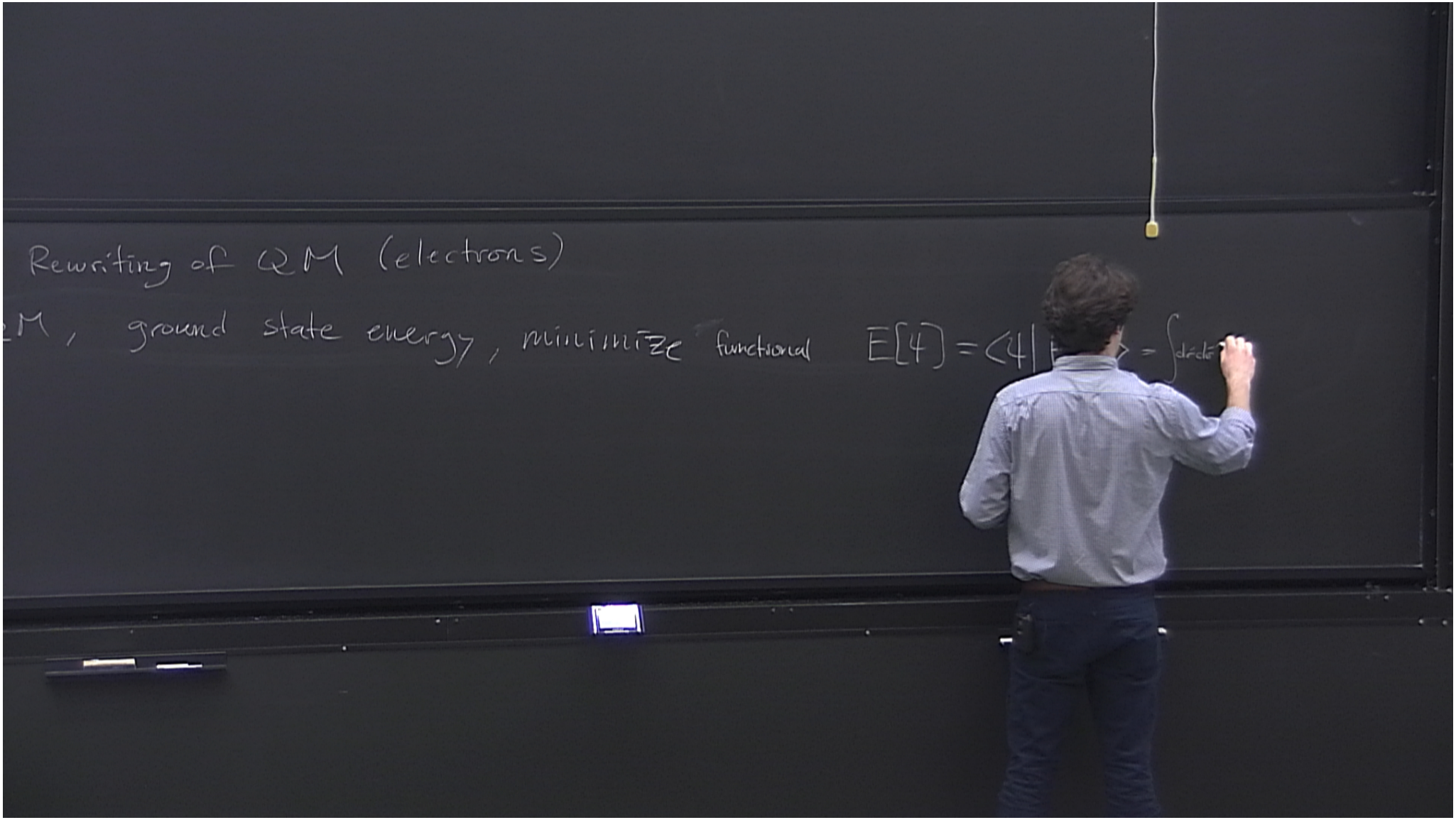
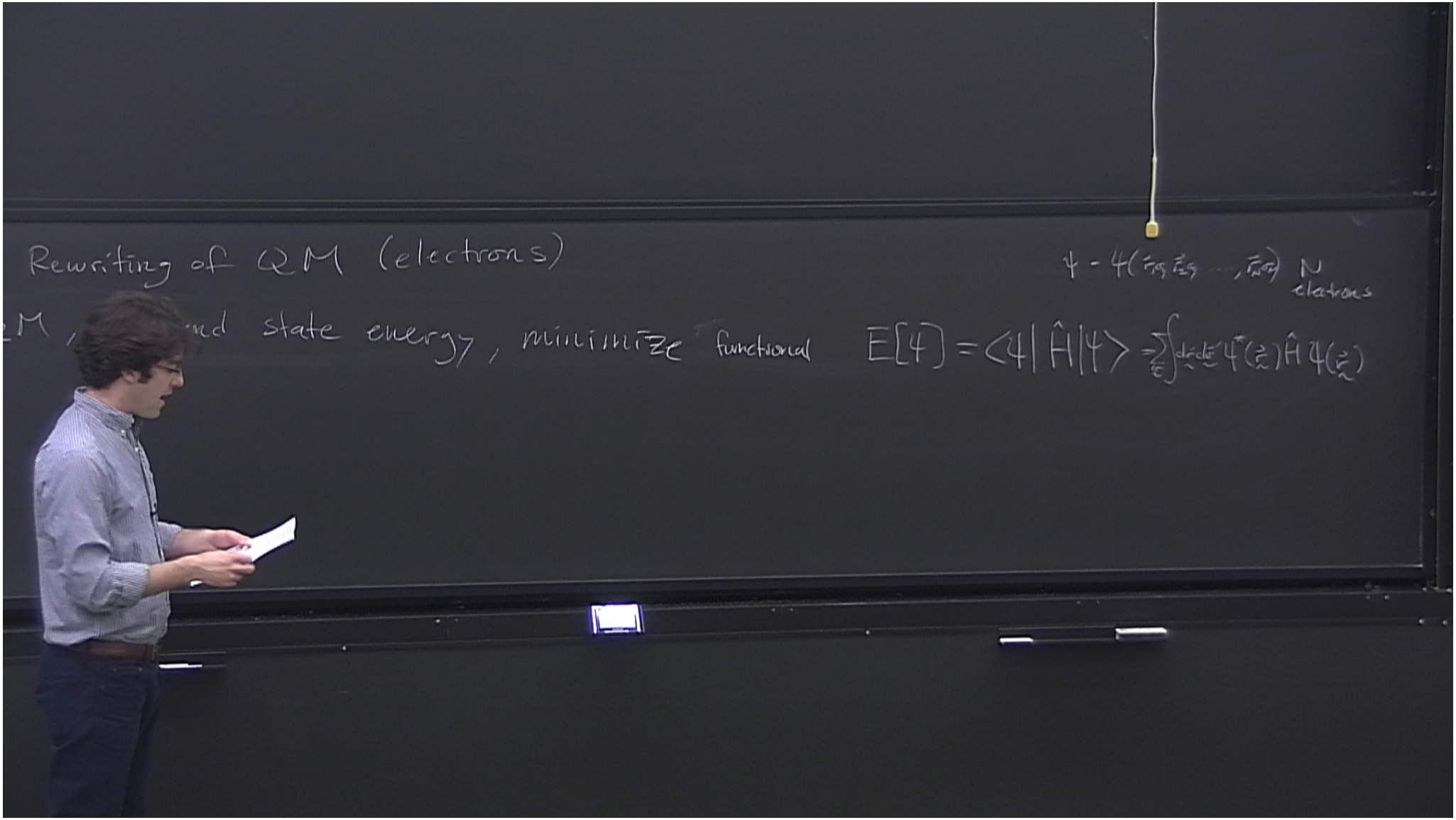
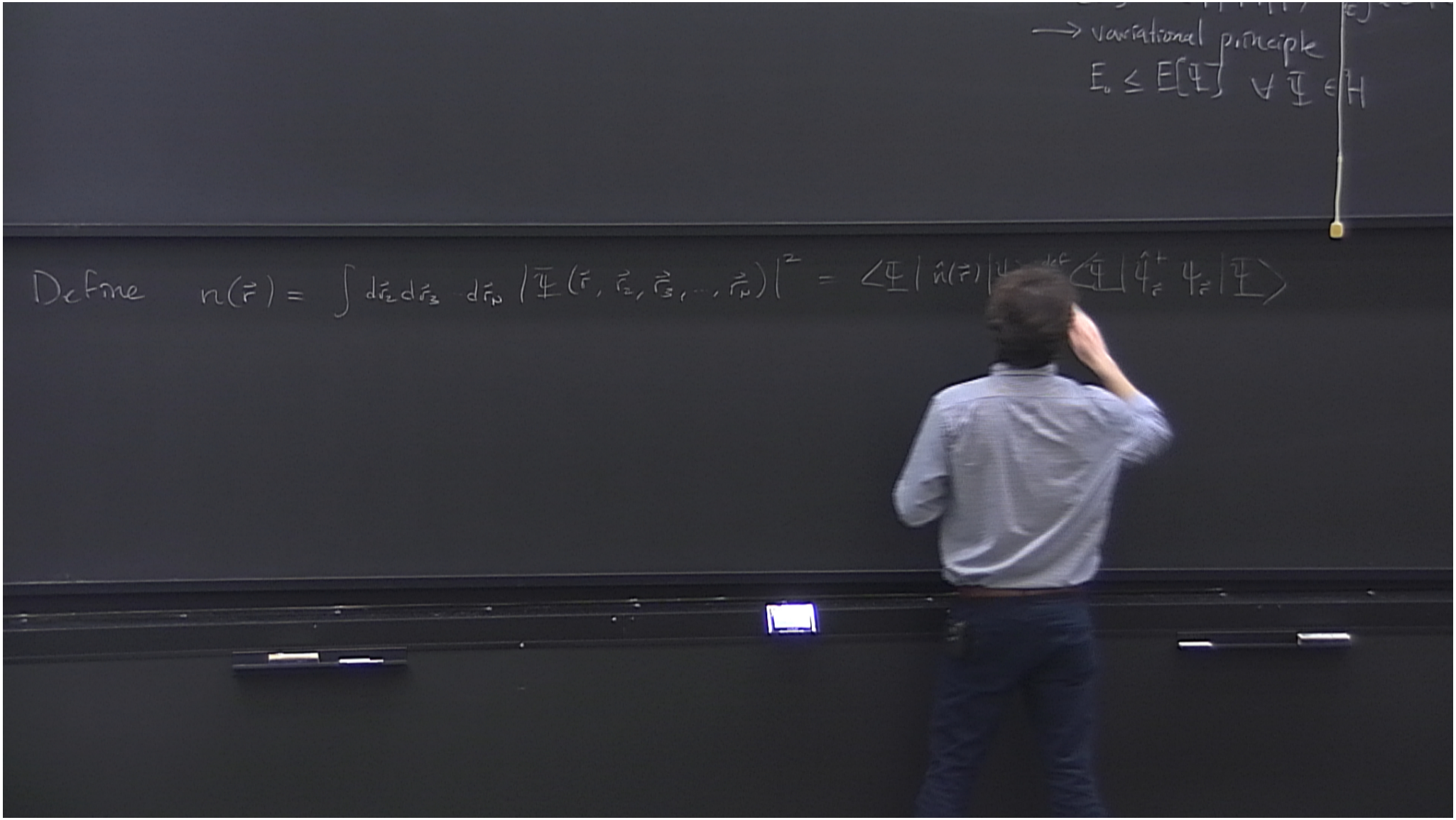
URL: http://pirsa.org/15030035

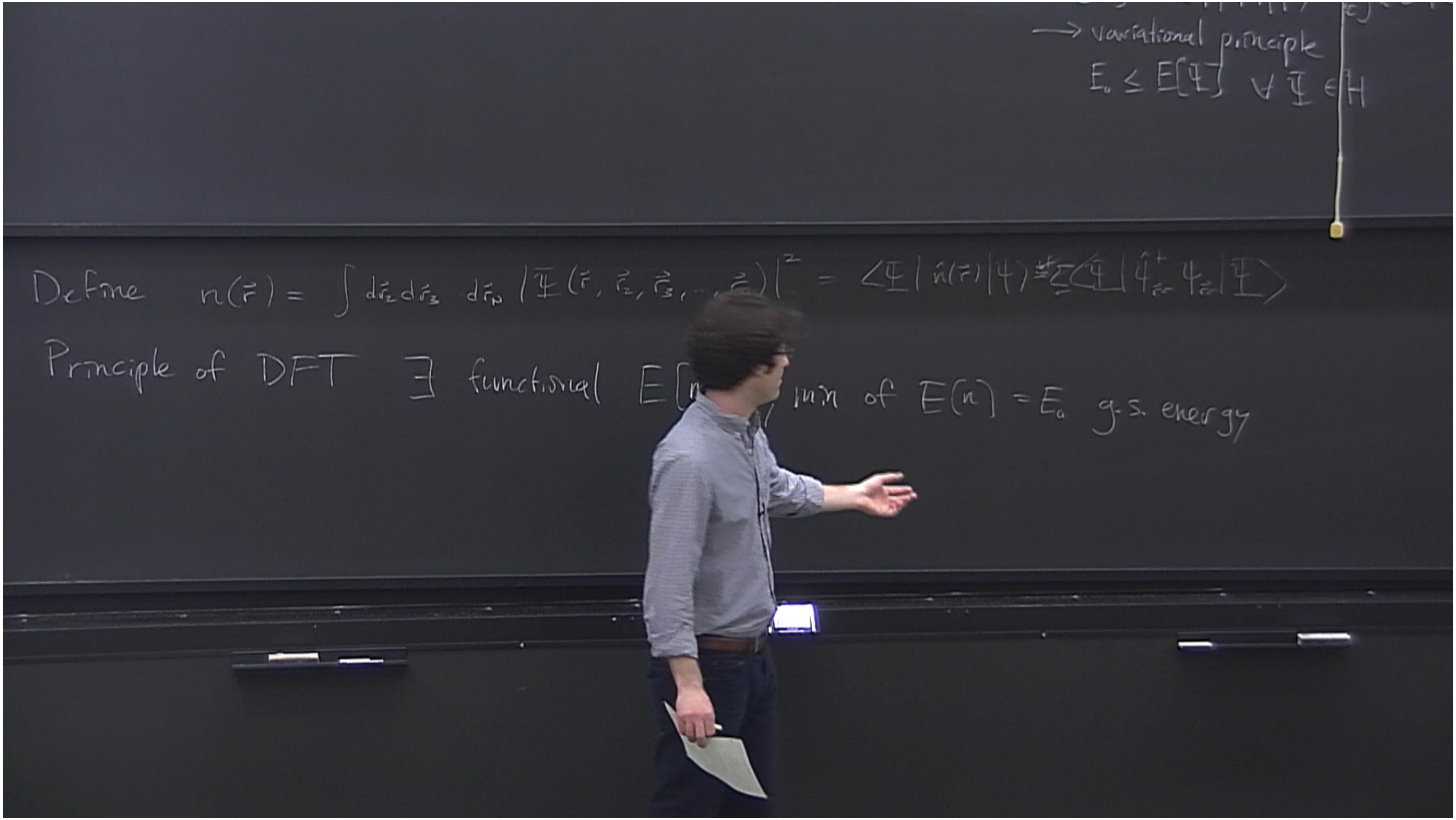
Abstract:


Review
Hartree-Fock


Rewriting of QM (electrons)
QM, ground state energy, minimize functional


Rewriting of QM (electrons)
$\psi = \psi(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_N)$ N electrons
QM, ...nd state energy, minimize functional $E[\psi] = \langle\psi|\hat{H}|\psi\rangle = \int d\vec{r}_1 \ldots d\vec{r}_N \psi^*(\vec{r}_N)\hat{H}\psi(\vec{r}_N)$


→ variational principle
$E_0 \leq E[\Psi] \quad \forall \Psi \in \mathcal{H}$
Define $n(\vec{r}) = \int d\vec{r}_2 d\vec{r}_3 \cdots d\vec{r}_N |\Psi(\vec{r}, \vec{r}_2, \vec{r}_3, \ldots, \vec{r}_N)|^2 = \langle \Psi | \hat{n}(\vec{r}) | \Psi \rangle \overset{\text{def}}{=} \langle \Psi | \hat{\psi}^\dagger_\sigma \psi_\sigma | \Psi \rangle$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Principle of DFT $\exists$ functional $E[n]$ min of $E(n) = E_0$ g.s. energy

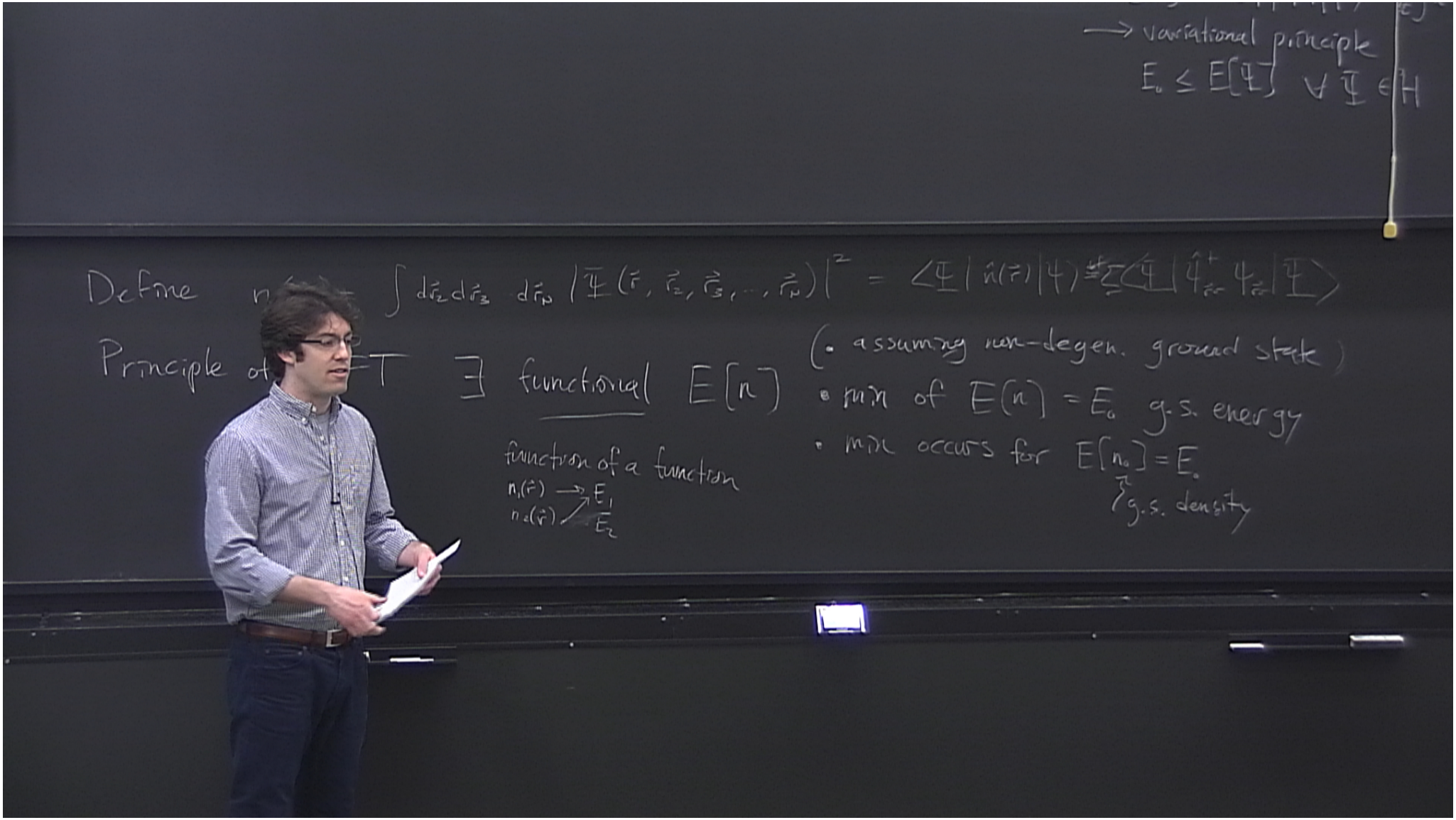
→ variational principle

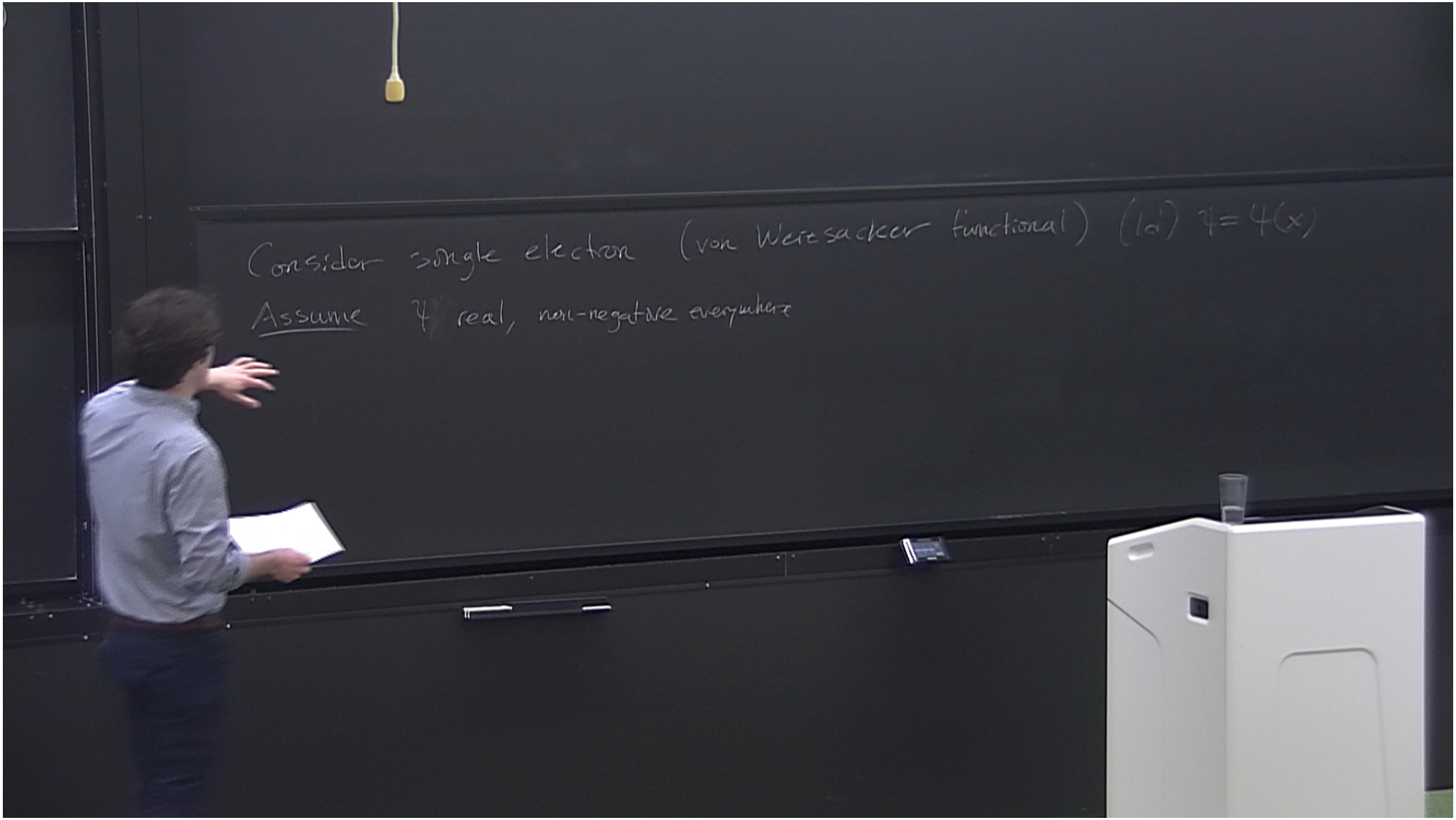
$E_0 \leq E[\Psi] \quad \forall \Psi \in \mathcal{H}$

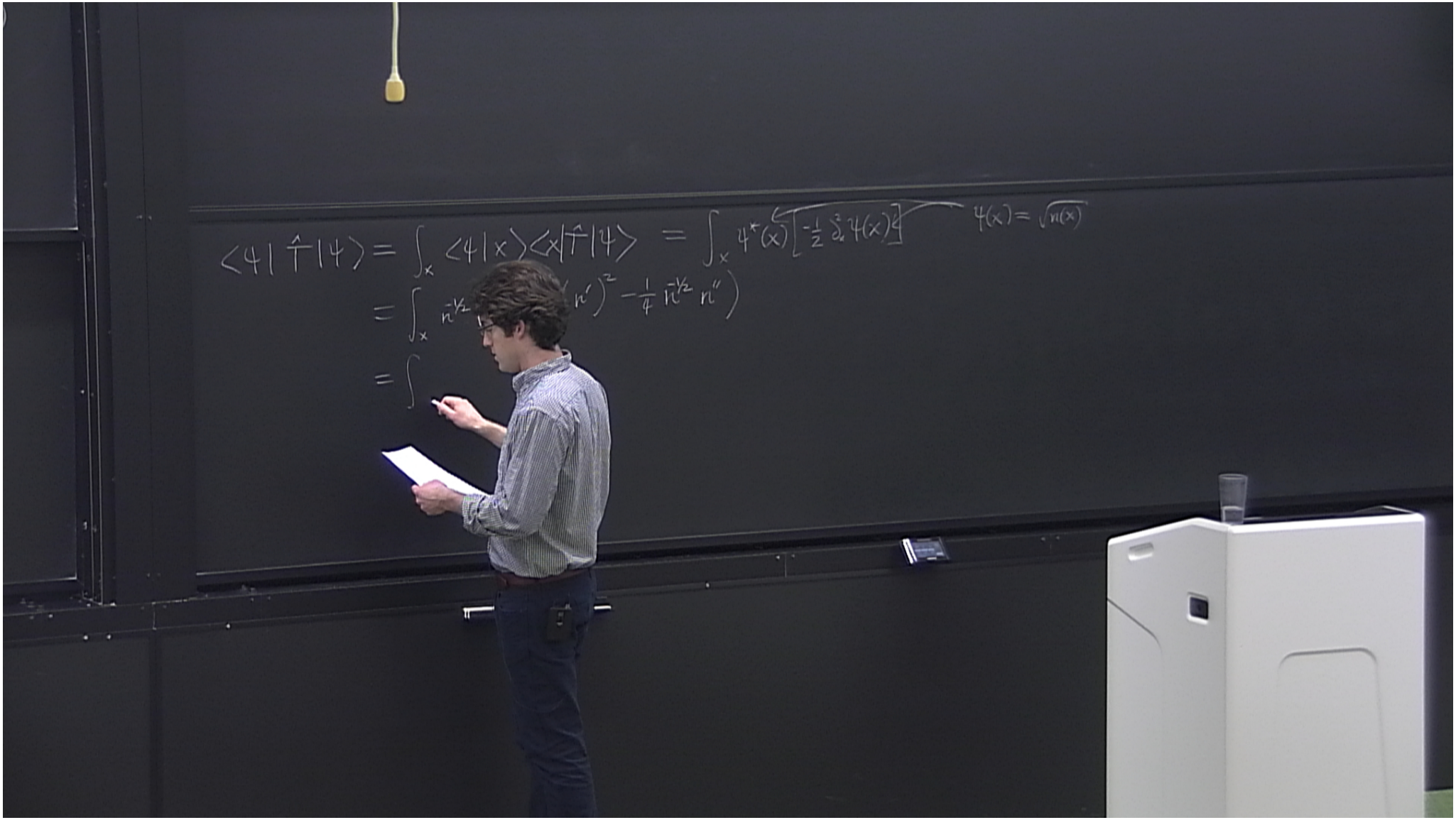
Define $n(\vec{r}) = \int d\vec{r}_2 d\vec{r}_3 \ldots d\vec{r}_N \, |\Psi(\vec{r}, \vec{r}_2, \vec{r}_3, \ldots, \vec{r}_N)|^2 = \langle \Psi | \hat{n}(\vec{r}) | \Psi \rangle = \sum \langle \Psi | \hat{\psi}^\dagger_{\vec{r}\sigma} \psi_{\vec{r}\sigma} | \Psi \rangle$

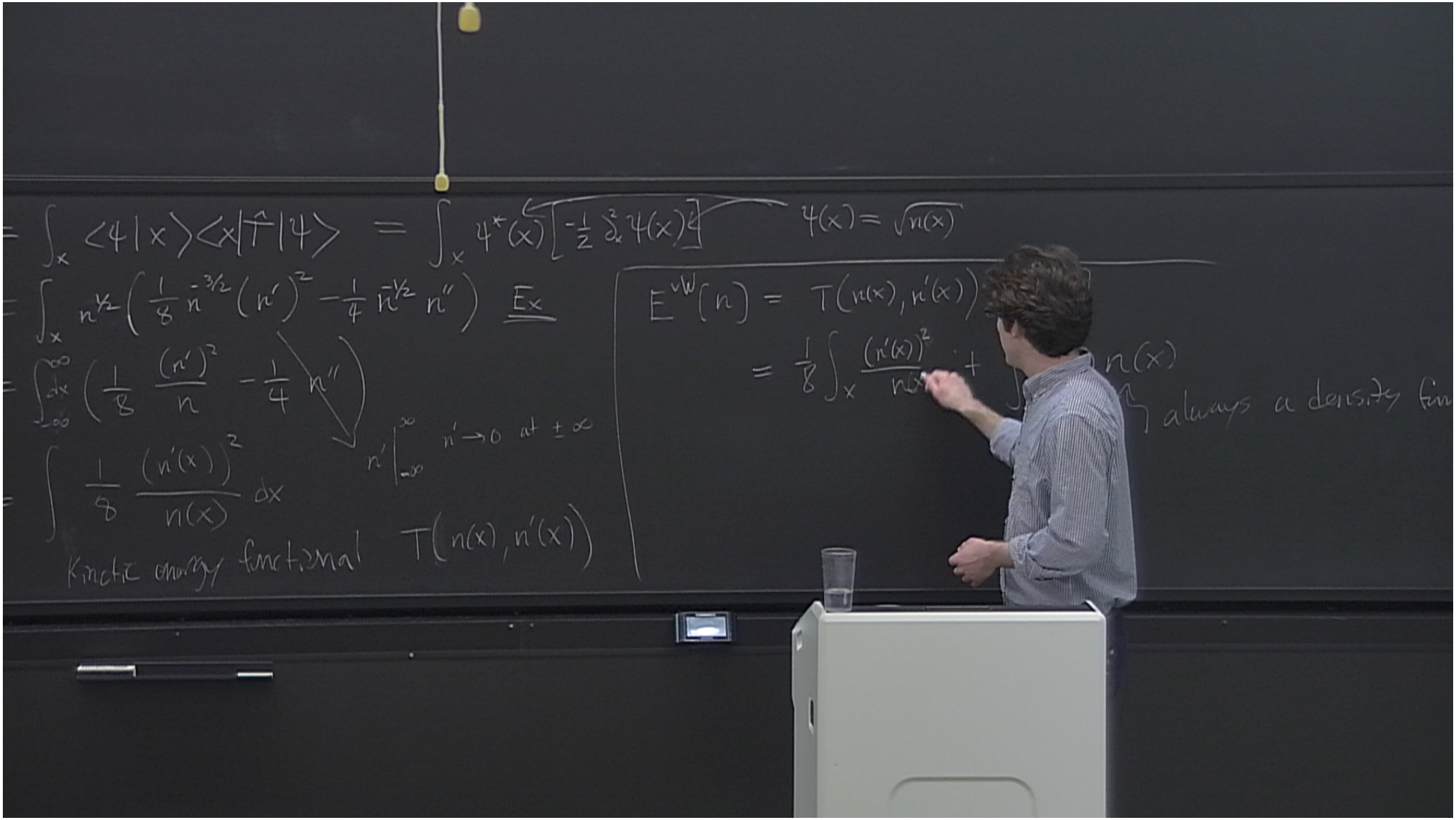
Principle of DFT $\exists$ functional $E[n]$ (• assuming non-degen. ground state)

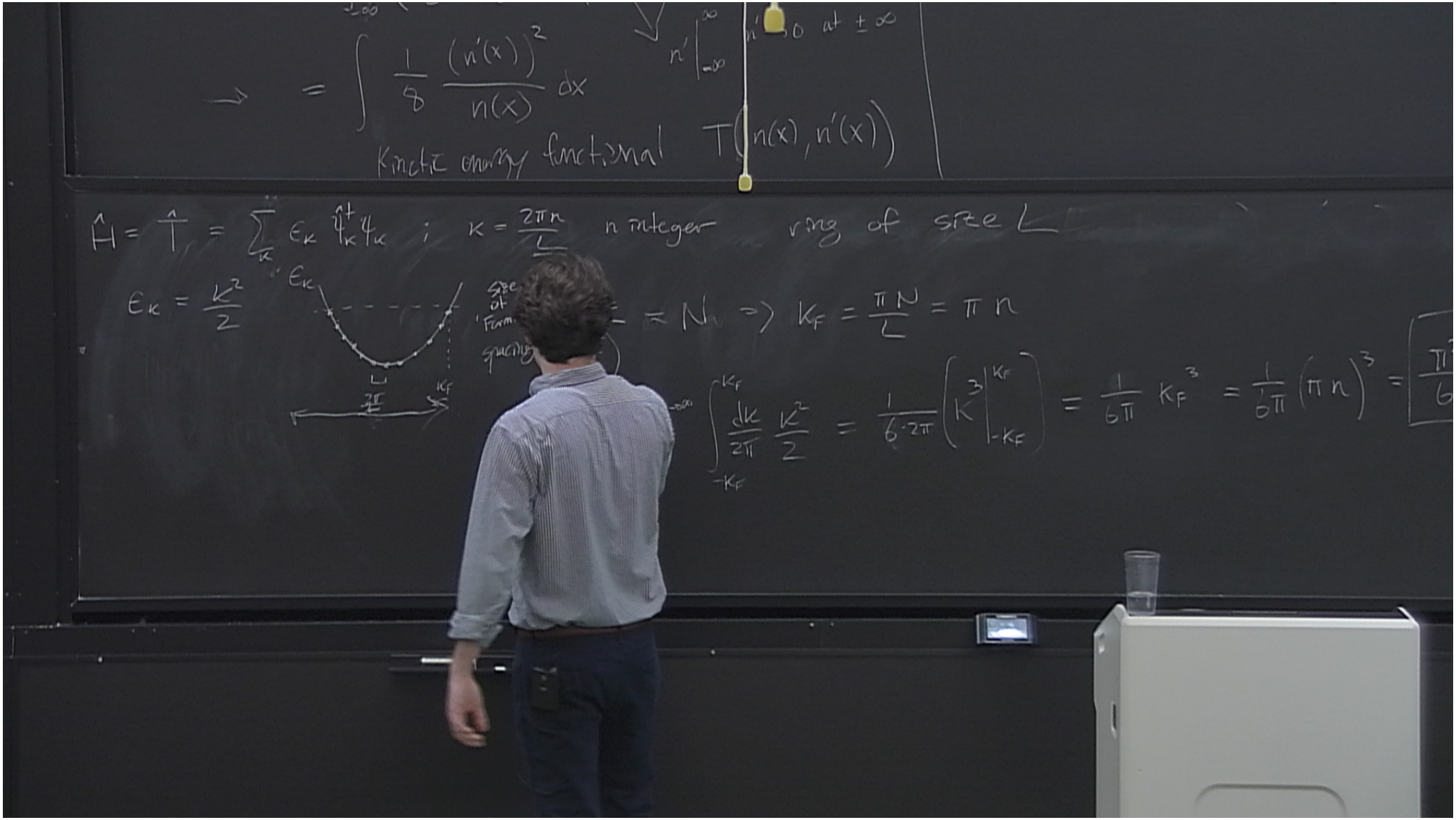
- min of $E(n) = E_0$ g.s. energy
- min occurs for $E[n_0] = E_0$, n_0 g.s. density

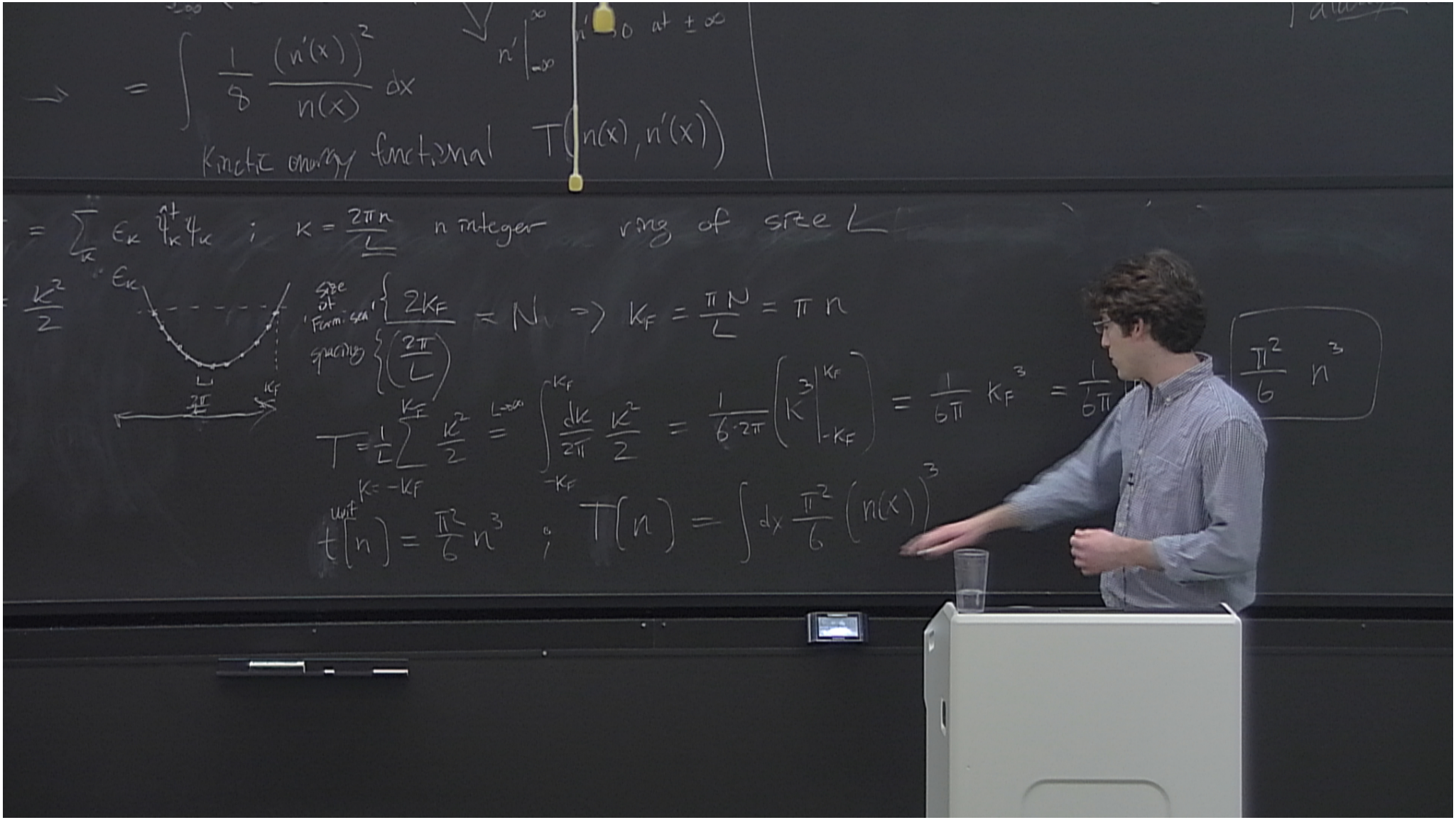

→ variational principle
$E_0 \leq E[\Psi] \quad \forall \Psi \in \mathcal{H}$
Define $n(\vec{r}) = \int d\vec{r}_2 d\vec{r}_3 \ldots d\vec{r}_N |\Psi(\vec{r}, \vec{r}_2, \vec{r}_3, \ldots, \vec{r}_N)|^2 = \langle \Psi | \hat{n}(\vec{r}) | \Psi \rangle = \sum \langle \Psi | \hat{\psi}^\dagger_{\sigma r} \hat{\psi}_{\sigma r} | \Psi \rangle$
Principle of ET $\exists$ functional $E[n]$
(• assuming non-degen. ground state)
• min of $E(n) = E_0$ g.s. energy
• min occurs for $E[n_0] = E_0$
n_0 g.s. density
function of a function
$n_1(\vec{r}) \rightarrow E_1$
$n_2(\vec{r}) \rightarrow E_2$

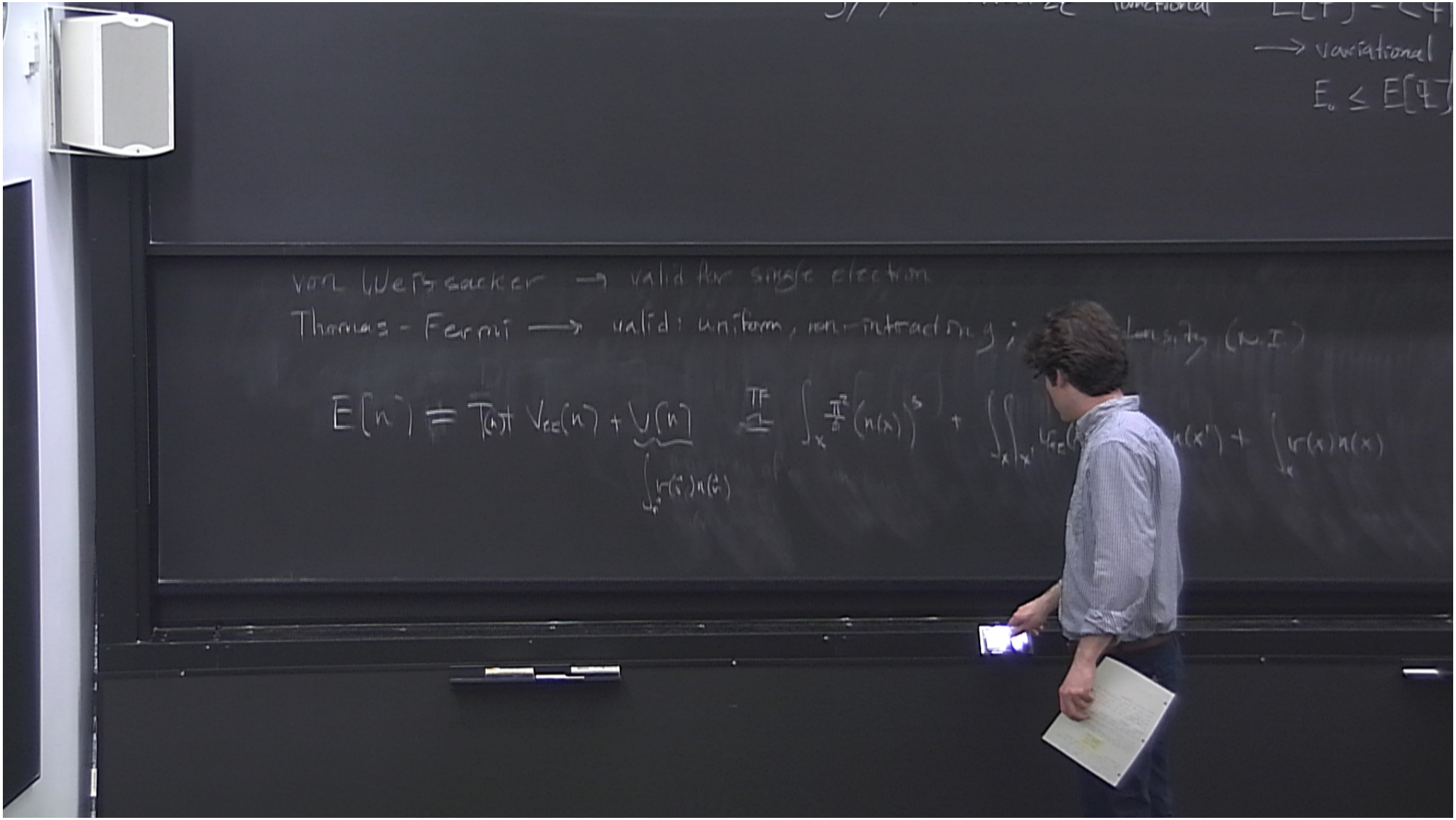

Consider single electron (von Weizsäcker functional) (1d) $\gamma = 4(x)$
Assume γ real, non-negative everywhere

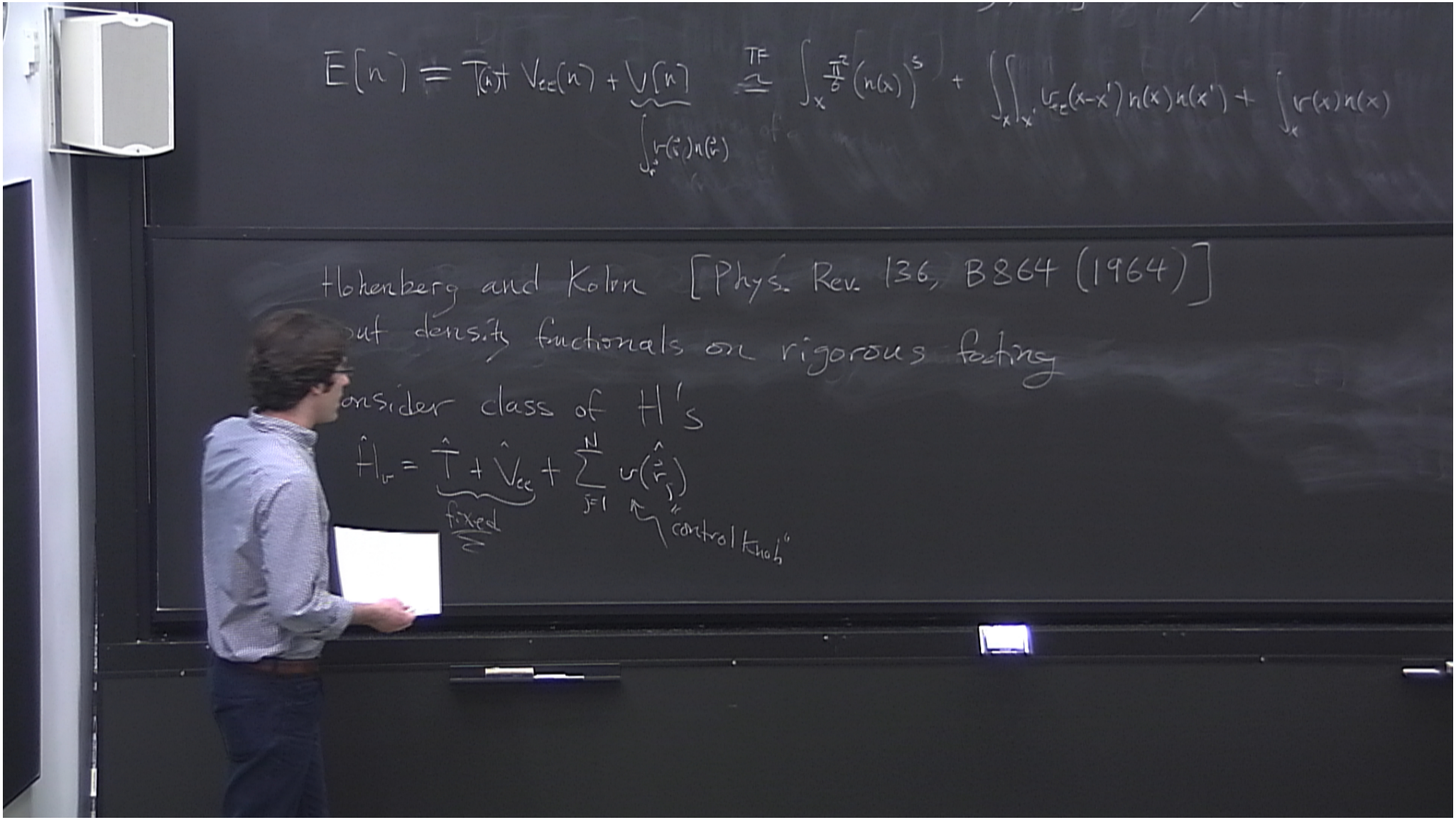

$\langle \psi | \hat{T} | \psi \rangle = \int_x \langle \psi | x \rangle \langle x | \hat{T} | \psi \rangle = \int_x \psi^*(x) \left[-\frac{1}{2} \partial_x^2 \psi(x) \right]$
$\psi(x) = \sqrt{n(x)}$


$= \int_x \langle \psi | x \rangle \langle x | \hat{T} | \psi \rangle = \int_x \psi^*(x) \left[-\frac{1}{2} \partial_x^2 \psi(x) \right]$
$\psi(x) = \sqrt{n(x)}$
$= \int_x n^{1/2} \left(\frac{1}{8} n^{-3/2} (n')^2 - \frac{1}{4} n^{-1/2} n'' \right)$ Ex
$= \int_{-\infty}^{\infty} dx \left(\frac{1}{8} \frac{(n')^2}{n} - \frac{1}{4} n'' \right)$
$n' \Big|_{-\infty}^{\infty}$ $n' \to 0$ at $\pm\infty$
$= \int \frac{1}{8} \frac{(n'(x))^2}{n(x)} dx$
Kinetic energy functional $T(n(x), n'(x))$
$E^{vW}(n) = T(n(x), n'(x))$
$= \frac{1}{8} \int_x \frac{(n'(x))^2}{n(x)}$ +
$n(x)$
always a density fun


$= \int \frac{1}{8} \frac{(n'(x))^2}{n(x)} dx$
$n' \Big|_{-\infty}^{\infty}$
$n' = 0$ at $\pm\infty$
Kinetic energy functional $T[n(x), n'(x)]$
$\hat{H} = \hat{T} = \sum_k \epsilon_k \hat{\psi}_k^\dagger \hat{\psi}_k$; $k = \frac{2\pi n}{L}$ n integer ring of size L
$\epsilon_k = \frac{k^2}{2}$
ϵ_k
k_F
$\frac{2\pi}{L}$
$= N \Rightarrow k_F = \frac{\pi N}{L} = \pi n$
$\int_{-k_F}^{k_F} \frac{dk}{2\pi} \frac{k^2}{2} = \frac{1}{6 \cdot 2\pi} \left(k^3 \Big|_{-k_F}^{k_F} \right) = \frac{1}{6\pi} k_F^3 = \frac{1}{6\pi} (\pi n)^3 =$


$= \int \frac{1}{8} \frac{(n'(x))^2}{n(x)} dx$
$n' \Big|_{-\infty}^{\infty}$
$n' \to 0$ at $\pm\infty$
Kinetic energy functional $T(n(x), n'(x))$
$= \sum_k \epsilon_k \hat{\psi}_k^\dagger \psi_k$; $k = \frac{2\pi n}{L}$ n integer ring of size L
$\frac{k^2}{2}$
ϵ_k
$-k_F$ k_F $\frac{2\pi}{L}$
size of Fermi sea $\begin{cases} 2k_F \\ \text{spacing} \left(\frac{2\pi}{L}\right) \end{cases} = N \Rightarrow k_F = \frac{\pi N}{L} = \pi n$
$T = \frac{1}{L} \sum_{k=-k_F}^{k_F} \frac{k^2}{2} \xrightarrow{L\to\infty} \int_{-k_F}^{k_F} \frac{dk}{2\pi} \frac{k^2}{2} = \frac{1}{6\cdot 2\pi} \left(k^3 \Big|_{-k_F}^{k_F} \right) = \frac{1}{6\pi} k_F^3 = \frac{1}{6\pi}$
$\frac{\pi^2}{6} n^3$
Unit $t(n) = \frac{\pi^2}{6} n^3$; $T(n) = \int dx \frac{\pi^2}{6} (n(x))^3$


→ variational
von Weizsäcker → valid for single electron
Thomas - Fermi → valid: uniform, non-interacting;
$E[n] = T[n] + V_{ee}(n) + V[n] \overset{TF}{=} \int_x \frac{3}{10}(3\pi^2)^{2/3} n(x)^{5/3} + \iint_{x,x'} \ldots + \int_x v(x) n(x)$


$E[n] = T[n] + V_{ee}[n] + \int v(\vec{r})n(\vec{r})$
TF
$\frac{3}{10}(3\pi^2)^{2/3}\int n(x)^{5/3} + \iint v_{ee}(x-x')n(x)n(x') + \int v(x)n(x)$
Hohenberg and Kohn [Phys. Rev. 136, B864 (1964)]
out density functionals on rigorous footing
onsider class of H's
$\hat{H}_v = \hat{T} + \hat{V}_{ee} + \sum_{j=1}^{N} v(\hat{r}_j)$
fixed
control knob

uniform, non-interacting; high density (N.I.)

$$E[n] = T[n] + V_{ee}[n] + \underbrace{V[n]}_{\int_r v(\vec{r})n(\vec{r})} \overset{TF}{\approx} \int_x \frac{\hbar^2}{6}\left(n(x)\right)^3 + \iint_x v_{ee}(x-x')n(x)n(x') + \int_x v(x)n(x)$$

Hohenberg and Kohn [Phys. Rev. 136, B864 (1964)]
put density functionals on rigorous footing

Consider class of H's

$$\hat{H}_v = \underbrace{\hat{T} + \hat{V}_{ee}}_{\text{fixed}} + \int_r v(\vec{r})\hat{n}(\vec{r})$$

"control knob"

Typically $\hat{T} = -\frac{1}{2}\sum_{i=1}^{N}\nabla^2$

$\hat{V}_{ee} = \frac{1}{2}\sum_{i\neq j}\frac{1}{|\vec{r}_i - \vec{r}_j|}$

HK showed:
two H's $\hat{H}_v$, $\hat{H}_{v'}$ (H, H')
- assuming each has non-degen. ground state
- ground states ψ, ψ' same density

$\Rightarrow$ v, v' differ by const shift

$v(\vec{r}) = v'(\vec{r}) + C$