Title: Explorations in Condensed Matter-4

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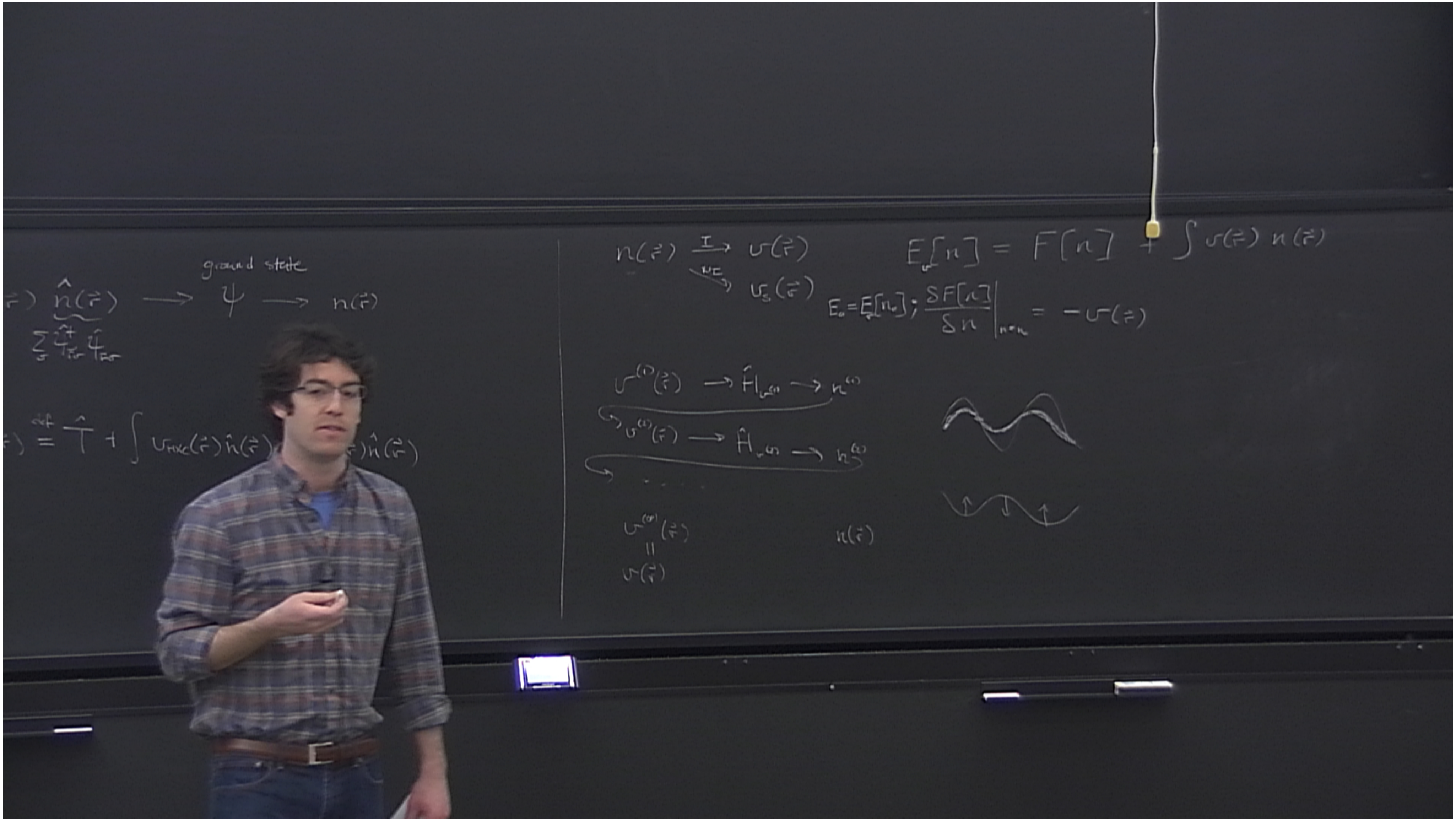
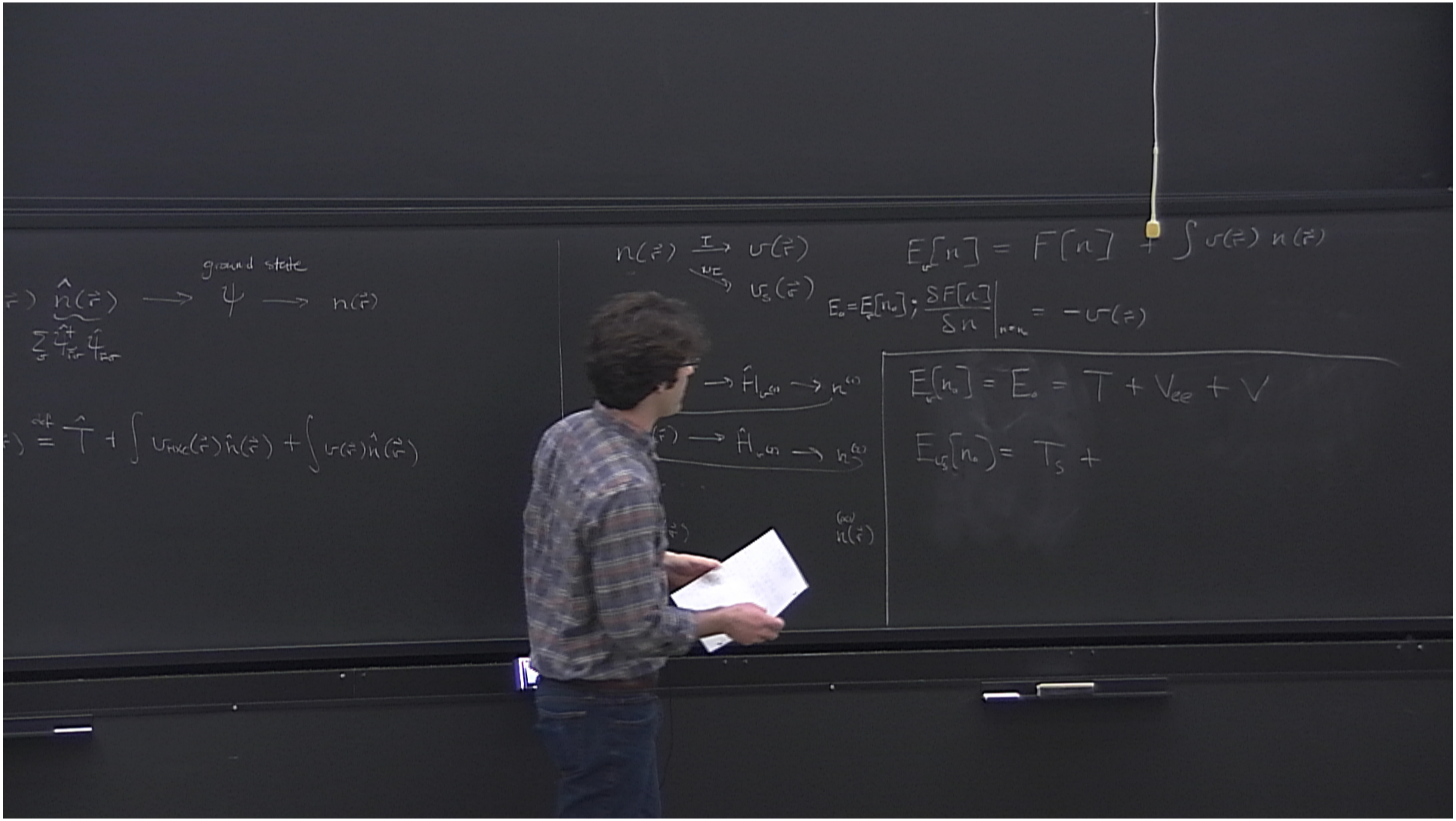
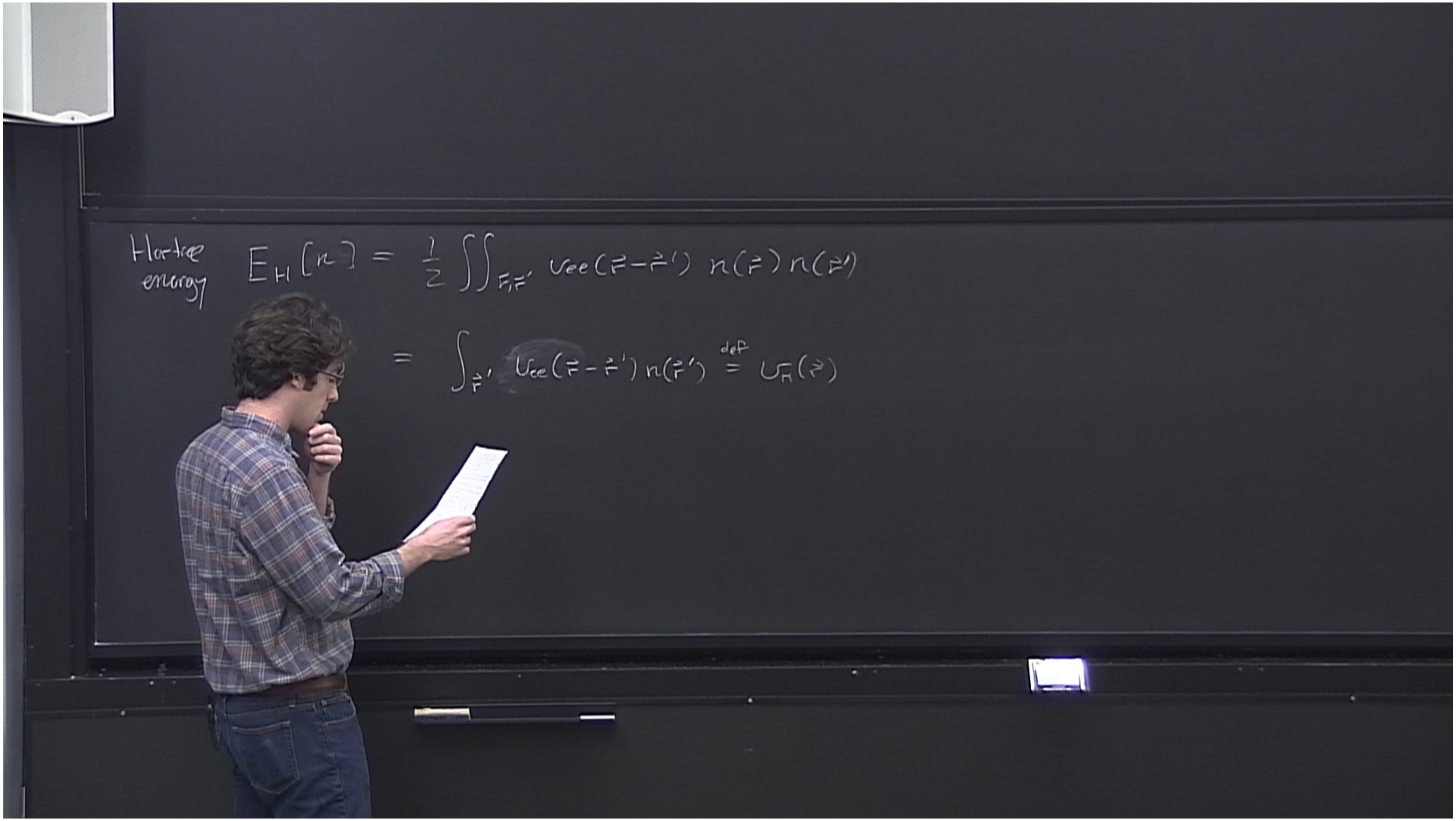
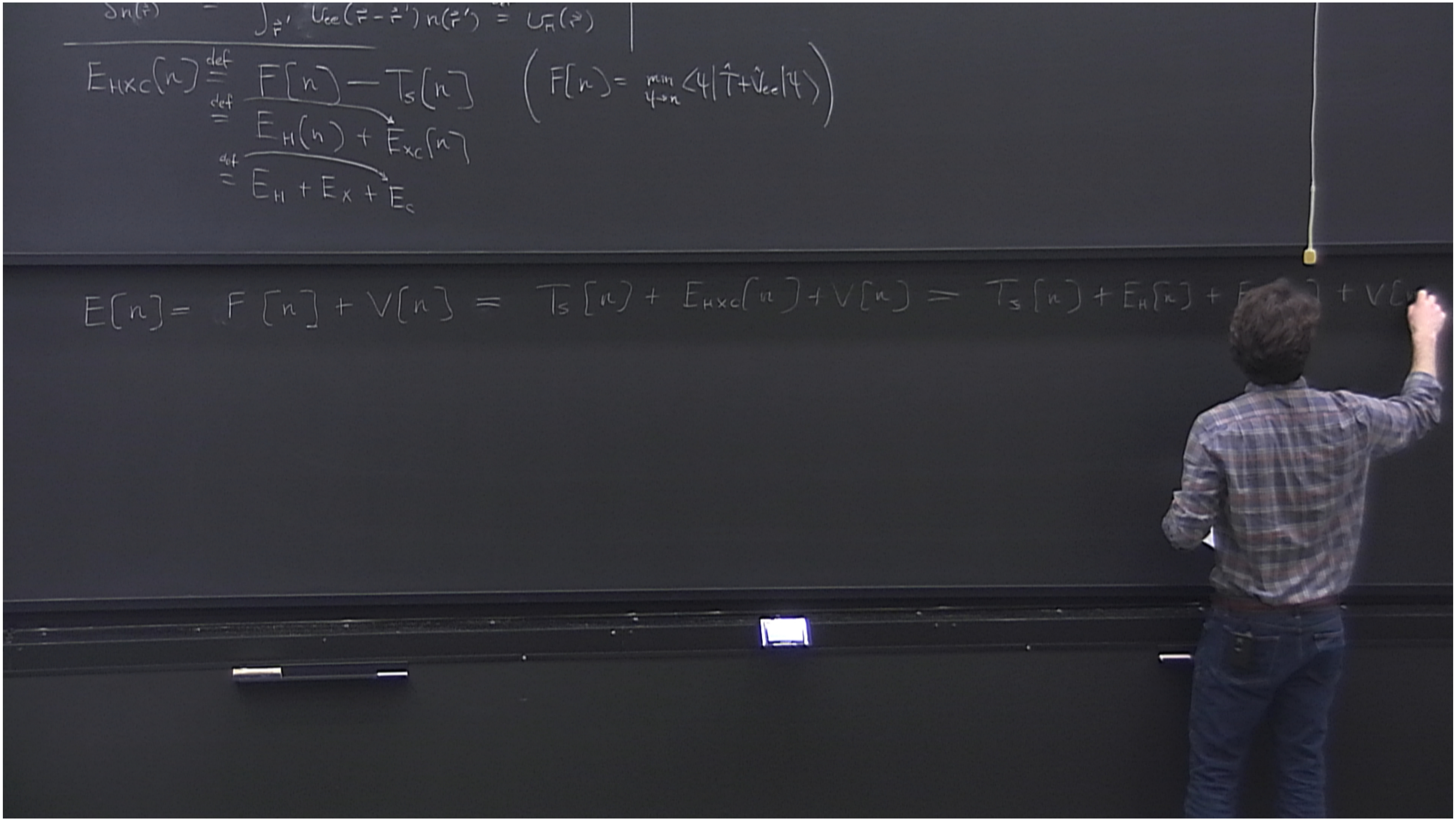
URL: http://pirsa.org/15030037

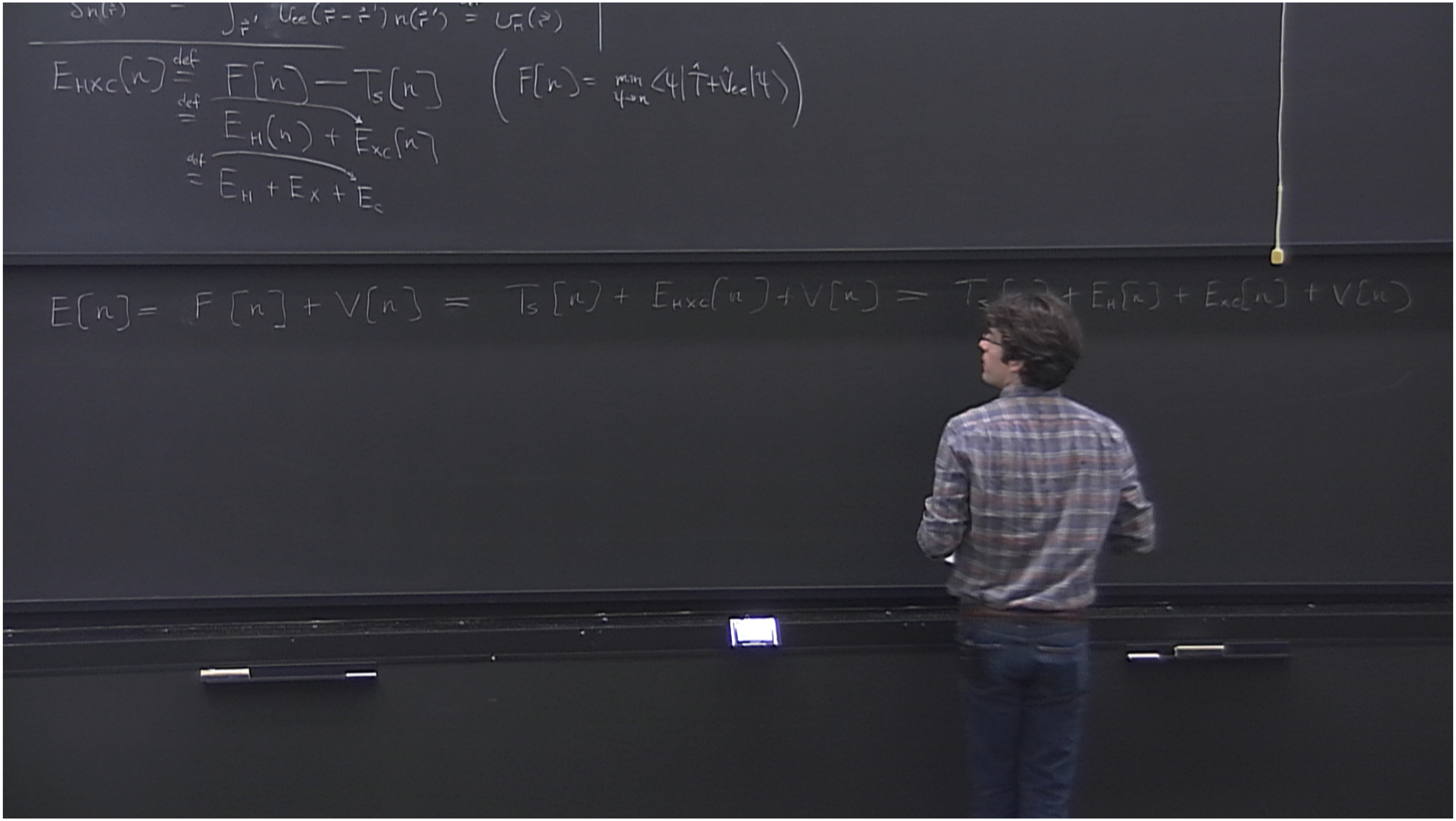
Abstract:


ground state
E[n] = F[n] + ∫ v(r) n(r)

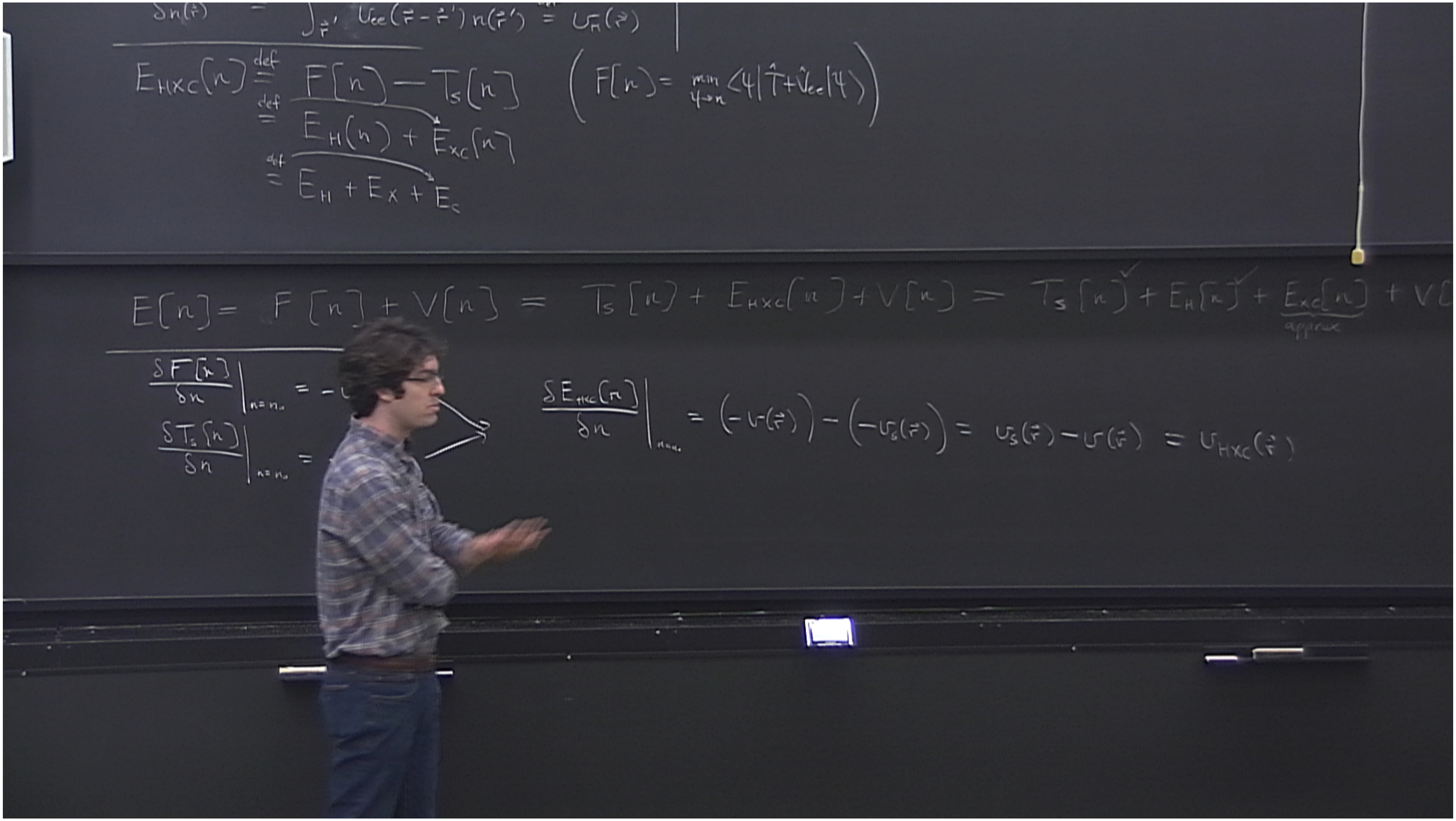

ground state
n(r) → v(r)
v_s(r)
E_v[n] = F[n] + ∫ v(r) n(r)
E_v[n_0] = E_0 = T + V_ee + V
E_KS[n_0] = T_s +

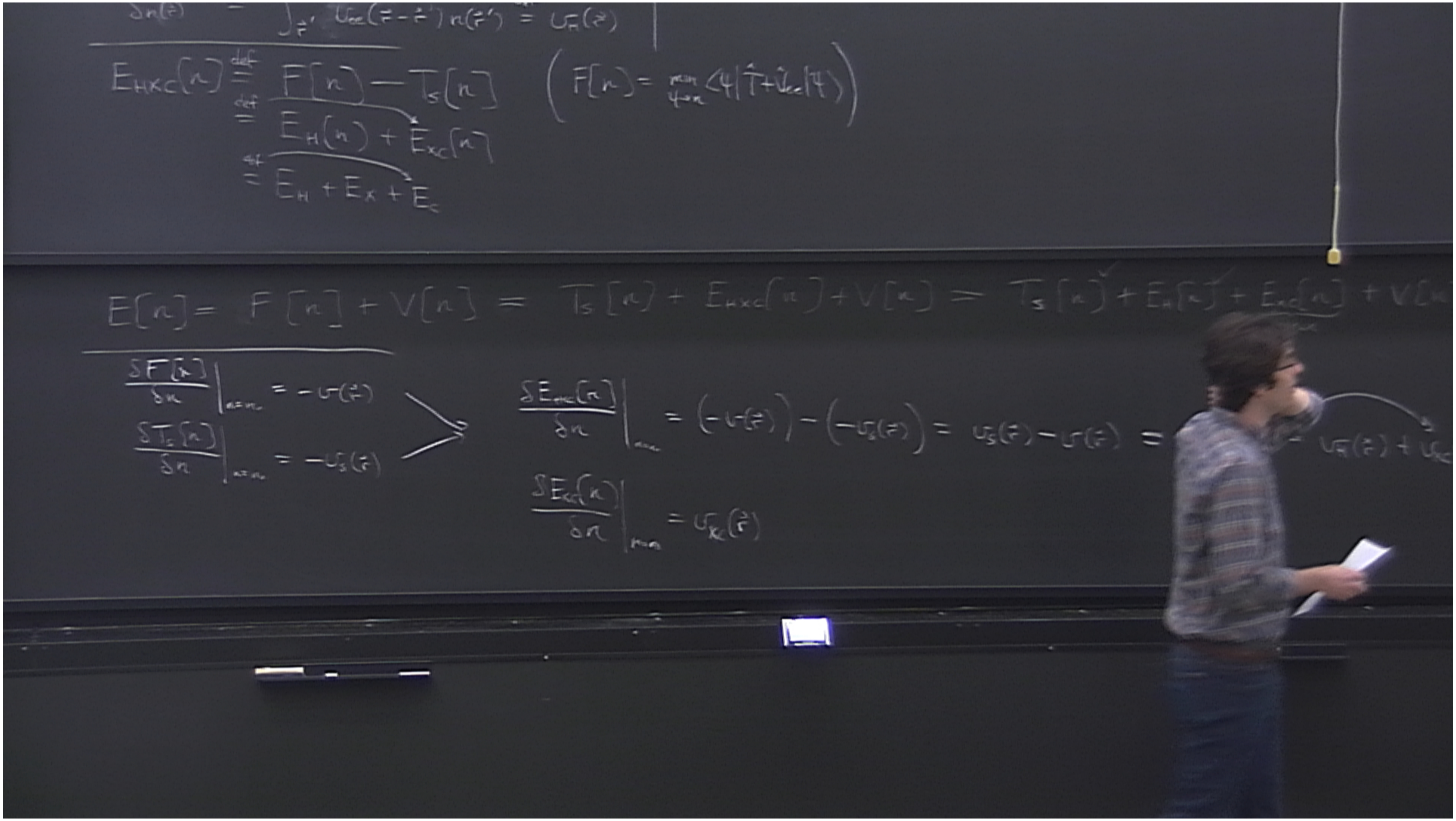

Hartree energy
$E_H[n] = \frac{1}{2} \iint_{\vec{r},\vec{r}'} v_{ee}(\vec{r}-\vec{r}')\, n(\vec{r})\, n(\vec{r}')$
$= \int_{\vec{r}'} v_{ee}(\vec{r}-\vec{r}')\, n(\vec{r}') \overset{def}{=} v_H(\vec{r})$


$\delta n(\vec r) = \int_{\vec r'} v_{ee}(\vec r - \vec r')\, n(\vec r') = v_H(\vec r)$
$E_{Hxc}[n] \overset{def}{=} F[n] - T_s[n]$ $\left(F[n] = \min_{\Psi \to n} \langle \Psi | \hat T + \hat V_{ee} | \Psi \rangle \right)$
$\overset{def}{=} E_H[n] + E_{xc}[n]$
$\overset{def}{=} E_H + E_x + E_c$
$E[n] = F[n] + V[n] = T_s[n] + E_{Hxc}[n] + V[n] = T_s[n] + E_H[n] +$



δn(r) = ∫r' vee(r − r') n(r') = vH(r)
EHxc[n] ≝ F[n] − Ts[n]
(F[n] = min ψ→n ⟨ψ|T̂ + V̂ee|ψ⟩)
≝ EH[n] + Exc[n]
≝ EH + Ex + Ec
E[n] = F[n] + V[n] = Ts[n] + EHxc[n] + V[n] = Ts[n] + EH[n] + Exc[n] + V[n]


$\int_{\vec r'} v_{ee}(\vec r - \vec r')\, n(\vec r') = v_H(\vec r)$
$E_{HXC}[n] \overset{def}{=} F[n] - T_s[n]$
$\overset{def}{=} E_H[n] + E_{XC}[n]$
$\overset{def}{=} E_H + E_X + E_C$
$\left(F[n] = \min_{\Psi \to n} \langle \Psi | \hat T + \hat V_{ee} | \Psi \rangle \right)$
$E[n] = F[n] + V[n] = T_s[n] + E_{HXC}[n] + V[n] = T_s[n] + E_H[n] + \underbrace{E_{XC}[n]}_{approx} + V[$
$\left.\frac{\delta F[n]}{\delta n}\right|_{n=n_0} = -$
$\left.\frac{\delta T_s[n]}{\delta n}\right|_{n=n_0} =$
$\left.\frac{\delta E_{HXC}[n]}{\delta n}\right|_{n=n_0} = (-v(\vec r)) - (-v_s(\vec r)) = v_s(\vec r) - v(\vec r) = v_{HXC}(\vec r)$


$\int_{\vec r'} v_{ee}(\vec r - \vec r')\, n(\vec r') = v_H(\vec r)$
$E_{Hxc}[n] \stackrel{def}{=} F[n] - T_s[n] \quad \left(F[n] = \min_{\Psi \to n} \langle \Psi | \hat T + \hat V_{ee} | \Psi \rangle \right)$
$\stackrel{def}{=} E_H[n] + E_{xc}[n]$
$\stackrel{def}{=} E_H + E_x + E_c$
$E[n] = F[n] + V[n] = T_s[n] + E_{Hxc}[n] + V[n] = T_s[n] + E_H[n] + E_{xc}[n] + V[n]$
$\left.\frac{\delta F[n]}{\delta n}\right|_{n=n_0} = -v(\vec r)$
$\left.\frac{\delta T_s[n]}{\delta n}\right|_{n=n_0} = -v_s(\vec r)$
$\left.\frac{\delta E_{Hxc}[n]}{\delta n}\right|_{n=n_0} = (-v(\vec r)) - (-v_s(\vec r)) = v_s(\vec r) - v(\vec r) = v_H(\vec r) + v_{xc}$
$\left.\frac{\delta E_{xc}[n]}{\delta n}\right|_{n=n_0} = v_{xc}(\vec r)$

$$\int d\vec r' \, v_{ee}(\vec r - \vec r')\, n(\vec r') = v_H(\vec r)$$

$$F[n] - T_s[n] \qquad \left(F[n] = \min_{\psi \to n} \langle \psi | \hat T + \hat V_{ee} | \psi \rangle \right)$$

$$E_H(n) + E_{xc}[n]$$

$$E_H + E_x + E_c$$

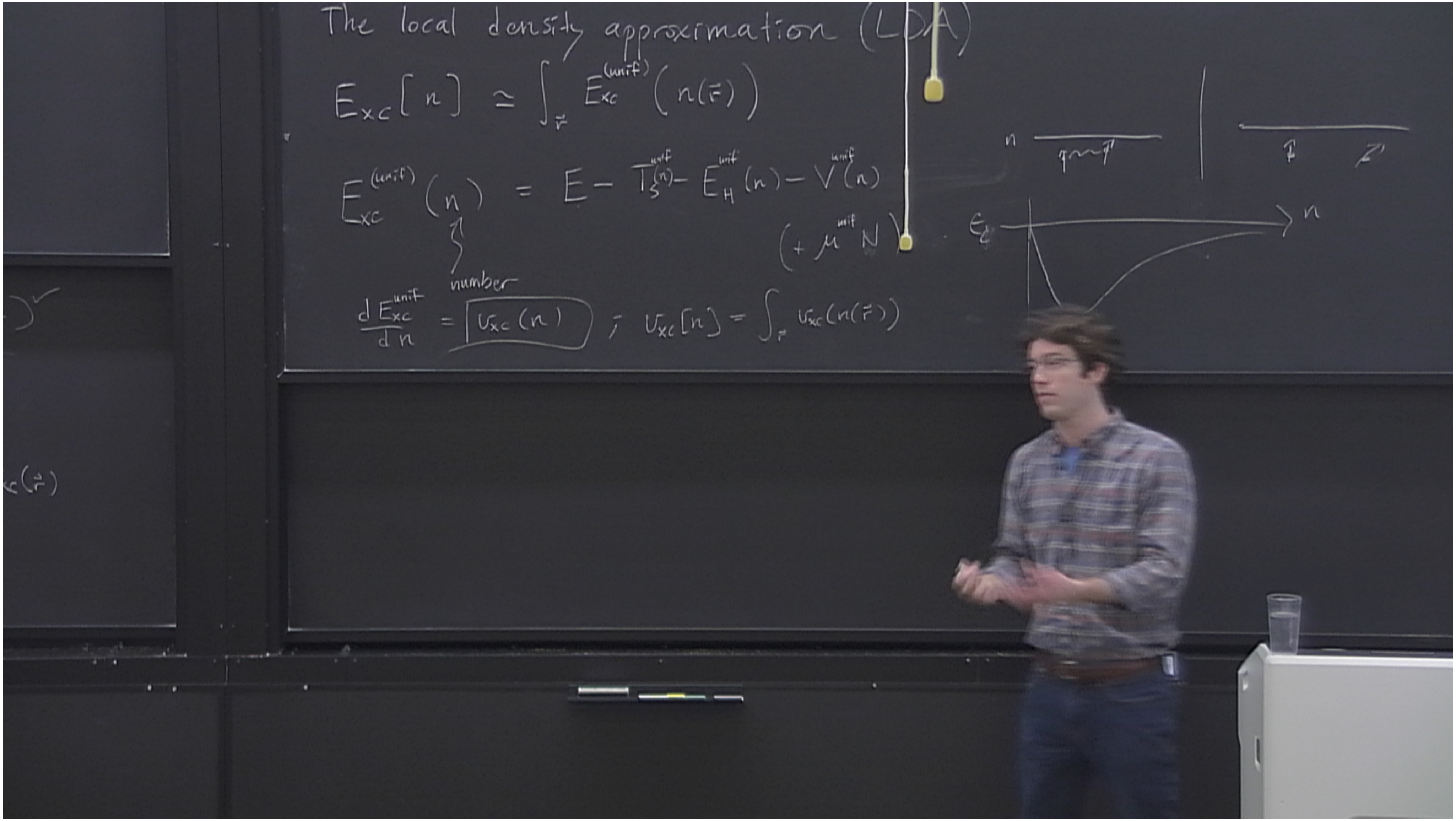
$$F[n] + V[n] = T_s[n] + E_{Hxc}[n] + V[n] = T_s[n] + E_H[n] + \underbrace{E_{xc}[n]}_{\text{approx}} + V[n]$$

$$= -v(\vec r)$$

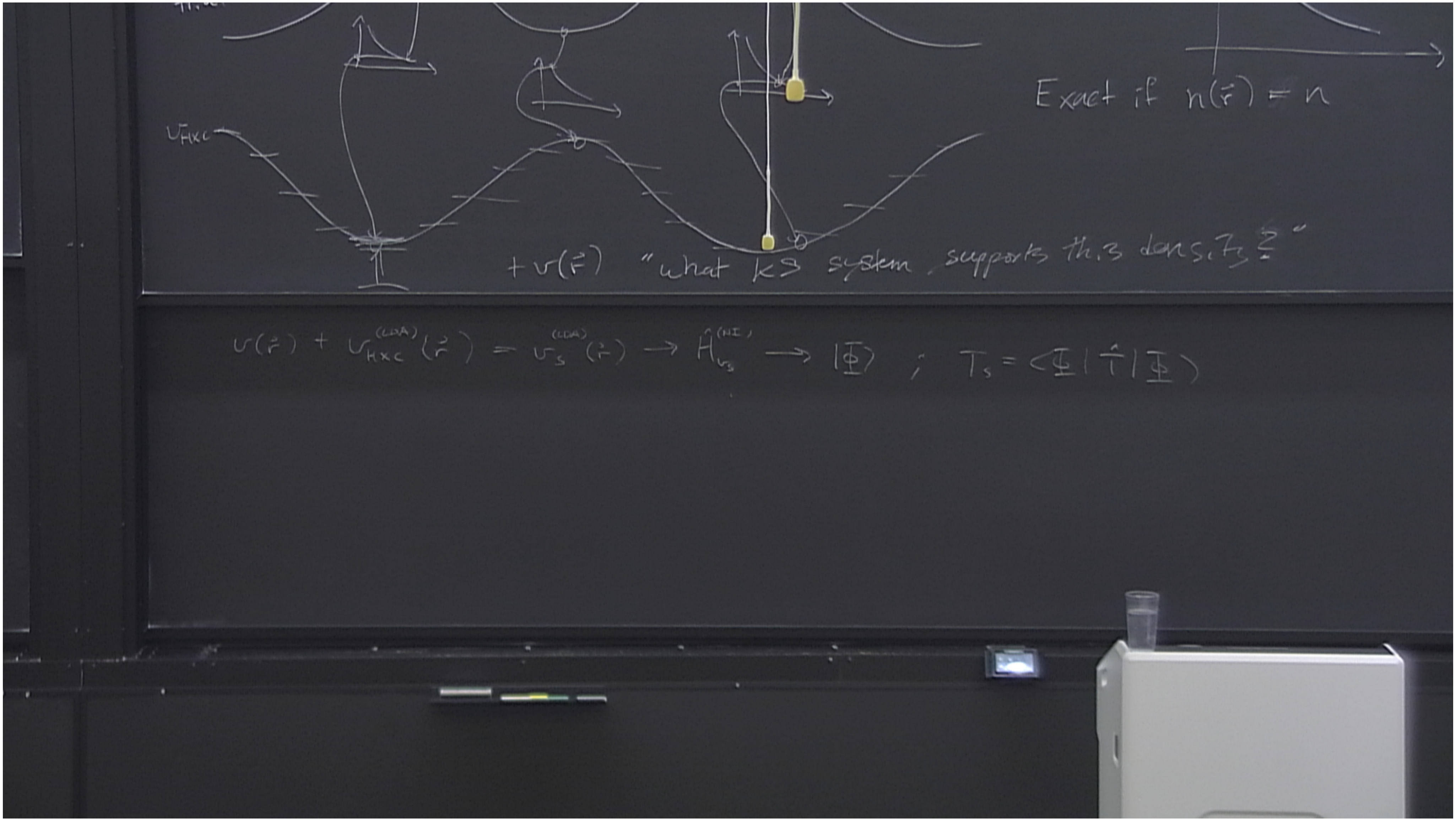
$$= -v_s(\vec r)$$

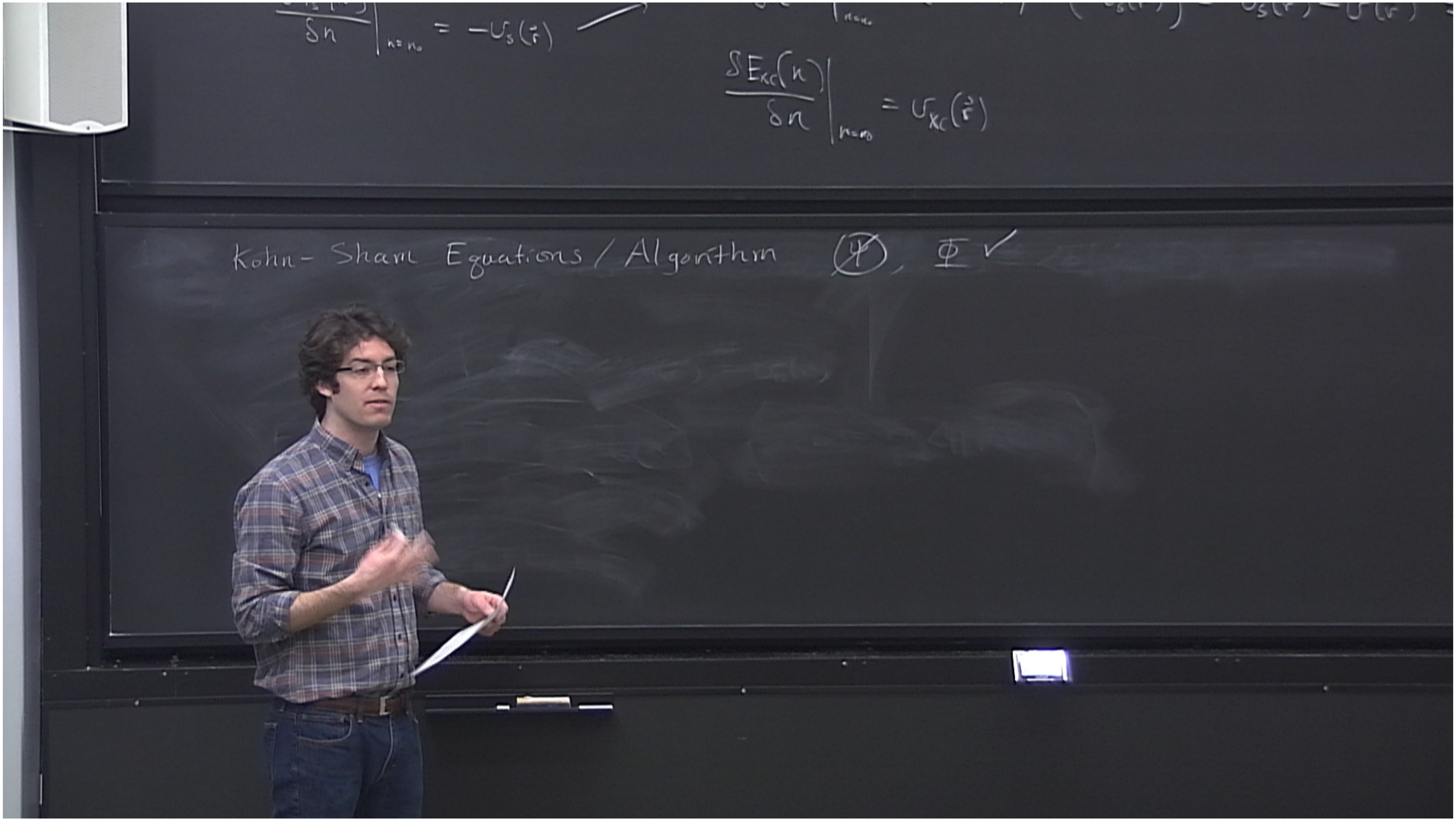
$$\left.\frac{\delta E_{Hxc}[n]}{\delta n}\right|_{n=n_0} = \left(-v(\vec r)\right) - \left(-v_s(\vec r)\right) = v_s(\vec r) - v(\vec r) = v_{Hxc}(\vec r) \overset{\text{def}}{=} v_H(\vec r) + v_{xc}(\vec r)$$

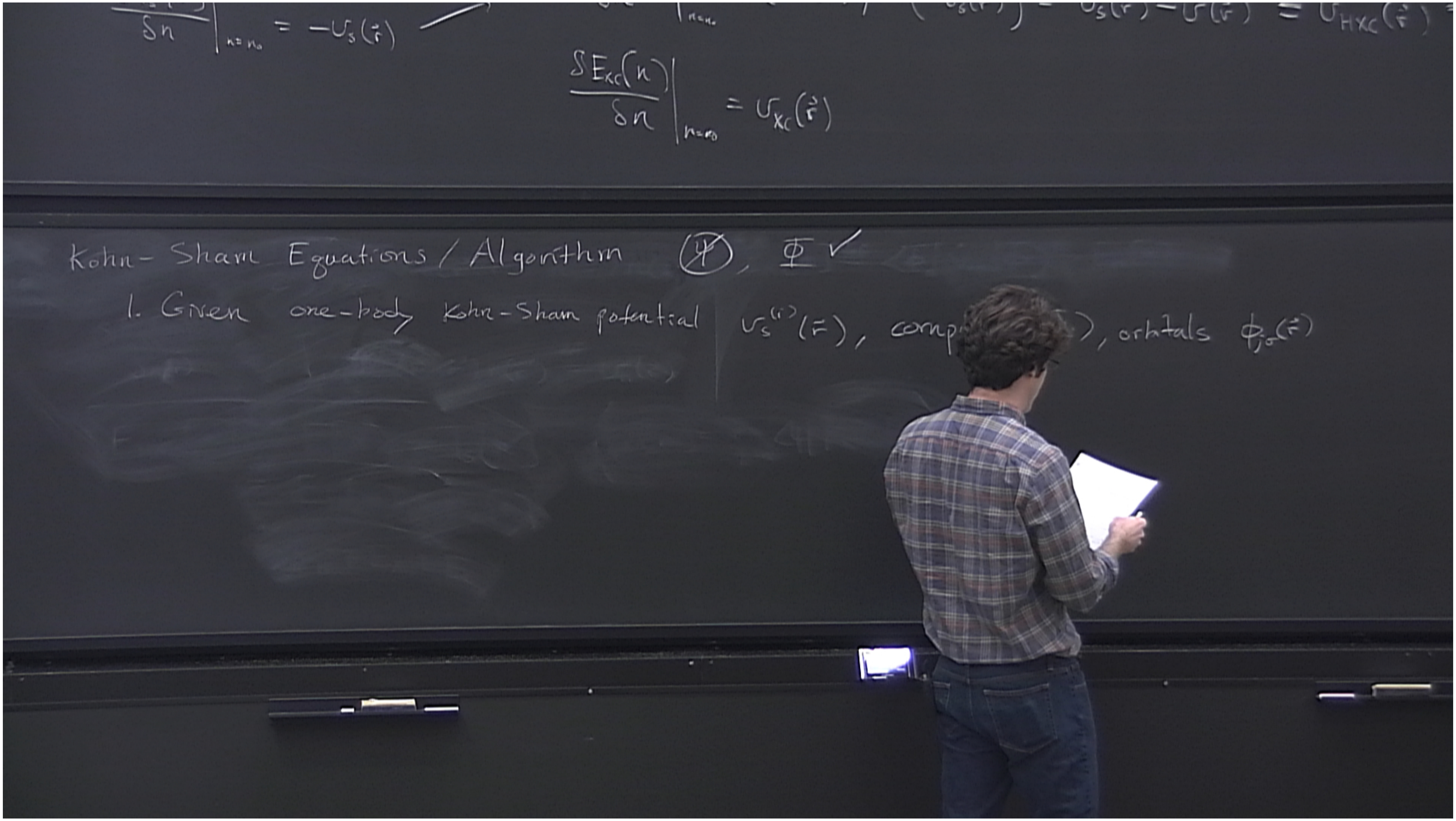
$$\left.\frac{\delta E_{xc}[n]}{\delta n}\right|_{n=n_0} = v_{xc}(\vec r)$$

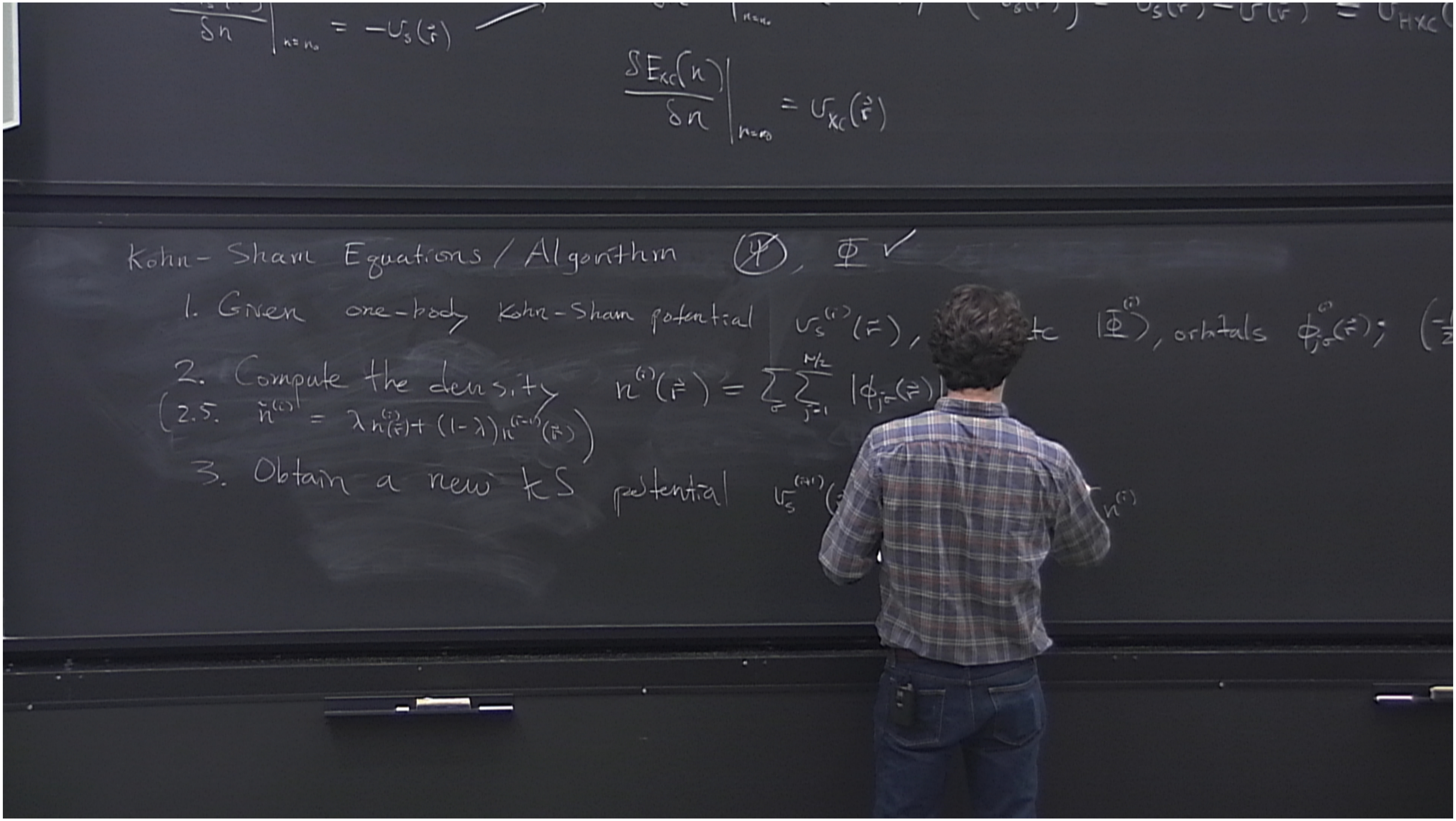

The local density approximation (LDA)
Exc[n] ≃ ∫r Exc(unif)(n(r))
Exc(unif)(n) = E − Ts unif(n) − EH unif(n) − V unif(n)
(+ μ unif N)
number
d Exc unif / dn = Vxc(n) ; Vxc[n] = ∫r Vxc(n(r))
n
εc
n

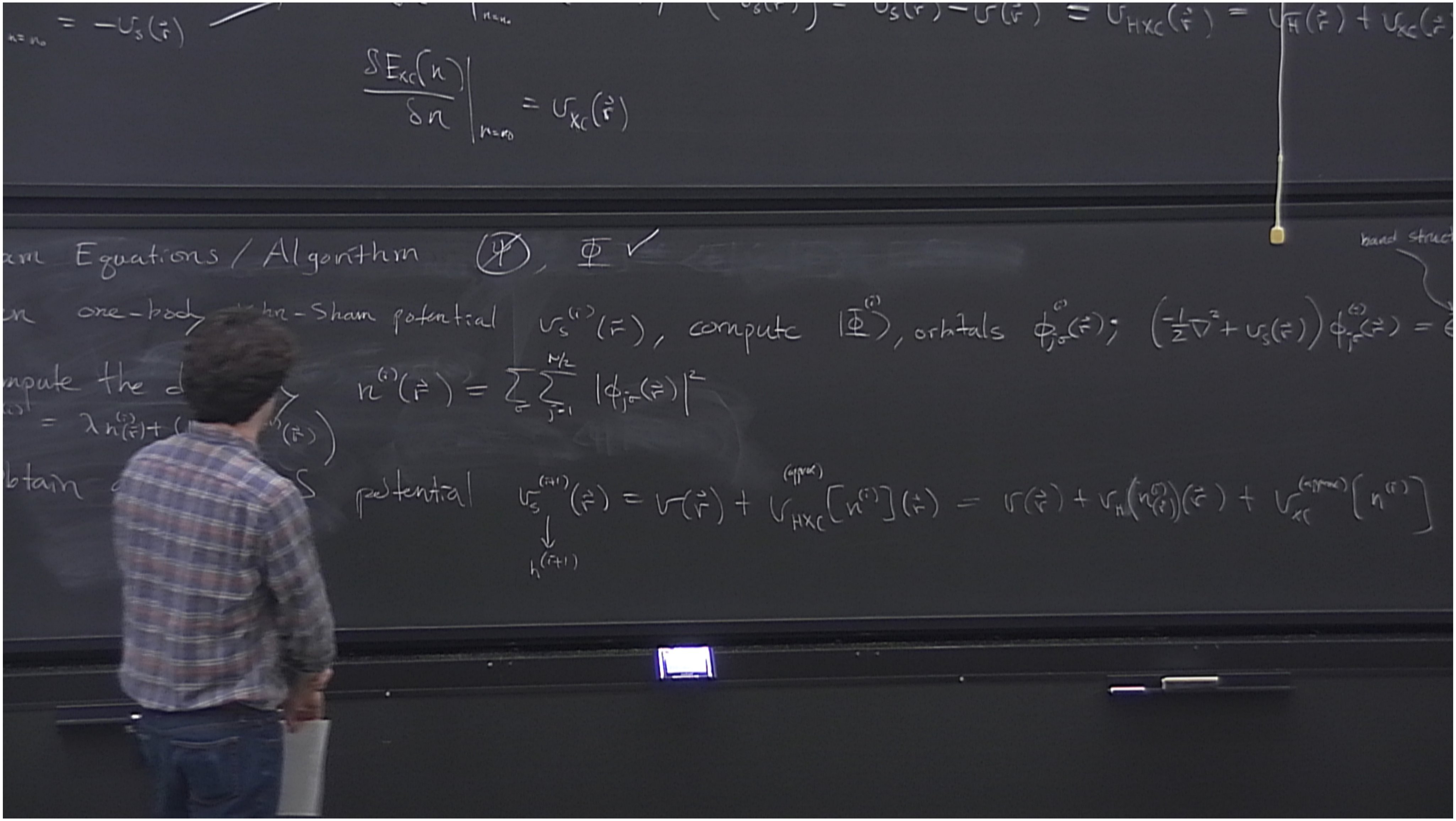

number
propose


v_HXC
Exact if n(r) = n
+ v(r) "what KS system supports this density?"
v(r) + v_HXC^(LDA)(r) = v_s^(LDA)(r) → Ĥ^(NI)_{v_s} → |Φ⟩ ; T_s = ⟨Φ| T̂ |Φ⟩


= −v_s(r)
δE_xc(n)/δn |_{n=n_0} = v_xc(r)
Kohn-Sham Equations / Algorithm


δE_xc(n)/δn |_{n=n_0} = v_xc(r)
Kohn-Sham Equations / Algorithm Ψ, Φ
1. Given one-body Kohn-Sham potential v_s^(i)(r), orbitals φ_jσ(r)


δE_xc(n)/δn |_{n=n₀} = v_xc(r)
Kohn-Sham Equations / Algorithm
1. Given one-body Kohn-Sham potential v_s^(i)(r),
orbitals φ_jσ^(i)(r);
2. Compute the density n^(i)(r) = Σ_σ Σ_{j=1}^{N/2} |φ_jσ(r)|
(2.5. ñ^(i) = λ n^(i)(r) + (1-λ) n^(i-1)(r))
3. Obtain a new KS potential v_s^(i+1)(


$= -v_s(\vec r)$
$= v_{HXC}(\vec r) = v_H(\vec r) + v_{xc}(\vec r)$
$\frac{\delta E_{xc}(n)}{\delta n}\Big|_{n=n_0} = v_{xc}(\vec r)$
Equations / Algorithm
band struct
one-body Kohn-Sham potential $v_s^{(i)}(\vec r)$, compute $|\Phi^{(i)}\rangle$, orbitals $\phi_{j\sigma}^{(i)}(\vec r)$; $\left(-\frac{1}{2}\nabla^2 + v_s(\vec r)\right)\phi_{j\sigma}^{(i)}(\vec r) =$
$n^{(i)}(\vec r) = \sum_\sigma \sum_{j=1}^{N/2} |\phi_{j\sigma}(\vec r)|^2$
potential $v_s^{(i+1)}(\vec r) = v(\vec r) + v_{HXC}^{(approx)}[n^{(i)}](\vec r) = v(\vec r) + v_H(n^{(i)}(\vec r))(\vec r) + v_{xc}^{(approx)}[n^{(i)}]$
$h^{(i+1)}$

$$\left.\frac{\delta}{\delta n}\right|_{n=n_0} = -v_s(\vec{r}) \qquad \left. \right|_{n=n_0} \qquad \left(v_s(\vec{r}) \right) = v_s(\vec{r}) - v(\vec{r}) \equiv v_{HXC}(\vec{r}) =$$

$$\left.\frac{\delta E_{XC}(n)}{\delta n}\right|_{n=n_0} = v_{XC}(\vec{r})$$

Kohn-Sham Equations / Algorithm $\cancel{\Psi}$, Φ ✓

1. Given one-body Kohn-Sham potential $v_s^{(i)}(\vec{r})$, compute $|\Phi^{(i)}\rangle$, orbitals $\phi^{(i)}_{j\sigma}(\vec{r})$; $\left(-\frac{1}{2}\nabla^2 + \right.$

2. Compute the density $n^{(i)}(\vec{r}) = \sum_\sigma \sum_{j=1}^{N/2} |\phi_{j\sigma}(\vec{r})|^2$

(2.5. $\tilde{n}^{(i)} = \lambda n^{(i)}(\vec{r}) + (1-\lambda) n^{(i-1)}(\vec{r})$)

3. Obtain a new KS potential $v_s^{(i+1)}(\vec{r}) = v(\vec{r}) + v^{(approx)}_{HXC}[n^{(i)}](\vec{r}) = v(\vec{r}) + v_H(n^{(i)}(\vec{r}))(\vec{r}) +$

$v_s^{(i+1)} \downarrow n^{(i+1)}$

∞ : $E^{(approx)}[n^{(\infty)}] = E_0^{(\infty)} \neq 2\sum_j \epsilon_j$