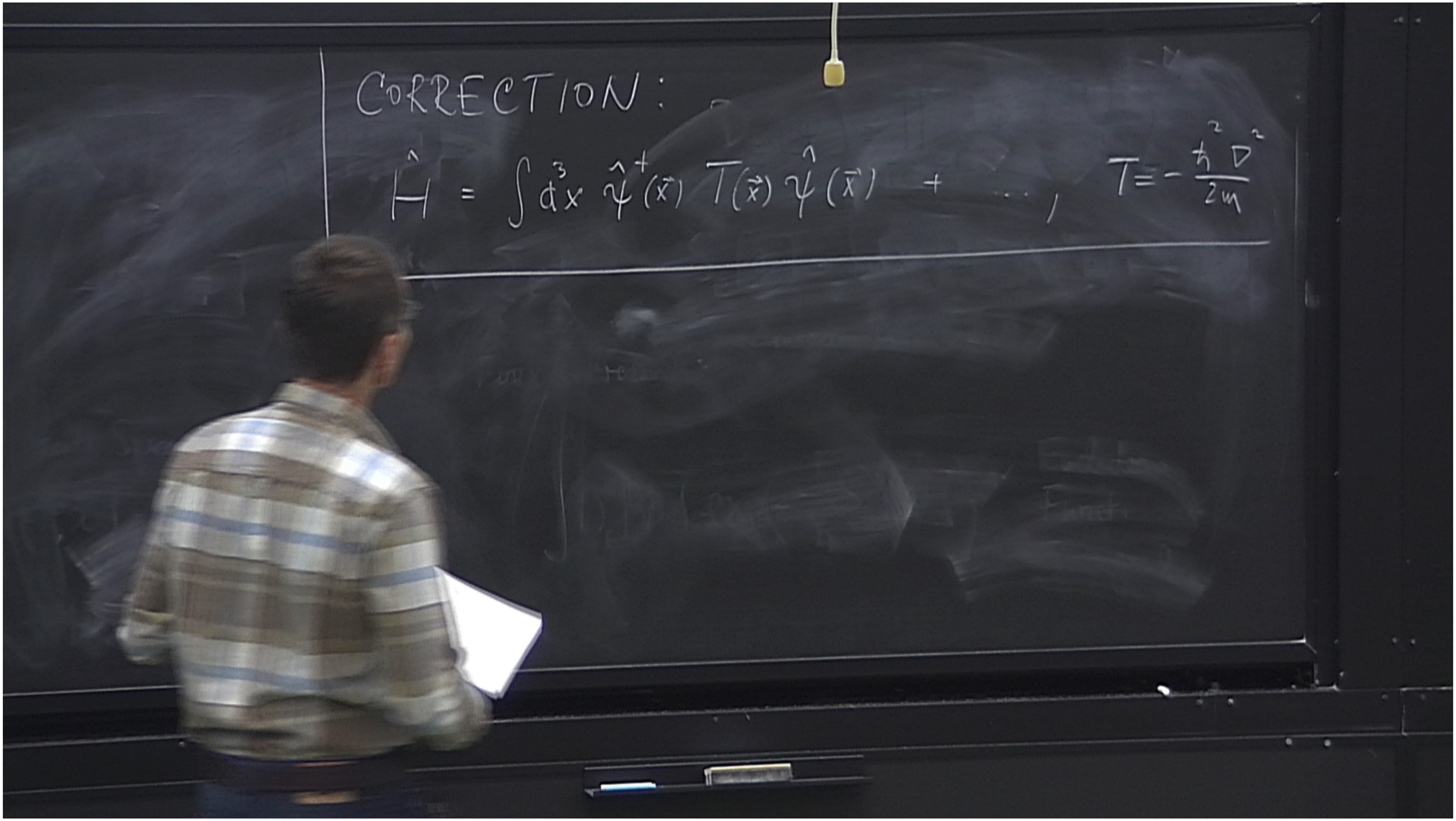
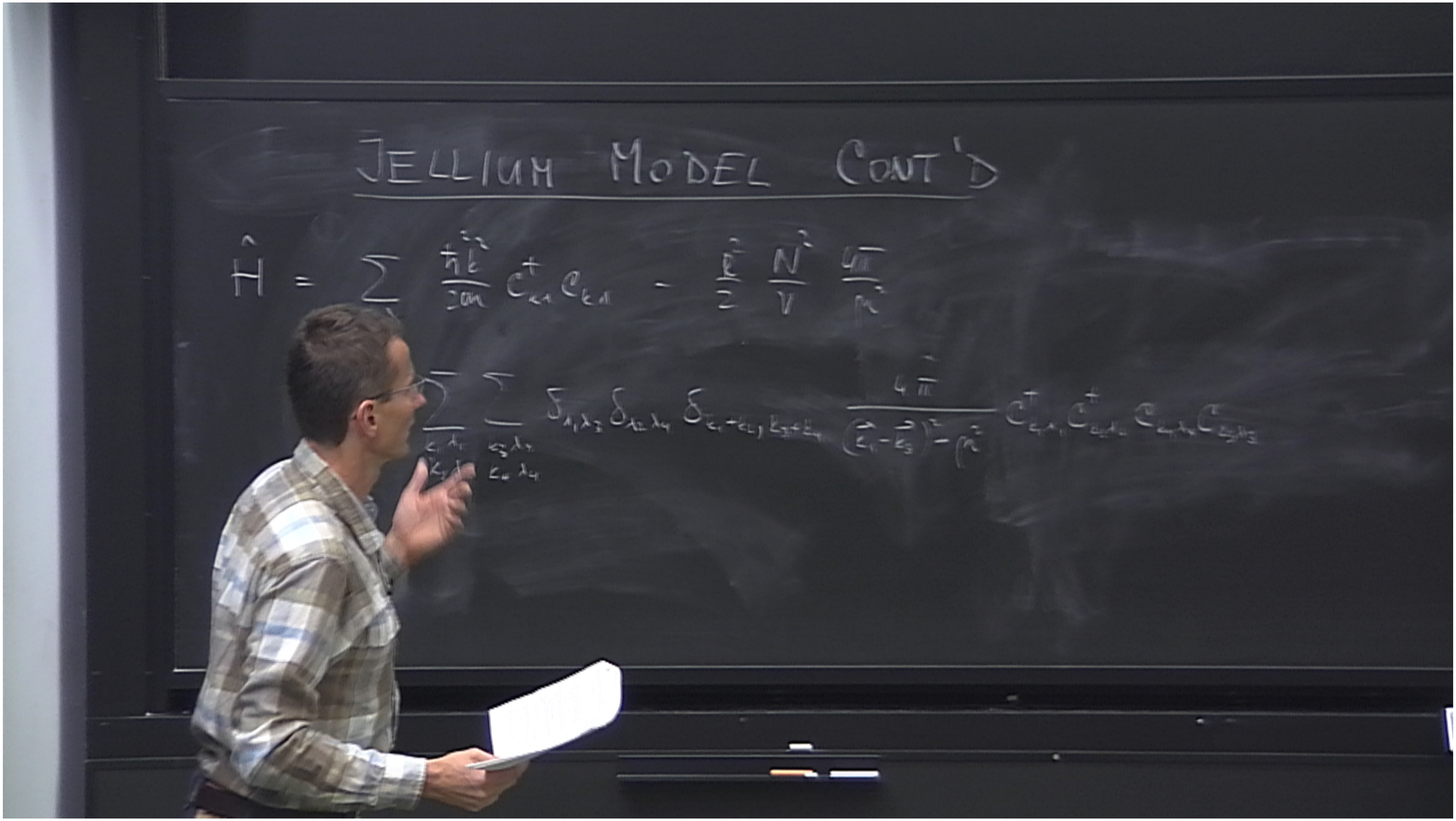
Title: 14/15 PSI - Condensed Matter-Lecture 3

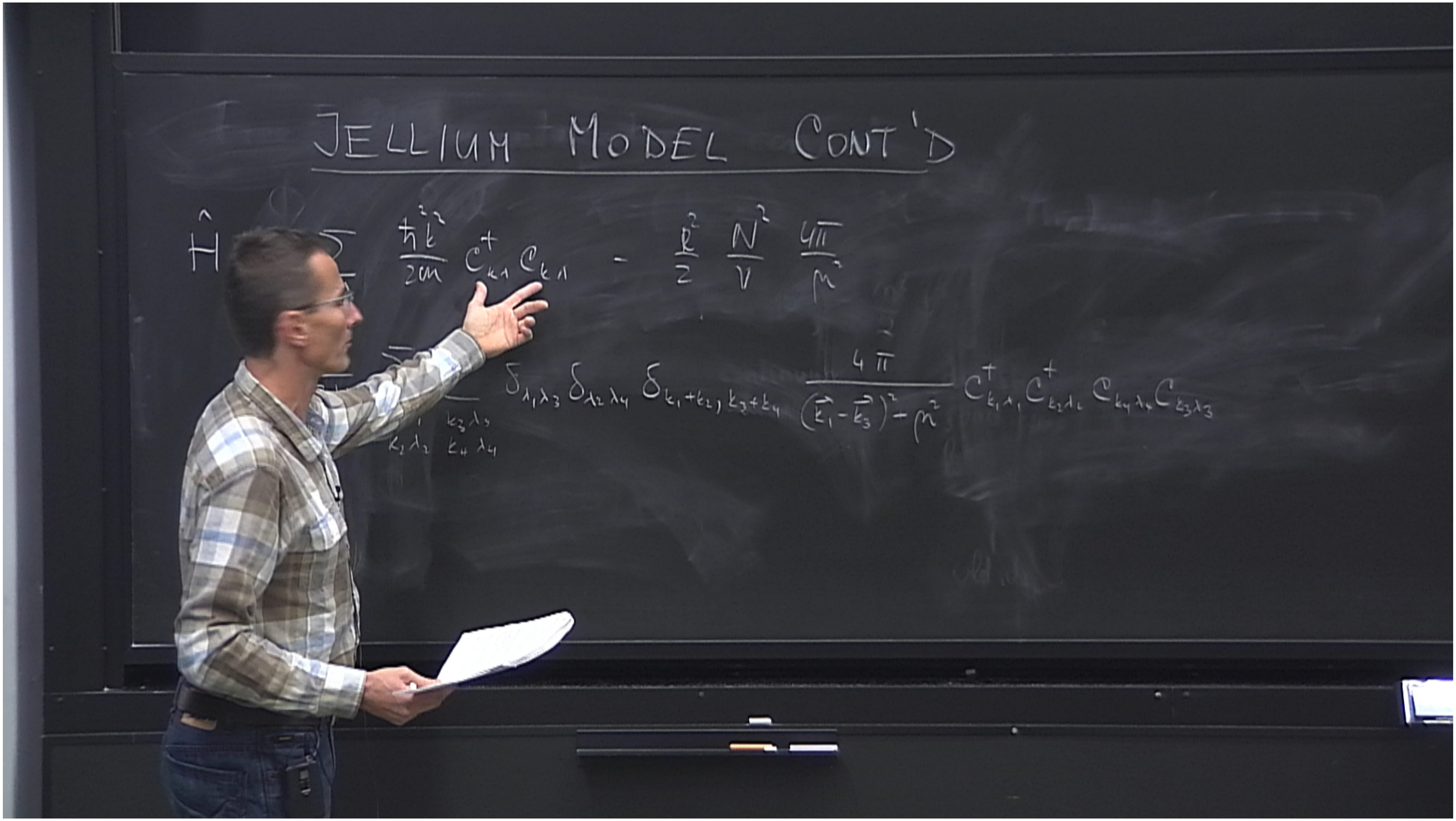
Date: Nov 12, 2014 10:45 AM

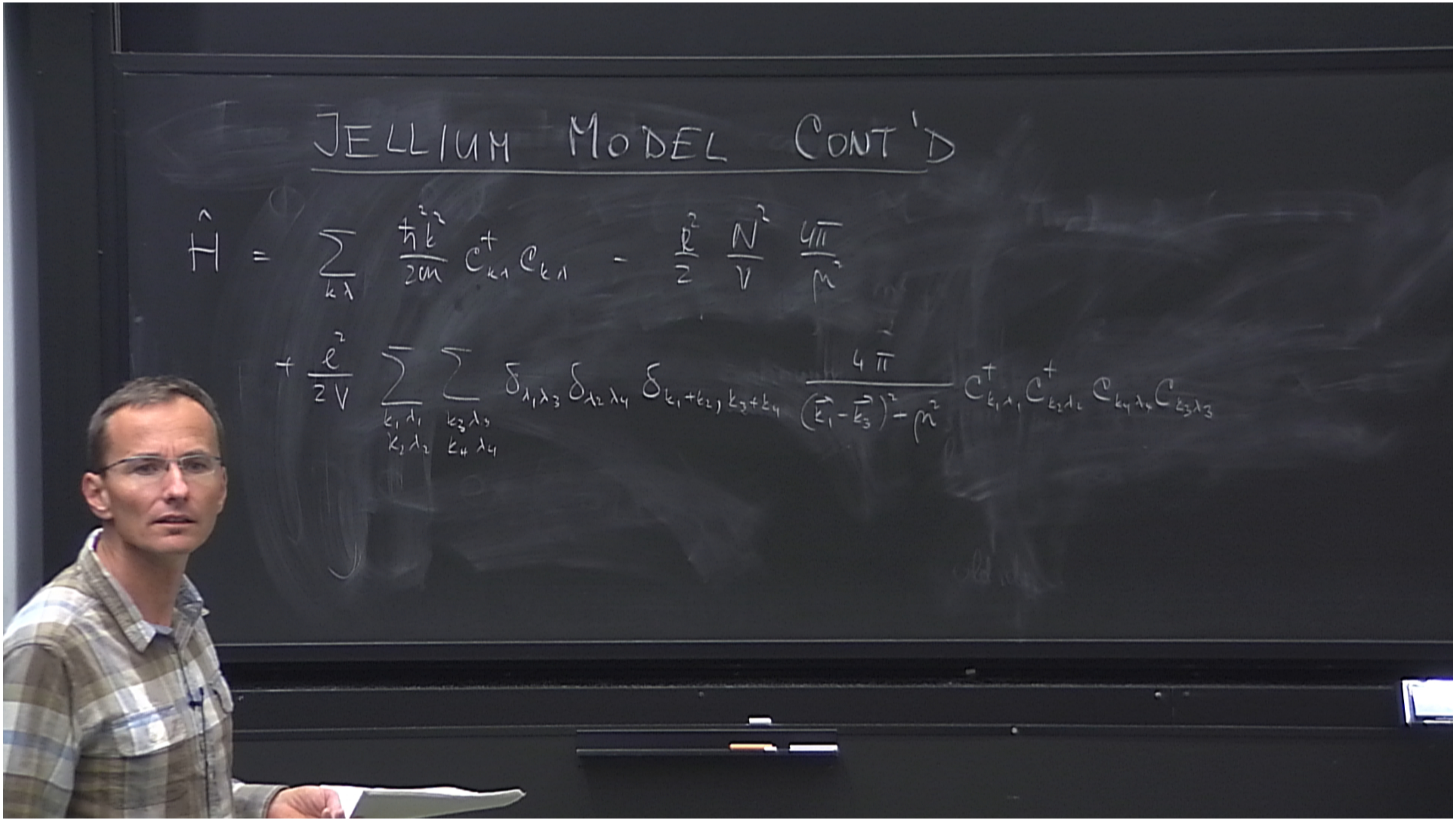
URL: http://pirsa.org/14110027

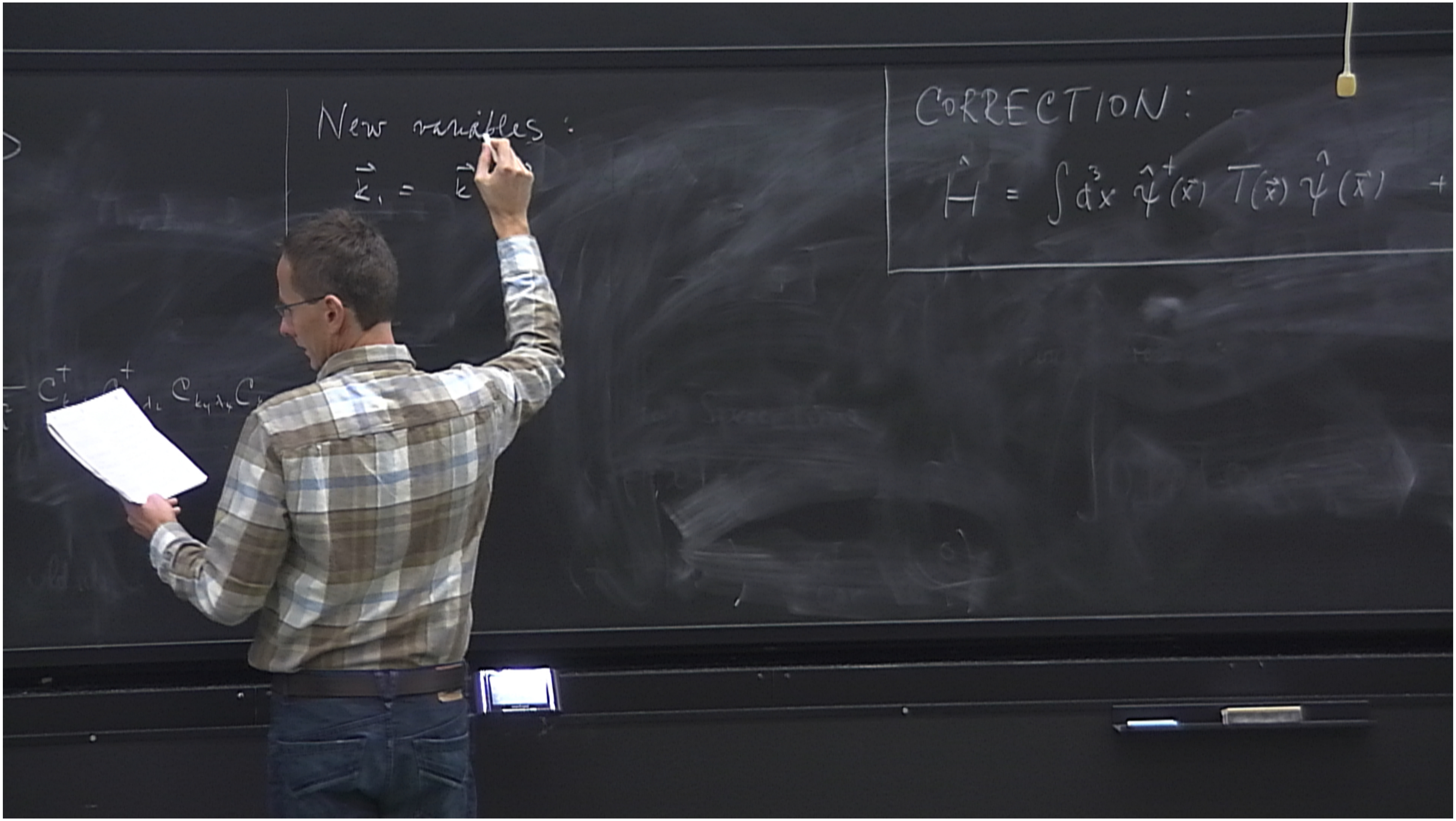
Abstract:

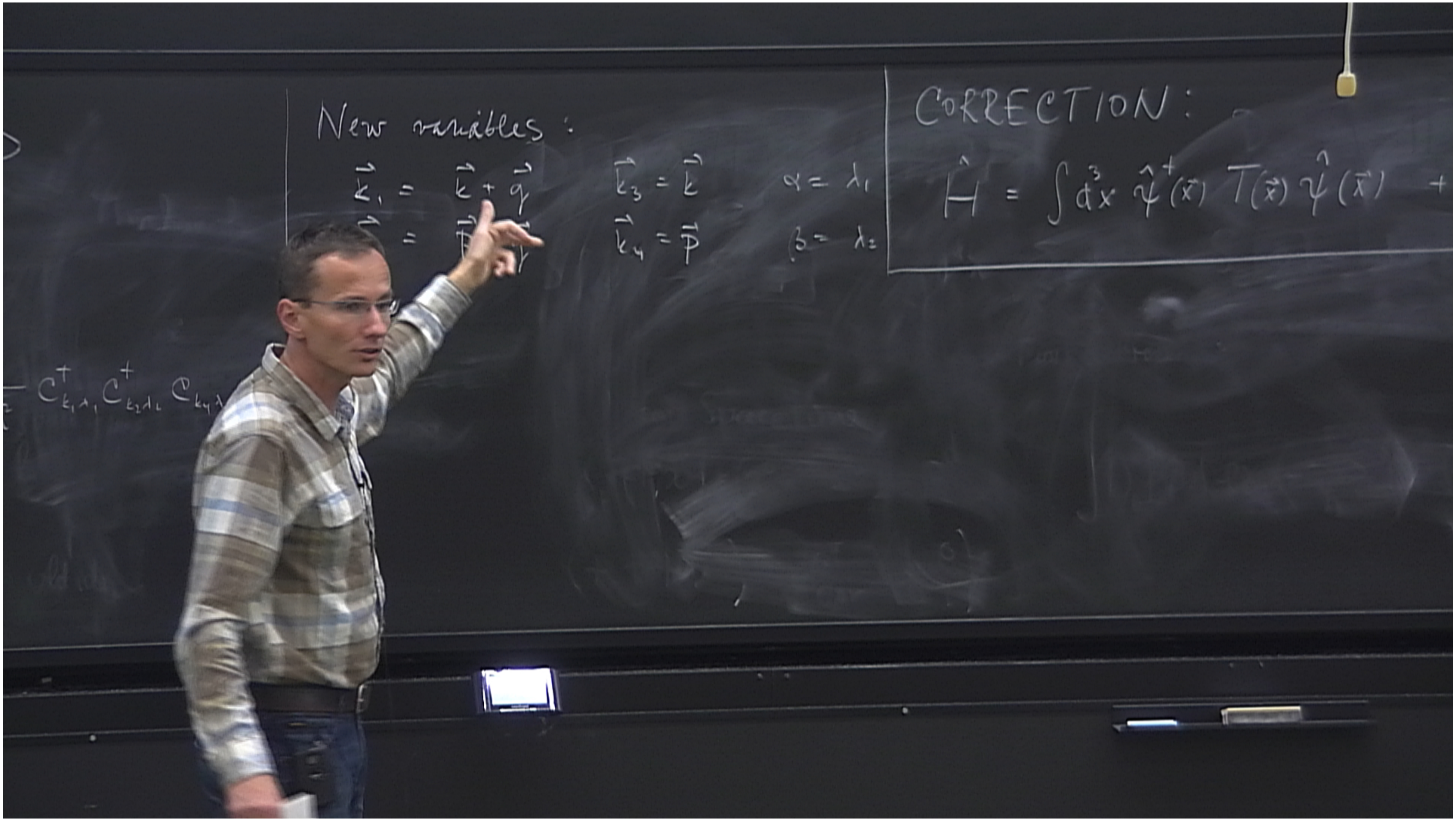

CORRECTION :
$\hat{H} = \int d^3x \, \hat{\psi}^+(\vec{x}) \, T(\vec{x}) \, \hat{\psi}(\vec{x}) \; + \; \ldots \, , \quad T = -\frac{\hbar^2 \nabla^2}{2m}$

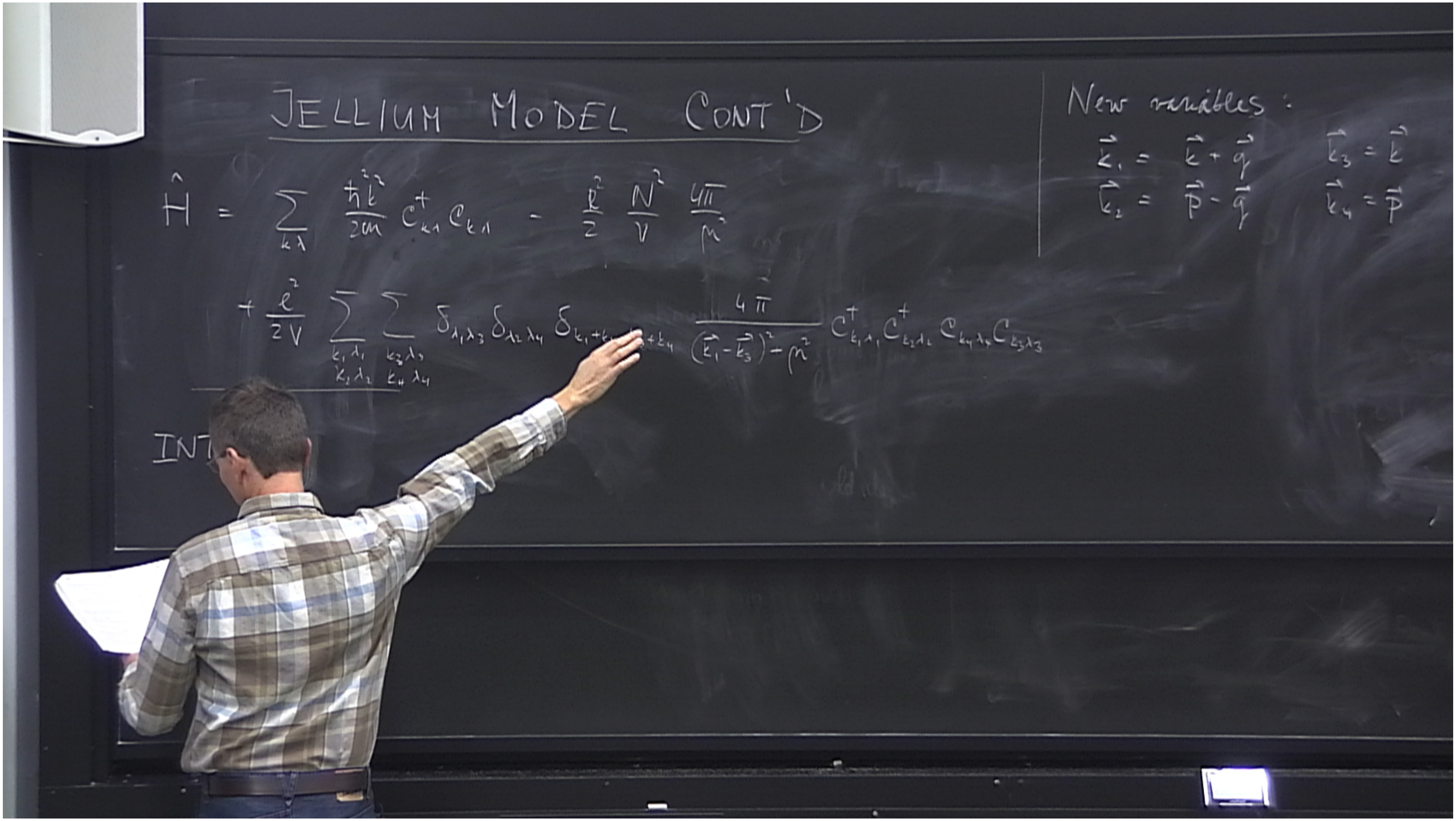

JELLIUM MODEL CONT'D
$\hat{H} = \sum_{k\lambda} \frac{\hbar^2 k^2}{2m} c^\dagger_{k\lambda} c_{k\lambda} - \frac{e^2}{2} \frac{N^2}{V} \frac{4\pi}{\mu^2}$
$\sum_{k_1\lambda_1, k_3\lambda_3} \sum_{k_2\lambda_2, k_4\lambda_4} \delta_{\lambda_1\lambda_3} \delta_{\lambda_2\lambda_4} \delta_{k_1+k_2, k_3+k_4} \frac{4\pi}{(\vec{k}_1-\vec{k}_3)^2-\mu^2} c^\dagger_{k_1\lambda_1} c^\dagger_{k_2\lambda_2} c_{k_4\lambda_4} c_{k_3\lambda_3}$

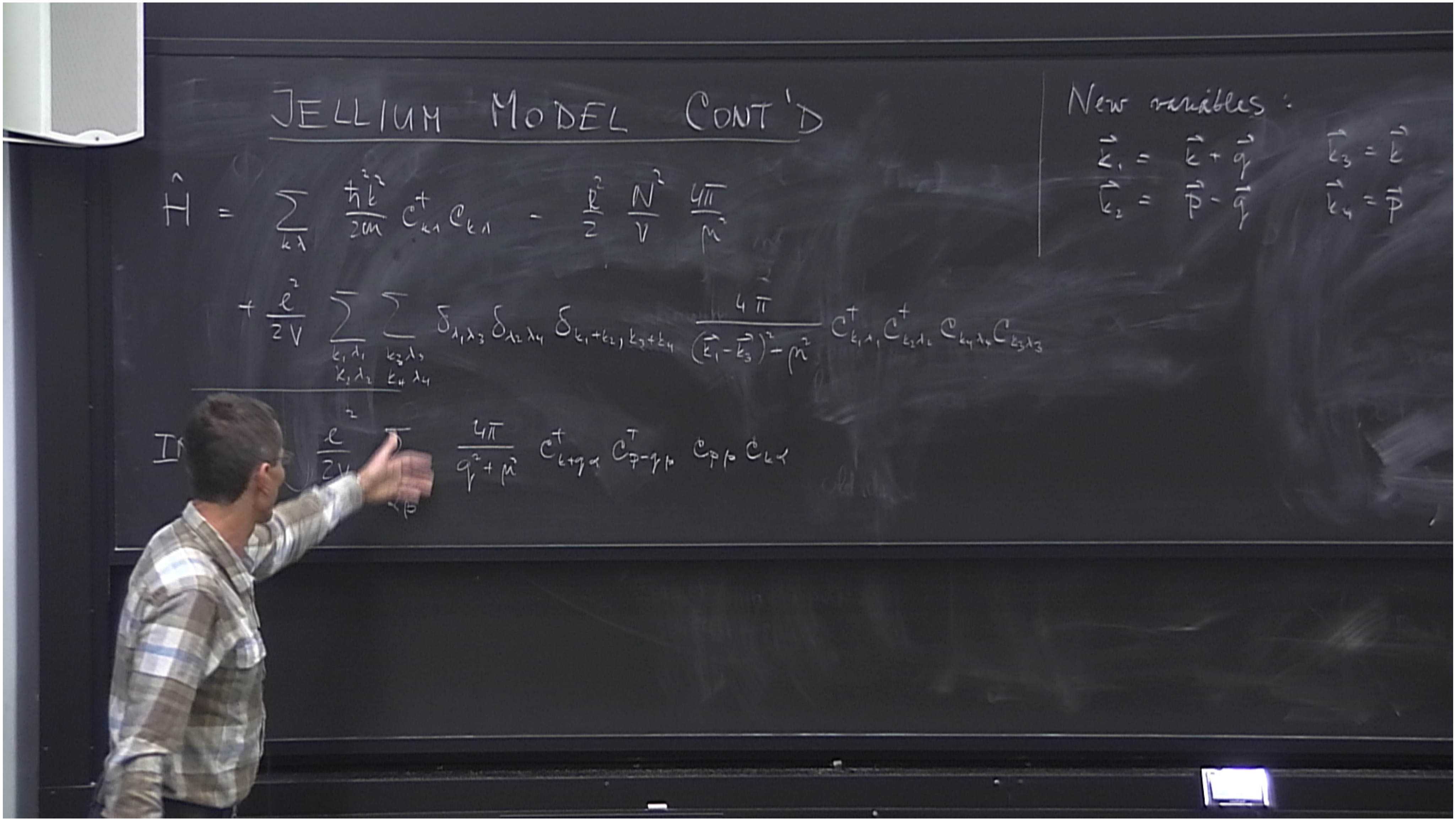

JELLIUM MODEL CONT'D

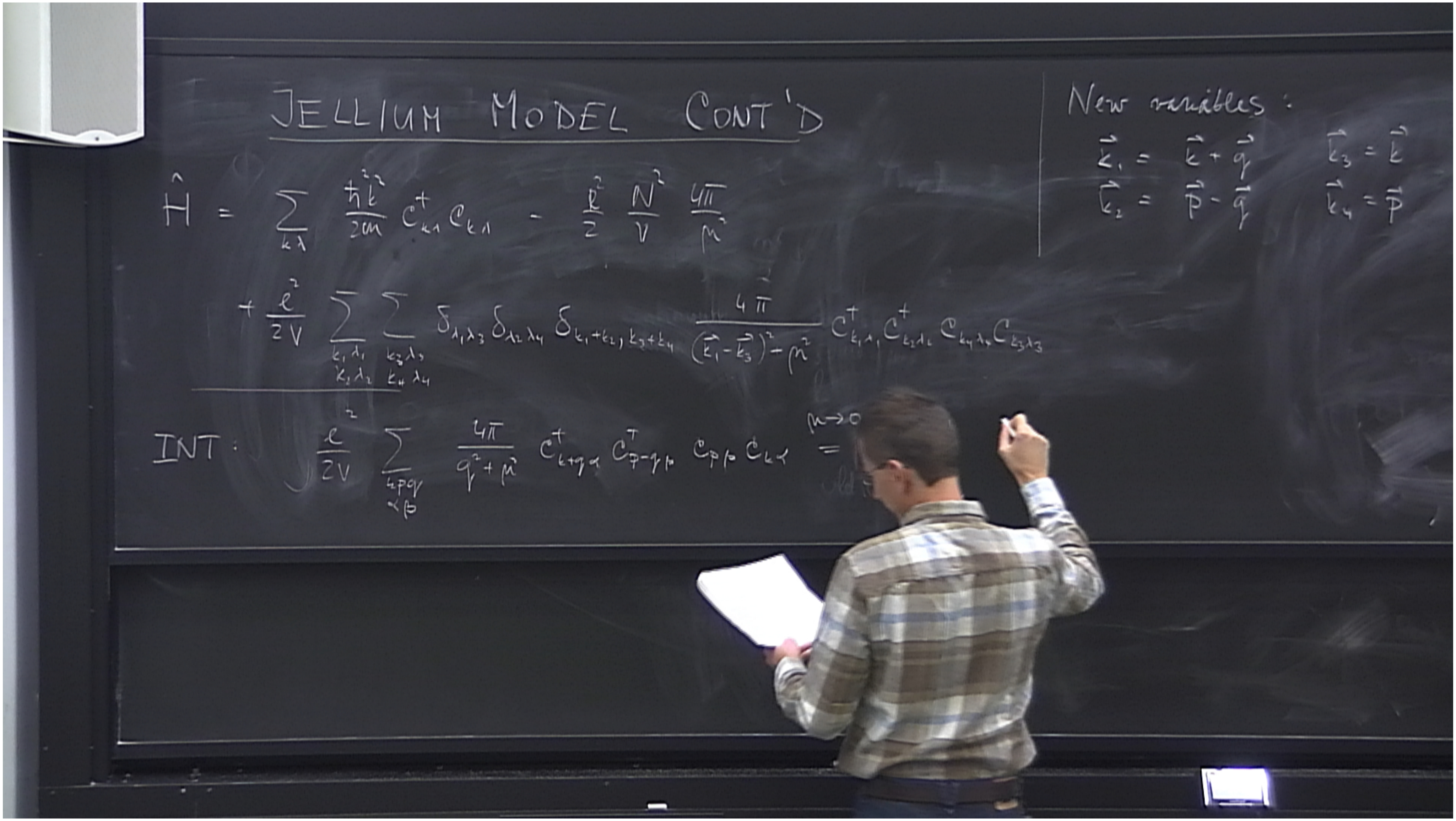

JELLIUM MODEL CONT'D
$\hat{H} = \sum_{k\lambda} \frac{\hbar^2 k^2}{2m} c^{\dagger}_{k\lambda} c_{k\lambda} - \frac{e^2}{2} \frac{N^2}{V} \frac{4\pi}{\mu^2}$
$+ \frac{e^2}{2V} \sum_{\substack{k_1\lambda_1 \\ k_2\lambda_2}} \sum_{\substack{k_3\lambda_3 \\ k_4\lambda_4}} \delta_{\lambda_1\lambda_3} \delta_{\lambda_2\lambda_4} \delta_{k_1+k_2, k_3+k_4} \frac{4\pi}{(\vec{k}_1 - \vec{k}_3)^2 + \mu^2} c^{\dagger}_{k_1\lambda_1} c^{\dagger}_{k_2\lambda_2} c_{k_4\lambda_4} c_{k_3\lambda_3}$

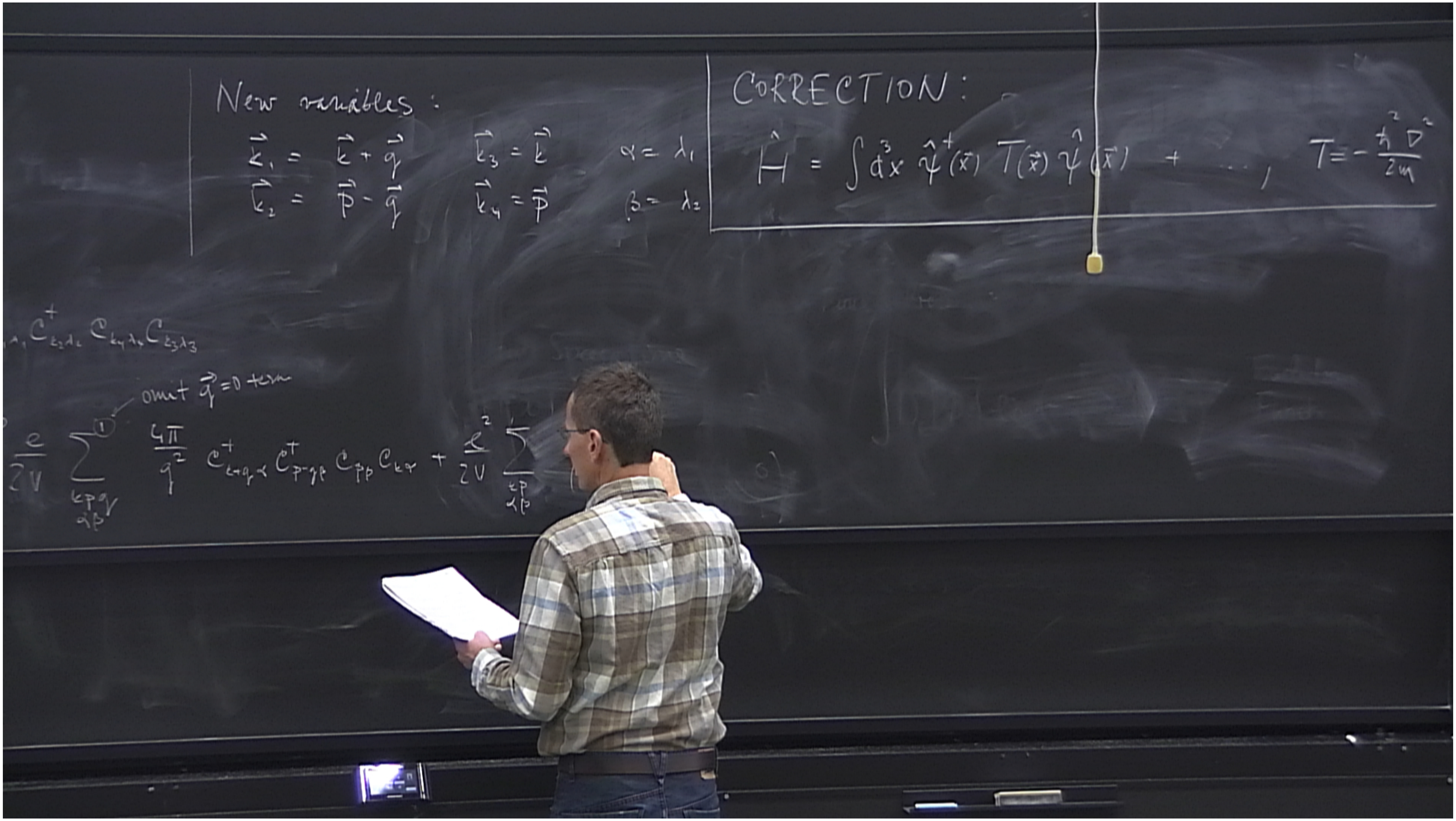

New variables :
CORRECTION :
$\hat{H} = \int d^3x\, \hat{\psi}^\dagger(\vec{x})\, T(\vec{x})\, \hat{\psi}(\vec{x}) +$

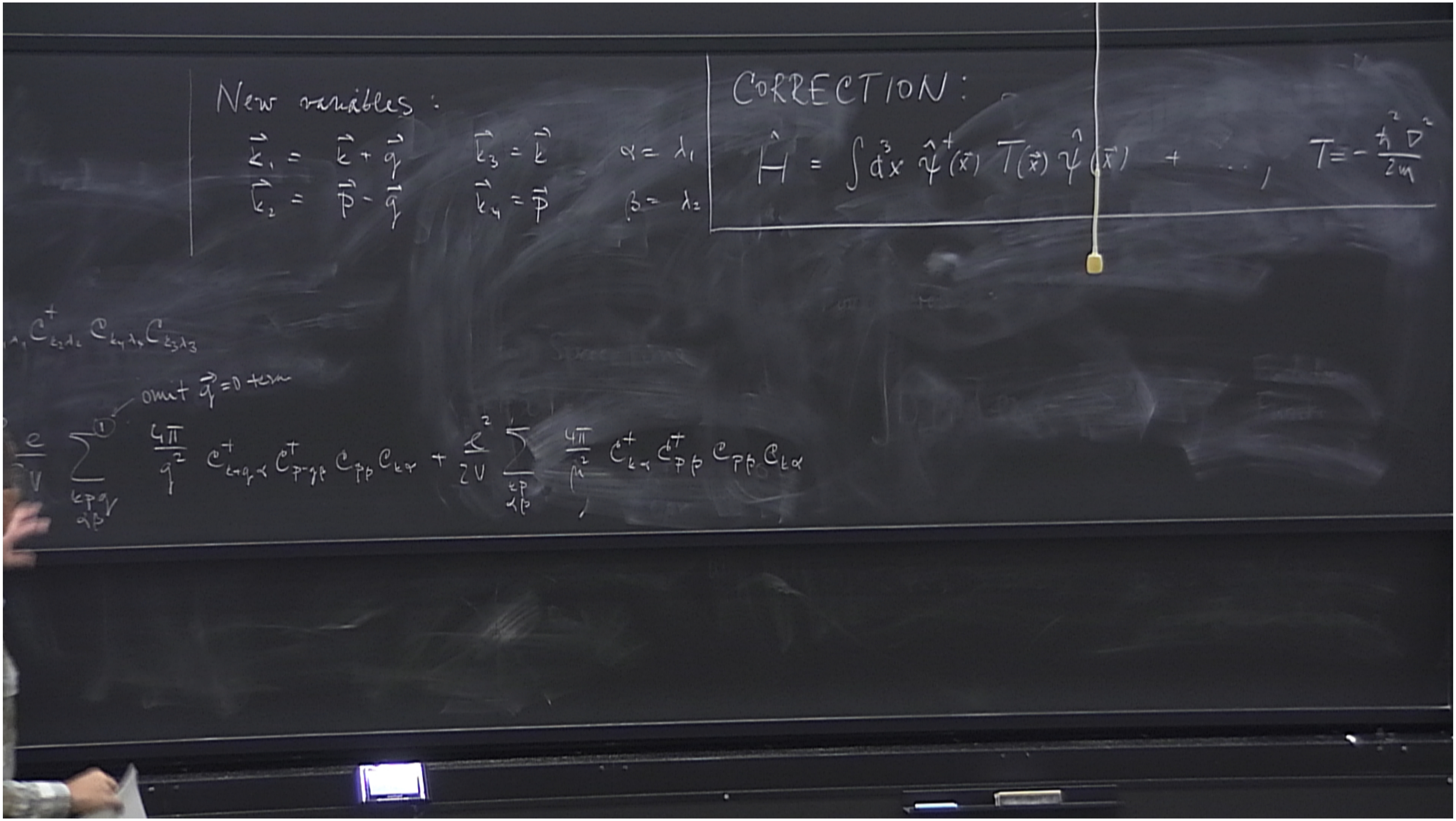

New variables :
k1 = k + q
k3 = k
α = λ1
k4 = p
β = λ2
CORRECTION :
H = ∫ d3x ψ†(x) T(x) ψ(x) +

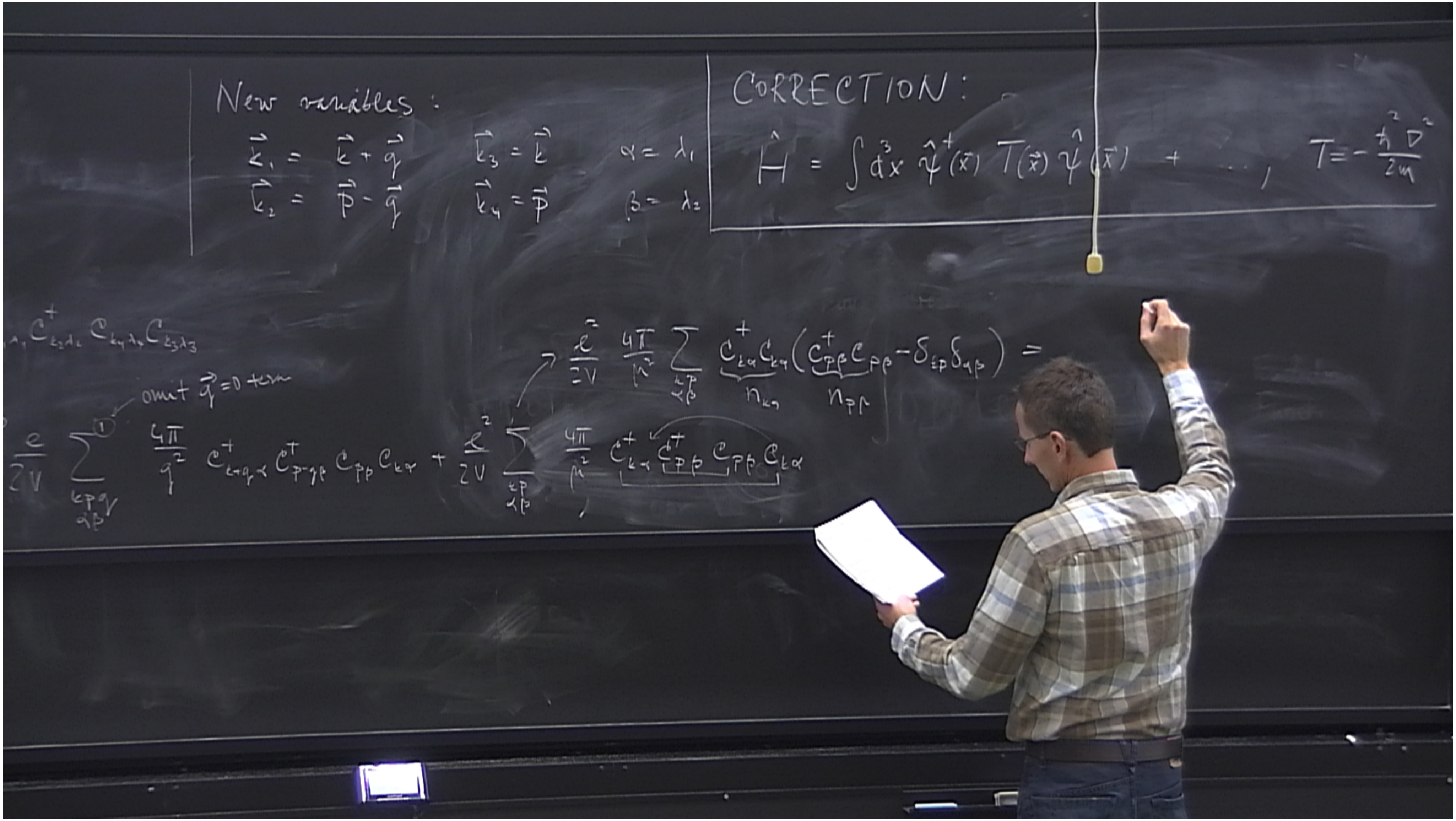

JELLIUM MODEL CONT'D
$\hat{H} = \sum_{k\lambda} \frac{\hbar^2 k^2}{2m} c^+_{k\lambda} c_{k\lambda} - \frac{e^2}{2} \frac{N^2}{V} \frac{4\pi}{\mu^2}$
$+ \frac{e^2}{2V} \sum_{k_1\lambda_1, k_2\lambda_2} \sum_{k_3\lambda_3, k_4\lambda_4} \delta_{\lambda_1\lambda_3} \delta_{\lambda_2\lambda_4} \delta_{k_1+k_2, k_3+k_4} \frac{4\pi}{(\vec{k}_1-\vec{k}_3)^2-\mu^2} c^+_{k_1\lambda_1} c^+_{k_2\lambda_2} c_{k_4\lambda_4} c_{k_3\lambda_3}$
INT
New variables :
$\vec{k}_1 = \vec{k} + \vec{q}$
$\vec{k}_2 = \vec{p} - \vec{q}$
$\vec{k}_3 = \vec{k}$
$\vec{k}_4 = \vec{p}$

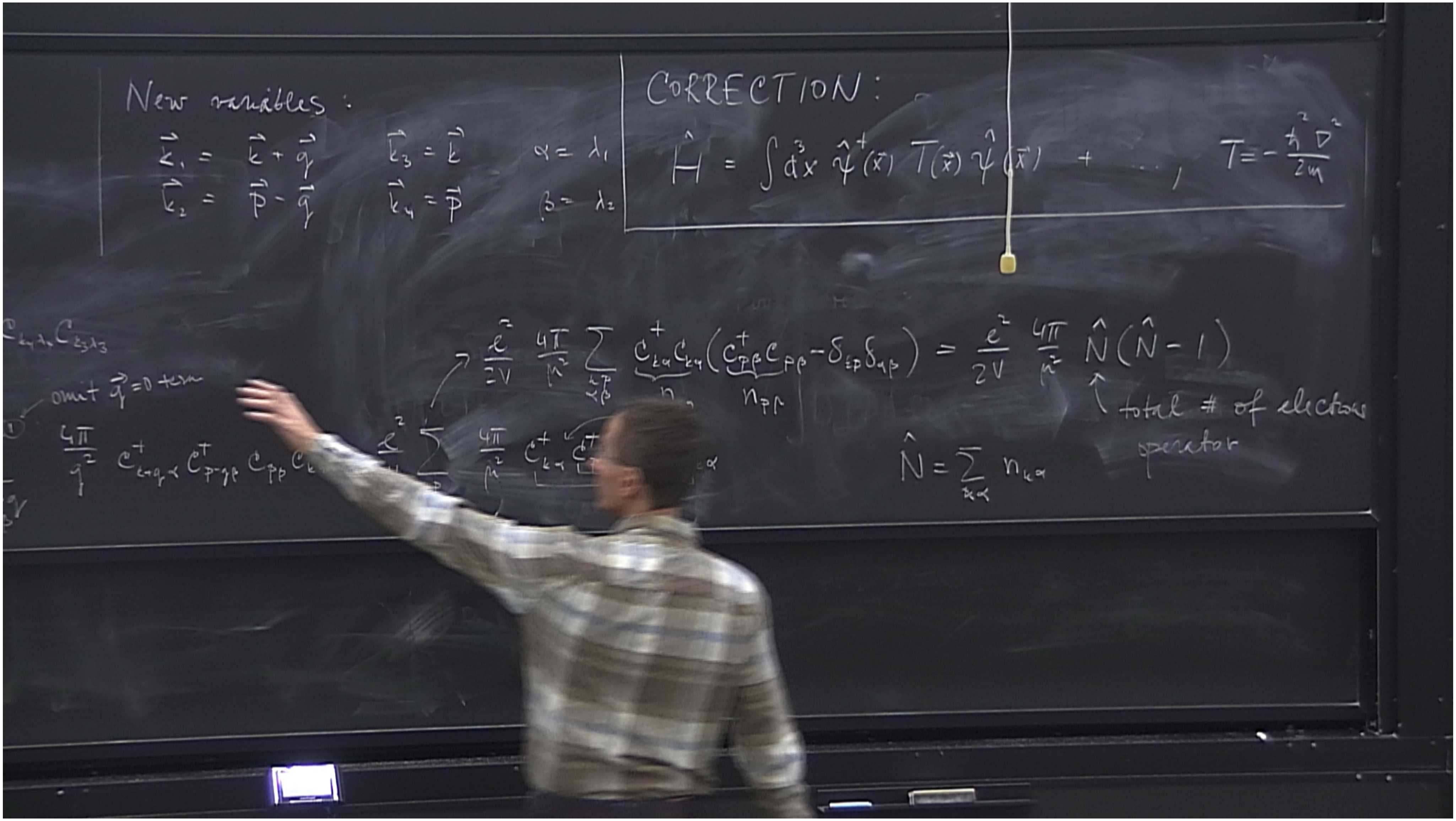

JELLIUM MODEL CONT'D
$\hat{H} = \sum_{k\lambda} \frac{\hbar^2 k^2}{2m} c^\dagger_{k\lambda} c_{k\lambda} - \frac{e^2}{2} \frac{N^2}{V} \frac{4\pi}{\mu^2}$
$+ \frac{e^2}{2V} \sum_{k_1\lambda_1, k_2\lambda_2} \sum_{k_3\lambda_3, k_4\lambda_4} \delta_{\lambda_1\lambda_3} \delta_{\lambda_2\lambda_4} \delta_{k_1+k_2, k_3+k_4} \frac{4\pi}{(\vec{k}_1-\vec{k}_3)^2-\mu^2} c^\dagger_{k_1\lambda_1} c^\dagger_{k_2\lambda_2} c_{k_4\lambda_4} c_{k_3\lambda_3}$
$\frac{e^2}{2V} \sum \frac{4\pi}{q^2+\mu^2} c^\dagger_{k+q\alpha} c^\dagger_{p-q\beta} c_{p\beta} c_{k\alpha}$
New variables :
$\vec{k}_1 = \vec{k} + \vec{q}$
$\vec{k}_3 = \vec{k}$
$\vec{k}_2 = \vec{p} - \vec{q}$
$\vec{k}_4 = \vec{p}$

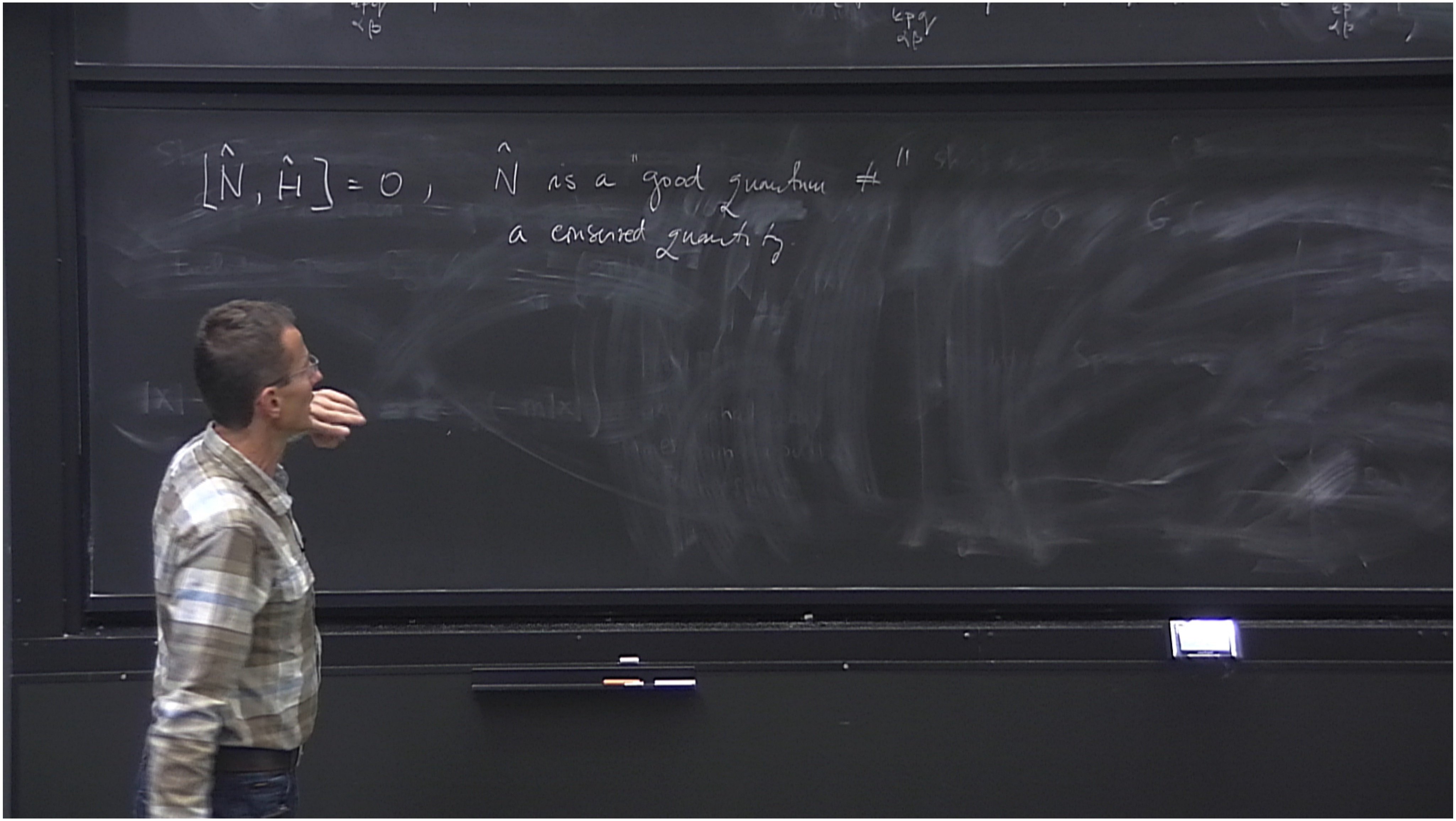

JELLIUM MODEL CONT'D
$\hat{H} = \sum_{k\lambda} \frac{\hbar^2 k^2}{2m} c^\dagger_{k\lambda} c_{k\lambda} - \frac{e^2}{2} \frac{N^2}{V} \frac{4\pi}{\mu^2}$
$+ \frac{e^2}{2V} \sum_{\substack{k_1\lambda_1 \\ k_2\lambda_2}} \sum_{\substack{k_3\lambda_3 \\ k_4\lambda_4}} \delta_{\lambda_1\lambda_3} \delta_{\lambda_2\lambda_4} \delta_{k_1+k_2, k_3+k_4} \frac{4\pi}{(\vec{k}_1-\vec{k}_3)^2 - \mu^2} c^\dagger_{k_1\lambda_1} c^\dagger_{k_2\lambda_2} c_{k_4\lambda_4} c_{k_3\lambda_3}$
INT: $\frac{e^2}{2V} \sum_{\substack{kpq \\ \alpha\beta}} \frac{4\pi}{q^2+\mu^2} c^\dagger_{k+q\alpha} c^\dagger_{p-q\beta} c_{p\beta} c_{k\alpha} \overset{\mu\to 0}{=}$
New variables:
$\vec{k}_1 = \vec{k} + \vec{q}$ $\vec{k}_3 = \vec{k}$
$\vec{k}_2 = \vec{p} - \vec{q}$ $\vec{k}_4 = \vec{p}$

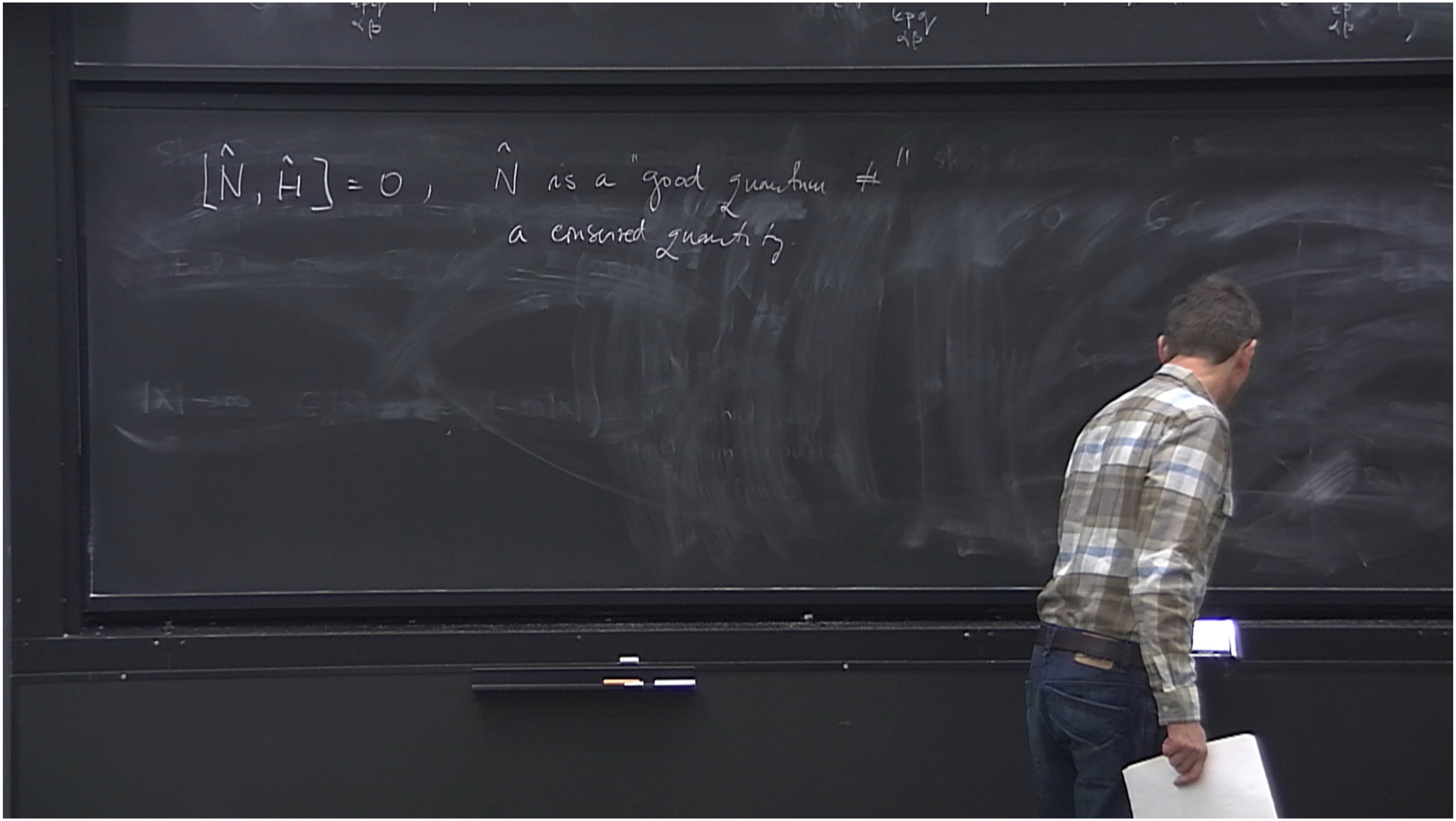

New variables :
CORRECTION :
omit q = 0 term

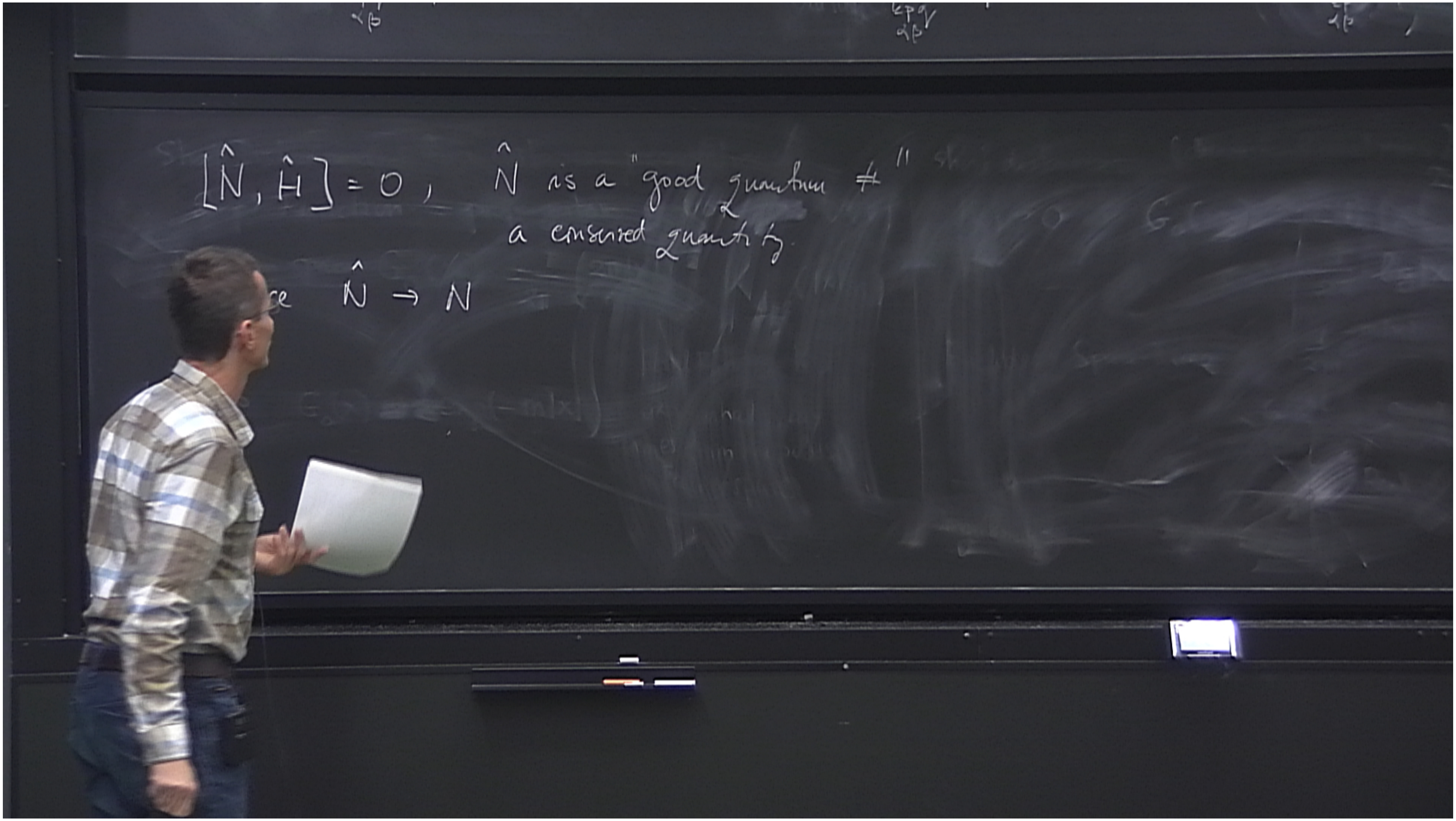

New variables:
k1 = k + q
k2 = p - q
k3 = k
k4 = p
α = λ1
β = λ2
CORRECTION:
Ĥ = ∫d³x ψ̂†(x) T(x) ψ̂(x) + ... , T = - ħ²∇²/2m
omit q = 0 term

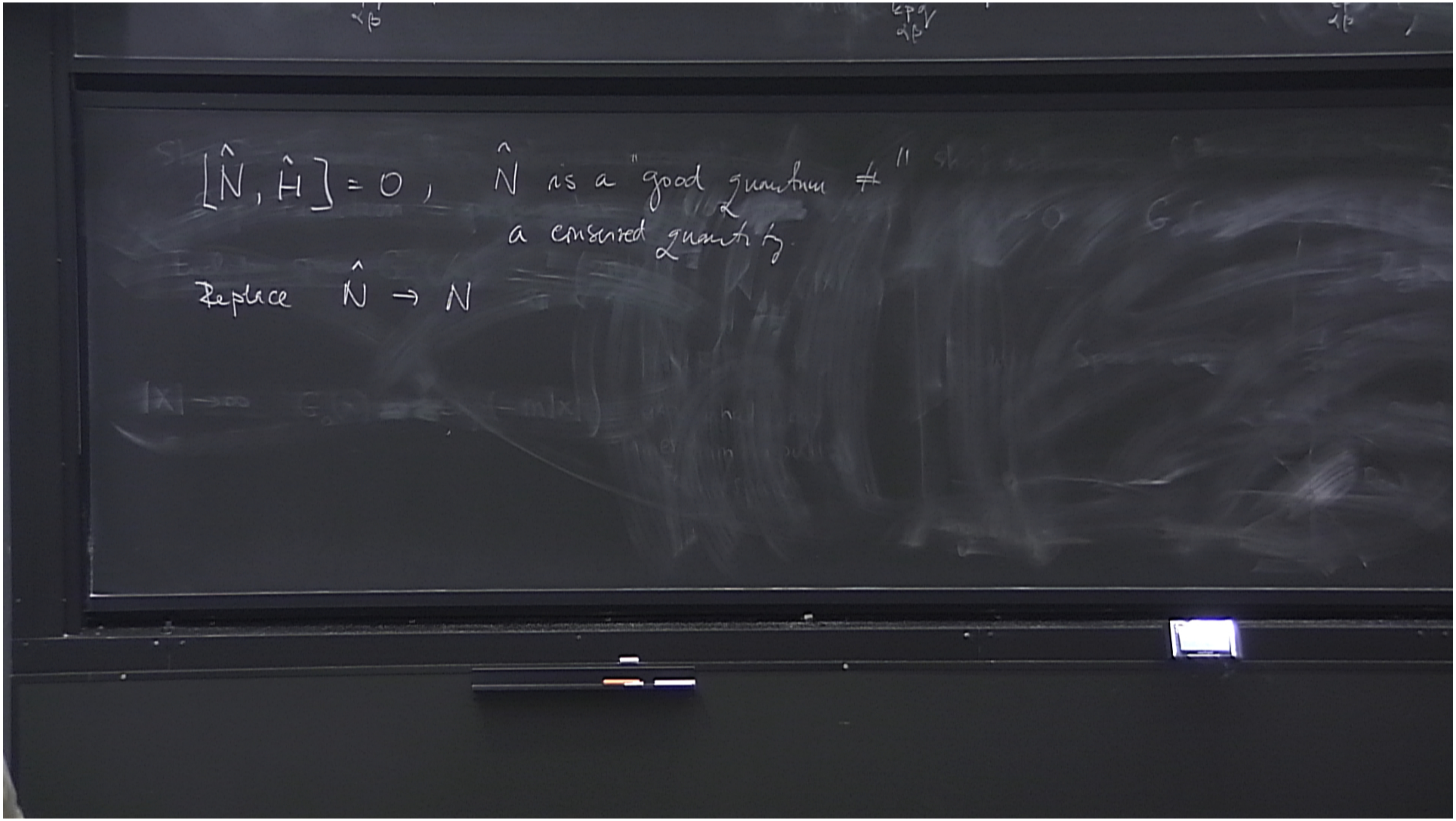

New variables :
CORRECTION :

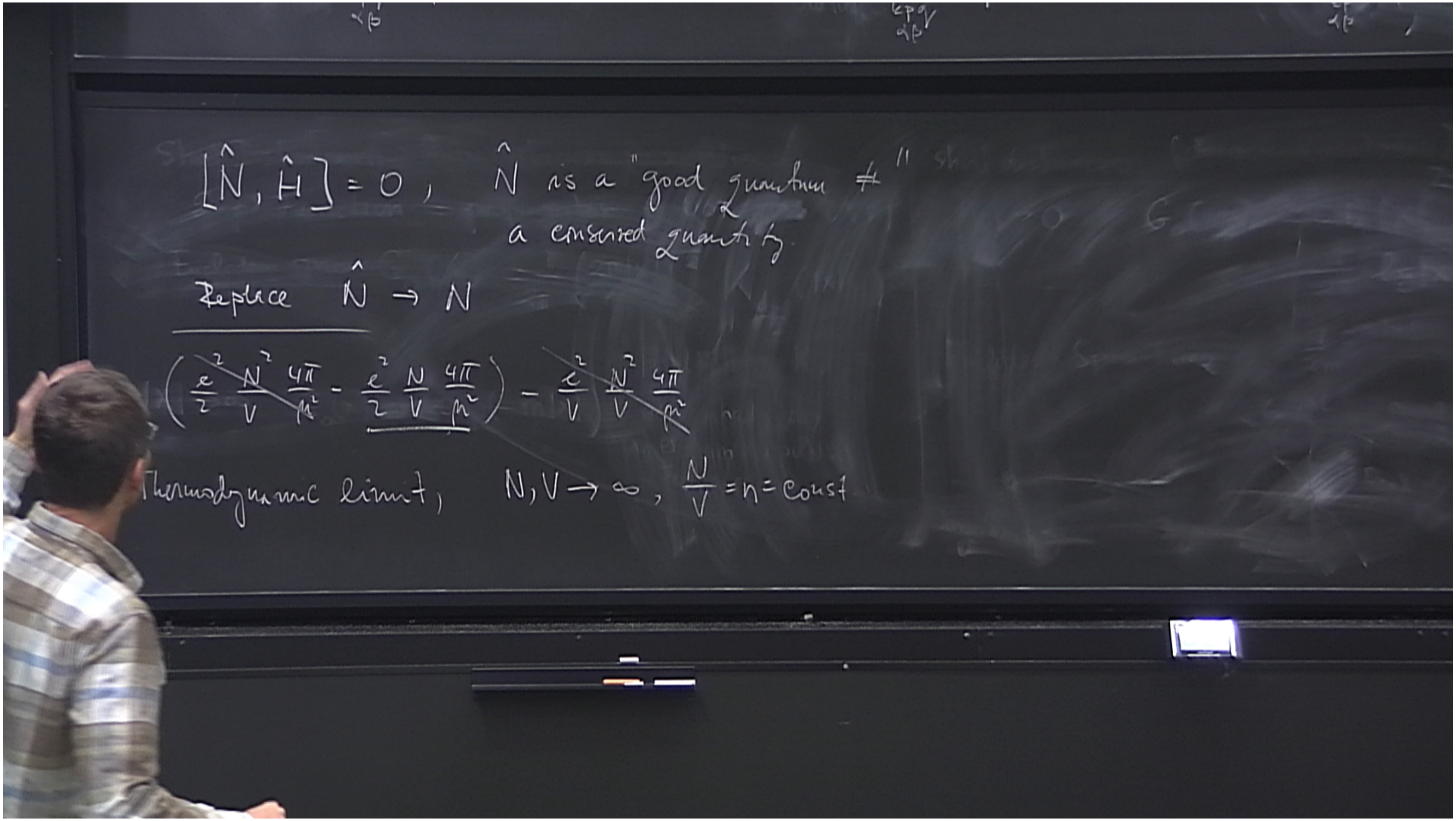

New variables :
CORRECTION :
omit q=0 term
total # of electrons operator

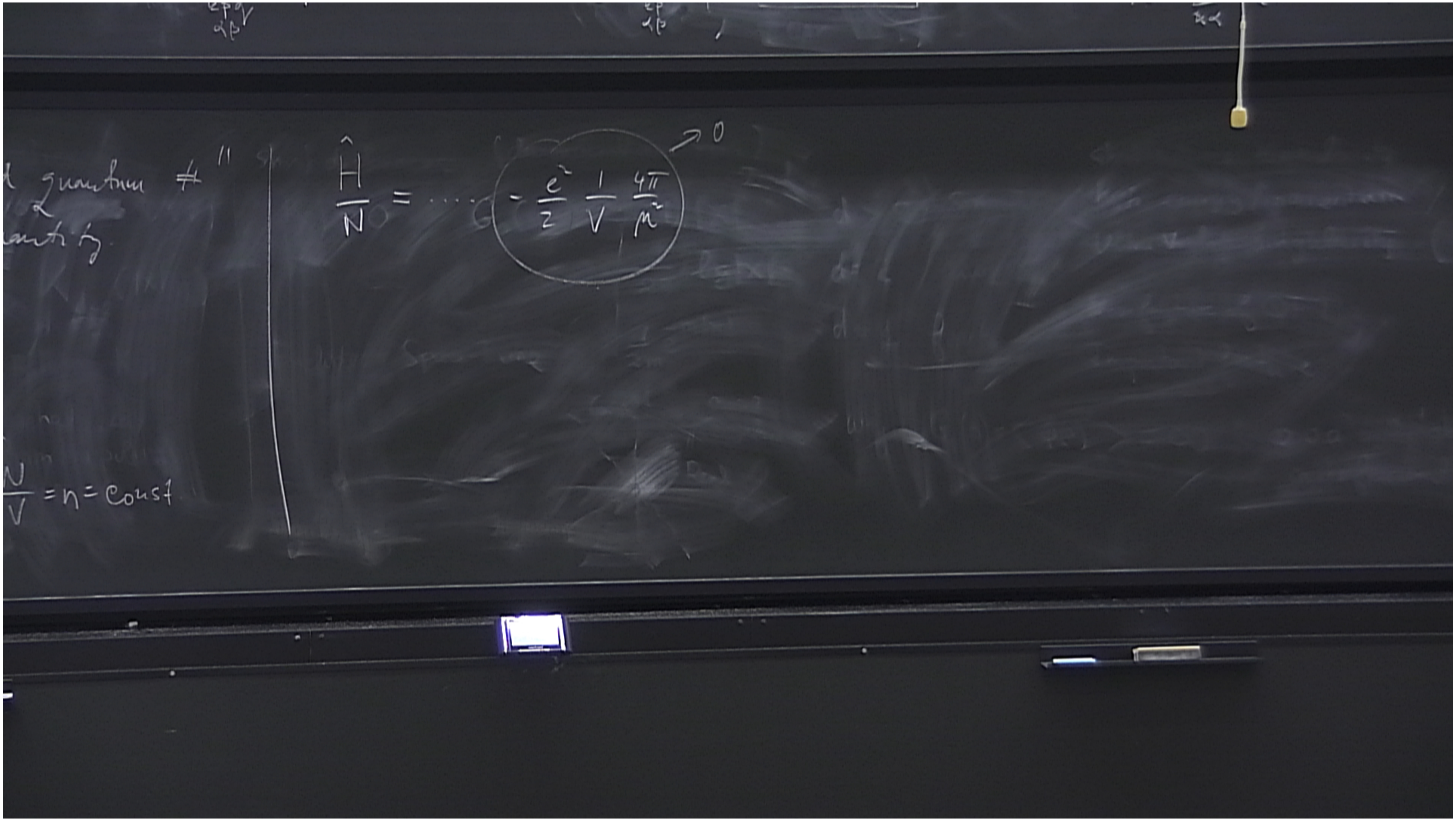

[N̂, Ĥ] = 0 , N̂ is a "good quantum #"
a conserved quantity

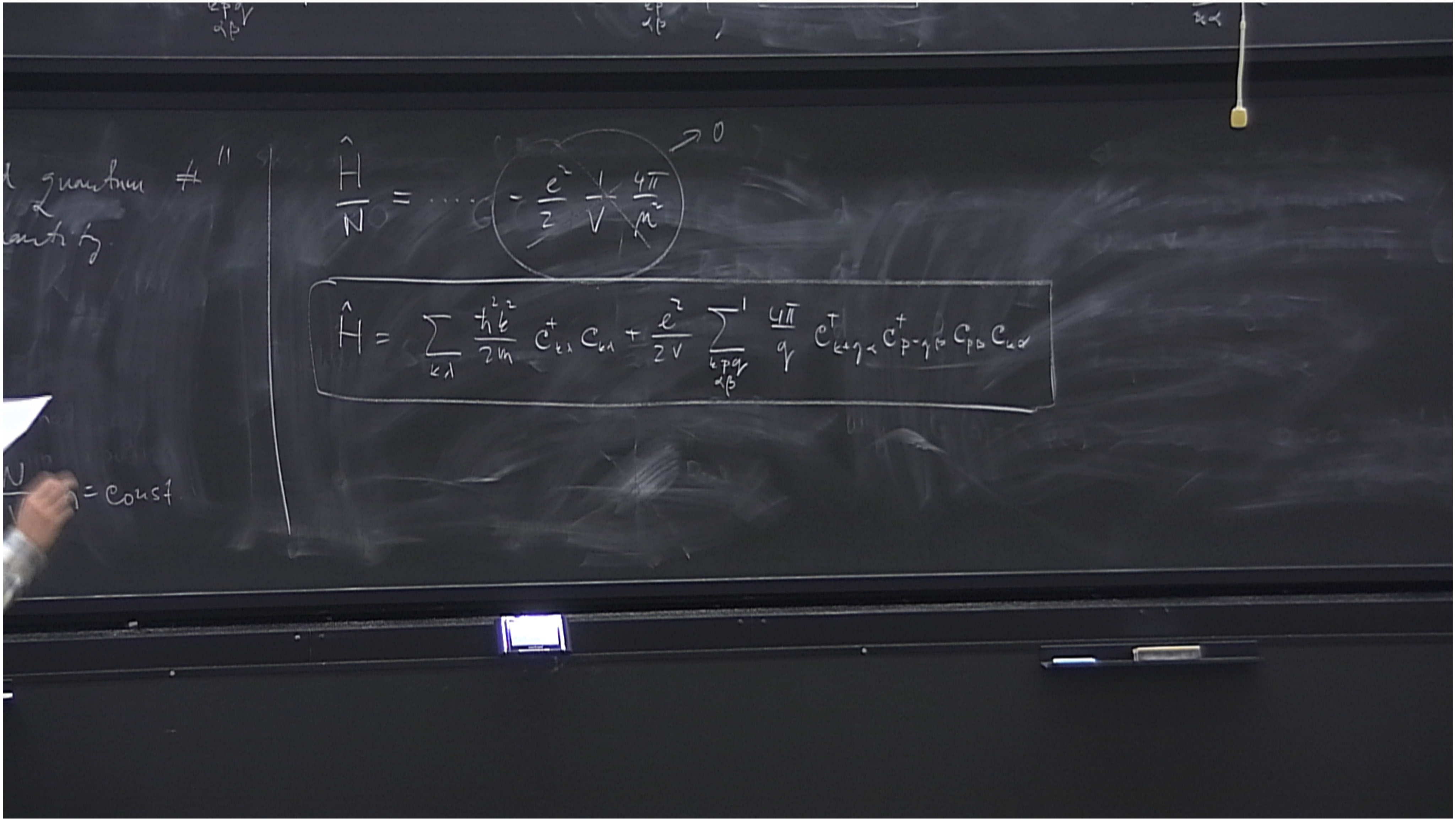

$[\hat{N}, \hat{H}] = 0$, $\hat{N}$ is a "good quantum #"
& a conserved quantity

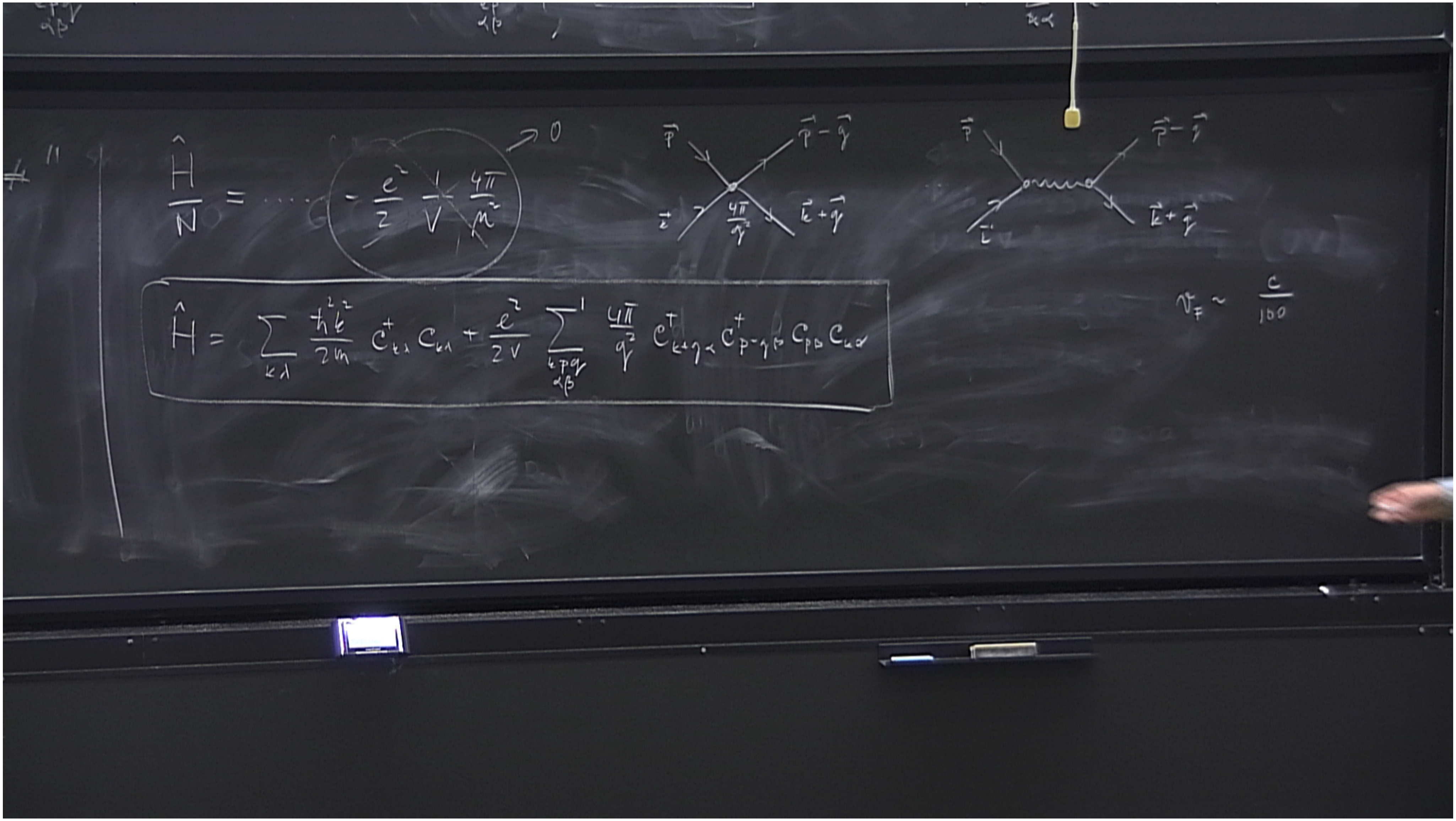

[N̂, Ĥ] = 0 , N̂ is a "good quantum #"
a conserved quantity
ce N̂ → N


[N̂, Ĥ] = 0 , N̂ is a "good quantum #"
a conserved quantity
Replace N̂ → N

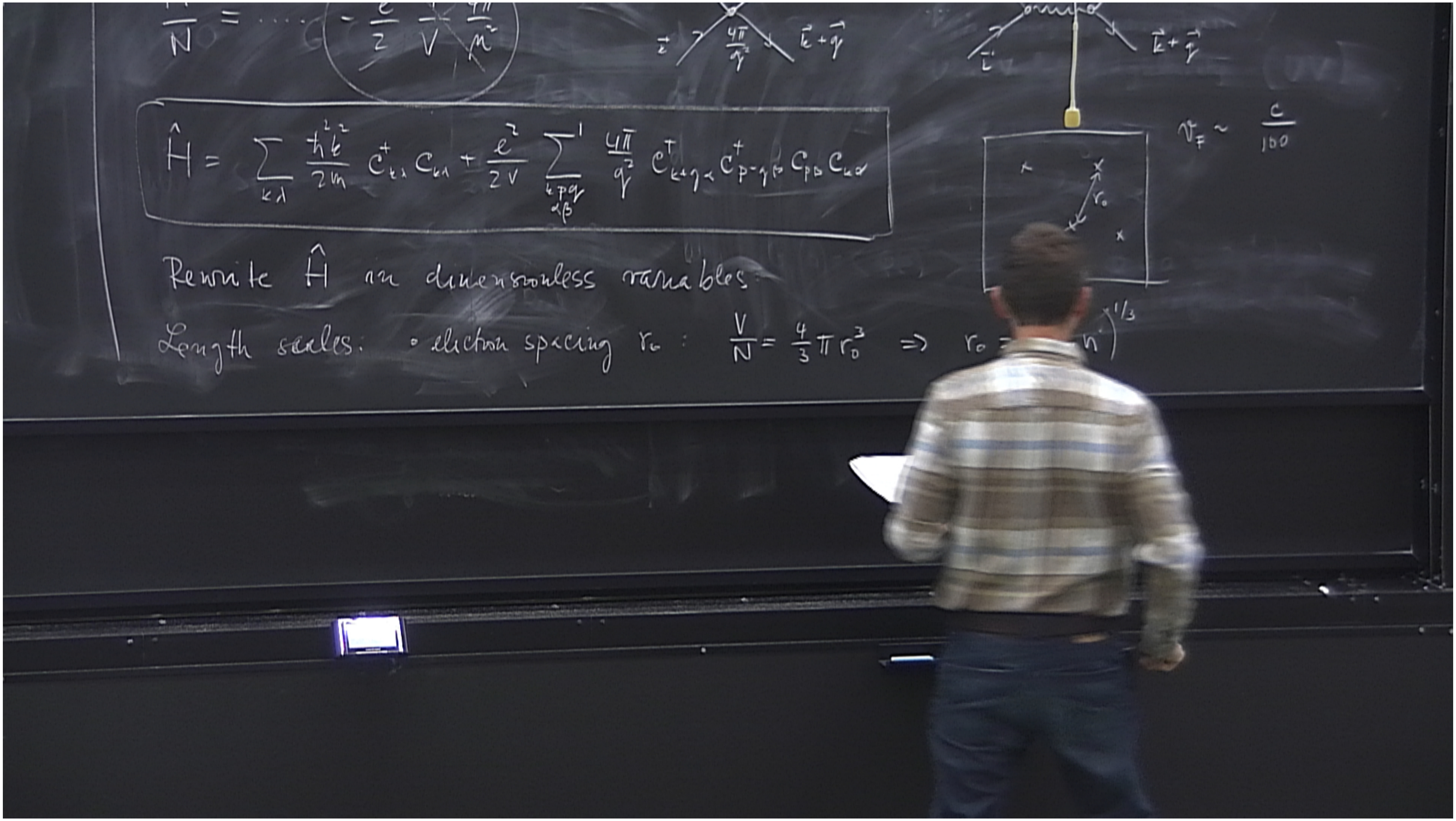

$[\hat{N}, \hat{H}] = 0$, $\hat{N}$ is a "good quantum #"
a conserved quantity
Replace $\hat{N} \to N$
$\left(\frac{e^2}{2} \frac{N^2}{V} \frac{4\pi}{\mu^2} - \frac{e^2}{2} \frac{N}{V} \frac{4\pi}{\mu^2} \right) - \frac{e^2}{V} \frac{N^2}{V} \frac{4\pi}{\mu^2}$
Thermodynamic limit, $N, V \to \infty$, $\frac{N}{V} = n = \text{const}$

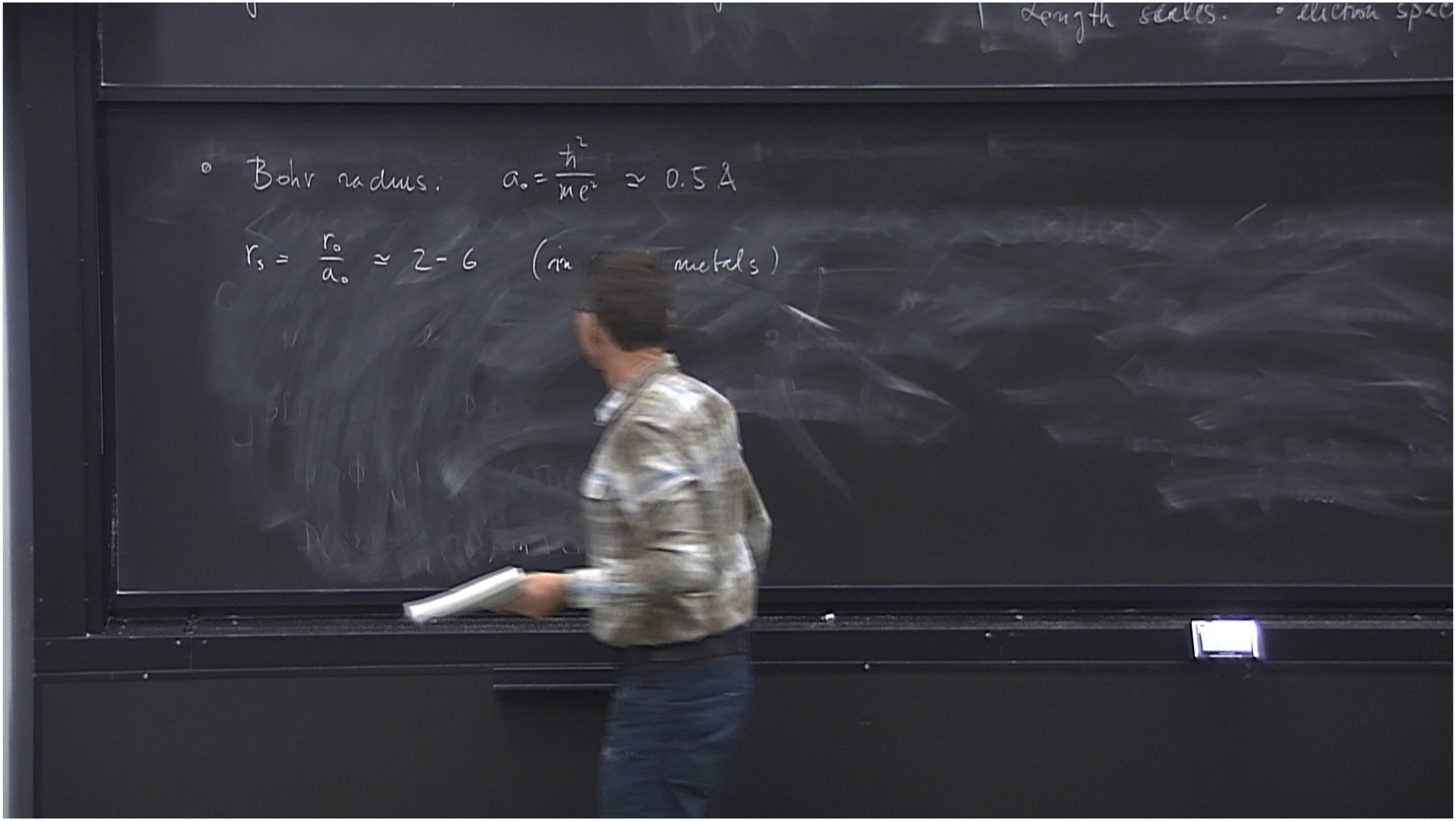

quantum #"
quantity.
Ĥ/N = ... − e²/2 · 1/V · 4π/μ² → 0
N/V = n = const

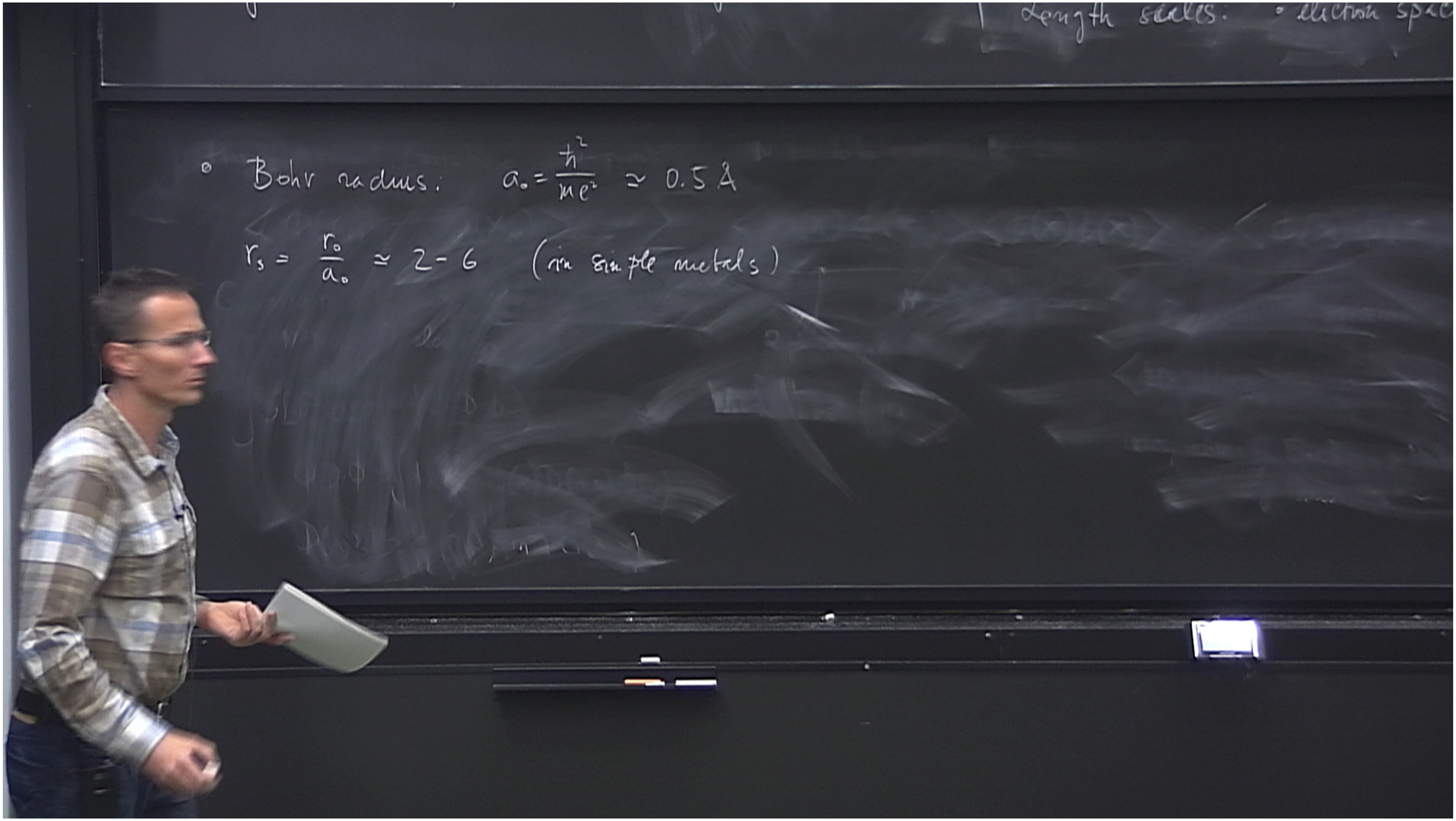

Ĥ/N = ... - e²/2 · 1/V · 4π/μ² → 0
Ĥ = Σ_{kλ} ħ²k²/2m c†_{kλ} c_{kλ} + e²/2V Σ'_{kpq, αβ} 4π/q c†_{k+q α} c†_{p-q β} c_{pβ} c_{kα}

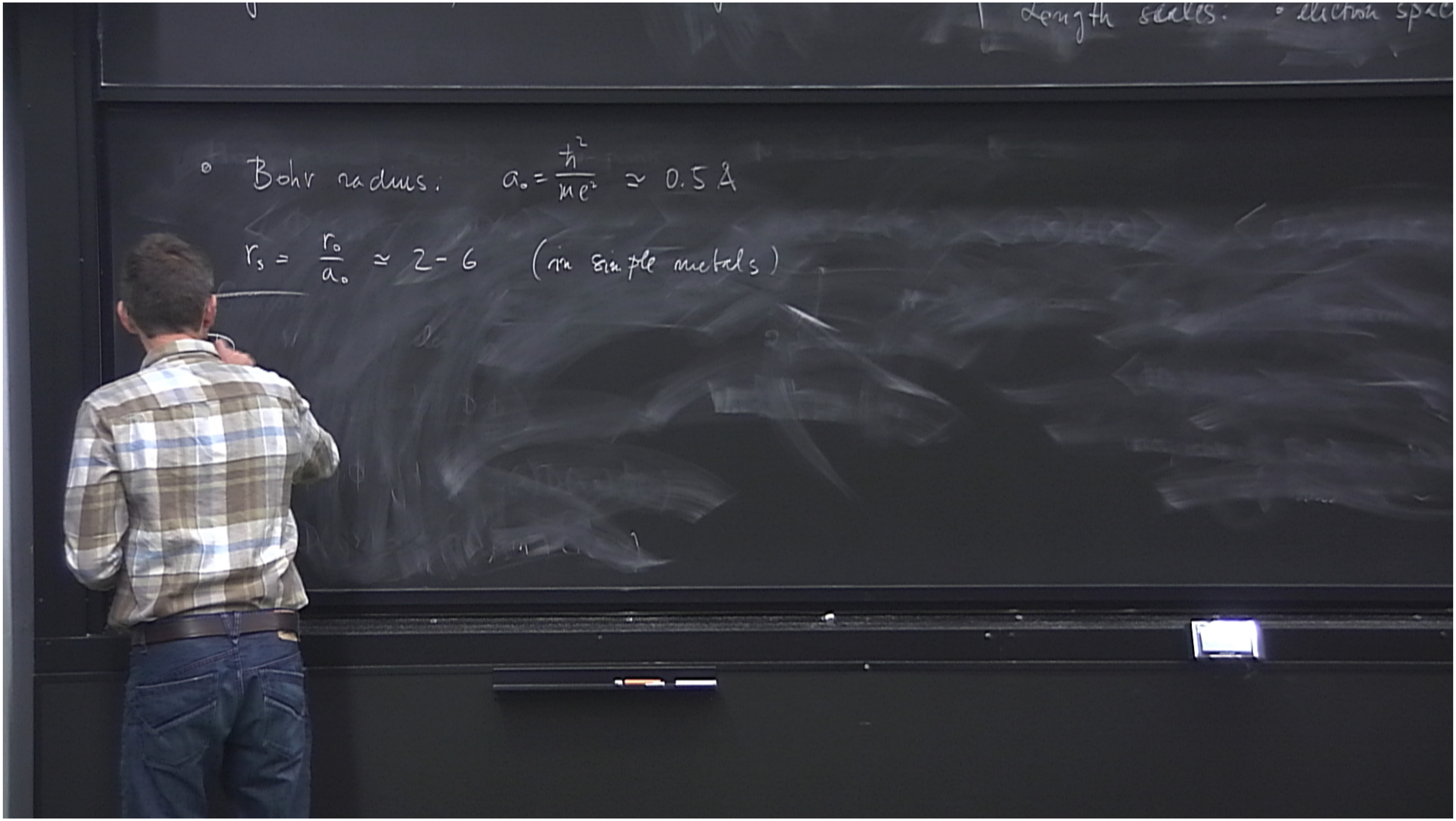


$\frac{\hat{H}}{N} = \cdots - \frac{e^2}{2}\frac{1}{V}\frac{4\pi}{\mu^2} \to 0$
$\vec{p}$ $\vec{p}-\vec{q}$ $\vec{k}$ $\vec{k}+\vec{q}$ $\frac{4\pi}{q^2}$
$\hat{H} = \sum_{k\lambda} \frac{\hbar^2 k^2}{2m} c^\dagger_{k\lambda} c_{k\lambda} + \frac{e^2}{2V} \sum'_{kpq\,\alpha\beta} \frac{4\pi}{q^2} c^\dagger_{k+q\,\alpha} c^\dagger_{p-q\,\beta} c_{p\beta} c_{k\alpha}$
$v_F \sim \frac{c}{100}$


Ĥ = Σ ħ²k²/2m c†kλ ckλ + e²/2V Σ' 4π/q² c†k+q α c†p-q β cpβ ckα
vF ~ c/100
Rewrite Ĥ in dimensionless variables
Length scales: • electron spacing r0 : V/N = 4/3 π r0³ =>


Length scales:
Bohr radius: $a_0 = \frac{\hbar^2}{me^2} \simeq 0.5$ Å
$r_s = \frac{r_0}{a_0} \simeq 2-6$ (in metals)


Length scales: • electron spac
• Bohr radius: a₀ = ħ²/me² ≃ 0.5 Å
r_s = r₀/a₀ ≃ 2 - 6 (in simple metals)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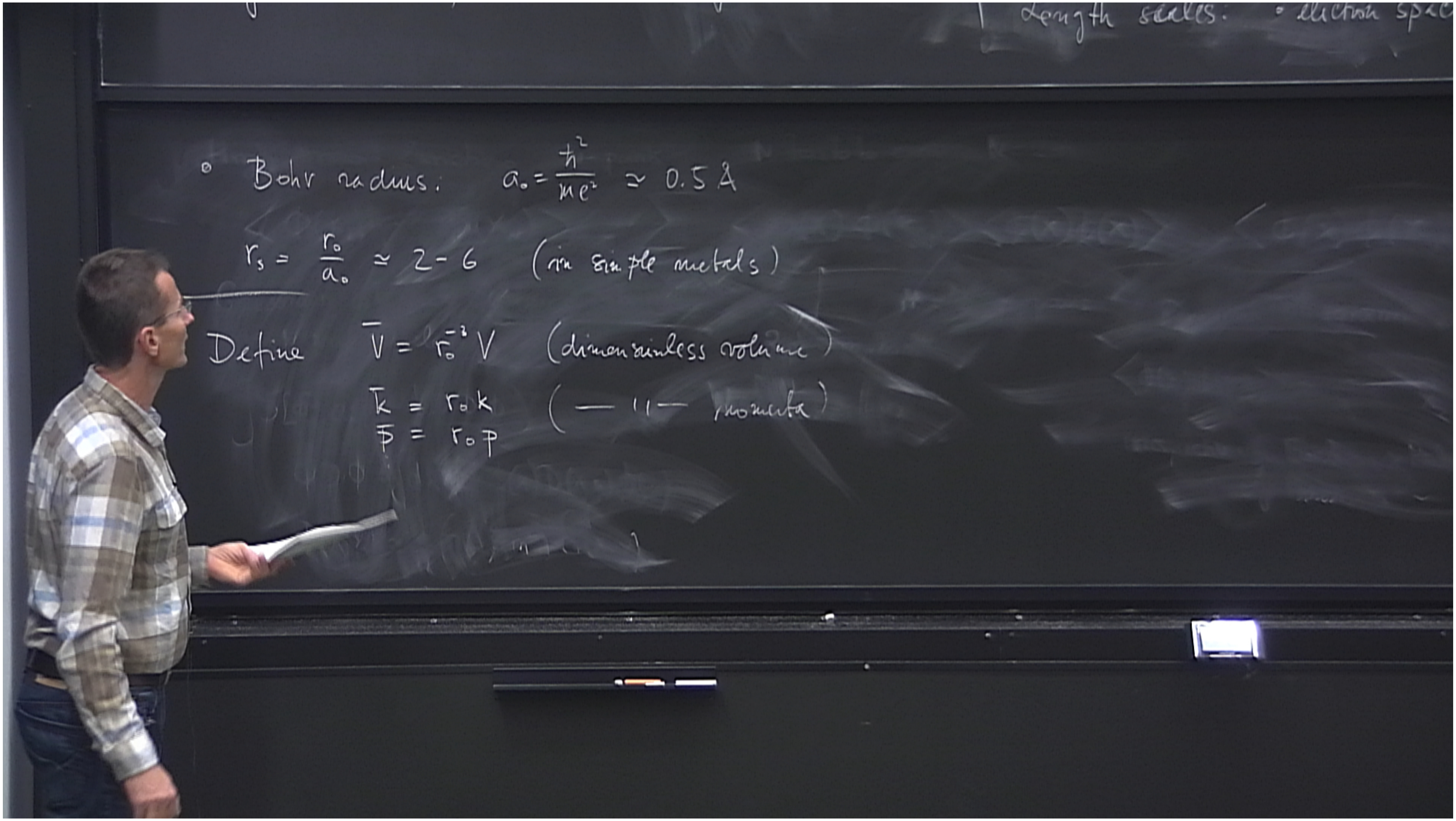
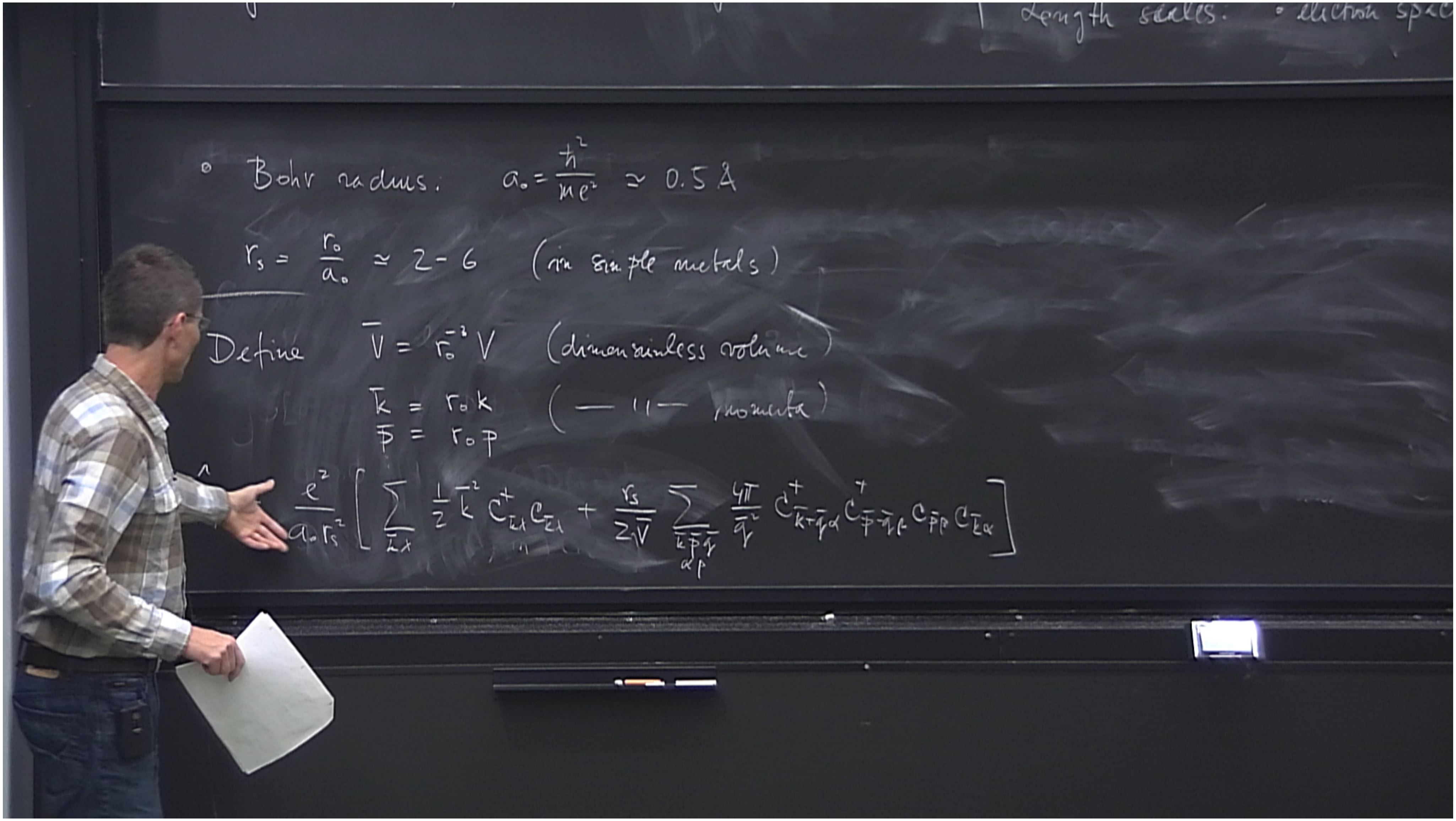
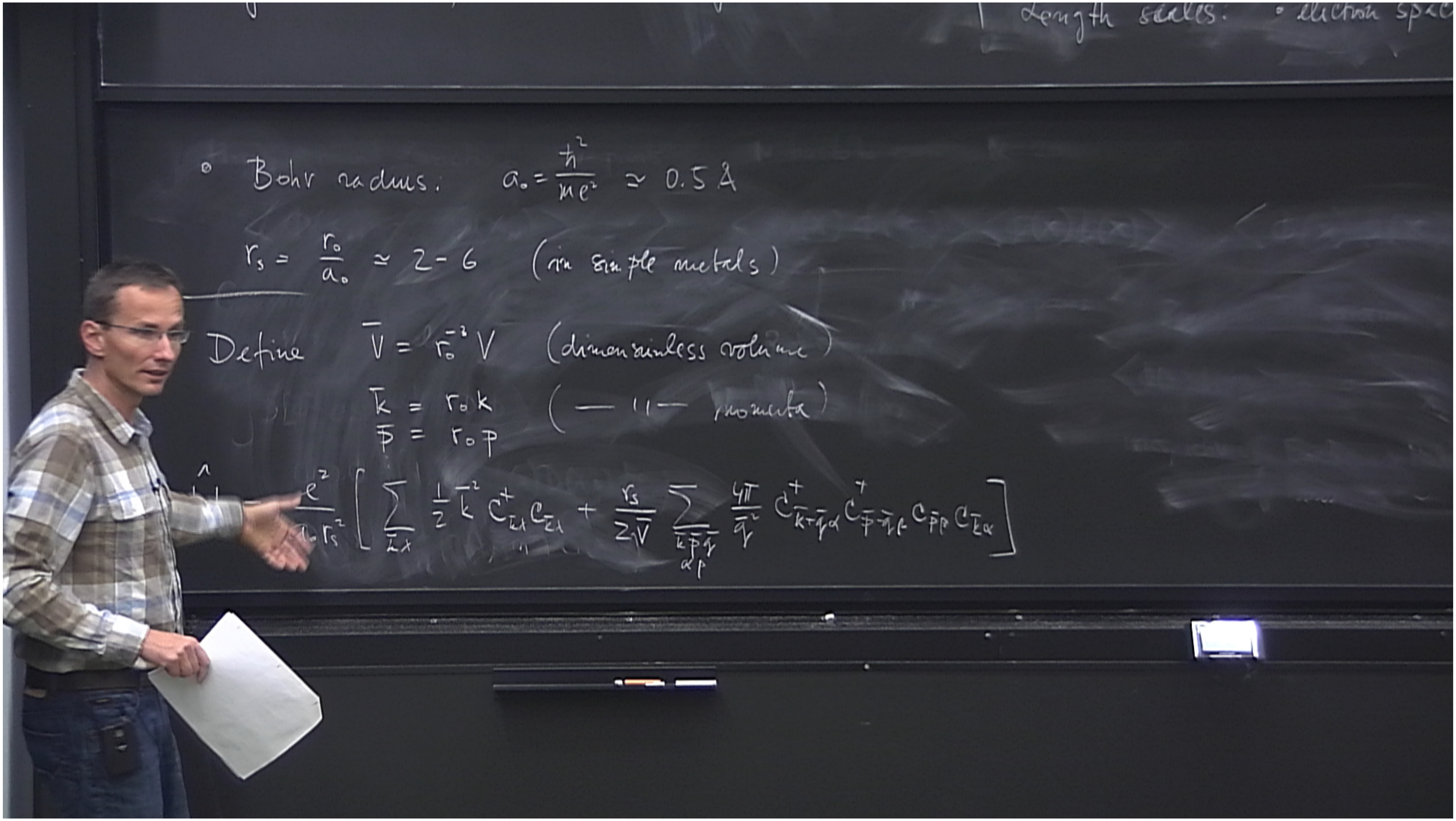

Length scales: • electron
• Bohr radius: $a_0 = \frac{\hbar^2}{me^2} \simeq 0.5$ Å
$r_s = \frac{r_0}{a_0} \simeq 2-6$ (in simple metals)
Define $\bar{V} = r_0^{-3} V$ (dimensionless volume)
$\bar{k} = r_0 k$ (—"— momenta)
$\bar{p} = r_0 p$


Length scales: • electron spac
• Bohr radius: $a_0 = \frac{\hbar^2}{me^2} \simeq 0.5$ Å
$r_s = \frac{r_0}{a_0} \simeq 2-6$ (in simple metals)
Define $\bar{V} = r_0^{-3} V$ (dimensionless volume)
$\bar{k} = r_0 k$ (— " — momenta)
$\bar{p} = r_0 p$
$\frac{e^2}{a_0 r_s^2}\left[\sum_{\bar{k}\alpha} \frac{1}{2}\bar{k}^2 c^\dagger_{\bar{k}\alpha} c_{\bar{k}\alpha} + \frac{r_s}{2\bar{V}} \sum_{\substack{\bar{k}\bar{p}\bar{q}\\ \alpha\beta}} \frac{4\pi}{\bar{q}^2} c^\dagger_{\bar{k}+\bar{q}\alpha} c^\dagger_{\bar{p}-\bar{q}\beta} c_{\bar{p}\beta} c_{\bar{k}\alpha}\right]$


Length scales:
• Bohr radius: $a_0 = \frac{\hbar^2}{me^2} \simeq 0.5$ Å
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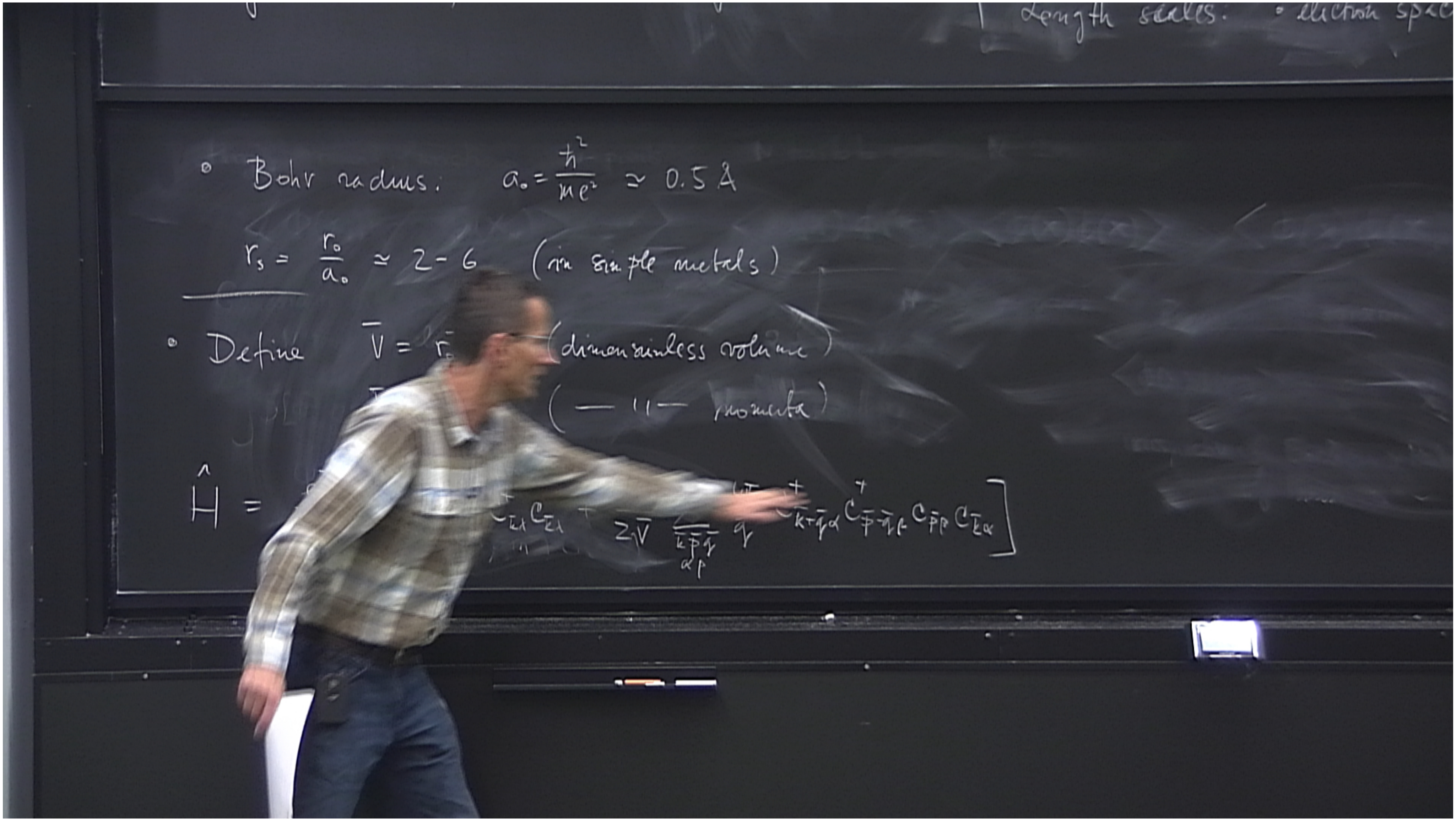
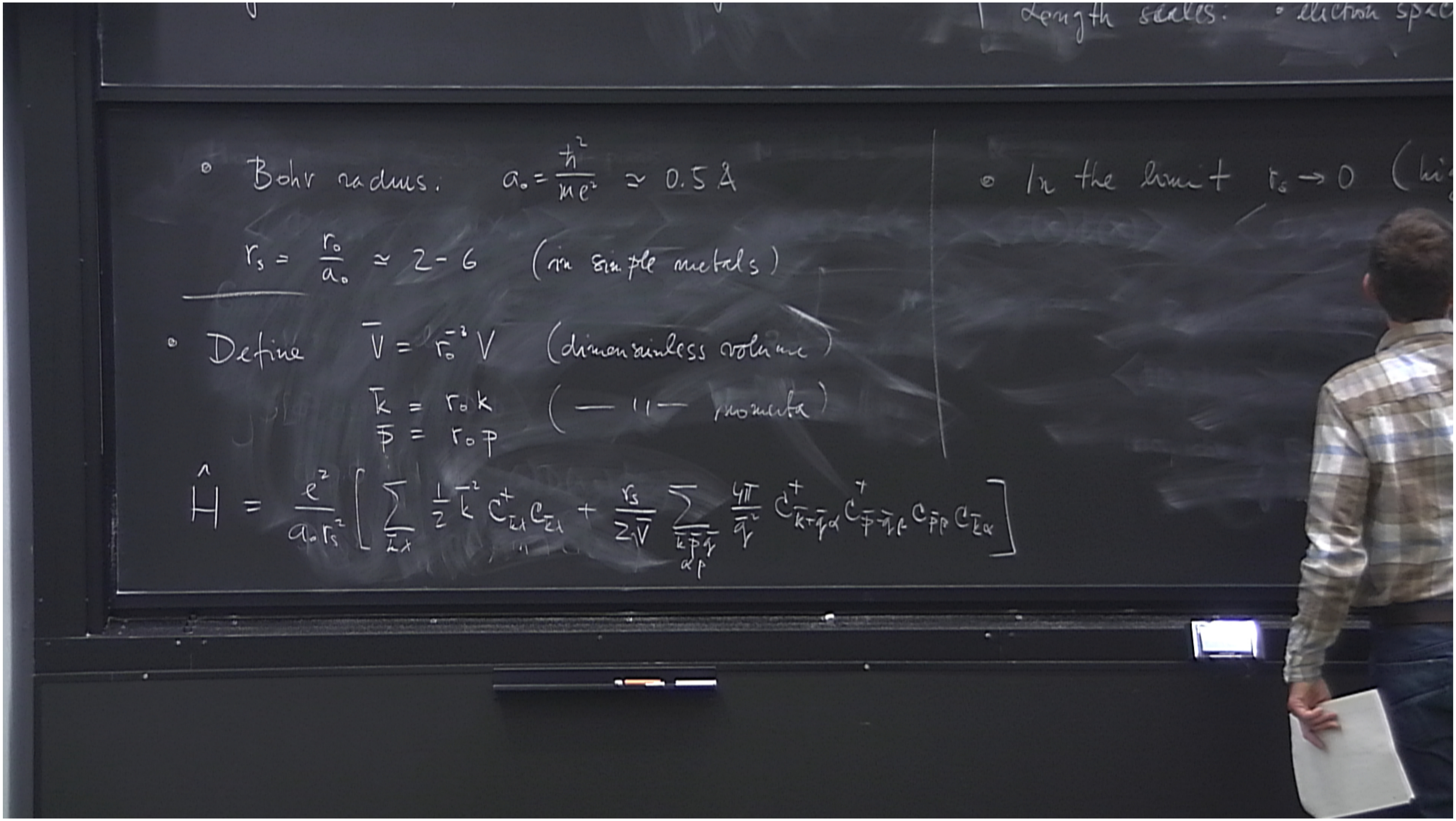
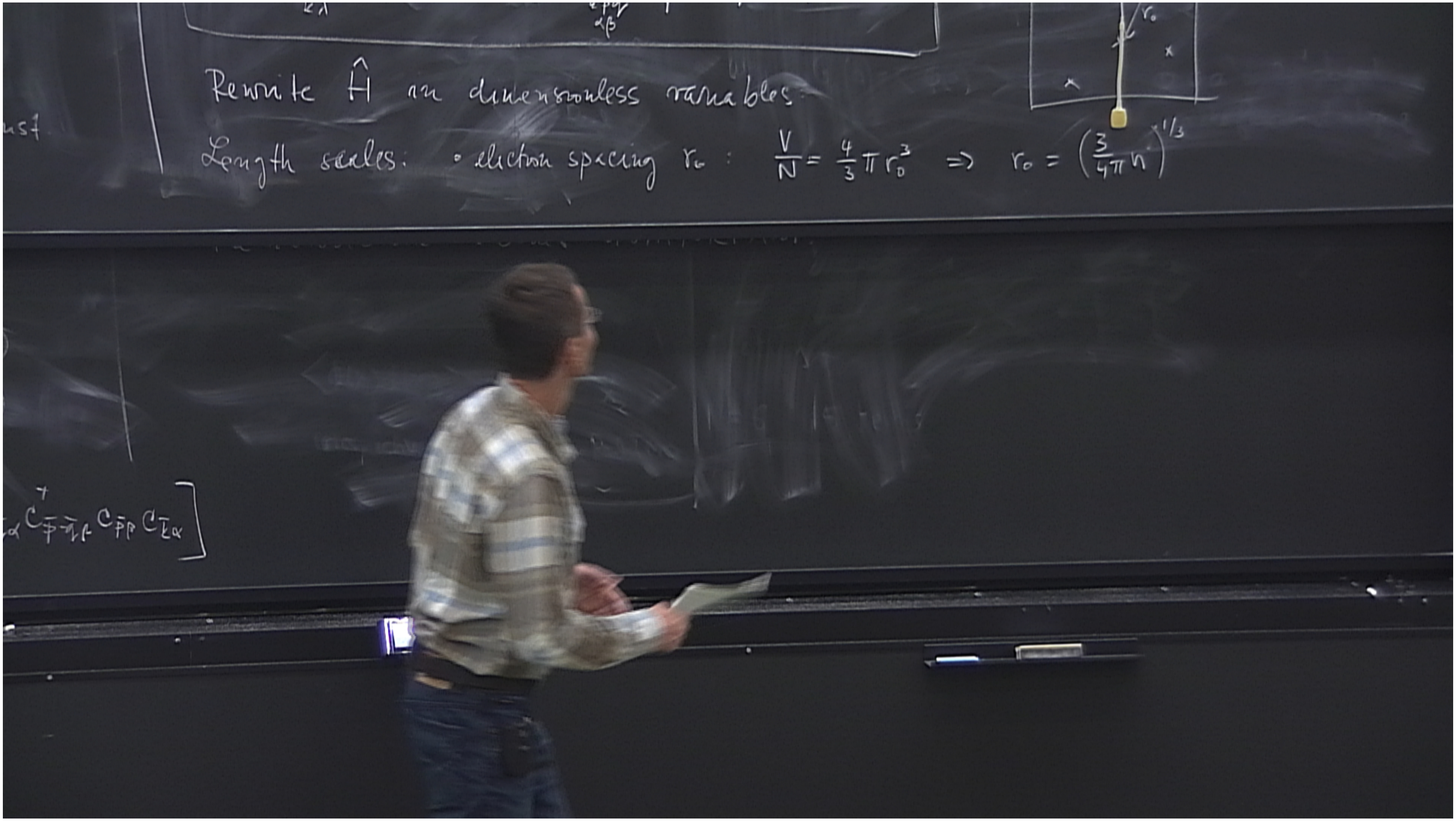
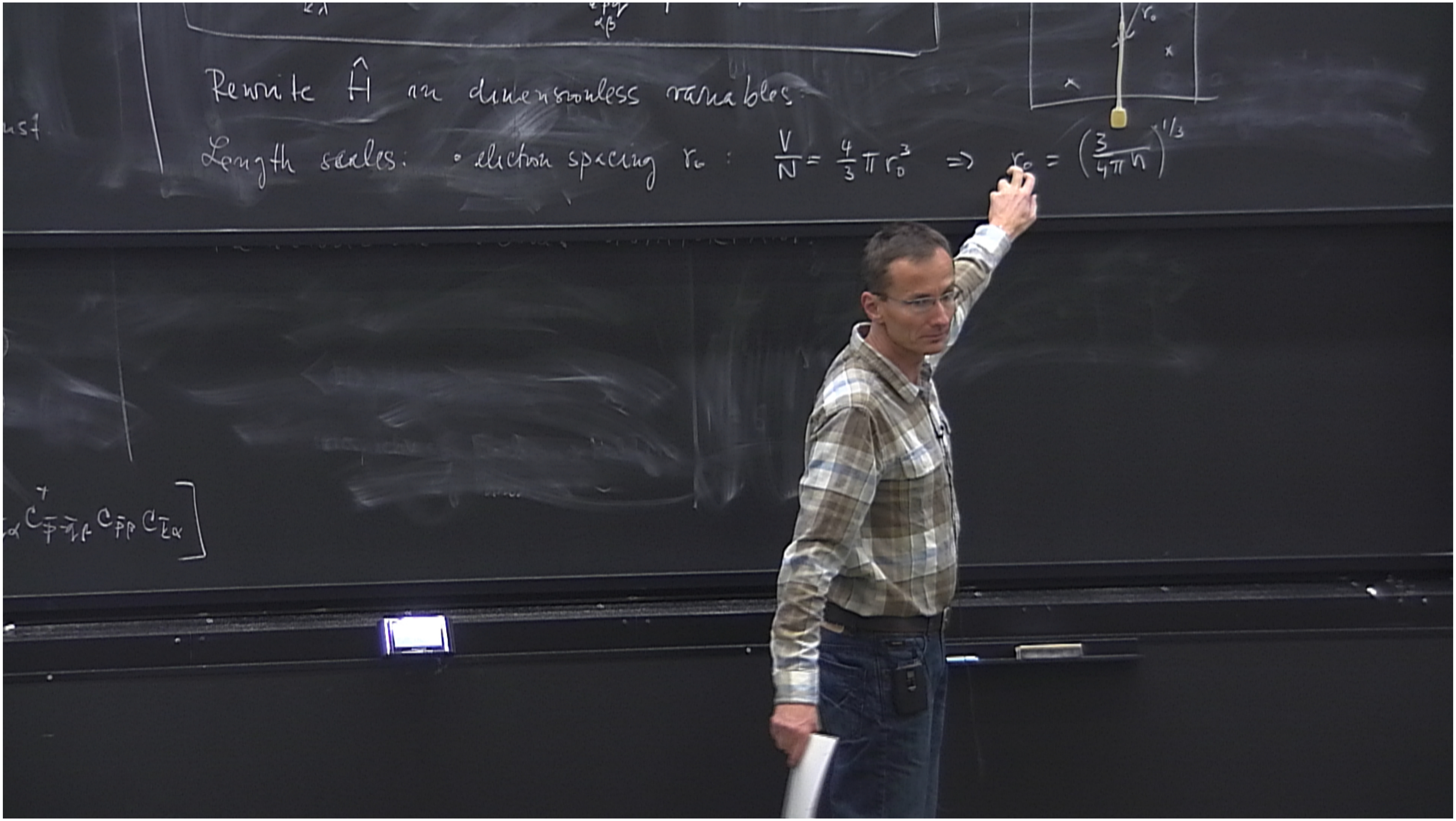
$\frac{e^2}{a_0 r_s^2}\left[\sum_{\bar{k}\alpha} \frac{1}{2}\bar{k}^2 c^\dagger_{\bar{k}\alpha} c_{\bar{k}\alpha} + \frac{r_s}{2\bar{V}} \sum_{\bar{k}\bar{p}\bar{q}, \alpha\beta} \frac{4\pi}{\bar{q}^2} c^\dagger_{\bar{k}+\bar{q}\alpha} c^\dagger_{\bar{p}-\bar{q}\beta} c_{\bar{p}\beta} c_{\bar{k}\alpha} \right]$


Length scales: • electron spac
• Bohr radius: $a_0 = \frac{\hbar^2}{me^2} \simeq 0.5$ Å
$r_s = \frac{r_0}{a_0} \simeq 2-6$ (in simple metals)
• Define
(dimensionless volume)
(— " — momenta)


Length scales: ∘ electron spac
∘ Bohr radius: $a_0 = \frac{\hbar^2}{me^2} \simeq 0.5\,Å$
$r_s = \frac{r_0}{a_0} \simeq 2-6$ (in simple metals)
∘ Define $\bar{V} = r_0^{-3} V$ (dimensionless volume)
$\bar{k} = r_0 k$ (— " — momenta)
$\bar{p} = r_0 p$
$\hat{H} = \frac{e^2}{a_0 r_s^2}\left[\sum_{\bar{k}\alpha} \frac{1}{2}\bar{k}^2 c^\dagger_{\bar{k}\alpha} c_{\bar{k}\alpha} + \frac{r_s}{2\bar{V}} \sum_{\substack{\bar{k}\bar{p}\bar{q}\\ \alpha\beta}} \frac{4\pi}{\bar{q}^2} c^\dagger_{\bar{k}+\bar{q}\alpha} c^\dagger_{\bar{p}-\bar{q}\beta} c_{\bar{p}\beta} c_{\bar{k}\alpha}\right]$
∘ In the limit $r_s \to 0$ (hi


Rewrite Ĥ in dimensionless variables:
Length scales: • electron spacing r0 : V/N = 4/3 π r0^3 => r0 = (3/4πn)^1/3


Rewrite Ĥ in dimensionless variables:
Length scales: • electron spacing r0 : V/N = 4/3 π r0^3 => r0 = (3/4πn)^1/3

- In the limit $r_s \to 0$ (high density) the interaction becomes UNIMPORTANT.
- Treat $\hat{H}_{int}$ perturbatively in r_s
- Expand physical quantities in powers of r_s.

$$E_g = \frac{Ne^2}{a_0 r_s^2}\left[a + b r_s + c r_s^2 \ln r_s + d r_s^2 + \dots\right]$$

$$\frac{4\pi}{\bar{q}^2} c^{\dagger}_{\bar{k}+\bar{q}\alpha} c^{\dagger}_{\bar{p}-\bar{q}\beta} c_{\bar{p}\beta} c_{\bar{k}\alpha} \Big]$$

- In the limit $r_s \to 0$ (high density) the interaction becomes UNIMPORTANT.
- Treat $\hat{H}_{int}$ perturbatively in r_s
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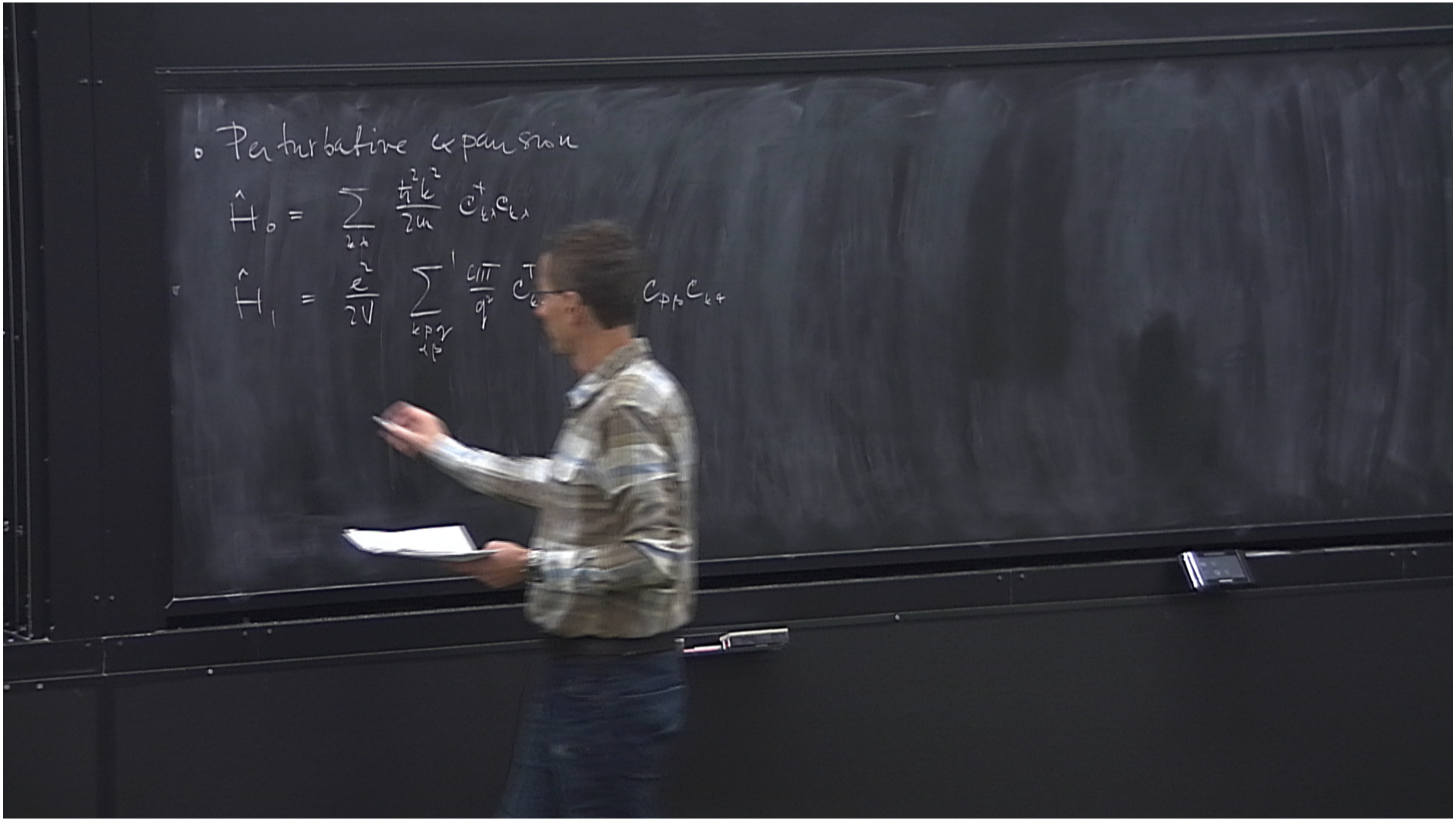
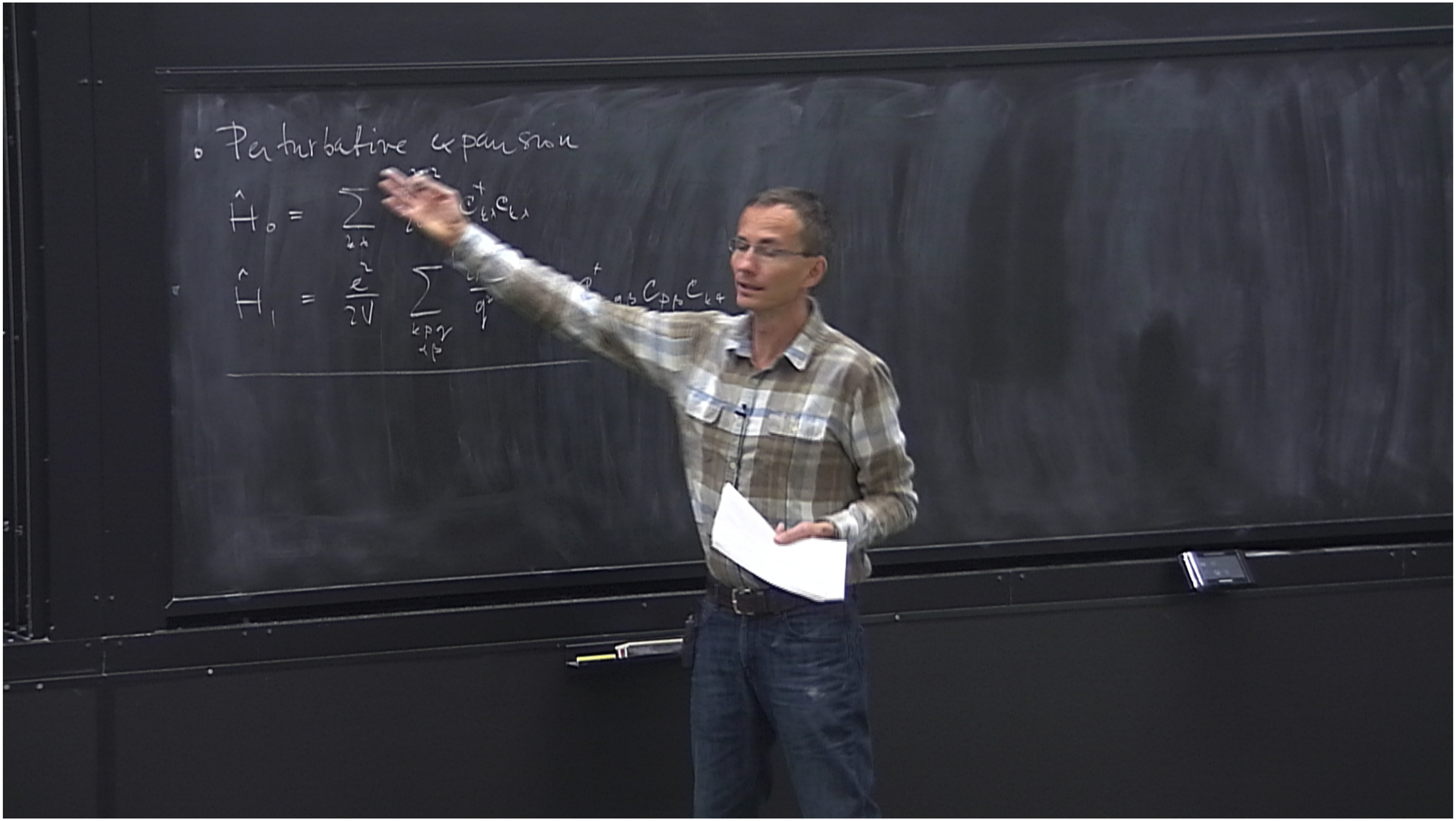
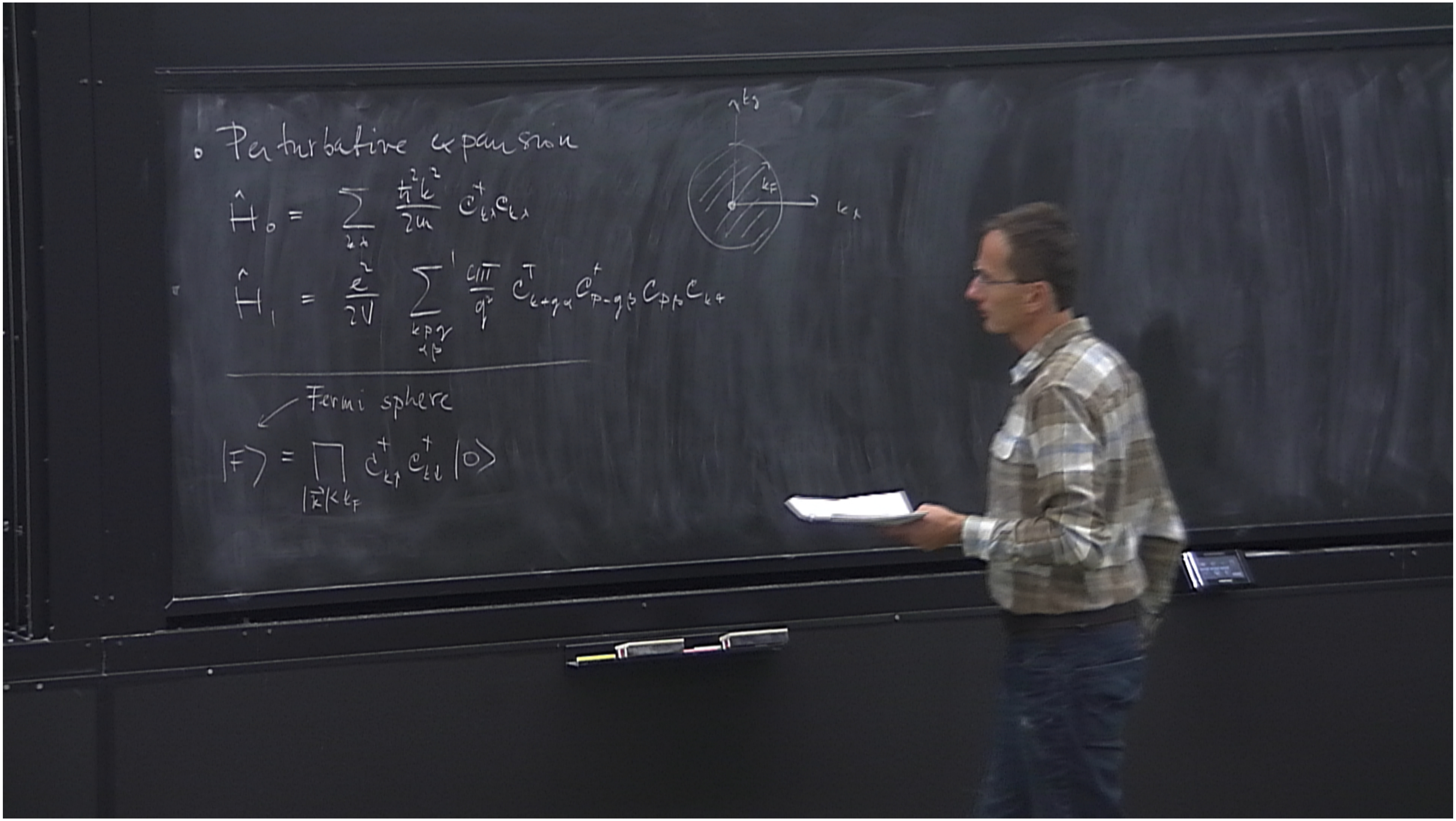
$$E_g = \frac{Ne^2}{a_0 r_s^2}\left[\underline{a} + \underline{b} r_s + \underline{c} r_s^2 \ln r_s + \underline{d} r_s^2 + \dots\right]$$

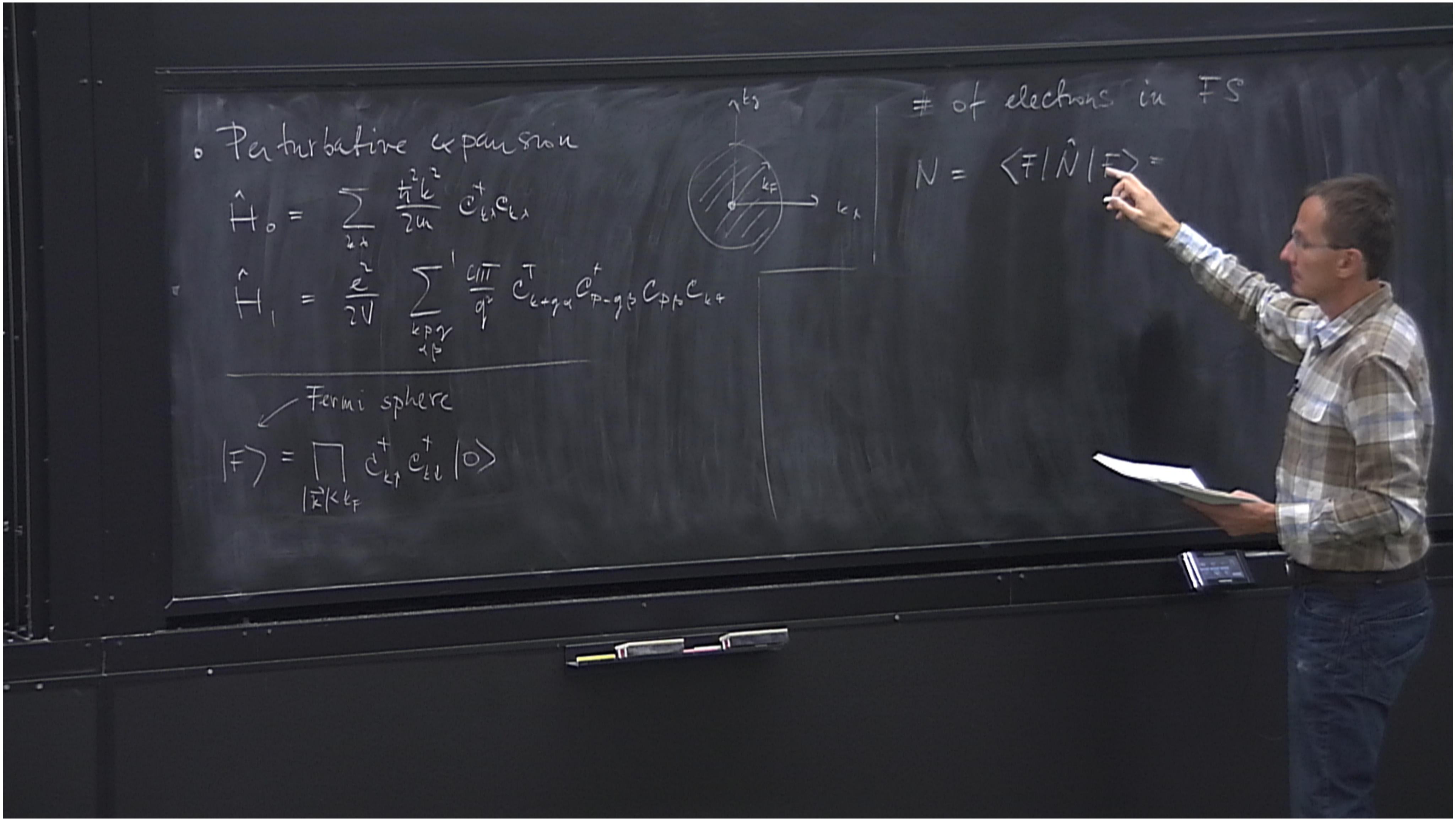
$$\frac{4\pi}{\bar{q}^2} c^{\dagger}_{\bar{k}+\bar{q}\alpha} c^{\dagger}_{\bar{p}-\bar{q}\beta} c_{\bar{p}\beta} c_{\bar{k}\alpha}\Big]$$


Perturbative expansion

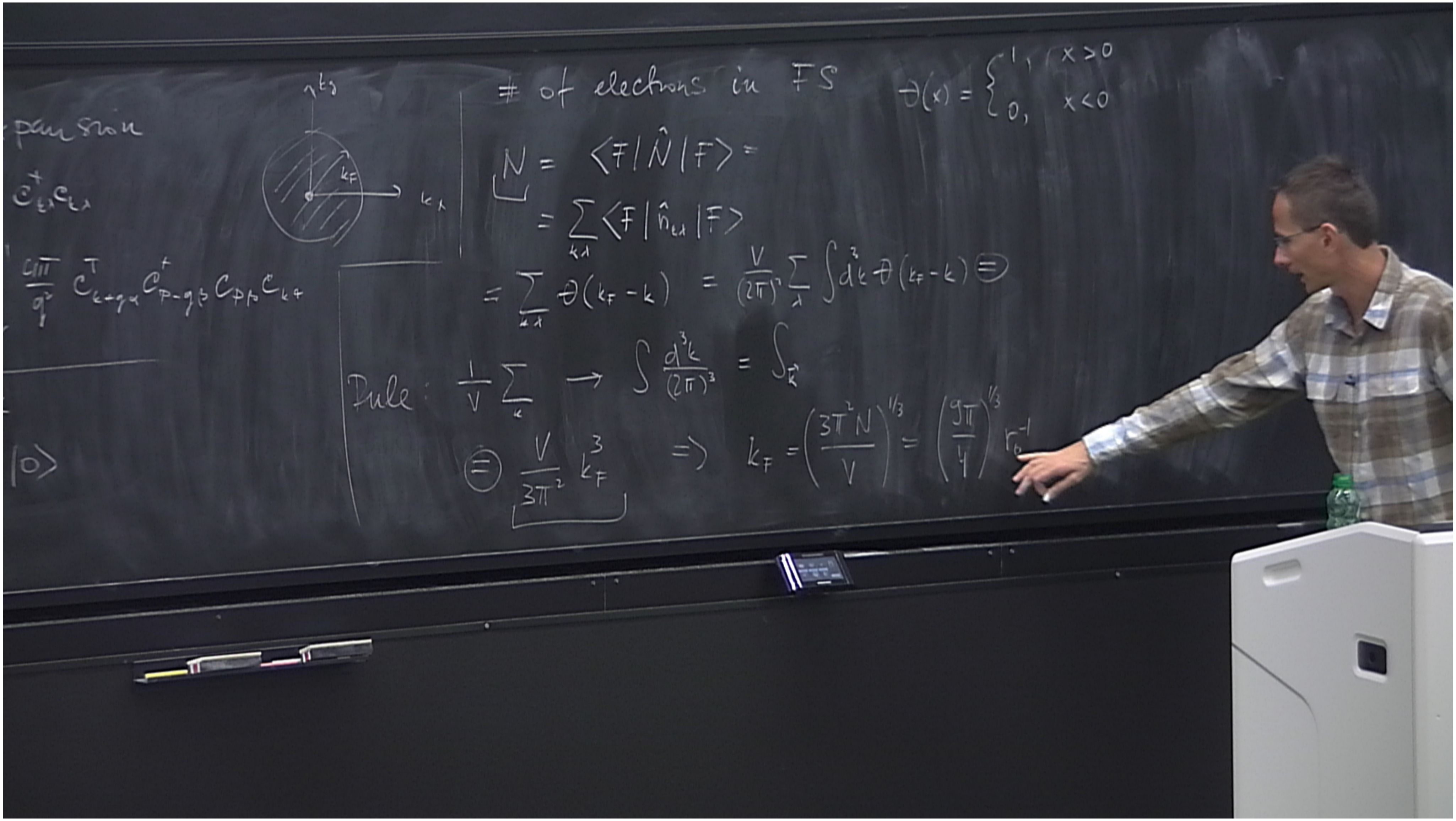

Perturbative expansion

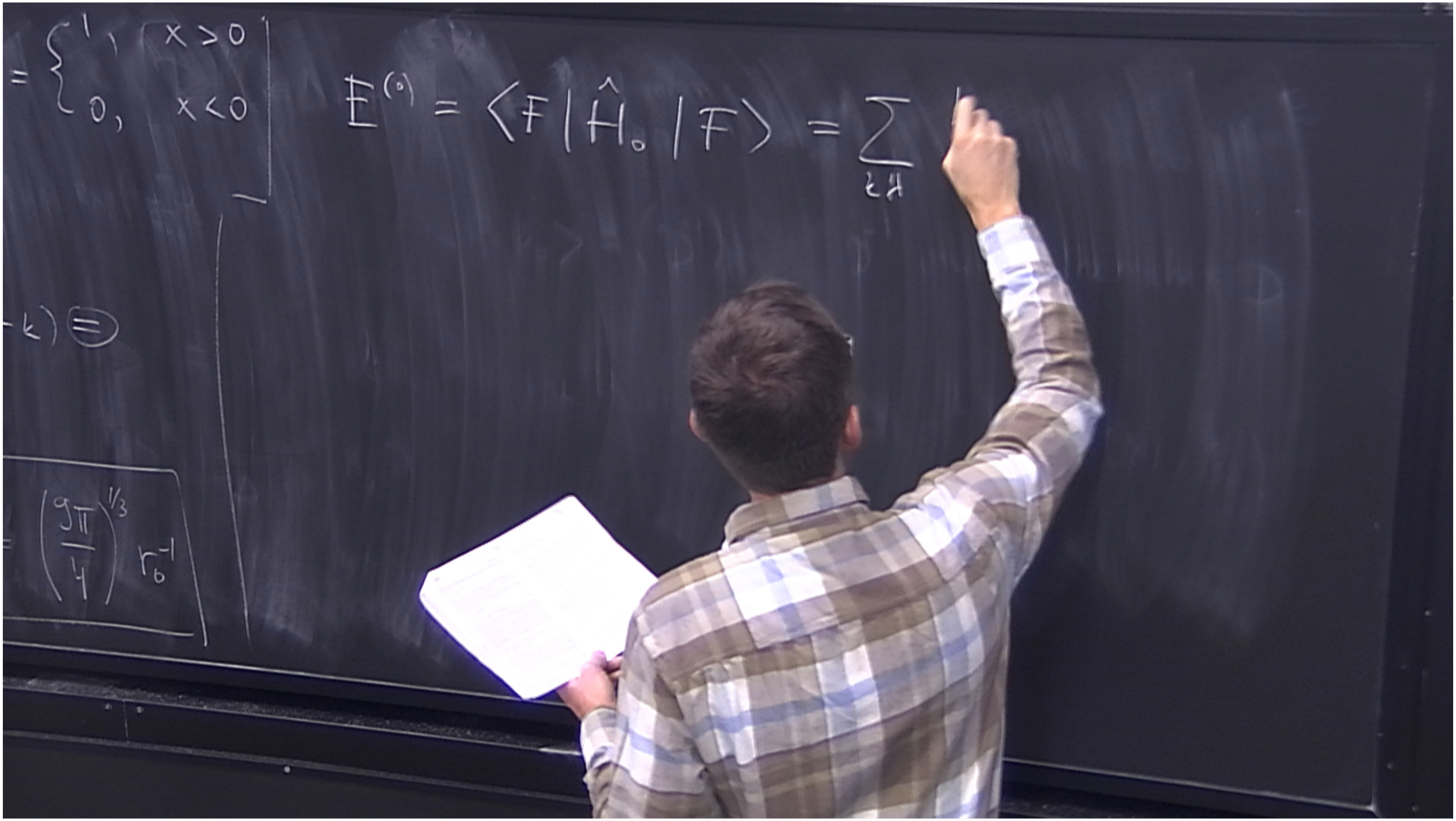


Perturbative expansion
$\hat{H}_0 = \sum_{k\lambda} \frac{\hbar^2 k^2}{2m} c^\dagger_{k\lambda} c_{k\lambda}$
$\hat{H}_1 = \frac{e^2}{2V} \sum'_{kpq\,\alpha\beta} \frac{4\pi}{q^2} c^\dagger_{k+q\alpha} c^\dagger_{p-q\beta} c_{p\beta} c_{k\alpha}$
Fermi sphere
$|F\rangle = \prod_{|\vec{k}|<k_F} c^\dagger_{k\uparrow} c^\dagger_{k\downarrow} |0\rangle$
k_y
k_F
k_x

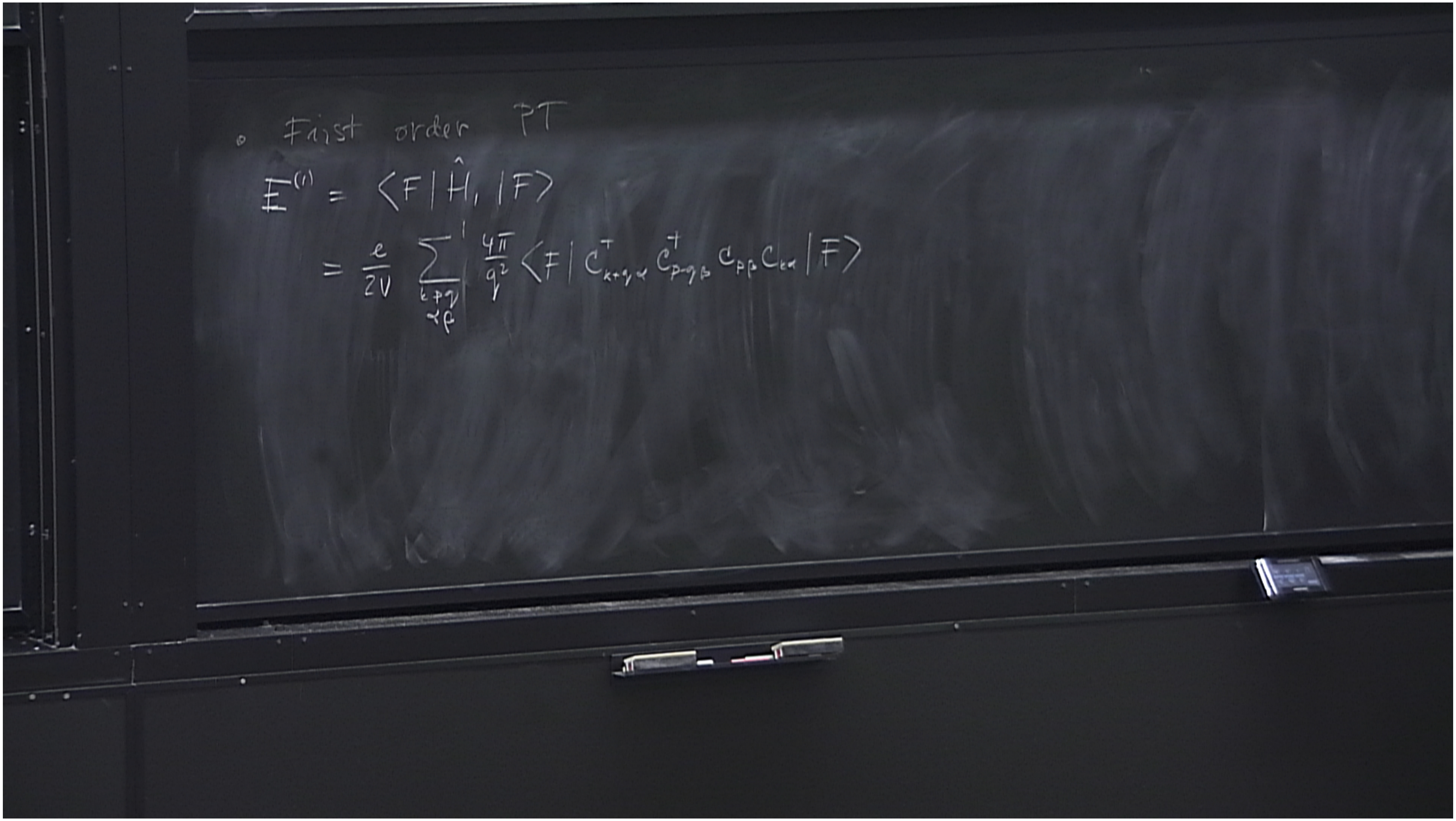


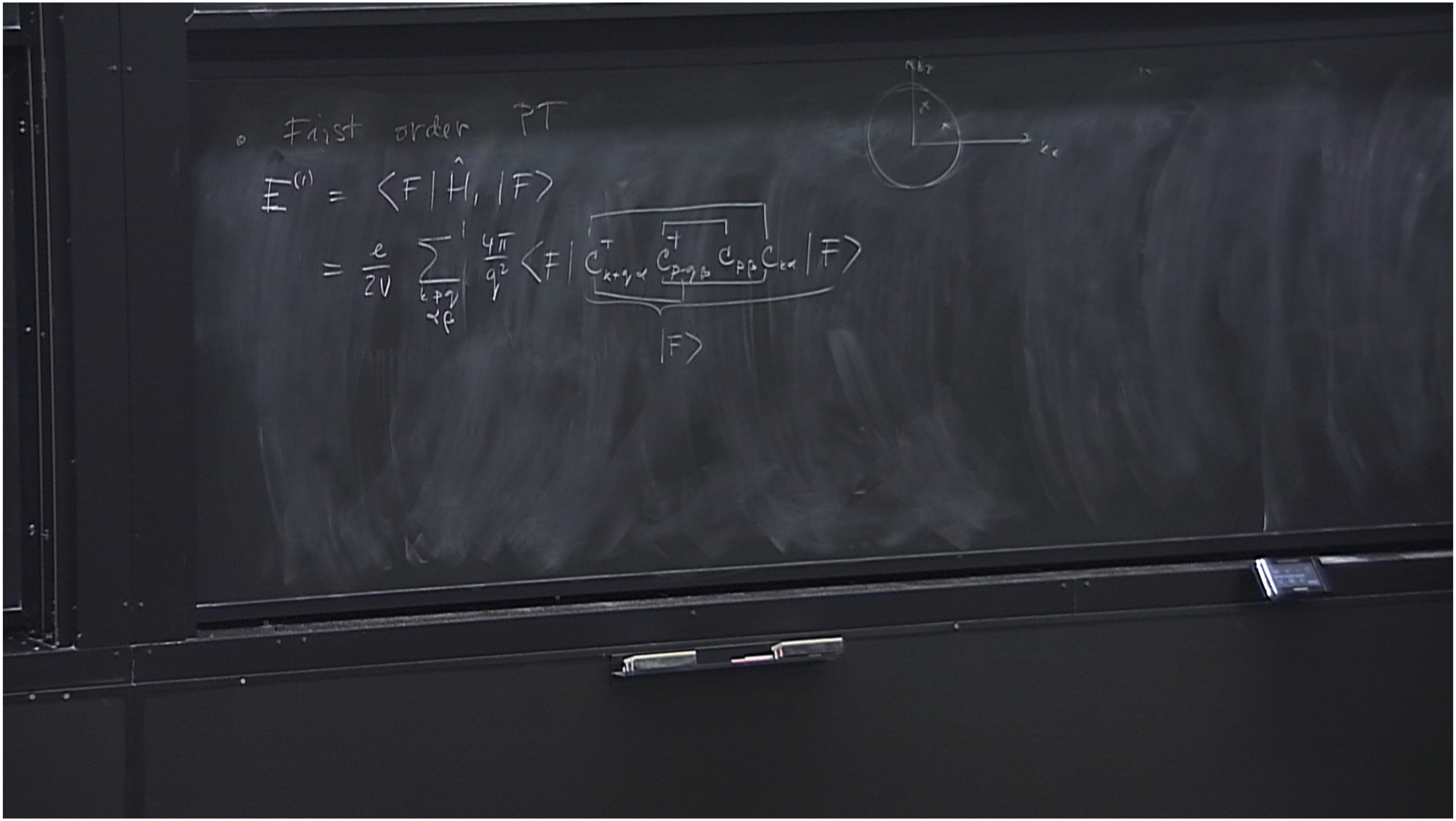
• Perturbative expansion
$\hat{H}_0 = \sum_{k\lambda} \frac{\hbar^2 k^2}{2m} c^\dagger_{k\lambda} c_{k\lambda}$
$\hat{H}_1 = \frac{e^2}{2V} \sum'_{kpq,\alpha\beta} \frac{4\pi}{q^2} c^\dagger_{k+q\alpha} c^\dagger_{p-q\beta} c_{p\beta} c_{k\alpha}$
Fermi sphere
$|F\rangle = \prod_{|\vec{k}|<k_F} c^\dagger_{k\uparrow} c^\dagger_{k\downarrow} |0\rangle$
k_y
k_F
k_x
# of electrons in FS
$N = \langle F|\hat{N}|F\rangle =$


# of electrons in FS
$\theta(x) = \begin{cases} 1, & x>0 \\ 0, & x<0 \end{cases}$
$N = \langle F | \hat{N} | F \rangle =$
$= \sum_{k\lambda} \langle F | \hat{n}_{k\lambda} | F \rangle$
$= \sum_{k\lambda} \theta(k_F - k) = \frac{V}{(2\pi)^3} \sum_\lambda \int d^3k \, \theta(k_F - k)$
Rule: $\frac{1}{V} \sum_k \rightarrow \int \frac{d^3k}{(2\pi)^3} = \int_{\vec{k}}$
$= \frac{V}{3\pi^2} k_F^3 \Rightarrow k_F = \left(\frac{3\pi^2 N}{V} \right)^{1/3} = \left(\frac{9\pi}{4} \right)^{1/3} r_0^{-1}$
k_F
k_x
k_y
$|0\rangle$



x > 0
x < 0
E^(0) = ⟨F| Ĥ₀ |F⟩ = Σ

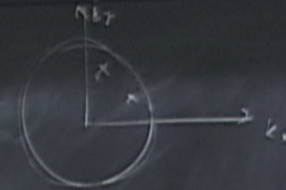

First order PT
$E^{(1)} = \langle F | \hat{H}_1 | F \rangle$
$= \frac{e}{2V} \sum'_{\substack{k p q \\ \alpha \beta}} \frac{4\pi}{q^2} \langle F | c^\dagger_{k+q\alpha} c^\dagger_{p-q\beta} c_{p\beta} c_{k\alpha} | F \rangle$


First order PT
E^(1) = ⟨F| Ĥ_1 |F⟩
= e/2V Σ' (k p q, α β) 4π/q² ⟨F| c†_{k+q α} c†_{p-q β} c_{p β} c_{k α} |F⟩
|F⟩

• First order PT

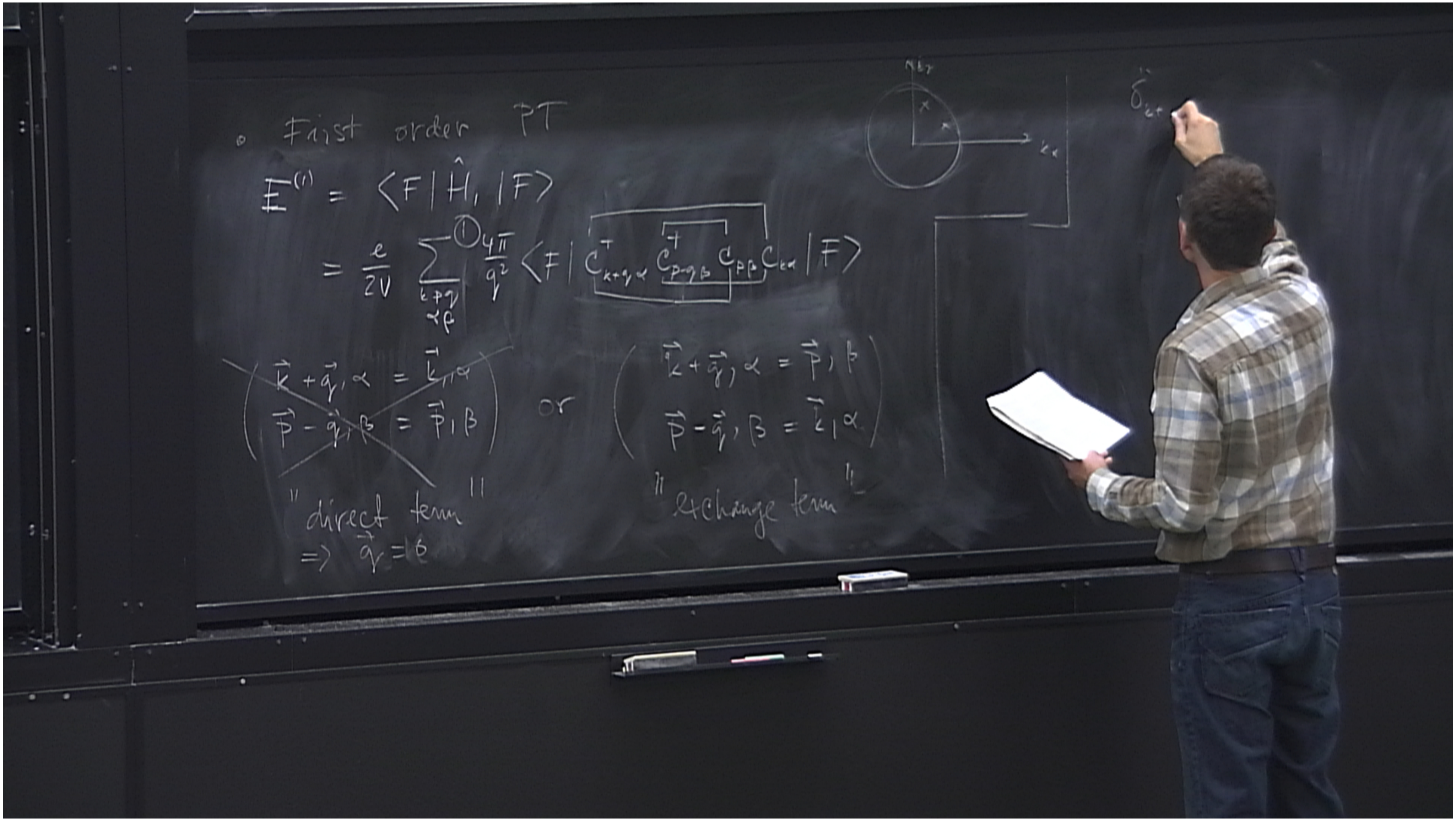
$$E^{(1)} = \langle F | \hat{H}_1 | F \rangle$$

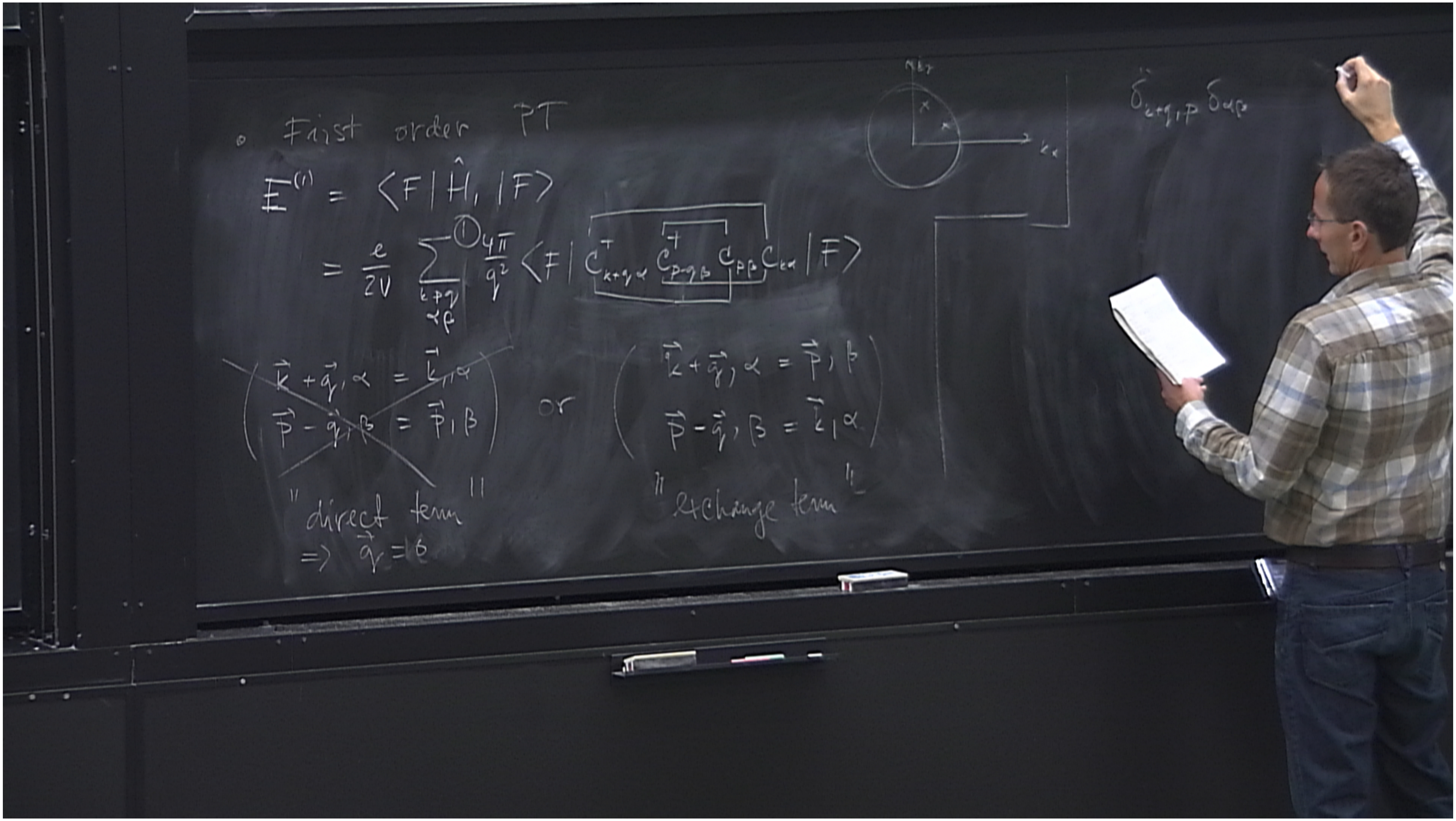
$$= \frac{e}{2V} \sum_{\substack{k\,p\,q \\ \alpha\beta}}{}' \frac{4\pi}{q^2} \langle F | c^\dagger_{k+q\,\alpha} \, c^\dagger_{p-q\,\beta} \, c_{p\beta} \, c_{k\alpha} | F \rangle$$

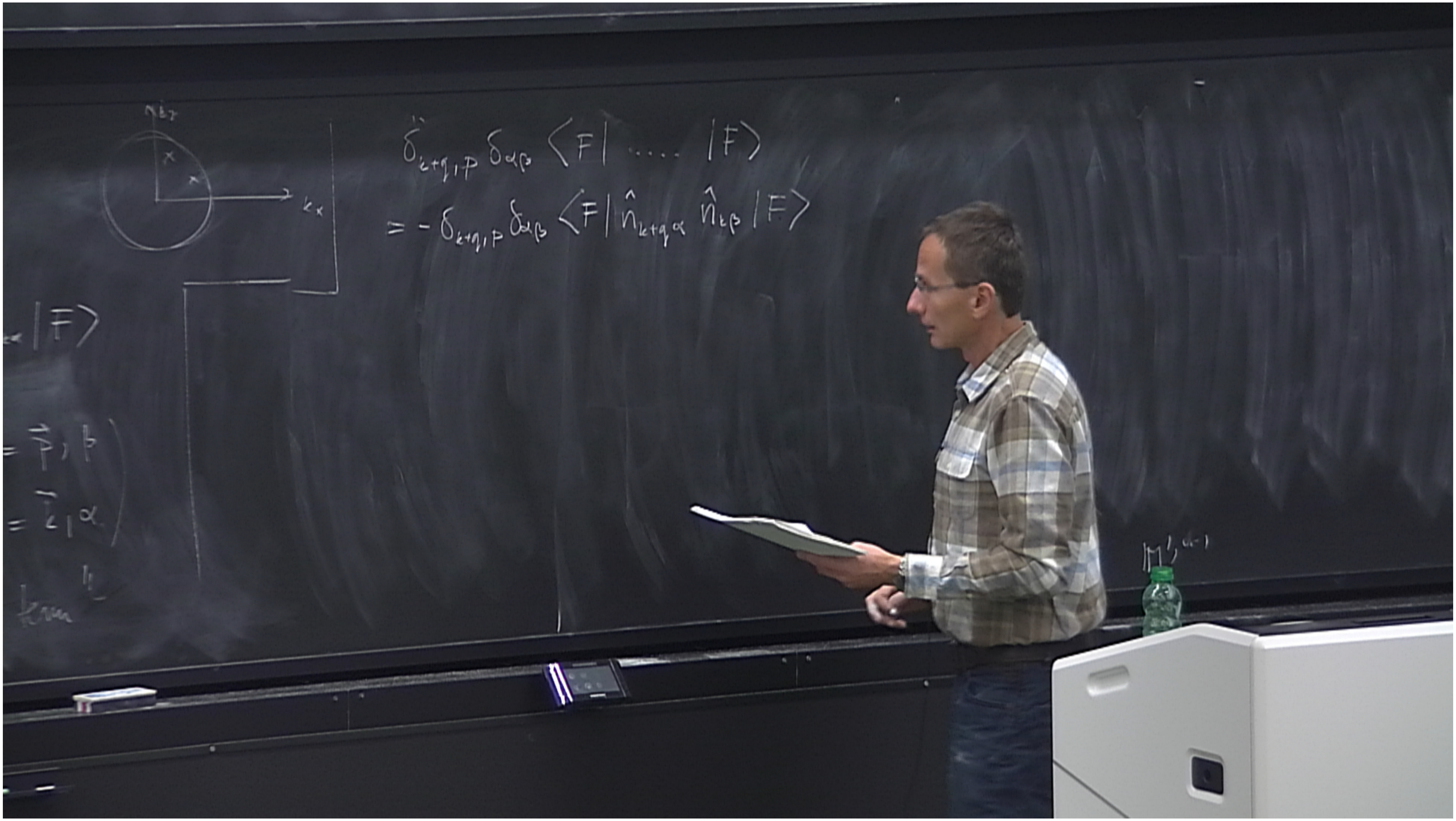


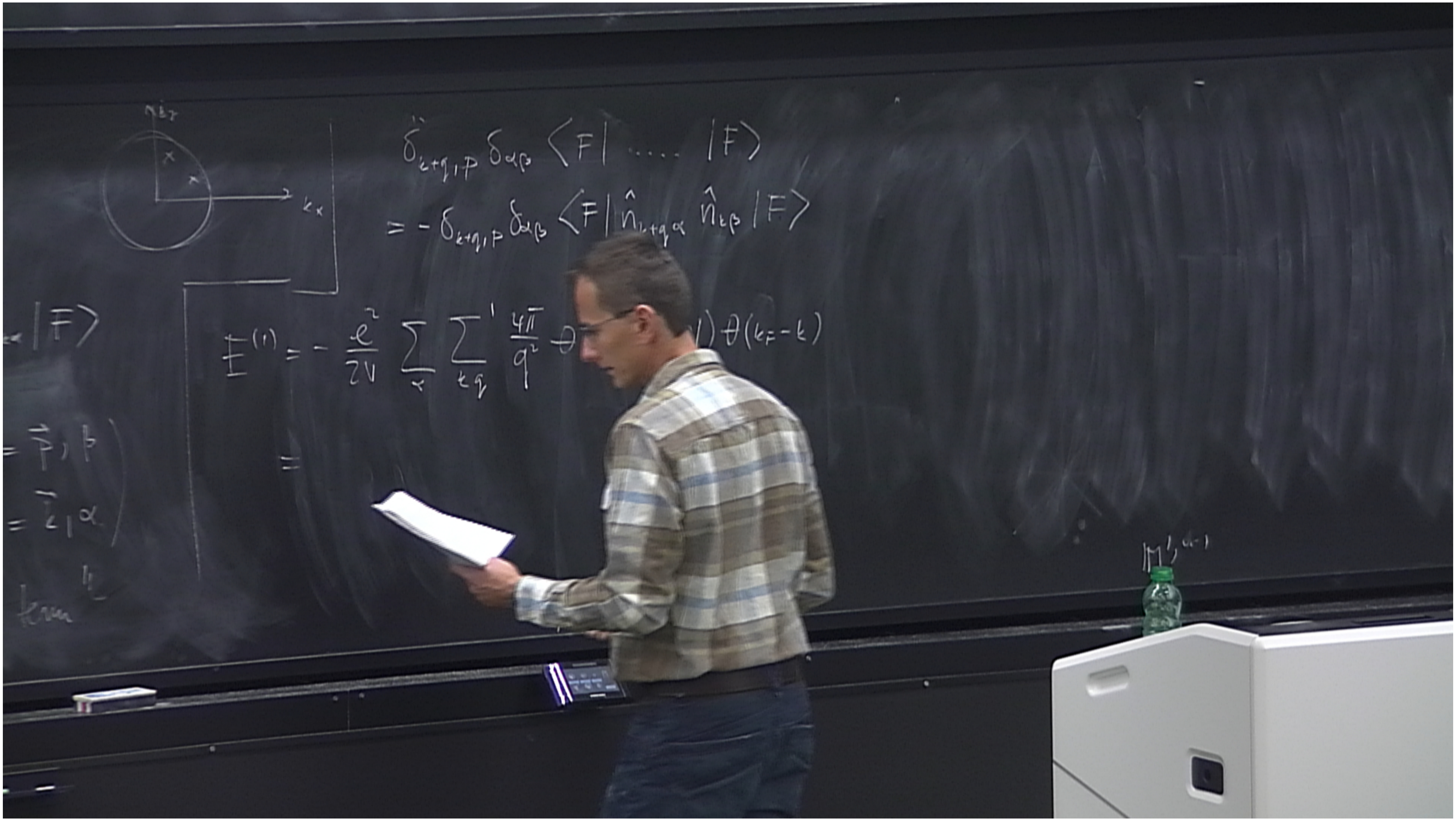
$$\begin{pmatrix} \vec{k}+\vec{q},\alpha = \vec{k},\alpha \\ \vec{p}-\vec{q},\beta = \vec{p},\beta \end{pmatrix} \quad \text{or} \quad \begin{pmatrix} \vec{k}+\vec{q},\alpha = \vec{p},\beta \\ \vec{p}-\vec{q},\beta = \vec{k},\alpha \end{pmatrix}$$

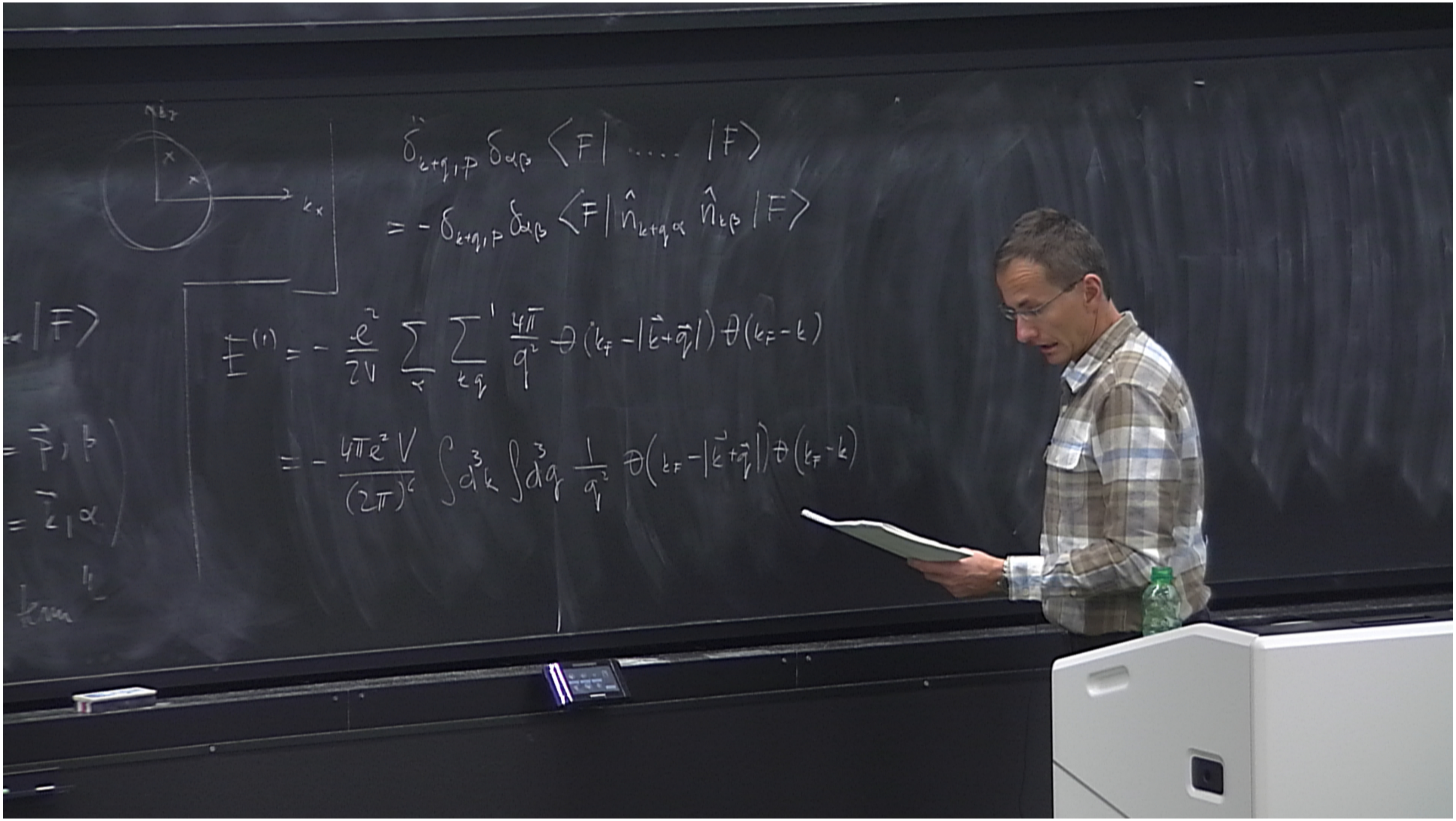
"direct term" "exchange term"

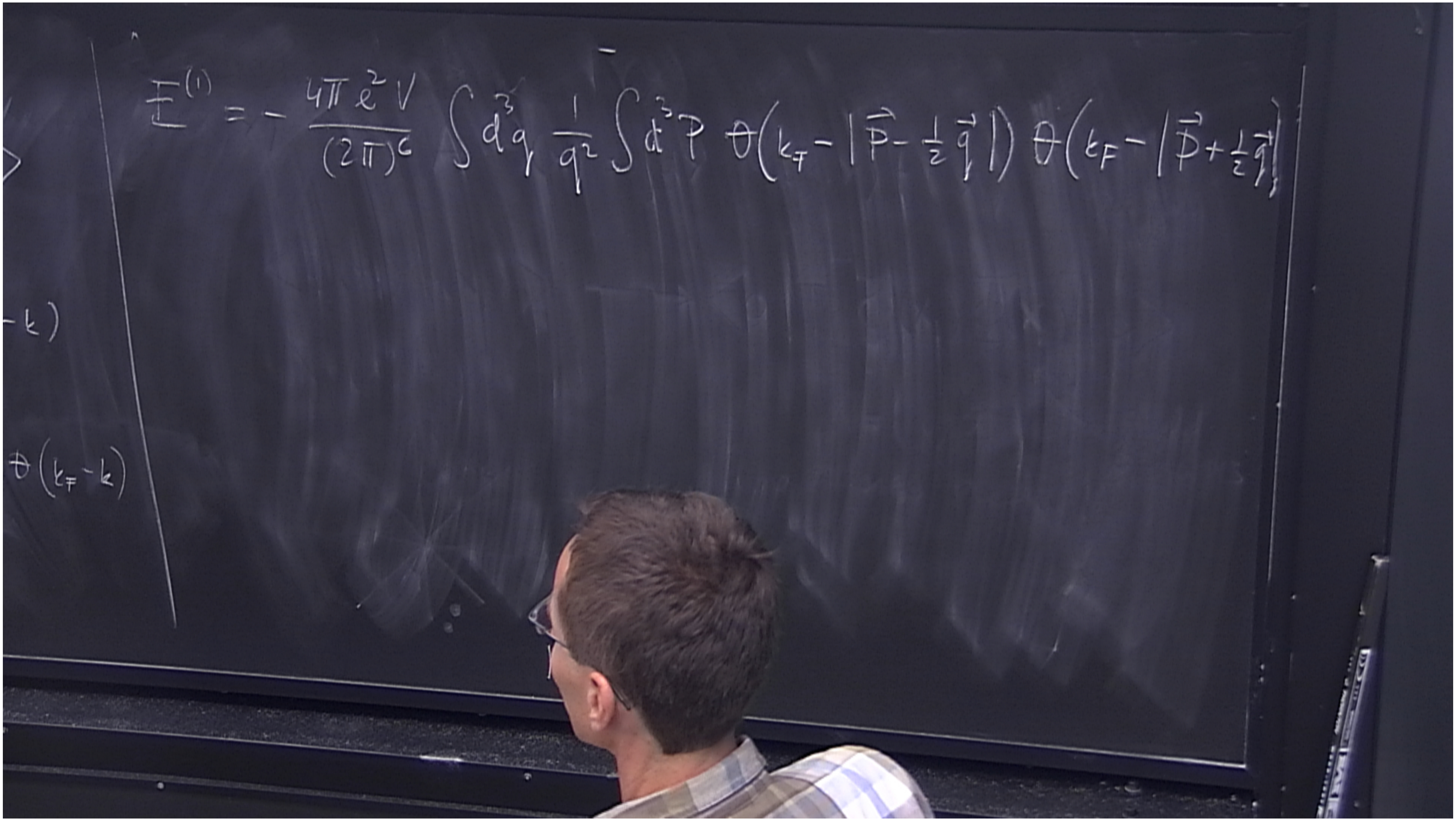

First order PT
E(1) = ⟨F| Ĥ1 |F⟩
= e/2V Σ 4π/q² ⟨F| c†k+q α c†p-q β cp β ck α |F⟩
k + q, α = k, α
p - q, β = p, β
or
k + q, α = p, β
p - q, β = k, α
"direct term"
=> q = 0
"exchange term"

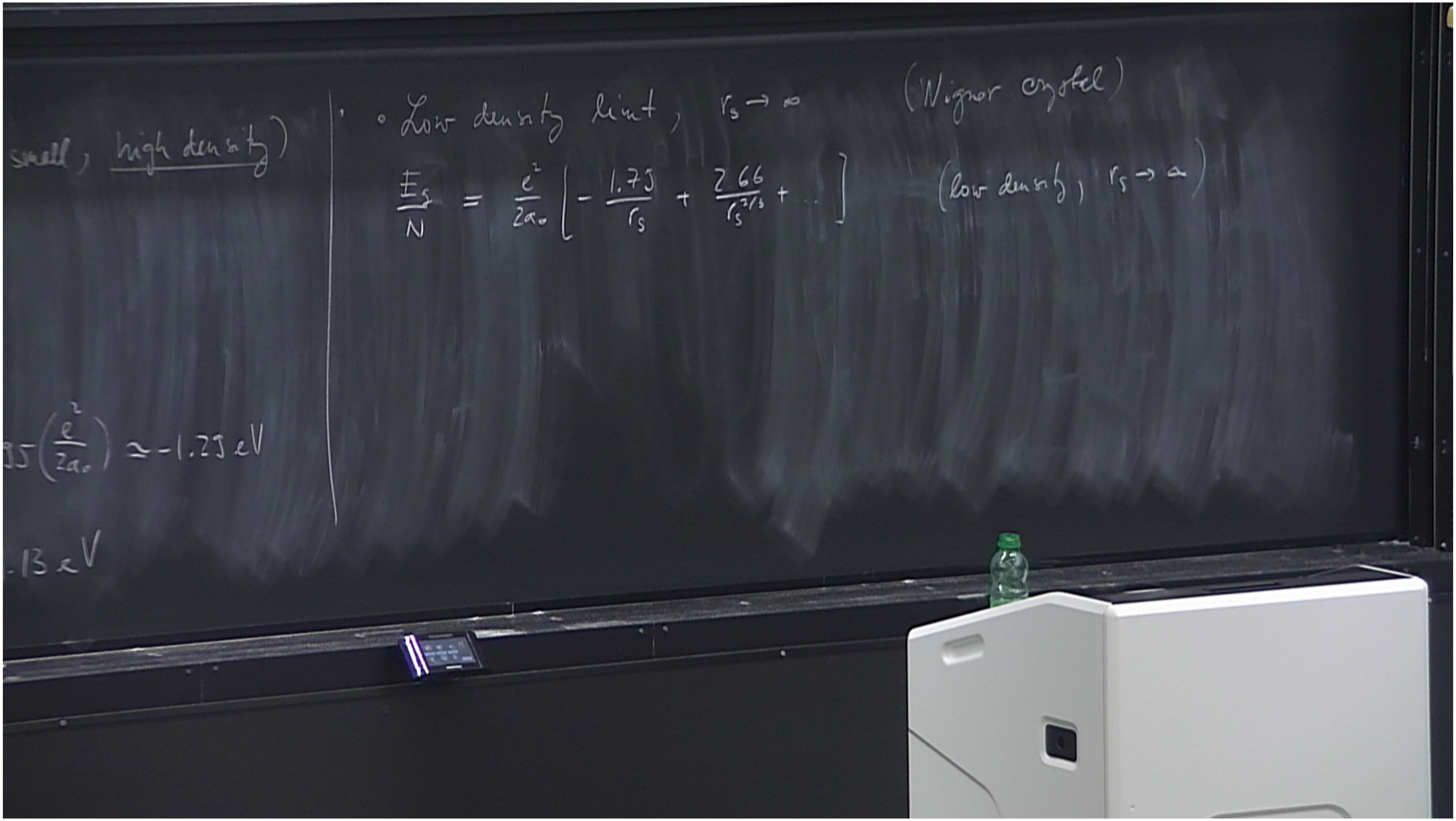

First order PT
E^(1) = ⟨F| Ĥ₁ |F⟩
= e/2V Σ_{k p q α β} 4π/q² ⟨F| c†_{k+q α} c†_{p−q β} c_{p β} c_{k α} |F⟩
(k + q, α = k, α ; p − q, β = p, β)
or
(k + q, α = p, β ; p − q, β = k, α)
"direct term"
=> q = 0
"exchange term"
δ_{k+q, p} δ_{αβ}


δ_{k+q,p} δ_{αβ} ⟨F| .... |F⟩
= - δ_{k+q,p} δ_{αβ} ⟨F| n̂_{k+q α} n̂_{p β} |F⟩






E^(1) = - 4π e² V / (2π)⁶ ∫d³q 1/q² ∫d³p θ(k_F - |p⃗ - ½q⃗|) θ(k_F - |p⃗ + ½q⃗|)
- k)
θ(k_F - k)


small, high density)
• Low density limit, $r_s \to \infty$
(Wigner crystal)
$\frac{E_g}{N} = \frac{e^2}{2a_0}\left[-\frac{1.79}{r_s} + \frac{2.66}{r_s^{3/2}} + \dots\right]$
(low density, $r_s \to \infty$)
$95\left(\frac{e^2}{2a_0}\right) \simeq -1.29\,eV$
.13 eV