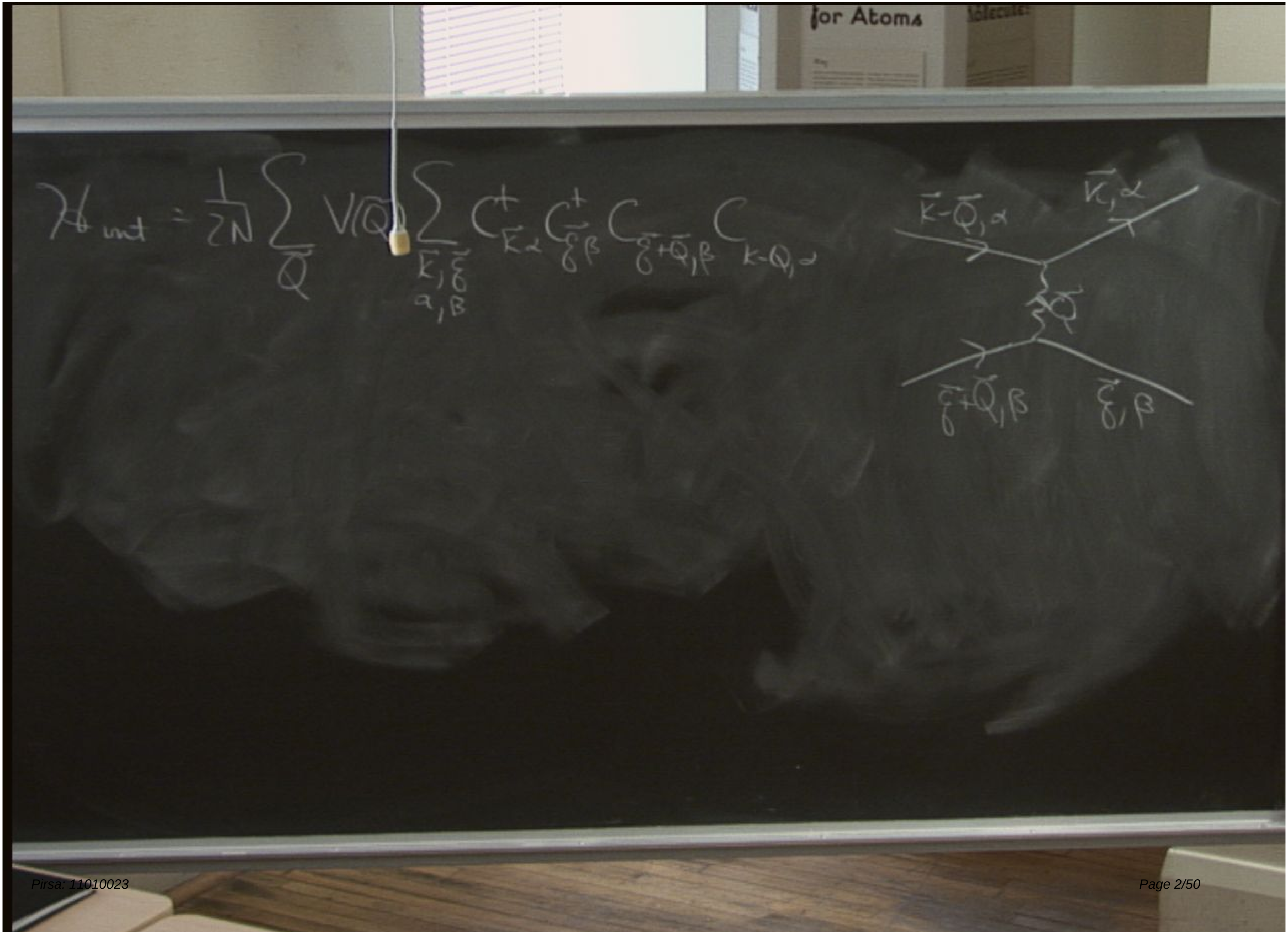
Title: Condensed Matter Review - Lecture 5

Date: Jan 07, 2011 10:15 AM

URL: http://pirsa.org/11010023

Abstract:


for Atoms
Molecules
$\mathcal{H}_{int} = \frac{1}{2N}\sum_{\vec{Q}} V(\vec{Q}) \sum_{\substack{\vec{k},\vec{\xi}\\ \alpha,\beta}} c^{\dagger}_{\vec{k}\alpha}\, c^{\dagger}_{\vec{\xi}\beta}\, c_{\vec{\xi}+\vec{Q},\beta}\, c_{k-Q,\alpha}$
$\vec{k}-\vec{Q},\alpha$
$\vec{k},\alpha$
$\vec{Q}$
$\vec{\xi}+\vec{Q},\beta$
$\vec{\xi},\beta$

To do Hartree-Fock for $\mathcal{H}$

consider a variational Hamiltonian

$$\mathcal{H}_V = \sum_{\vec{k},\sigma} (E_\sigma(\vec{k}) - \mu)\, C^{+}_{\vec{k},\sigma} C_{\vec{k},\sigma}$$

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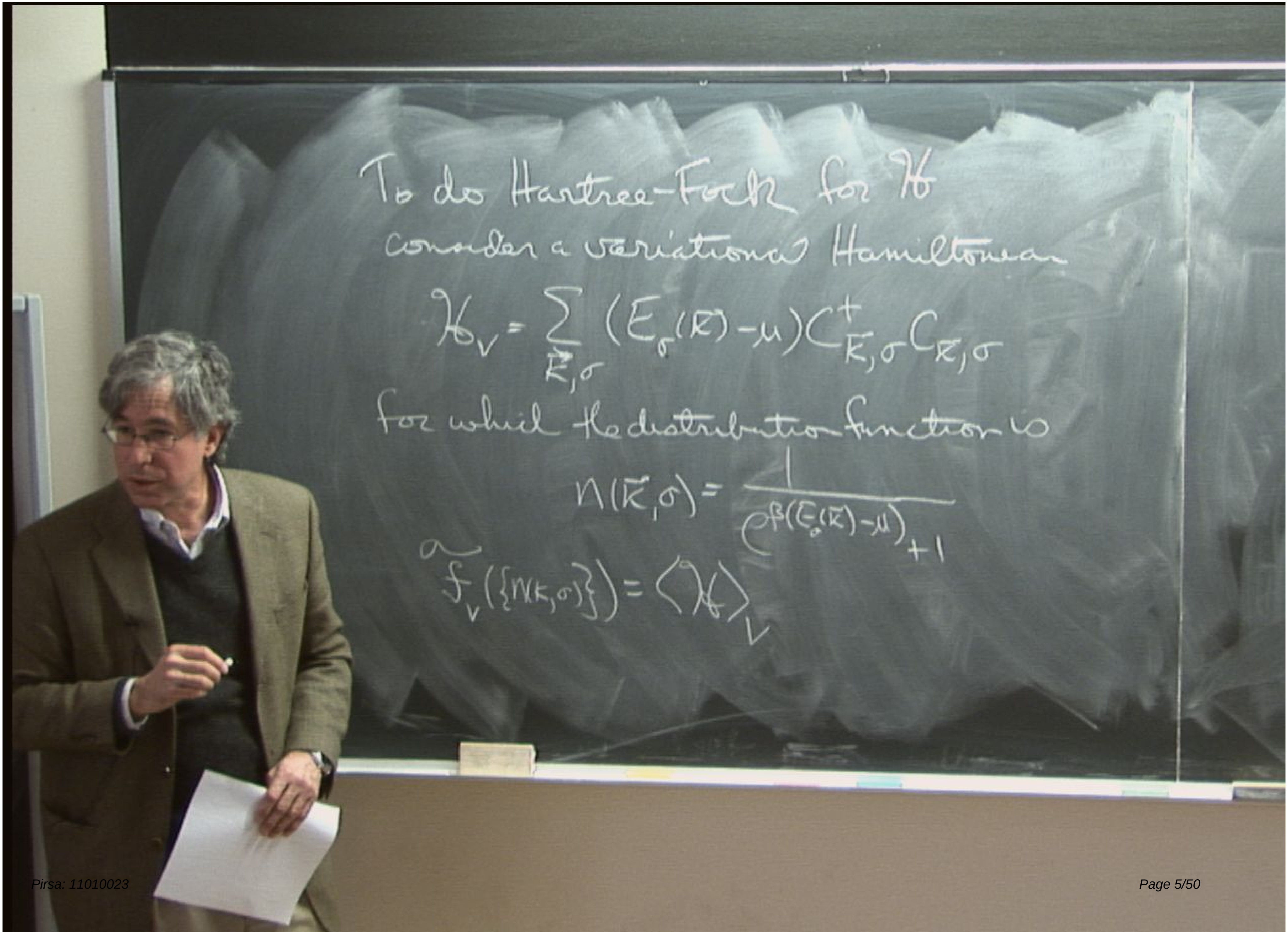
$$\mathcal{H}_V = \sum_{\vec{k},\sigma} (E_\sigma(\vec{k}) - \mu) C^{+}_{\vec{k},\sigma} C_{\vec{k},\sigma}$$

for which the distribution function is

$$n(\vec{k},\sigma) = \frac{1}{e^{\beta(E_\sigma(\vec{k}) - \mu)} + 1}$$



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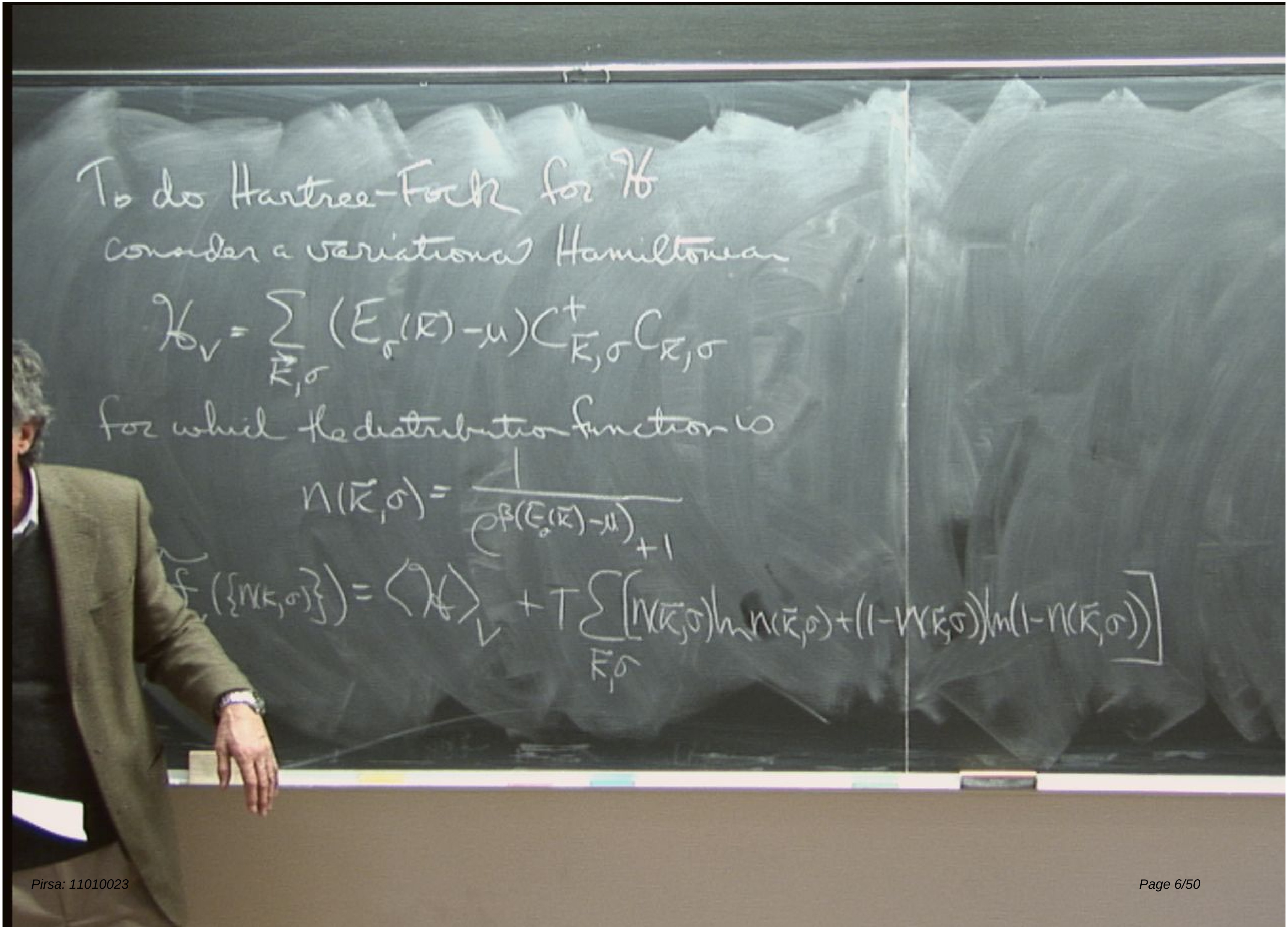
$n(\vec{k},\sigma) = \frac{1}{e^{\beta(E_\sigma(\vec{k})-\mu)}+1}$
$\tilde{f}_V(\{n(\vec{k},\sigma)\}) = \langle \mathcal{H} \rangle_V$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$n(\vec{k},\sigma) = \frac{1}{e^{\beta(E_\sigma(\vec{k})-\mu)}+1}$
$f_v(\{n(\vec{k},\sigma)\}) = \langle \mathcal{H} \rangle_V + T \sum_{\vec{k},\sigma} [n(\vec{k},\sigma) \ln n(\vec{k},\sigma) + (1-n(\vec{k},\sigma)) \ln(1-n(\vec{k},\sigma))]$

To do Hartree-Fock for $\mathcal{H}$

consider a variational Hamiltonian

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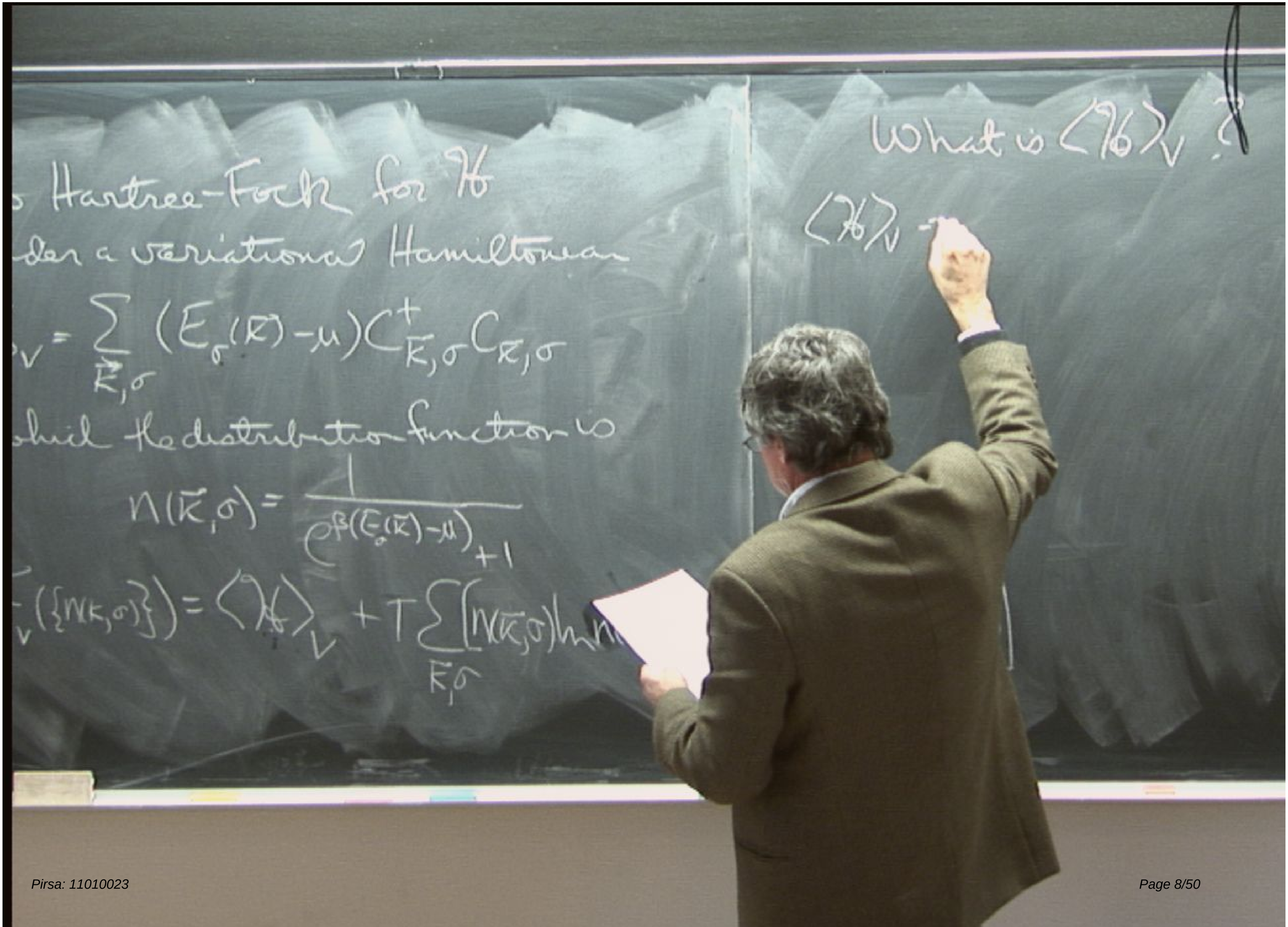
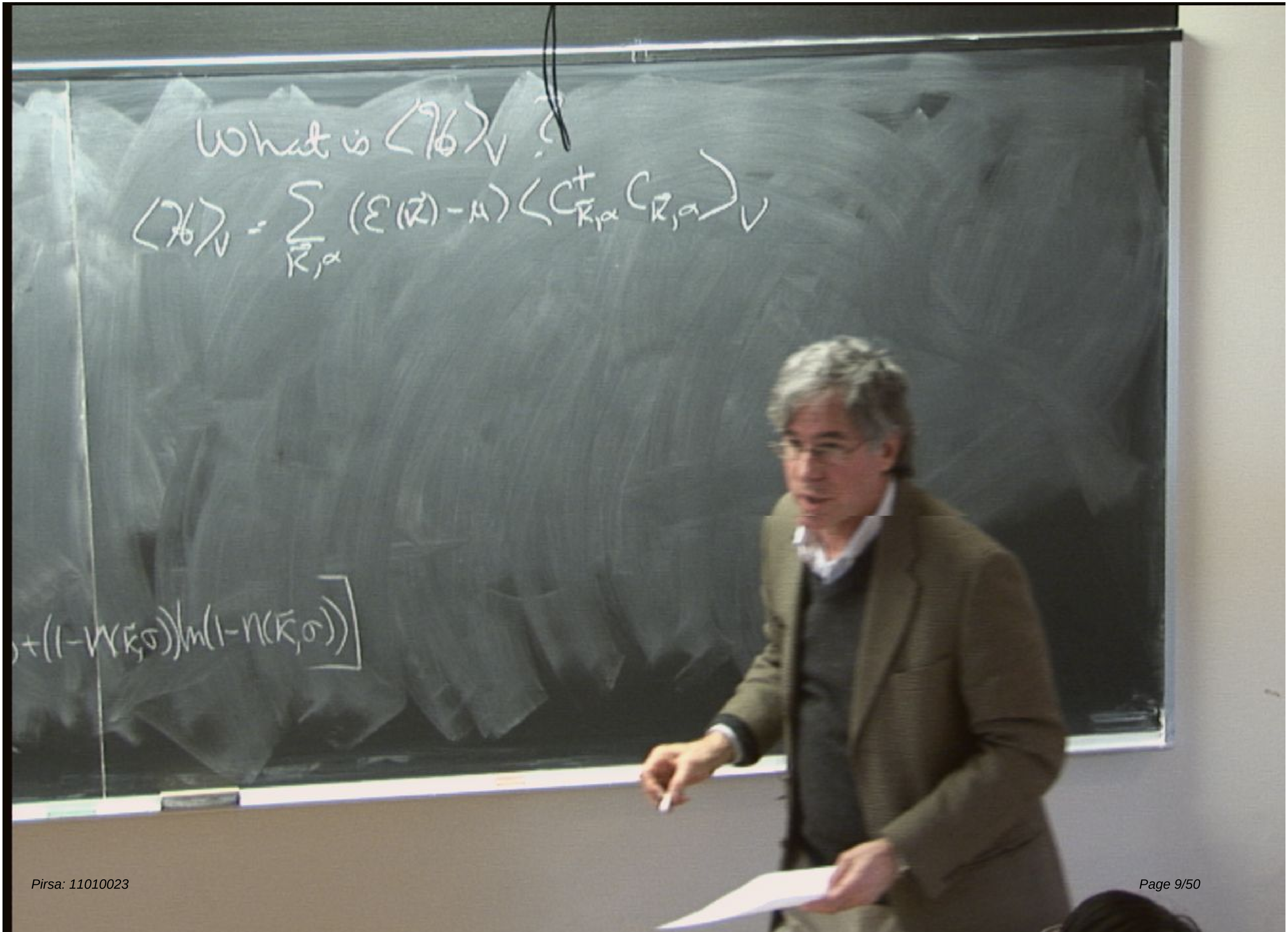
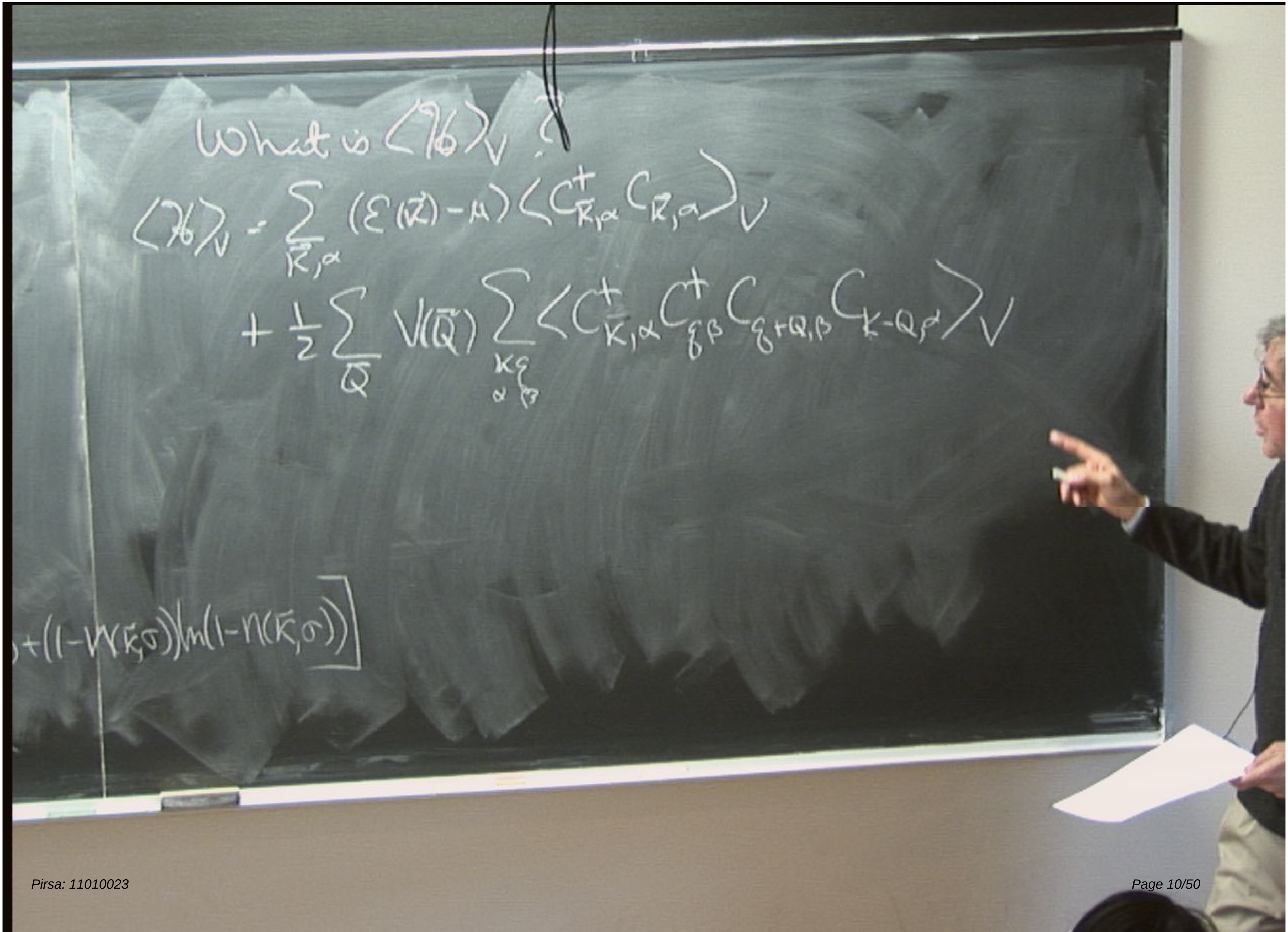
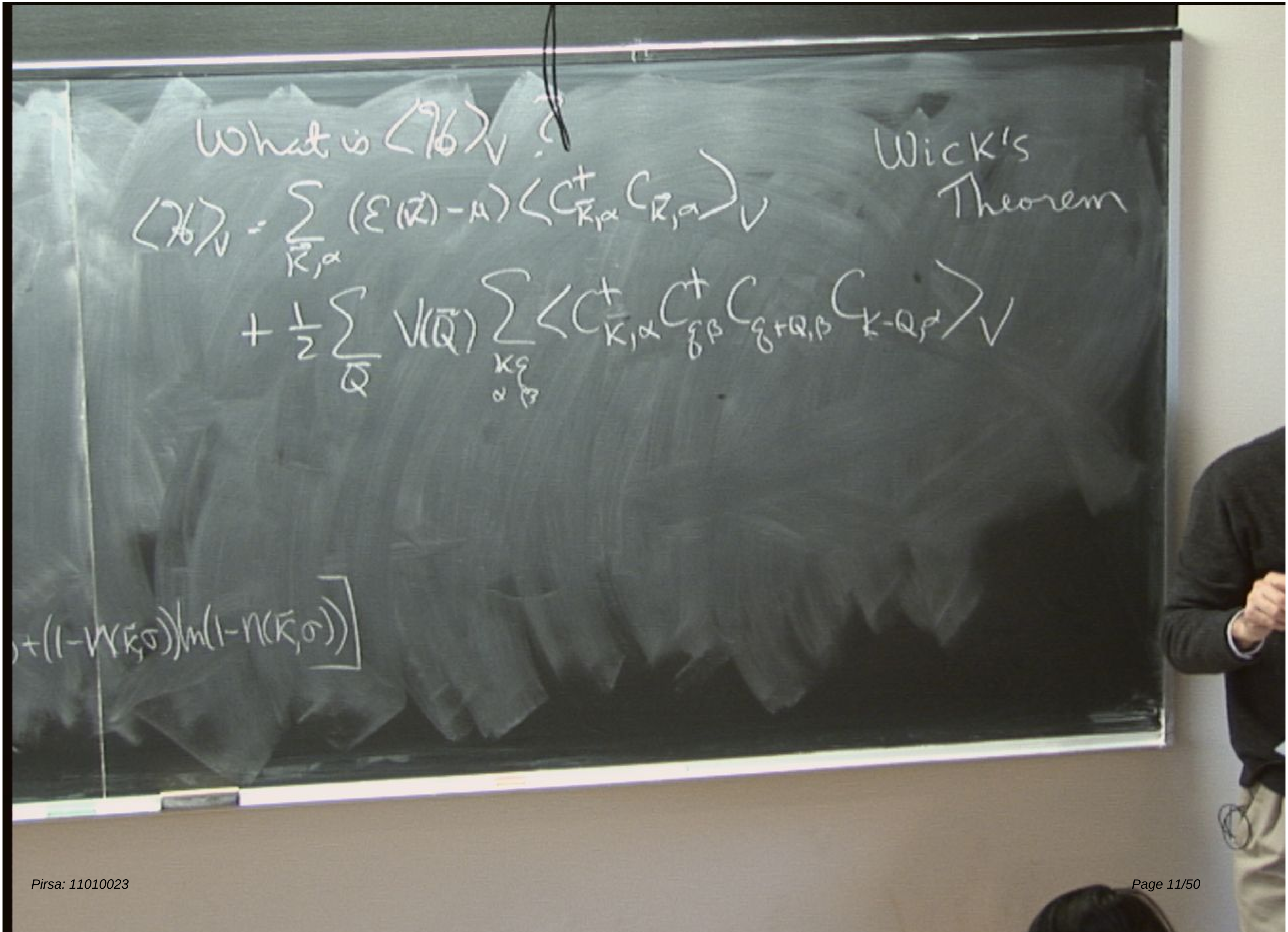

What is ⟨H⟩_V ?
Hartree-Fock for H
der a variational Hamiltonian
which the distribution function is
n(k,σ) = 1 / (e^{β(E_σ(k)−μ)} + 1)


What is ⟨H⟩_V ?
⟨H⟩_V = Σ_{k,α} (ε(k) − μ) ⟨c†_{k,α} c_{k,α}⟩_V
+(1−n(k,σ))ln(1−n(k,σ))]


What is $\langle \mathcal{H} \rangle_V$?
$\langle \mathcal{H} \rangle_V = \sum_{\vec{k},\alpha} (\varepsilon(\vec{k}) - \mu) \langle c^{\dagger}_{\vec{k},\alpha} c_{\vec{k},\alpha} \rangle_V$
$+ \frac{1}{2} \sum_{\vec{Q}} V(\vec{Q}) \sum_{\substack{k\xi \\ \alpha\beta}} \langle c^{\dagger}_{k,\alpha} c^{\dagger}_{\xi\beta} c_{\xi+Q,\beta} c_{k-Q,\alpha} \rangle_V$
$+ (1 - n(\vec{k},\sigma)) \ln(1 - n(\vec{k},\sigma))]$


What is ⟨H⟩_V ?
Wick's Theorem
⟨H⟩_V = Σ_{k,α} (ε(k) − μ) ⟨C†_{k,α} C_{k,α}⟩_V
+ 1/2 Σ_Q V(Q) Σ_{k ξ α β} ⟨C†_{k,α} C†_{ξ β} C_{ξ+Q,β} C_{k−Q,α}⟩_V
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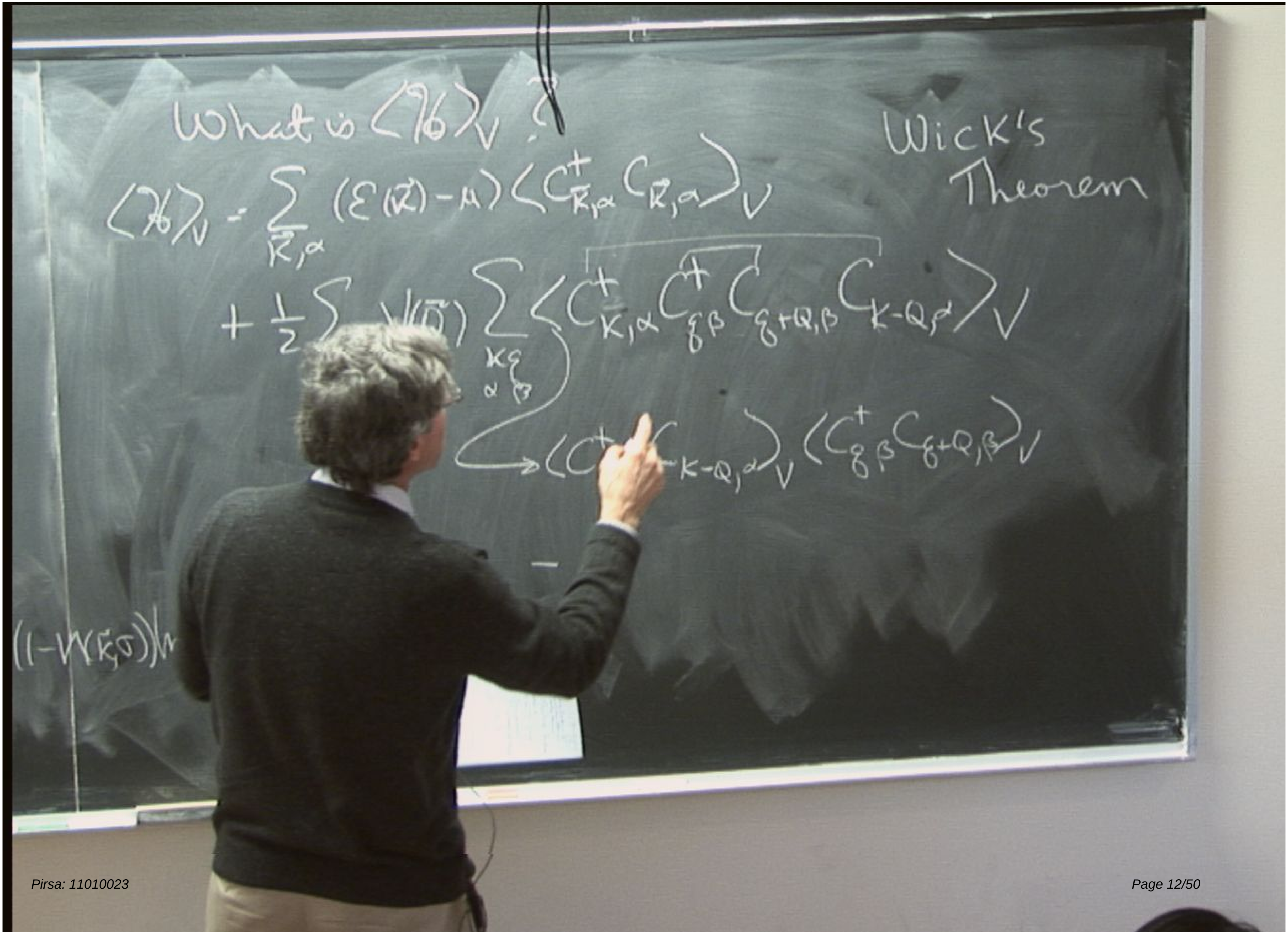
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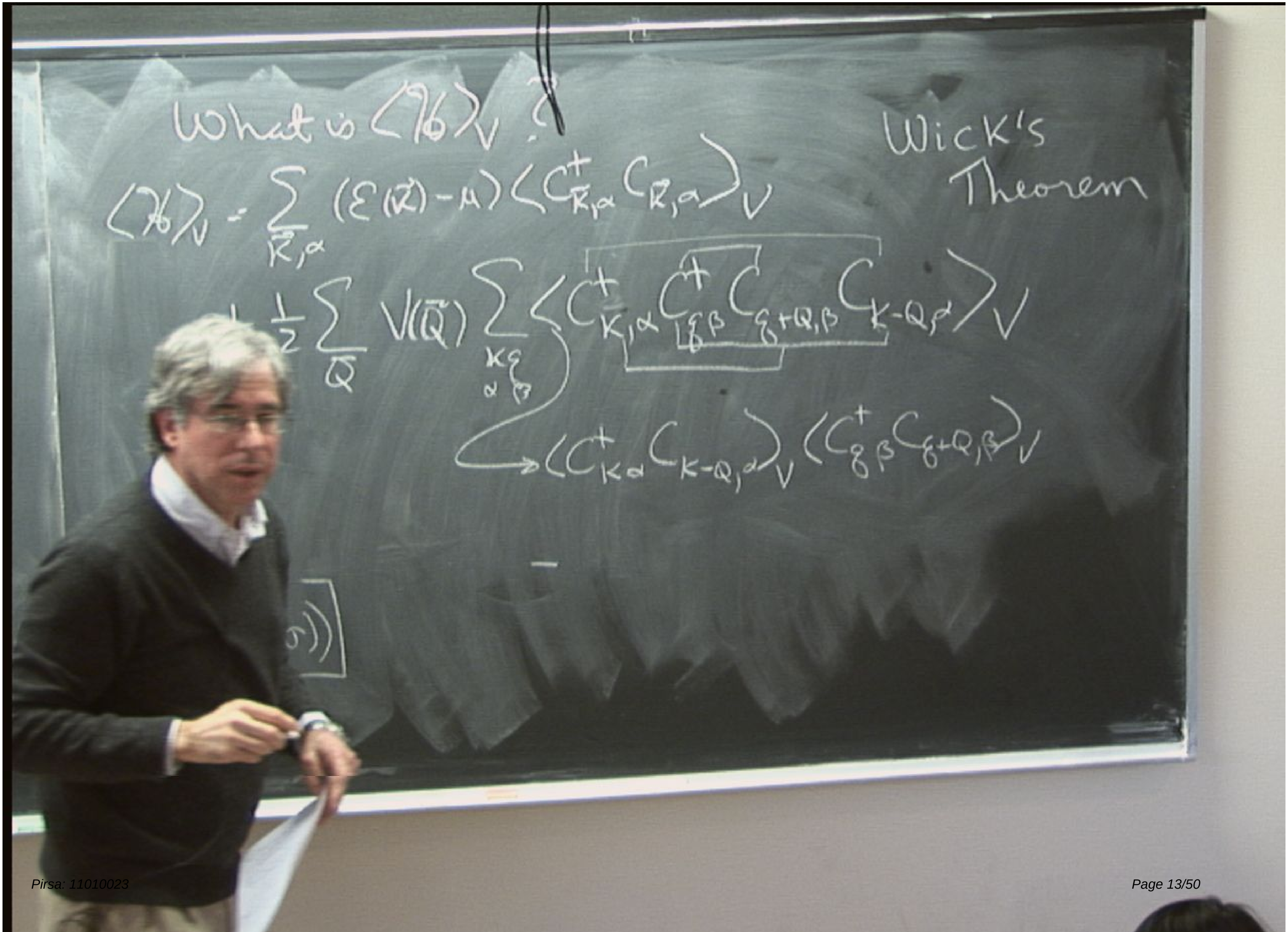
⟨C† C_{k−Q,α}⟩_V ⟨C†_{ξ β} C_{ξ+Q,β}⟩_V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What is $\langle \mathcal{H} \rangle_V$?

Wick's Theorem

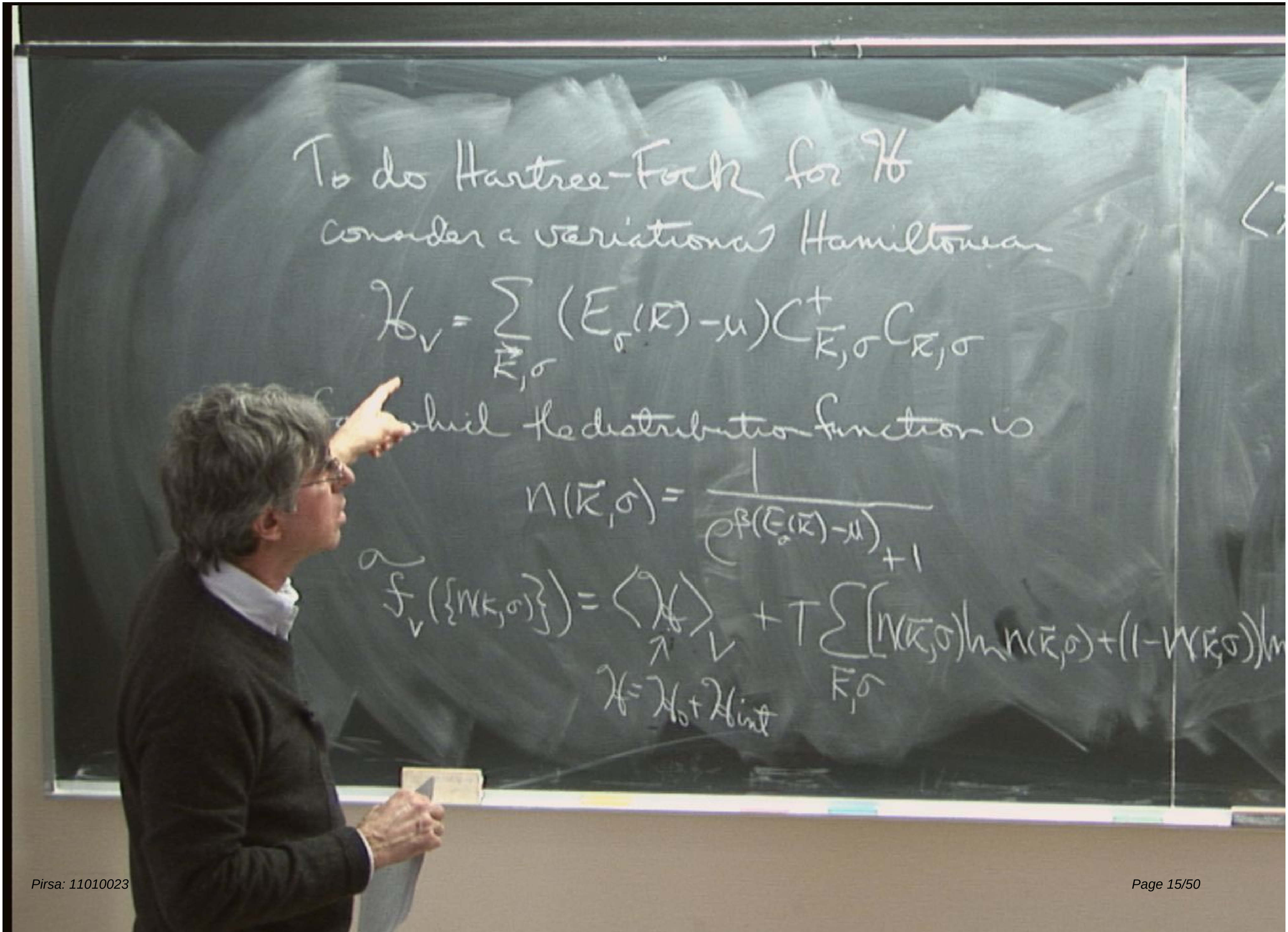
$$\langle \mathcal{H}\rangle_V = \sum_{\vec{k},\alpha} (\varepsilon(\vec{k})-\mu)\langle c^\dagger_{\vec{k},\alpha} c_{\vec{k},\alpha}\rangle_V$$

$$+ \frac{1}{2}\sum_{\vec{Q}} V(\vec{Q}) \sum_{\substack{k q \\ \alpha \beta}} \langle c^\dagger_{k,\alpha} c^\dagger_{q\beta} c_{q+Q,\beta} c_{k-Q,\alpha}\rangle_V$$

$$\to \langle c^\dagger_{k\alpha} c_{k-Q,\alpha}\rangle_V \langle c^\dagger_{q\beta} c_{q+Q,\beta}\rangle_V$$

$$- \langle c^\dagger_{k,\alpha} c_{q+Q,\beta}\rangle_V \langle c^\dagger_{q\beta} c_{k-Q,\alpha}\rangle_V$$

$(1-n(\vec{k},\sigma))\ln(1-n(\vec{k},\sigma))]$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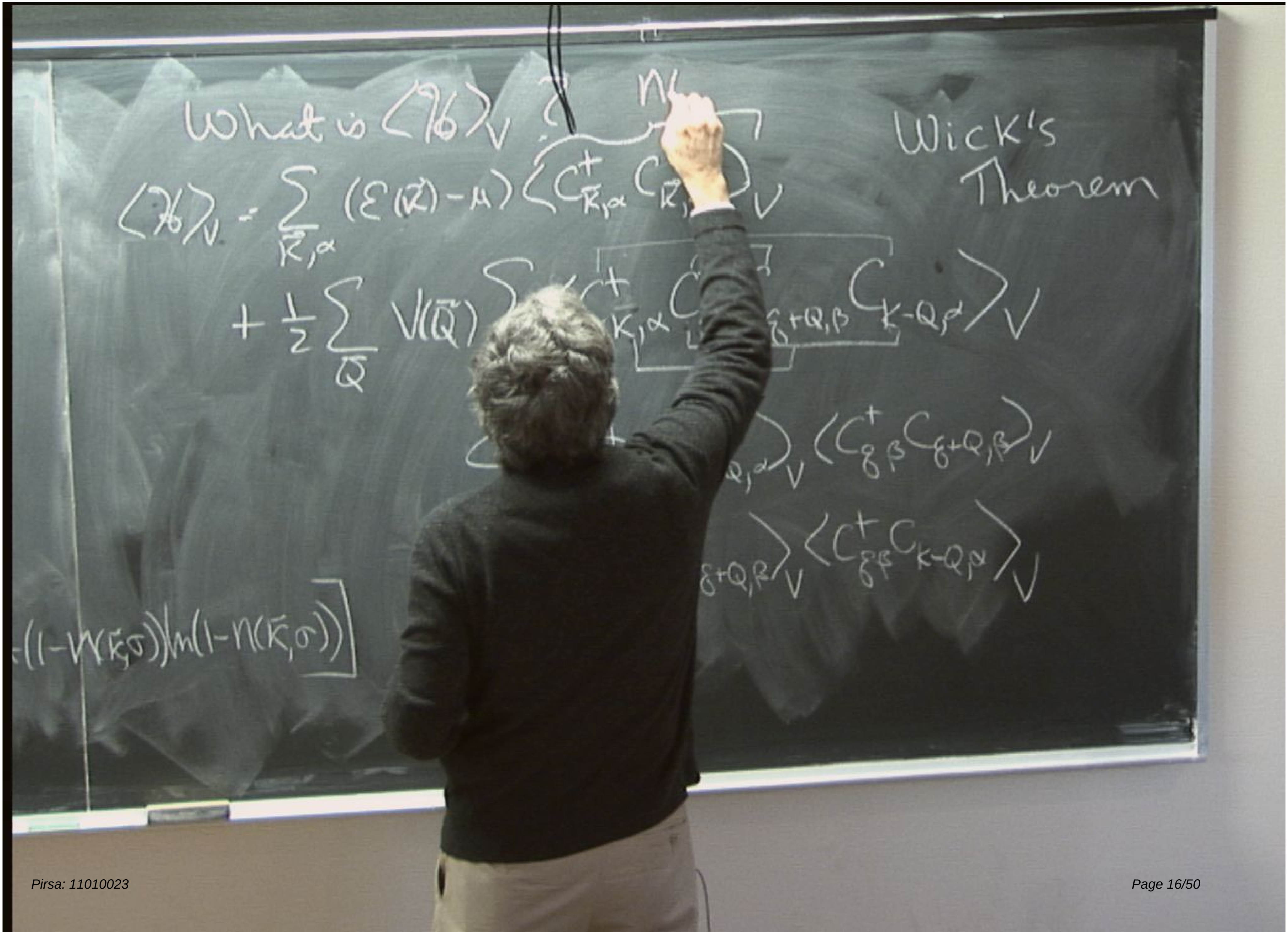
$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_{int}$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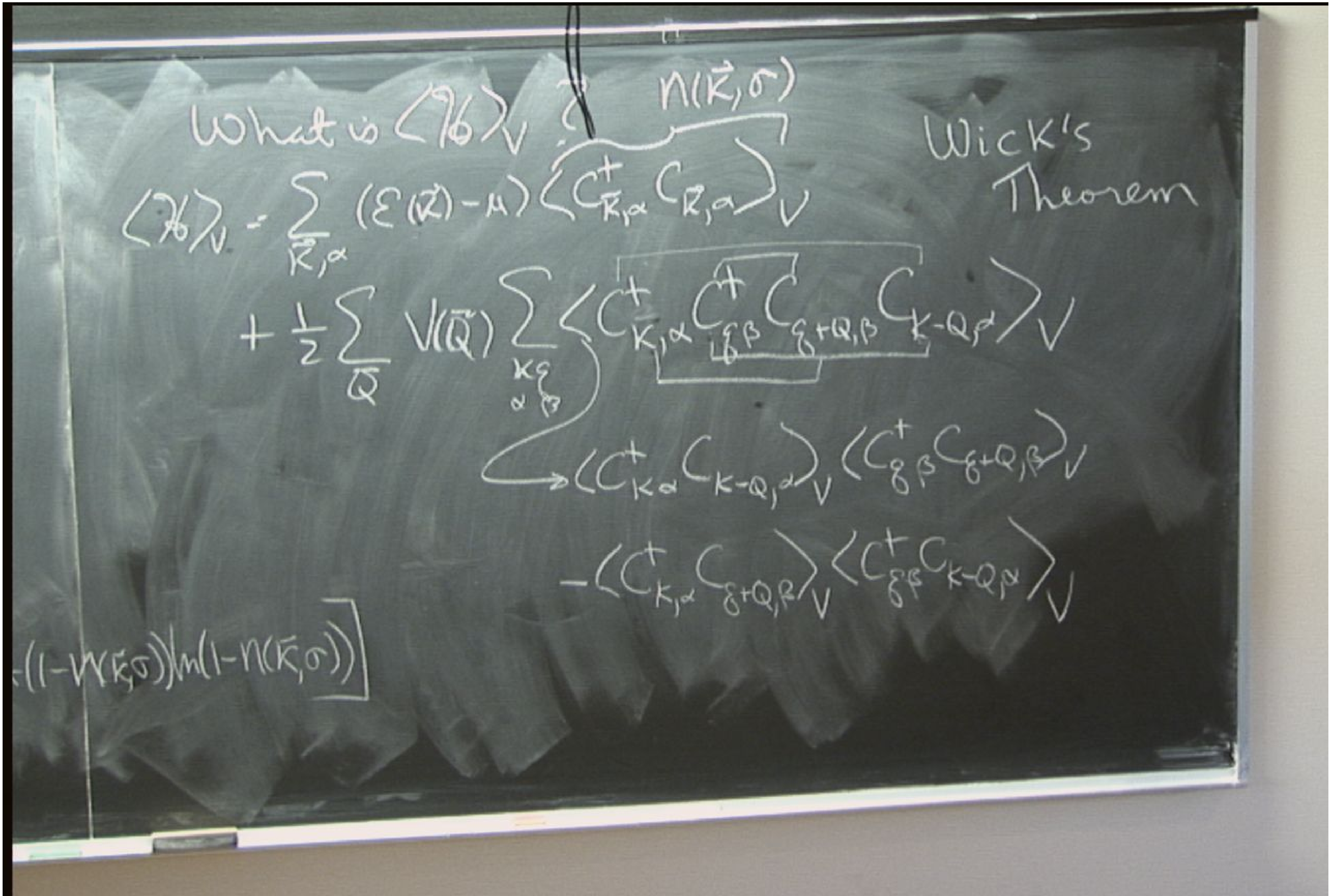

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$n(\vec{k},\sigma)$
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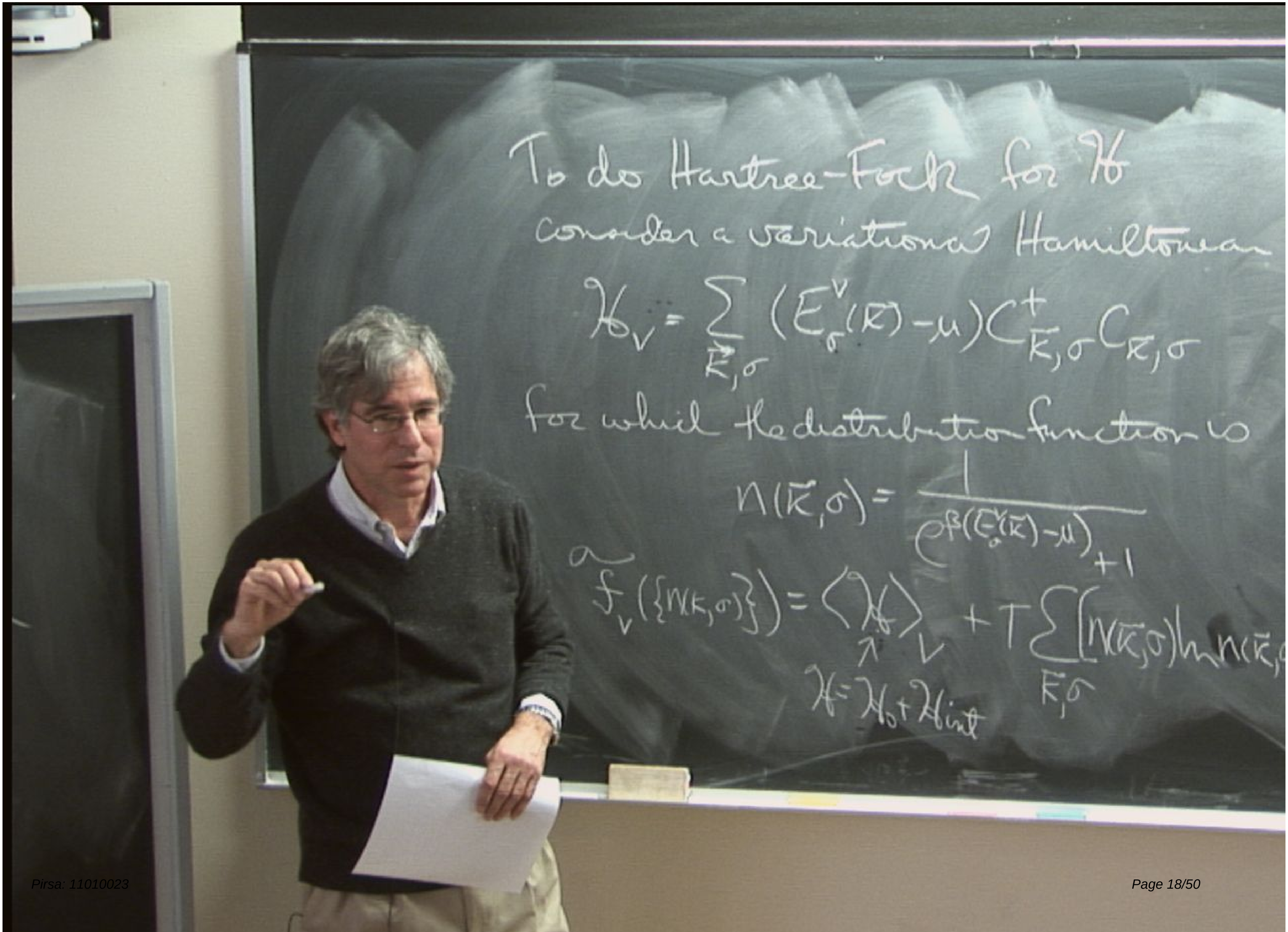
$\langle C^\dagger_{k\alpha} C_{k-Q,\alpha} \rangle_V \langle C^\dagger_{\xi\beta} C_{\xi+Q,\beta} \rangle_V$
$- \langle C^\dagger_{k,\alpha} C_{\xi+Q,\beta} \rangle_V \langle C^\dagger_{\xi\beta} C_{k-Q,\alpha} \rangle_V$
$(1-n(\vec{k},\sigma)) \ln(1-n(\vec{k},\sigma))$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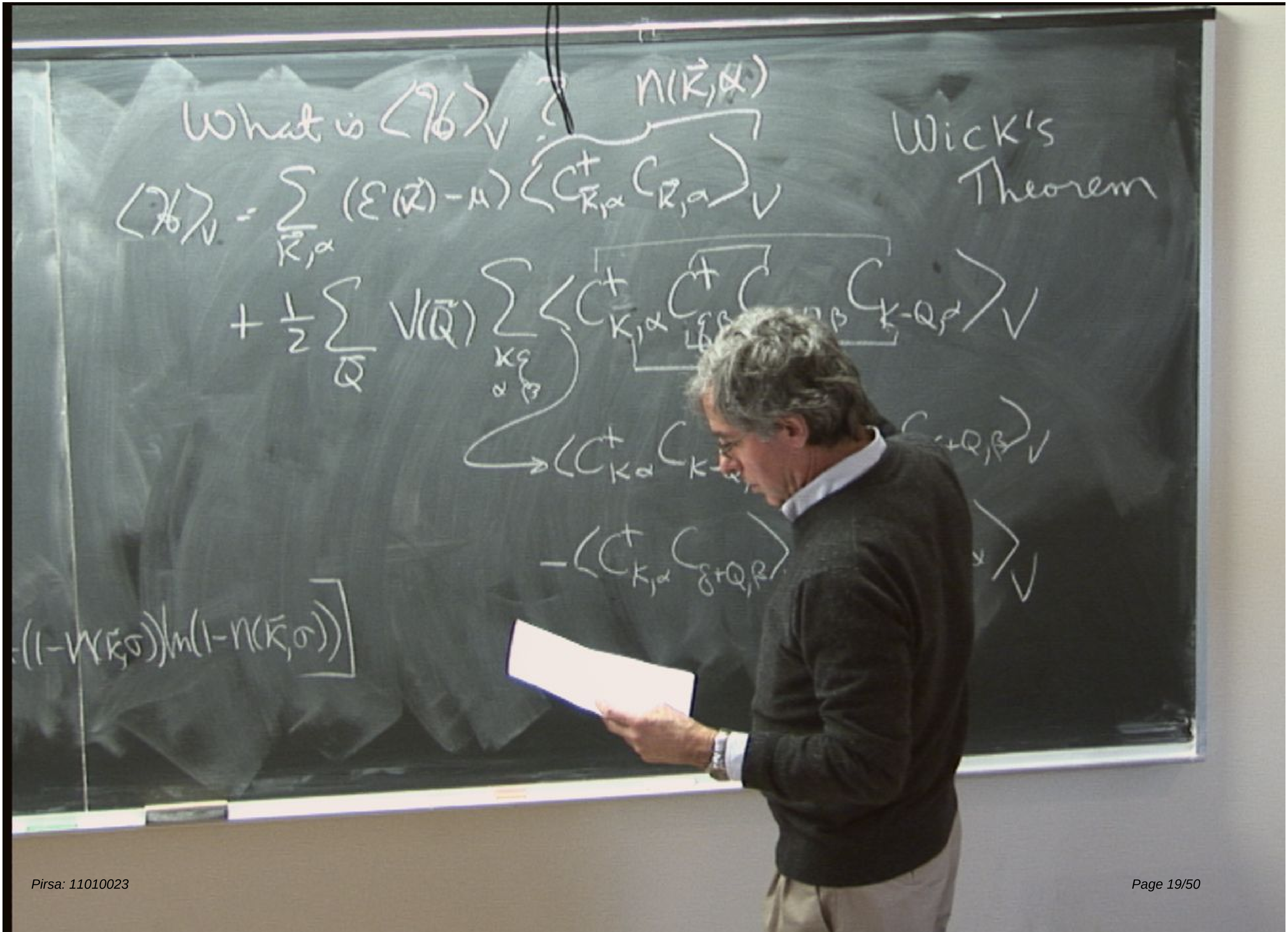
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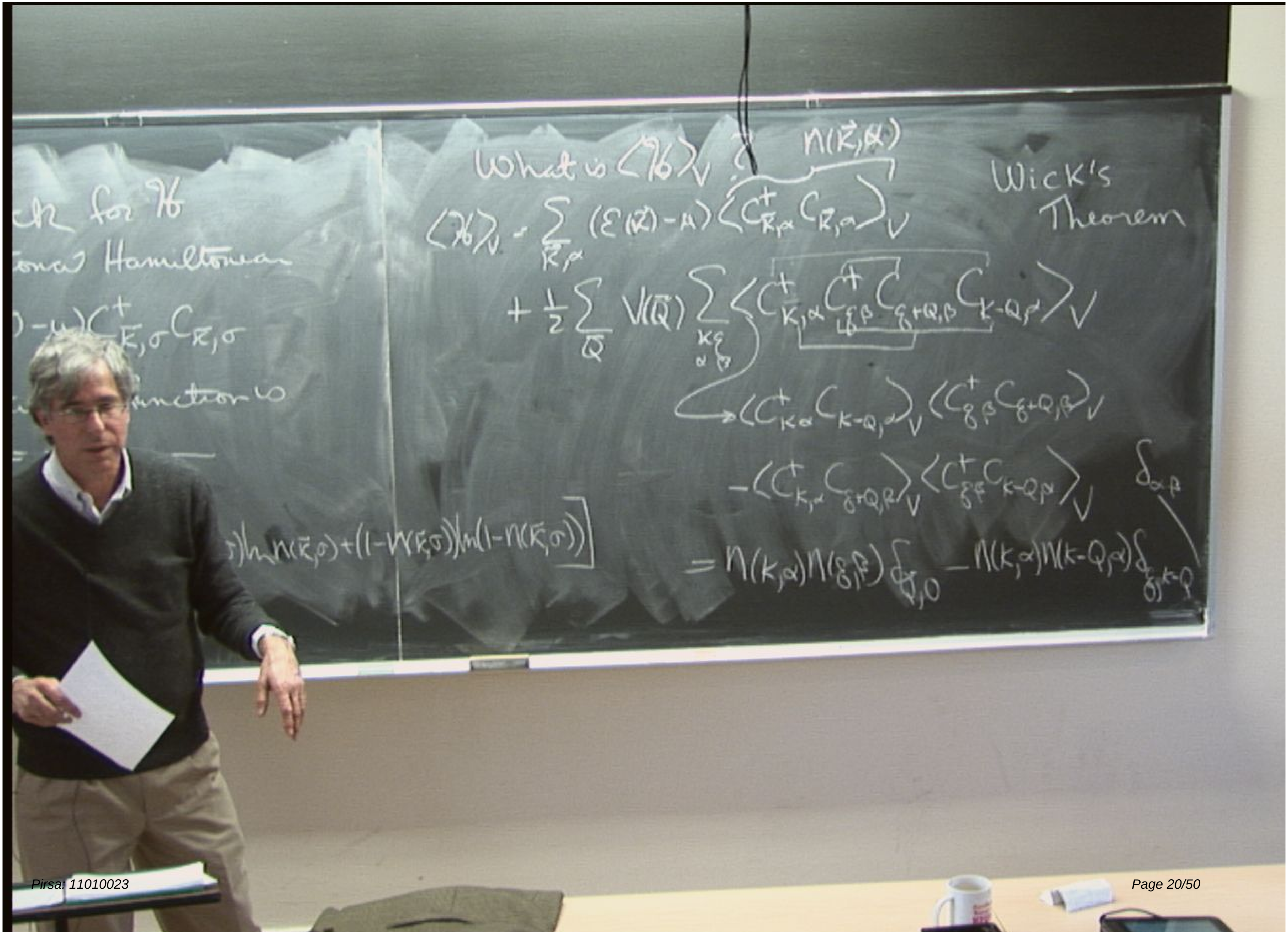
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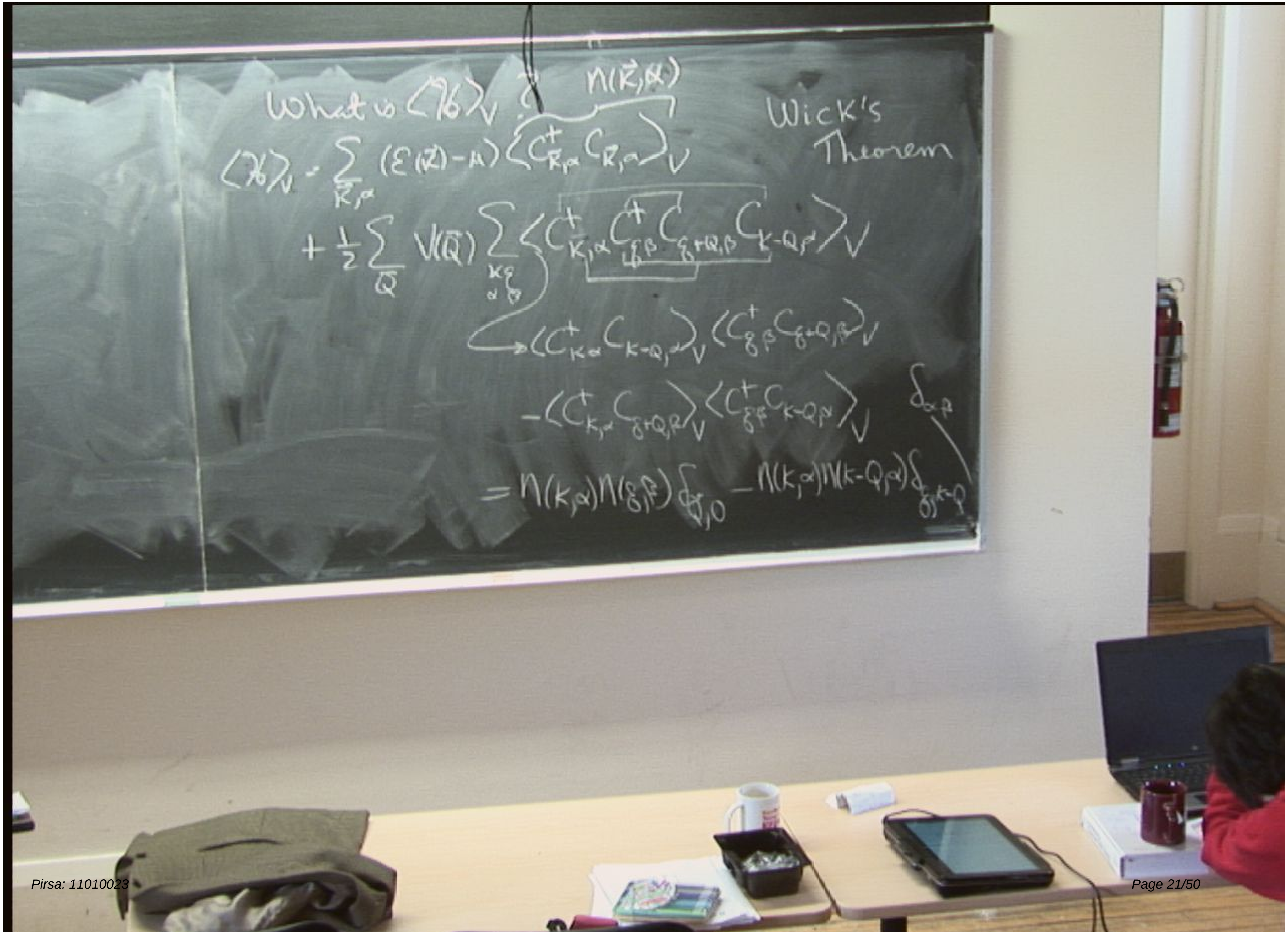
⟨C†_{k,α} C_{k−Q,α}⟩_V ⟨C†_{ξ,β} C_{ξ+Q,β}⟩_V
− ⟨C†_{k,α} C_{ξ+Q,β}⟩_V ⟨C†_{ξ,β} C_{k−Q,α}⟩_V
δ_{α,β}
= n(k,α) n(ξ,β) δ_{Q,0} − n(k,α) n(k−Q,α) δ_{ξ,k−Q}
Hamiltonian
function is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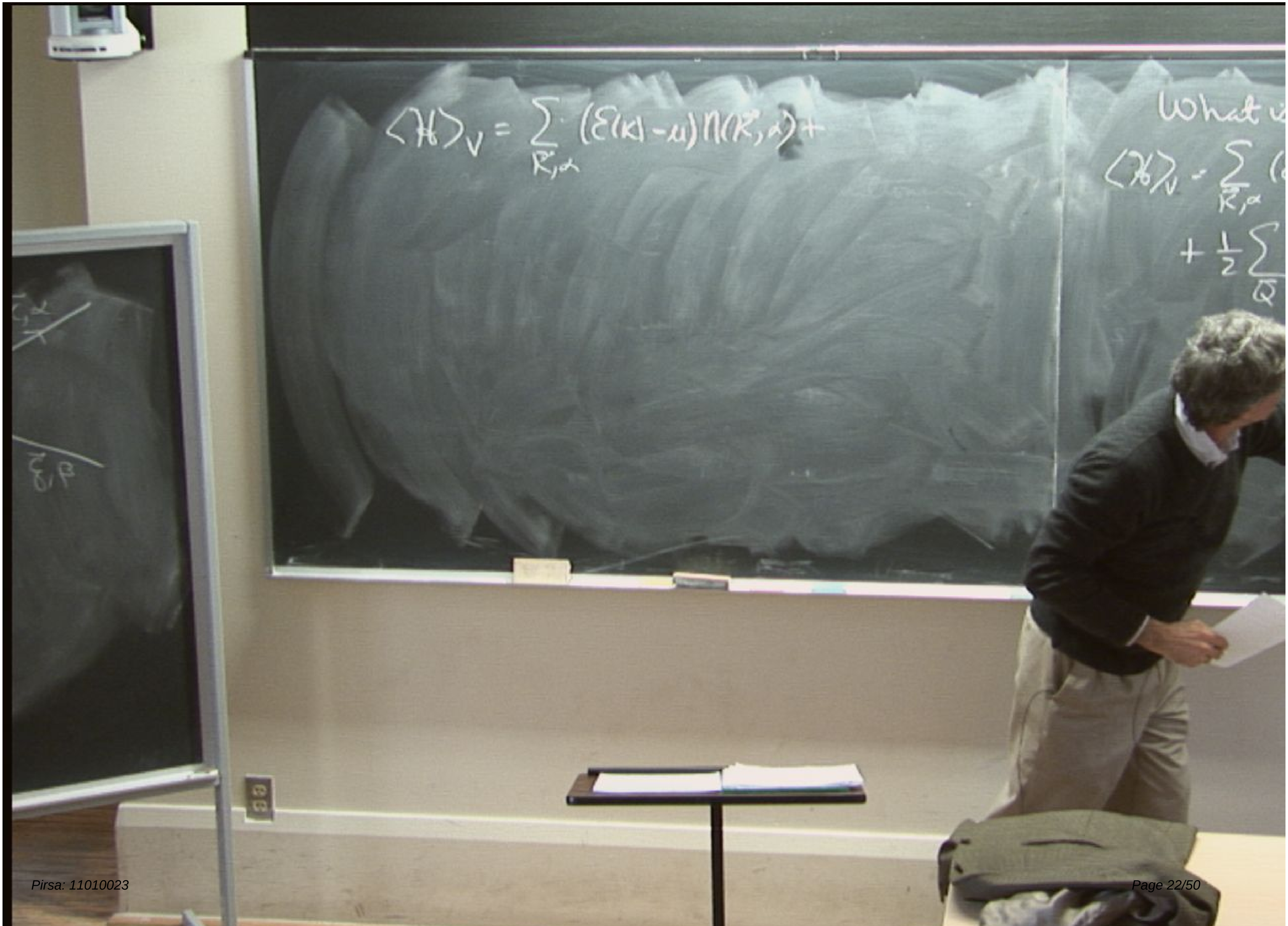
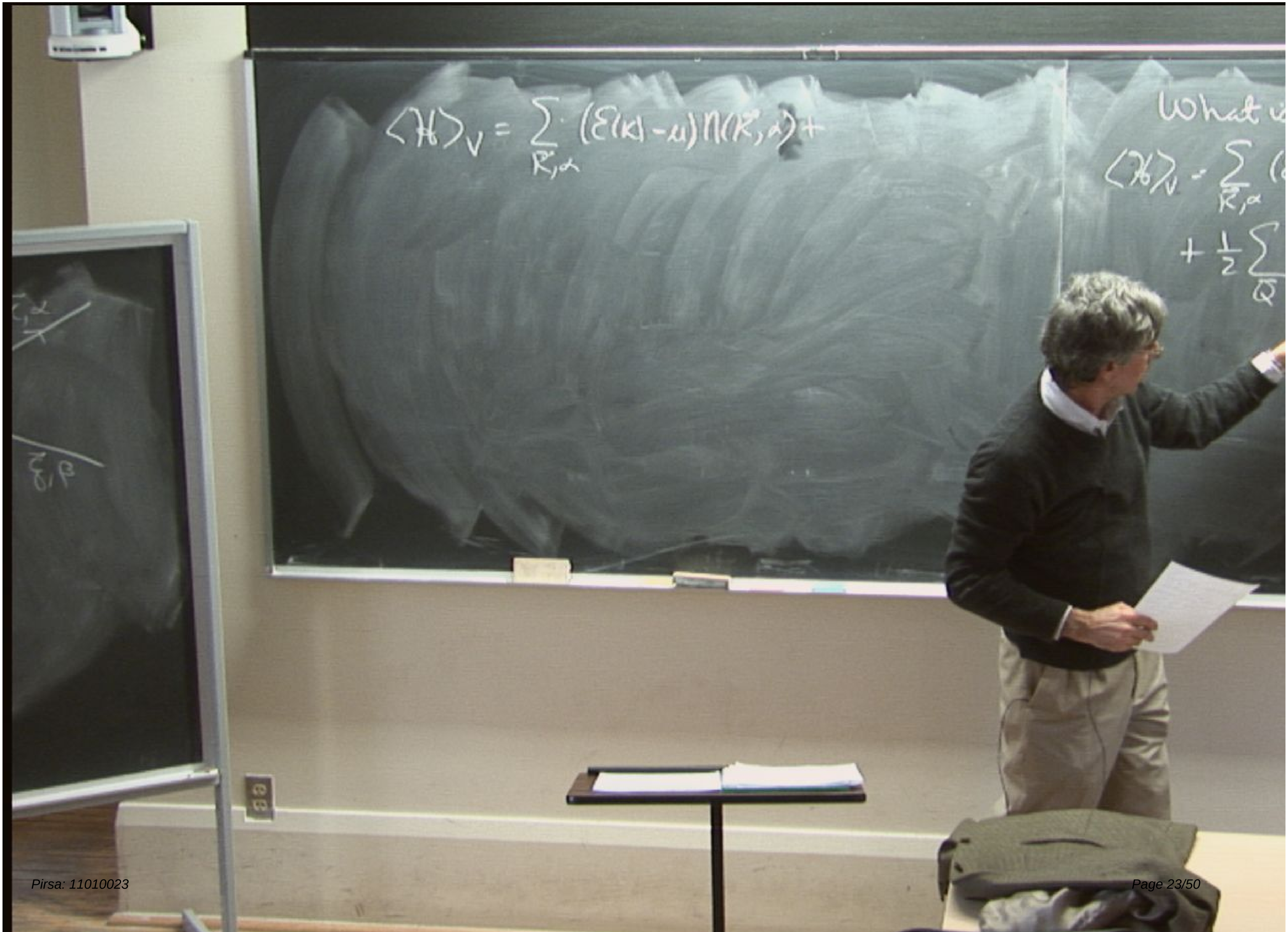
⟨c†_{kα} c_{k−Q,α}⟩_V ⟨c†_{qβ} c_{q+Q,β}⟩_V
− ⟨c†_{k,α} c_{q+Q,β}⟩_V ⟨c†_{qβ} c_{k−Q,α}⟩_V
δ_{αβ}
= n(k,α) n(q,β) δ_{Q,0} − n(k,α) n(k−Q,α) δ_{q,k−Q}


⟨H⟩_V = Σ_{k,α} (ε(k) − μ) n(k, α) +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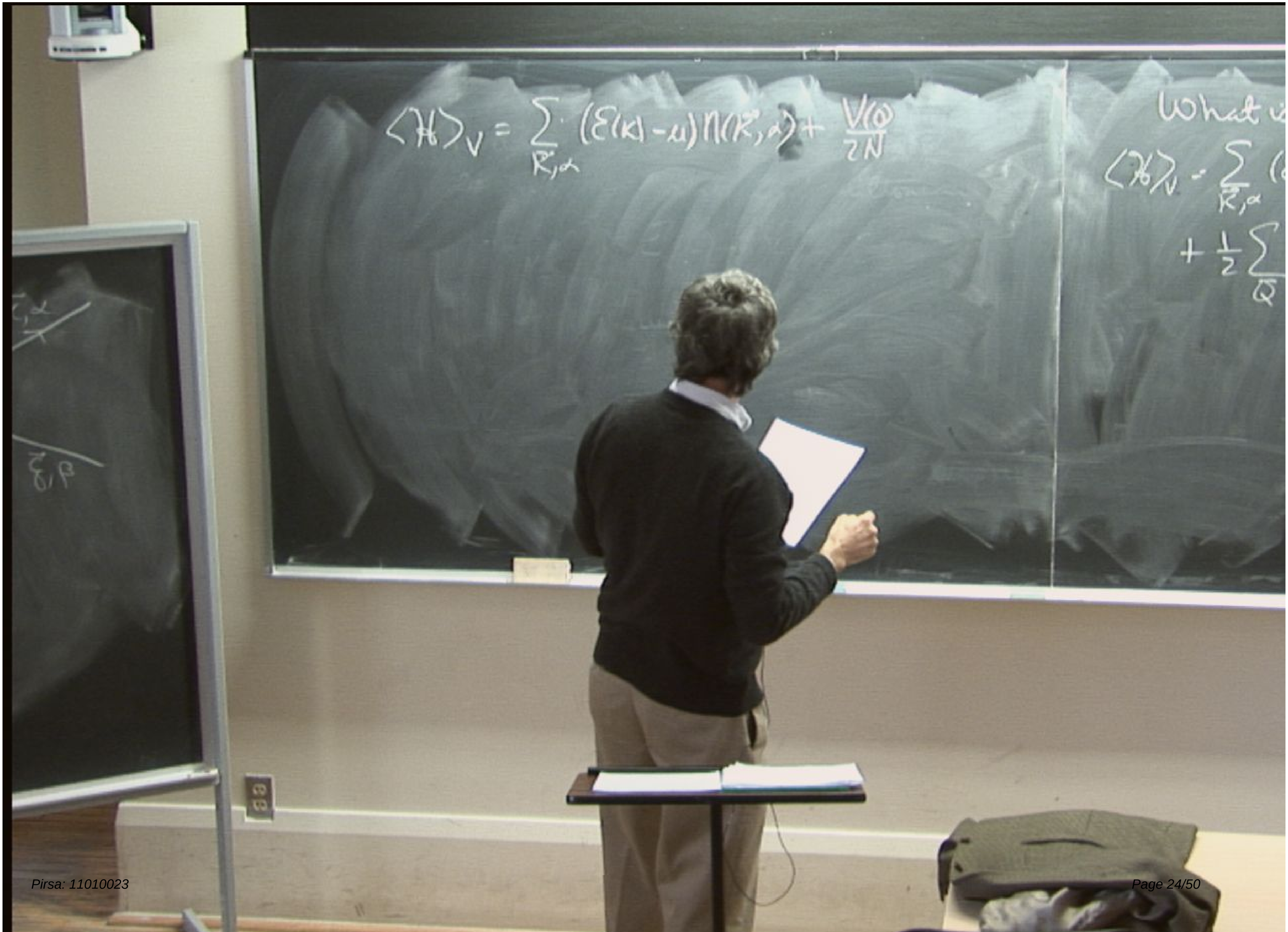
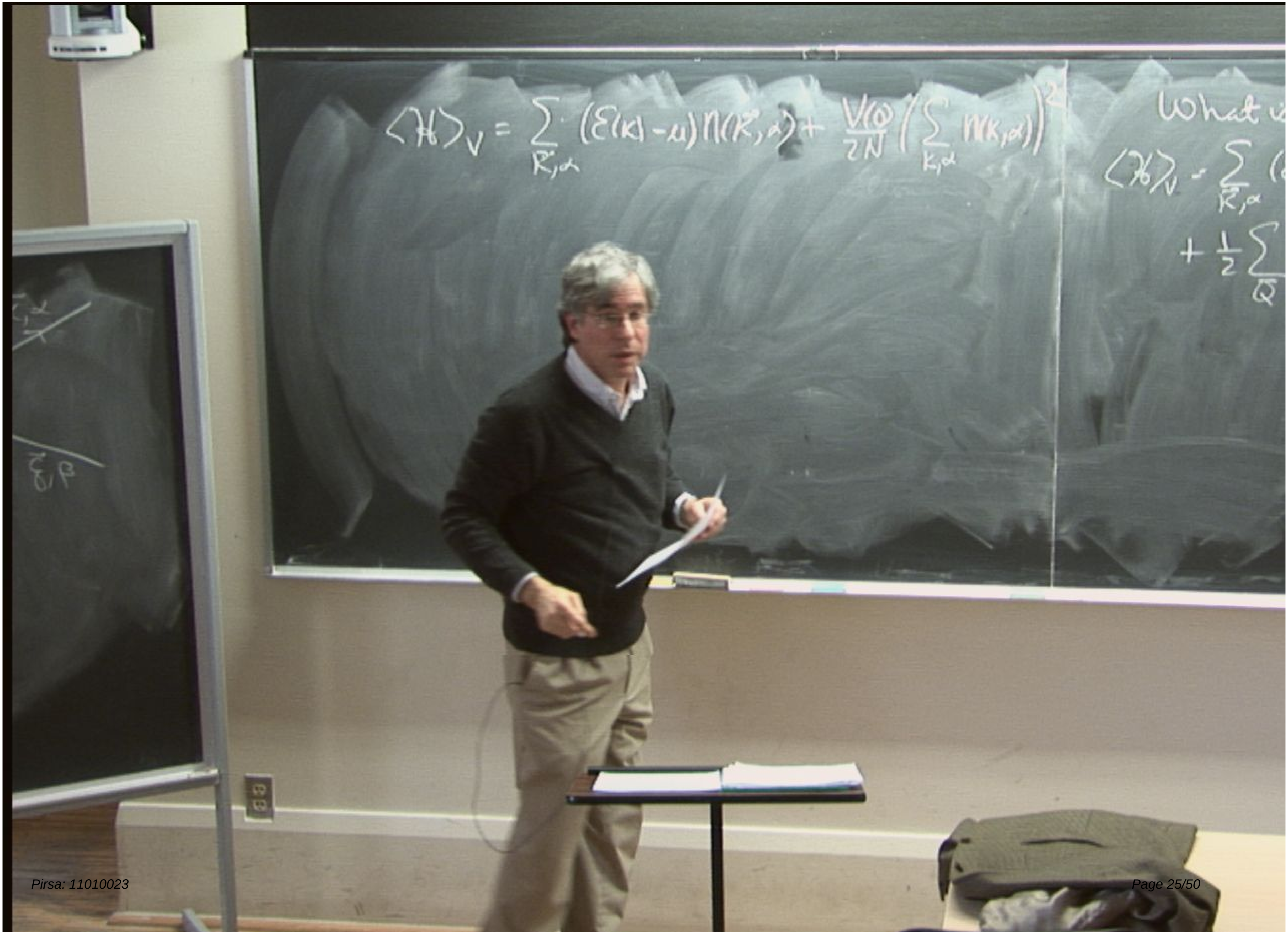
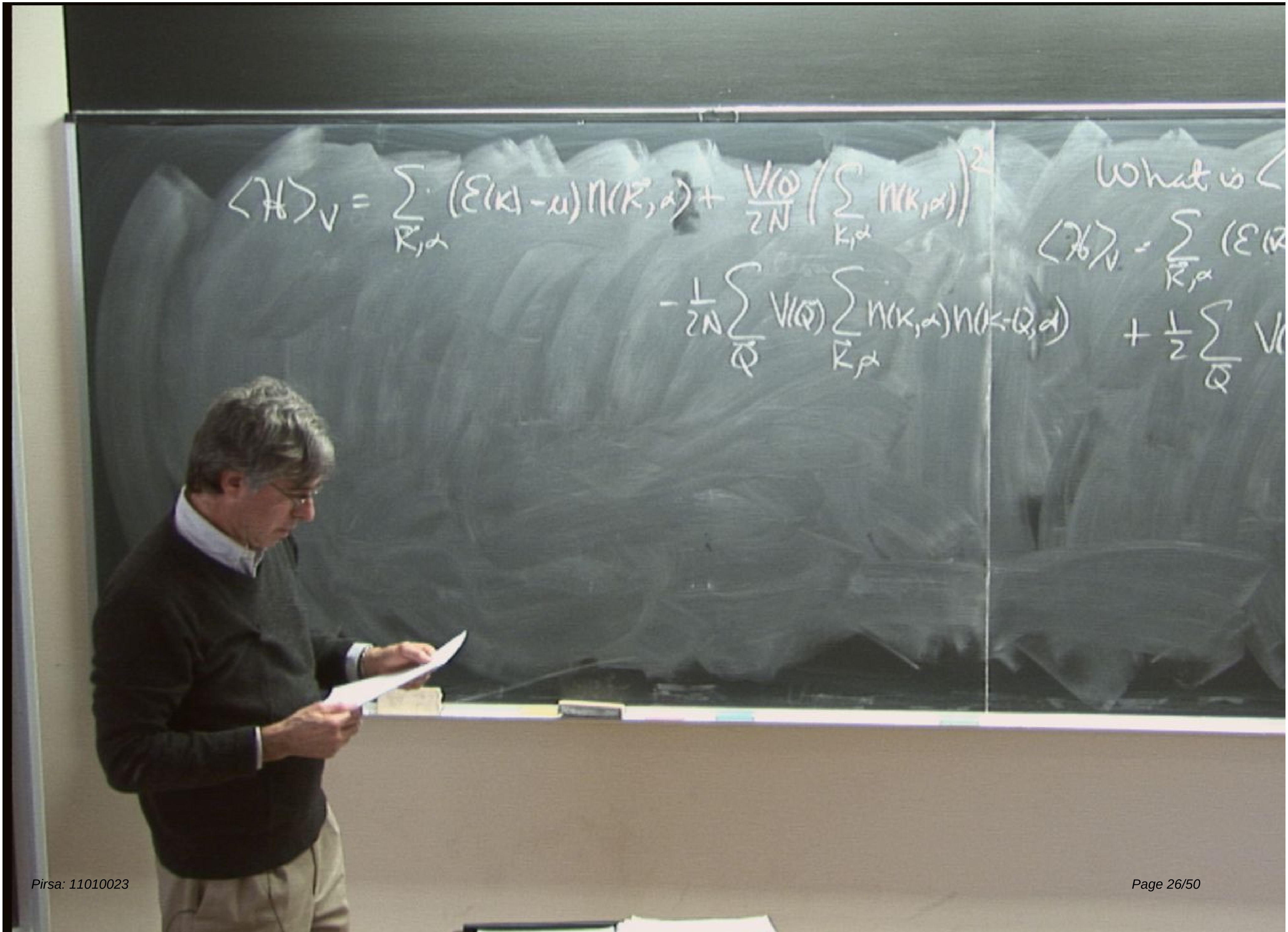


$\langle \mathcal{H} \rangle_V = \sum_{\vec{k},\alpha} (\varepsilon(k) - \mu) n(\vec{k},\alpha) + \frac{V(0)}{2N}$
What i


⟨H⟩_V = Σ_{k,α} (ε(k) − μ) n(k,α) + V(0)/2N (Σ_{k,α} n(k,α))²
What i
⟨H⟩_V = Σ_{k,α} (
+ 1/2 Σ_Q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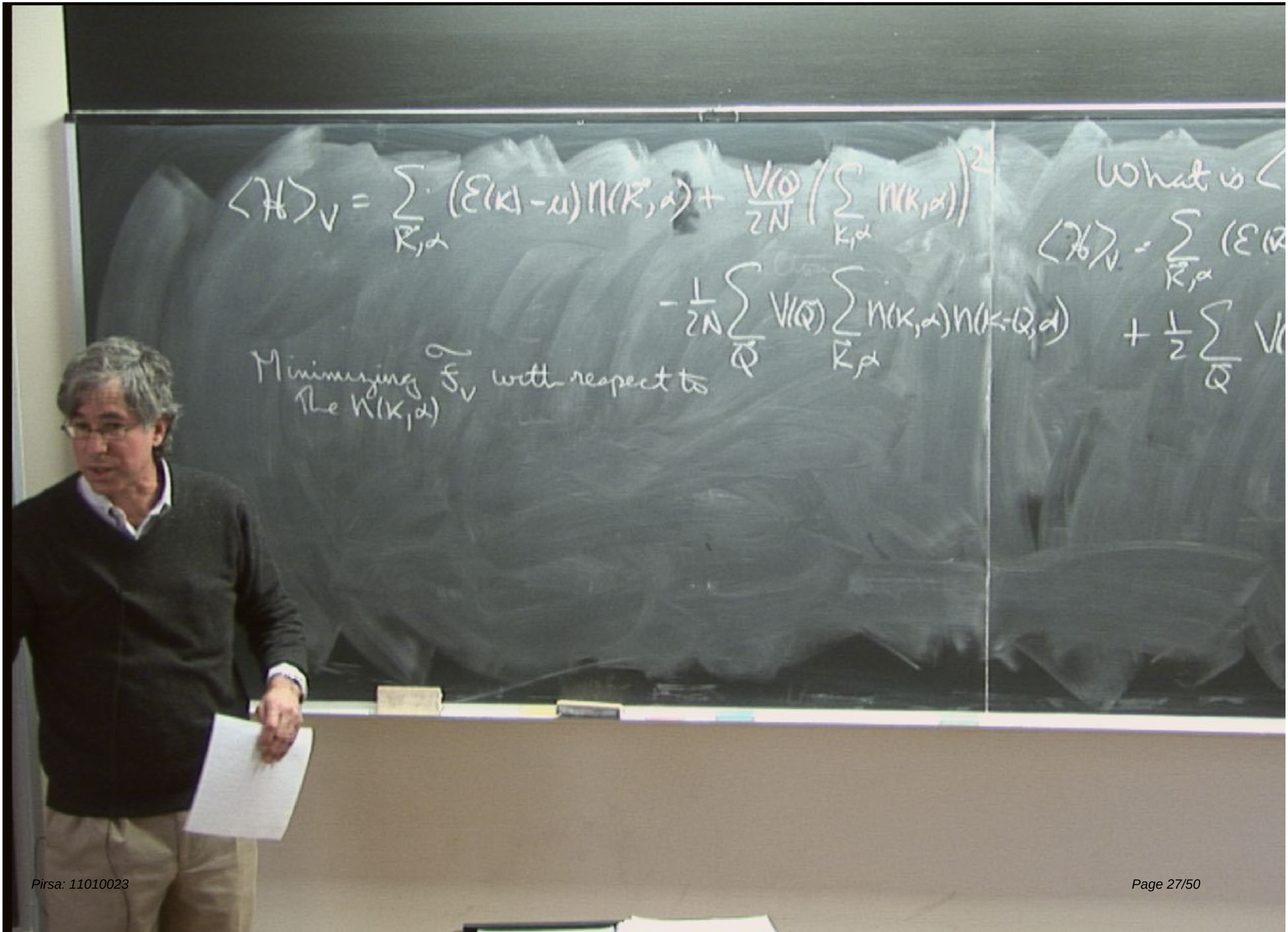
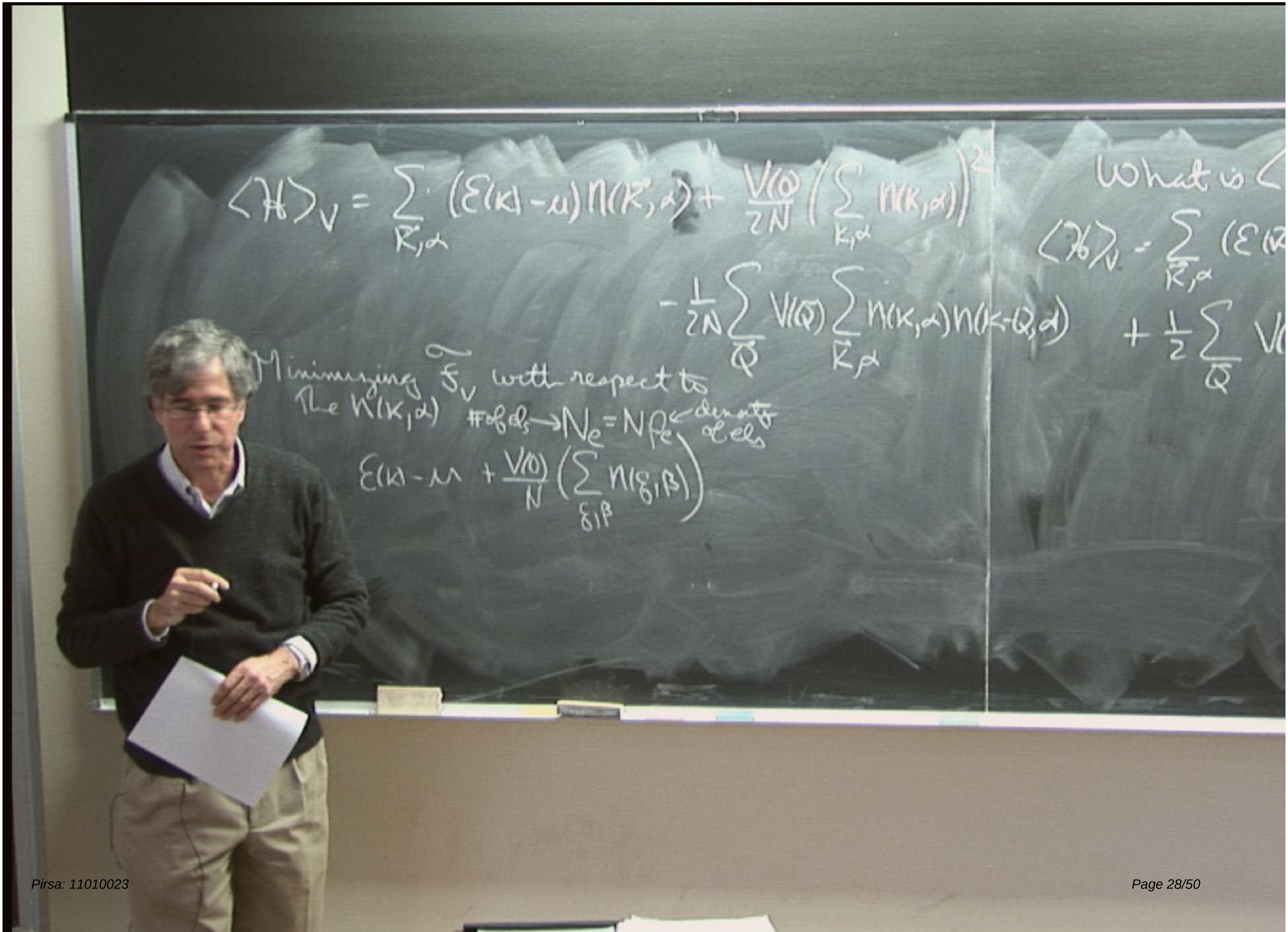
− 1/2N Σ_Q V(Q) Σ_{K,α} n(K,α) n(K−Q,α)
What is ⟨
⟨H⟩_V = Σ_{K,α} (ε(K
+ 1/2 Σ_Q V(


$\langle \mathcal{H} \rangle_V = \sum_{\vec{K},\alpha} (\varepsilon(K) - \mu) n(\vec{K},\alpha) + \frac{V(0)}{2N} \left(\sum_{K,\alpha} n(K,\alpha) \right)^2$
$- \frac{1}{2N} \sum_{\vec{Q}} V(\vec{Q}) \sum_{\vec{K},\alpha} n(K,\alpha) n(K-Q,\alpha)$
Minimizing $\tilde{F}_V$ with respect to the $n(K,\alpha)$
What is $\langle$
$\langle \mathcal{H} \rangle_V = \sum_{\vec{K},\alpha} (\varepsilon(\vec{K}$
$+ \frac{1}{2} \sum_{\vec{Q}} V($



What is
Minimizing with respect to
The n(k, α)
# of els
density of els

$$\langle H \rangle_V = \sum_{\vec{K},\alpha} \left(\mathcal{E}(K) - \mu\right) n(\vec{K},\alpha) + \frac{V(0)}{2N}\left(\sum_{K,\alpha} n(K,\alpha)\right)^2$$

$$- \frac{1}{2N}\sum_{\vec{Q}} V(\vec{Q}) \sum_{\vec{K},\alpha} n(K,\alpha)\, n(K-Q,\alpha)$$

What is $\langle$ …

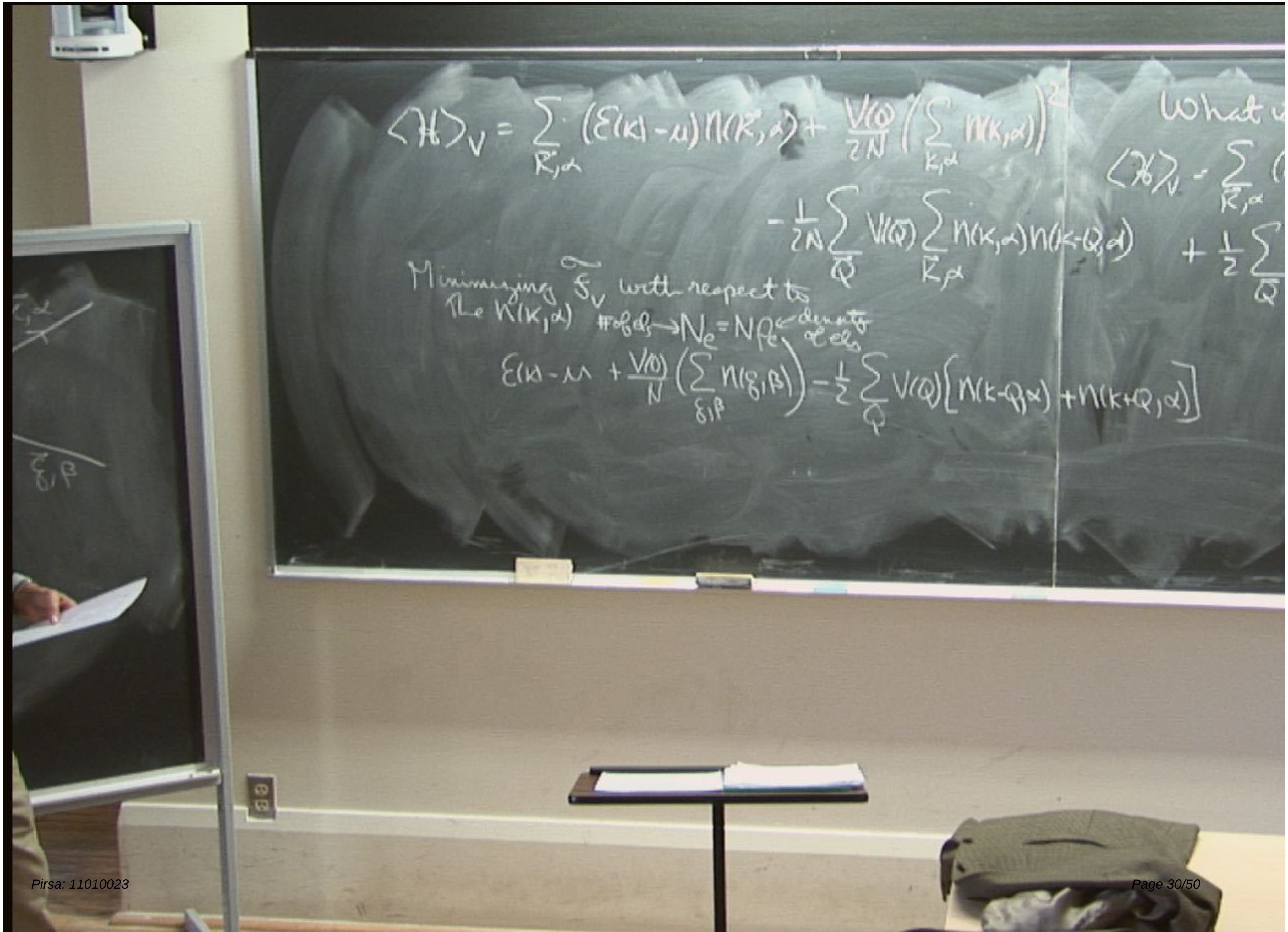
$$\langle H \rangle_V = \sum_{\vec{K},\alpha} (\mathcal{E}(K \ldots$$

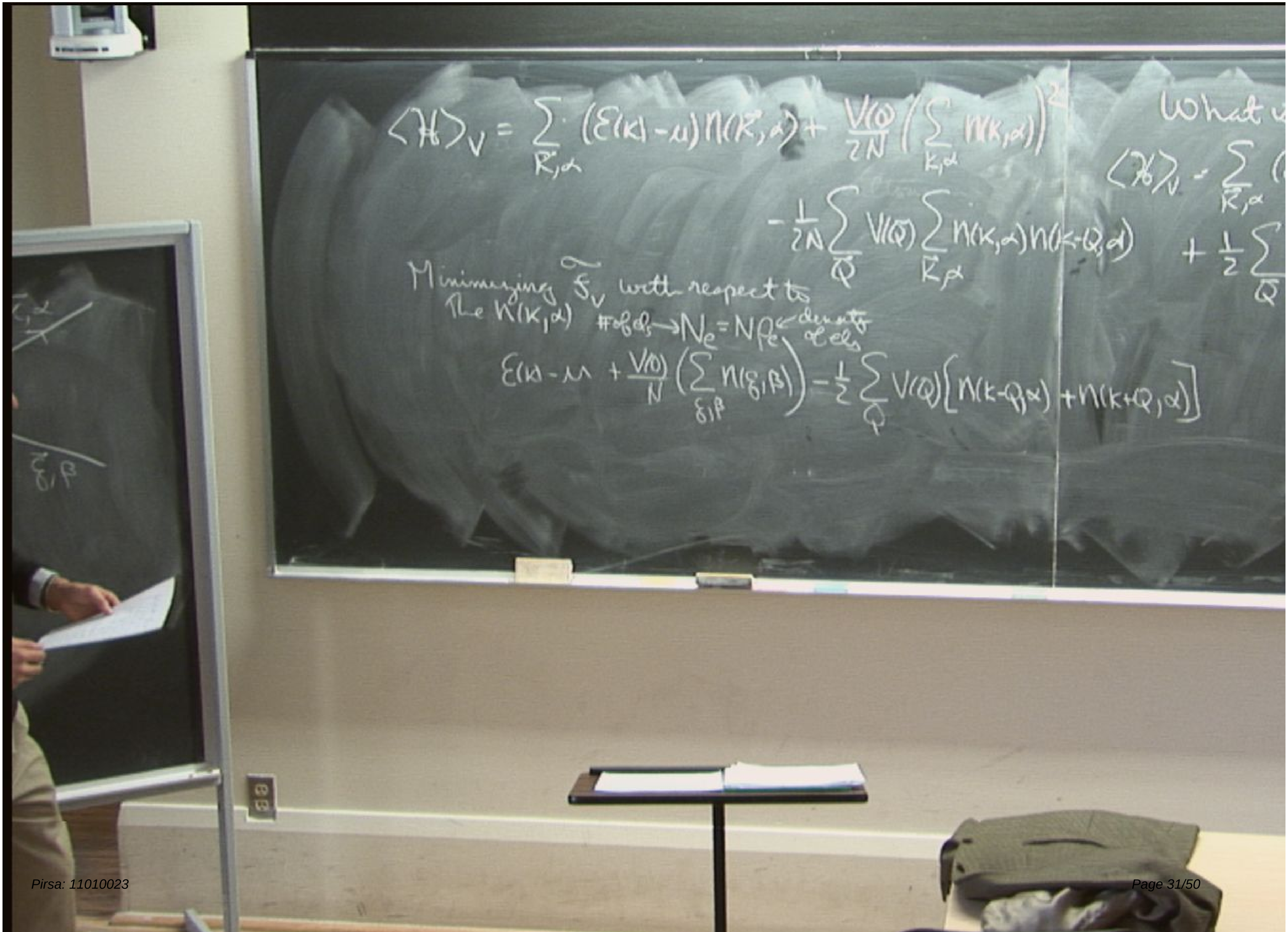
$$+ \frac{1}{2}\sum_{\vec{Q}} V(\ldots$$

Minimizing $\tilde{F}_V$ with respect to the $n(K,\alpha)$

\# of els $\rightarrow N_e = N\rho_e \leftarrow$ density of els

$$\mathcal{E}(K) - \mu + \frac{V(0)}{N}\left(\sum_{\delta,\beta} n(\delta,\beta)\right) - \frac{1}{2}\sum_{Q} V(Q)\left[n(K-Q,\alpha) + n(K+Q,\alpha)\right]$$


⟨H⟩_V = Σ_{k,α} (ε(k) − μ) n(k,α) + V(0)/2N (Σ_{k,α} n(k,α))^2
− 1/2N Σ_Q V(Q) Σ_{k,α} n(k,α) n(k−Q,α)
What i
Minimizing F̃_V with respect to
the n(k,α)
# of els → N_e = N ρ_e ← density of els
ε(k) − μ + V(0)/N (Σ_{q,β} n(q,β)) − 1/2 Σ_Q V(Q) [n(k−Q,α) + n(k+Q,α)]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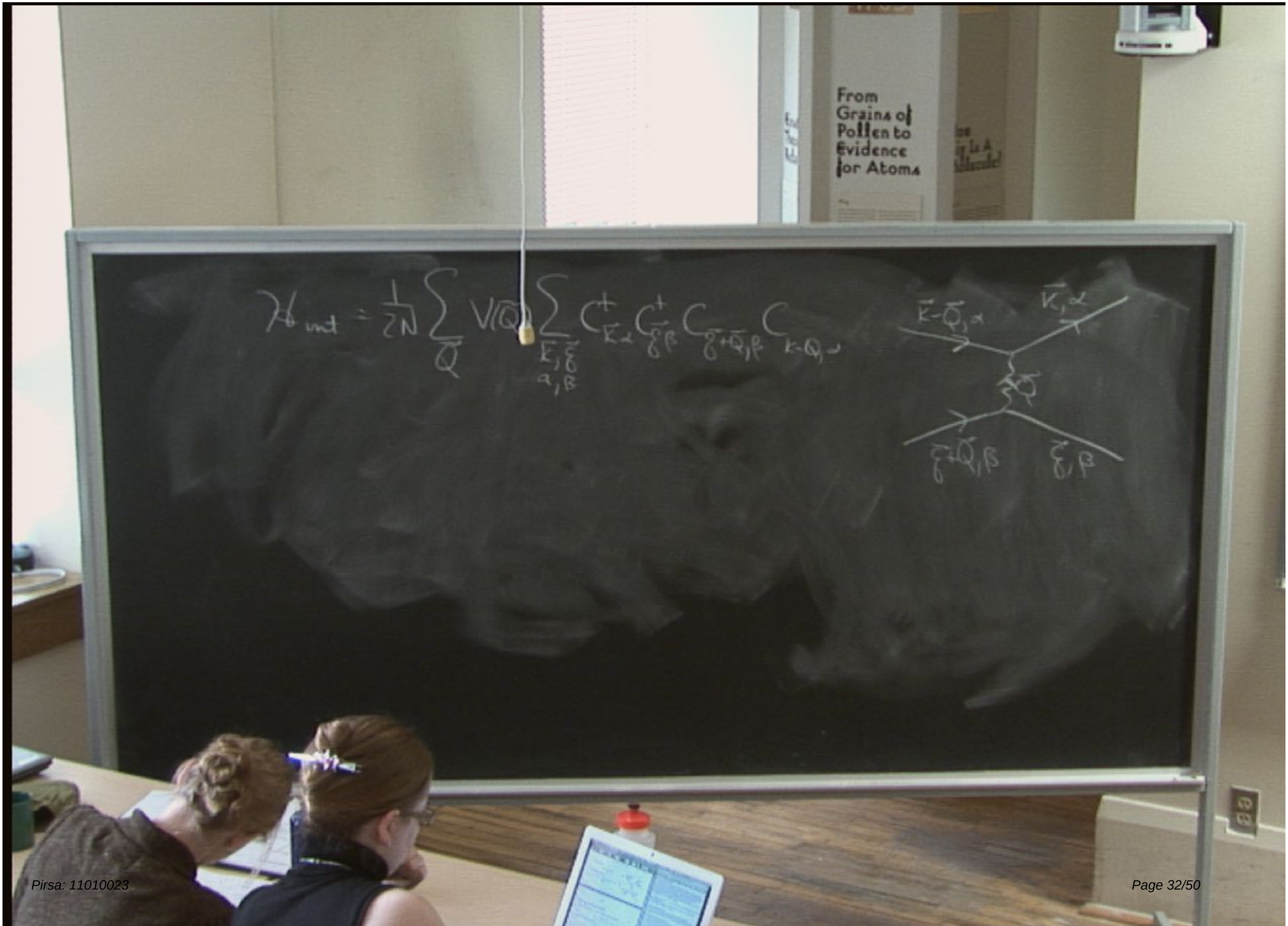
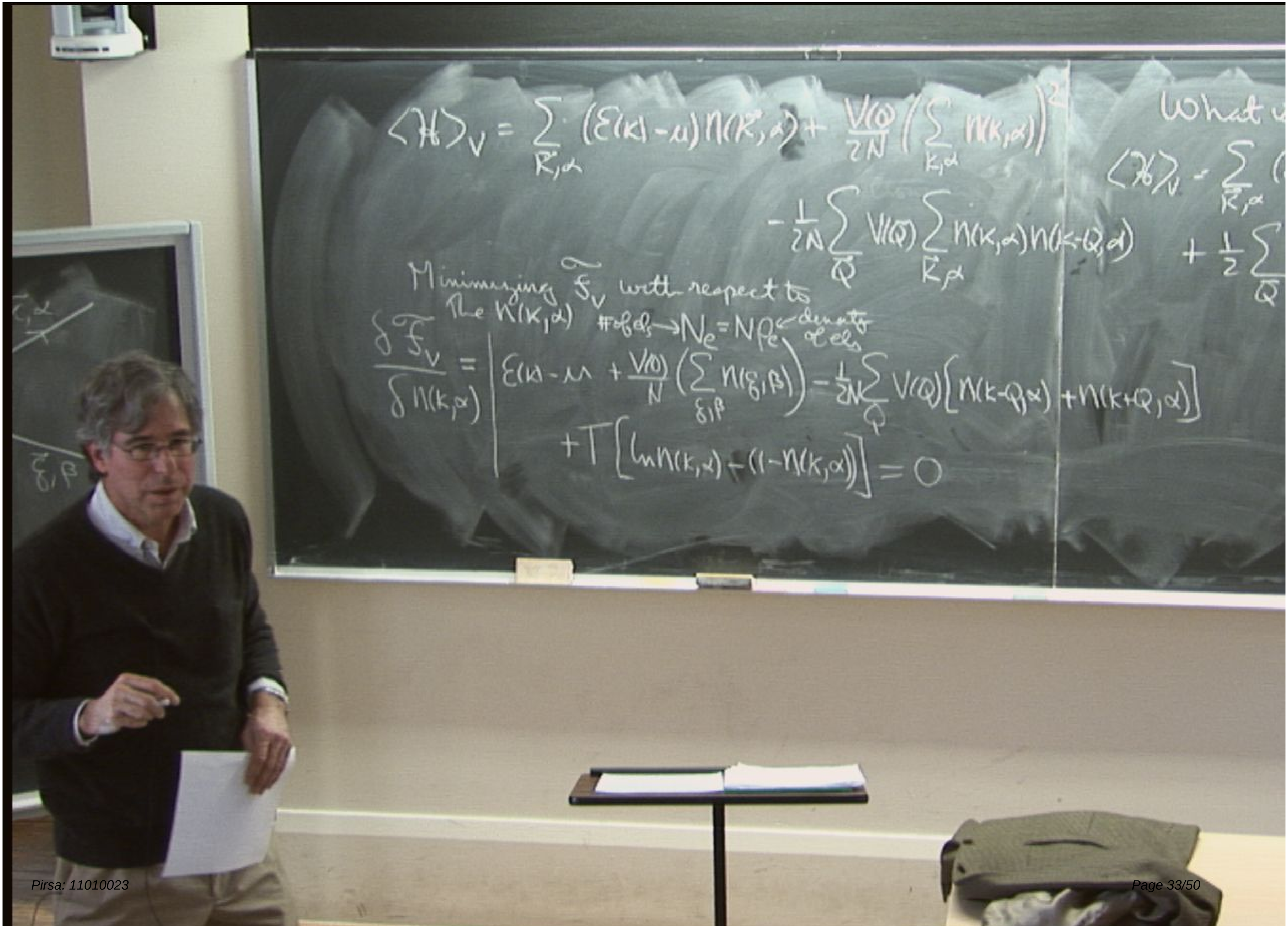
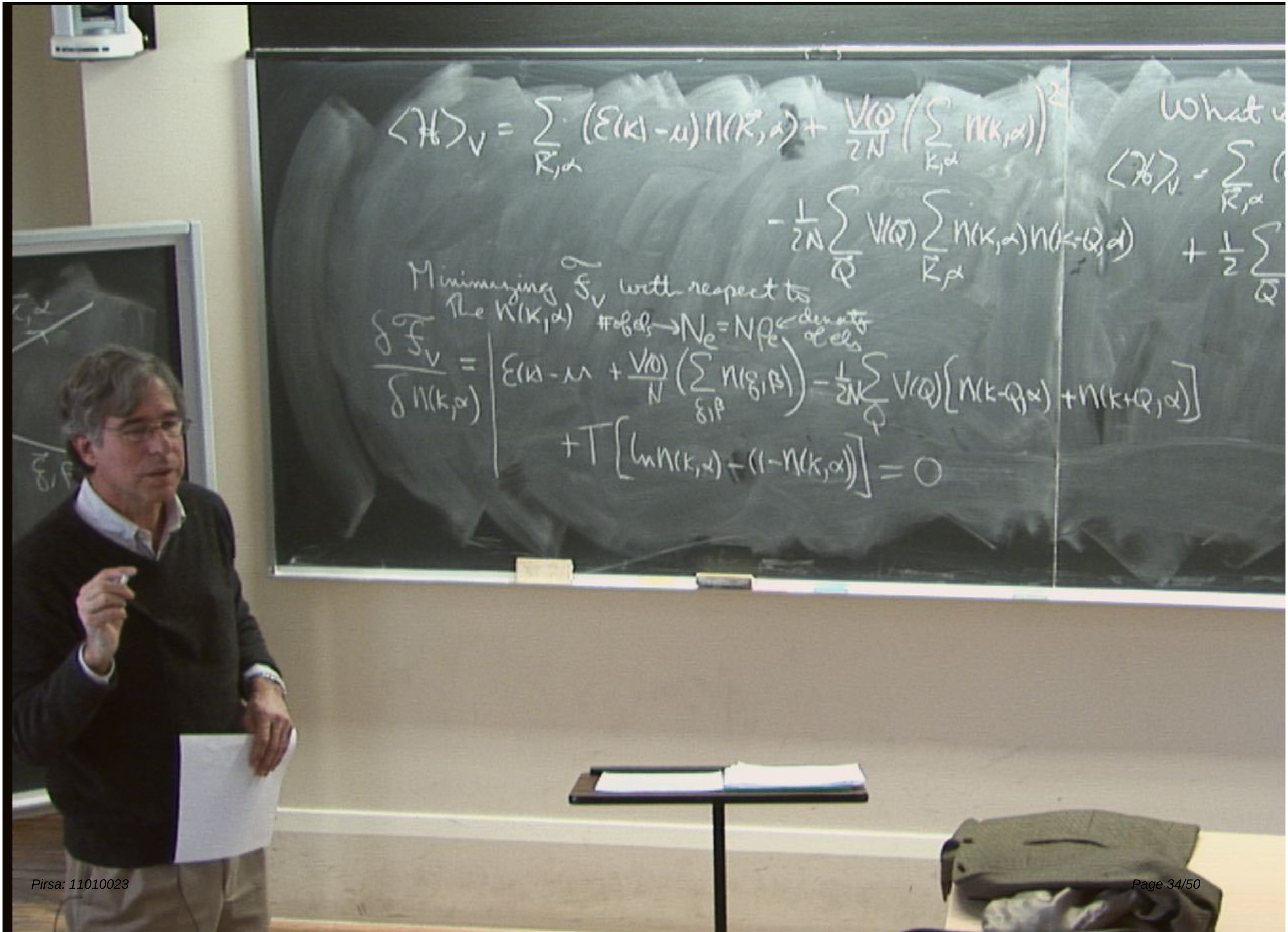
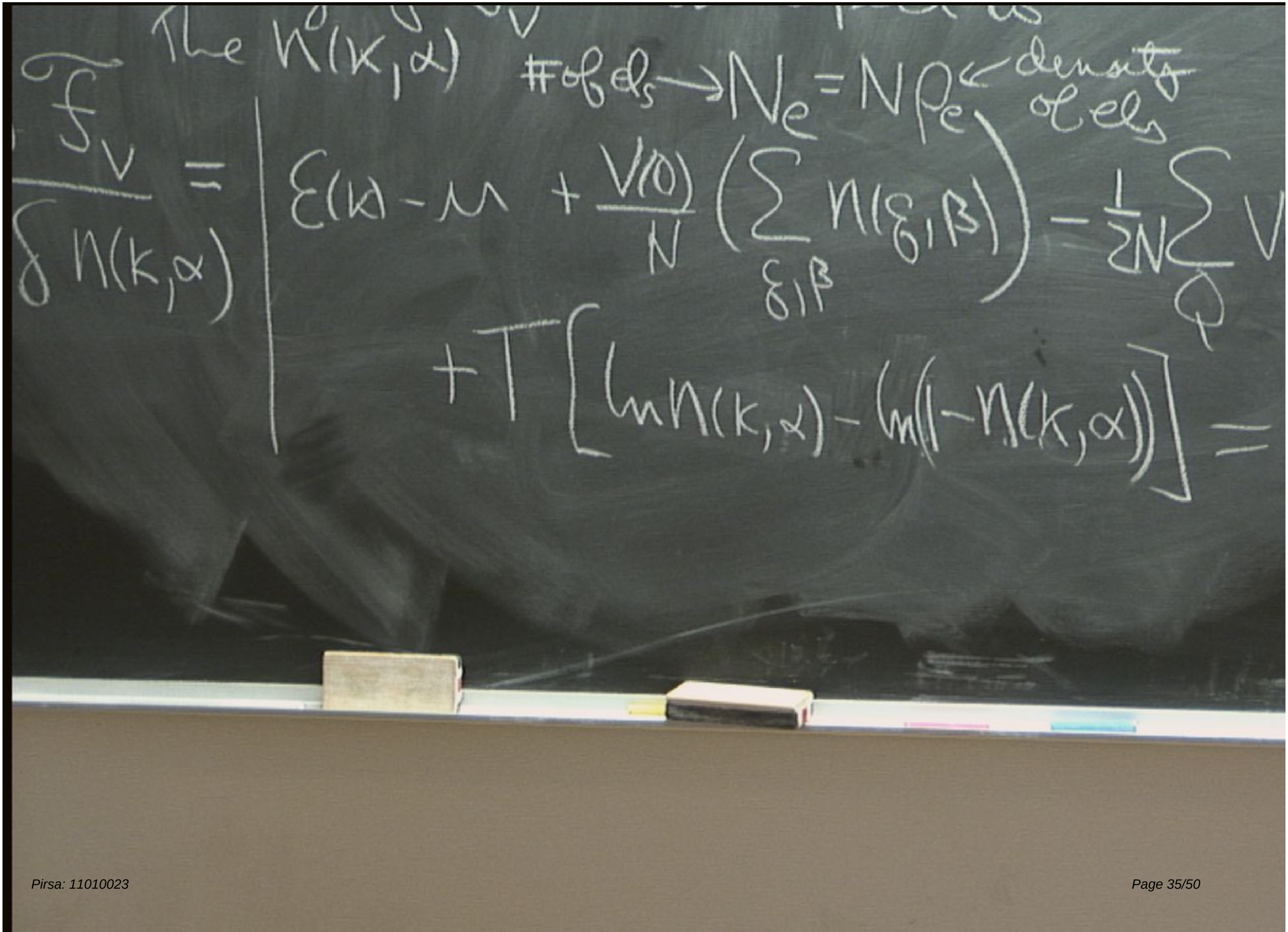
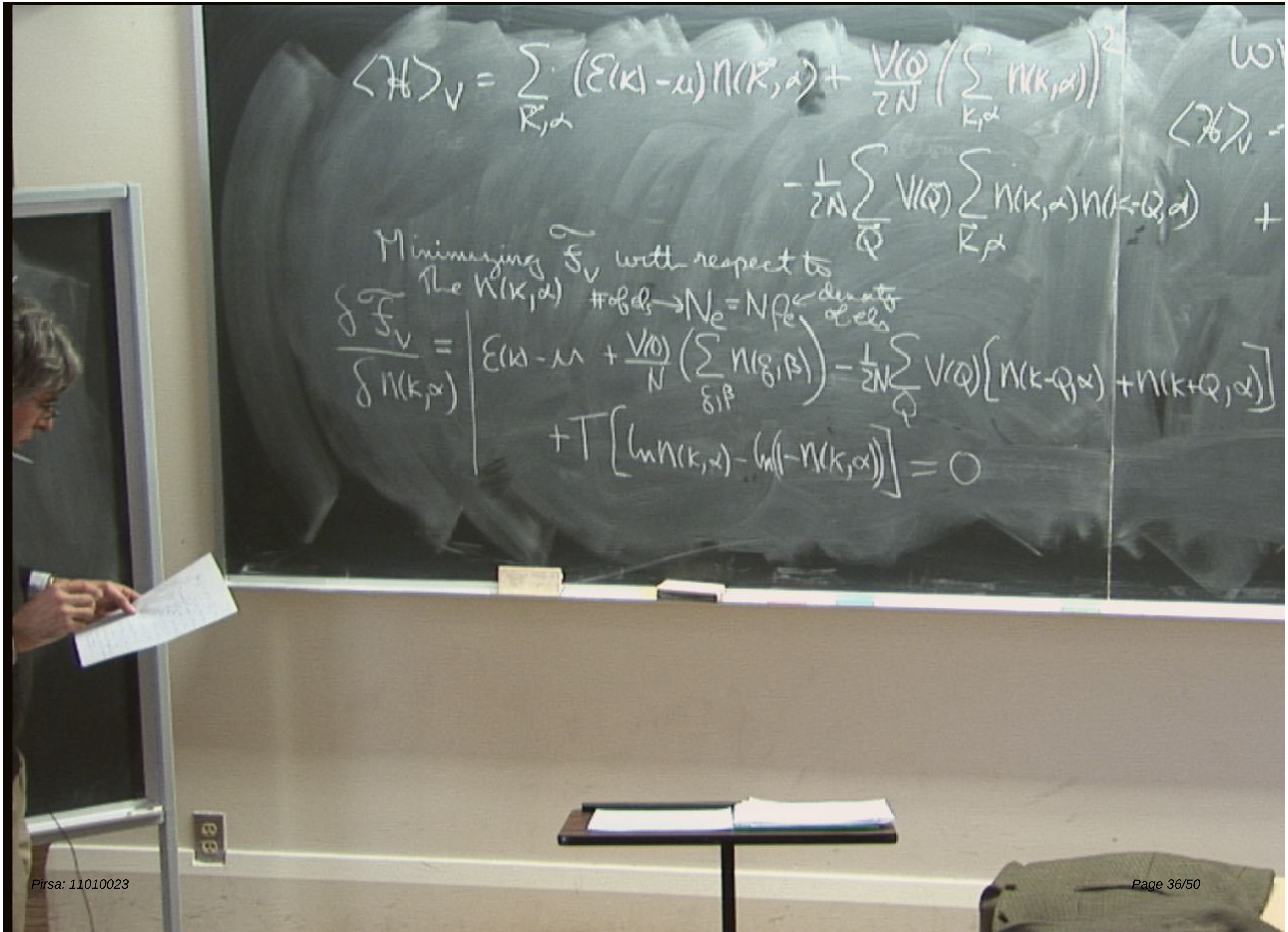
Minimizing F̃_V with respect to
the n(k,α)   # of els → N_e = Nρ_e ← density of els
ε(k) − μ + V(0)/N (Σ_{q,β} n(q,β)) − 1/2 Σ_Q V(Q)[n(k−Q,α) + n(k+Q,α)]
What is
⟨H⟩_V − Σ_{k,α}
+ 1/2 Σ_Q


From
Grains of
Pollen to
Evidence
for Atoms


Minimizing F_V with respect to
the n(k,α)
# of els → N_e = Nρ_e ← density of els
What is


What is
Minimizing $\tilde{\mathcal{F}}_V$ with respect to
the $n(k,\alpha)$
# of els → $N_e = N\rho_e$ ← density of els


The n(k,α)
# of els → N_e = N ρ_e ← density of els
δF_V / δn(k,α) = ε(k) − μ + V(0)/N (Σ_{δ,β} n(δ,β)) − 1/(2N) Σ_Q V
+ T [ln n(k,α) − ln(1 − n(k,α))] =



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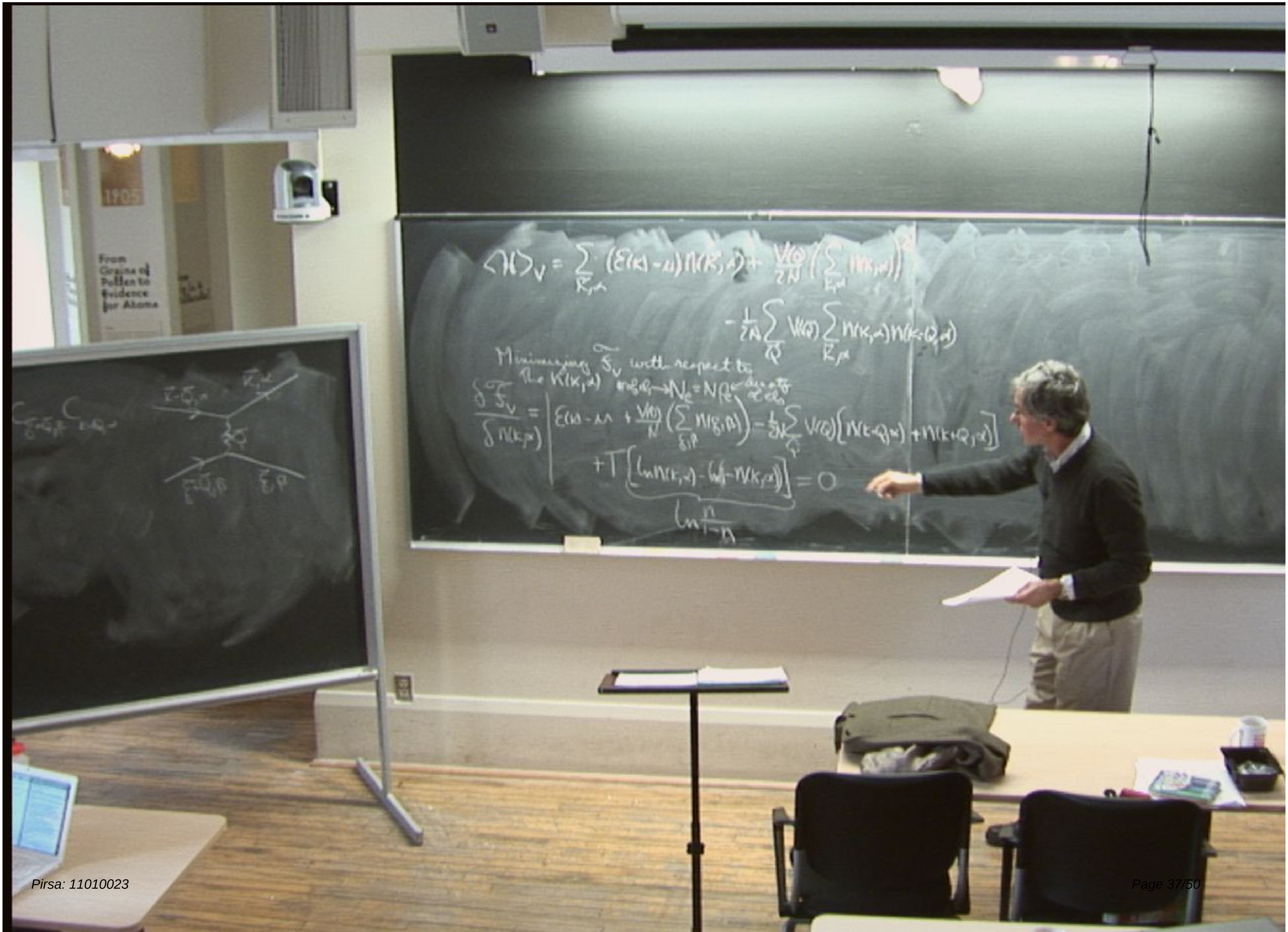
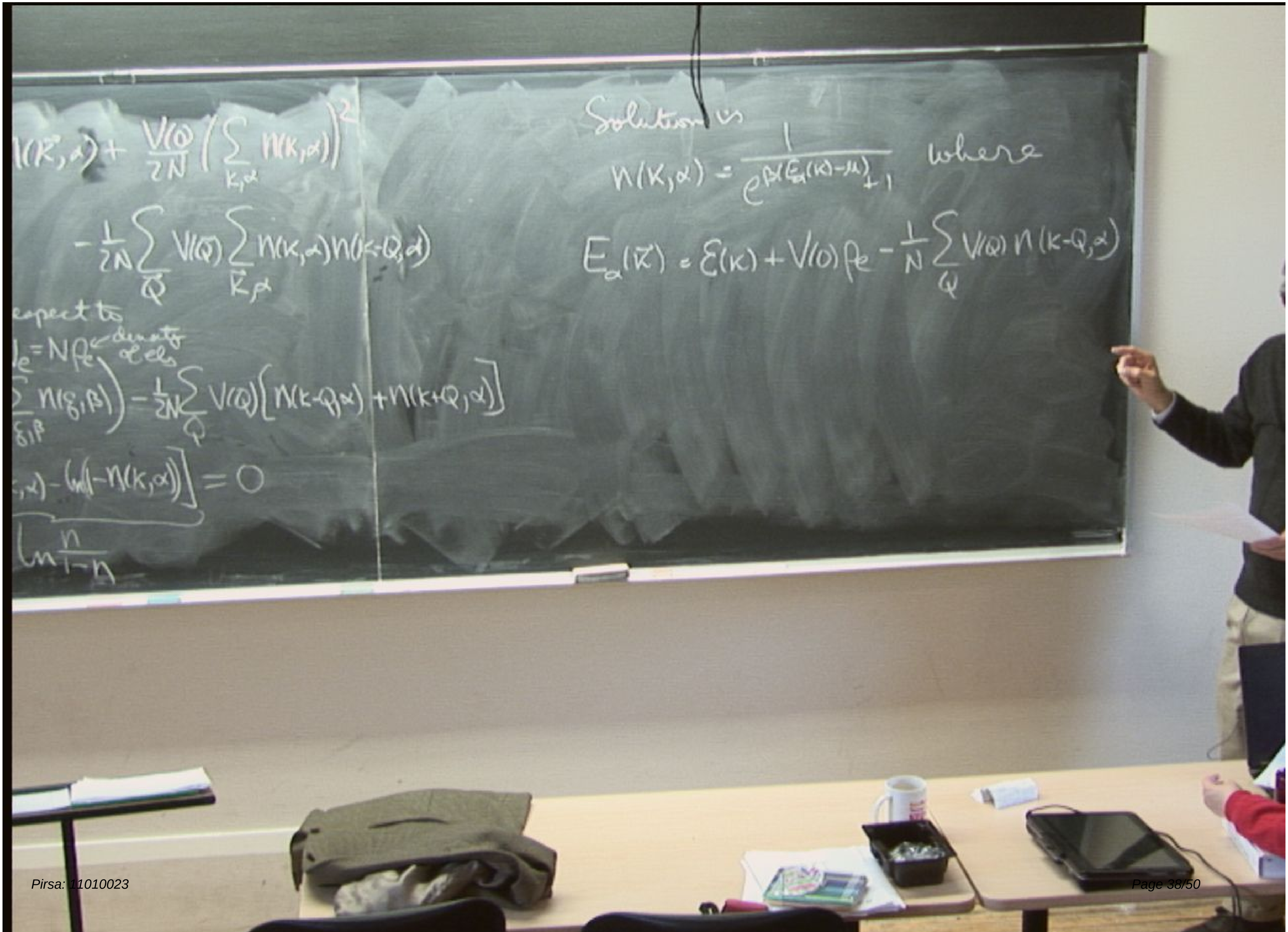
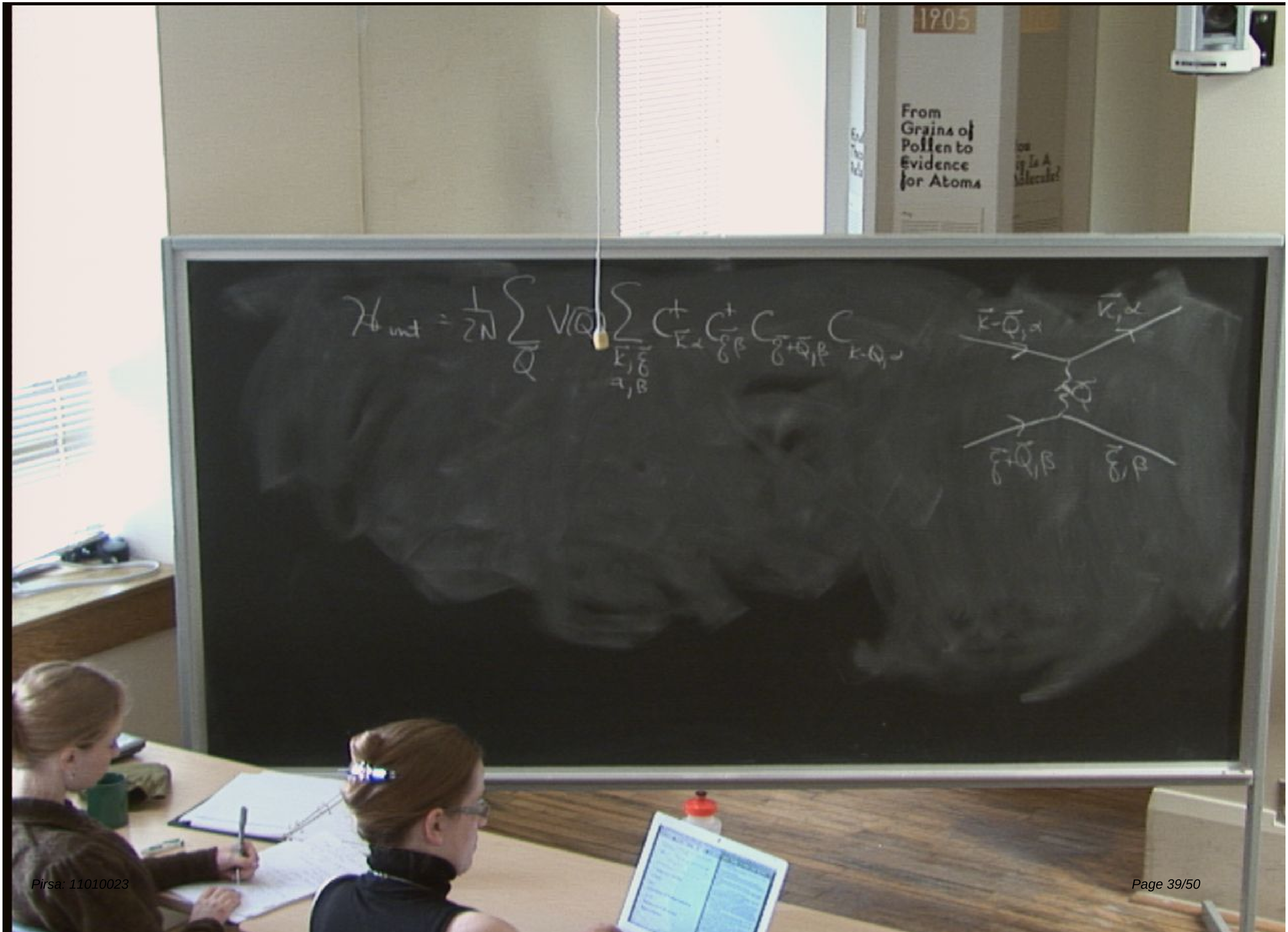
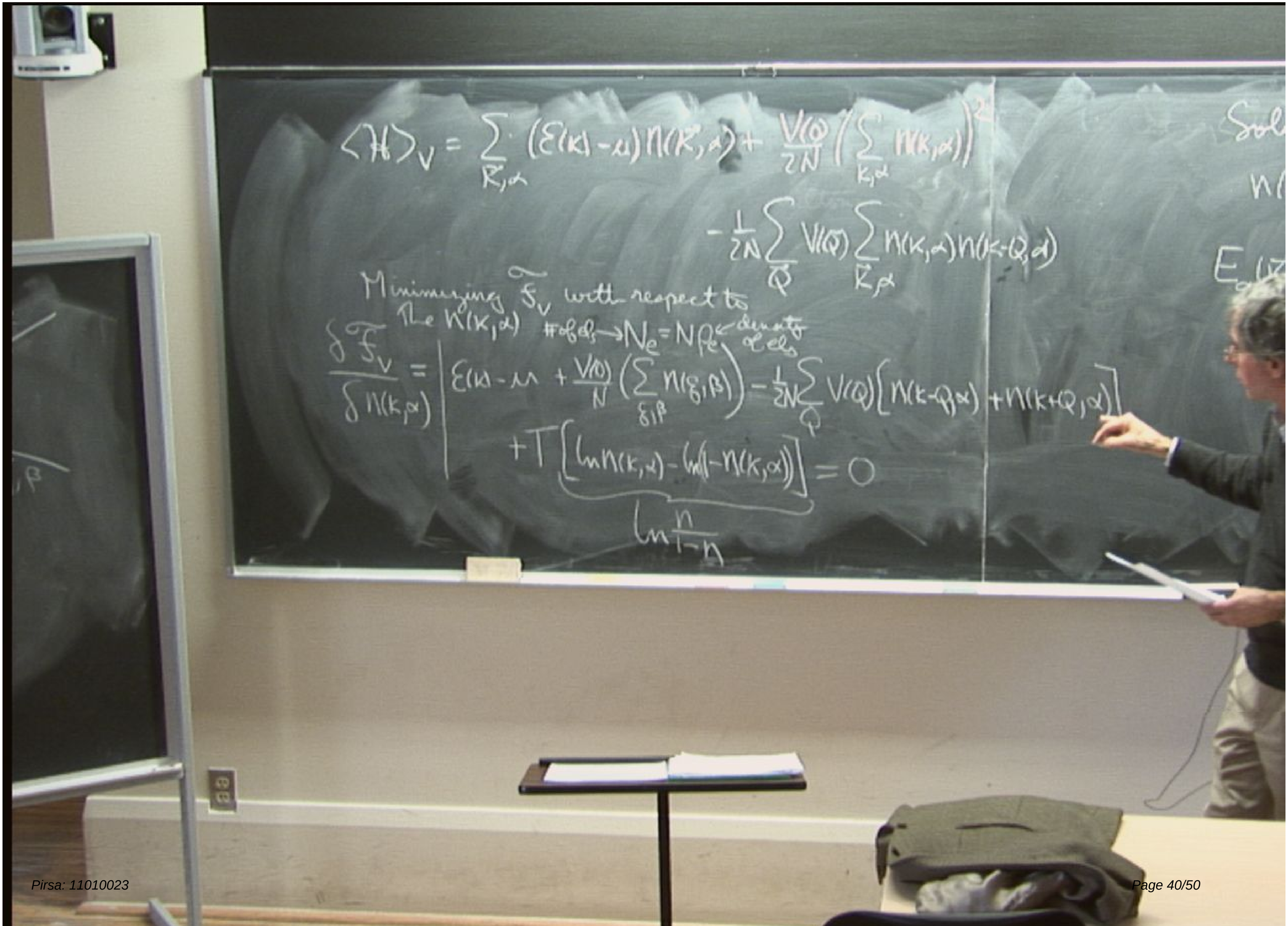
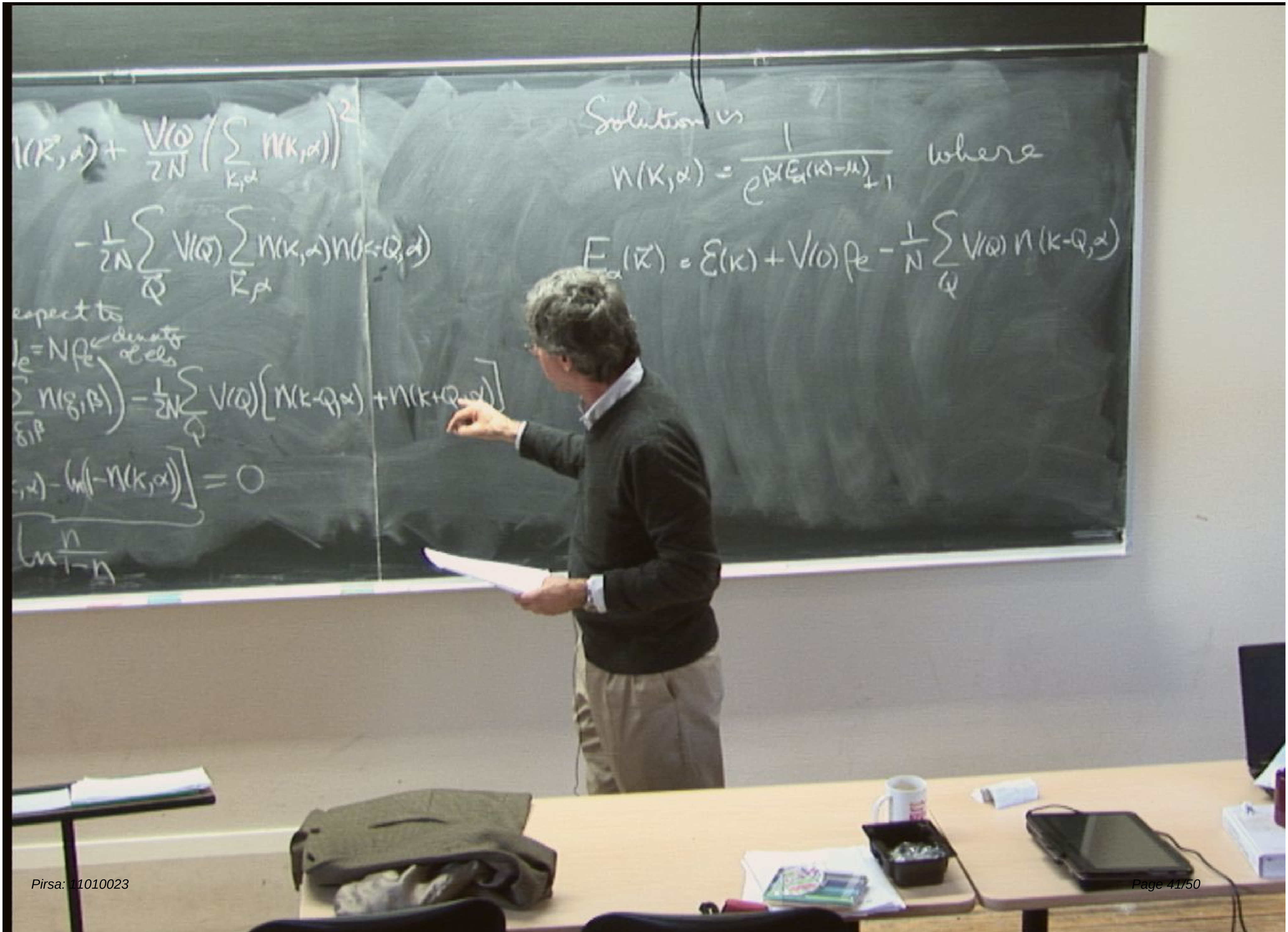
$- \frac{1}{2N} \sum_{\vec{Q}} V(\vec{Q}) \sum_{\vec{k},\alpha} n(k,\alpha)\, n(k-Q,\alpha)$
Minimizing $\tilde{\mathcal{F}}_V$ with respect to the $n(k,\alpha)$
# of els → $N_e = N\rho_e$ ← density of els
$\frac{\delta \tilde{\mathcal{F}}_V}{\delta n(k,\alpha)} = \varepsilon(k) - \mu + \frac{V(0)}{N} \left(\sum_{q,\beta} n(q,\beta) \right) - \frac{1}{2N} \sum_{Q} V(Q) \left[n(k-Q,\alpha) + n(k+Q,\alpha) \right]$
$+ T \left[\ln n(k,\alpha) - \ln(1 - n(k,\alpha)) \right] = 0$
$\langle \mathcal{H} \rangle_V$

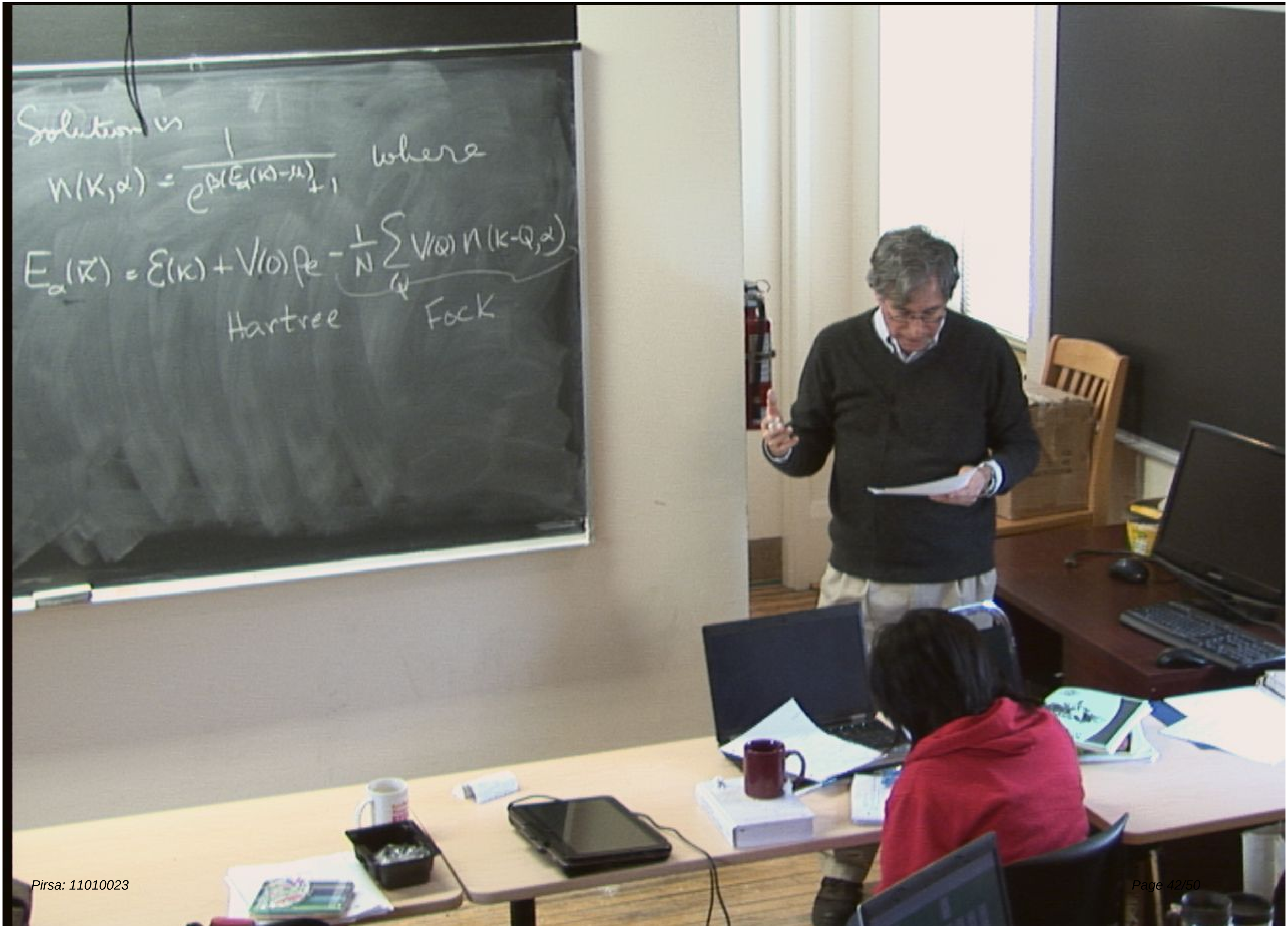

1905
From Grains of Pollen to Evidence for Atoms
Minimizing with respect to

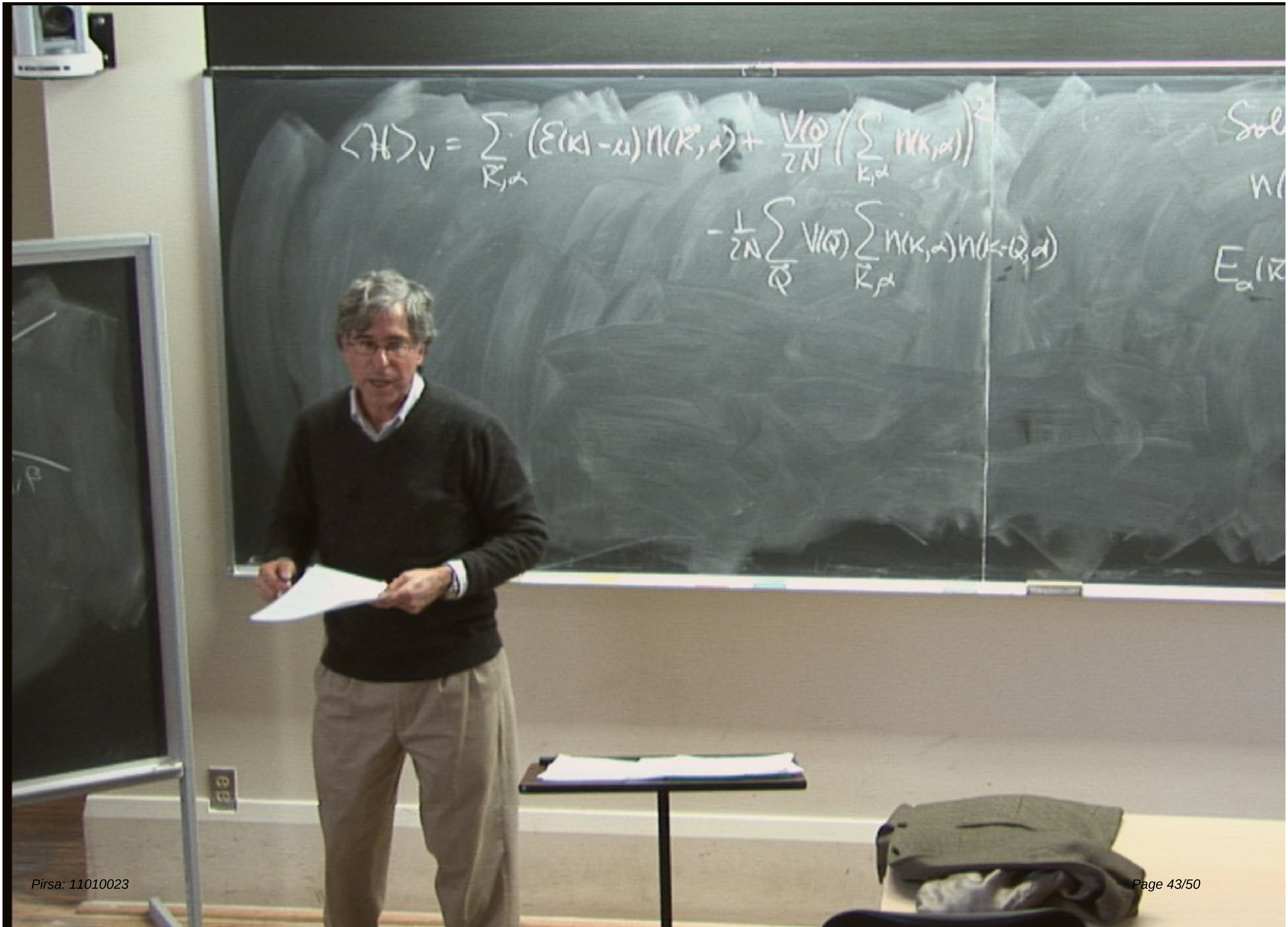

Solution is
where
respect to
density of els

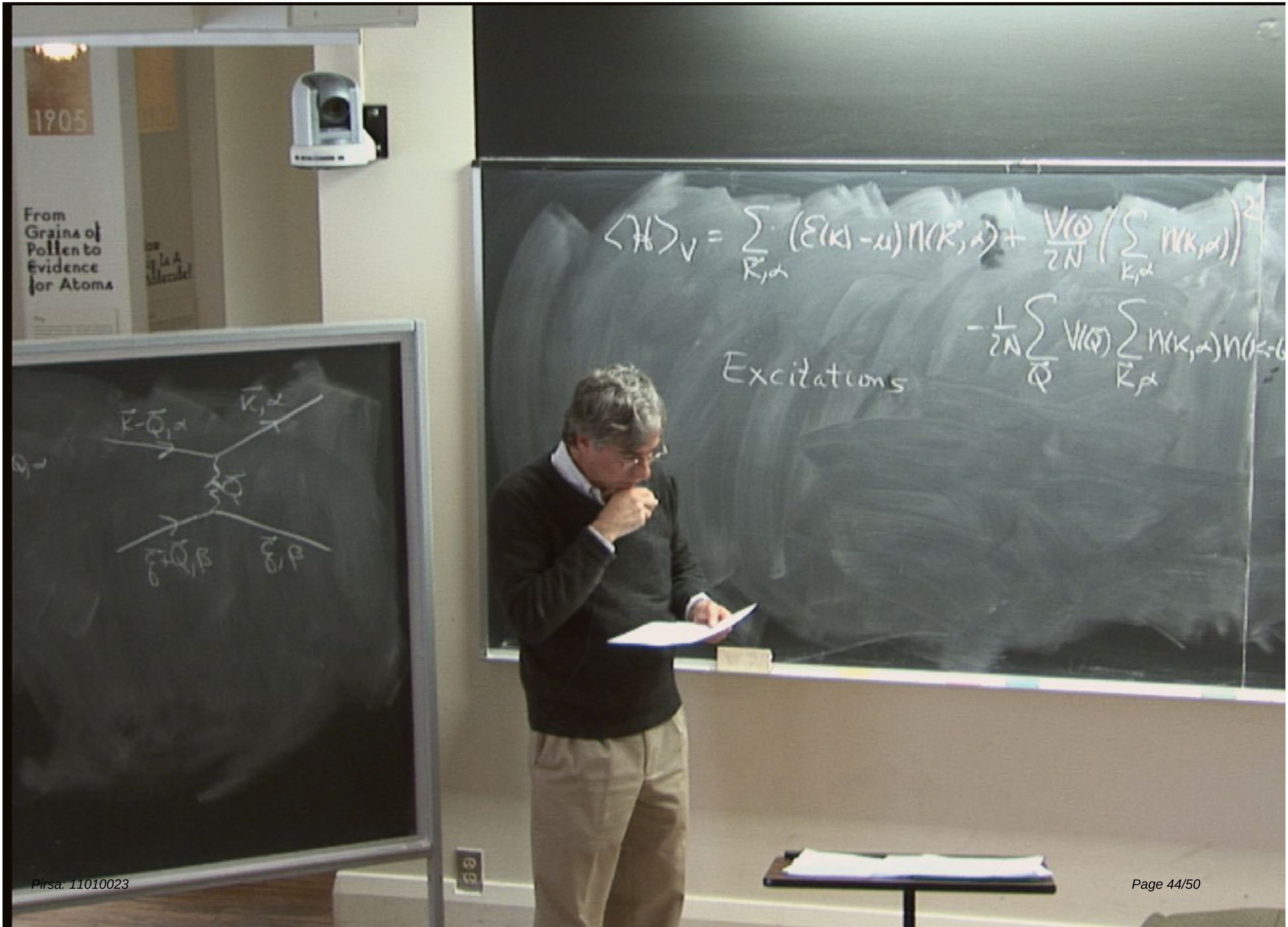

1905
From Grains of Pollen to Evidence for Atoms
$\mathcal{H}_{int} = \frac{1}{2N} \sum_{\vec{Q}} V(\vec{Q}) \sum_{\vec{k},\vec{\xi},\alpha,\beta} c^\dagger_{\vec{k}\alpha} c^\dagger_{\vec{\xi}\beta} c_{\vec{\xi}+\vec{Q},\beta} c_{\vec{k}-\vec{Q},\alpha}$
$\vec{k}-\vec{Q},\alpha$
$\vec{k},\alpha$
$\vec{Q}$
$\vec{\xi}+\vec{Q},\beta$
$\vec{\xi},\beta$

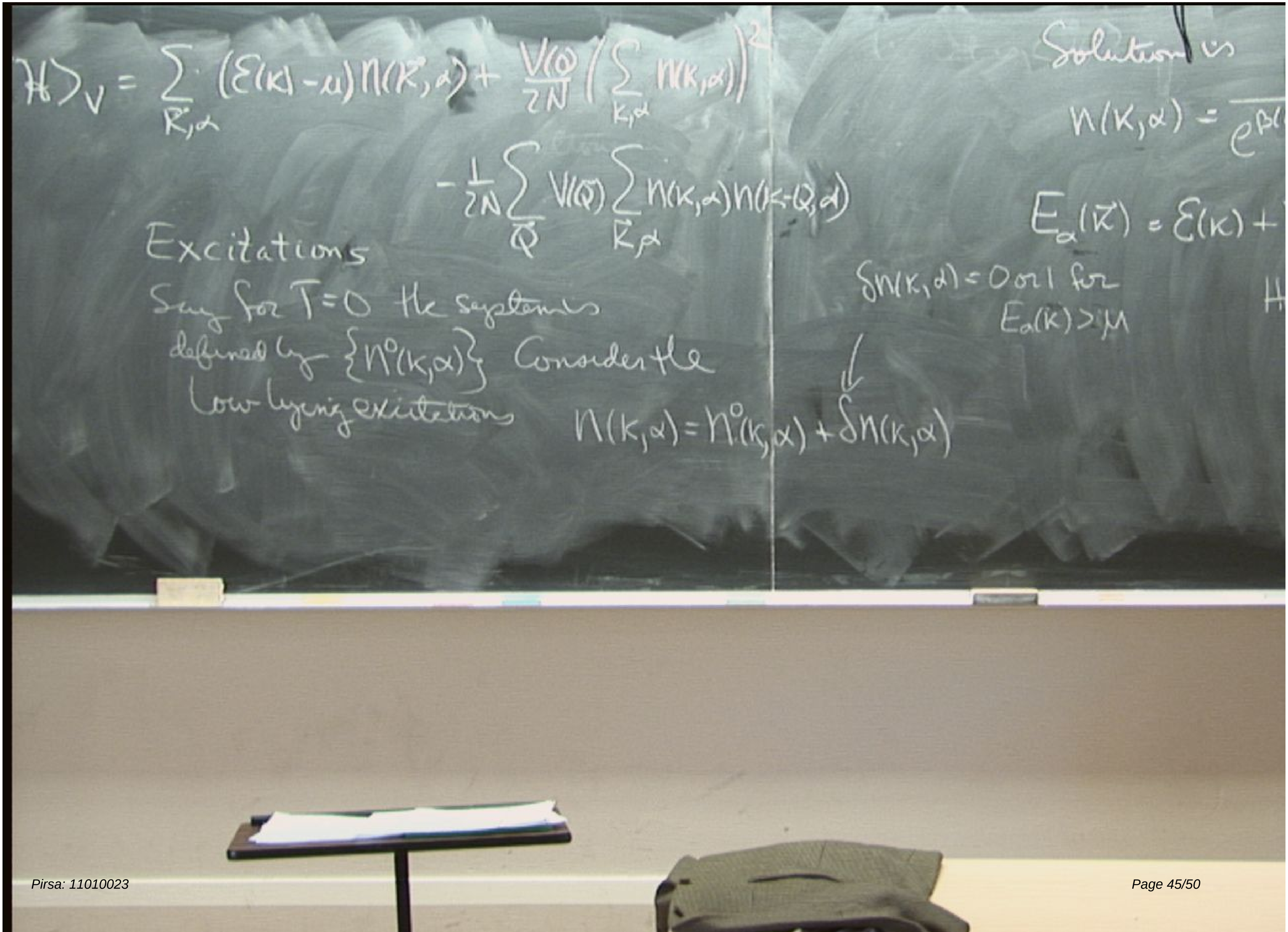

⟨H⟩_V = Σ_{K,α} (ε(K) − μ) n(K,α) + V(0)/2N (Σ_{K,α} n(K,α))²
− 1/2N Σ_Q V(Q) Σ_{K,α} n(K,α) n(K−Q,α)
Minimizing F̃_V with respect to the n(K,α)
# of els → N_e = N ρ_e ← density of els
δF̃_V / δn(K,α) = ε(K) − μ + V(0)/N (Σ_{g,β} n(g,β)) − 1/2N Σ_Q V(Q)[n(K−Q,α) + n(K+Q,α)]
+ T [ln n(K,α) − ln(1 − n(K,α))] = 0
ln n/(1−n)

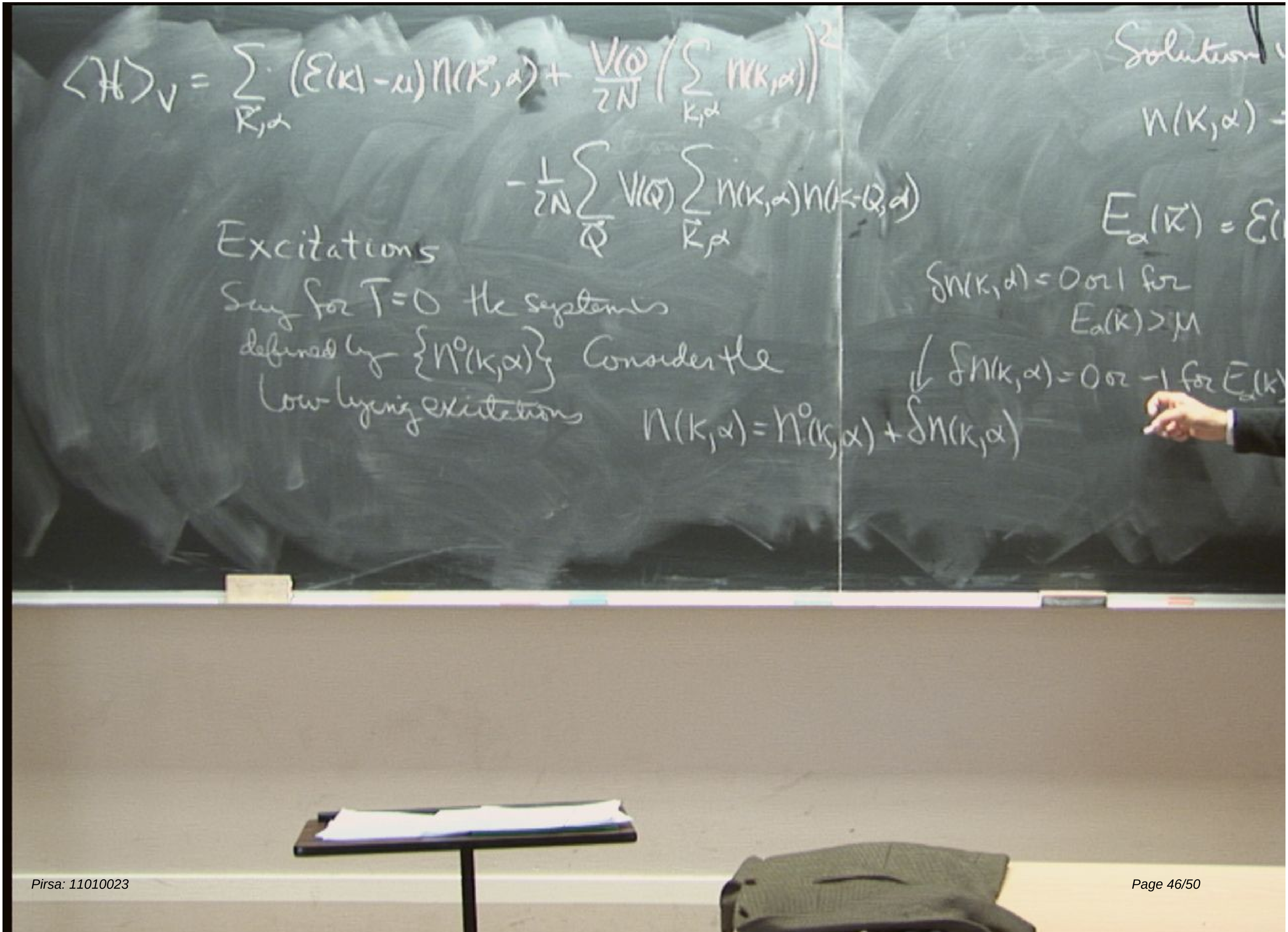

Solution is
where
respect to
density of els

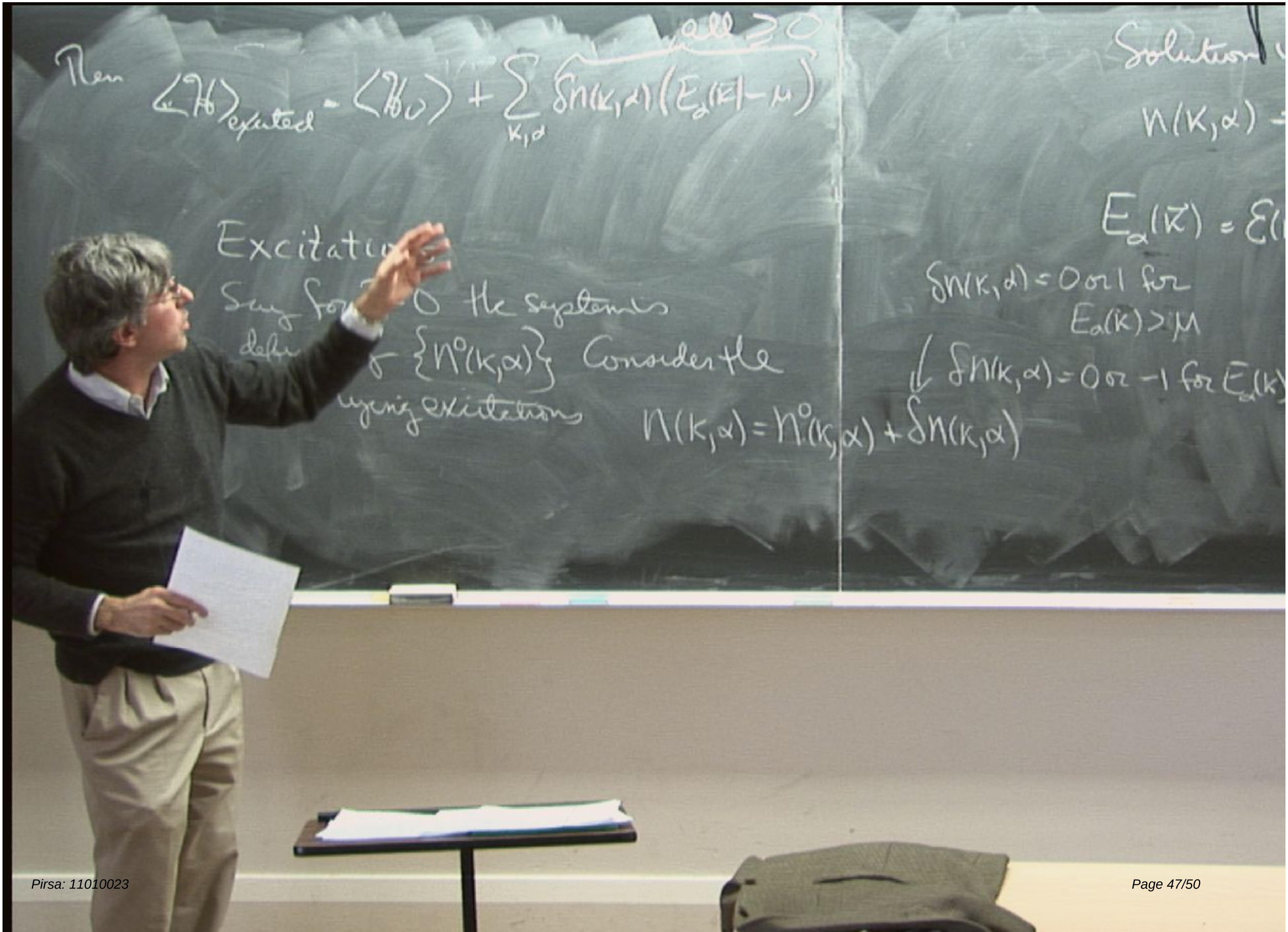

Solution is
n(K,α) = 1/(e^{β(E_α(K)−μ)}+1) where
E_α(K) = ε(K) + V(0)ρe − (1/N) Σ_Q V(Q) n(K−Q,α)
Hartree
Fock


⟨H⟩_V = Σ_{k,α} (ε(k) − μ) n(k,α) + V(0)/2N (Σ_{k,α} n(k,α))^2
− 1/2N Σ_Q V(Q) Σ_{k,α} n(k,α) n(k+Q,α)

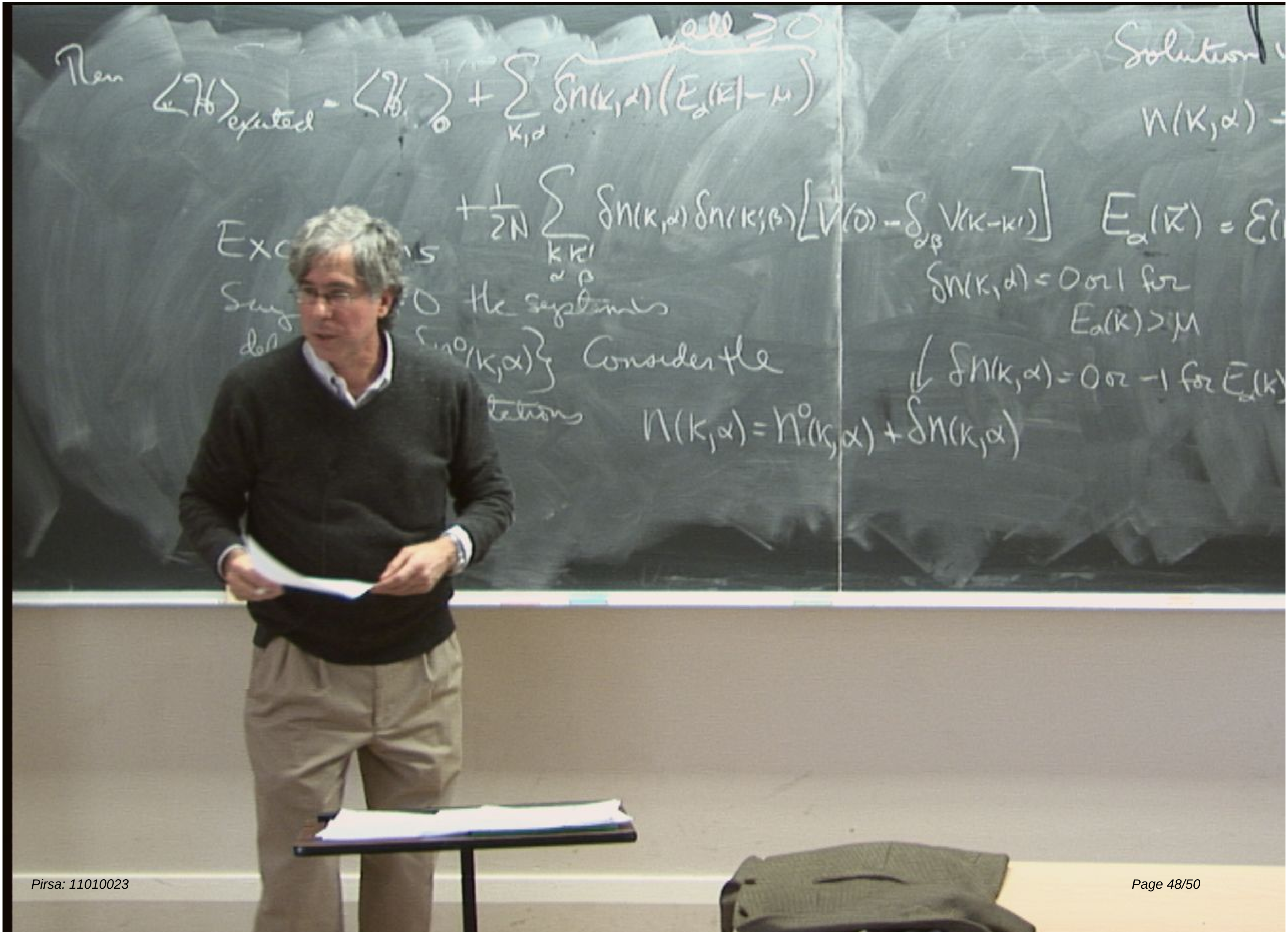

1905
From Grains of Pollen to Evidence for Atoms
Excitations

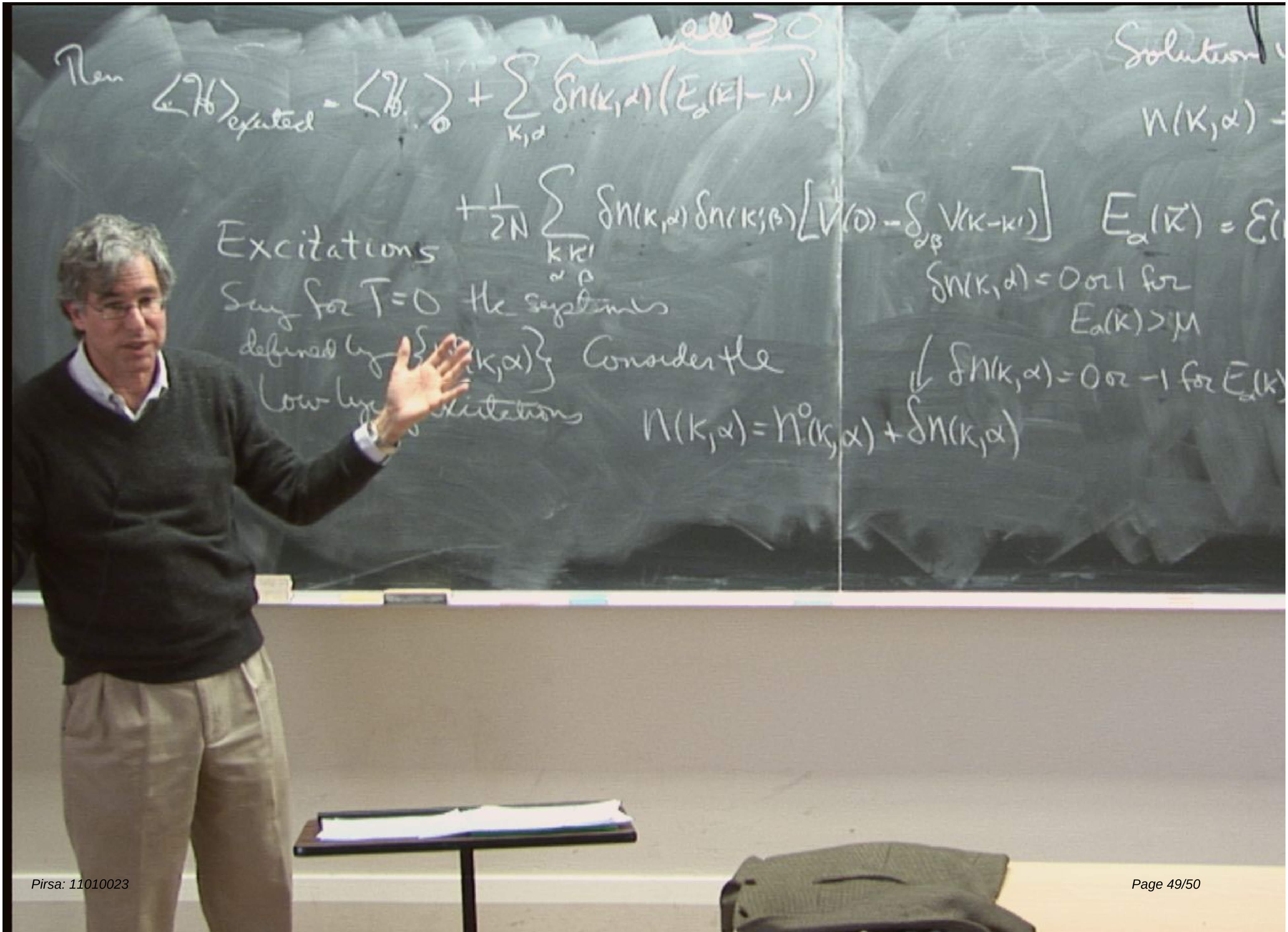

Excitations
Say for T=0 the system is
defined by {n°(k,α)} Consider the
low lying excitations
Solution is
δn(k,α) = 0 or 1 for

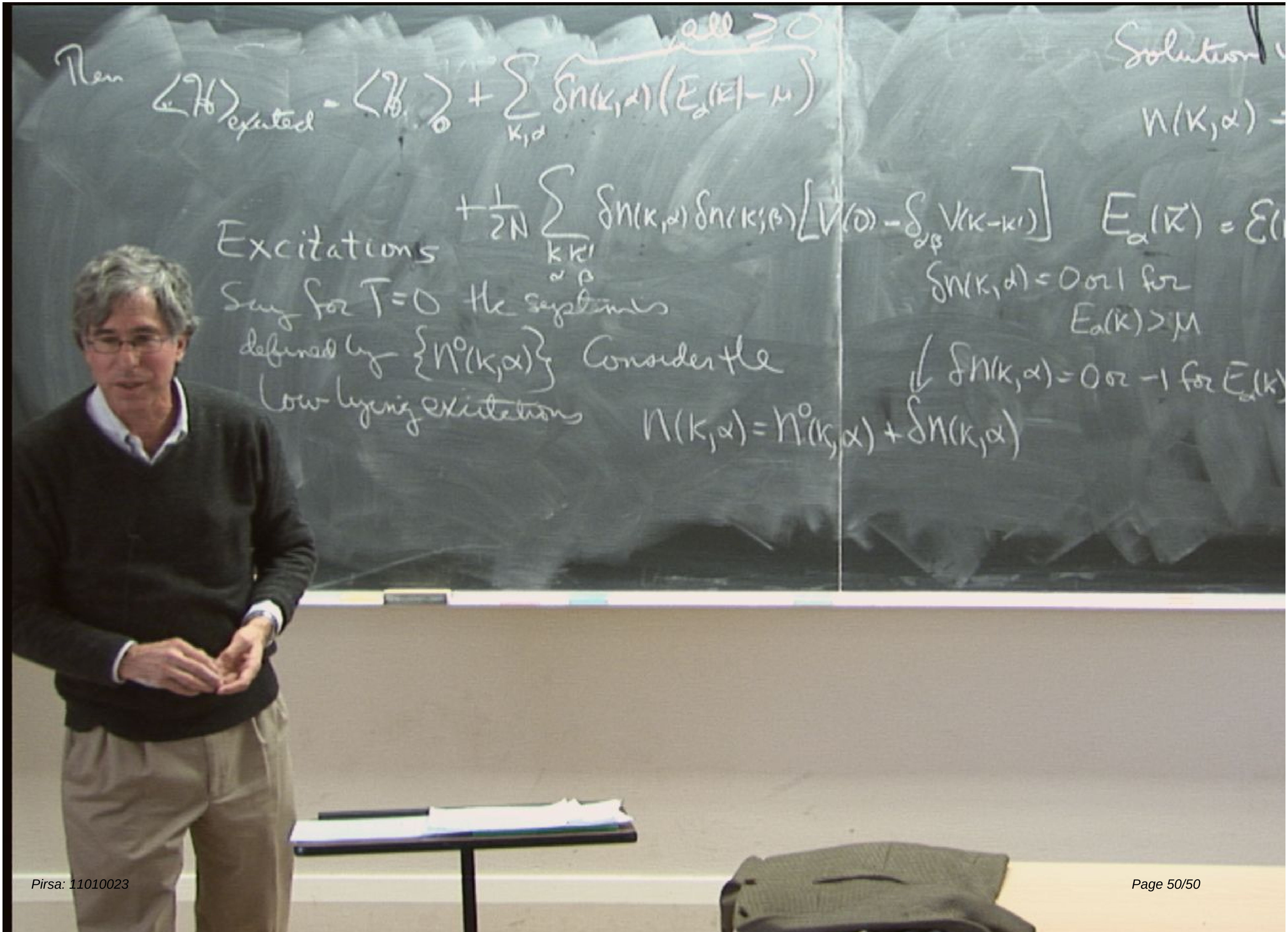

⟨H⟩_V = Σ_{K,α} (ε(K) − μ) n(K,α) + V(Q)/2N (Σ_{K,α} n(K,α))²
− 1/2N Σ_Q V(Q) Σ_{K,α} n(K,α) n(K−Q,α)
Excitations
Say for T=0 the system is
defined by {n°(k,α)} Consider the
low-lying excitations
n(k,α) = n°(k,α) + δn(k,α)
Solution
n(K,α) =
E_α(K) = ε(
δn(k,α) = 0 or 1 for
E_α(k) > μ
δn(k,α) = 0 or −1 for E_α(k)



Then
all ≥ 0
⟨H⟩excited = ⟨H0⟩ + Σk,α δn(k,α)(Eα(k) − μ)
Excitation
the system is
{n°(k,α)}
Consider the
excitations
n(k,α) = n°(k,α) + δn(k,α)
Solution
n(K,α) =
Eα(K) = ε(
δn(k,α) = 0 or 1 for
Eα(k) > μ
δn(k,α) = 0 or −1 for


Solution
n(k,α) = n°(k,α) + δn(k,α)
δn(k,α) = 0 or 1 for
Eα(k) > μ
δn(k,α) = 0 or −1 for
the system is
Consider the


Then ⟨H⟩excited = ⟨H0⟩ + Σ δn(k,α)(Eα(k) − μ)
all ≥ 0
+ 1/2N Σ δn(k,α) δn(k',β) [V(0) − δαβ V(k−k')]
Excitations
Say for T=0 the system is
defined by {n(k,α)} Consider the
Low lying excitations
n(k,α) = n°(k,α) + δn(k,α)
Solution
n(k,α) =
Eα(k) = ε(
δn(k,α) = 0 or 1 for
Eα(k) > μ
δn(k,α) = 0 or −1 for Eα(k)


Excitations
Say for T=0 the system is
defined by {n°(k,α)} Consider the
Low lying excitations
n(k,α) = n°(k,α) + δn(k,α)
δn(k,α) = 0 or 1 for
Eα(k) > μ
δn(k,α) = 0 or −1 for
Solution
n(k,α) =
Eα(k) = ε