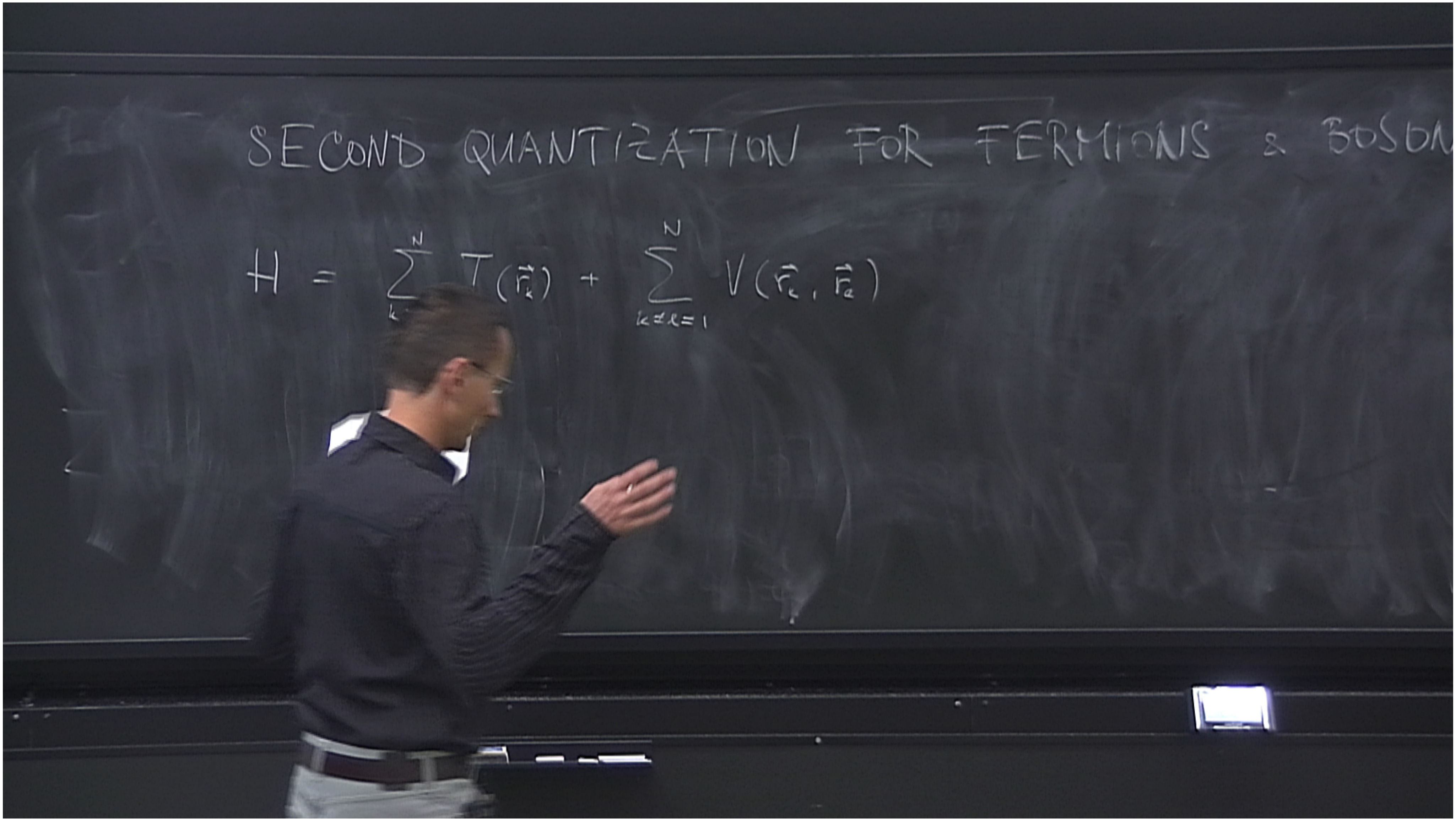
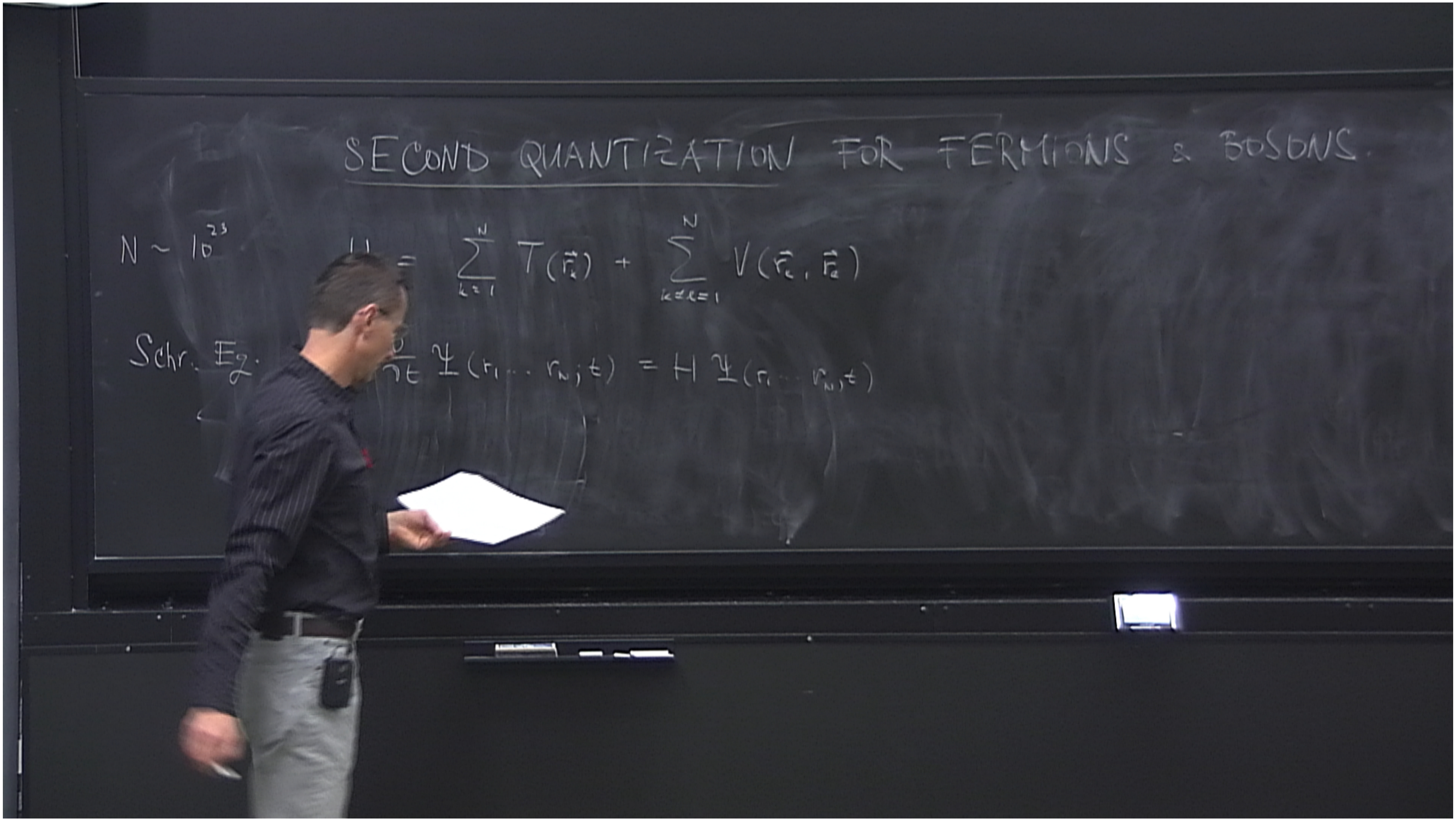
Title: 14/15 PSI - Condensed Matter-Lecture 2

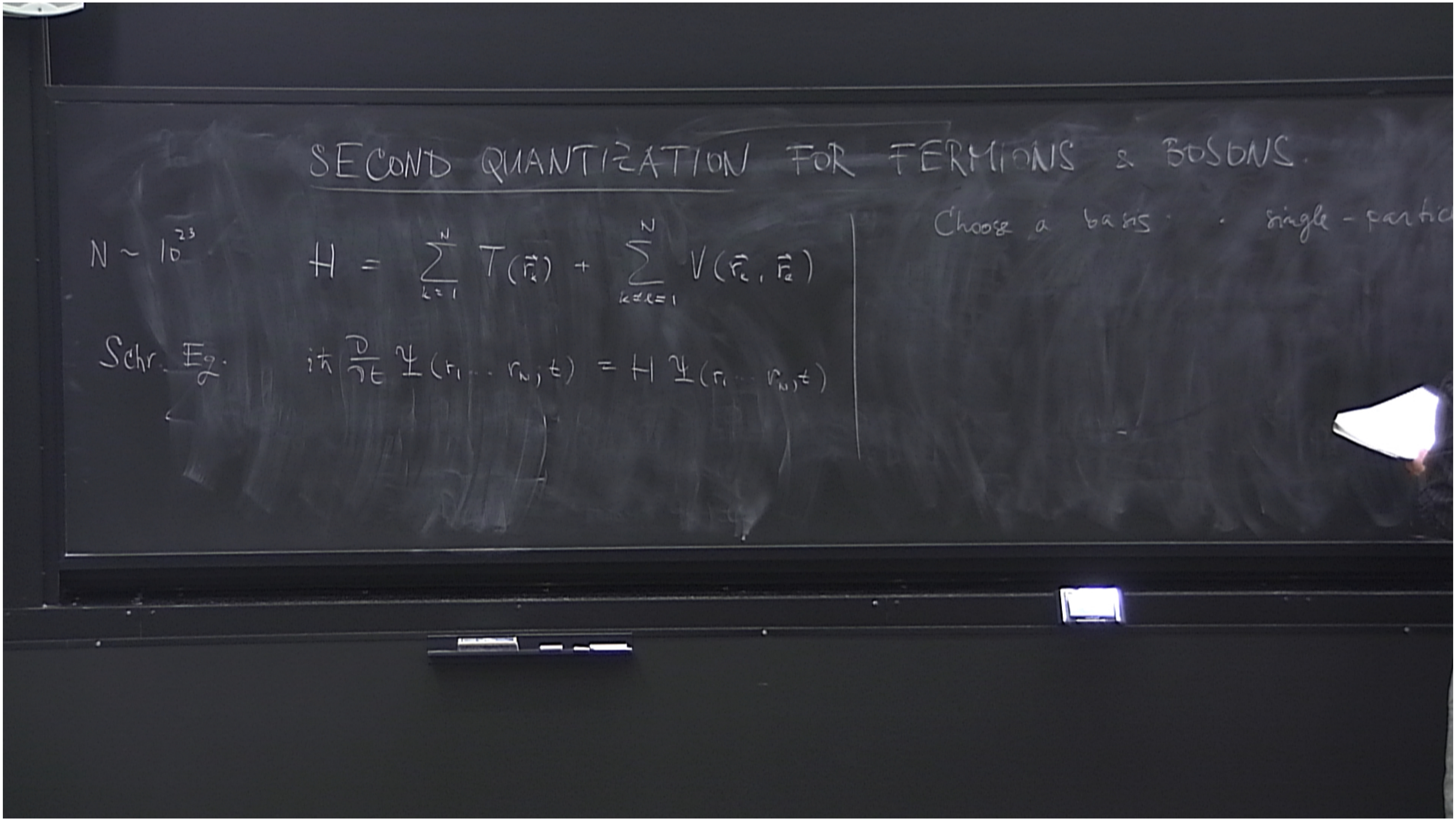
Date: Nov 11, 2014 10:45 AM

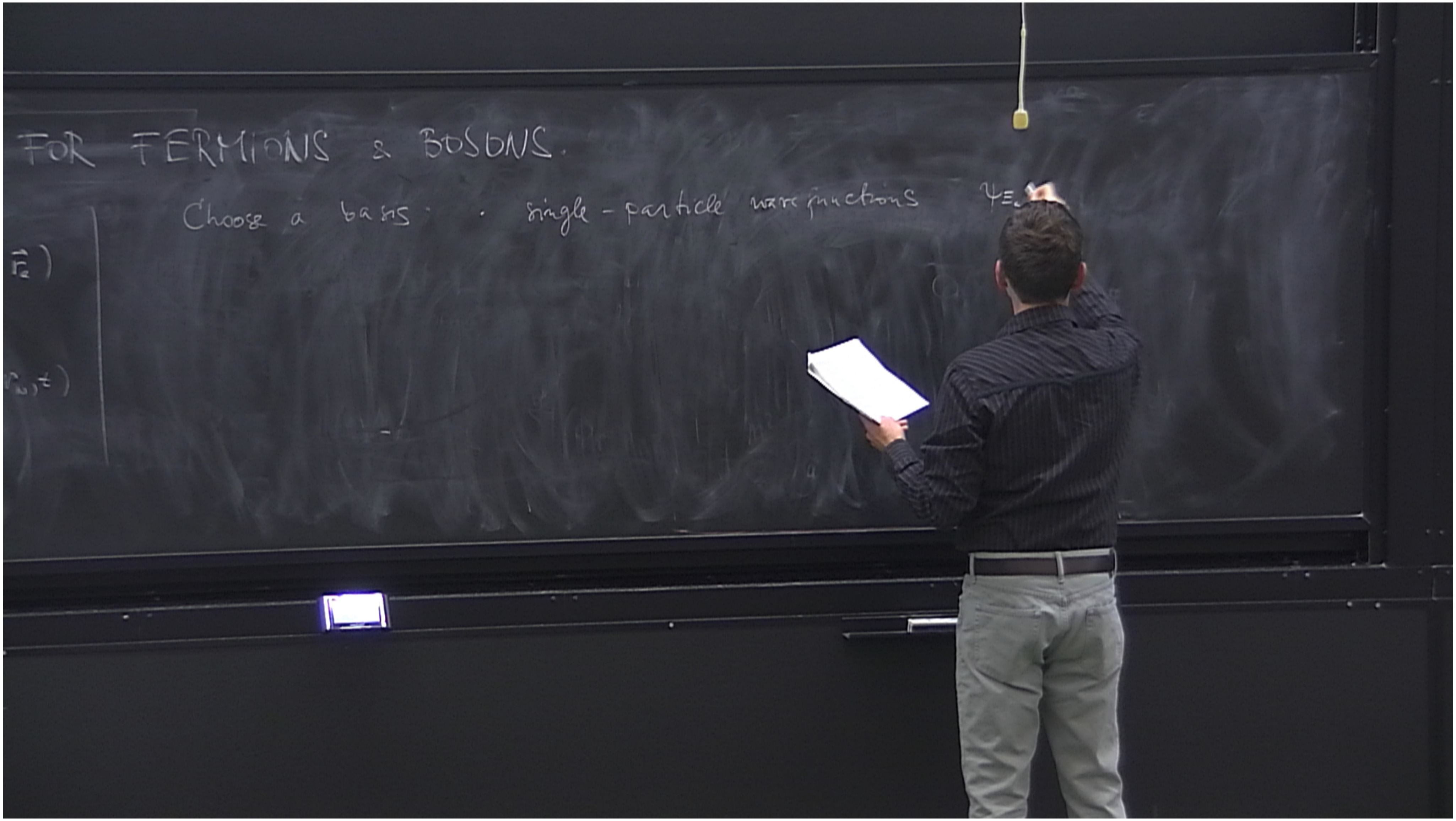
URL: http://pirsa.org/14110026

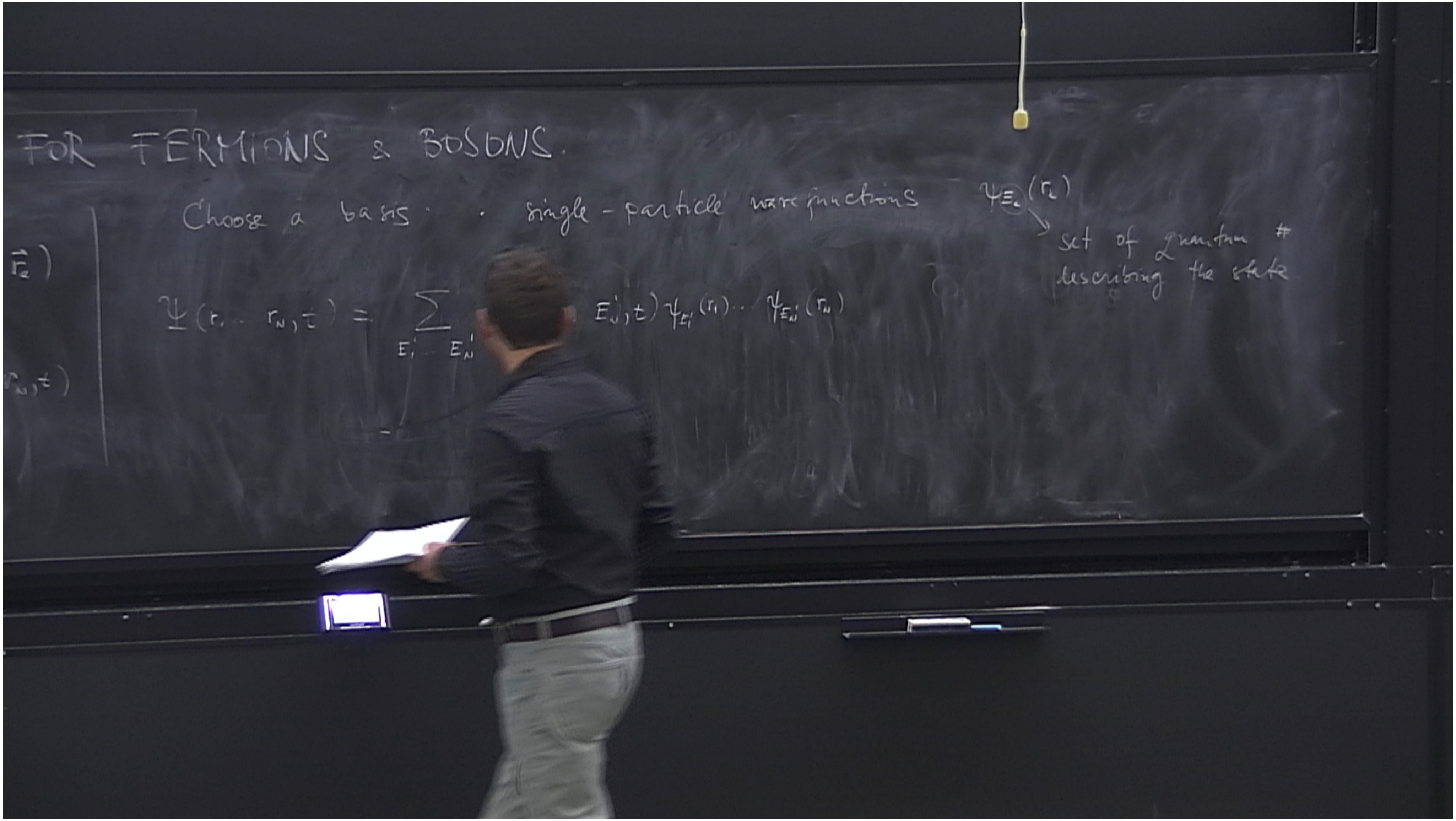
Abstract:

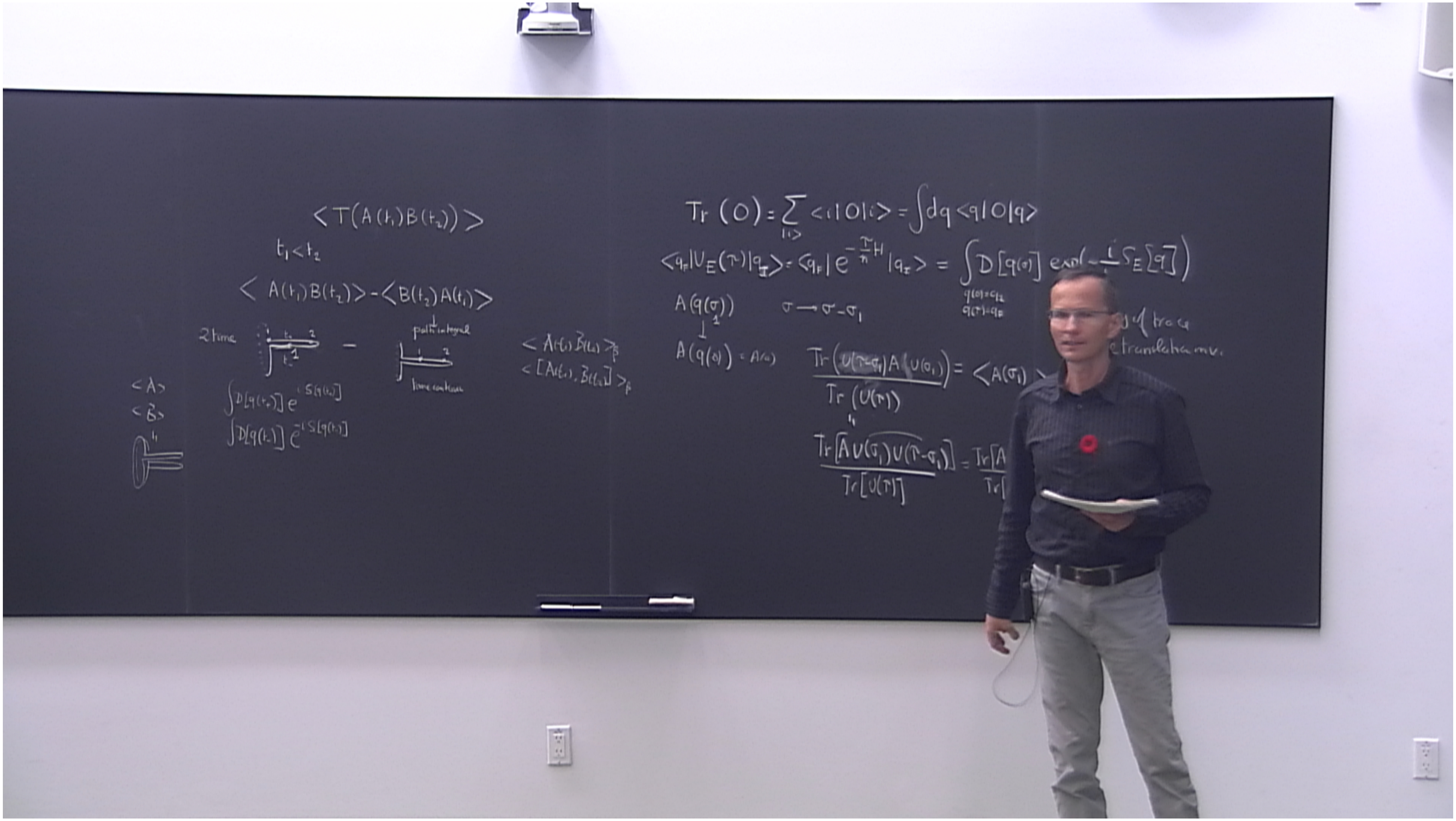

SECOND QUANTIZATION FOR FERMIONS & BOSON
$H = \sum^{N} T(\vec{r}_k) + \sum_{k\neq l=1}^{N} V(\vec{r}_k, \vec{r}_l)$


SECOND QUANTIZATION FOR FERMIONS & BOSONS
N ~ 10^23
Schr. Eq.

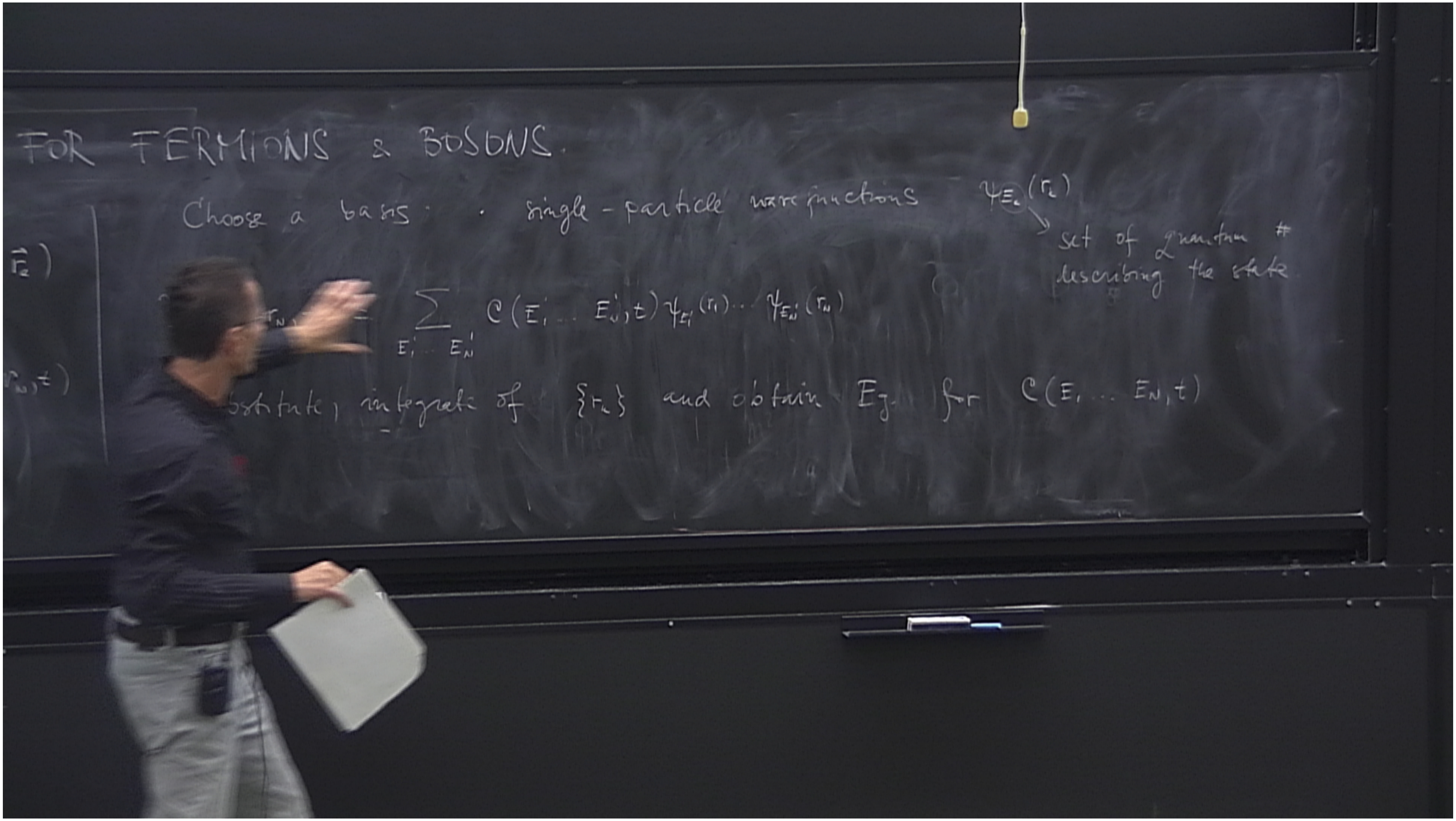

SECOND QUANTIZATION FOR FERMIONS & BOSONS.
$N \sim 10^{23}$
$H = \sum_{k=1}^{N} T(\vec{r}_k) + \sum_{k \neq \ell = 1}^{N} V(\vec{r}_k, \vec{r}_\ell)$
Schr. Eq.
$i\hbar \frac{\partial}{\partial t} \Psi(r_1 \dots r_N, t) = H \Psi(r_1 \cdots r_N, t)$
Choose a basis · single - partic

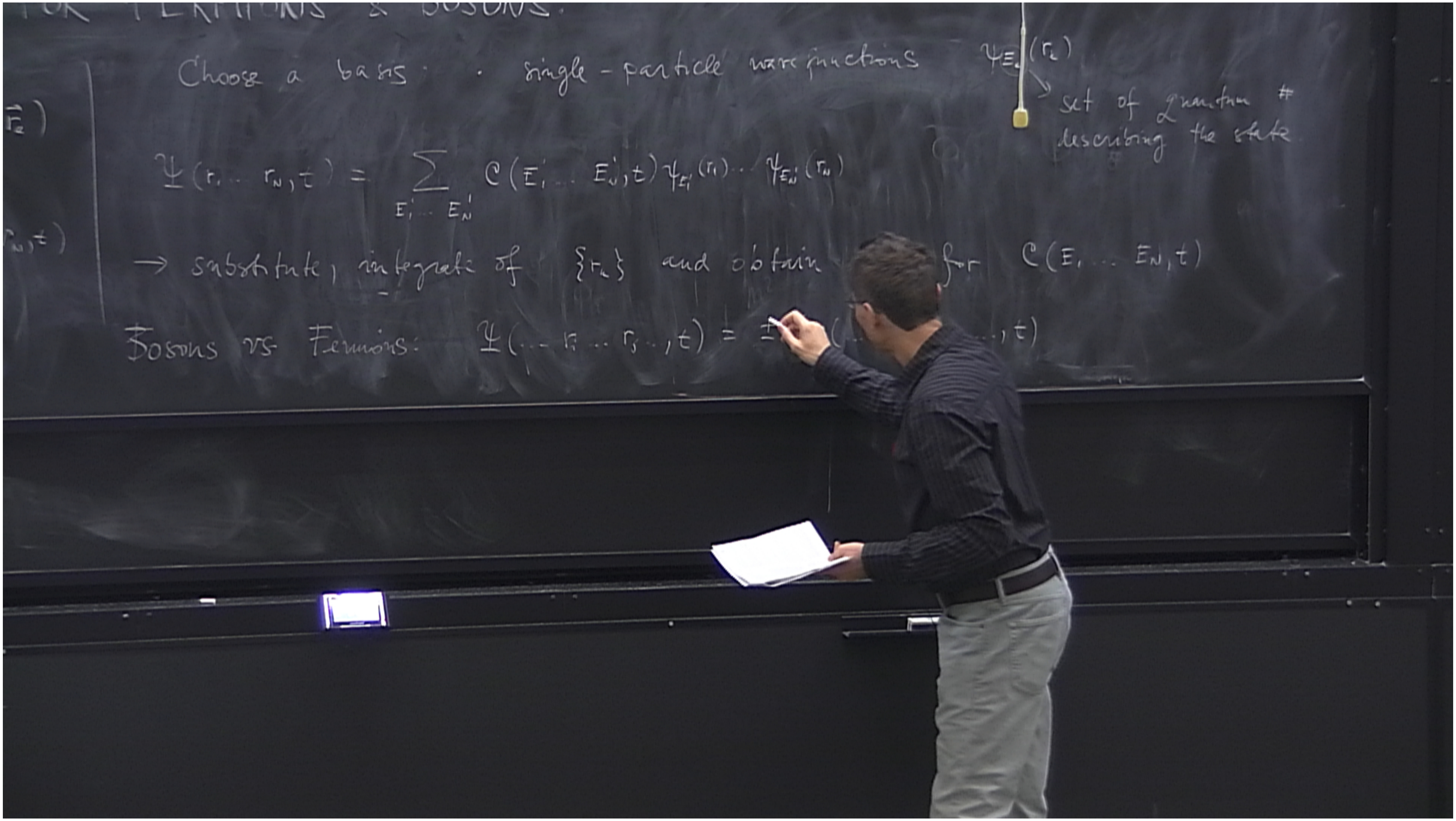

FOR FERMIONS & BOSONS.
Choose a basis · single-particle wave functions

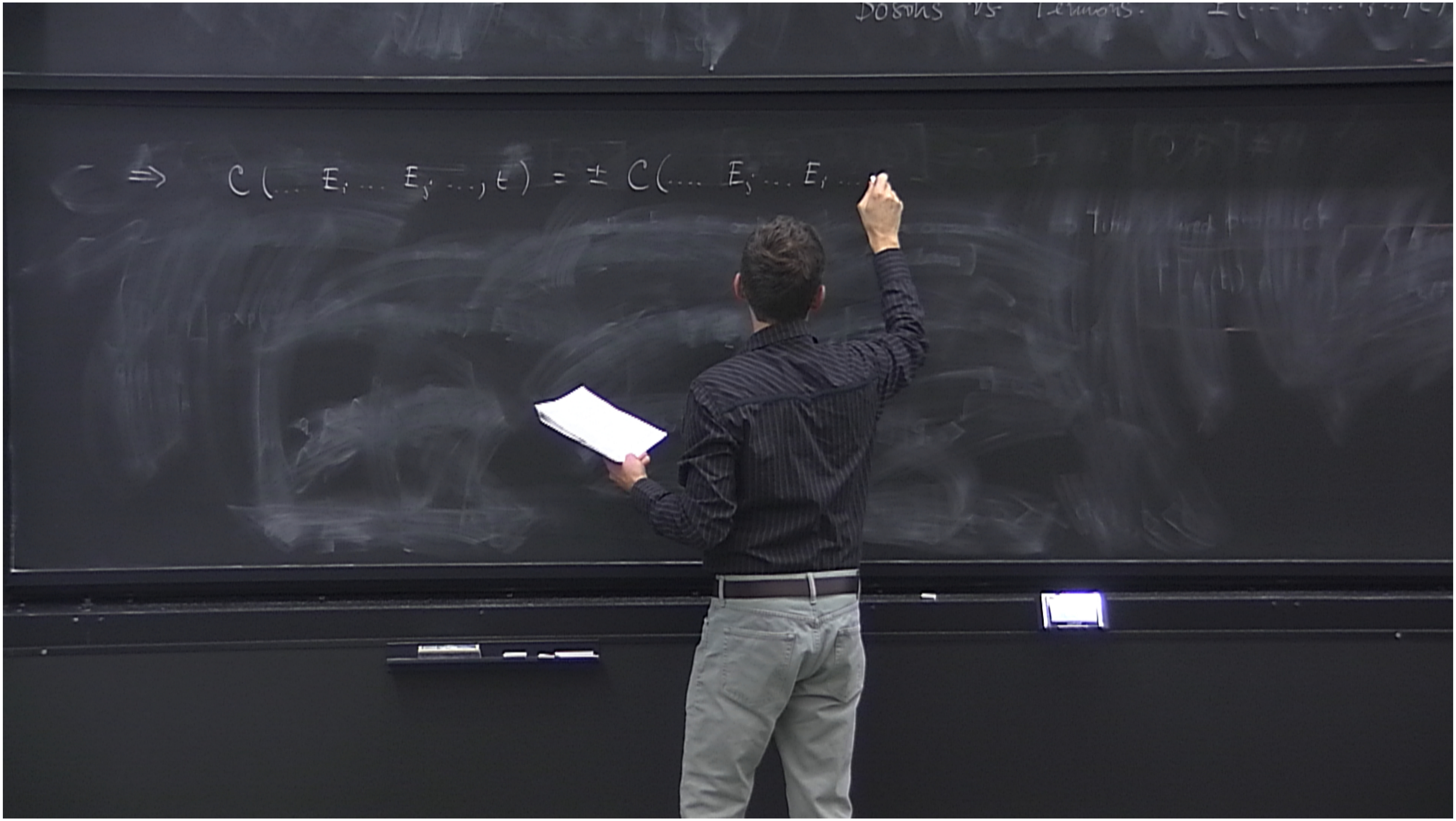

FOR FERMIONS & BOSONS.
Choose a basis · single-particle wave functions
set of quantum #
describing the state

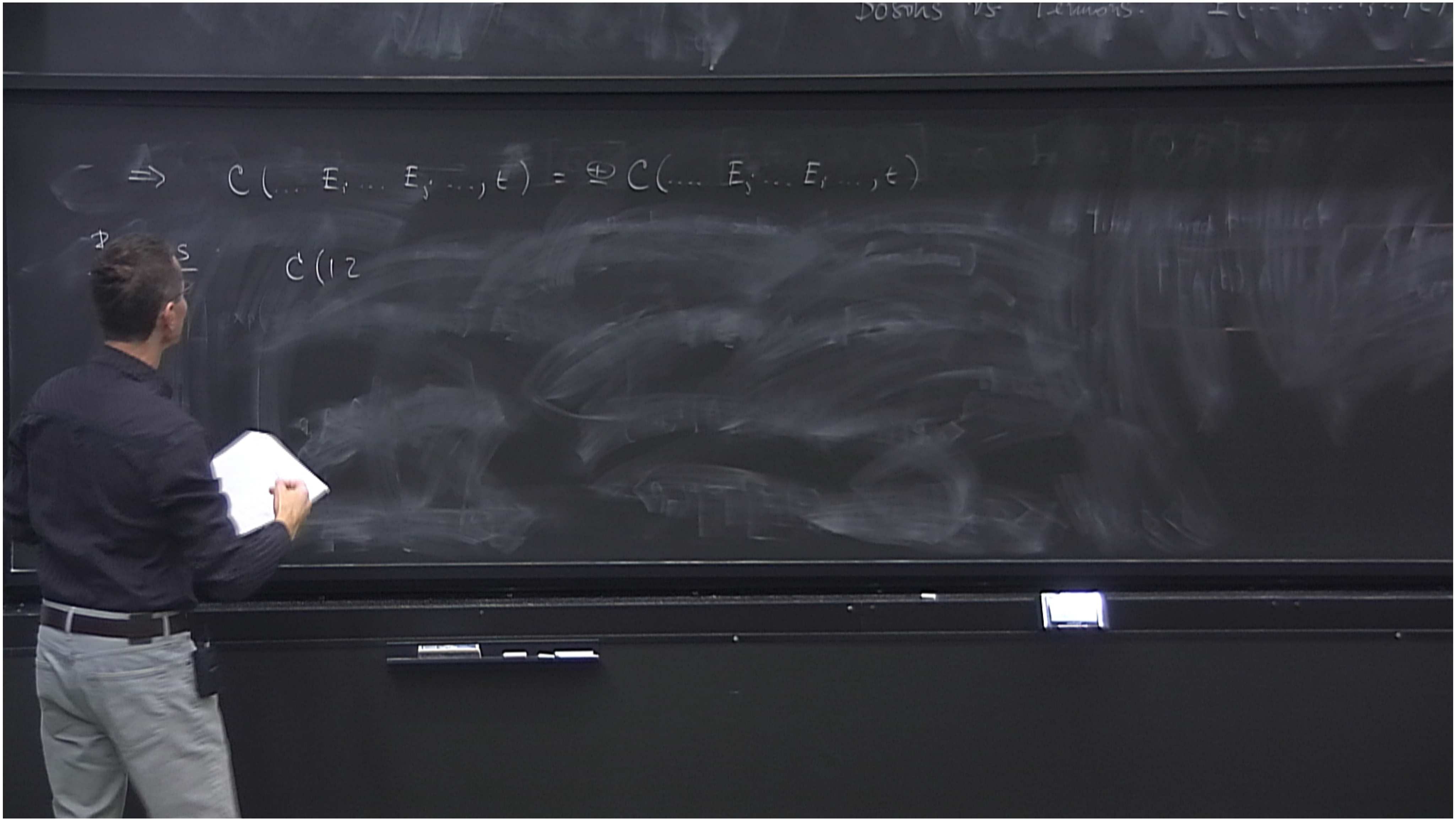


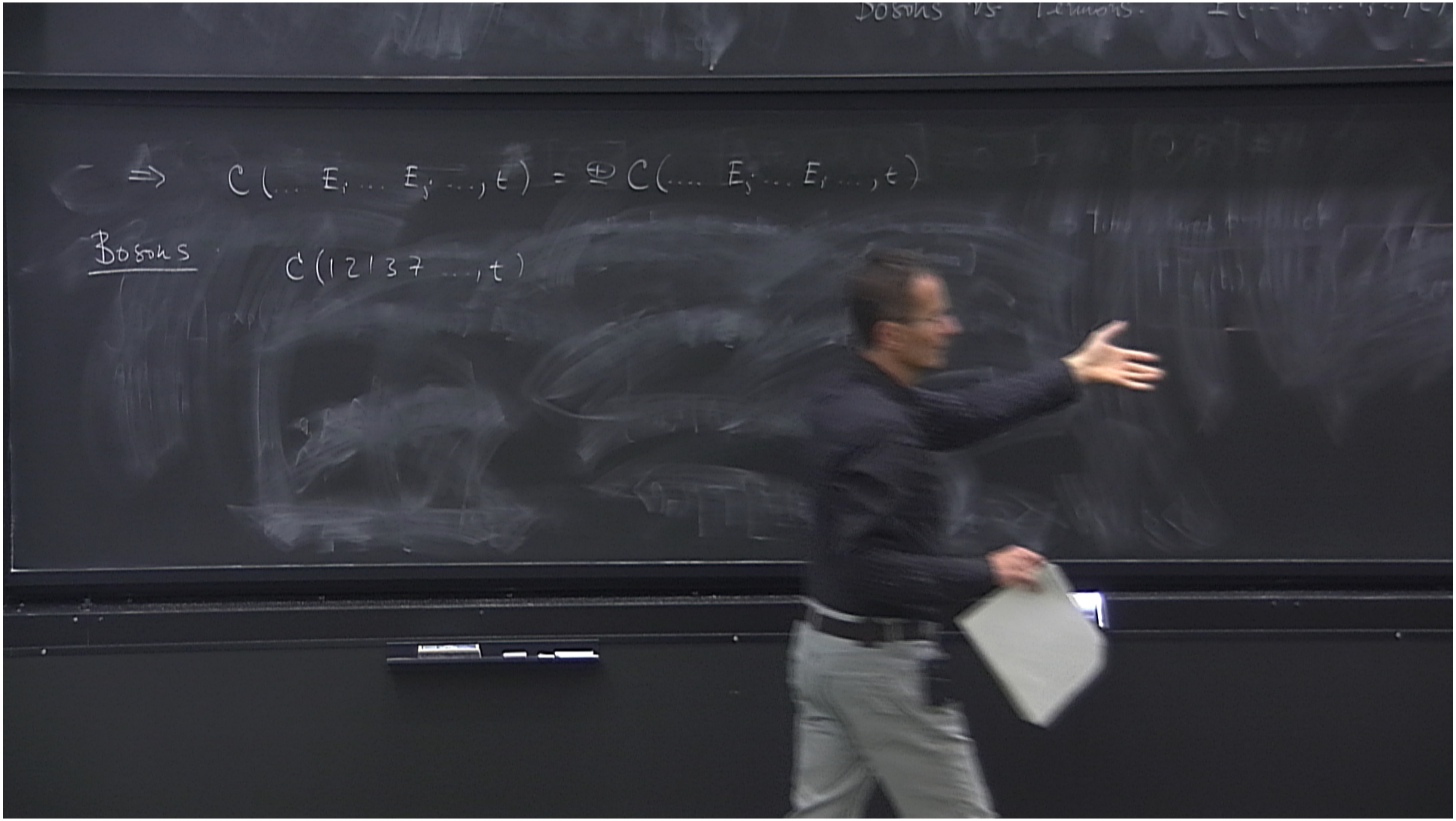
< T(A(t1)B(t2)) >
t1 < t2
< A(t1)B(t2) > - < B(t2)A(t1) >
2 time
path integral
time contour
Tr (O) = Σ < i|O|i > = ∫dq < q|O|q >
A(q(σ))
σ → σ - σ1

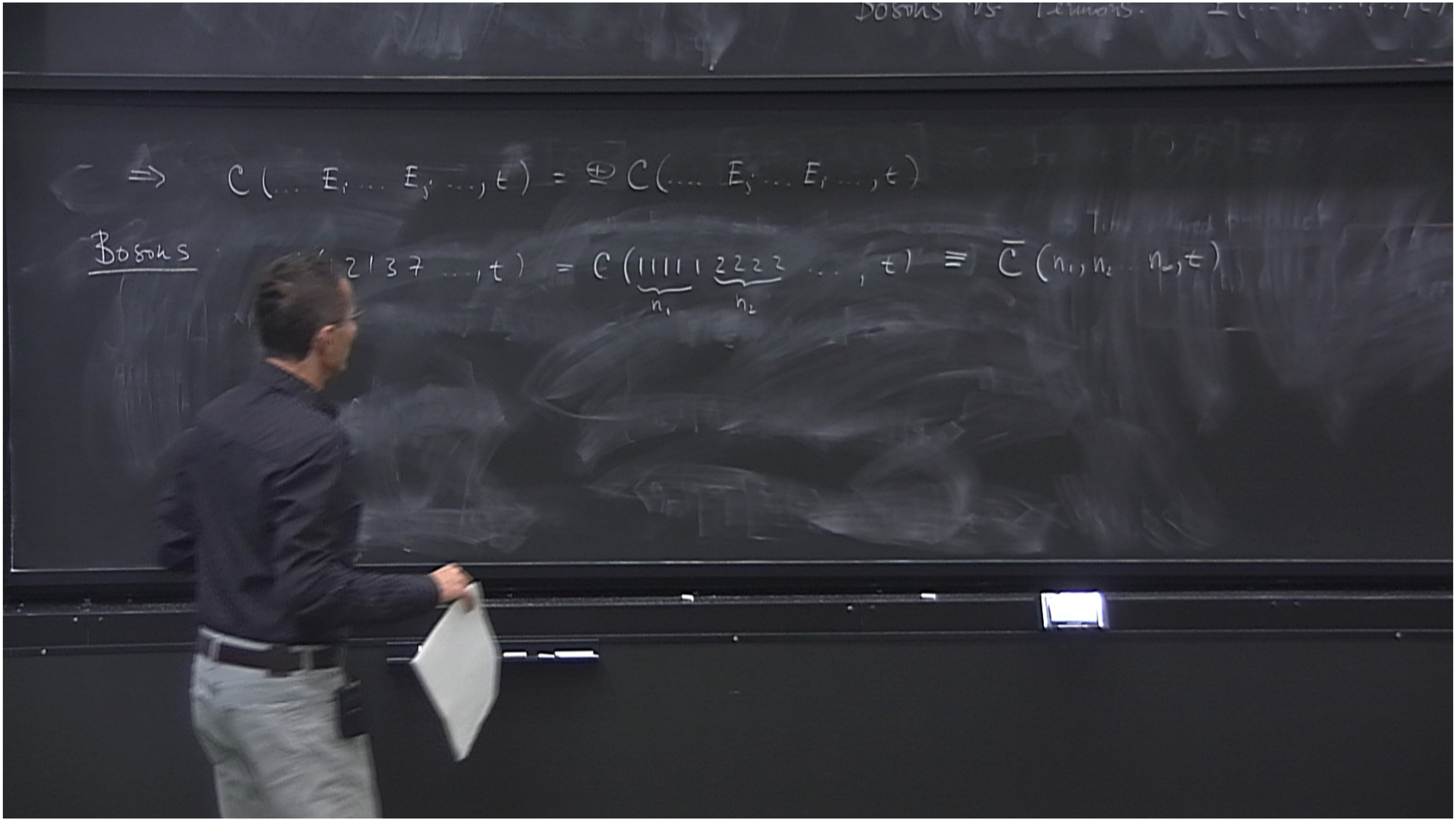

FOR FERMIONS & BOSONS.
Choose a basis: · single-particle wave functions $\psi_{E_\alpha}(r_\alpha)$
set of quantum # describing the state
$\sum_{E_1' \dots E_N'} C(E_1' \dots E_N', t)\, \psi_{E_1'}(r_1) \dots \psi_{E_N'}(r_N)$
bstitute, integrate of $\{r_\alpha\}$ and obtain Eq. for $C(E_1 \dots E_N, t)$

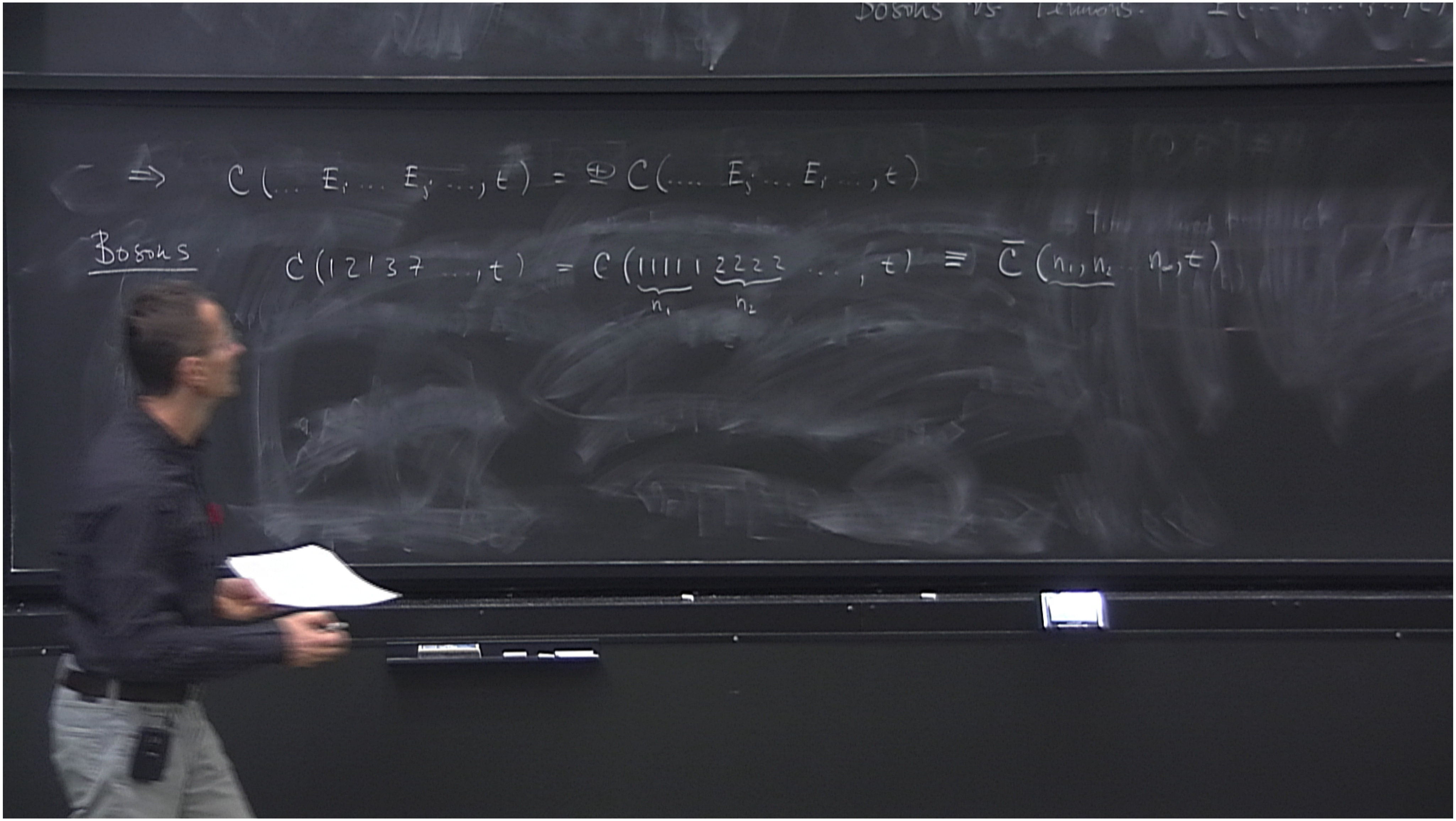

Choose a basis: · single-particle wave functions ψE(r)
set of quantum # describing the state
Ψ(r1 ... rN, t) = Σ C(E1' ... EN', t) ψE1'(r1) ... ψEN'(rN)
E1' ... EN'
→ substitute, integrate of {r} and obtain for C(E1 ... EN, t)
Bosons vs Fermions: Ψ(... ri ... rj ..., t) = ±

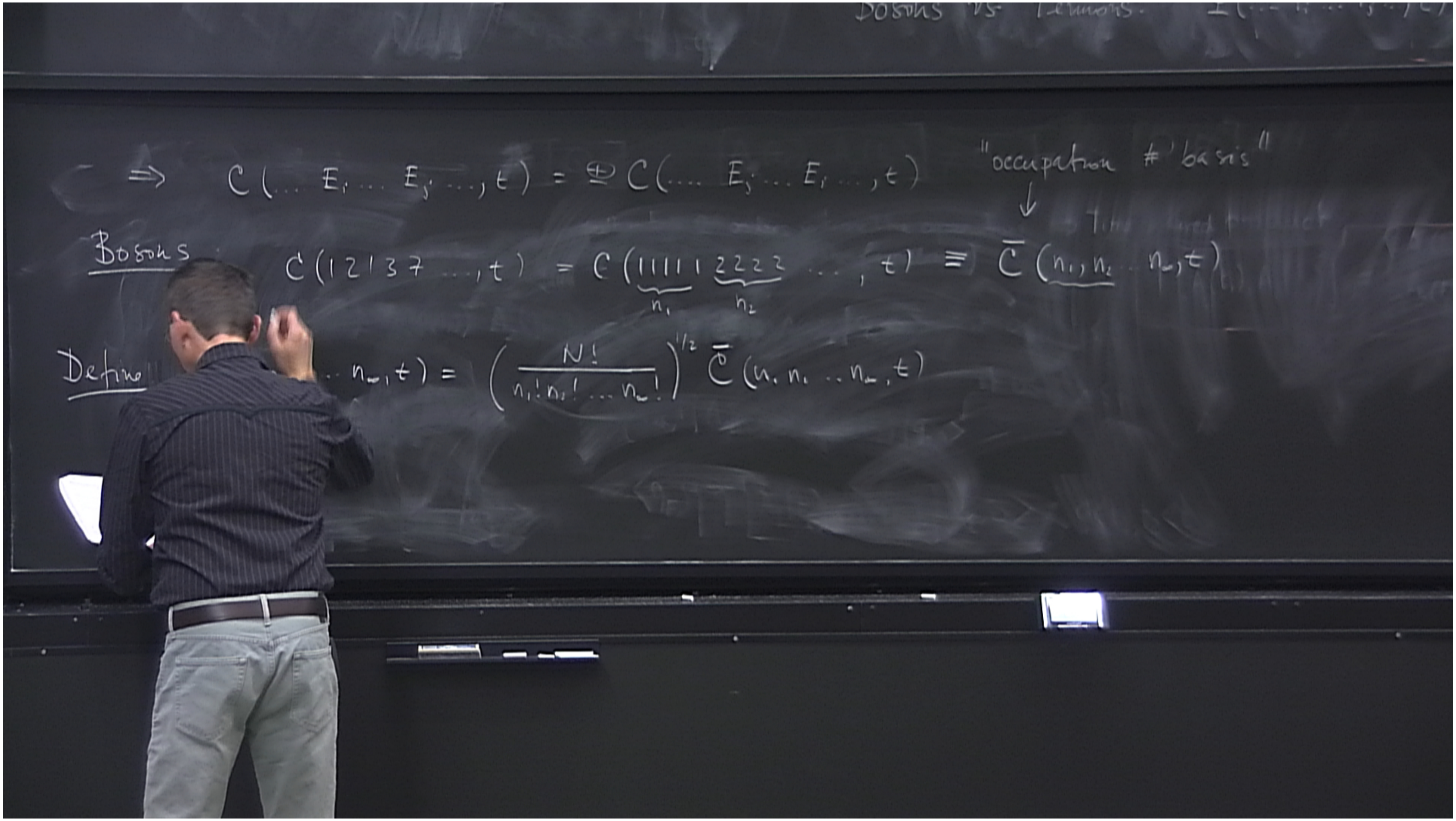

Bosons vs Fermions.
⇒ C(... E_i ... E_j ..., t) = ± C(... E_j ... E_i ...

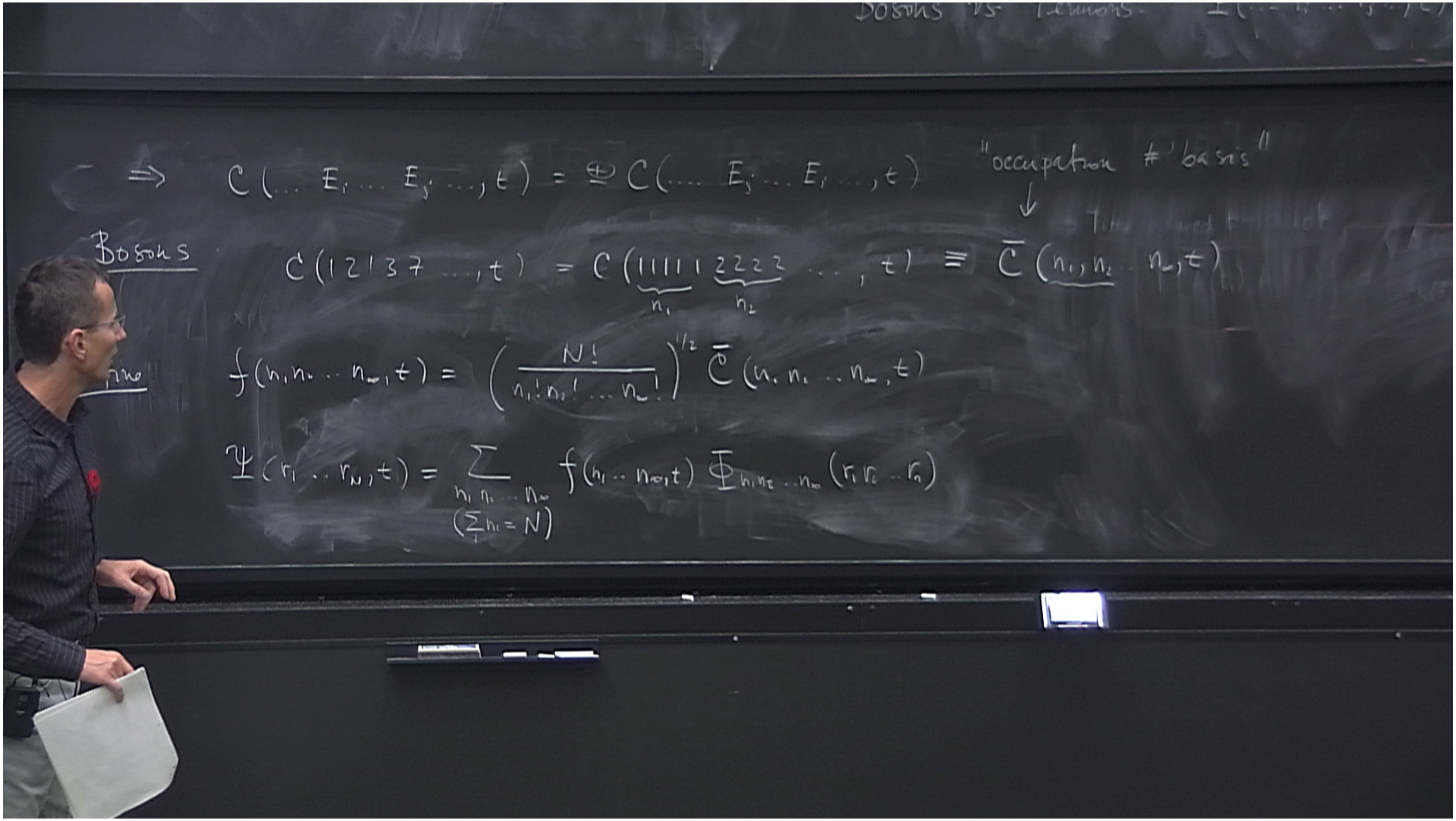

Bosons vs Fermions.
⇒ C(... E_i ... E_j ..., t) = ± C(.... E_j ... E_i ..., t)
C(12

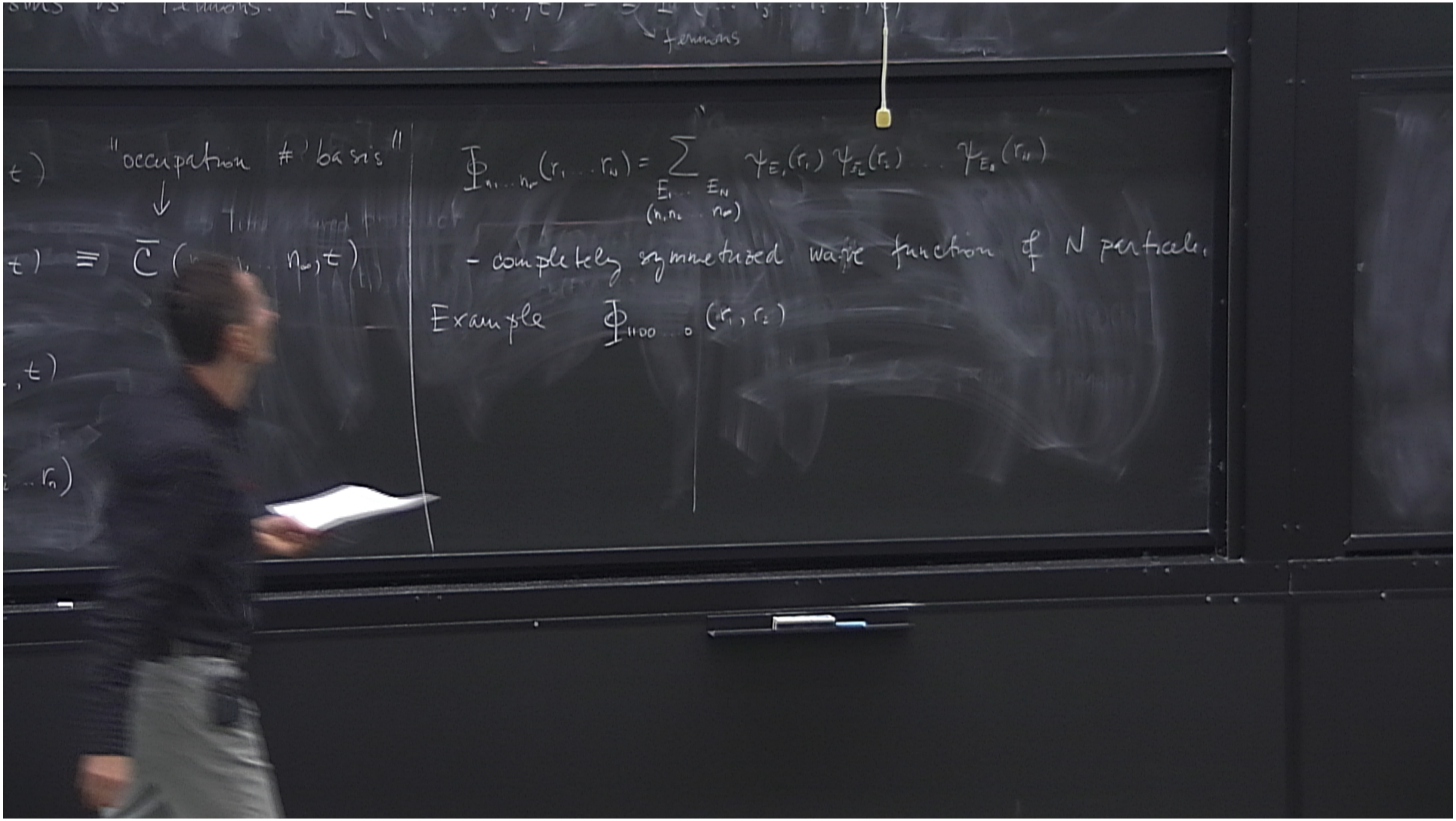

Bosons vs Fermions.
⇒ C(... E_i ... E_j ..., t) = ± C(... E_j ... E_i ..., t)
Bosons
C(1 2 1 3 7 ..., t)

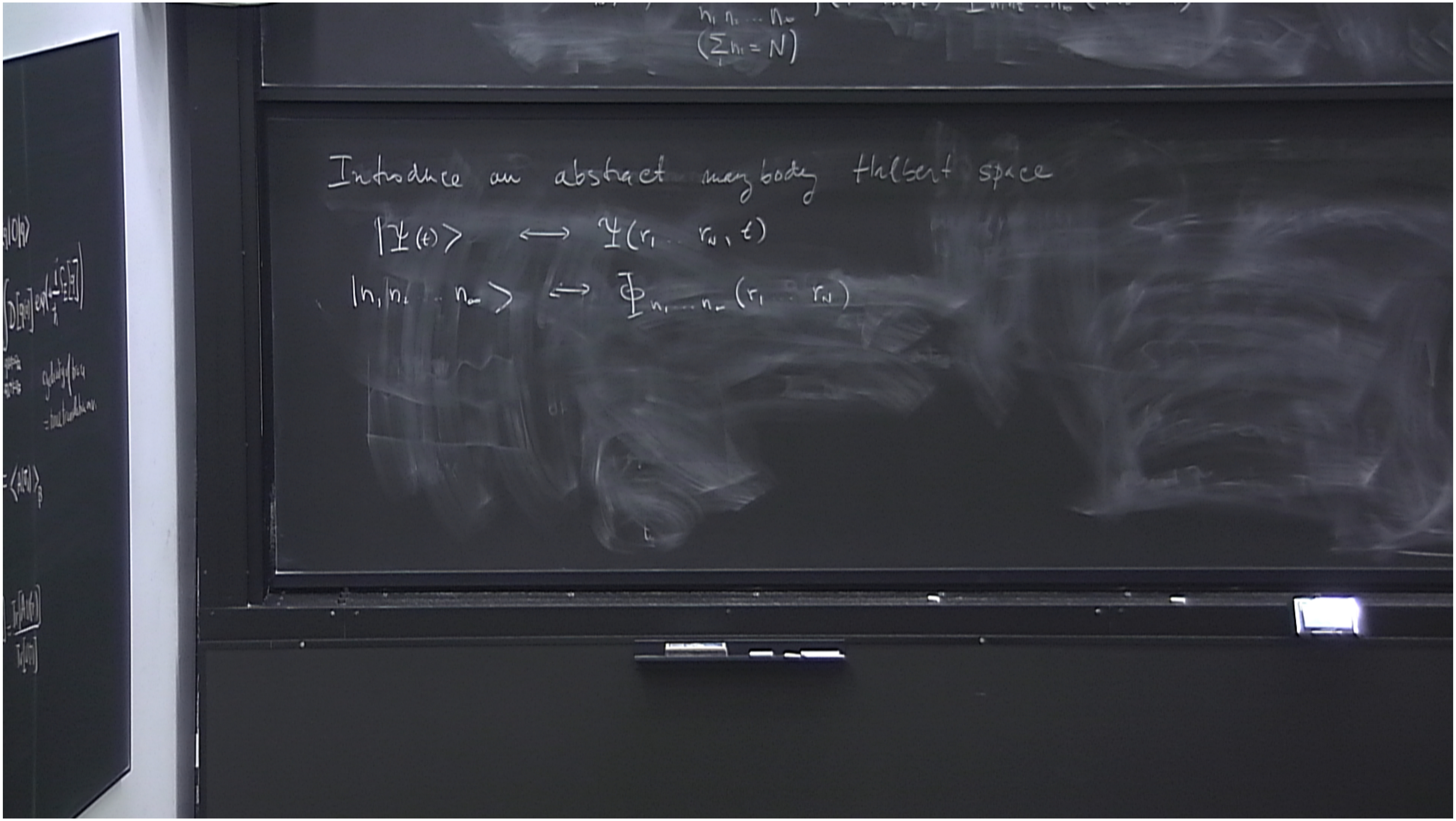

⇒ C(... E_i ... E_j ..., t) = ± C(... E_j ... E_i ..., t)
Bosons
= C(1111 2222 ..., t) ≡ C̄(n_1, n_2 ..., t)

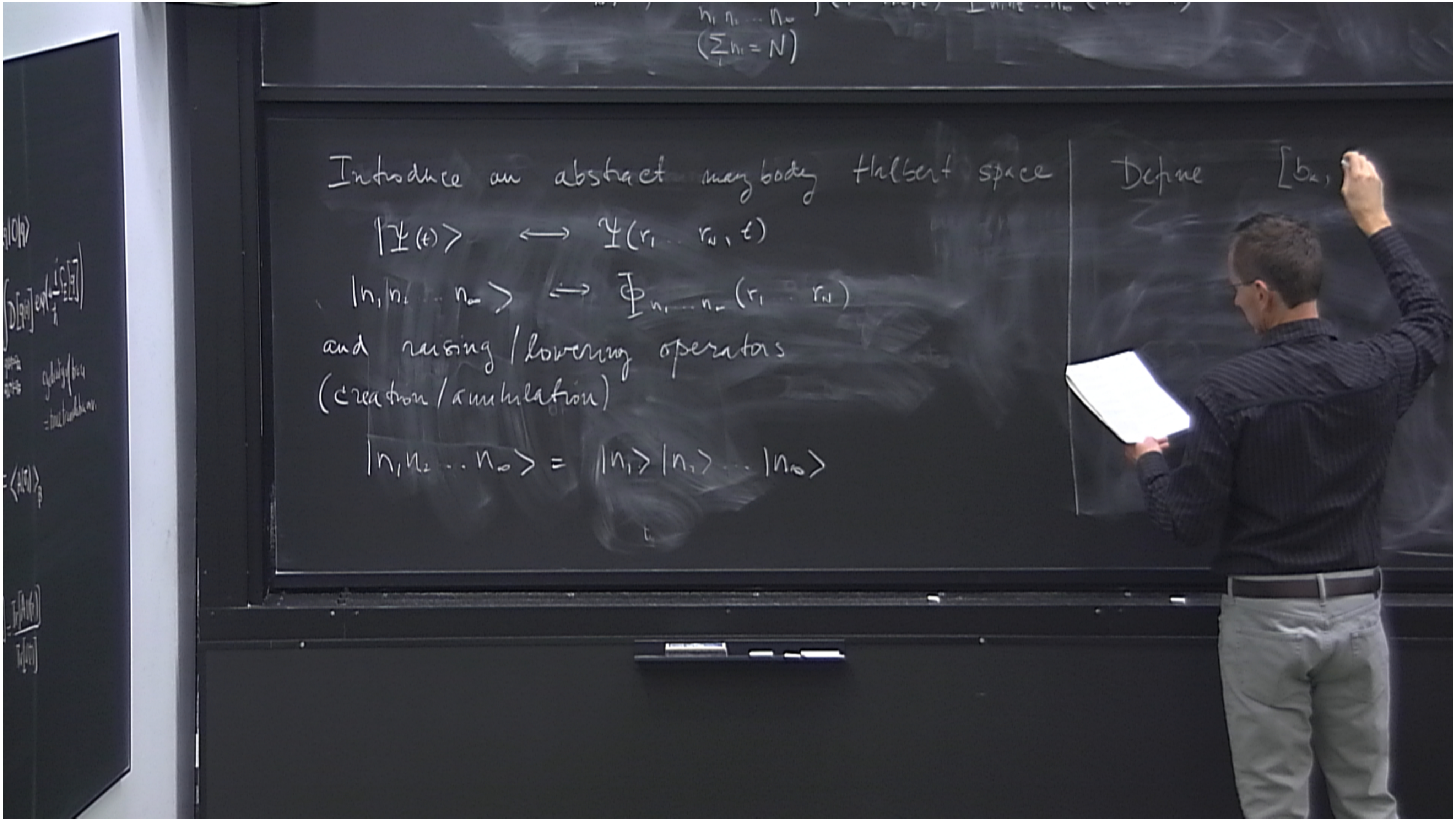

Bosons

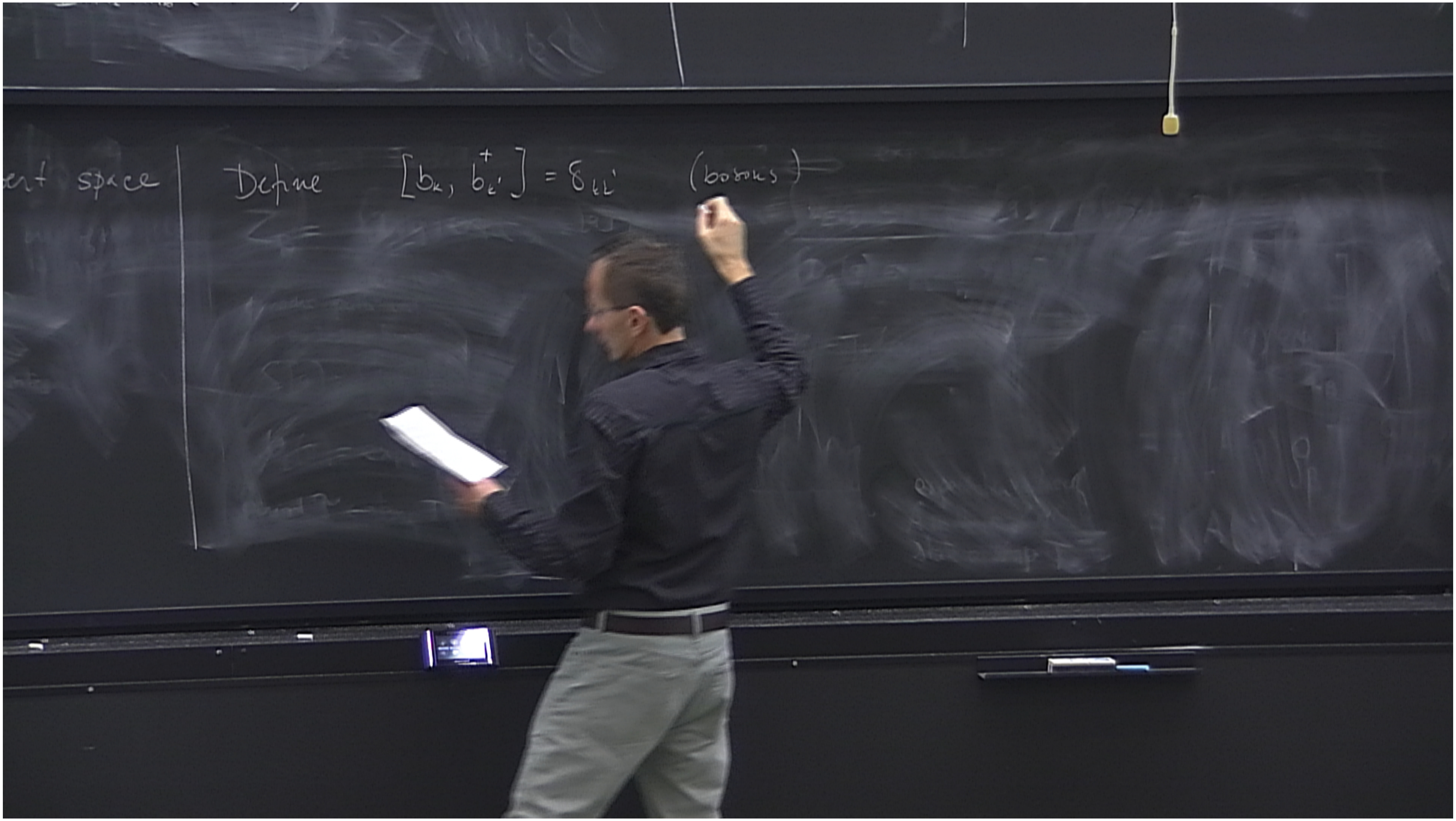

⇒ C(… E_i … E_j …, t) = ± C(… E_j … E_i …, t)
"occupation #" basis
Bosons
C(1 2 1 3 7 …, t) = C(1111 2222 …, t) ≡ C̄(n_1, n_2 … n_∞, t)
Define
n_∞, t) = (N! / n_1! n_2! … n_∞!)^{1/2} C̄(n_1 n_2 … n_∞, t)

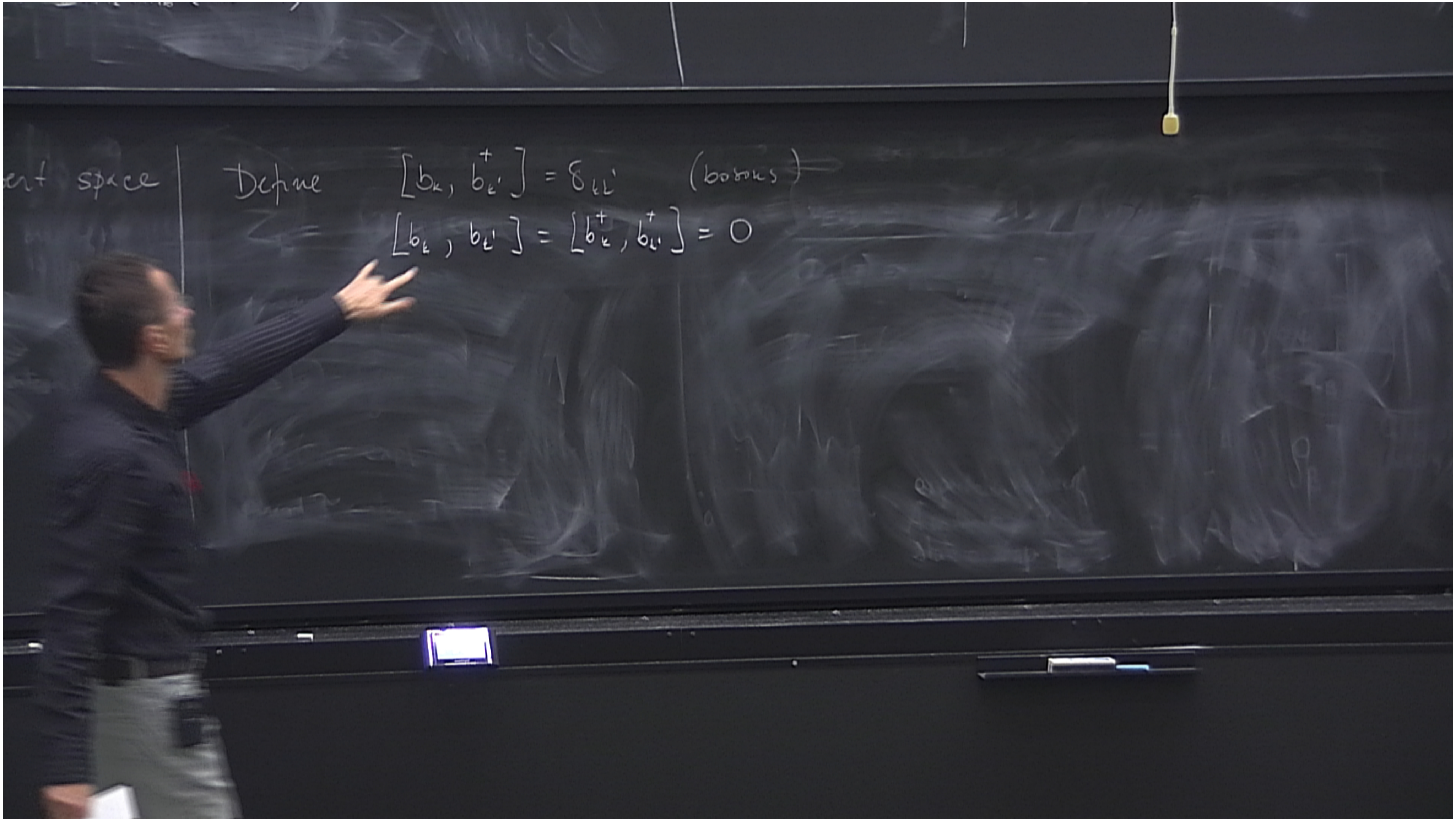

"occupation #' basis"
Bosons
C(12137 ..., t) = C(11111 2222 ..., t) ≡ C̄(n₁, n₂ ... n∞, t)
f(n₁ n₂ ... n∞, t) = (N! / n₁! n₂! ... n∞!)^1/2 C̄(n₁ n₂ ... n∞, t)
Ψ(r₁ ... r_N, t) = Σ f(n₁ ... n∞, t) Φ_{n₁n₂...n∞}(r₁ r₂ ... r_N)
(Σ nᵢ = N)

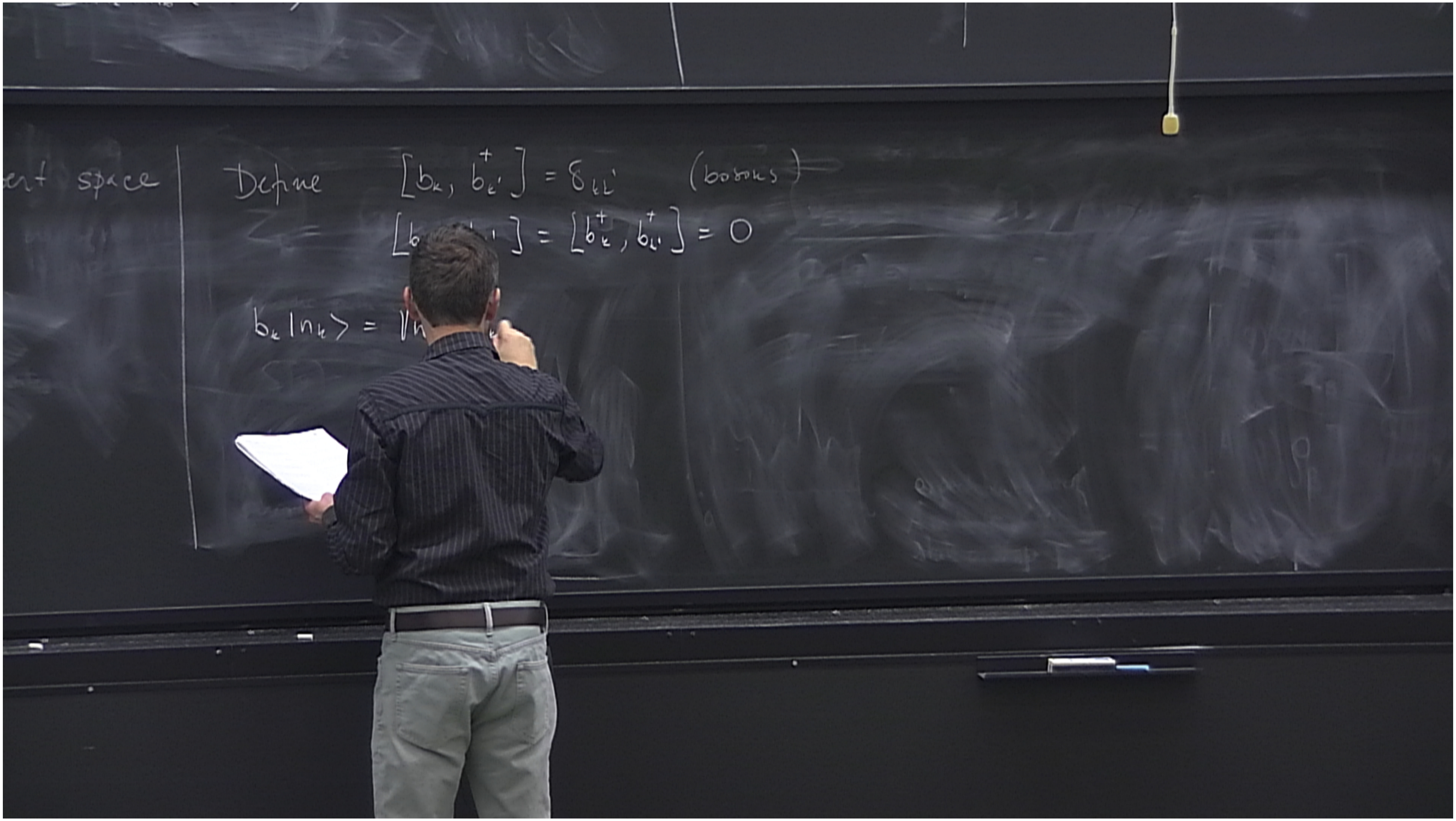

fermions
"occupation #' basis"
Φn1...n∞(r1 ... rN) = Σ ψE1(r1) ψE2(r2) ... ψEN(rN)
E1 ... EN
(n1, n2 ... n∞)
- completely symmetrized wave function of N particles.
Example Φ1100...0(r1, r2)


$(\sum_i n_i = N)$
Introduce an abstract manybody Hilbert space
$|\Psi(t)\rangle \longleftrightarrow \Psi(r_1 \ldots r_N, t)$
$|n_1 n_2 \ldots n_\infty\rangle \longleftrightarrow \Phi_{n_1 \ldots n_\infty}(r_1 \ldots r_N)$


Introduce an abstract many body Hilbert space
|Ψ(t)> ⟷ Ψ(r1 ... rN, t)
|n1 n2 ... n∞> ⟷ Φn1...n∞(r1 ... rN)
and raising/lowering operators
(creation/annihilation)
|n1 n2 ... n∞> = |n1>|n2> ... |n∞>
Define
(Σ ni = N)


ert space
Define [bk, bk'+] = δkk' (bosons)


ent space
Define [b_k, b_k'^+] = δ_kk' (bosons)
[b_k, b_k'] = [b_k^+, b_k'^+] = 0


space
Define
(bosons)

ert space

Define $[b_k, b_{k'}^{\dagger}] = \delta_{kk'}$ (bosons)

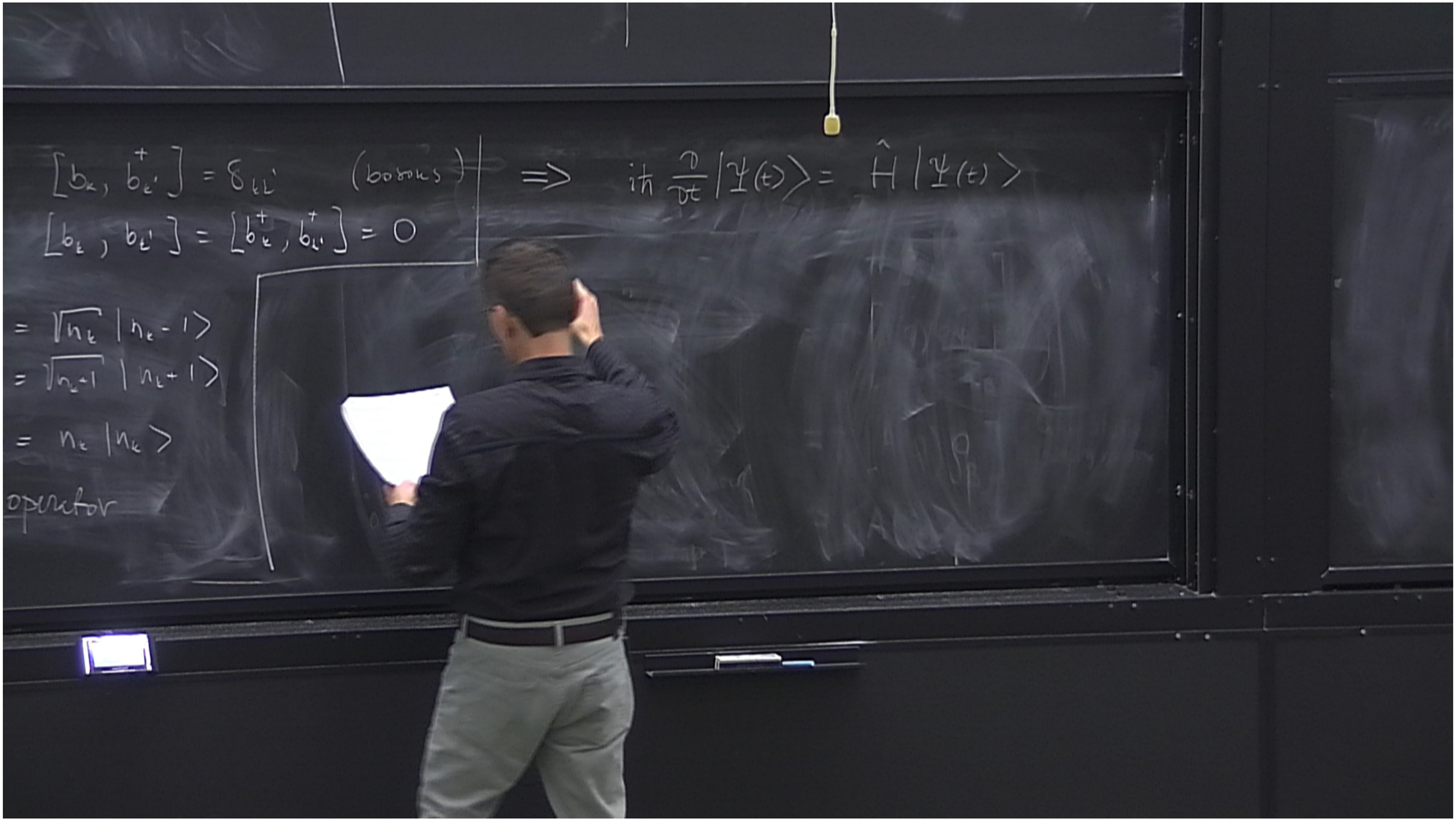
$$[b_k, b_{k'}] = [b_k^{\dagger}, b_{k'}^{\dagger}] = 0$$

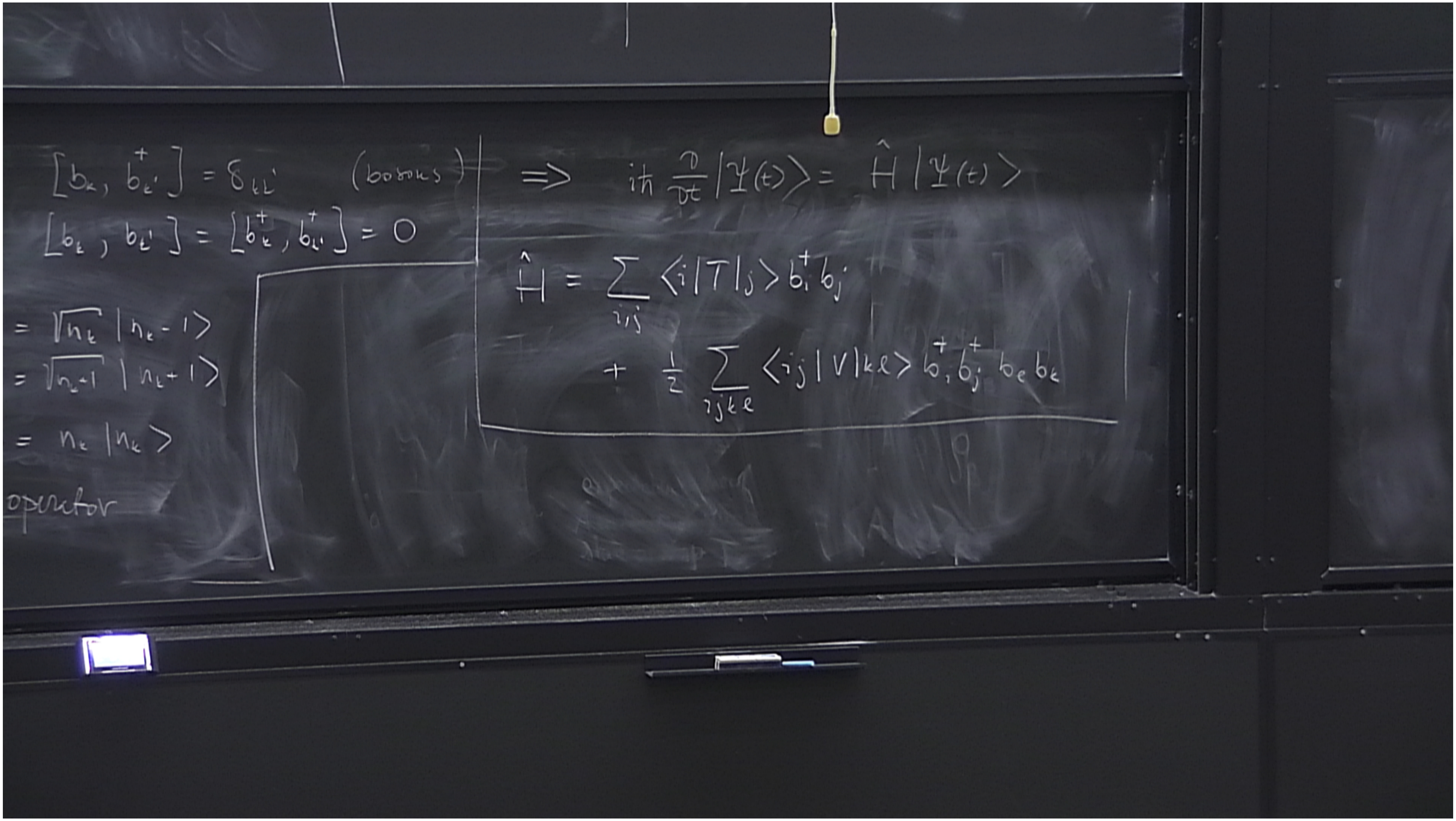
$$b_k |n_k\rangle = \sqrt{n_k}\, |n_k - 1\rangle$$

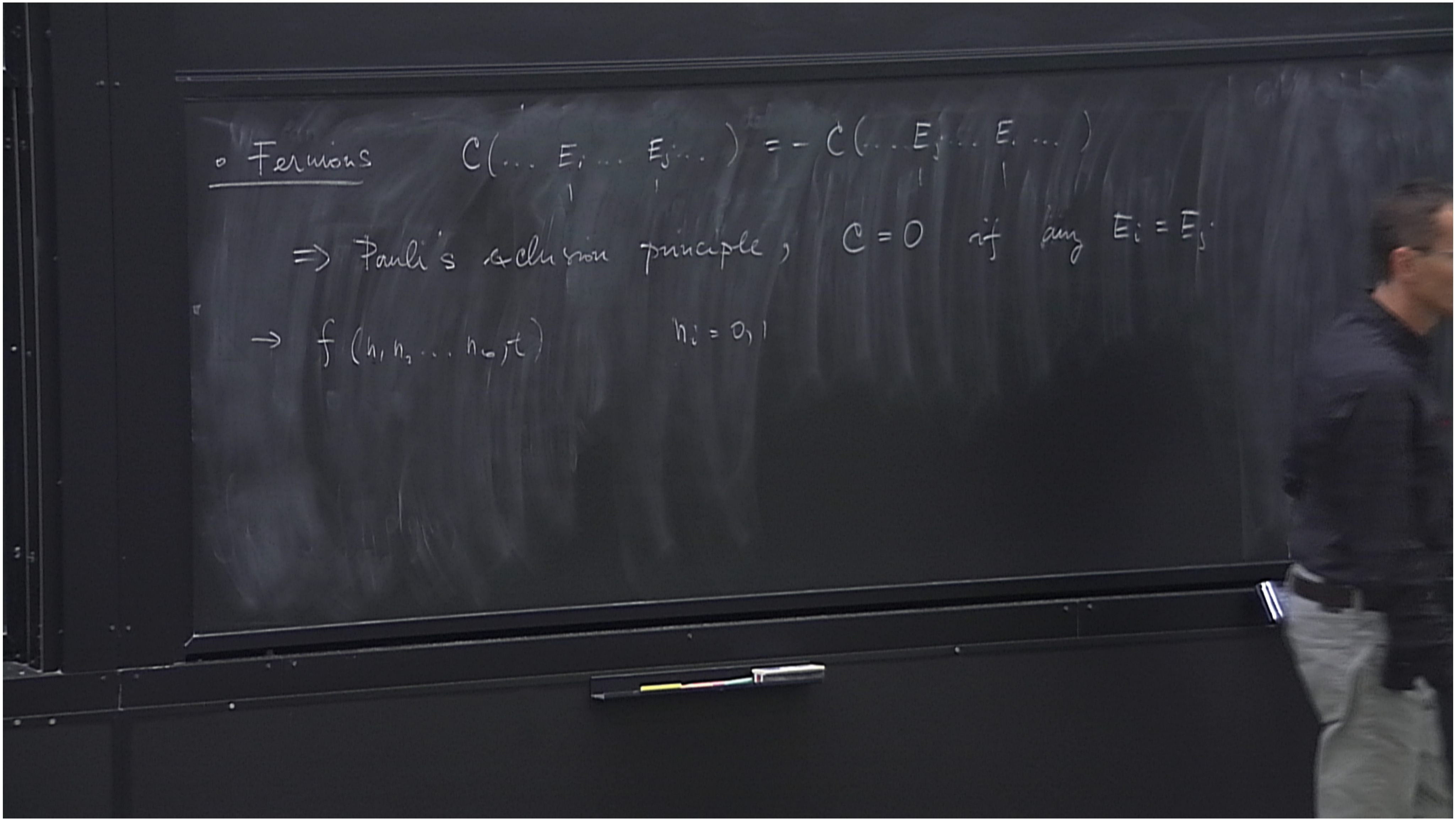
$$b_k^{\dagger} |n_k\rangle = \sqrt{n_k + 1}\, |n_k + 1\rangle$$

$$\underbrace{b_k^{\dagger} b_k}_{\hat{n}_k} |n_n\rangle = n_k |n_k\rangle$$

$\hat{n}_k$ - # operator


[b_k, b_k'^+] = δ_kk' (bosons)
[b_k, b_k'] = [b_k^+, b_k'^+] = 0
⇒ iħ ∂/∂t |Ψ(t)> = Ĥ |Ψ(t)>
= √n_k |n_k - 1>
= √(n_k+1) |n_k + 1>
= n_k |n_k>
operator


[b_k, b_k'^+] = δ_kk' (bosons)
[b_k, b_k'] = [b_k^+, b_k'^+] = 0
= √n_k |n_k - 1>
= √(n_k+1) |n_k + 1>
= n_k |n_k>
operator
⇒ iħ ∂/∂t |Ψ(t)> = Ĥ |Ψ(t)>
Ĥ = Σ_ij <i|T|j> b_i^+ b_j
+ 1/2 Σ_ijkl <ij|V|kl> b_i^+ b_j^+ b_l b_k

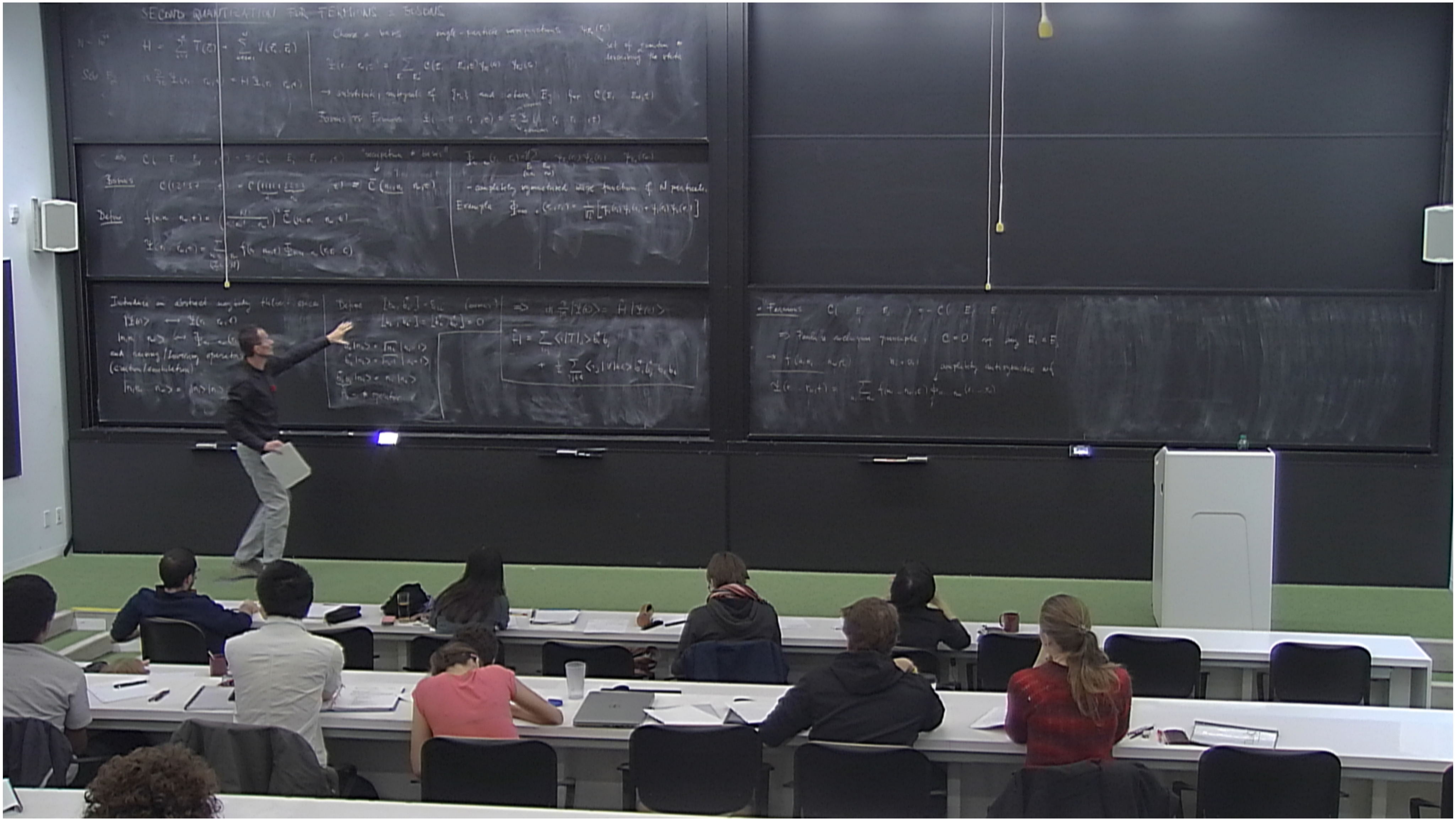

Fermions
C(... E_i ... E_j ...) = - C(... E_j ... E_i ...)
=> Pauli's exclusion principle, C = 0 if any E_i = E_j
-> f(n_1, n_2 ... n_∞, t)
n_i = 0, 1

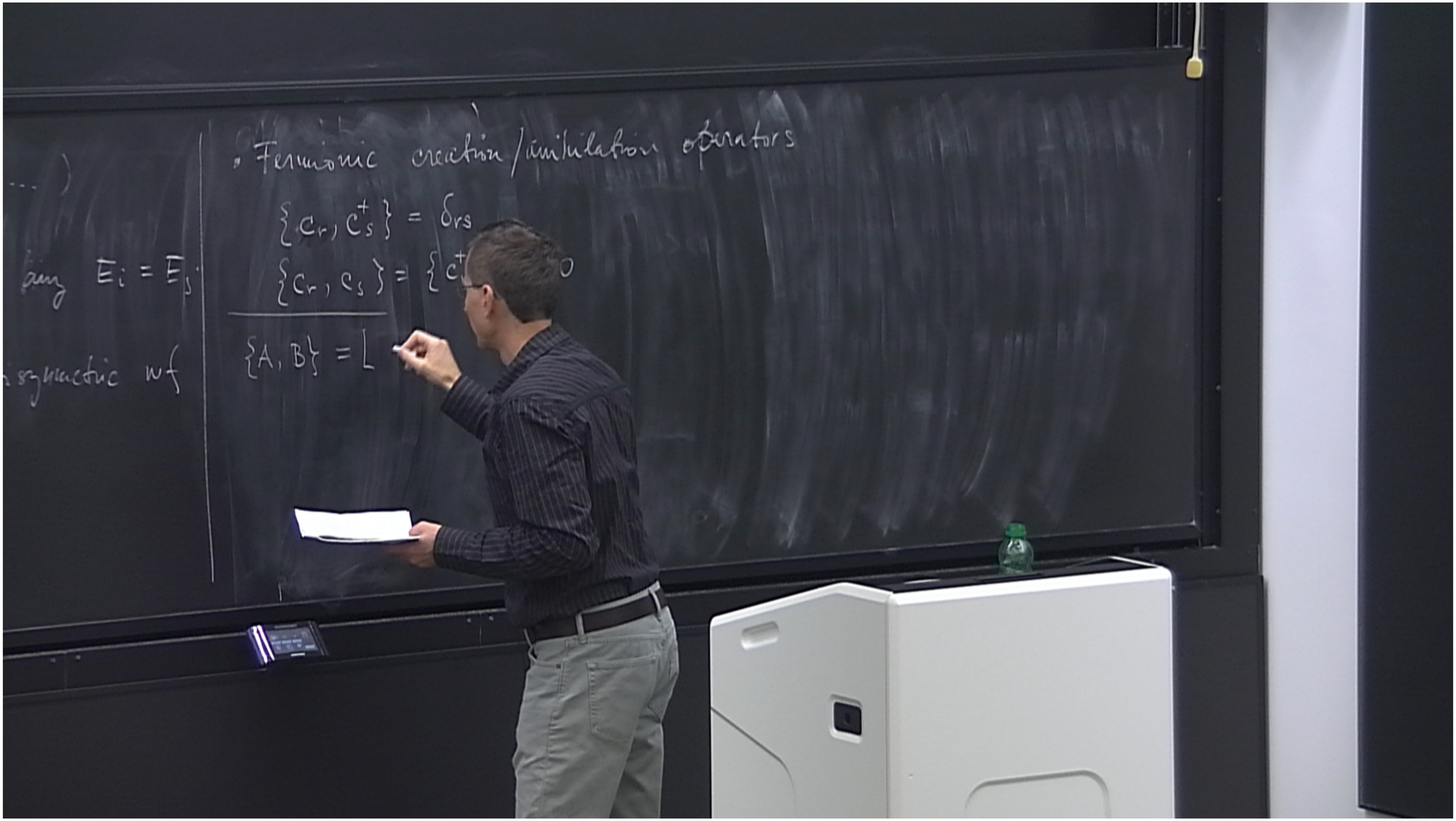
• **Fermions** $C(\ldots E_i \ldots E_j \ldots) = - C(\ldots E_j \ldots E_i \ldots)$

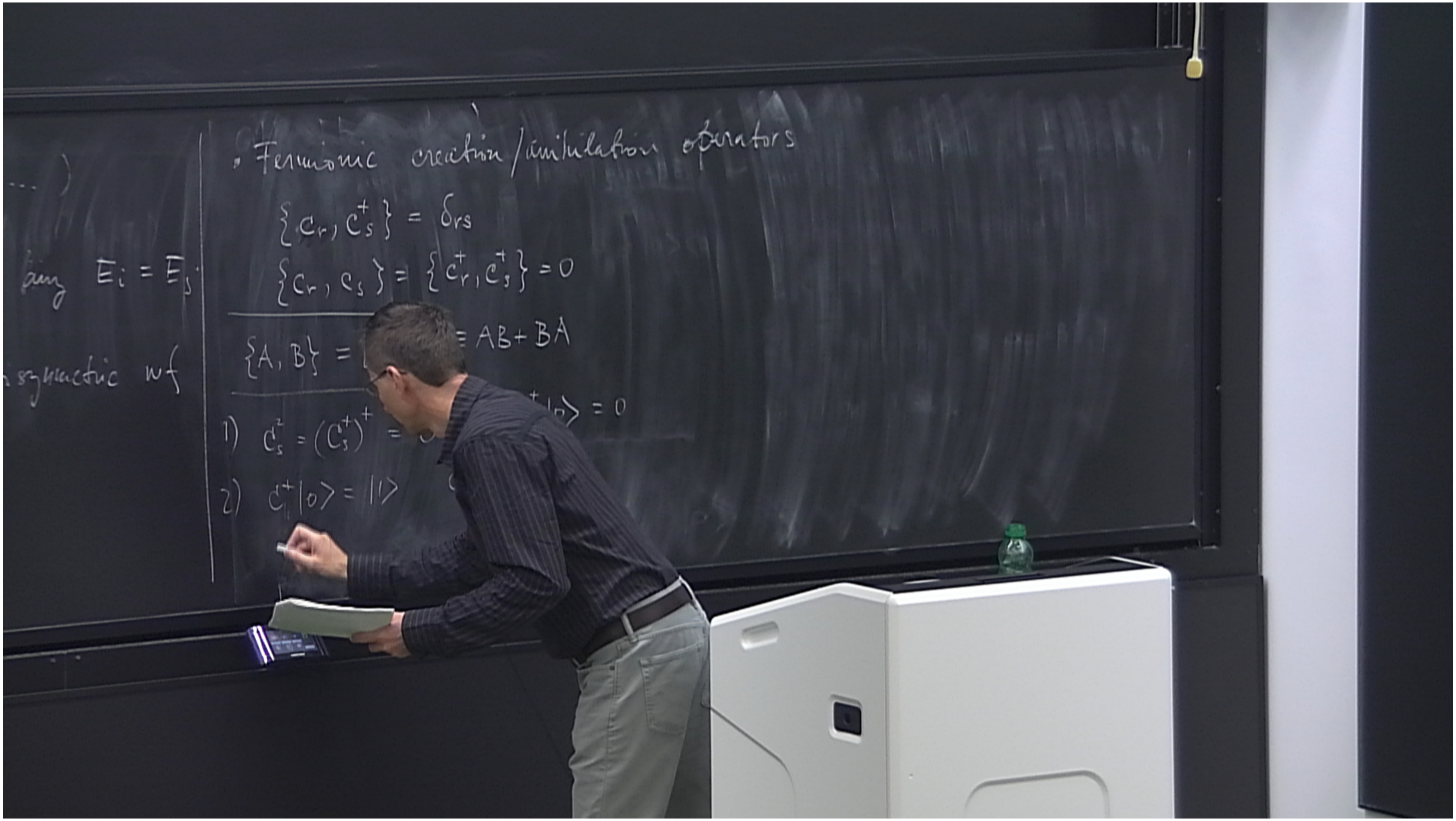
$\Rightarrow$ Pauli's exclusion principle, $C = 0$ if any $E_i = E_j$

$\rightarrow f(n_1, n_2 \ldots n_\infty, t)$ $n_i = 0, 1$ completely antisymmetric wf

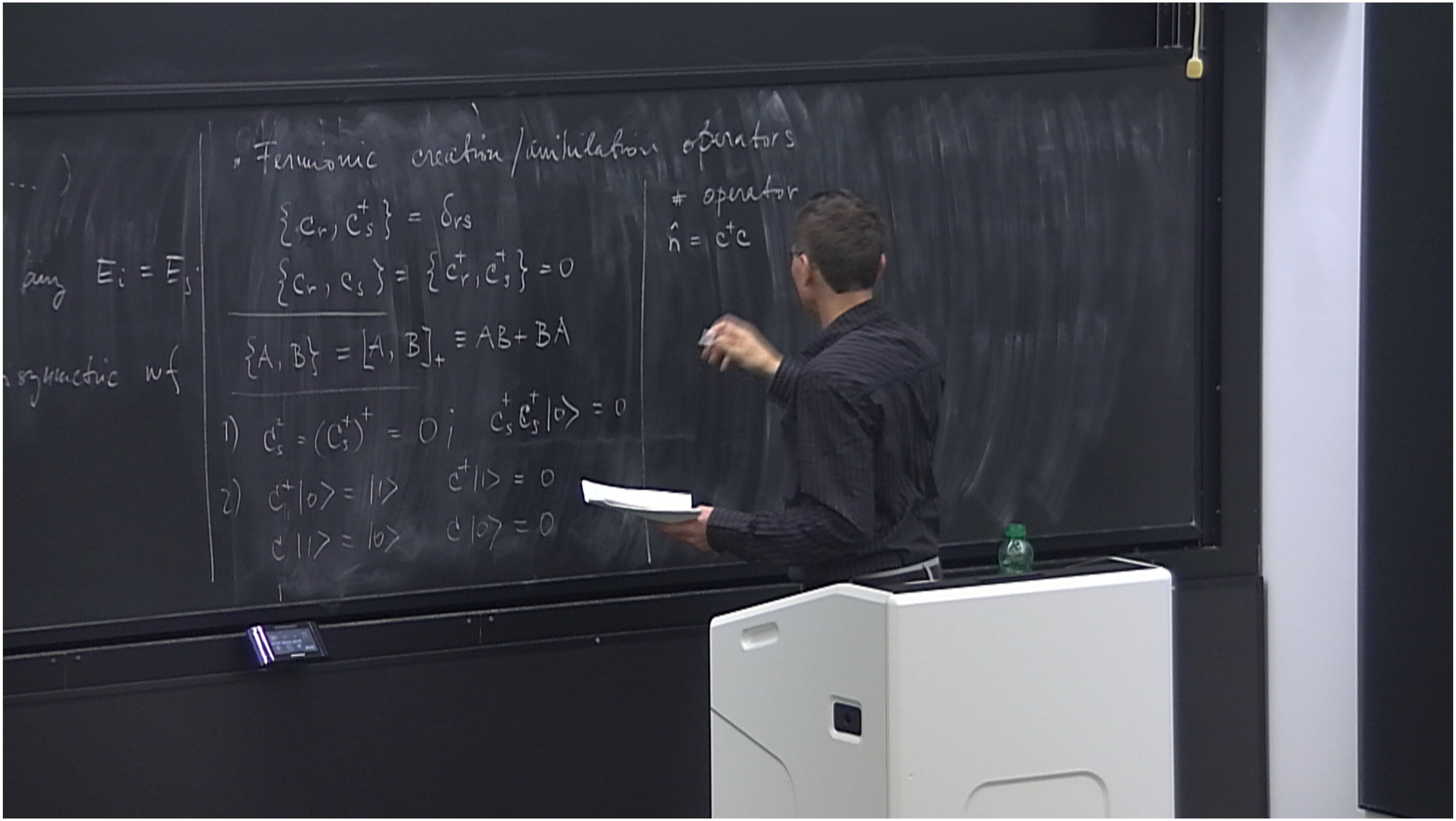
$$\Psi(r_1 \ldots r_N, t) = \sum_{n_1 \ldots n_\infty} f(n_1 \ldots n_\infty, t)\, \phi_{n_1 \ldots n_\infty}(x_1 \ldots x_N)$$

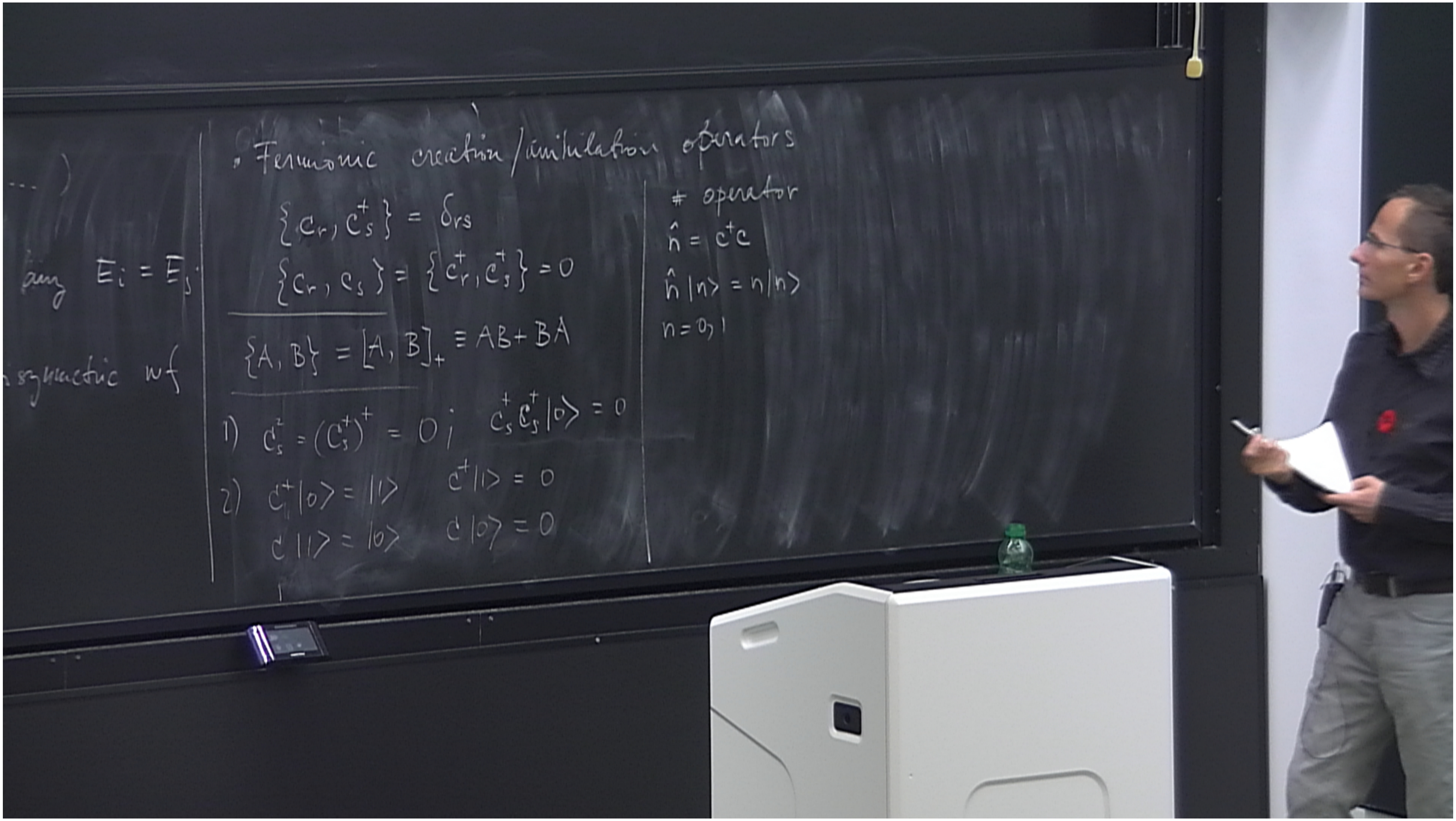

SECOND QUANTIZATION FOR FERMIONS & BOSONS

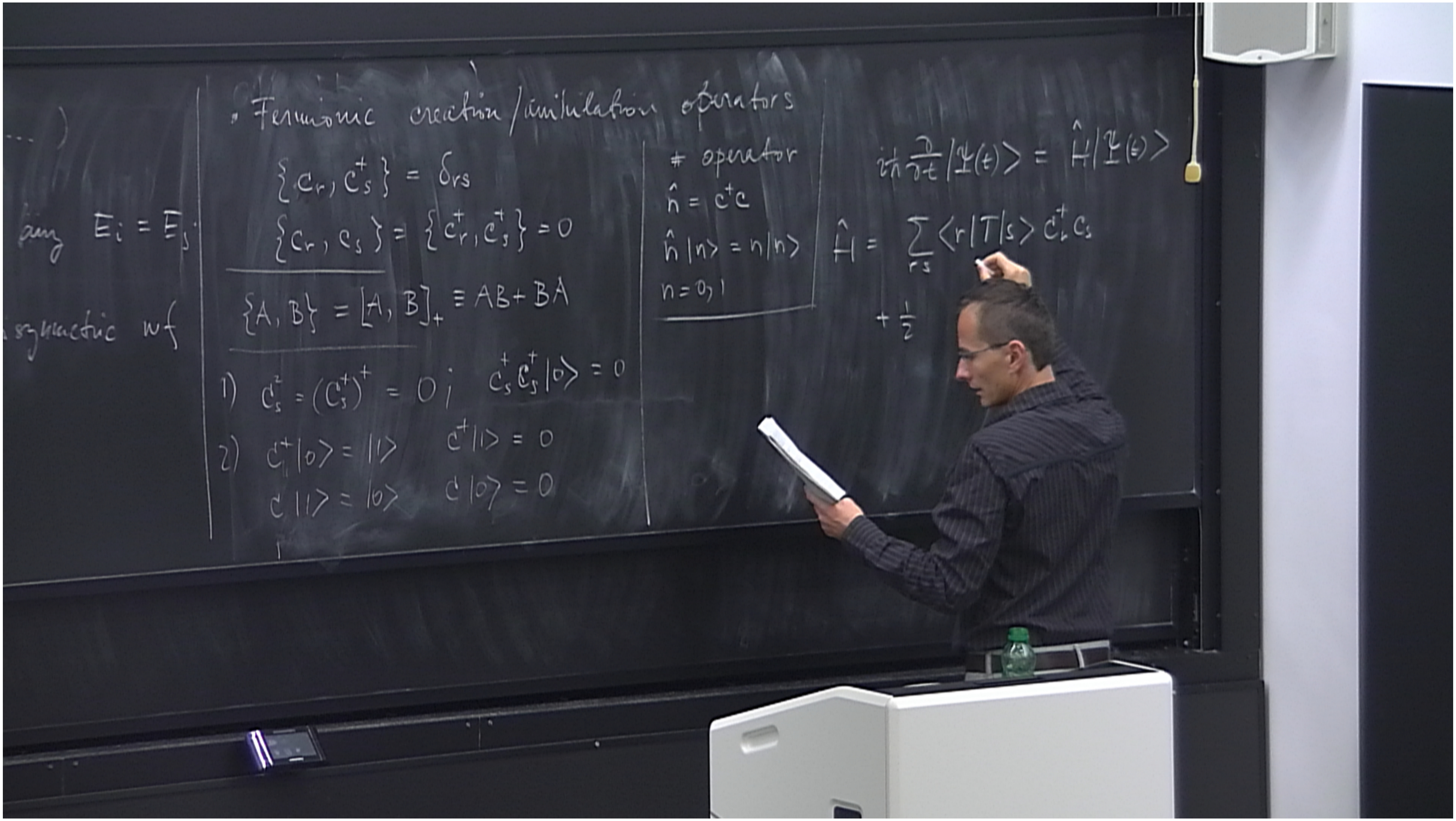

Fermionic creation/annihilation operators
$\{c_r, c_s^+\} = \delta_{rs}$
$\{A, B\} =$
$E_i = E_j$
symmetric wf

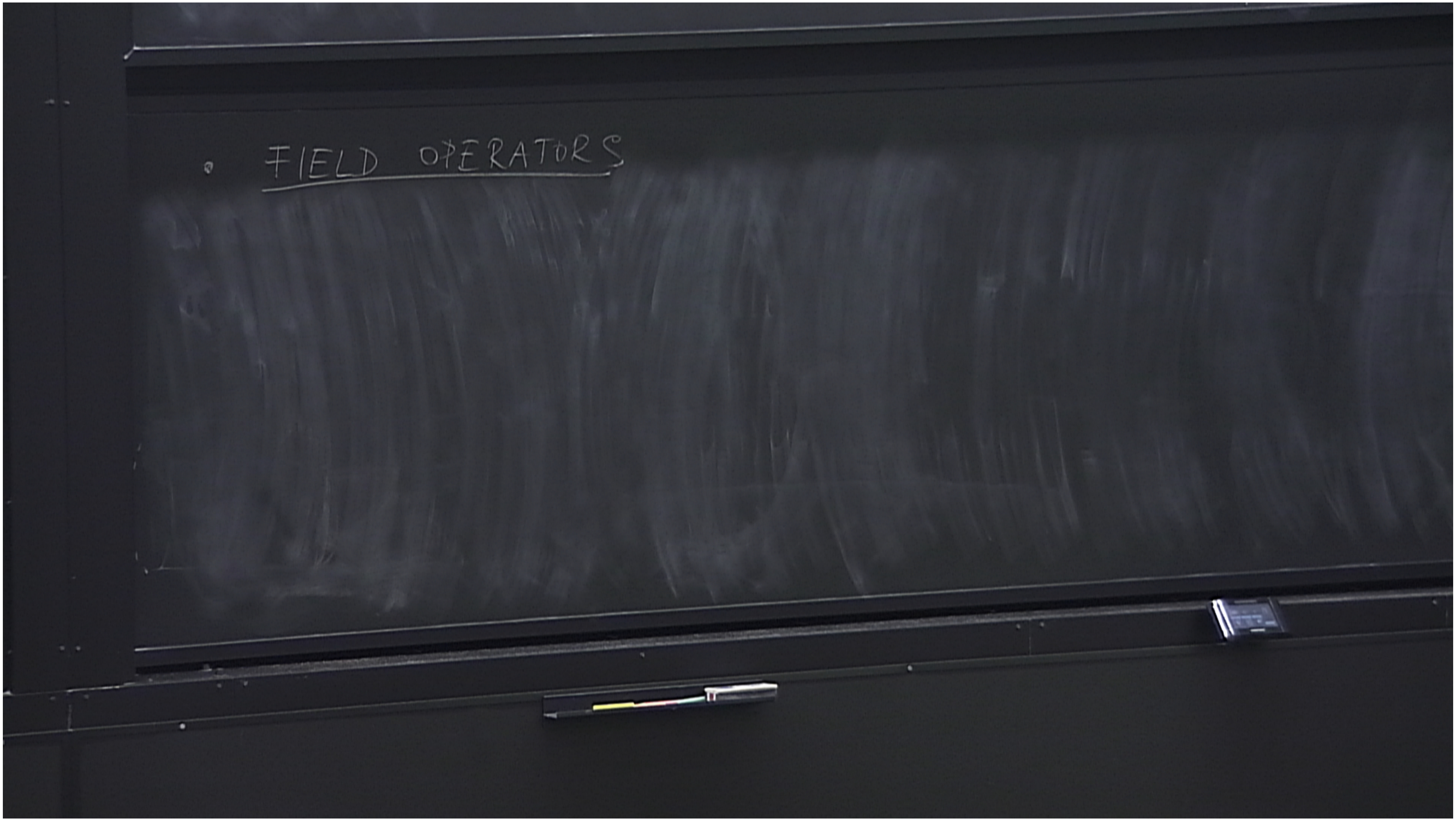


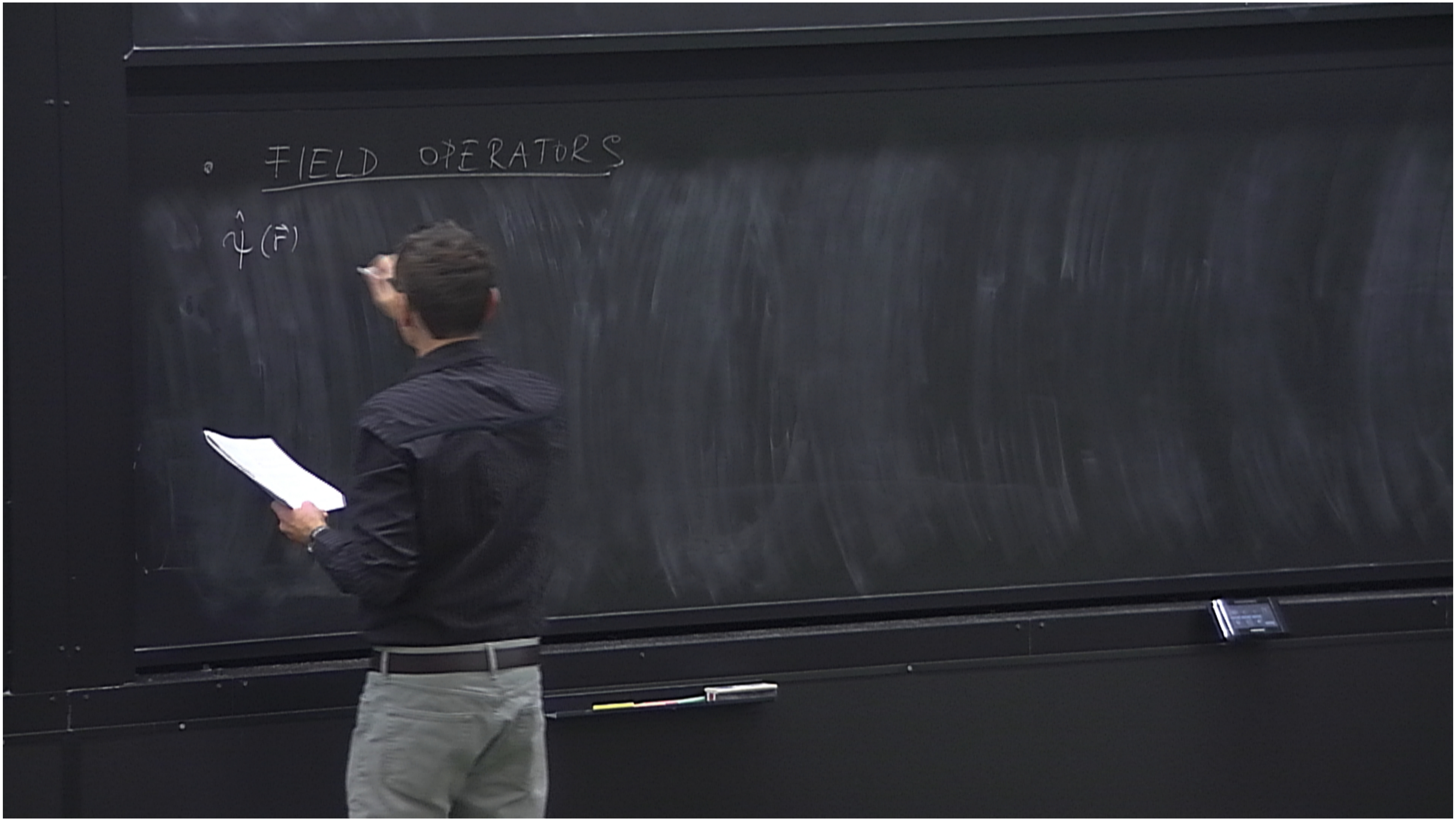
Fermionic creation/annihilation operators
{c_r, c_s^+} = δ_rs
{c_r, c_s} = {c_r^+, c_s^+} = 0
{A, B} =
= AB + BA
1) c_s^2 = (c_s^+)^+ =
2) c^+|0> = |1>
E_i = E_j
symmetric wf

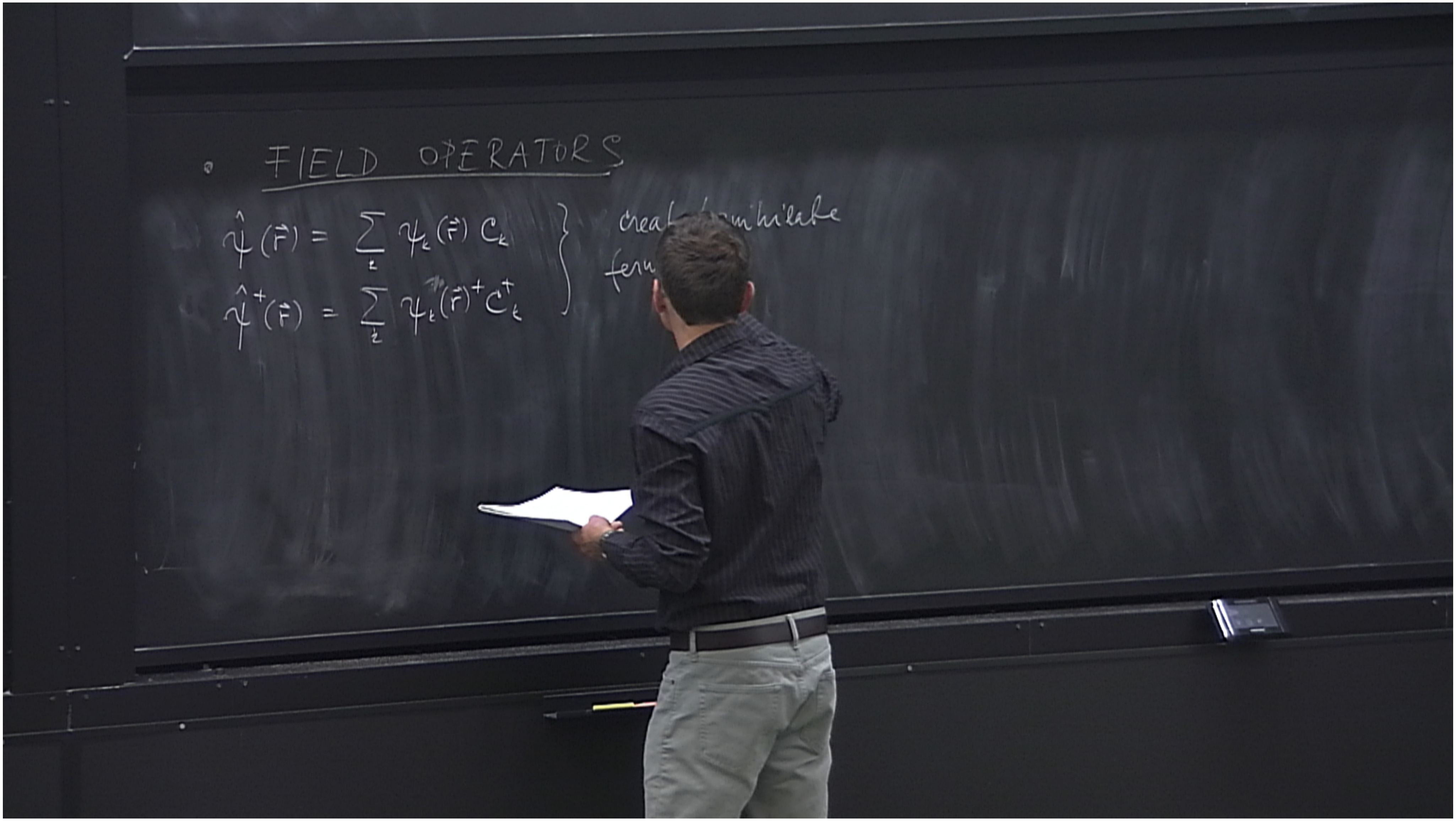

Fermionic creation/annihilation operators
{c_r, c_s^+} = δ_rs
{c_r, c_s} = {c_r^+, c_s^+} = 0
{A, B} = [A, B]_+ ≡ AB + BA
1) c_s^2 = (c_s^+)^+ = 0 ; c_s^+ c_s^+ |0> = 0
2) c^+|0> = |1> c^+|1> = 0
c|1> = |0> c|0> = 0
operator
n̂ = c^+c
E_i = E_j
wf

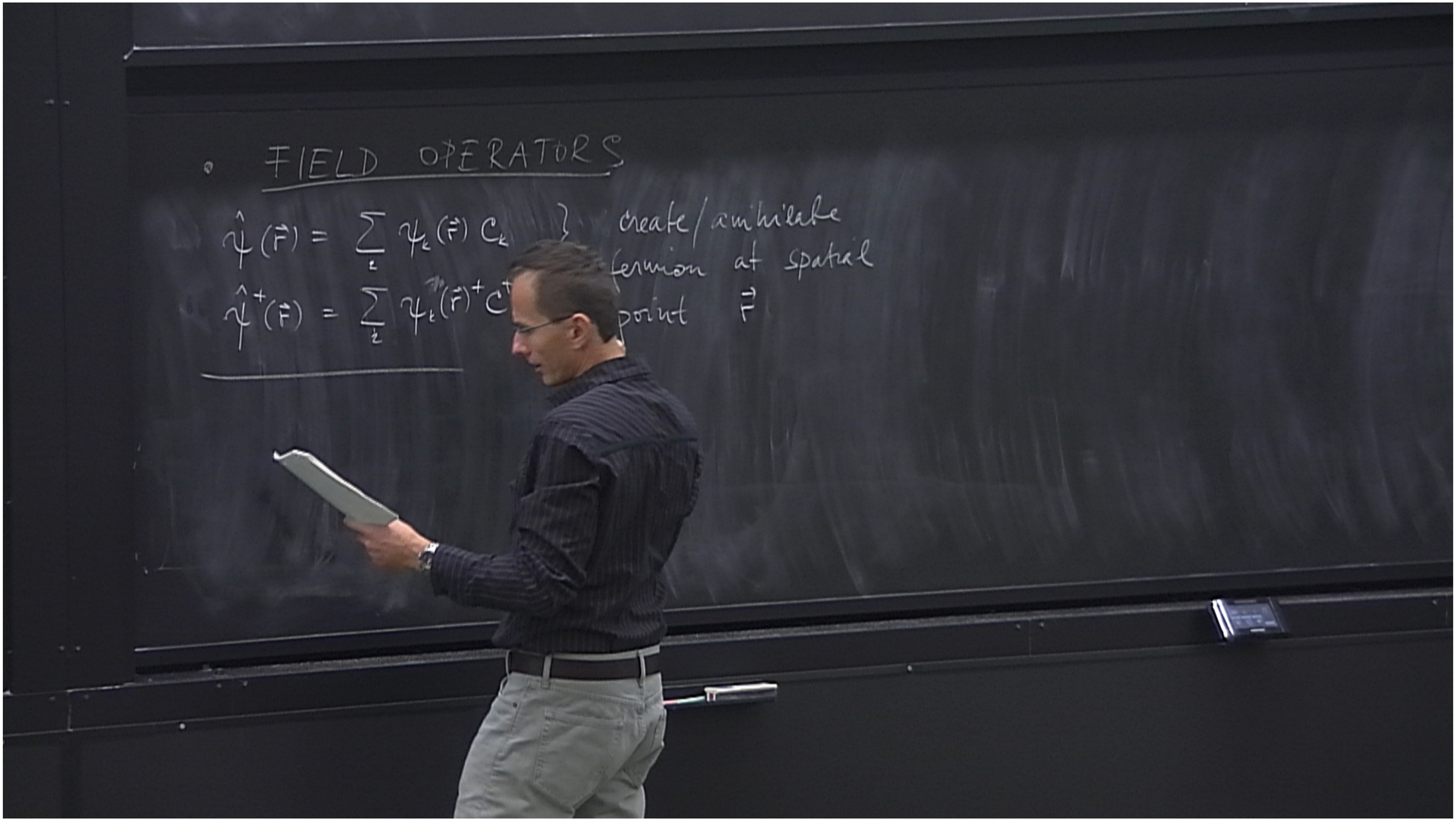

Fermionic creation/annihilation operators
{c_r, c_s^+} = δ_rs
{c_r, c_s} = {c_r^+, c_s^+} = 0
{A, B} = [A, B]_+ ≡ AB + BA
1) c_s^2 = (c_s^+)^+ = 0 ; c_s^+ c_s^+ |0> = 0
2) c^+ |0> = |1> c^+ |1> = 0
c |1> = |0> c |0> = 0
operator
n̂ = c^+ c
n̂ |n> = n |n>
n = 0, 1
E_i = E_j
symmetric wf

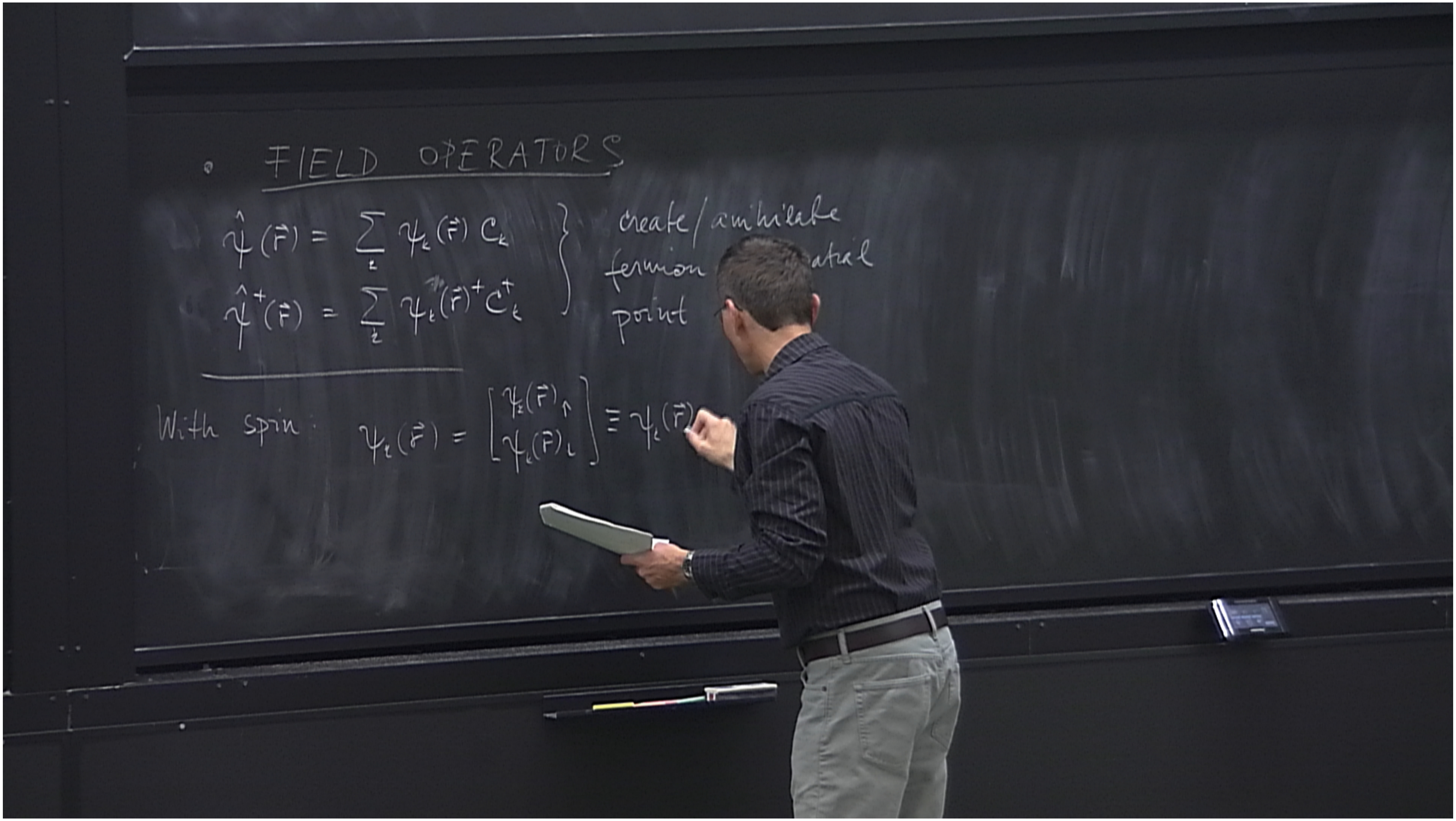

Fermionic creation/anihilation operators
operator

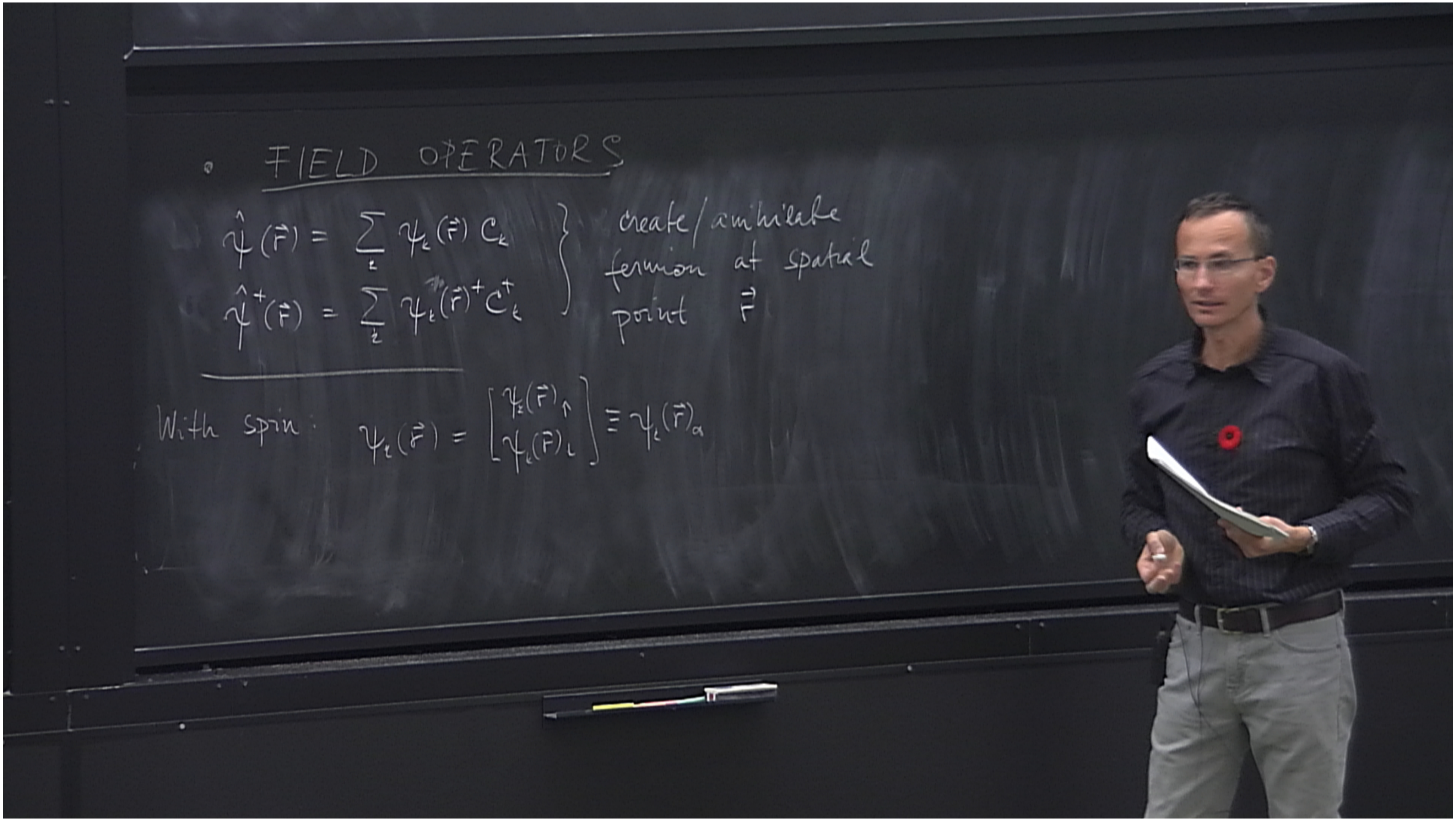

• FIELD OPERATORS

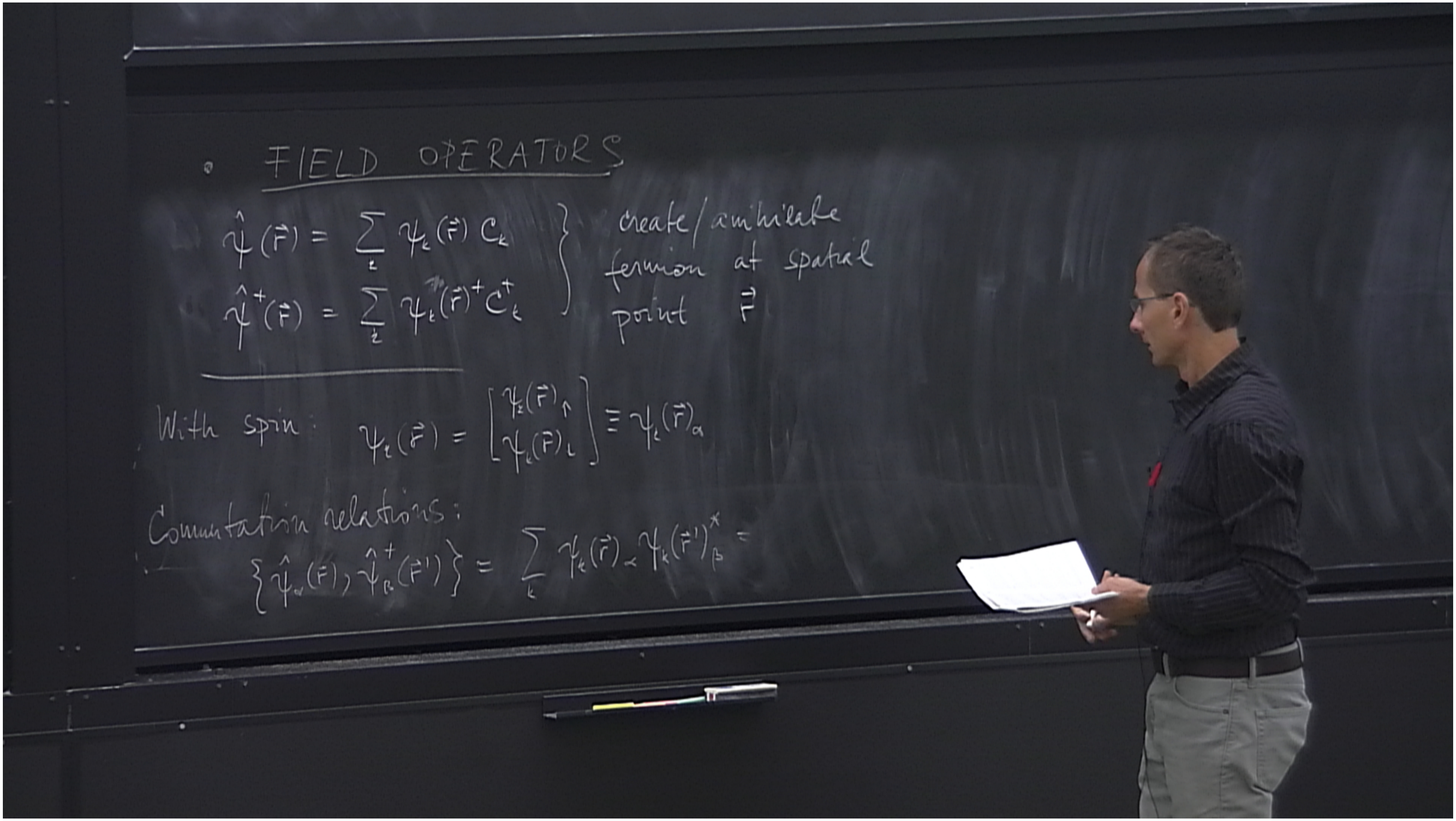

FIELD OPERATORS
$\hat{\psi}(\vec{r})$

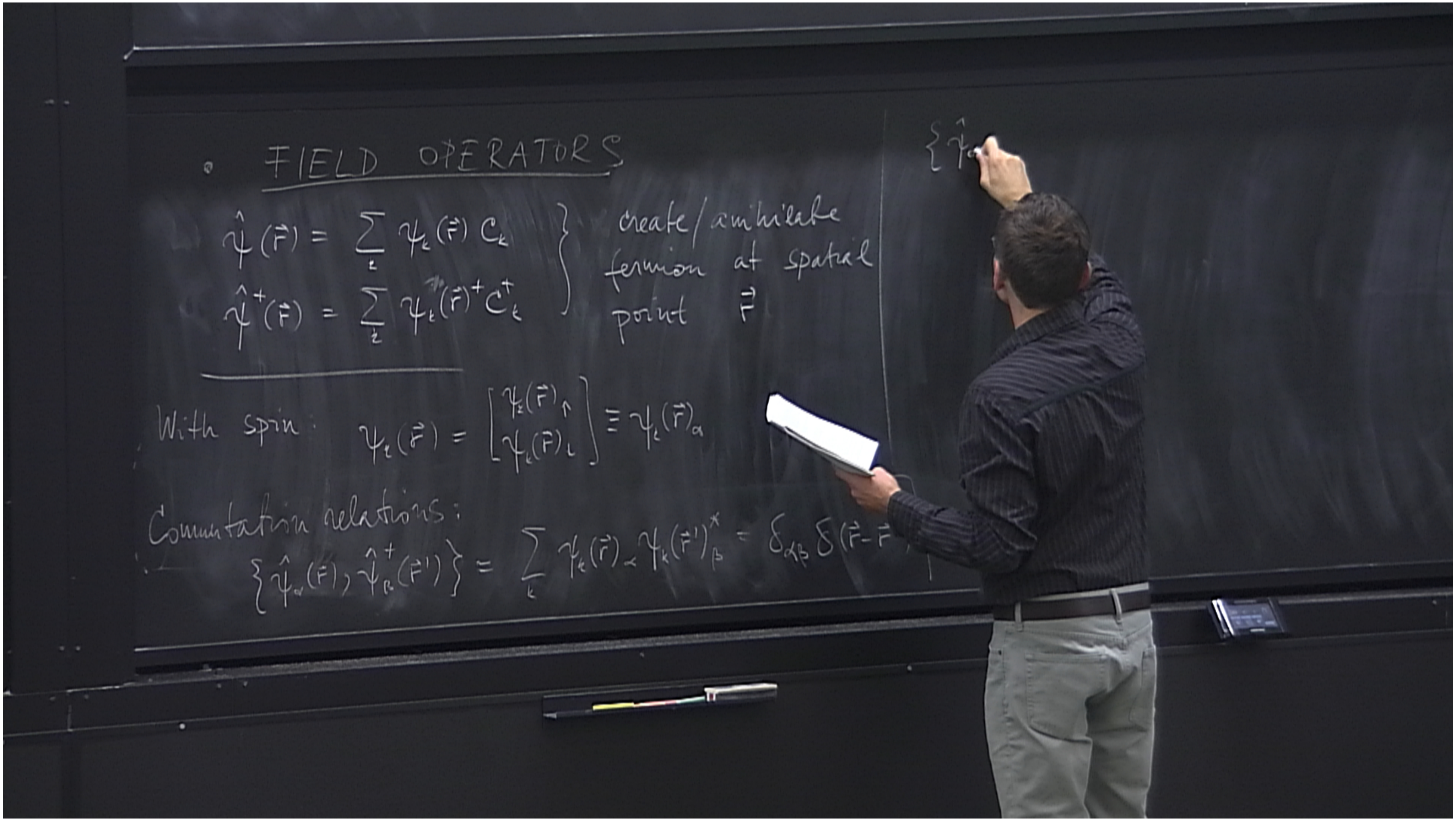

FIELD OPERATORS
$\hat{\psi}(\vec{r}) = \sum_k \psi_k(\vec{r})\, c_k$
$\hat{\psi}^+(\vec{r}) = \sum_k \psi_k(\vec{r})^+ c_k^+$

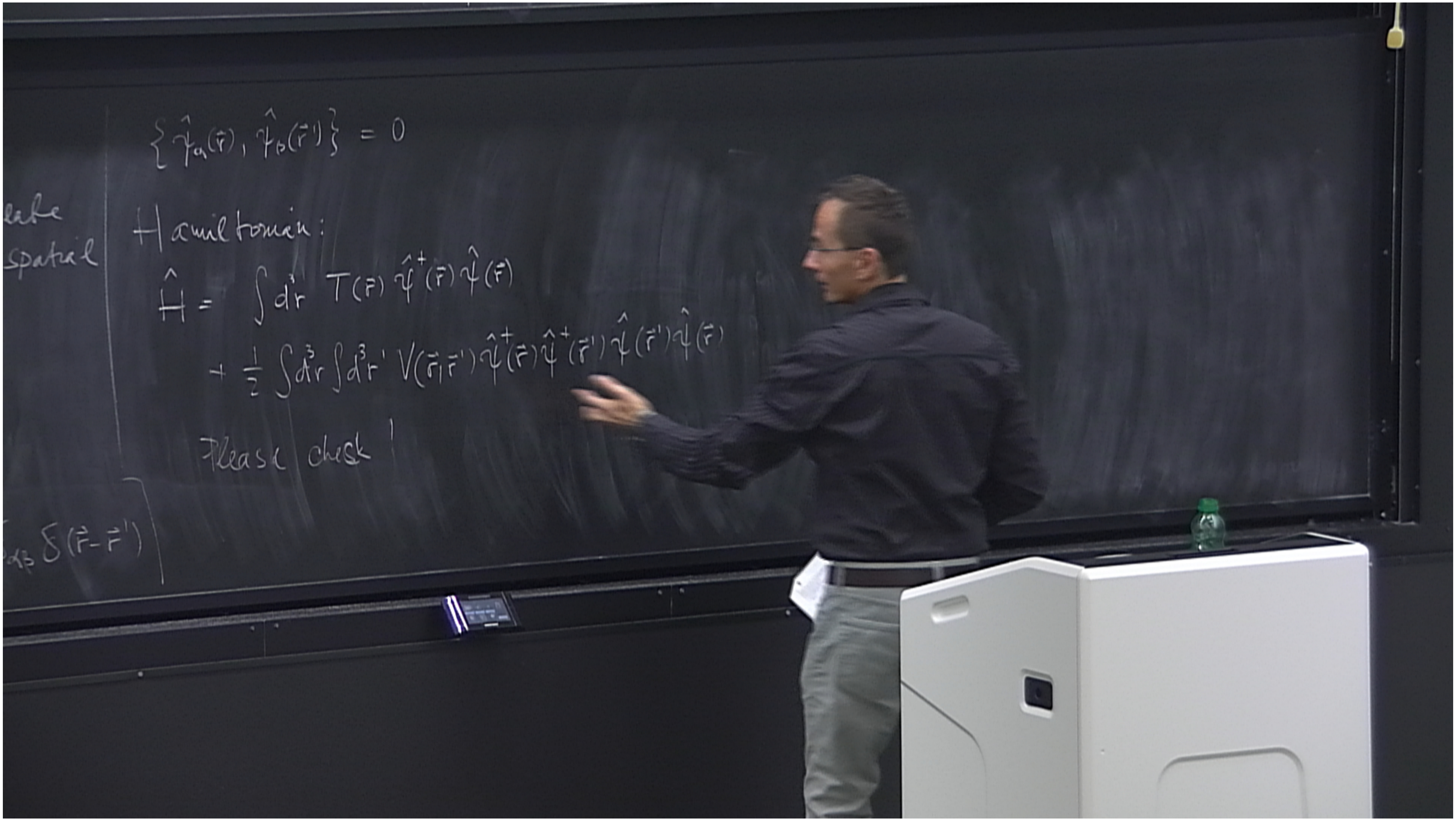

FIELD OPERATORS
create/annihilate
fermion at spatial
point

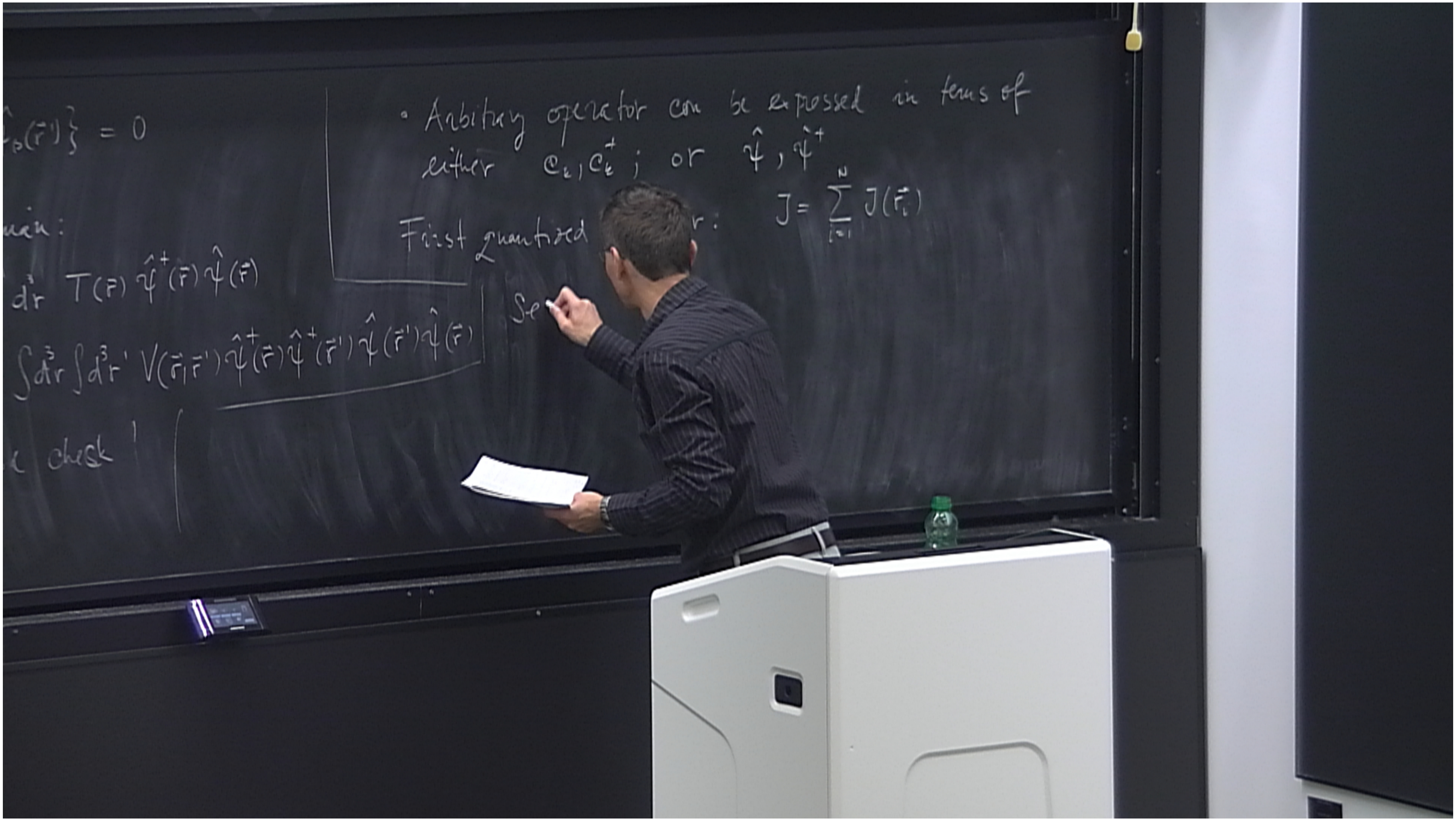

FIELD OPERATORS
create/annihilate
fermion
point
With spin


FIELD OPERATORS
$\hat{\psi}(\vec{r}) = \sum_k \psi_k(\vec{r})\, c_k$
$\hat{\psi}^+(\vec{r}) = \sum_k \psi_k(\vec{r})^+ c_k^+$
create/annihilate fermion at spatial point $\vec{r}$
With spin: $\psi_k(\vec{r}) = \begin{bmatrix} \psi_k(\vec{r})_\uparrow \\ \psi_k(\vec{r})_\downarrow \end{bmatrix} \equiv \psi_k(\vec{r})_\alpha$

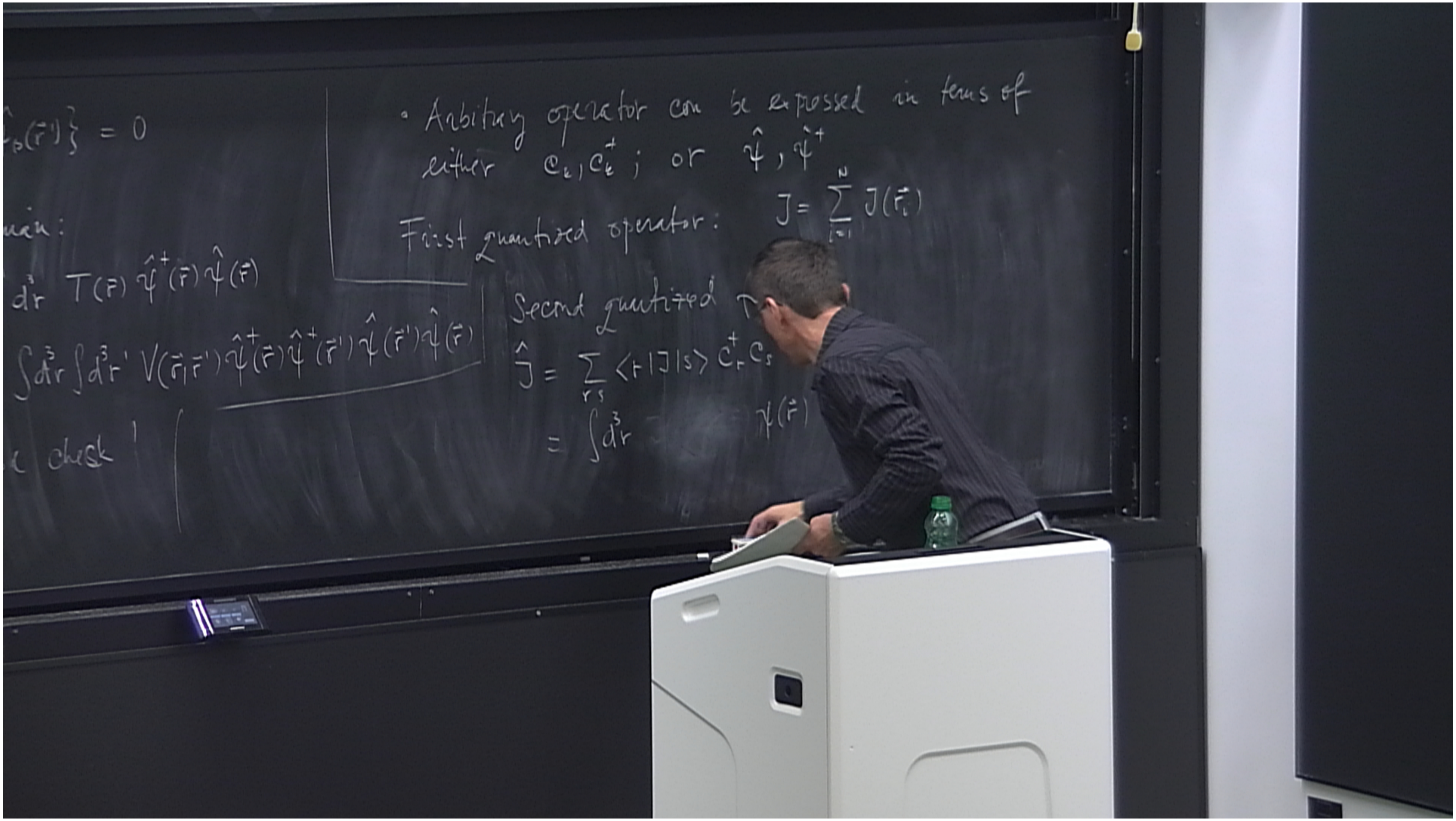

FIELD OPERATORS
$\hat{\psi}(\vec{r}) = \sum_k \psi_k(\vec{r})\, c_k$
$\hat{\psi}^+(\vec{r}) = \sum_k \psi_k(\vec{r})^+ c_k^+$
create/annihilate fermion at spatial point $\vec{r}$
With spin: $\psi_k(\vec{r}) = \begin{bmatrix} \psi_k(\vec{r})_\uparrow \\ \psi_k(\vec{r})_\downarrow \end{bmatrix} \equiv \psi_k(\vec{r})_\alpha$
Commutation relations:
$\{\hat{\psi}_\alpha(\vec{r}), \hat{\psi}^+_\beta(\vec{r}')\} = \sum_k \psi_k(\vec{r})_\alpha \psi_k(\vec{r}')^*_\beta =$


FIELD OPERATORS
$\hat{\psi}(\vec{r}) = \sum_k \psi_k(\vec{r})\, c_k$
$\hat{\psi}^+(\vec{r}) = \sum_k \psi_k(\vec{r})^+ c_k^+$
create/annihilate
fermion at spatial
point $\vec{r}$
With spin:
$\psi_k(\vec{r}) = \begin{bmatrix} \psi_k(\vec{r})_\uparrow \\ \psi_k(\vec{r})_\downarrow \end{bmatrix} \equiv \psi_k(\vec{r})_\alpha$
Commutation relations:
$\{\hat{\psi}_\alpha(\vec{r}), \hat{\psi}^+_\beta(\vec{r}\,')\} = \sum_k \psi_k(\vec{r})_\alpha \psi_k(\vec{r}\,')^*_\beta = \delta_{\alpha\beta}\,\delta(\vec{r}-\vec{r}\,')$

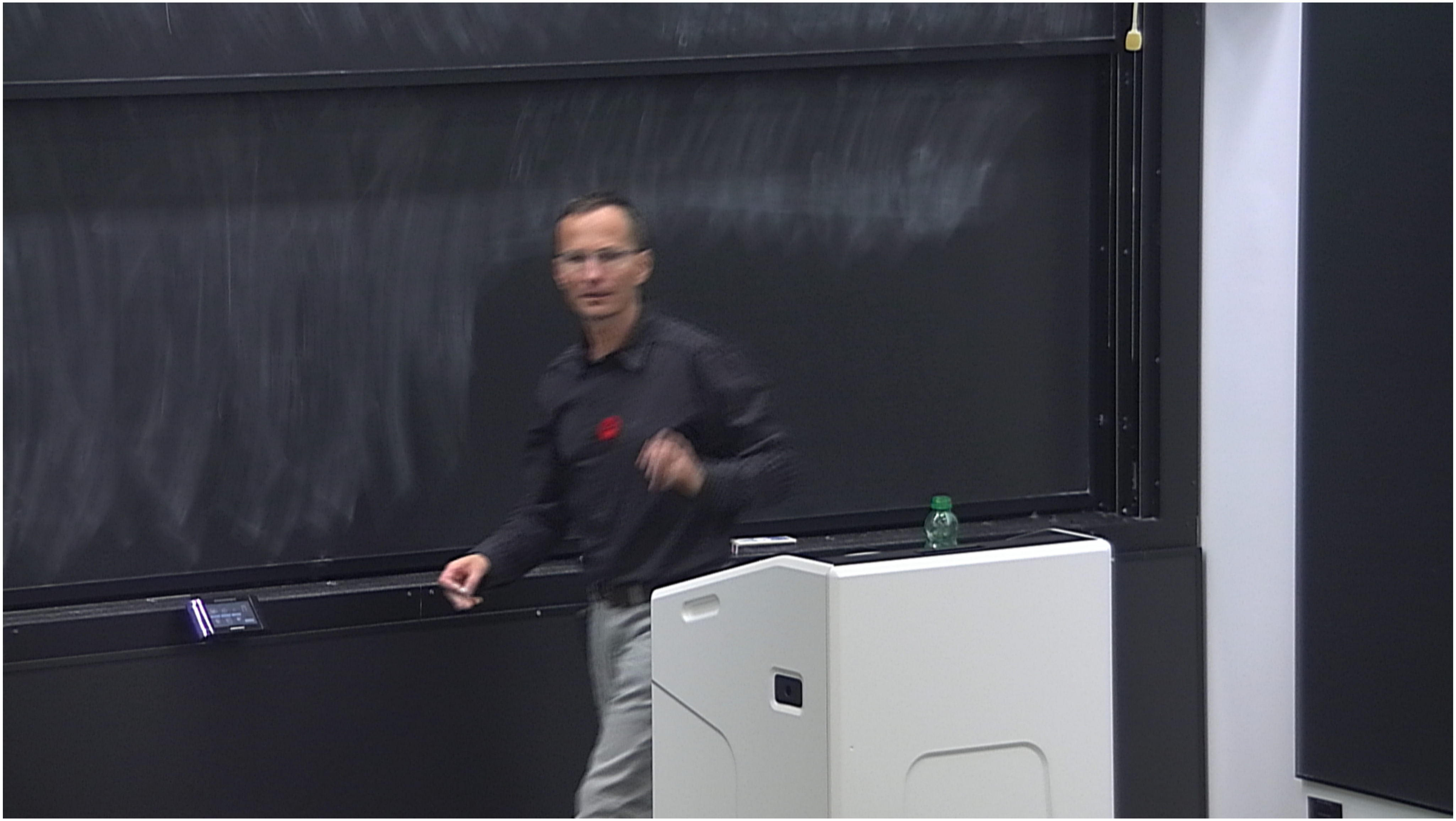

{ψ̂_α(r⃗), ψ̂_β(r⃗')} = 0
Hamiltonian:
Ĥ = ∫d³r T(r⃗) ψ̂†(r⃗) ψ̂(r⃗)
+ 1/2 ∫d³r ∫d³r' V(r⃗,r⃗') ψ̂†(r⃗) ψ̂†(r⃗') ψ̂(r⃗') ψ̂(r⃗)
Please check!

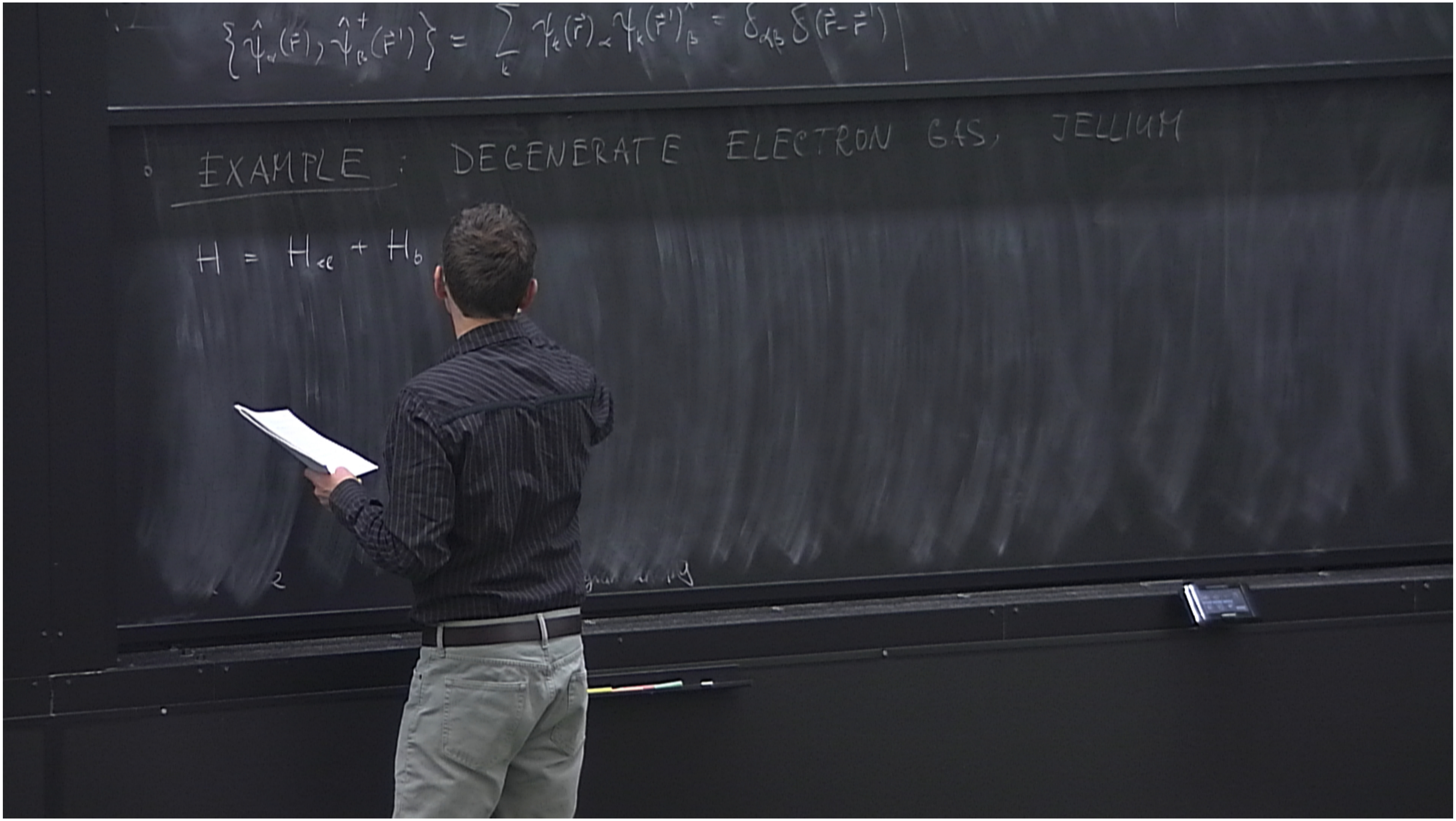


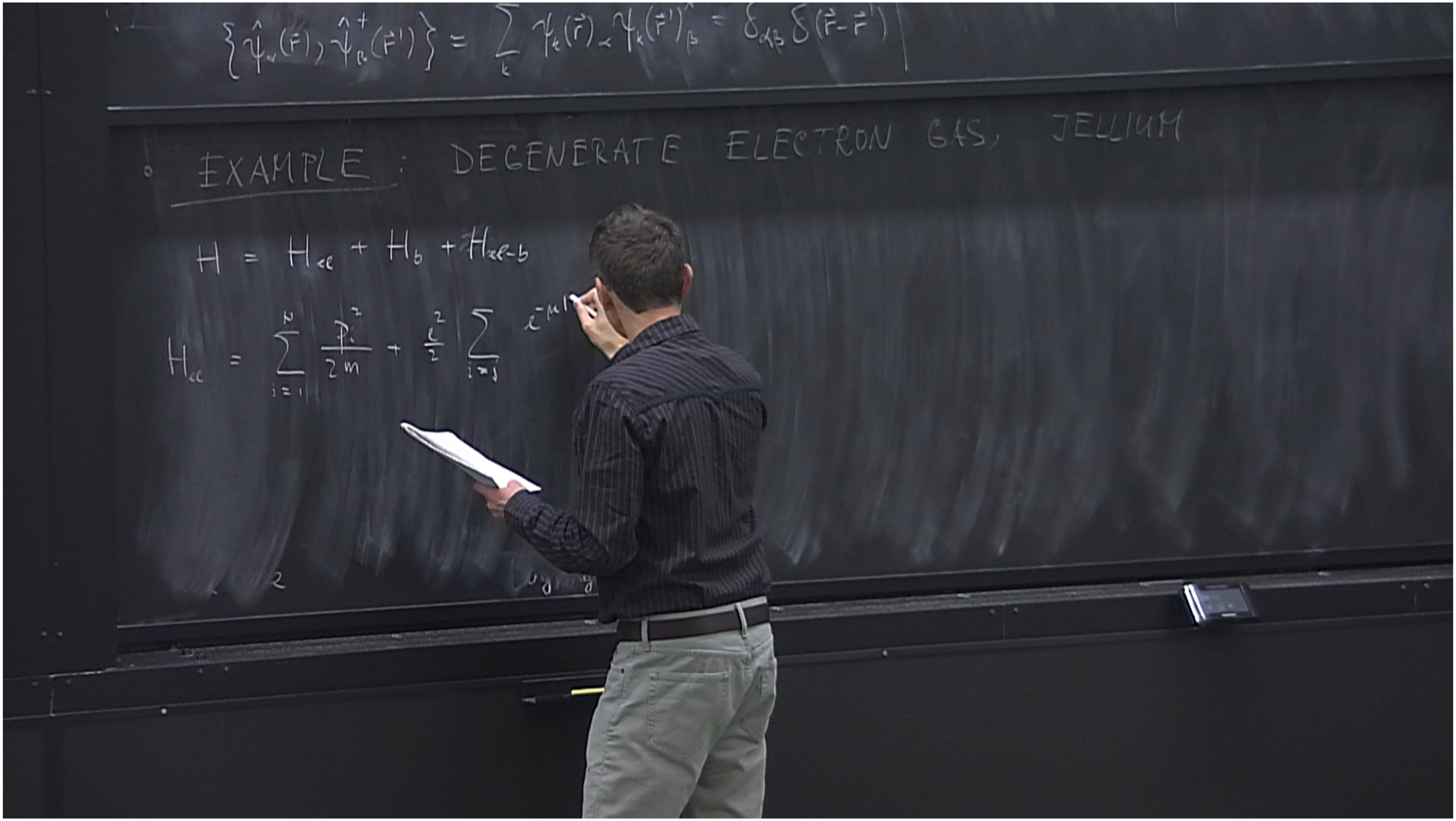
• Arbitrary operator can be expressed in terms of
either c_k, c_k^+ ; or $\hat{\psi}, \hat{\psi}^+$
First quantized
$J = \sum_{i=1}^{N} J(\vec{r}_i)$

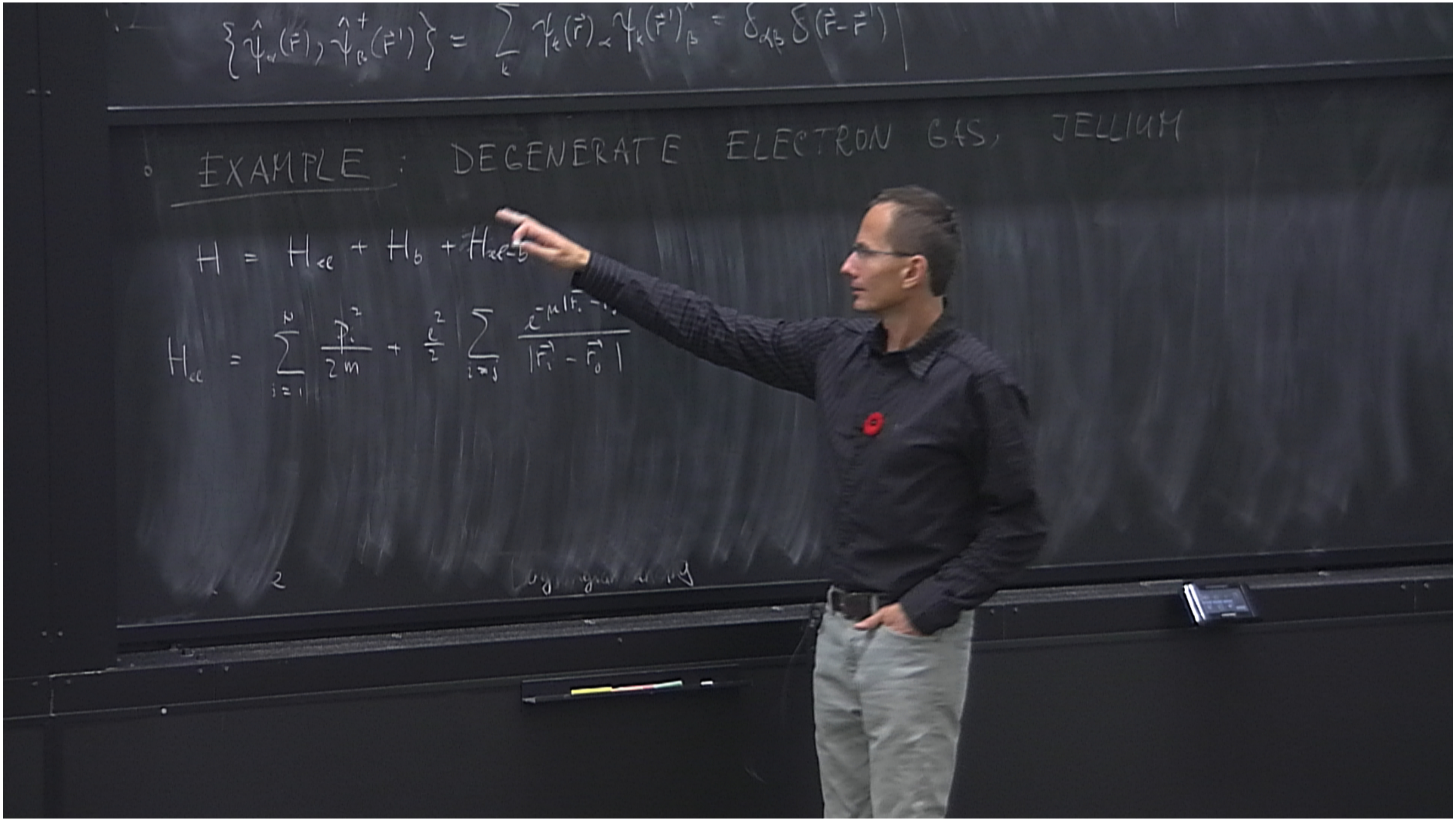


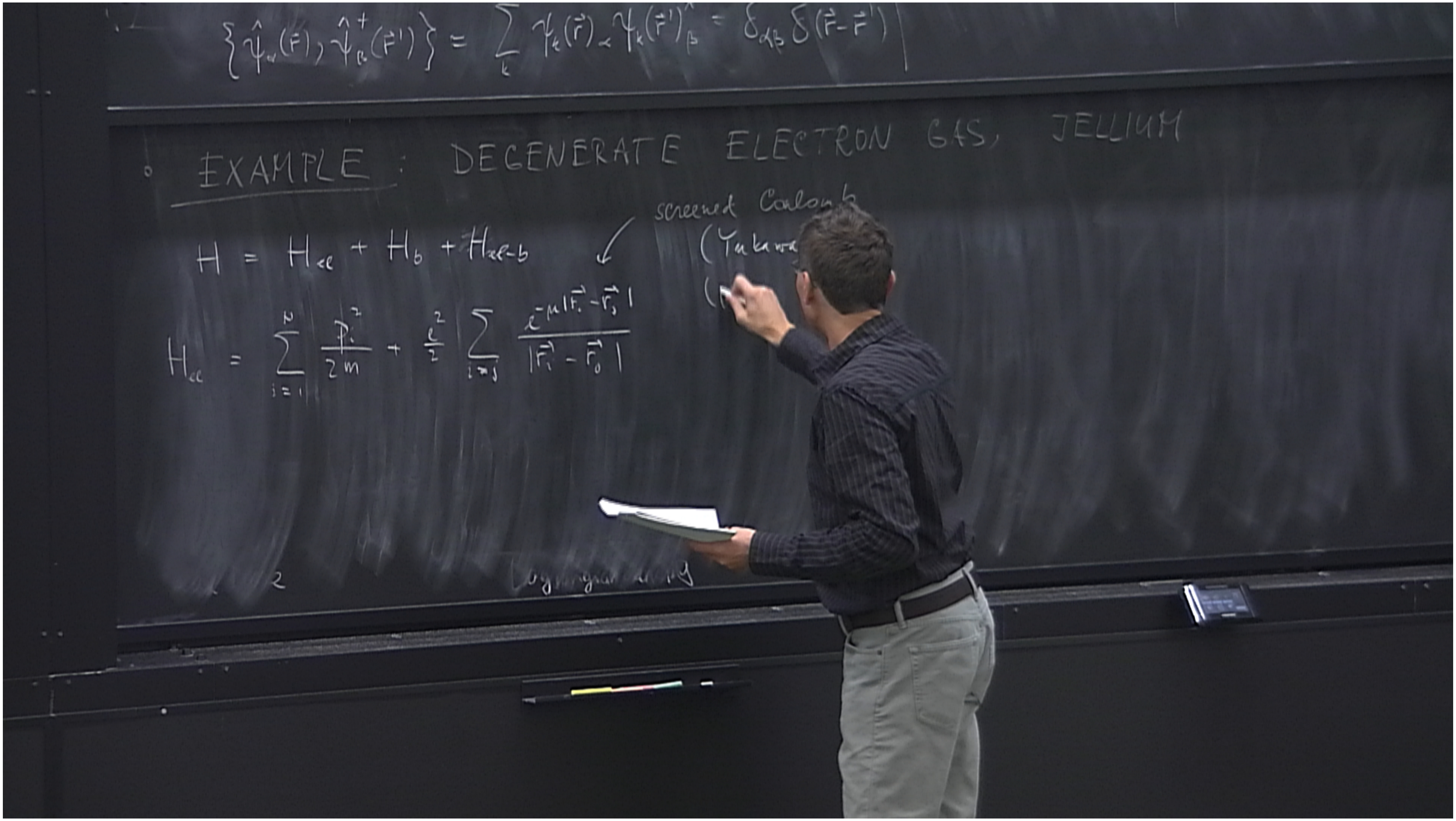
• Arbitrary operator can be expressed in terms of
either c_k, c_k^+ ; or ψ̂, ψ̂^+
First quantized operator: J = Σ_{i=1}^{N} J(r_i)
Second quantized
Ĵ = Σ_{rs} <r|J|s> c_r^+ c_s
= ∫d³r ψ(r)
∫d³r T(r) ψ̂^+(r) ψ̂(r)
∫d³r ∫d³r' V(r, r') ψ̂^+(r) ψ̂^+(r') ψ̂(r') ψ̂(r)
check!

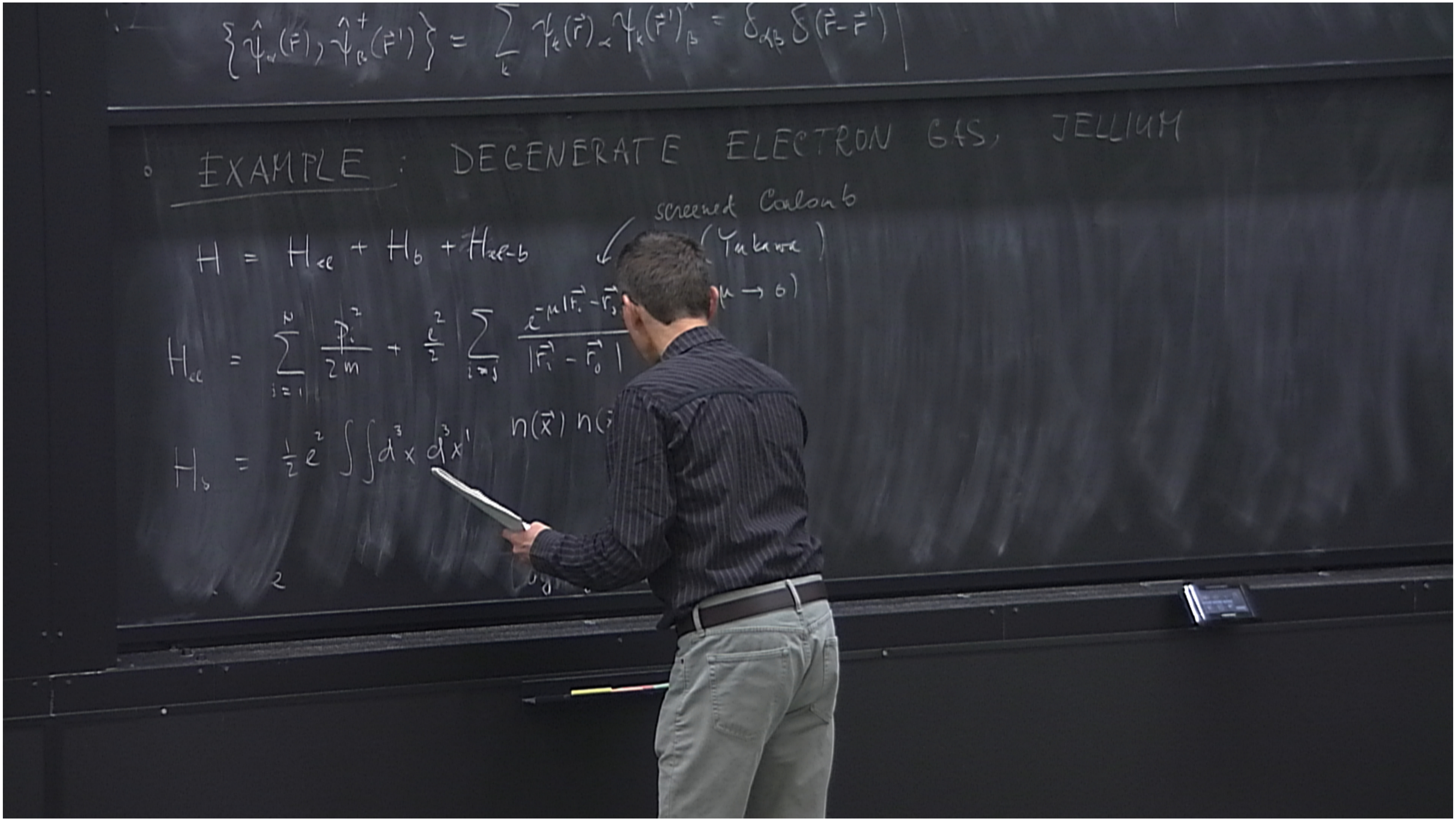


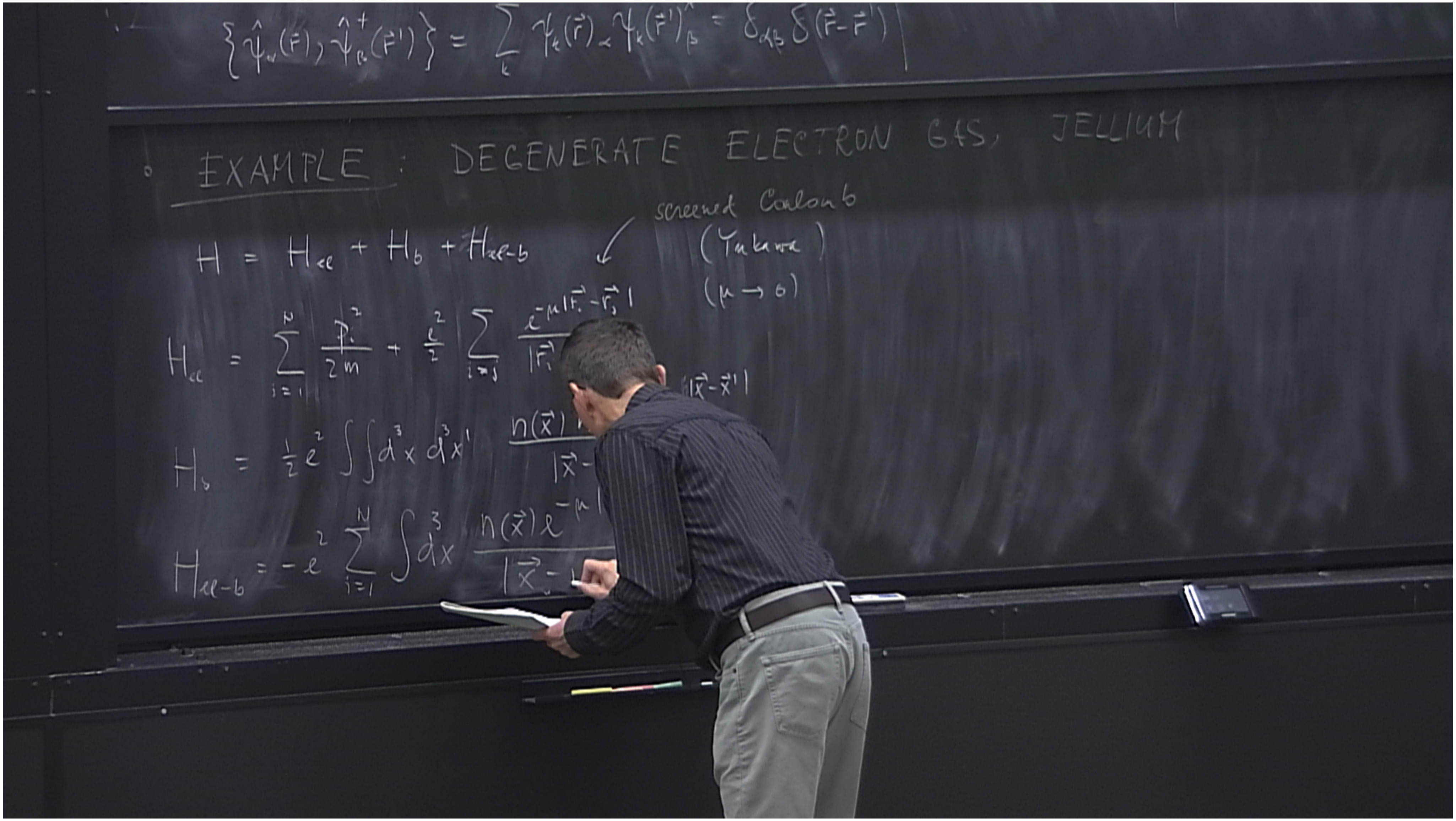

$\{\hat{\psi}_\alpha(\vec{r}), \hat{\psi}^\dagger_\beta(\vec{r}')\} = \sum_k \psi_k(\vec{r})_\alpha \psi_k(\vec{r}')^*_\beta = \delta_{\alpha\beta}\delta(\vec{r}-\vec{r}')$
EXAMPLE : DEGENERATE ELECTRON GAS, JELLIUM
$H = H_{el} + H_b$

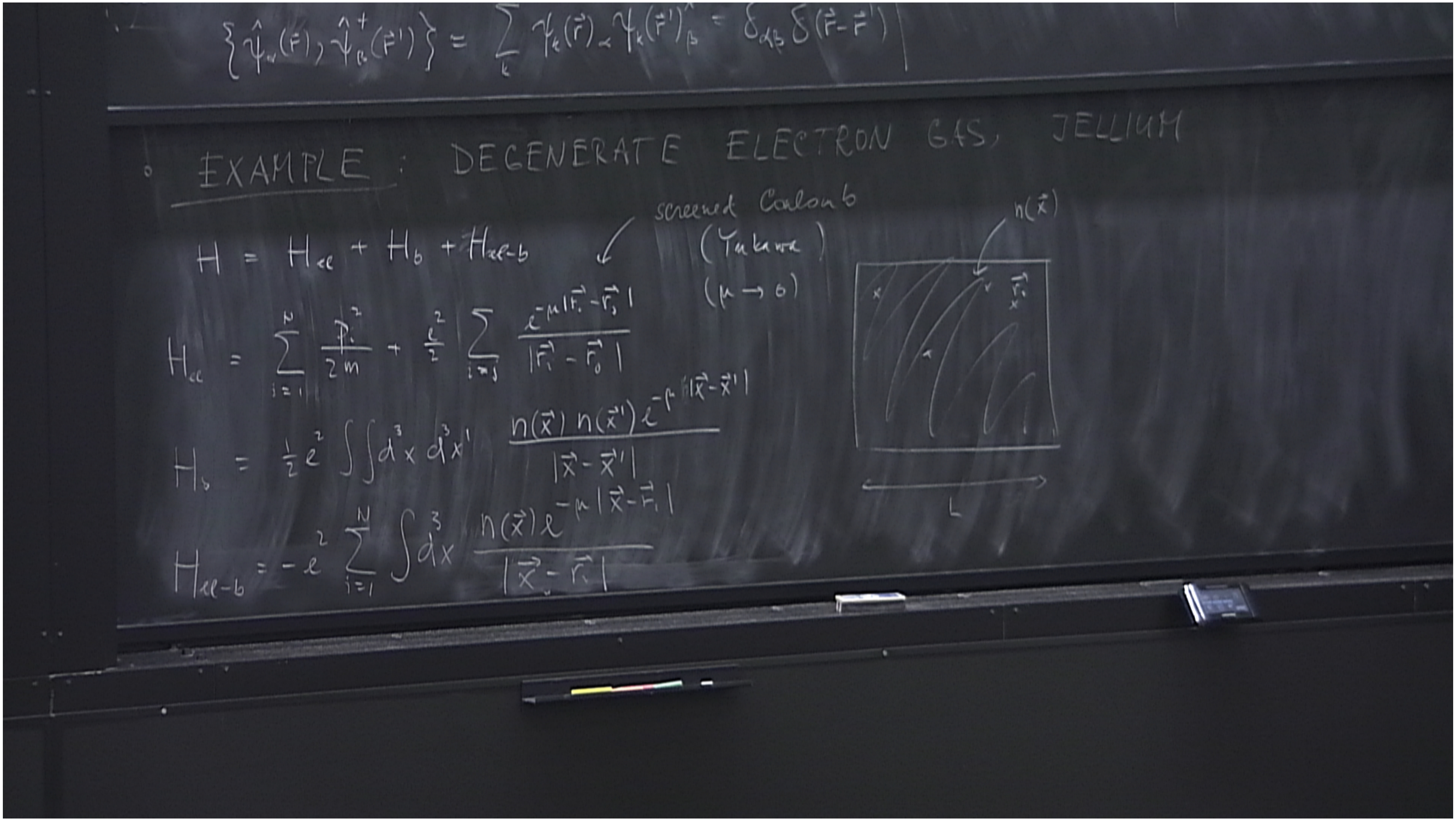

EXAMPLE: DEGENERATE ELECTRON GAS, JELLIUM
H = H_el + H_b + H_el-b

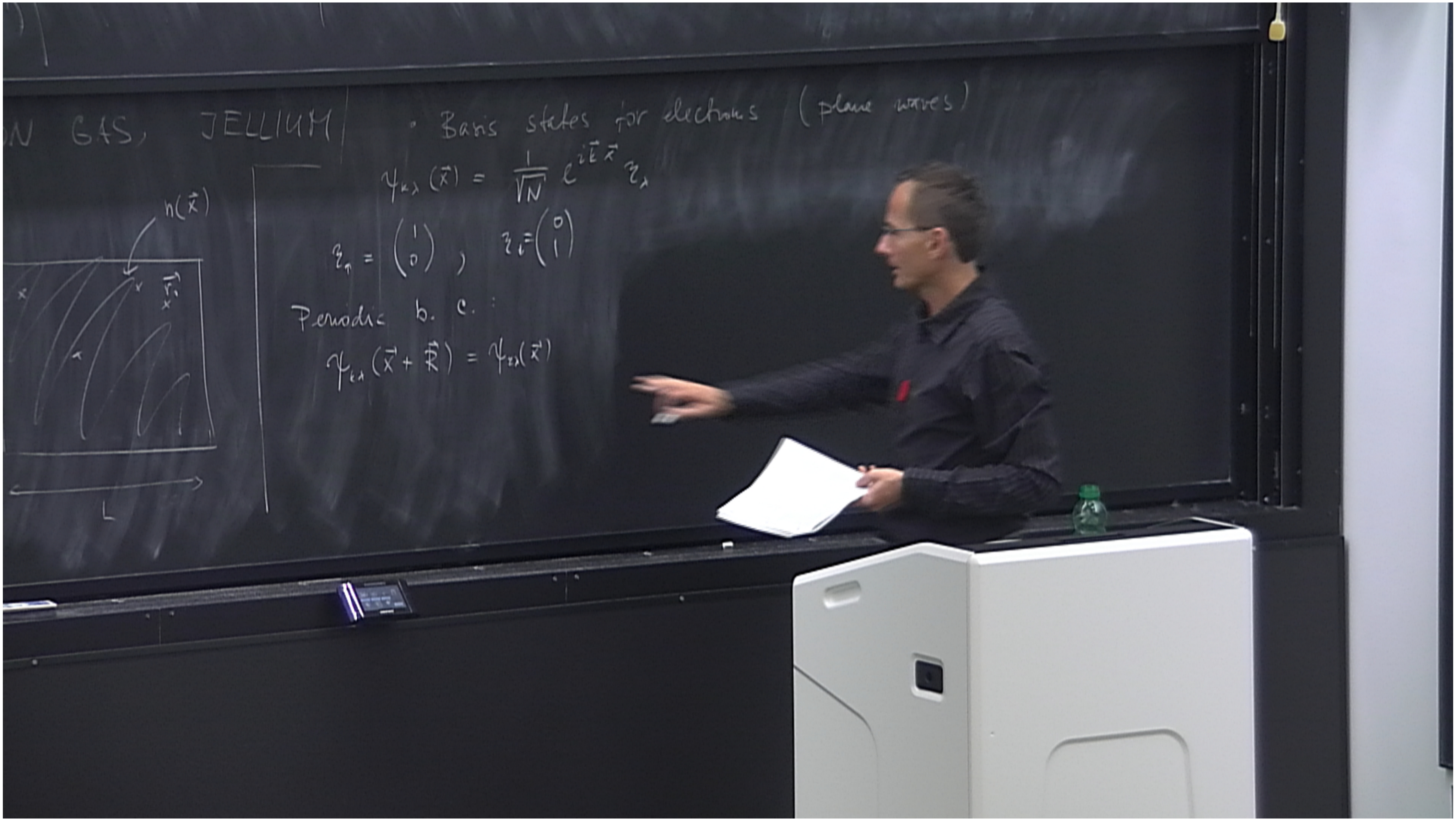

EXAMPLE : DEGENERATE ELECTRON GAS, JELLIUM

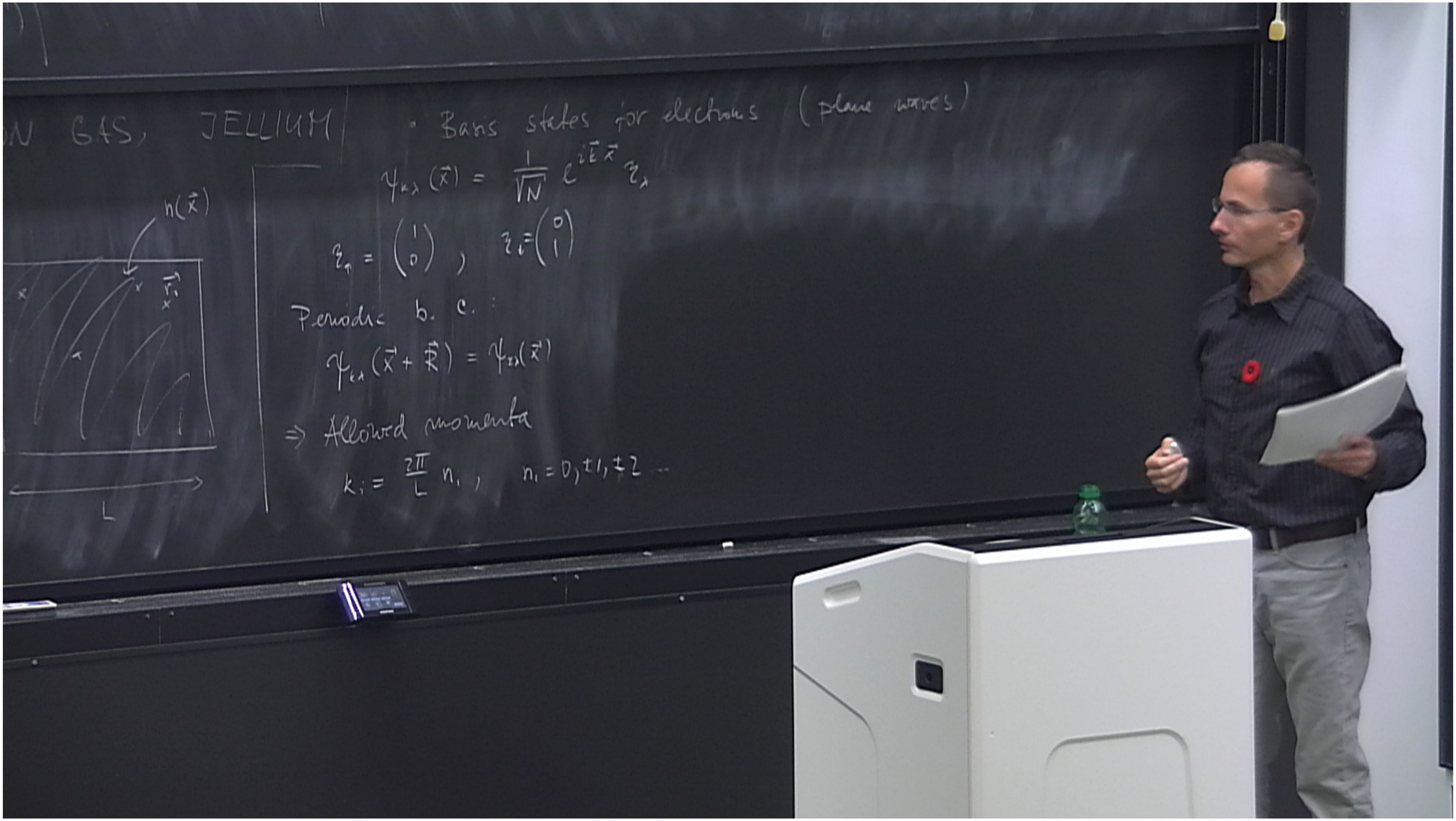

EXAMPLE : DEGENERATE ELECTRON GAS, JELLIUM
screened Coulomb
(Yukawa
H = H_ee + H_b + H_el-b

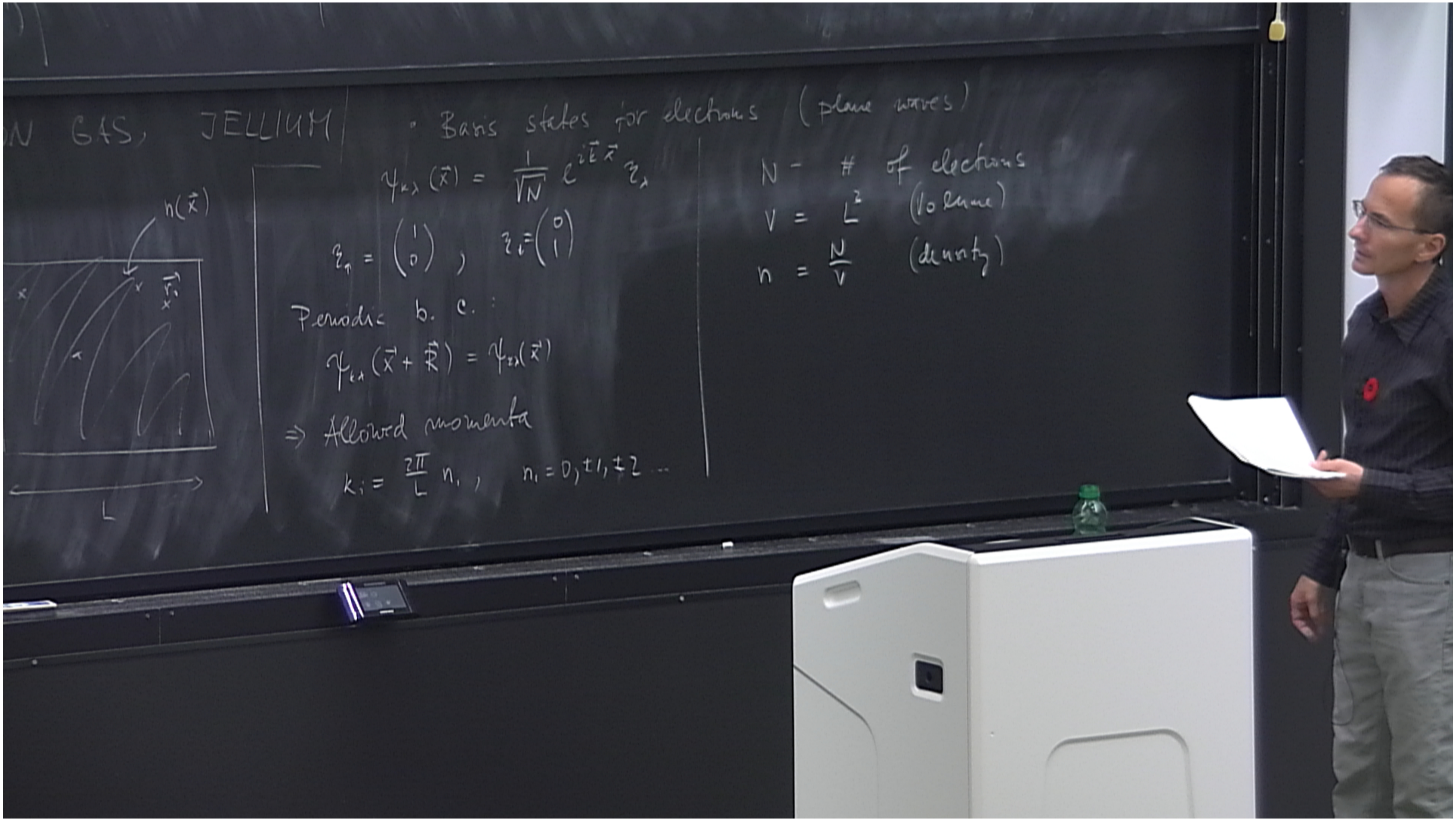

$\{\hat{\psi}_\alpha(\vec{r}), \hat{\psi}^\dagger_\beta(\vec{r}')\} = \sum_k \psi_k(\vec{r})_\alpha \psi_k(\vec{r}')^*_\beta = \delta_{\alpha\beta}\delta(\vec{r}-\vec{r}')$
EXAMPLE: DEGENERATE ELECTRON GAS, JELLIUM
screened Coulomb
(Yukawa)
$H = H_{el} + H_b + H_{el-b}$
$H_{el} = \sum_{i=1}^{N} \frac{p_i^2}{2m} + \frac{e^2}{2}\sum_{i \neq j} \frac{e^{-\mu|\vec{r}_i - \vec{r}_j|}}{|\vec{r}_i - \vec{r}_j|}$
$H_b = \frac{1}{2}e^2 \int\int d^3x\, d^3x'$


EXAMPLE : DEGENERATE ELECTRON GAS, JELLIUM
screened Coulomb
(Yukawa)
(μ → 0)
H = H_ee + H_b + H_ee-b

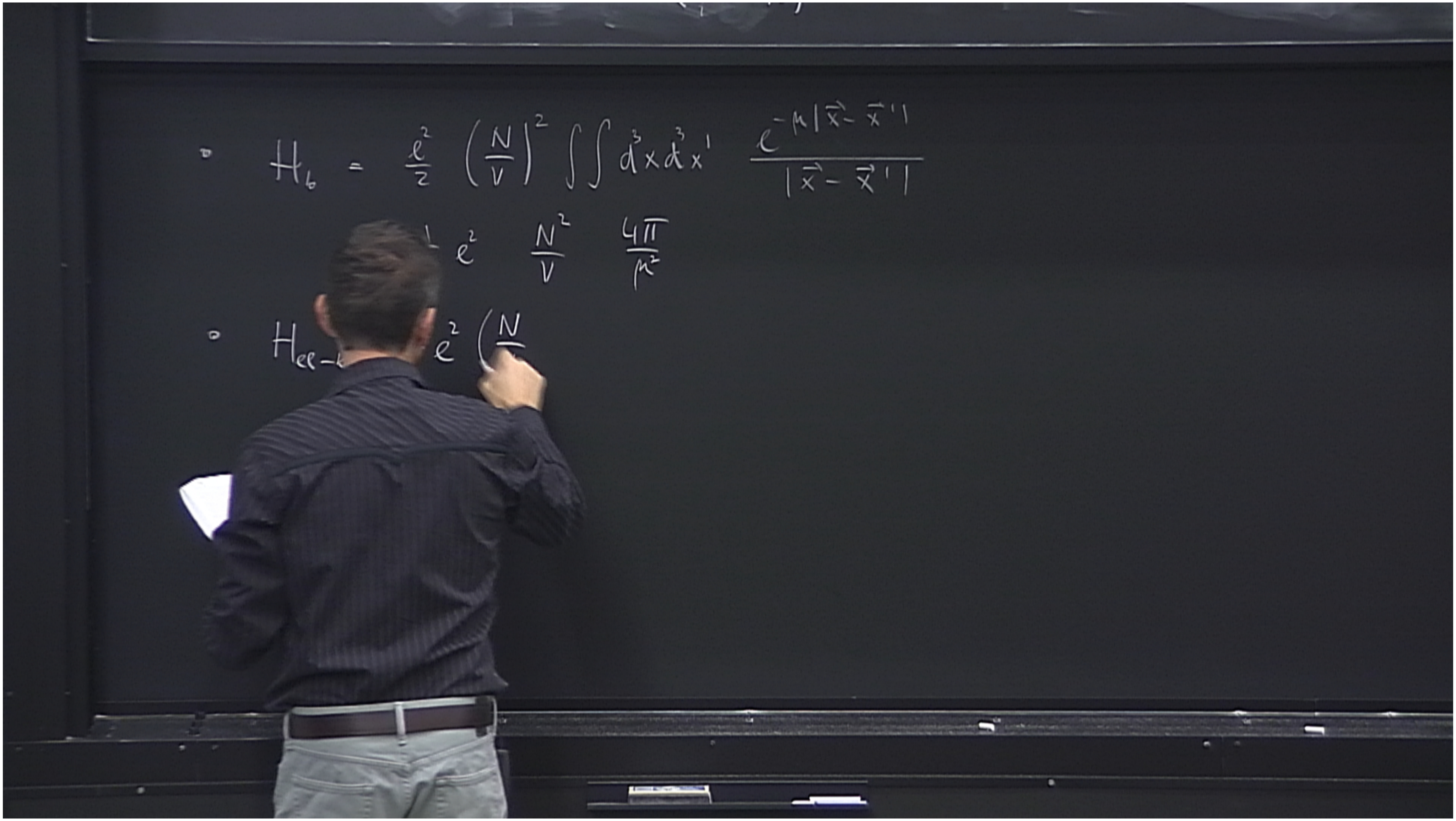

EXAMPLE: DEGENERATE ELECTRON GAS, JELLIUM
screened Coulomb
(Yukawa)
(μ → 0)
H = H_ee + H_b + H_ee-b
n(x)
L


ON GAS, JELLIUM
• Basis states for electrons (plane waves)
$\psi_{k\lambda}(\vec{x}) = \frac{1}{\sqrt{N}} e^{i\vec{k}\vec{x}} \xi_\lambda$
$\xi_\uparrow = \begin{pmatrix}1\\0\end{pmatrix}, \xi_\downarrow = \begin{pmatrix}0\\1\end{pmatrix}$
Periodic b. c.:
$\psi_{k\lambda}(\vec{x}+\vec{R}) = \psi_{k\lambda}(\vec{x})$
$n(\vec{x})$
$\vec{r}_i$
L


N GAS, JELLIUM
• Basis states for electrons (plane waves)
n(x)
Periodic b. c. :
⇒ Allowed momenta
L


GAS, JELLIUM
Basis states for electrons (plane waves)
Periodic b. c.
Allowed momenta
N - # of electrons
(volume)
(density)


$H_b = \frac{e^2}{2} \left(\frac{N}{V} \right.$


$H_b = \frac{e^2}{2} \left(\frac{N}{V}\right)^2 \iint d^3x\, d^3x' \frac{e^{-\mu|\vec{x}-\vec{x}'|}}{|\vec{x}-\vec{x}'|}$
$e^2 \quad \frac{N^2}{V} \quad \frac{4\pi}{\mu^2}$
H_{ee-} $e^2 \left(\frac{N}{\right.$

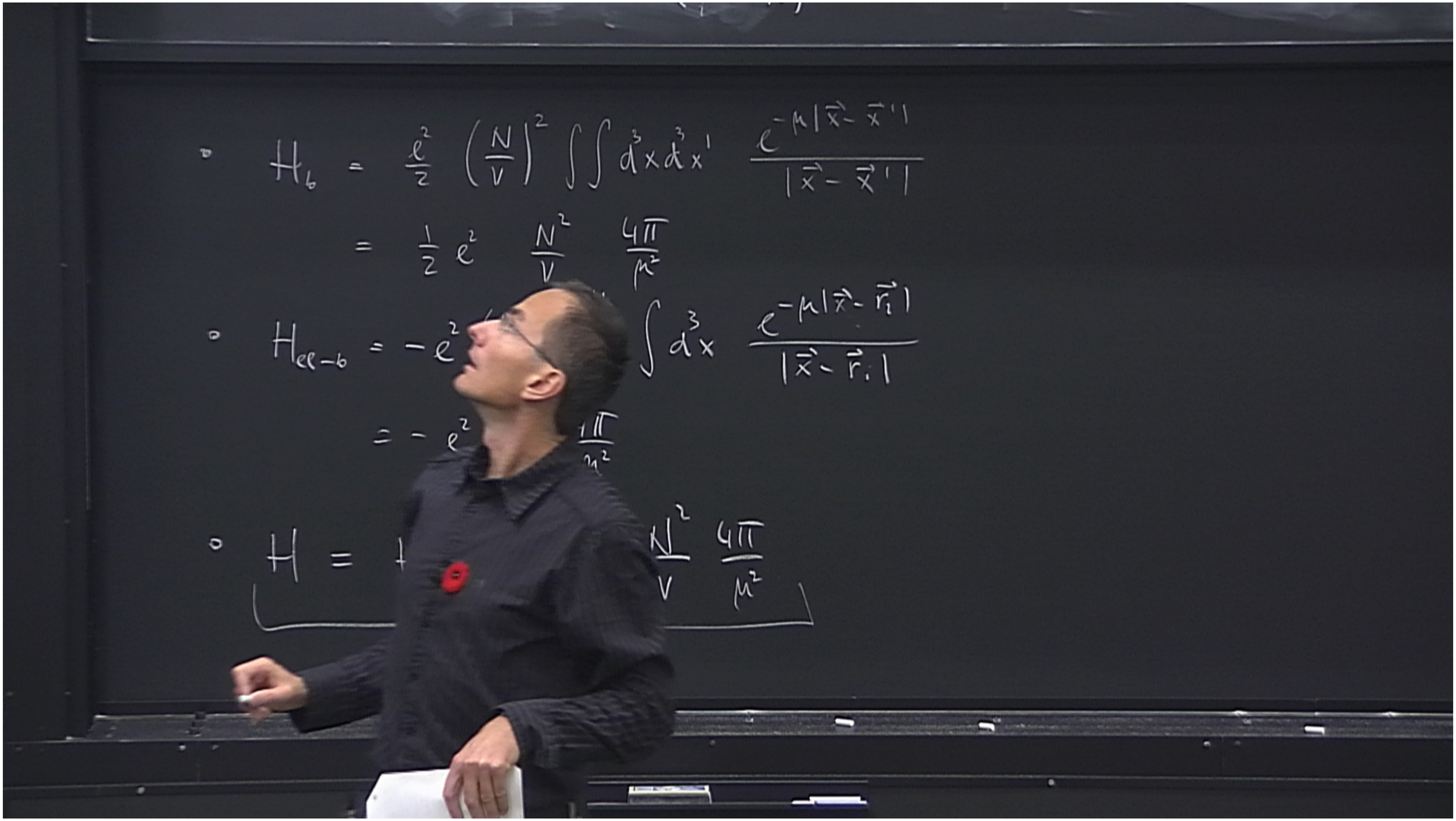
$$H_b = \frac{e^2}{2}\left(\frac{N}{V}\right)^2 \iint d^3x\, d^3x' \, \frac{e^{-\mu|\vec{x}-\vec{x}\,'|}}{|\vec{x}-\vec{x}\,'|}$$

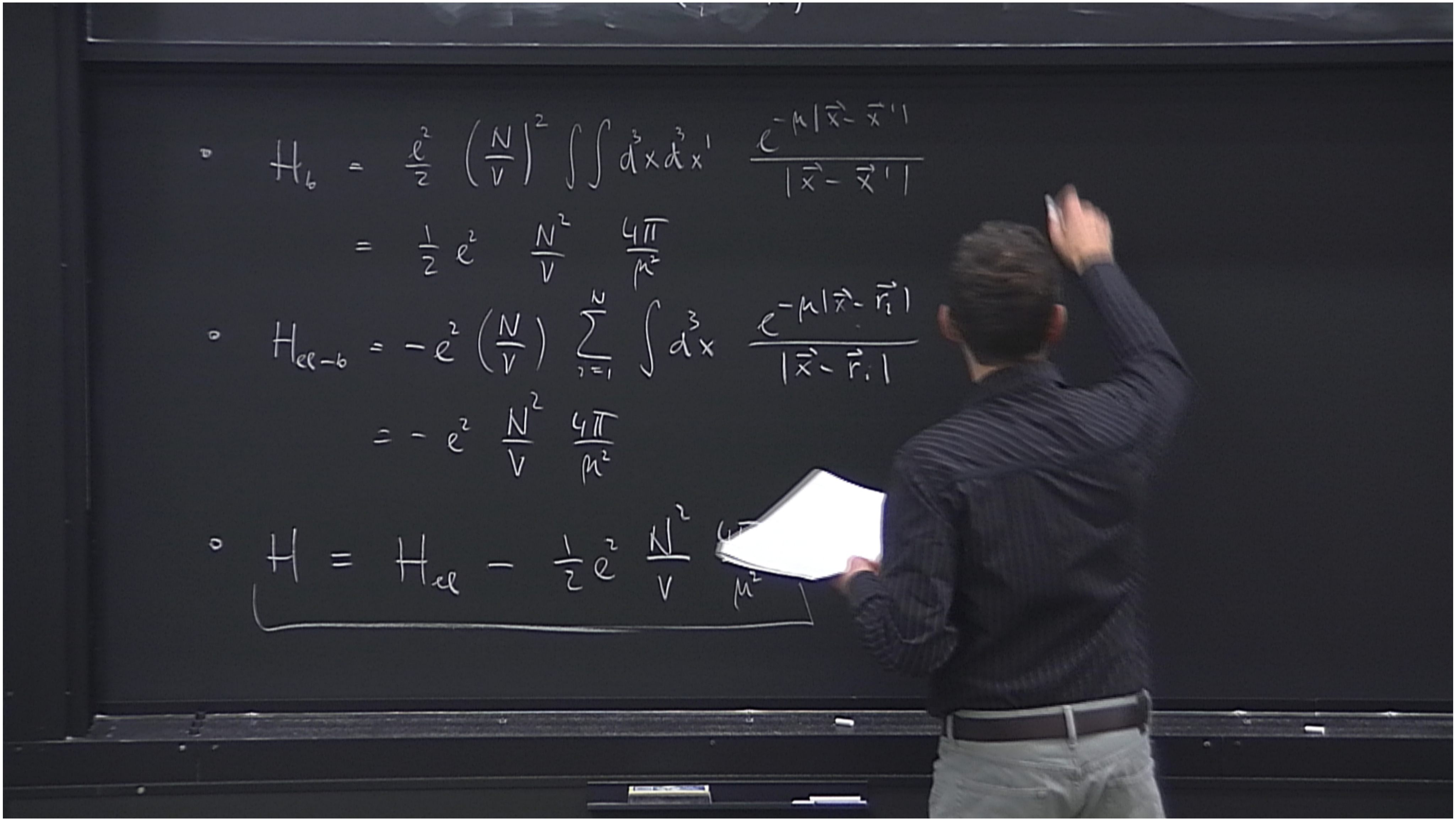
$$= \frac{1}{2} e^2 \, \frac{N^2}{V} \, \frac{4\pi}{\mu^2}$$

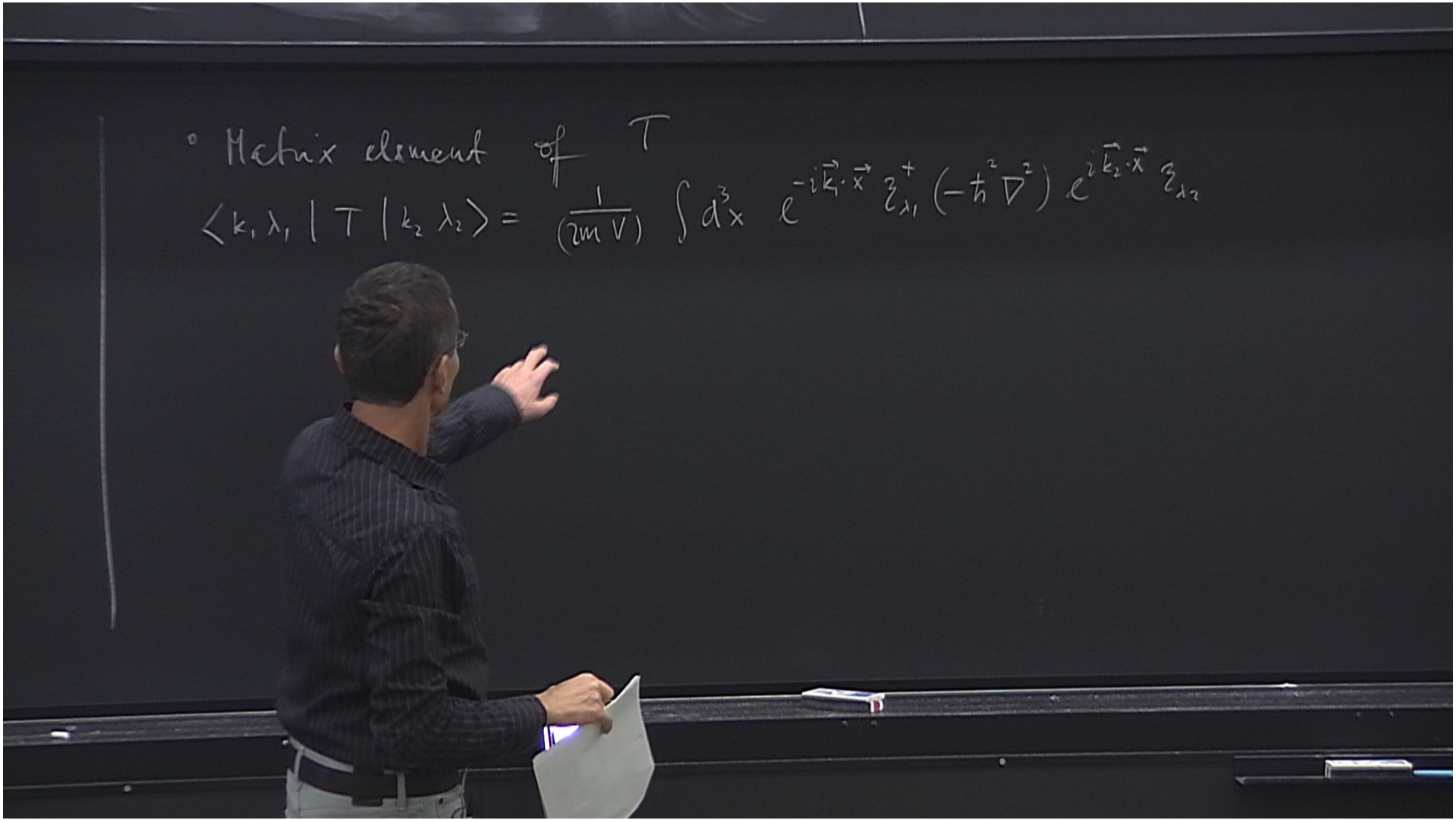
$$\ldots_b = -e^2 \left(\frac{N}{V}\right) \sum_{i=1}^{N} \int d^3x \, \frac{e^{-\mu|\vec{x}-\vec{r}_i|}}{|\vec{x}-\vec{r}_i|}$$

$$= -e^2 \, \frac{N^2}{V} \, \frac{4\pi}{\mu^2}$$

$$\ldots H_{ee} - \frac{1}{2} e^2 \, \frac{N^2}{V} \, \frac{4\pi}{\mu^2}$$


H_b = e^2/2 (N/V)^2 ∫∫ d^3x d^3x' e^{-μ|x - x'|} / |x - x'|
= 1/2 e^2 N^2/V 4π/μ^2
H_{el-b} = -e^2 ∫ d^3x e^{-μ|x - r_i|} / |x - r_i|
= - e^2
H =
N^2/V 4π/μ^2

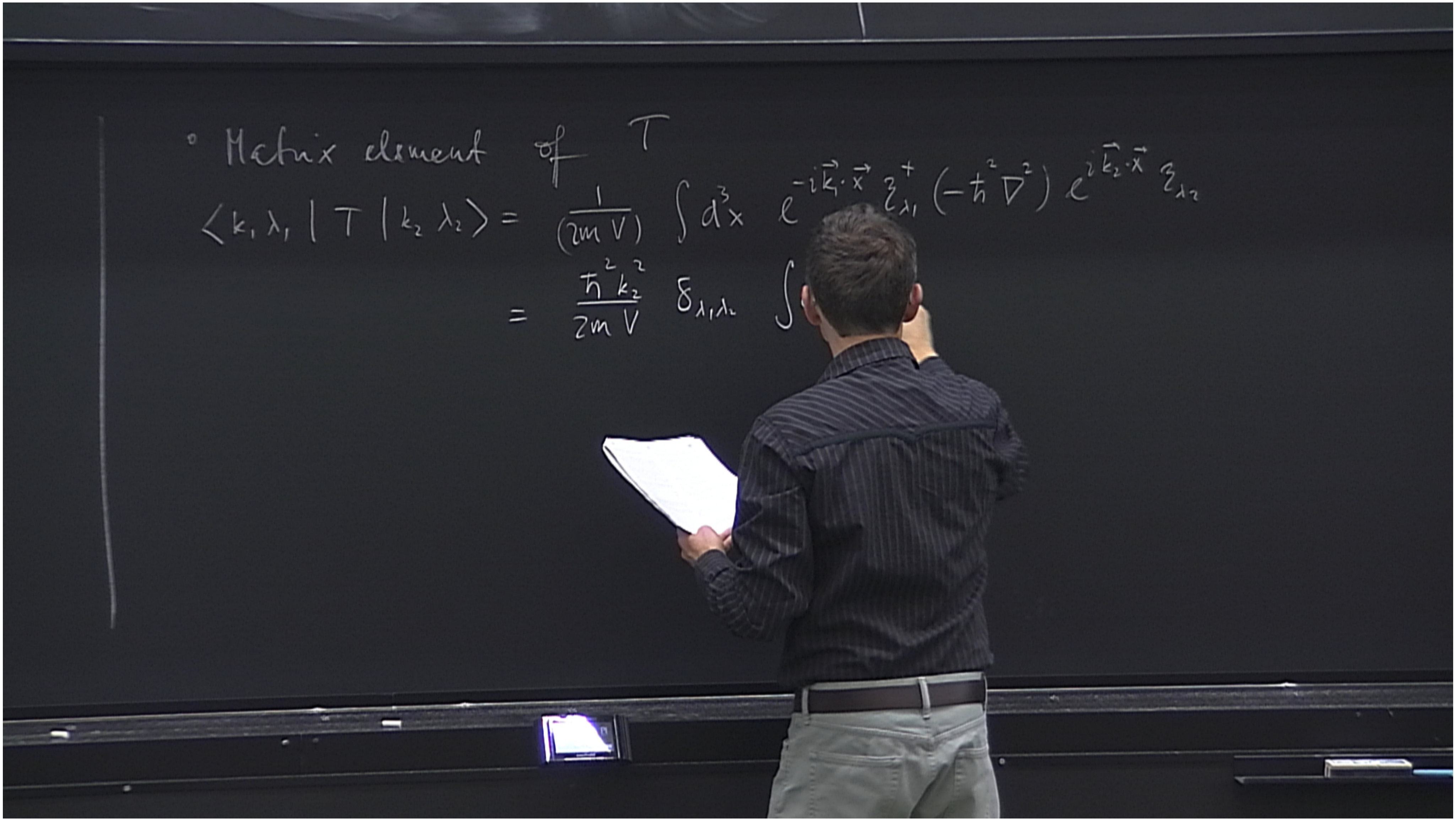

$H_b = \frac{e^2}{2} \left(\frac{N}{V}\right)^2 \iint d^3x\, d^3x' \frac{e^{-\mu|\vec{x}-\vec{x}'|}}{|\vec{x}-\vec{x}'|}$
$= \frac{1}{2} e^2 \frac{N^2}{V} \frac{4\pi}{\mu^2}$
$H_{el-b} = -e^2 \left(\frac{N}{V}\right) \sum_{i=1}^{N} \int d^3x \frac{e^{-\mu|\vec{x}-\vec{r}_i|}}{|\vec{x}-\vec{r}_i|}$
$= -e^2 \frac{N^2}{V} \frac{4\pi}{\mu^2}$
$H = H_{el} - \frac{1}{2} e^2 \frac{N^2}{V}$



• Matrix element of T
$\langle k_1 \lambda_1 | T | k_2 \lambda_2 \rangle = \frac{1}{(2mV)} \int d^3x \, e^{-i\vec{k}_1\cdot\vec{x}} \xi^{+}_{\lambda_1} (-\hbar^2 \nabla^2) e^{i\vec{k}_2\cdot\vec{x}} \xi_{\lambda_2}$

- Matrix element of T

$$\langle k_1 \lambda_1 | T | k_2 \lambda_2 \rangle = \frac{1}{(2mV)} \int d^3x \; e^{-i\vec{k}_1\cdot\vec{x}} \, \xi^{\dagger}_{\lambda_1} \left(-\hbar^2 \nabla^2\right) e^{i\vec{k}_2\cdot\vec{x}} \, \xi_{\lambda_2}$$


• Matrix element of T
$\langle k_1 \lambda_1 | T | k_2 \lambda_2 \rangle = \frac{1}{(2mV)} \int d^3x \, e^{-i\vec{k}_1\cdot\vec{x}} \xi^{+}_{\lambda_1} (-\hbar^2 \nabla^2) e^{i\vec{k}_2\cdot\vec{x}} \xi_{\lambda_2}$
$= \frac{\hbar^2 k_2^2}{2mV} \delta_{\lambda_1 \lambda_2} \int$

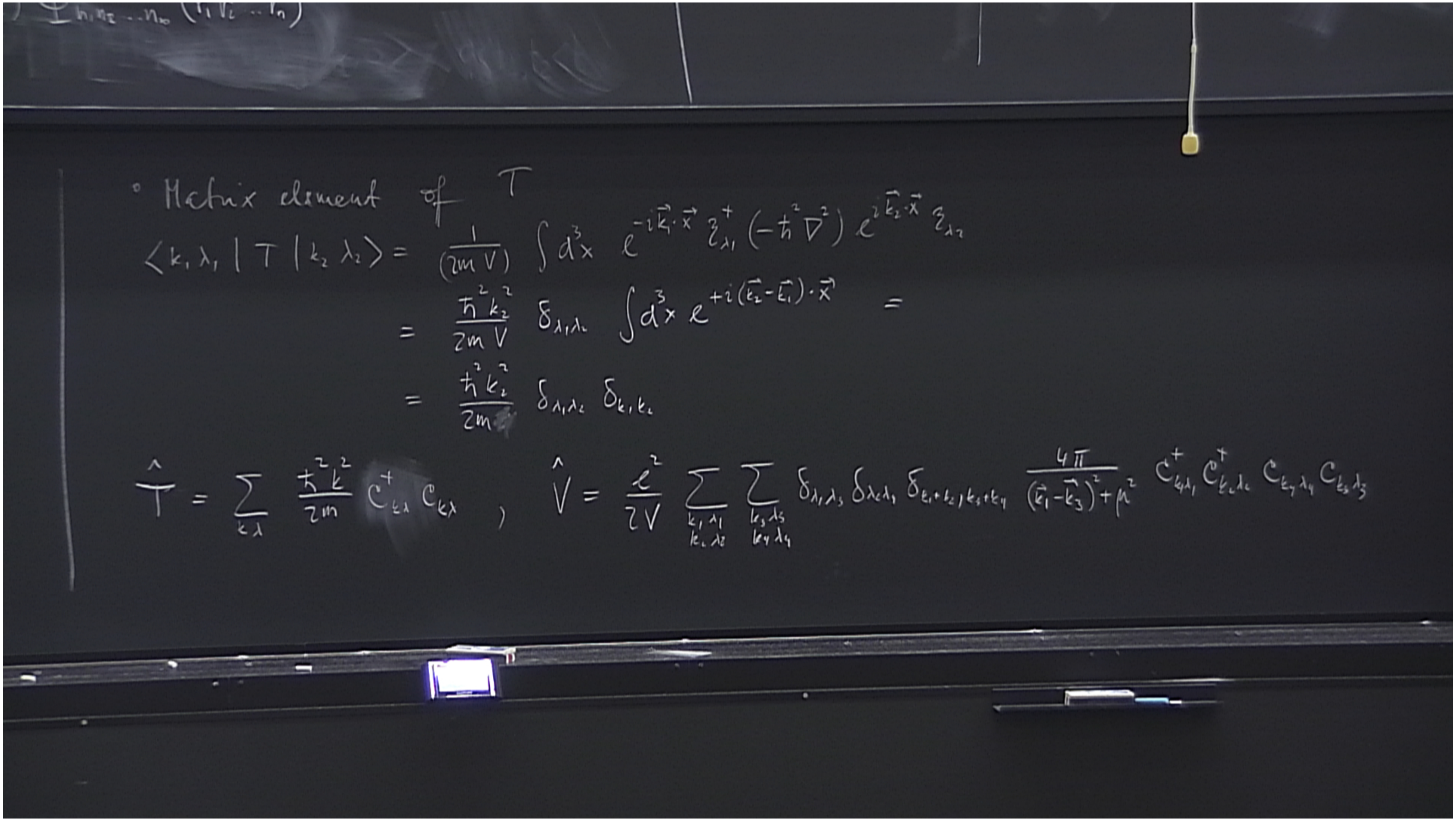
• Matrix element of T

$$\langle k_1 \lambda_1 | T | k_2 \lambda_2 \rangle = \frac{1}{(2mV)} \int d^3x \; e^{-i\vec{k}_1\cdot\vec{x}} \xi^+_{\lambda_1} \left(-\hbar^2 \nabla^2\right) e^{i\vec{k}_2\cdot\vec{x}} \xi_{\lambda_2}$$

$$= \frac{\hbar^2 k_2^2}{2mV} \delta_{\lambda_1\lambda_2} \int d^3x \, e^{+i(\vec{k}_2-\vec{k}_1)\cdot\vec{x}} =$$

$$= \frac{\hbar^2 k_2^2}{2m} \delta_{\lambda_1\lambda_2} \delta_{k_1 k_2}$$

$$\hat{T} = \sum_{k\lambda} \frac{\hbar^2 k^2}{2m} c^+_{k\lambda} c_{k\lambda} \; , \quad \hat{V} = \frac{e^2}{2V} \sum_{\substack{k_1\lambda_1 \\ k_2\lambda_2}} \sum_{\substack{k_3\lambda_3 \\ k_4\lambda_4}} \delta_{\lambda_1\lambda_3} \delta_{\lambda_2\lambda_4} \delta_{k_1+k_2, k_3+k_4} \frac{4\pi}{(\vec{k}_1-\vec{k}_3)^2+\mu^2}$$



$\Phi_{n_1 n_2 \ldots n_\infty}(r_1 r_2 \ldots r_n)$
• Matrix element of T
$\langle k_1 \lambda_1 | T | k_2 \lambda_2 \rangle = \frac{1}{(2mV)} \int d^3x \; e^{-i\vec{k}_1\cdot\vec{x}} \xi^\dagger_{\lambda_1} (-\hbar^2 \nabla^2) e^{i\vec{k}_2\cdot\vec{x}} \xi_{\lambda_2}$
$= \frac{\hbar^2 k_2^2}{2mV} \delta_{\lambda_1\lambda_2} \int d^3x \; e^{+i(\vec{k}_2-\vec{k}_1)\cdot\vec{x}} =$
$= \frac{\hbar^2 k_2^2}{2m} \delta_{\lambda_1\lambda_2} \delta_{k_1 k_2}$
$\hat{T} = \sum_{k\lambda} \frac{\hbar^2 k^2}{2m} c^\dagger_{k\lambda} c_{k\lambda}$, $\hat{V} = \frac{e^2}{2V} \sum_{\substack{k_1\lambda_1 \\ k_2\lambda_2}} \sum_{\substack{k_3\lambda_3 \\ k_4\lambda_4}} \delta_{\lambda_1\lambda_3} \delta_{\lambda_2\lambda_4} \delta_{k_1+k_2, k_3+k_4} \frac{4\pi}{(\vec{k}_1-\vec{k}_3)^2+\mu^2} c^\dagger_{k_1\lambda_1} c^\dagger_{k_2\lambda_2} c_{k_4\lambda_4} c_{k_3\lambda_3}$