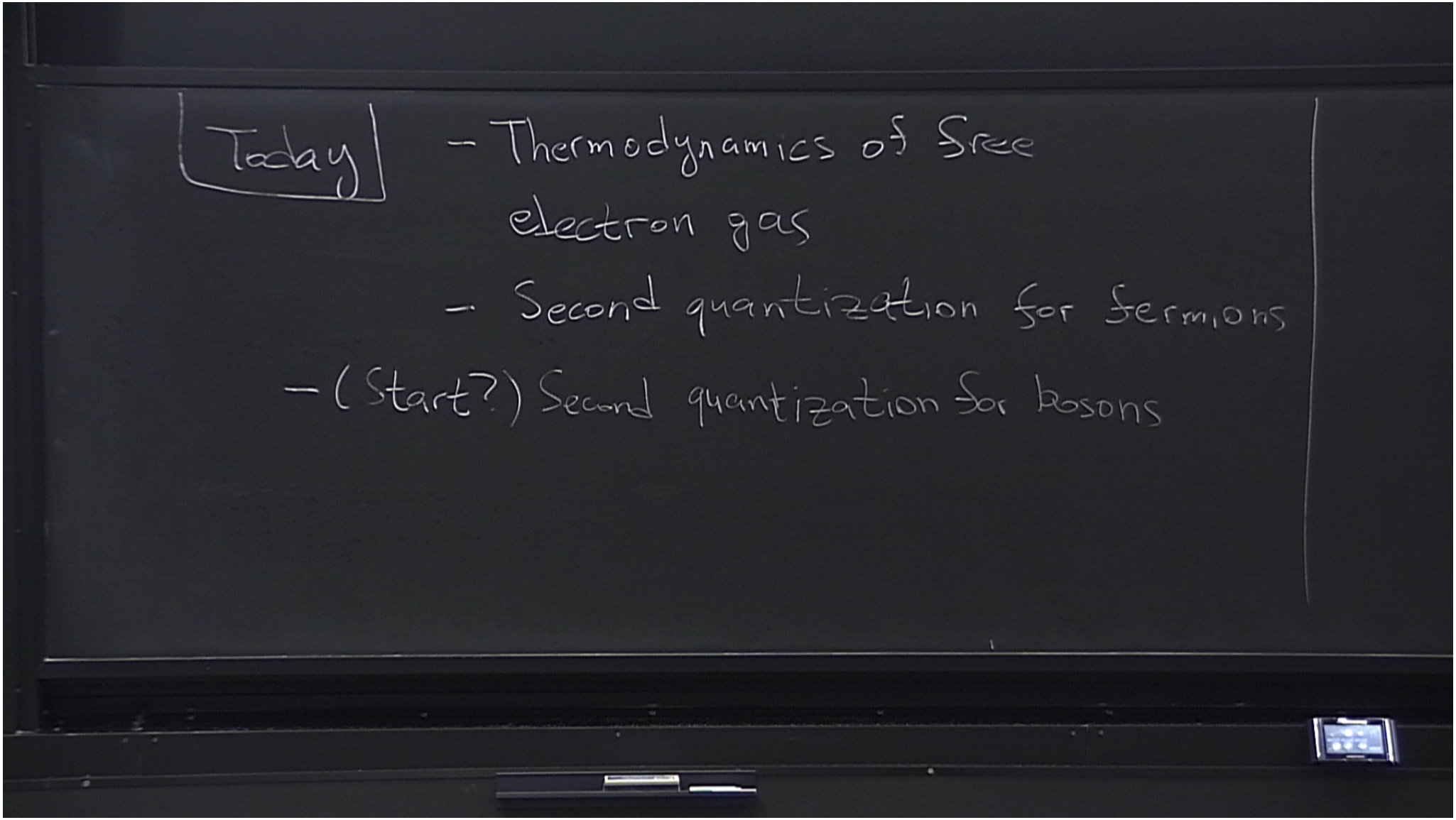
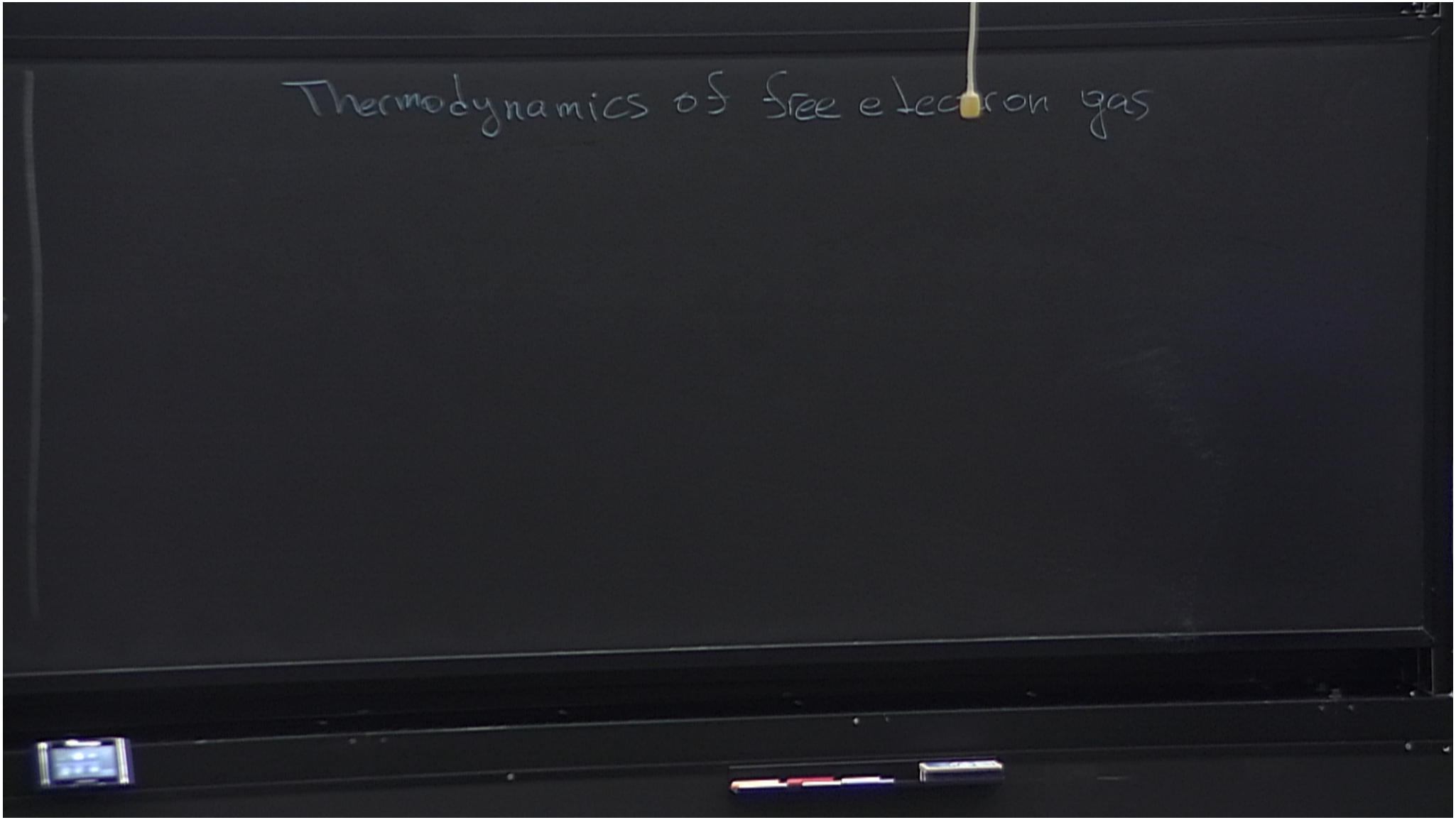
Title: Front End - Condensed Matter - 1

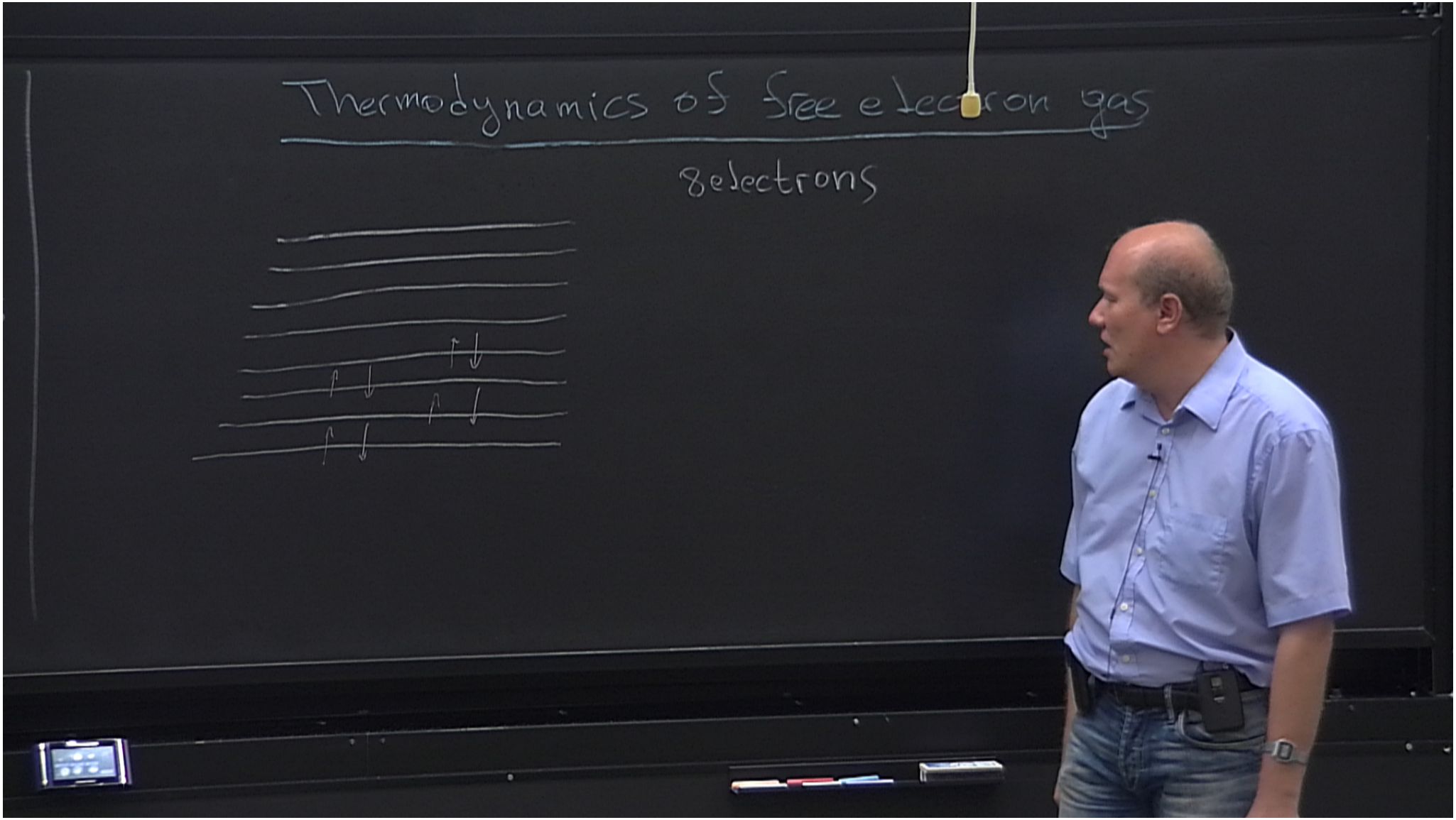
Date: Aug 30, 2016 10:30 AM

URL: http://pirsa.org/16080087

Abstract:

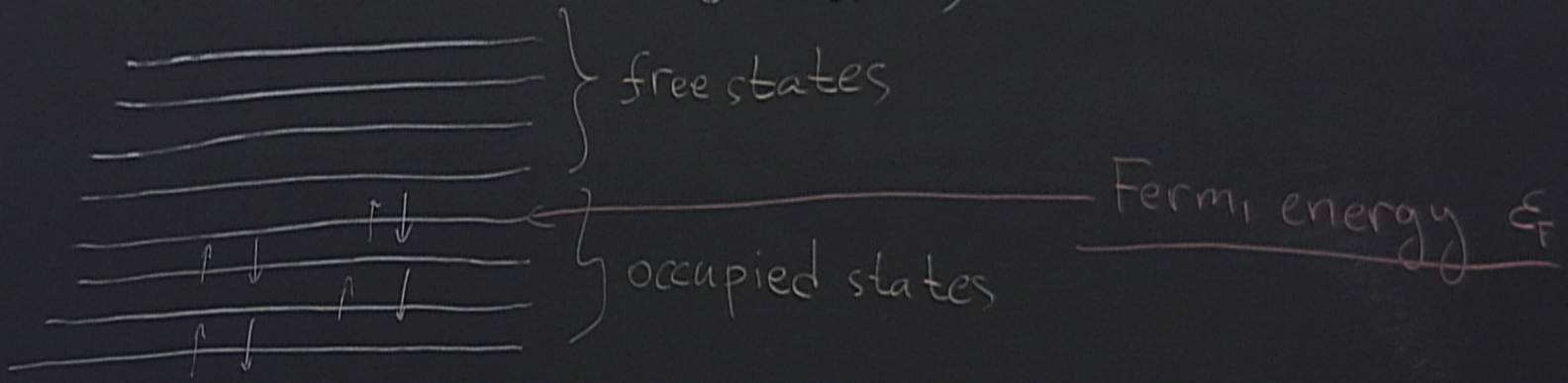

Today
- Thermodynamics of free electron gas
- Second quantization for fermions
- (Start?) Second quantization for bosons

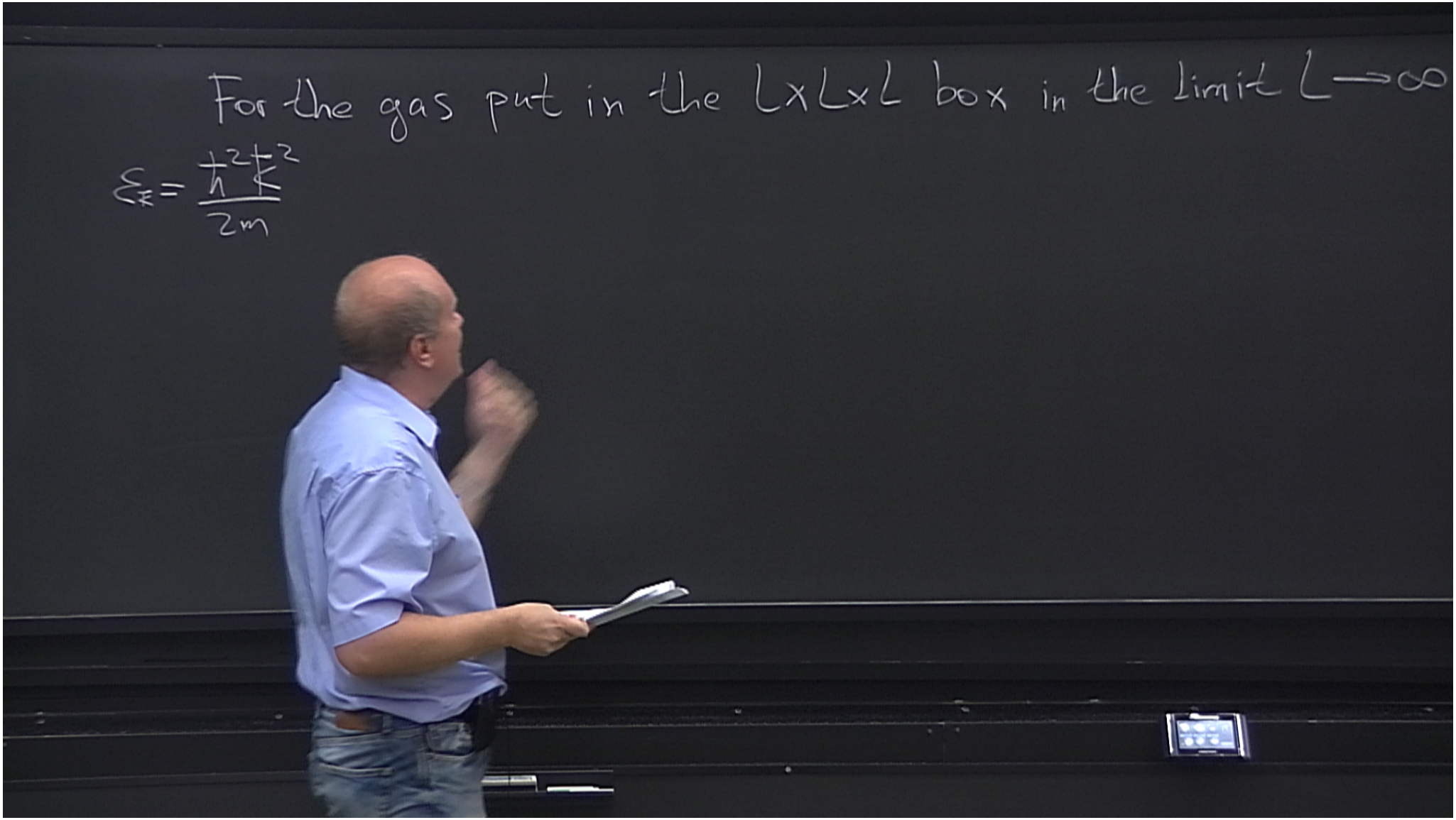

Thermodynamics of free electron gas


Thermodynamics of free electron gas
8 electrons

Thermodynamics of free electron gas

8 electrons

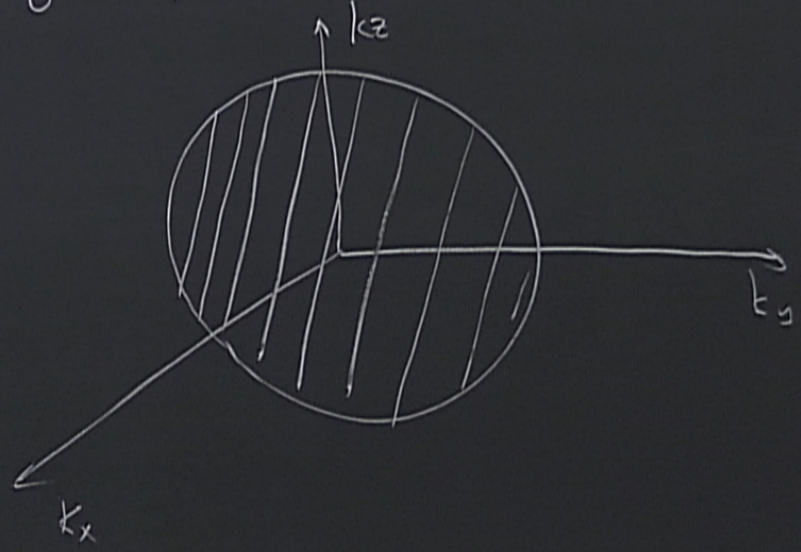



For the gas put in the L×L×L box in the limit L→∞
$\varepsilon_{\vec{k}} = \frac{\hbar^2 \vec{k}^2}{2m}$

For the gas put in the $L \times L \times L$ box in the limit $L \to \infty$

$$\varepsilon_{\vec{k}} = \frac{\hbar^2 \vec{k}^2}{2m}$$

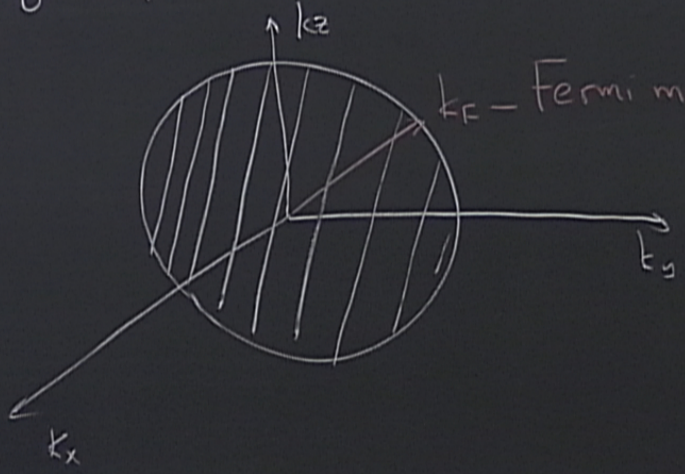
$|\vec{k}|$



For the gas put in the $L \times L \times L$ box in the limit $L \to \infty$

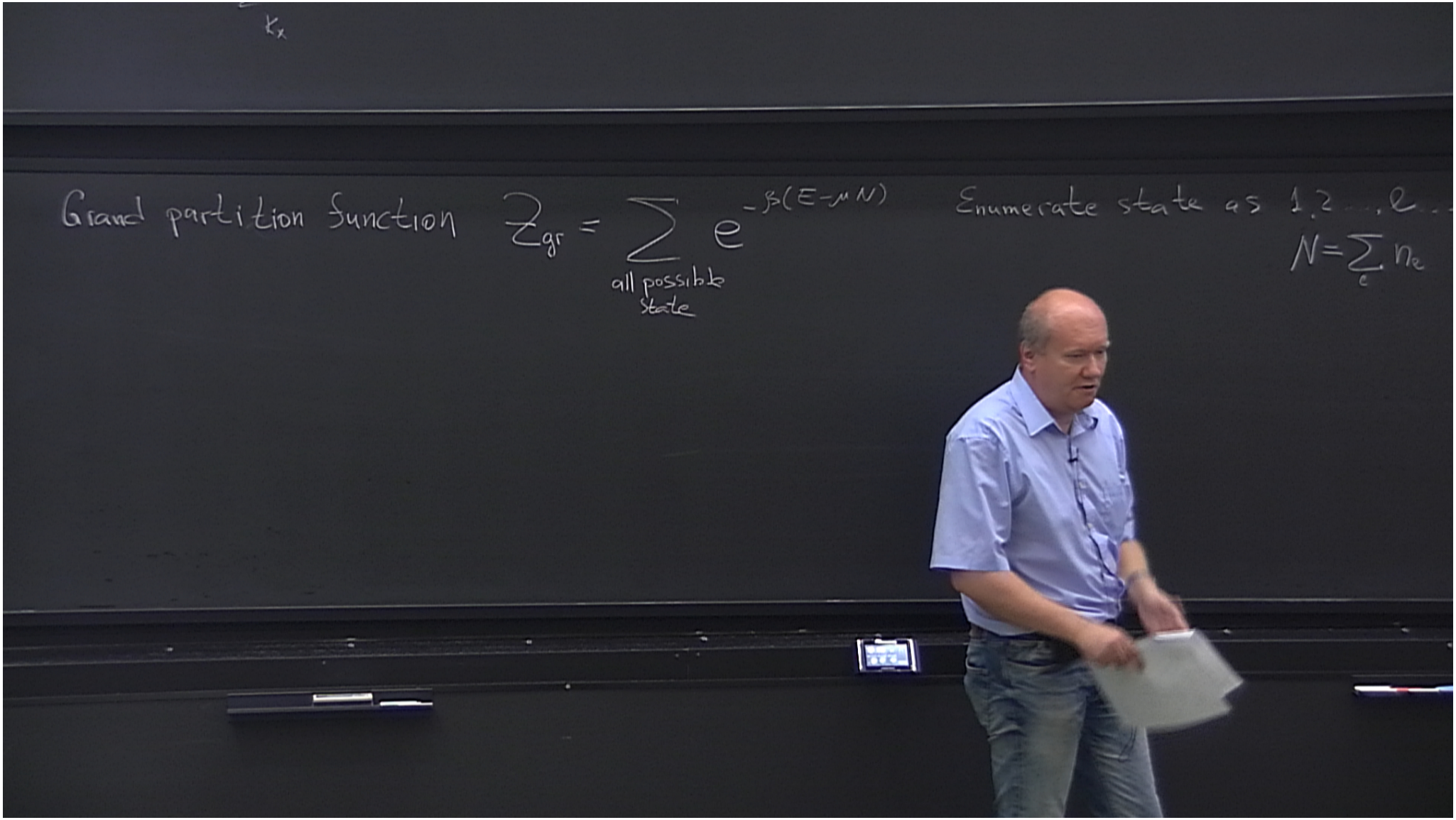
$$\varepsilon_{\vec{k}} = \frac{\hbar^2 \vec{k}^2}{2m}$$

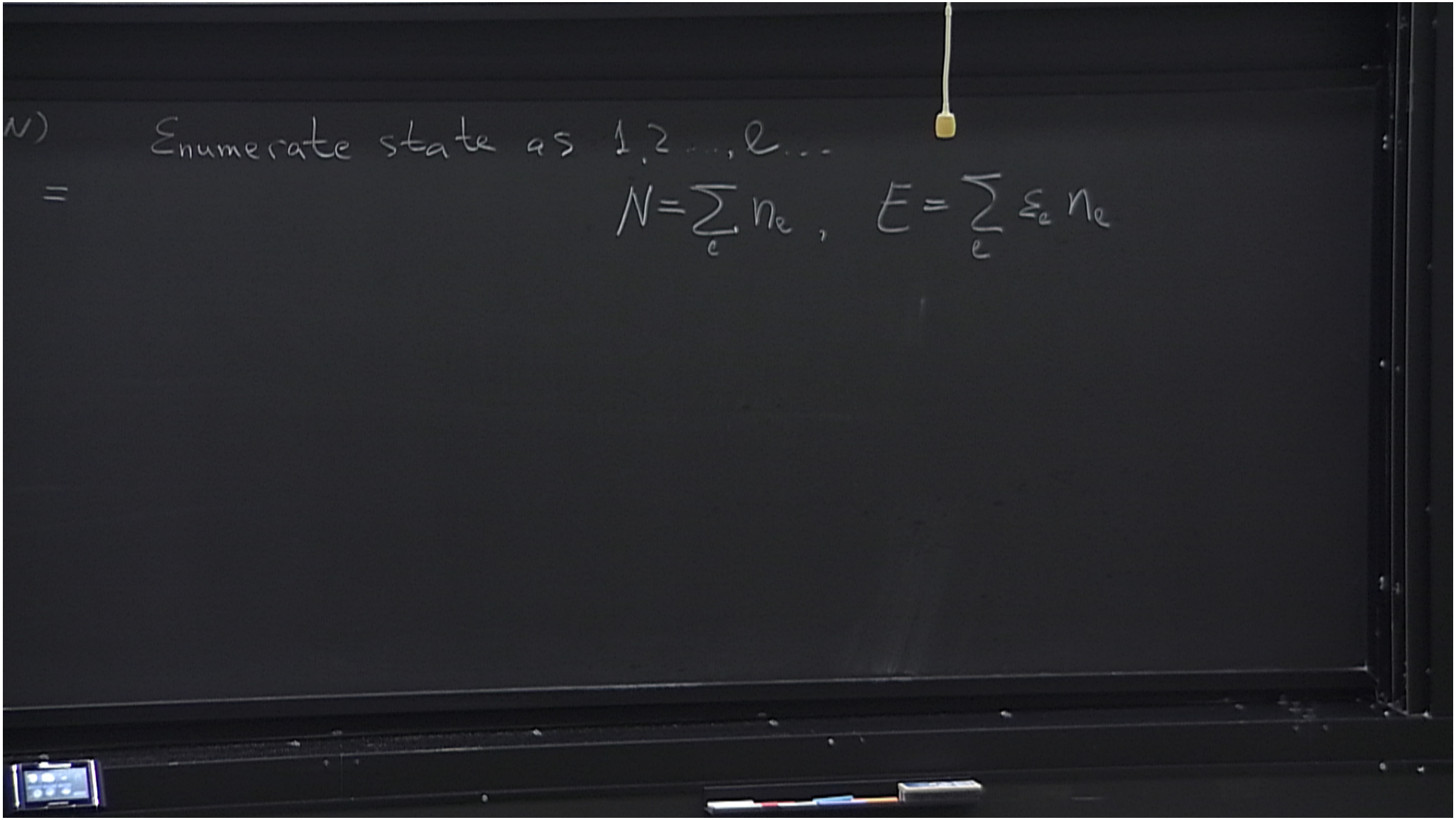
$|\vec{k}|$



$|\vec{k}| < k_F$ – states are occupied

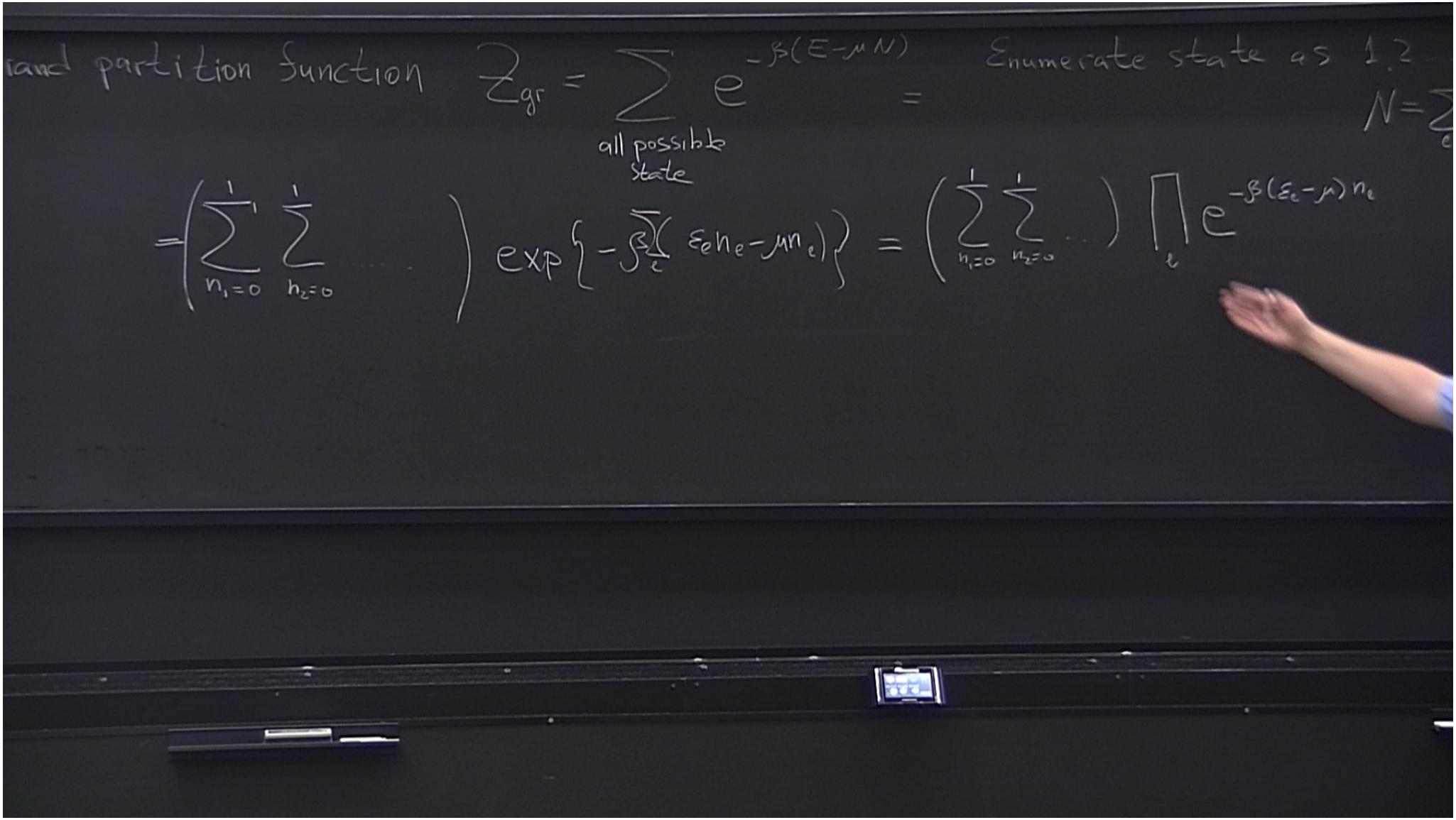
$$\varepsilon_F = \frac{\hbar^2 k_F^2}{2m}$$ – Fermi energy

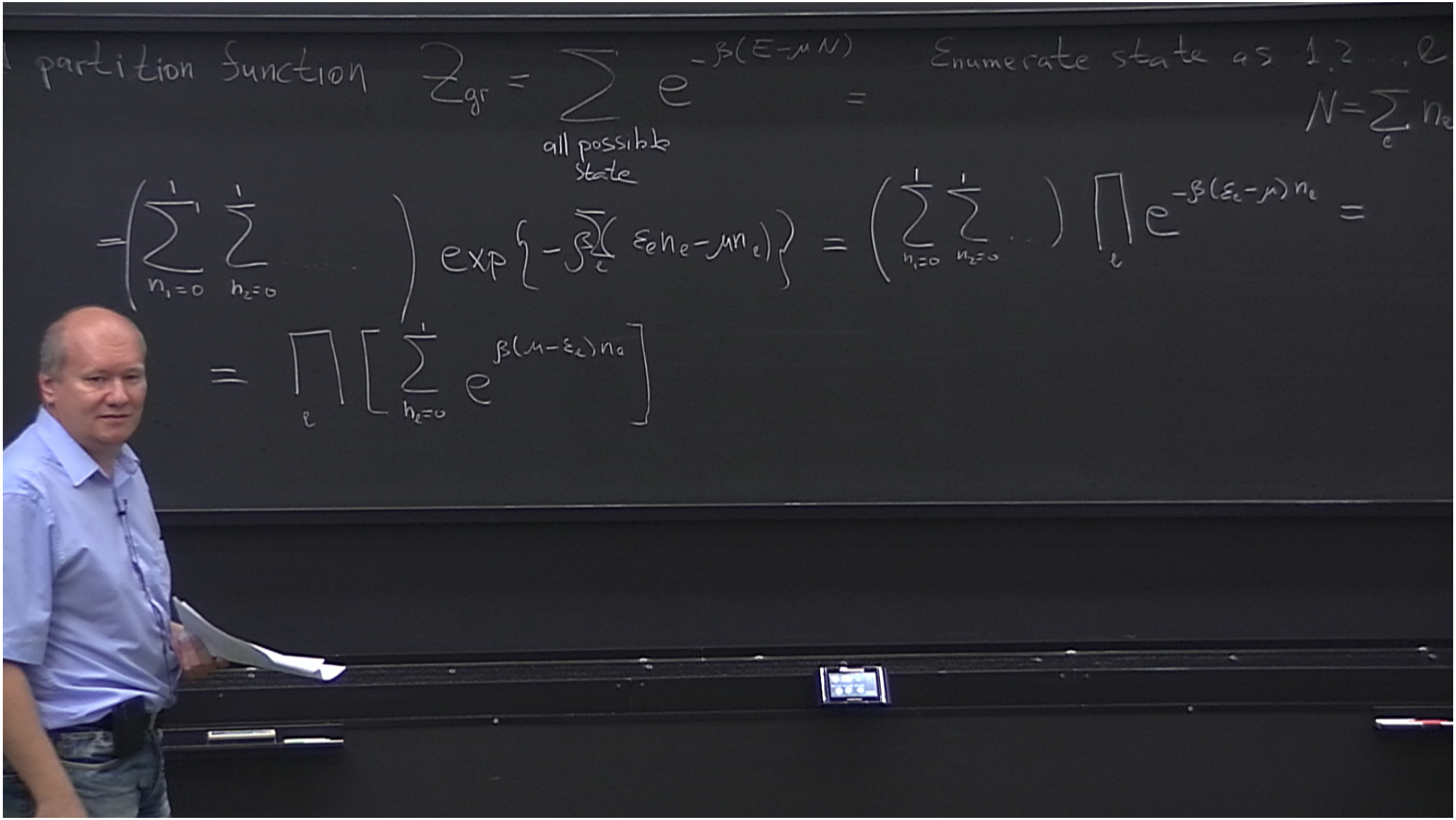

k_x
Grand partition function $Z_{gr} = \sum_{\text{all possible state}} e^{-\beta(E-\mu N)}$
Enumerate state as 1, 2, ..., ℓ, ...
$N = \sum_{\ell} n_\ell$

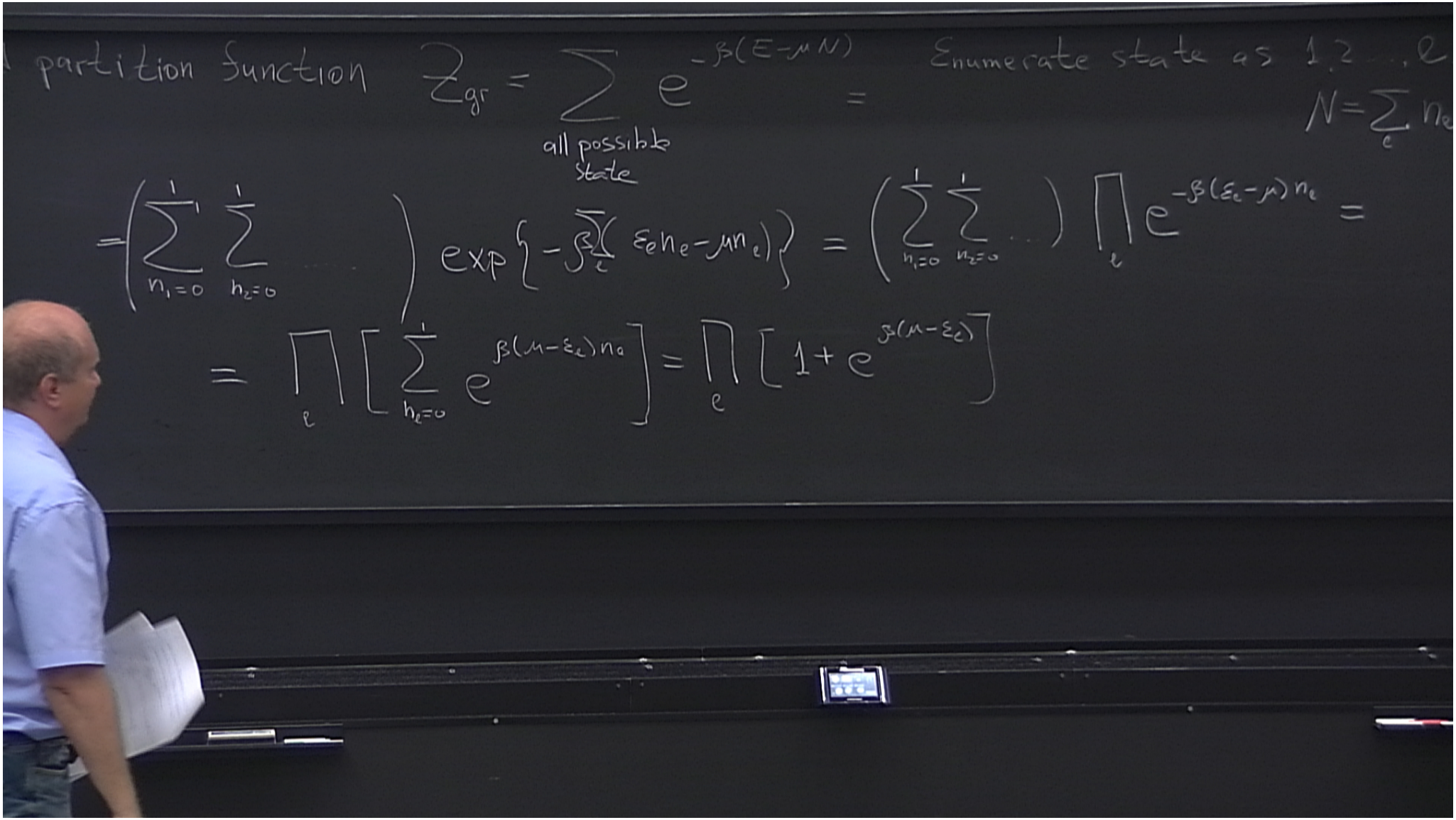

N)
Enumerate state as 1, 2 ..., ℓ ...
=
$N = \sum_\ell n_\ell$, $E = \sum_\ell \varepsilon_\ell n_\ell$

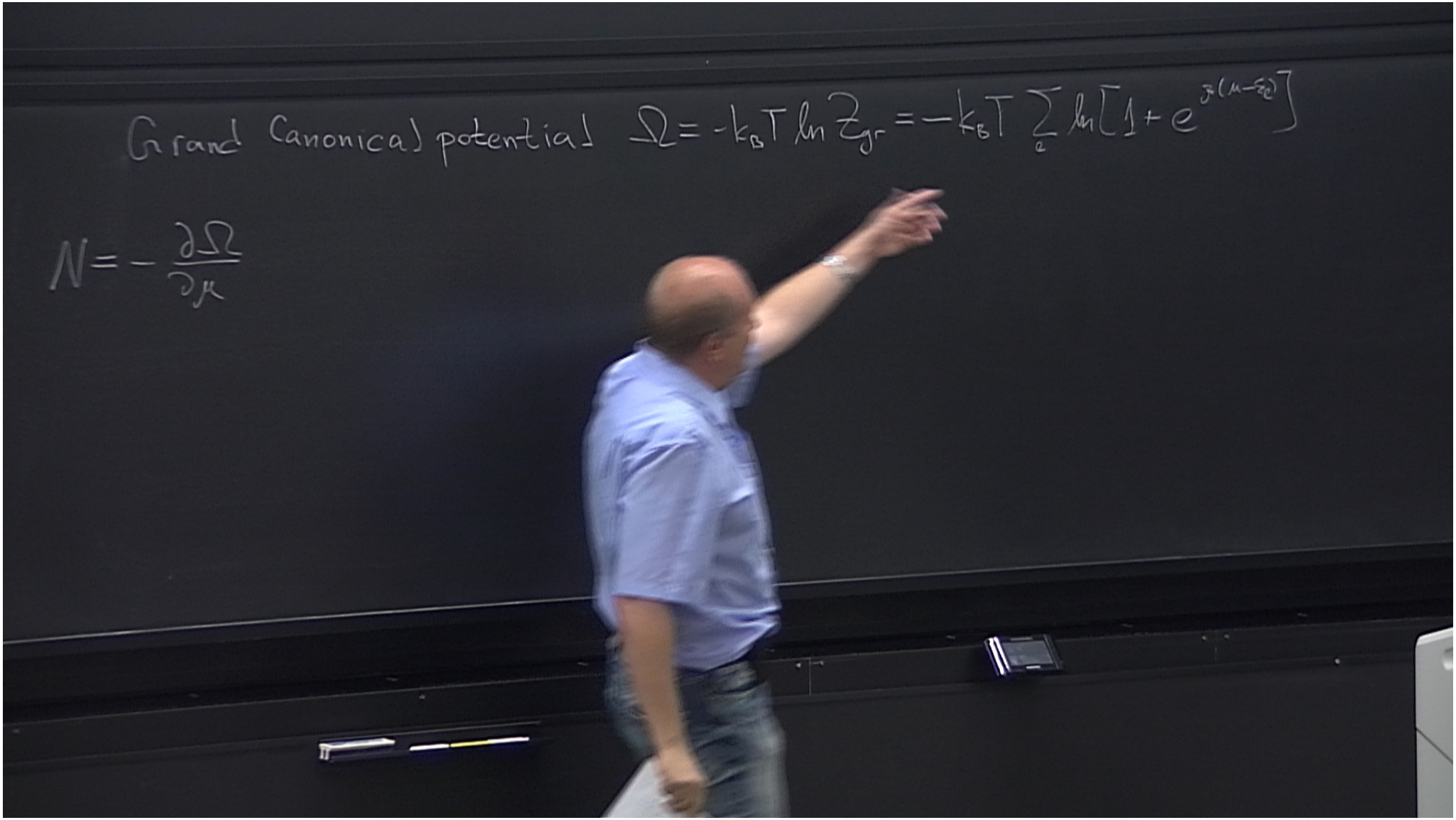
Grand partition function $Z_{gr} = \sum_{\text{all possible state}} e^{-\beta(E-\mu N)} =$

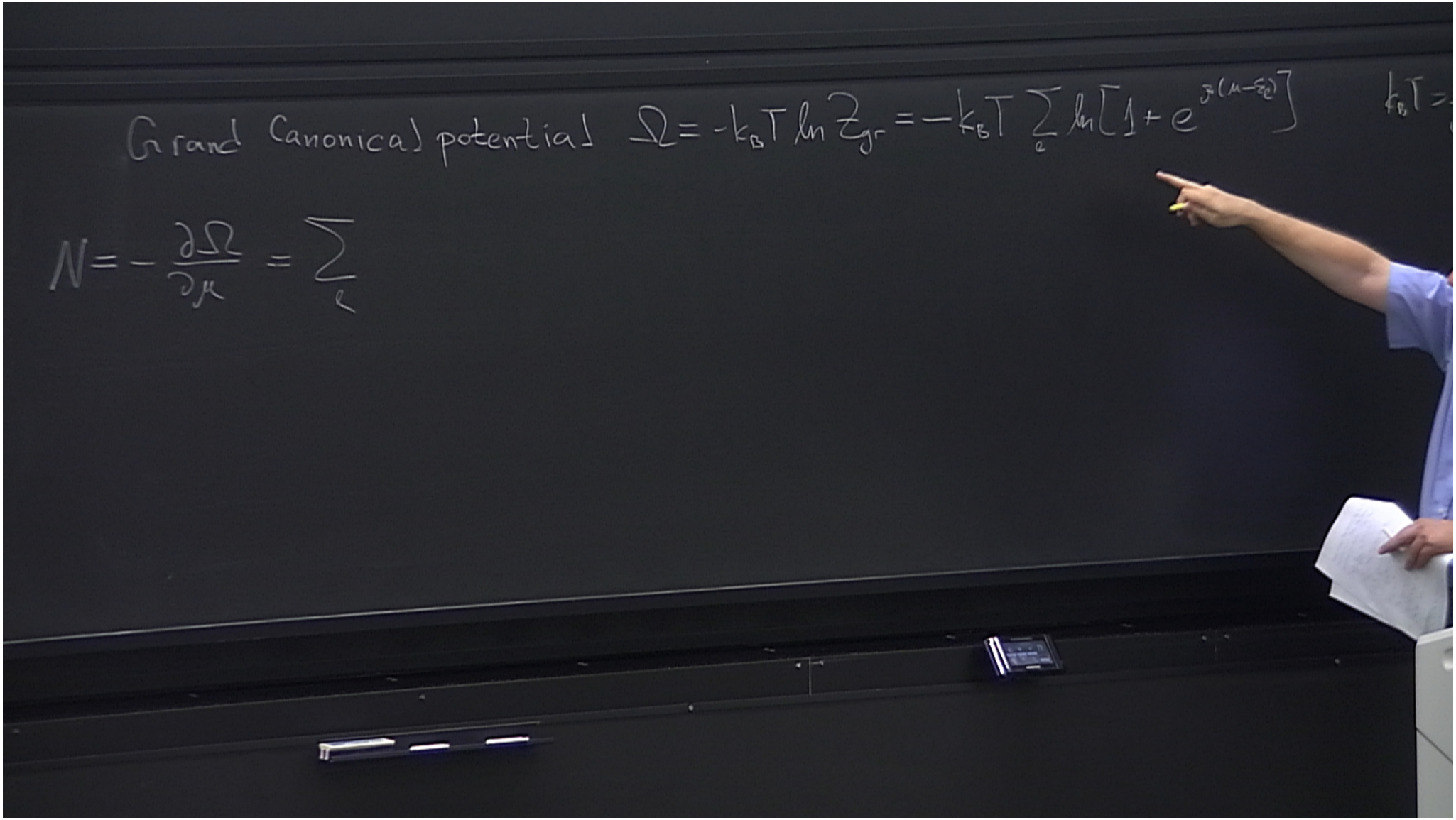
$$= \left(\sum_{n_1=0}^{1} \sum_{n_2=0}^{1} \cdots \right) \exp\left\{-\beta(\varepsilon_e n_e - \mu n_e)\right\}$$


and partition function $Z_{gr} = \sum_{\text{all possible state}} e^{-\beta(E-\mu N)}$
Enumerate state as 1, 2
$N = \sum$
$= \left(\sum_{n_1=0}^{1} \sum_{n_2=0}^{1} \cdots \right) \exp\left\{ -\beta \sum_i (\varepsilon_i n_i - \mu n_i) \right\} = \left(\sum_{n_1=0}^{1} \sum_{n_2=0}^{1} \cdots \right) \prod_i e^{-\beta(\varepsilon_i - \mu) n_i}$


partition function $Z_{gr} = \sum_{\text{all possible state}} e^{-\beta(E-\mu N)}$
Enumerate state as 1, 2, ..., ℓ
$N = \sum_\ell n_\ell$
$= \left(\sum_{n_1=0}^{1} \sum_{n_2=0}^{1} \cdots \right) \exp\left\{ -\beta \sum_\ell (\varepsilon_\ell n_\ell - \mu n_\ell) \right\} = \left(\sum_{n_1=0}^{1} \sum_{n_2=0}^{1} \cdots \right) \prod_\ell e^{-\beta(\varepsilon_\ell - \mu) n_\ell} =$
$= \prod_\ell \left[\sum_{n_\ell=0}^{1} e^{\beta(\mu-\varepsilon_\ell) n_\ell} \right]$

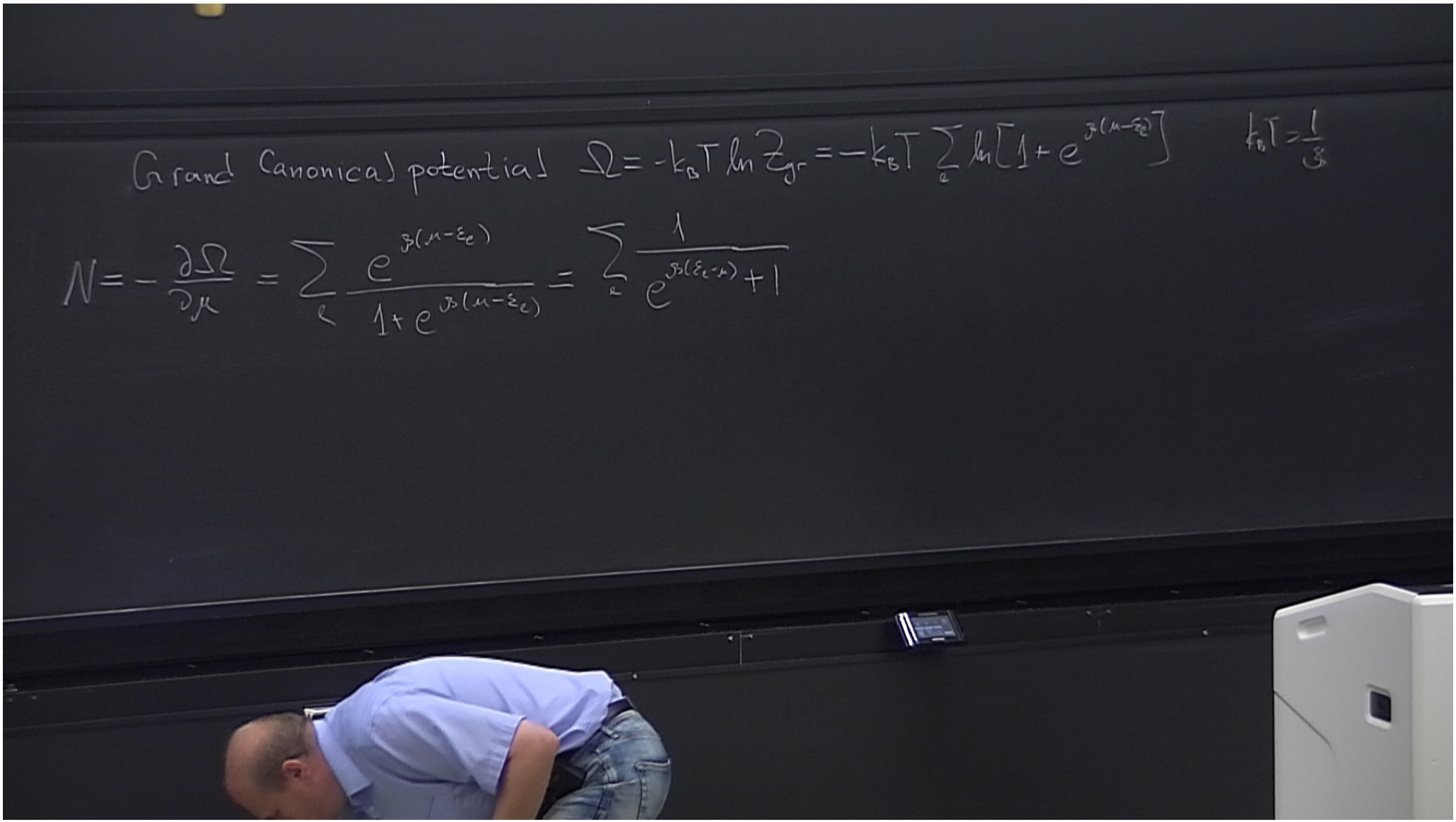

partition function $Z_{gr} = \sum_{\text{all possible state}} e^{-\beta(E-\mu N)}$
Enumerate state as 1, 2, ..., e
$N = \sum_e n_e$
$= \left(\sum_{n_1=0}^{1} \sum_{n_2=0}^{1} \dots \right) \exp\left\{ -\beta \sum_e (\varepsilon_e n_e - \mu n_e) \right\} = \left(\sum_{n_1=0}^{1} \sum_{n_2=0}^{1} \dots \right) \prod_e e^{-\beta(\varepsilon_e - \mu) n_e} =$
$= \prod_e \left[\sum_{n_e=0}^{1} e^{\beta(\mu-\varepsilon_e) n_e} \right] = \prod_e \left[1 + e^{\beta(\mu-\varepsilon_e)} \right]$

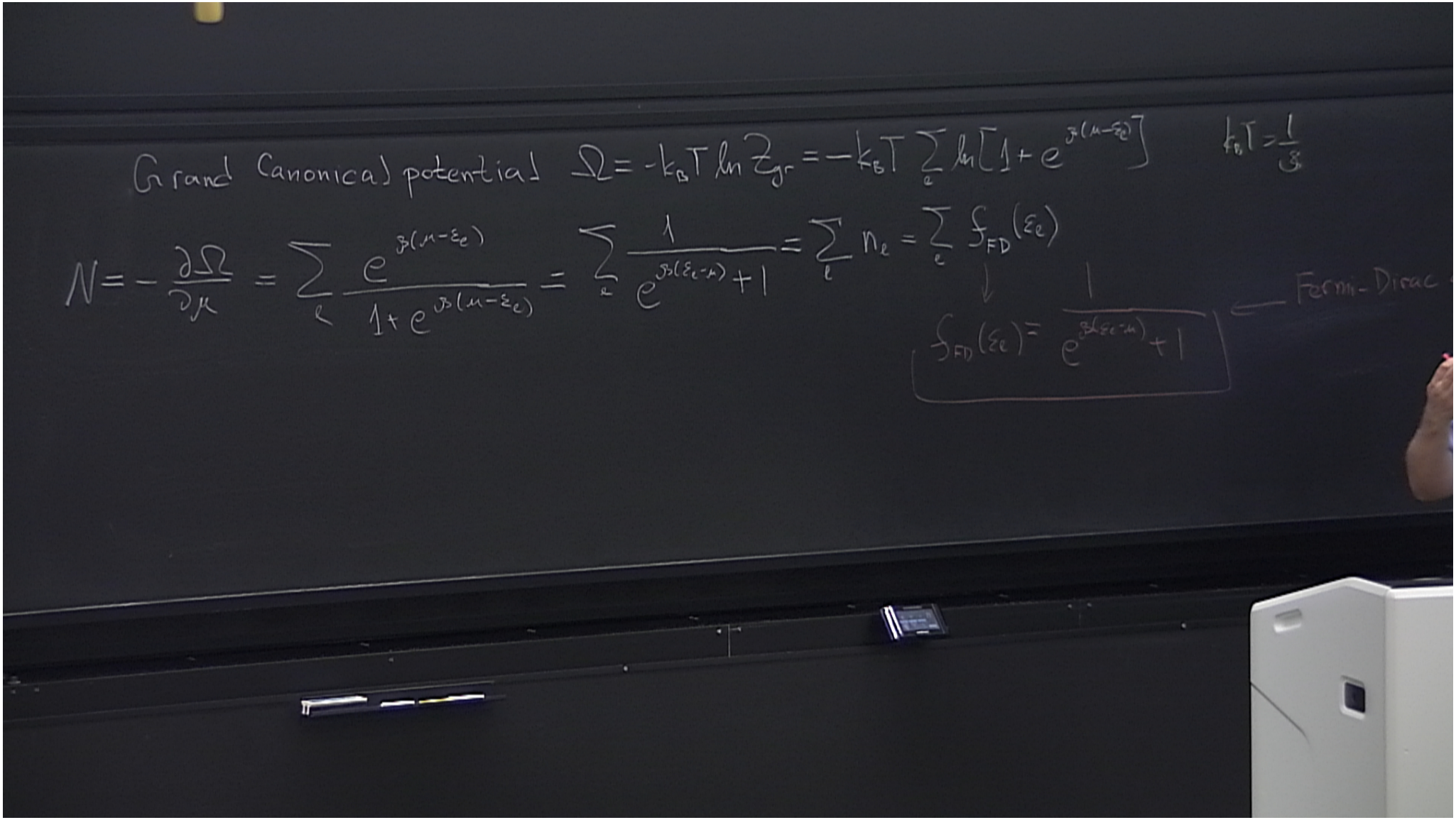

Grand Canonical potential $\Omega = -k_B T \ln Z_{gr} = -k_B T \sum_a \ln\left[1 + e^{\beta(\mu - \varepsilon_a)}\right]$
$N = -\frac{\partial \Omega}{\partial \mu}$

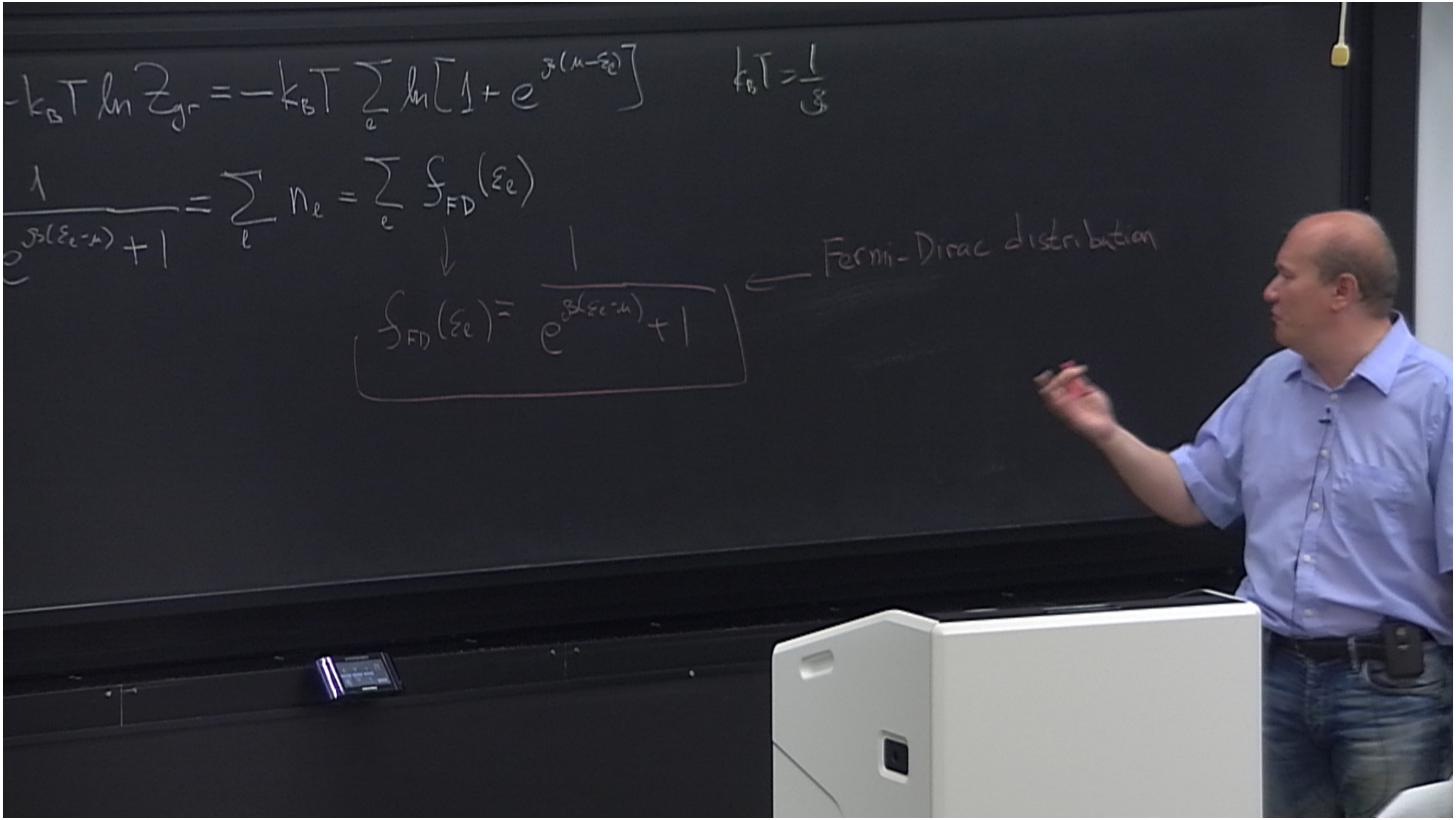

Grand Canonical potential $\Omega = -k_B T \ln Z_{gr} = -k_B T \sum_k \ln\left[1 + e^{\beta(\mu - \varepsilon_k)}\right]$
$N = -\frac{\partial \Omega}{\partial \mu} = \sum_k$

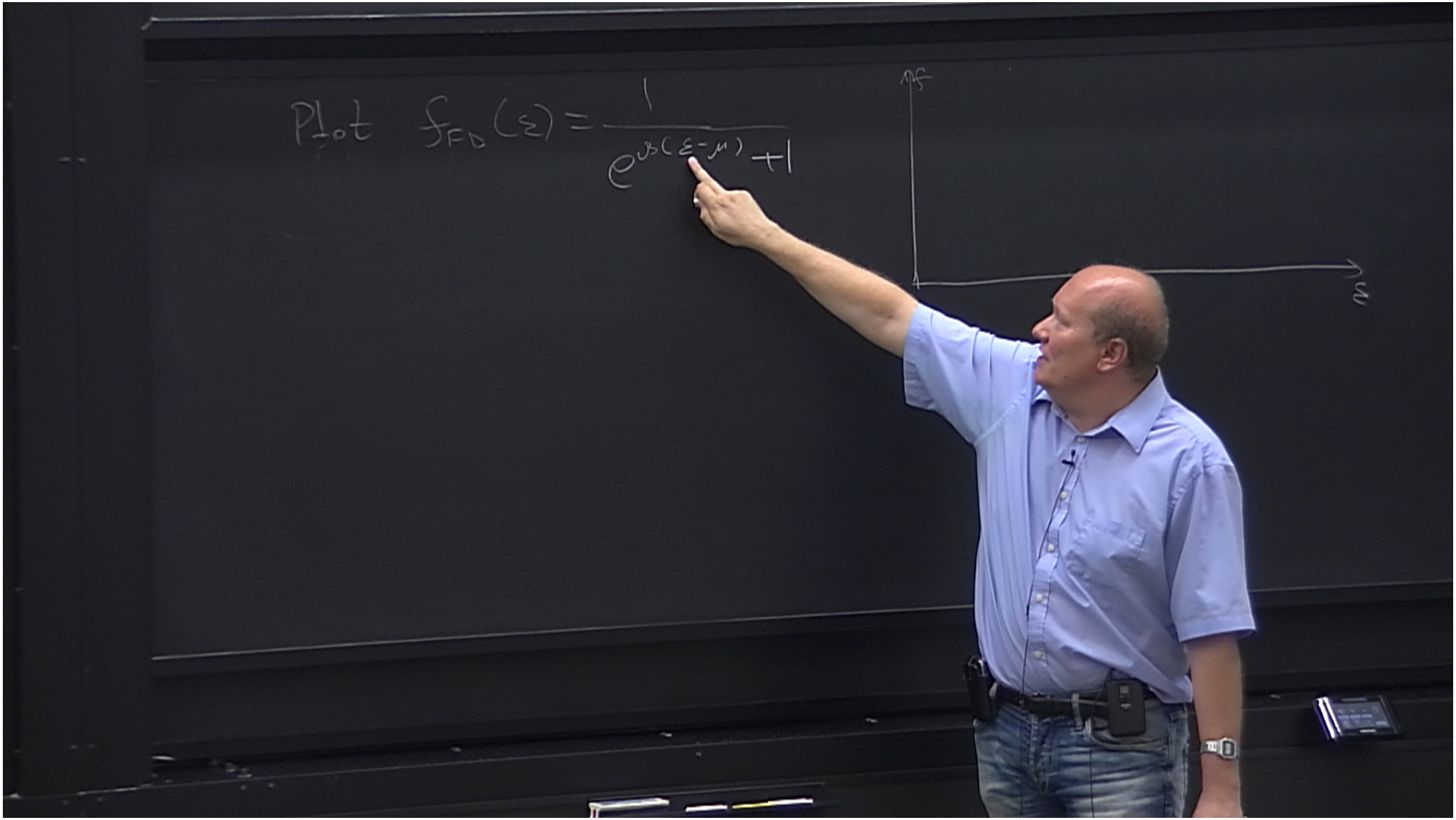
Grand Canonical potential $\Omega = -k_B T \ln Z_{gr} = -k_B T \sum_\epsilon \ln\left[1 + e^{\beta(\mu-\epsilon)}\right]$ $\quad k_B T = \frac{1}{\beta}$

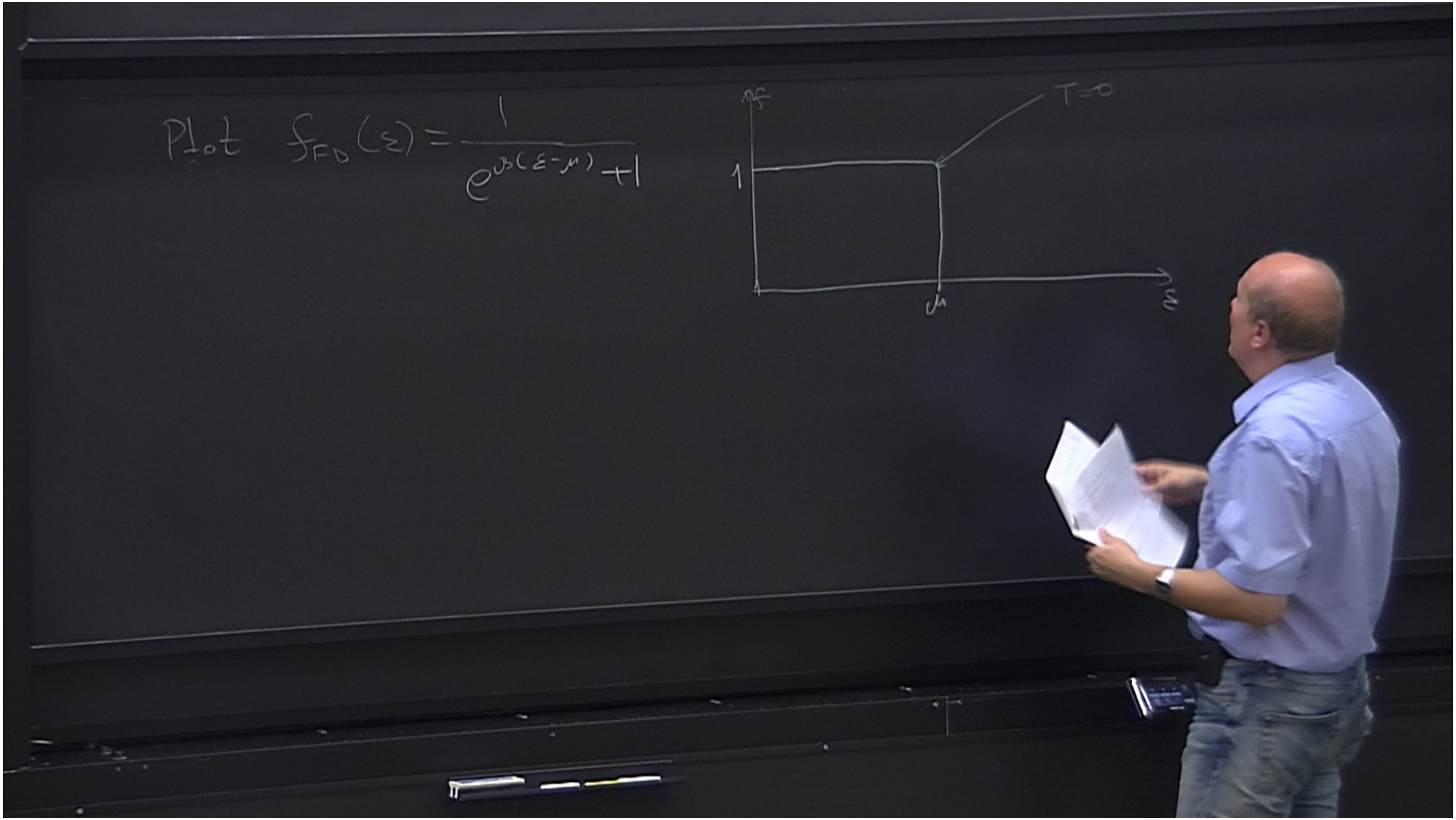
$$N = -\frac{\partial \Omega}{\partial \mu} = \sum_\epsilon \frac{e^{\beta(\mu-\epsilon)}}{1+e^{\beta(\mu-\epsilon)}} = \sum_\epsilon \frac{1}{e^{\beta(\epsilon-\mu)}+1}$$

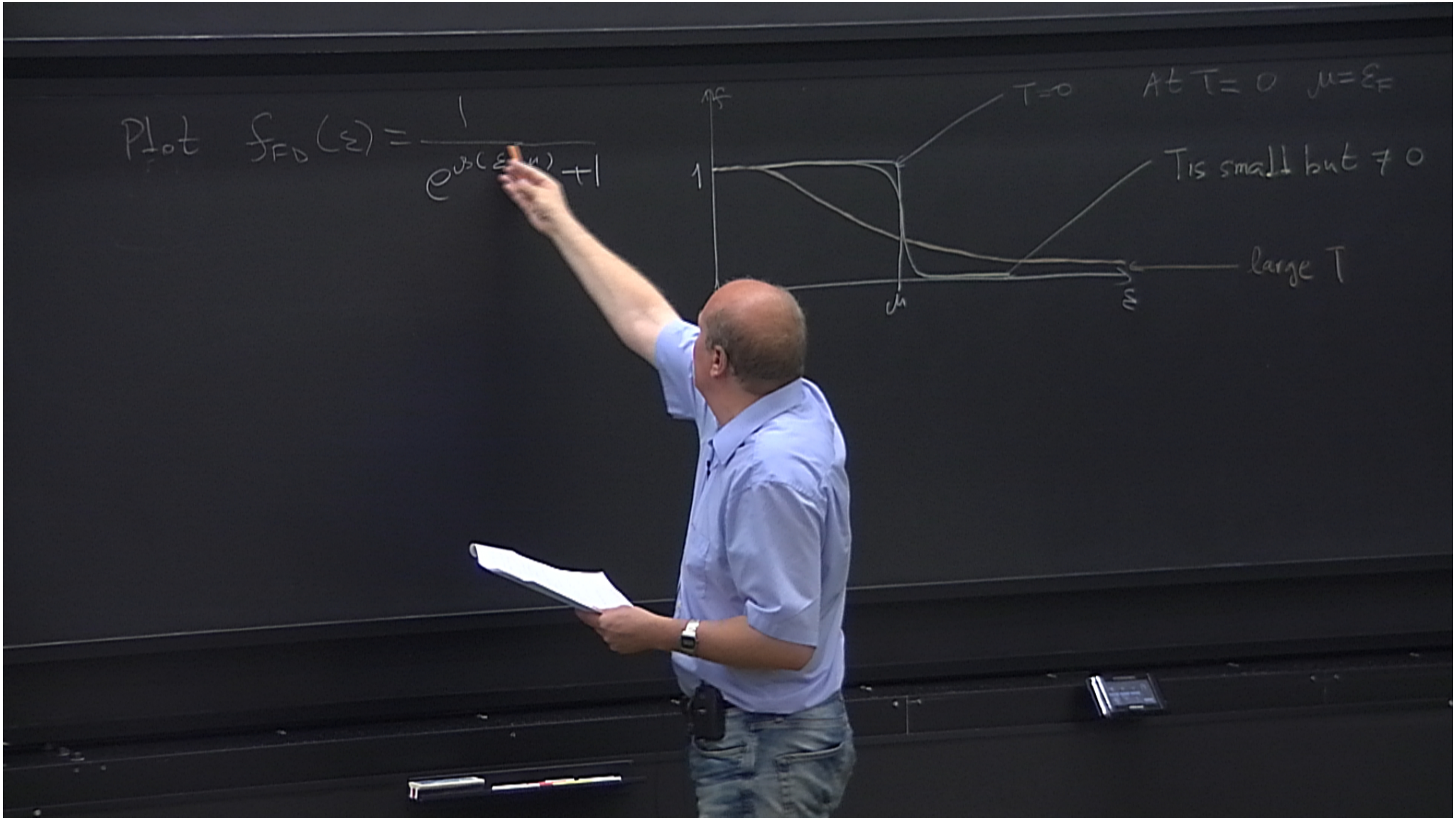



Grand Canonical potential $\Omega = -k_B T \ln Z_{gr} = -k_B T \sum_\ell \ln\left[1 + e^{\beta(\mu-\varepsilon_\ell)}\right]$ $k_B T = \frac{1}{\beta}$
$N = -\frac{\partial \Omega}{\partial \mu} = \sum_\ell \frac{e^{\beta(\mu-\varepsilon_\ell)}}{1+e^{\beta(\mu-\varepsilon_\ell)}} = \sum_\ell \frac{1}{e^{\beta(\varepsilon_\ell-\mu)}+1} = \sum_\ell n_\ell = \sum_\ell f_{FD}(\varepsilon_\ell)$
$f_{FD}(\varepsilon_\ell) = \frac{1}{e^{\beta(\varepsilon_\ell-\mu)}+1}$
Fermi-Dirac

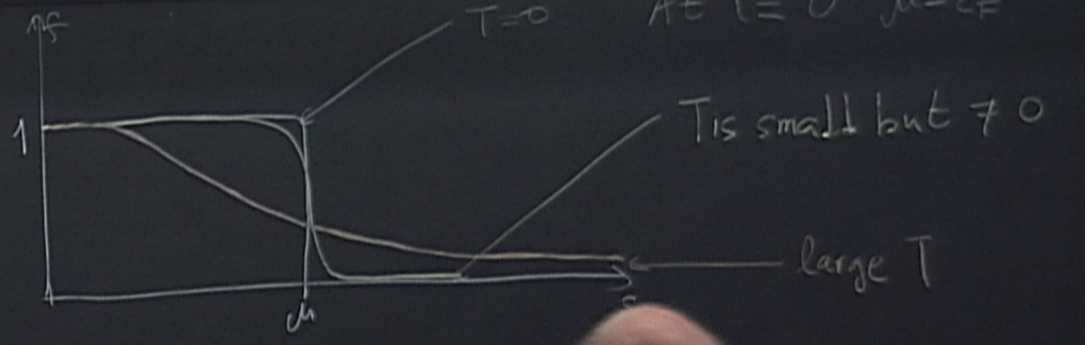

$-k_B T \ln Z_{gr} = -k_B T \sum_\ell \ln\left[1 + e^{\beta(\mu-\varepsilon_\ell)}\right]$
$k_B T = \frac{1}{\beta}$
$\frac{1}{e^{\beta(\varepsilon_\ell-\mu)}+1} = \sum_\ell n_\ell = \sum_\ell f_{FD}(\varepsilon_\ell)$
$f_{FD}(\varepsilon_\ell) = \frac{1}{e^{\beta(\varepsilon_\ell-\mu)}+1}$
← Fermi-Dirac distribution


Plot $f_{FD}(\varepsilon) = \frac{1}{e^{\beta(\varepsilon-\mu)}+1}$
f_{FD}
ε


Plot $f_{FD}(\varepsilon) = \frac{1}{e^{\beta(\varepsilon-\mu)}+1}$
f
T=0
1
μ
ε

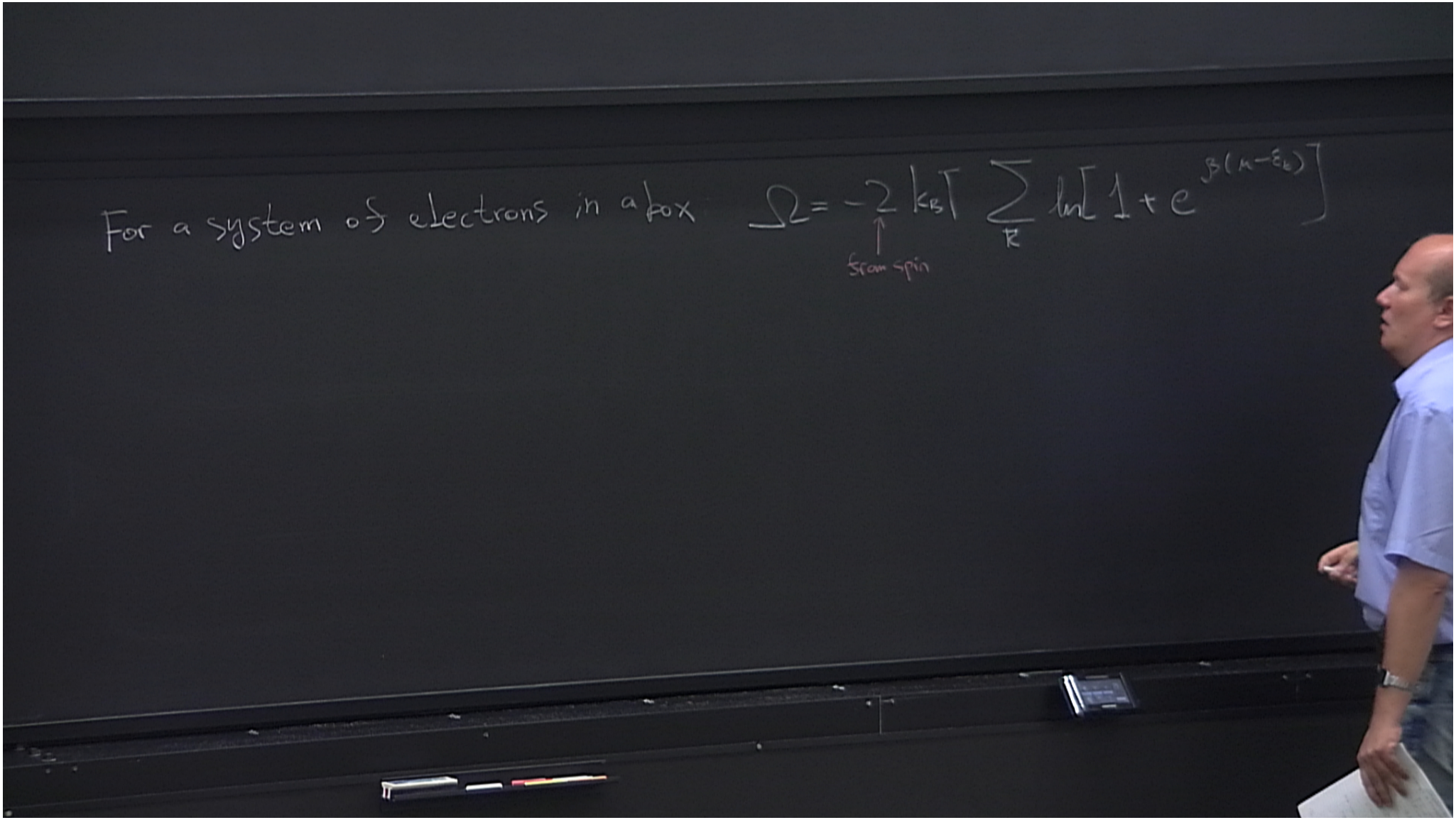

Plot $f_{FD}(\varepsilon) = \frac{1}{e^{\beta(\varepsilon-\mu)}+1}$
T=0
At T=0 $\mu=\varepsilon_F$
T is small but ≠ 0
large T
1
μ
ε

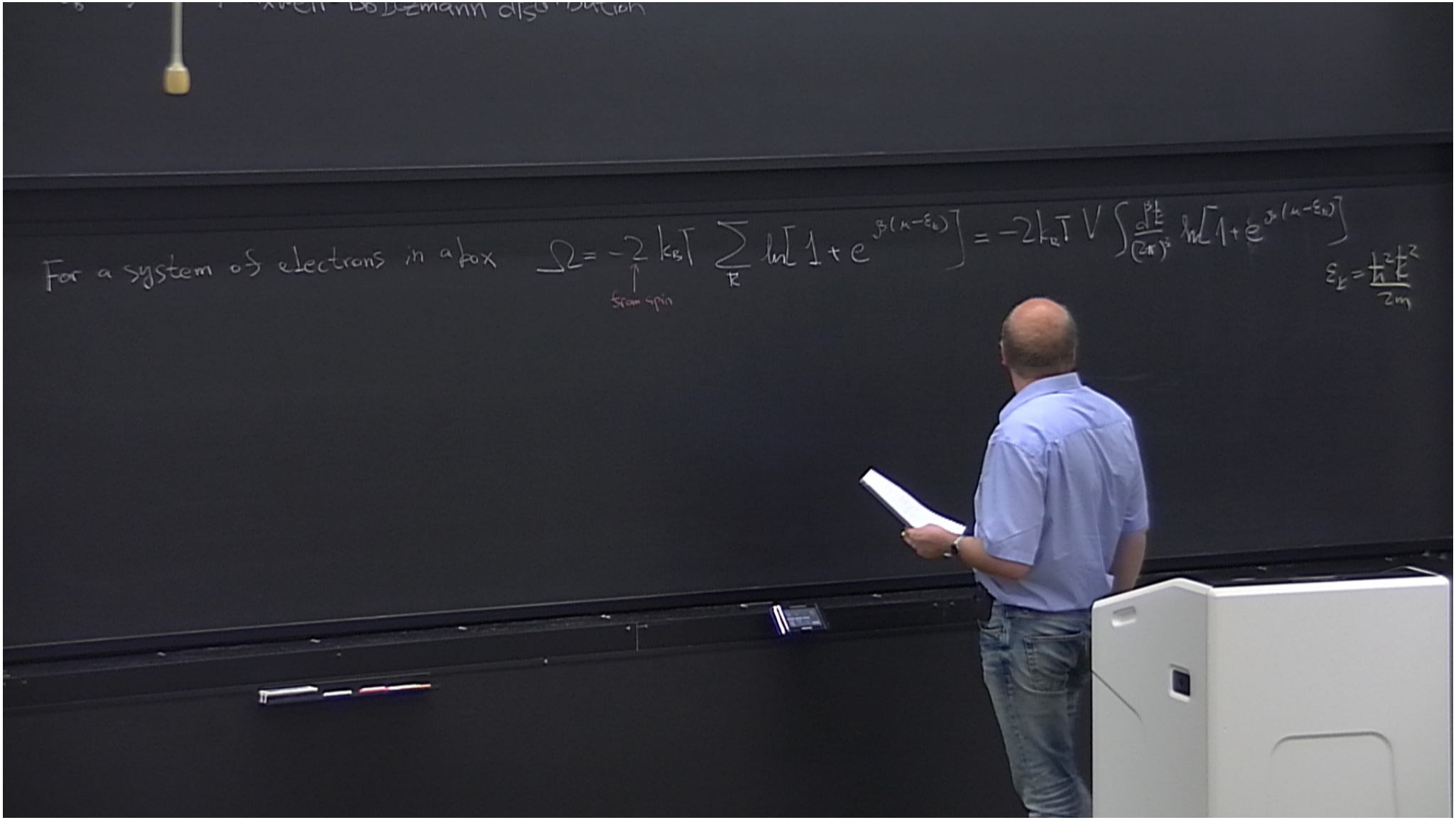
Plot $f_{FD}(\varepsilon) = \dfrac{1}{e^{\beta(\varepsilon-\mu)}+1}$

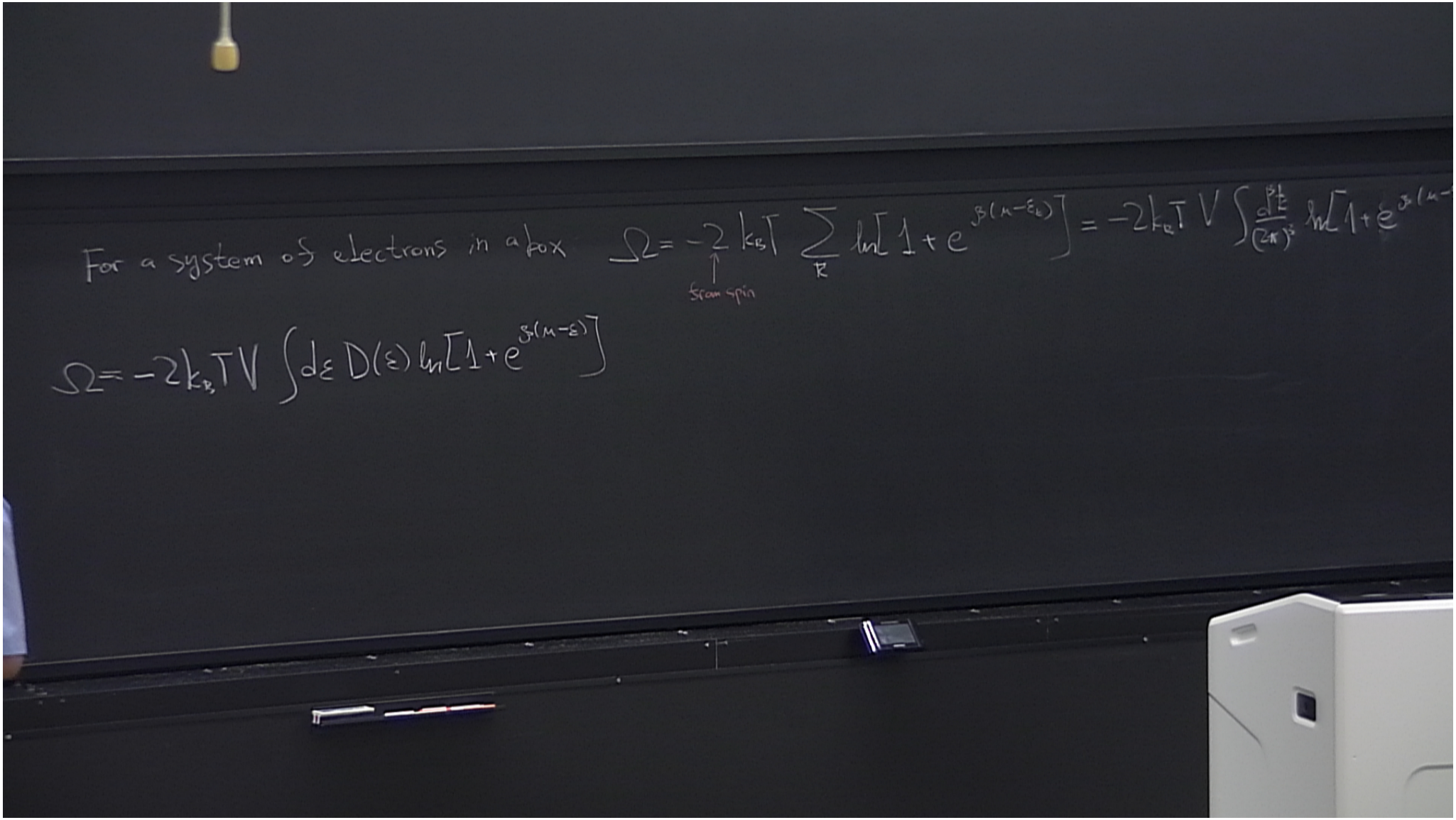


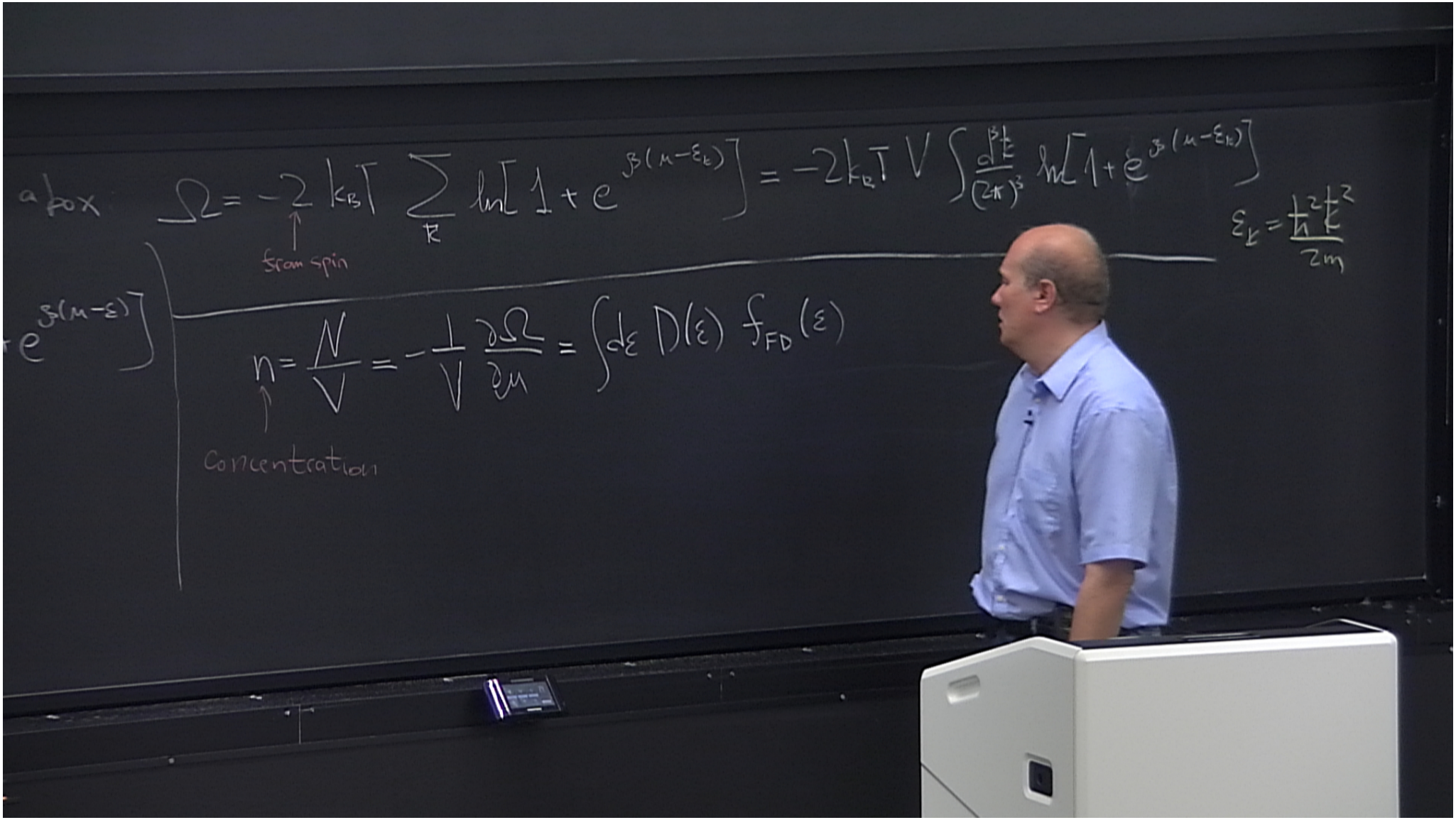
$f_{FD}(\varepsilon) \approx e^{-\beta(\varepsilon-\mu)}$

for $k_B T \gg \mu$ — Maxwell-Boltzmann distribution


For a system of electrons in a box $\Omega = -2 k_B T \sum_k \ln\left[1 + e^{\beta(\mu - \varepsilon_k)}\right]$
from spin


For a system of electrons in a box
$\Omega = -2 k_B T \sum_k \ln\left[1 + e^{\beta(\mu - \varepsilon_k)}\right] = -2 k_B T V \int \frac{d^3k}{(2\pi)^3} \ln\left[1 + e^{\beta(\mu - \varepsilon_k)}\right]$
from spin
$\varepsilon_k = \frac{\hbar^2 k^2}{2m}$


For a system of electrons in a box $\Omega = -2 k_B T \sum_k \ln\left[1 + e^{\beta(\mu - \varepsilon_k)}\right] = -2 k_B T V \int \frac{d^3k}{(2\pi)^3} \ln\left[1 + e^{\beta(\mu -$
from spin
$\Omega = -2 k_B T V \int d\varepsilon\, D(\varepsilon) \ln\left[1 + e^{\beta(\mu - \varepsilon)}\right]$


a box
$\Omega = -2 k_B T \sum_k \ln\left[1 + e^{\beta(\mu - \varepsilon_k)}\right] = -2 k_B T V \int \frac{d^3k}{(2\pi)^3} \ln\left[1 + e^{\beta(\mu - \varepsilon_k)}\right]$
from spin
$\varepsilon_k = \frac{\hbar^2 k^2}{2m}$
$e^{\beta(\mu-\varepsilon)}\Big]$
$n = \frac{N}{V} = -\frac{1}{V}\frac{\partial \Omega}{\partial \mu} = \int d\varepsilon\, D(\varepsilon)\, f_{FD}(\varepsilon)$
Concentration

a box $\Omega = -2 k_B T \sum_k \ln\left[1 + e^{\beta(\mu - \varepsilon_k)}\right] = -2 k_B T V \int \frac{d^3k}{(2\pi)^3} \ln\left[1 + e^{\beta(\mu - \varepsilon_k)}\right]$

2 from spin

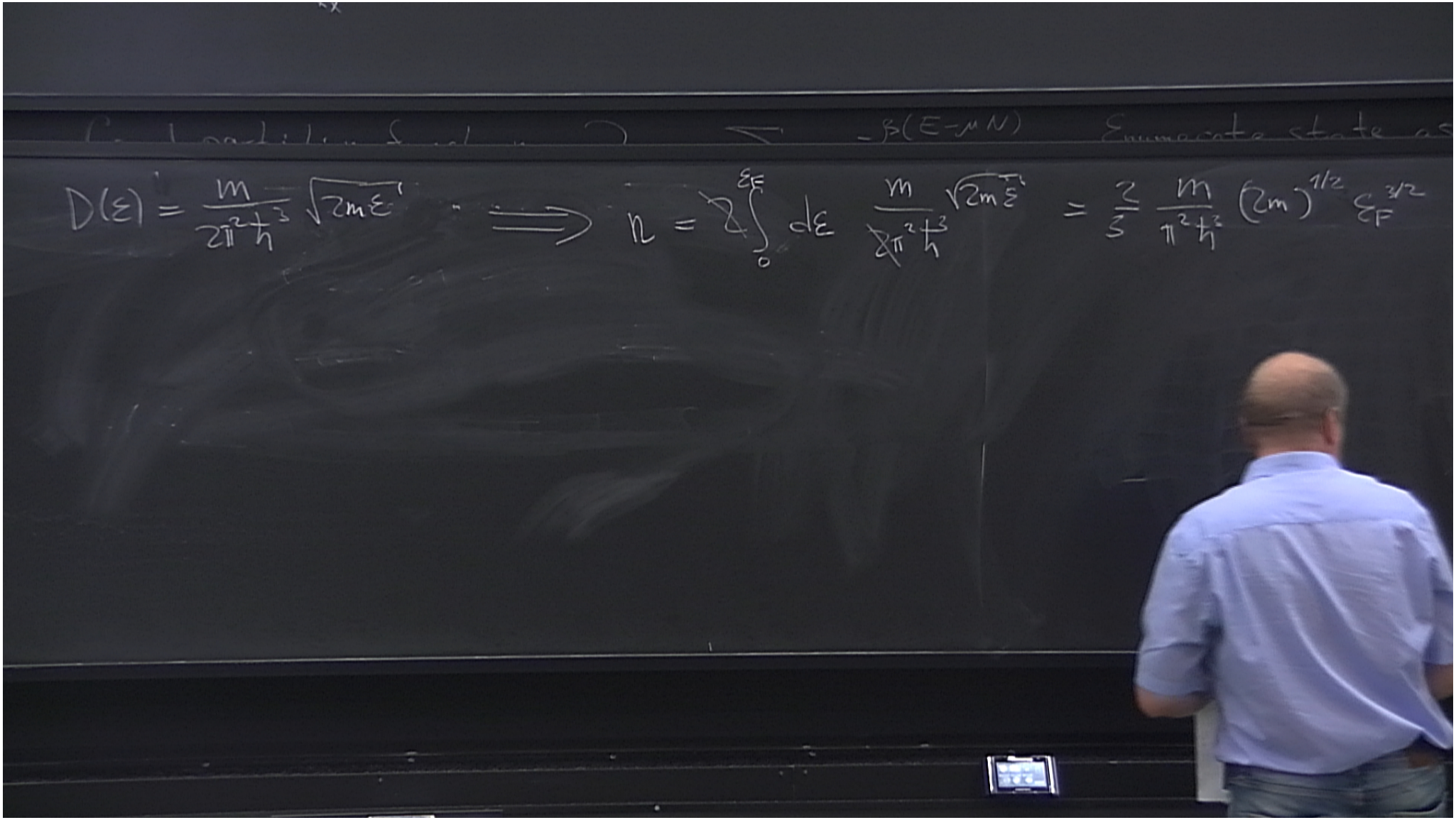
$\varepsilon_k = \frac{\hbar^2 k^2}{2m}$

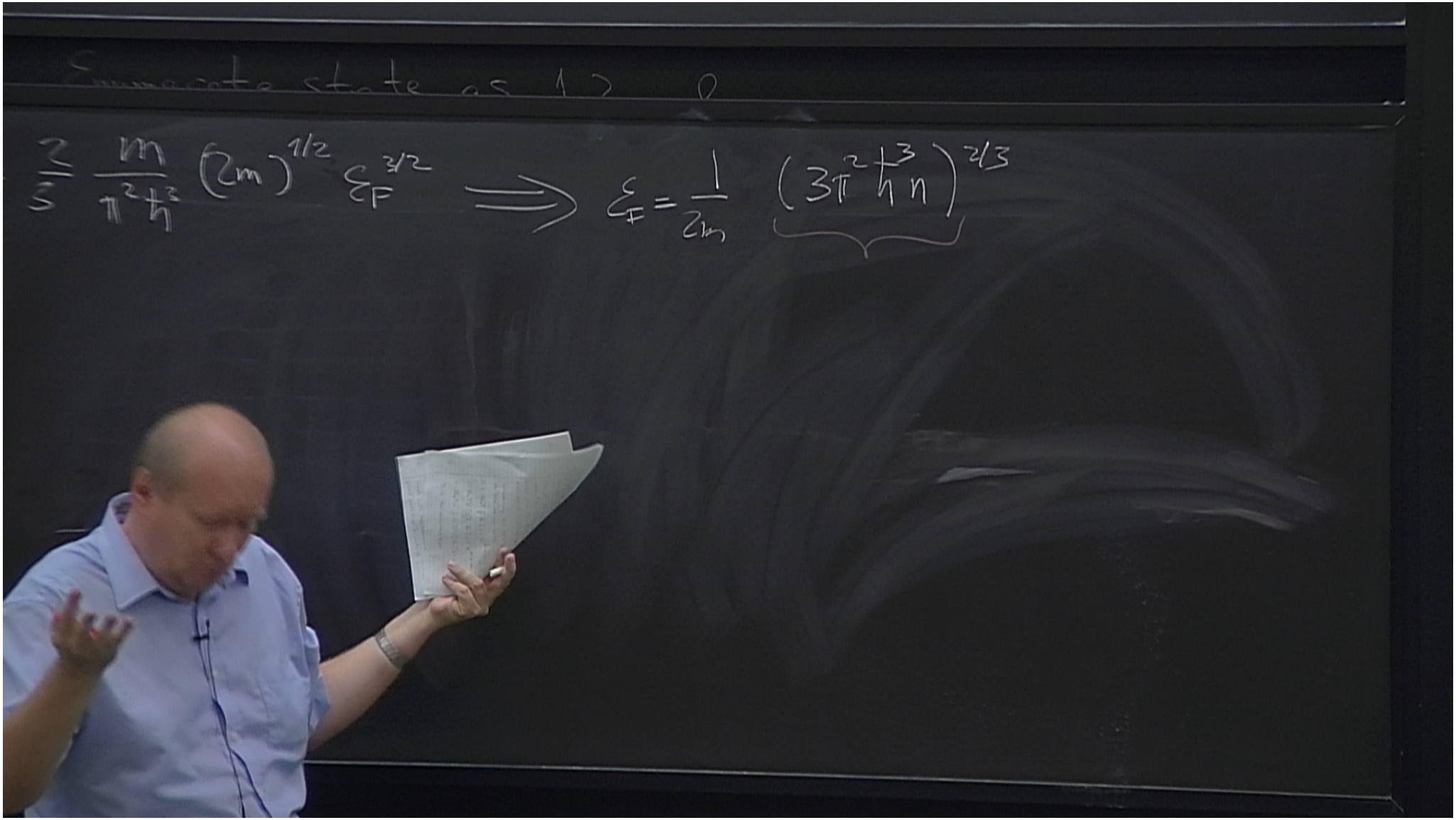
$e^{\beta(\mu - \varepsilon)}\Big]$

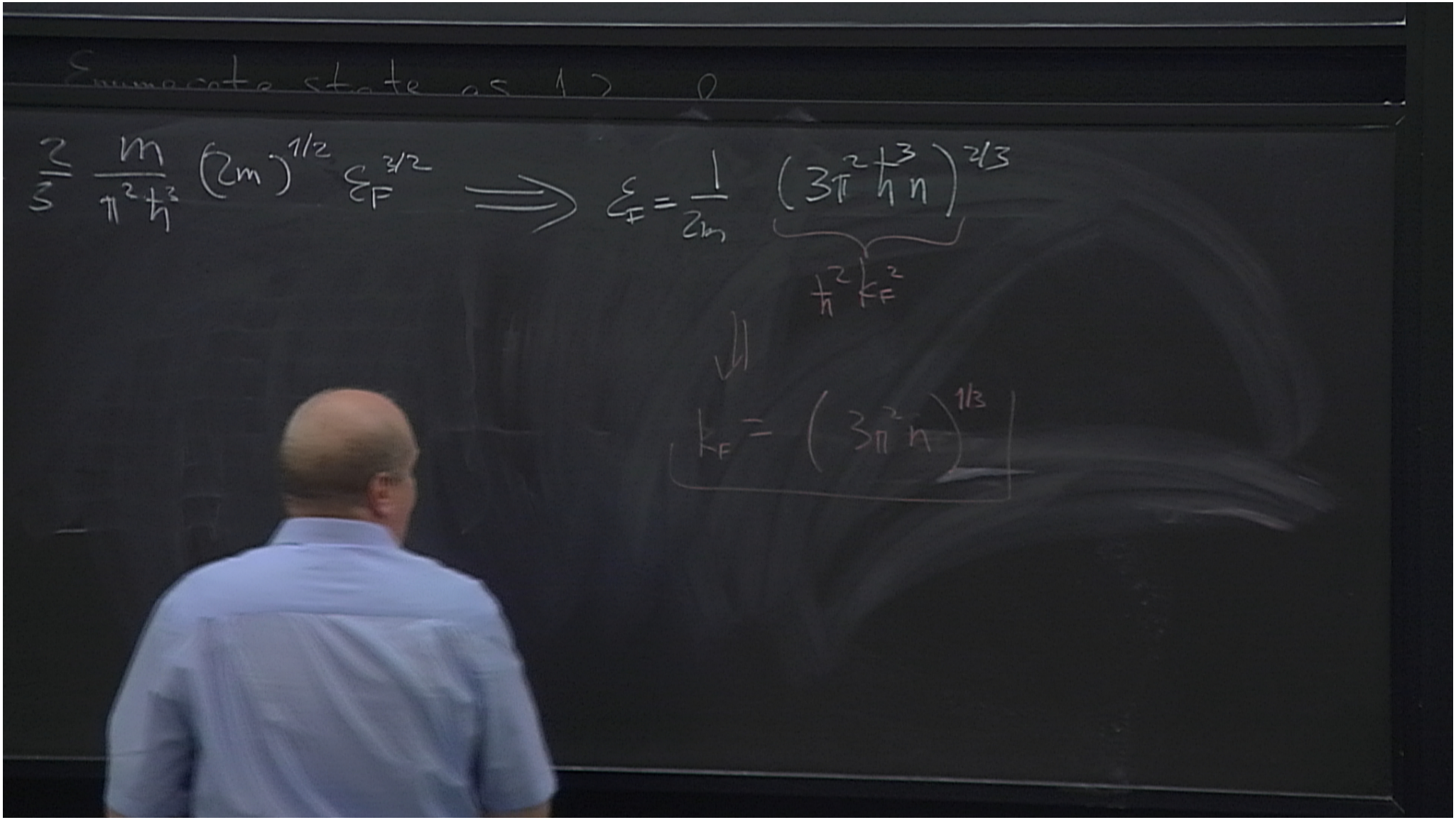
$n = \frac{N}{V} = -\frac{1}{V}\frac{\partial \Omega}{\partial \mu} = \int d\varepsilon\, D(\varepsilon)\, f_{FD}(\varepsilon)$

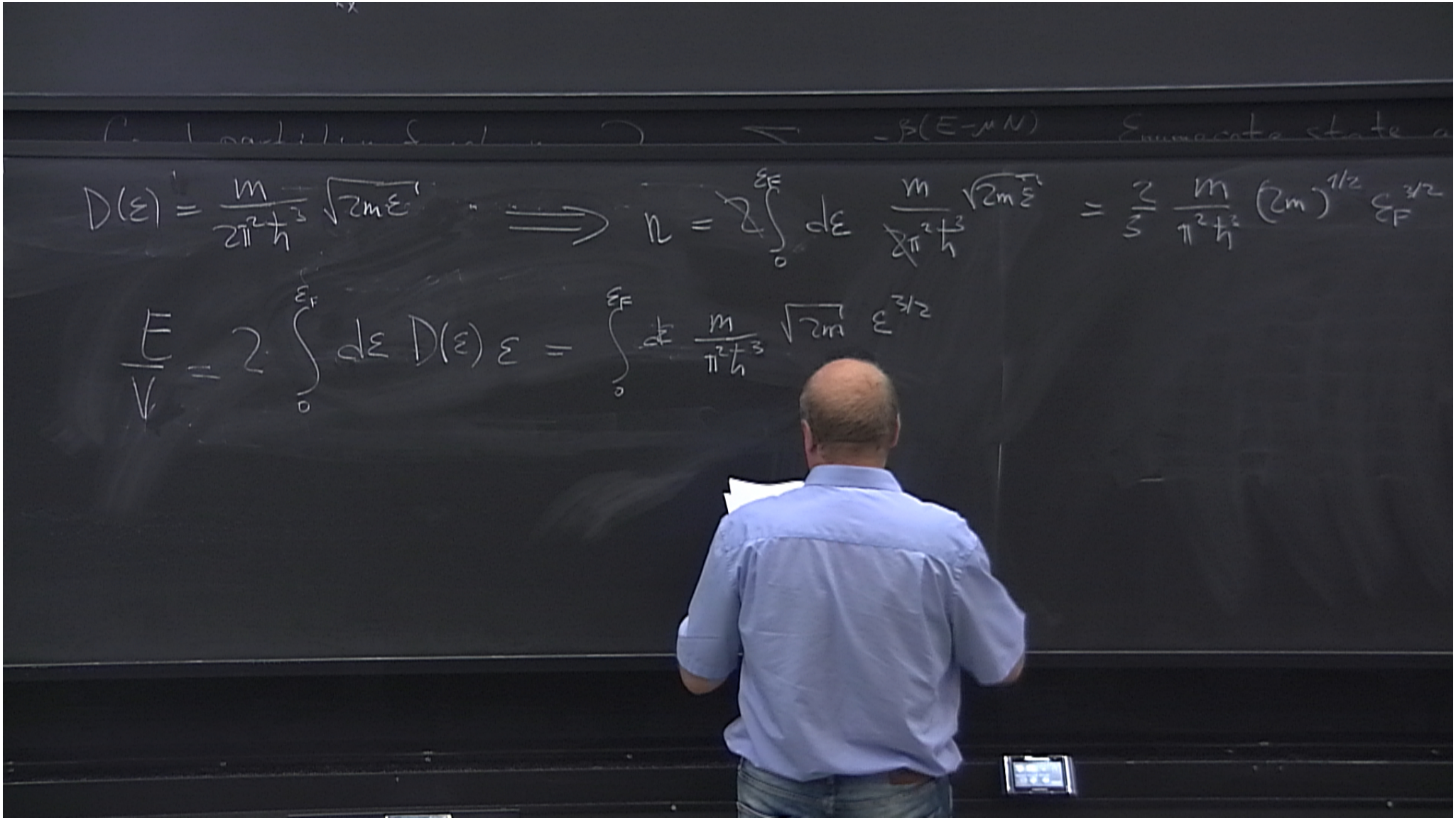
$\Theta(\mu - \varepsilon)$

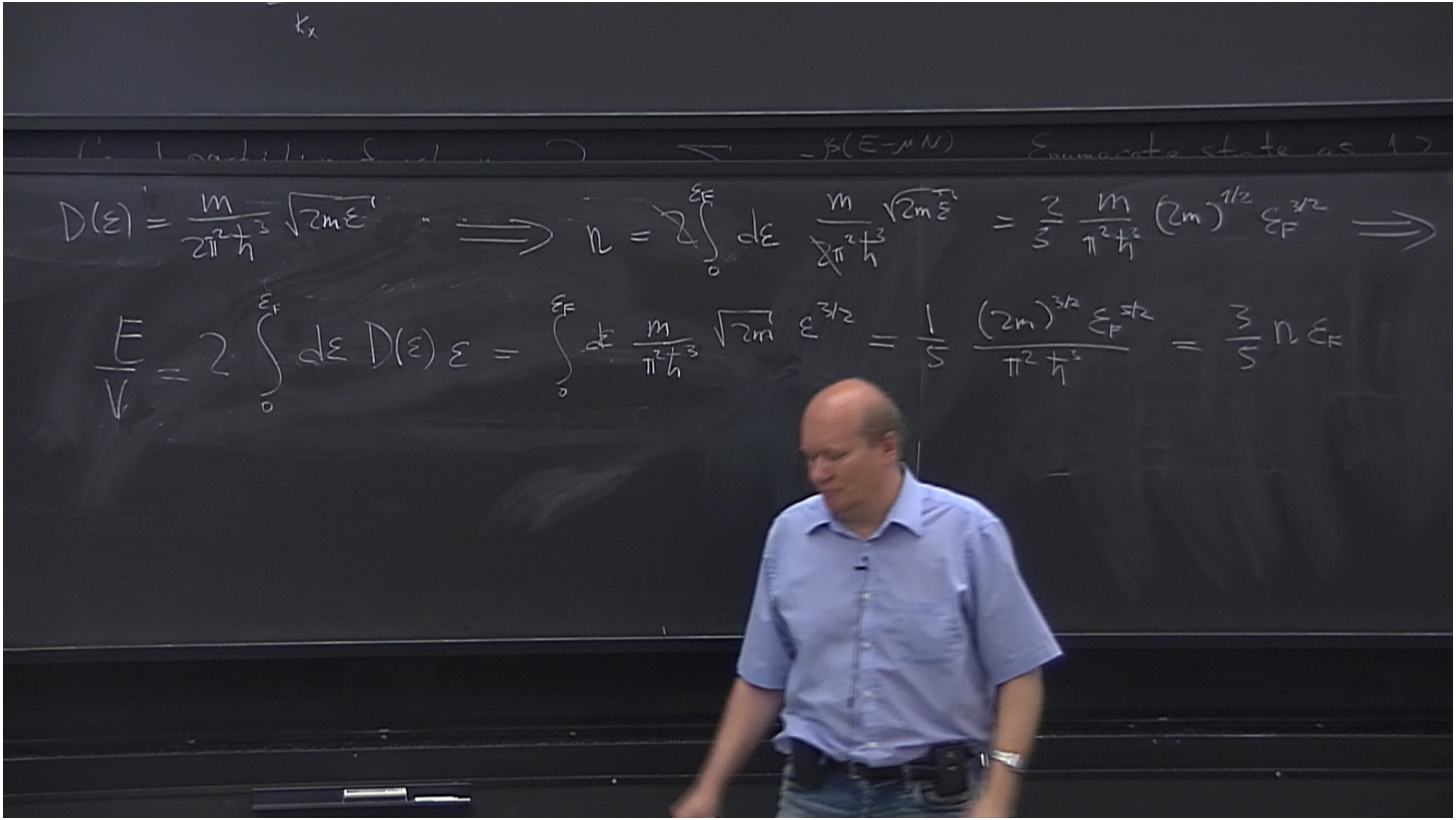
Concentration

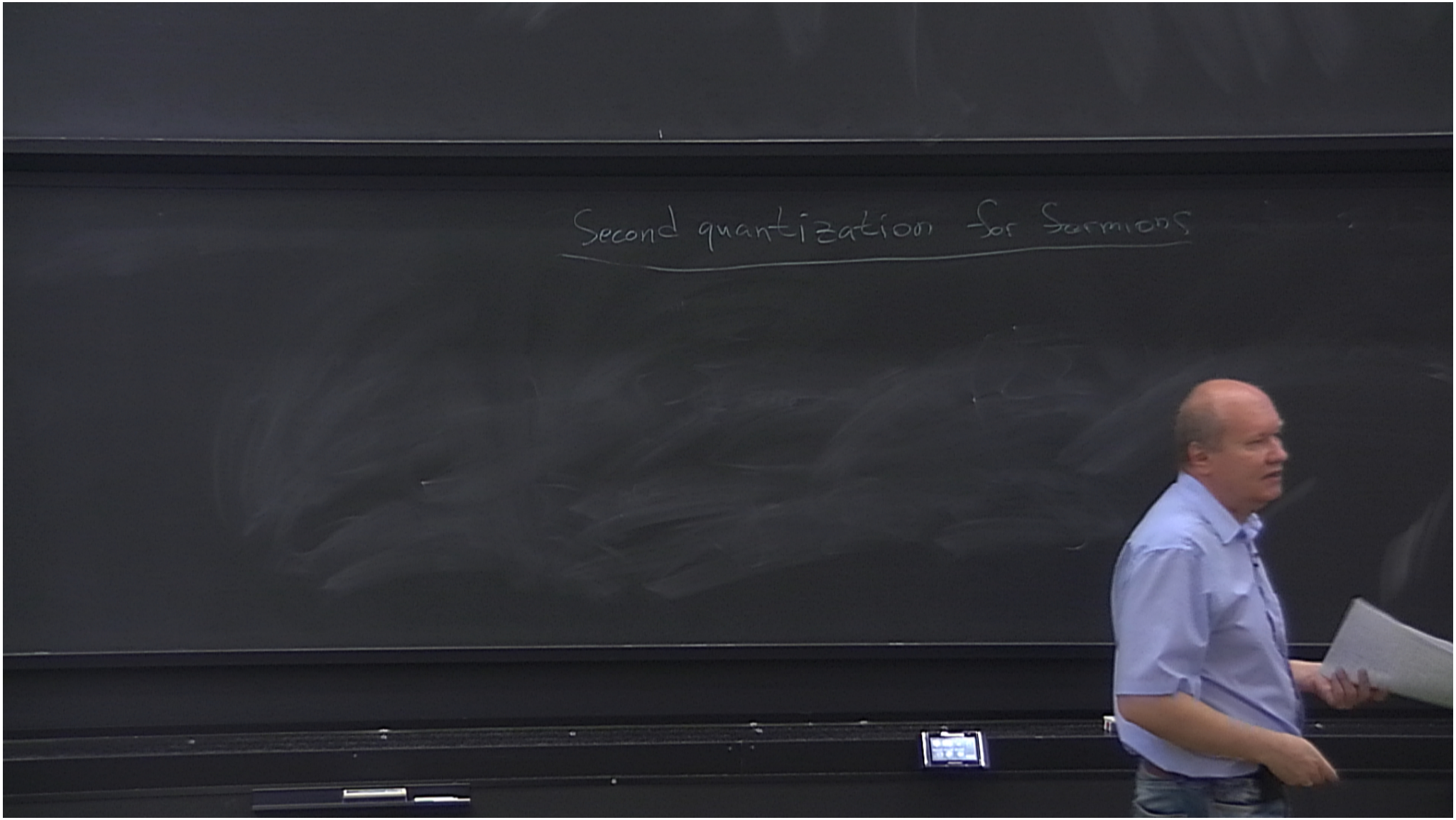

$D(\varepsilon) = \frac{m}{2\pi^2\hbar^3}\sqrt{2m\varepsilon}$
$\Longrightarrow n = 2\int_0^{\varepsilon_F} d\varepsilon \frac{m}{2\pi^2\hbar^3}\sqrt{2m\varepsilon} = \frac{2}{3}\frac{m}{\pi^2\hbar^3}(2m)^{1/2}\varepsilon_F^{3/2}$

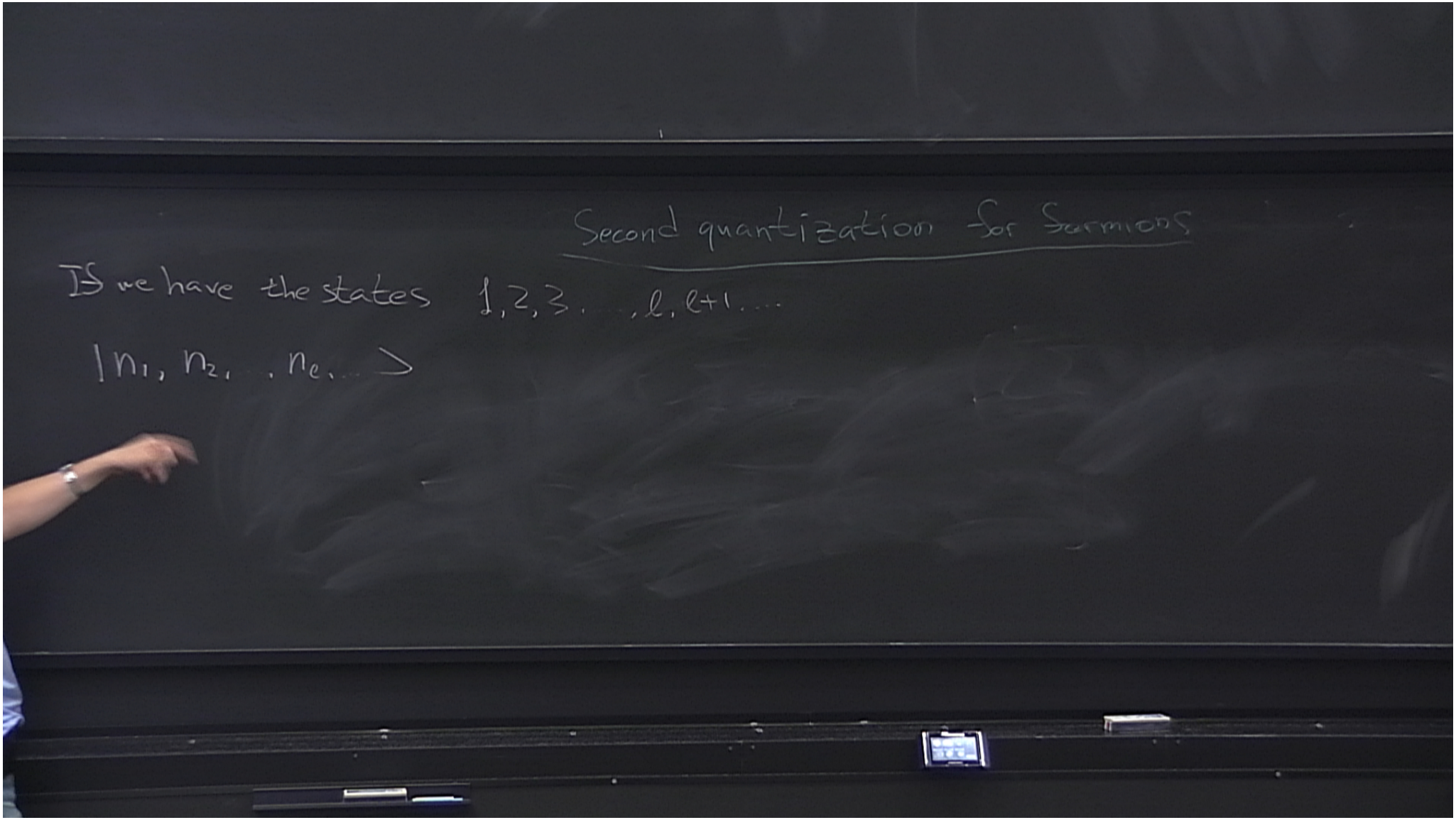

Summarize state as 1 > 0
$\frac{2}{5}\frac{m}{\pi^2\hbar^3}(2m)^{1/2}\varepsilon_F^{3/2} \Rightarrow \varepsilon_F = \frac{1}{2m}(3\pi^2\hbar^3 n)^{2/3}$

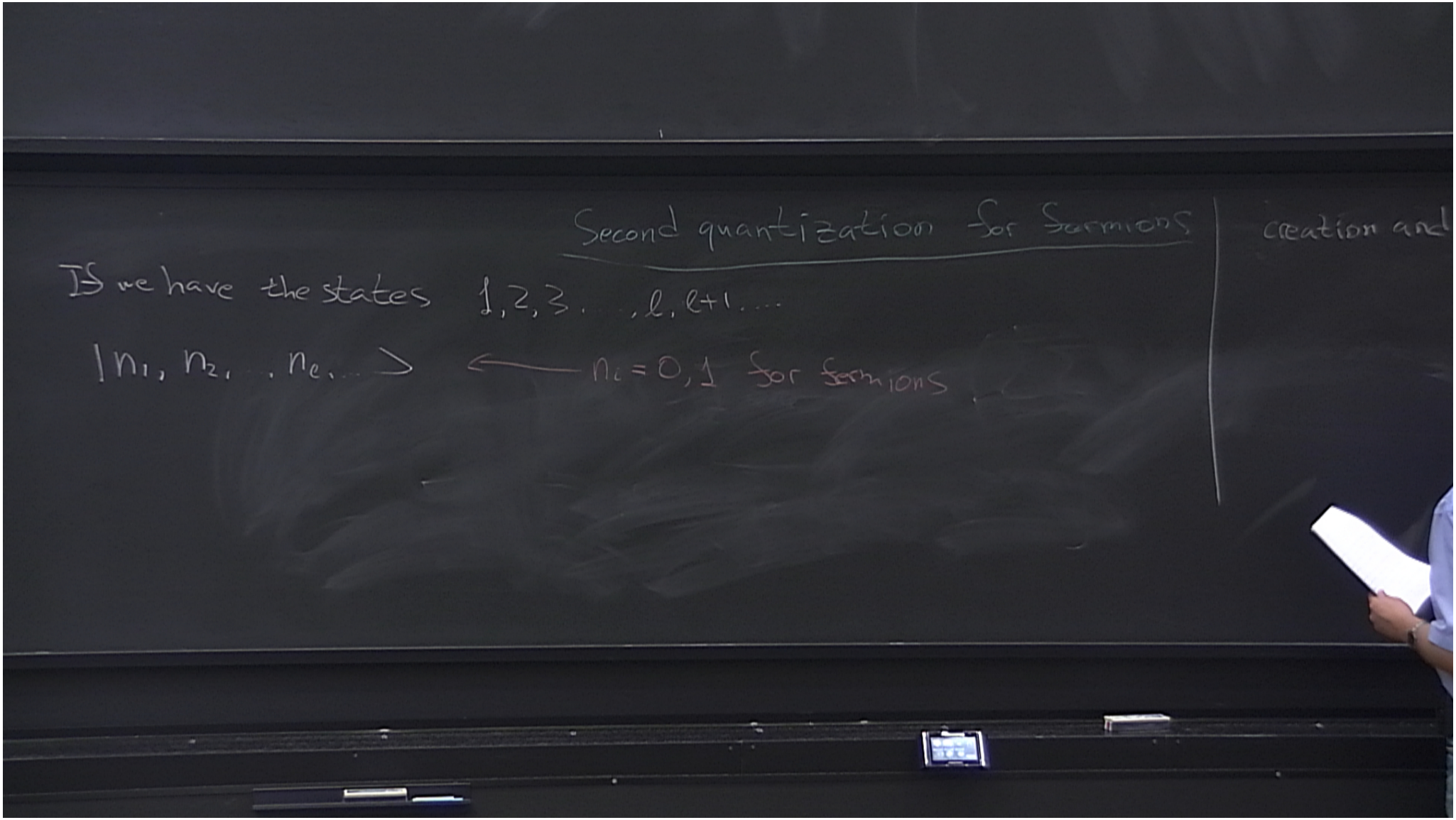

Evaporate state as 1 > 0
$\frac{2}{5}\frac{m}{\pi^2\hbar^3}(2m)^{1/2}\varepsilon_F^{3/2} \Longrightarrow \varepsilon_F = \frac{1}{2m}(3\pi^2\hbar^3 n)^{2/3}$
$\hbar^2 k_F^2$
$k_F = (3\pi^2 n)^{1/3}$

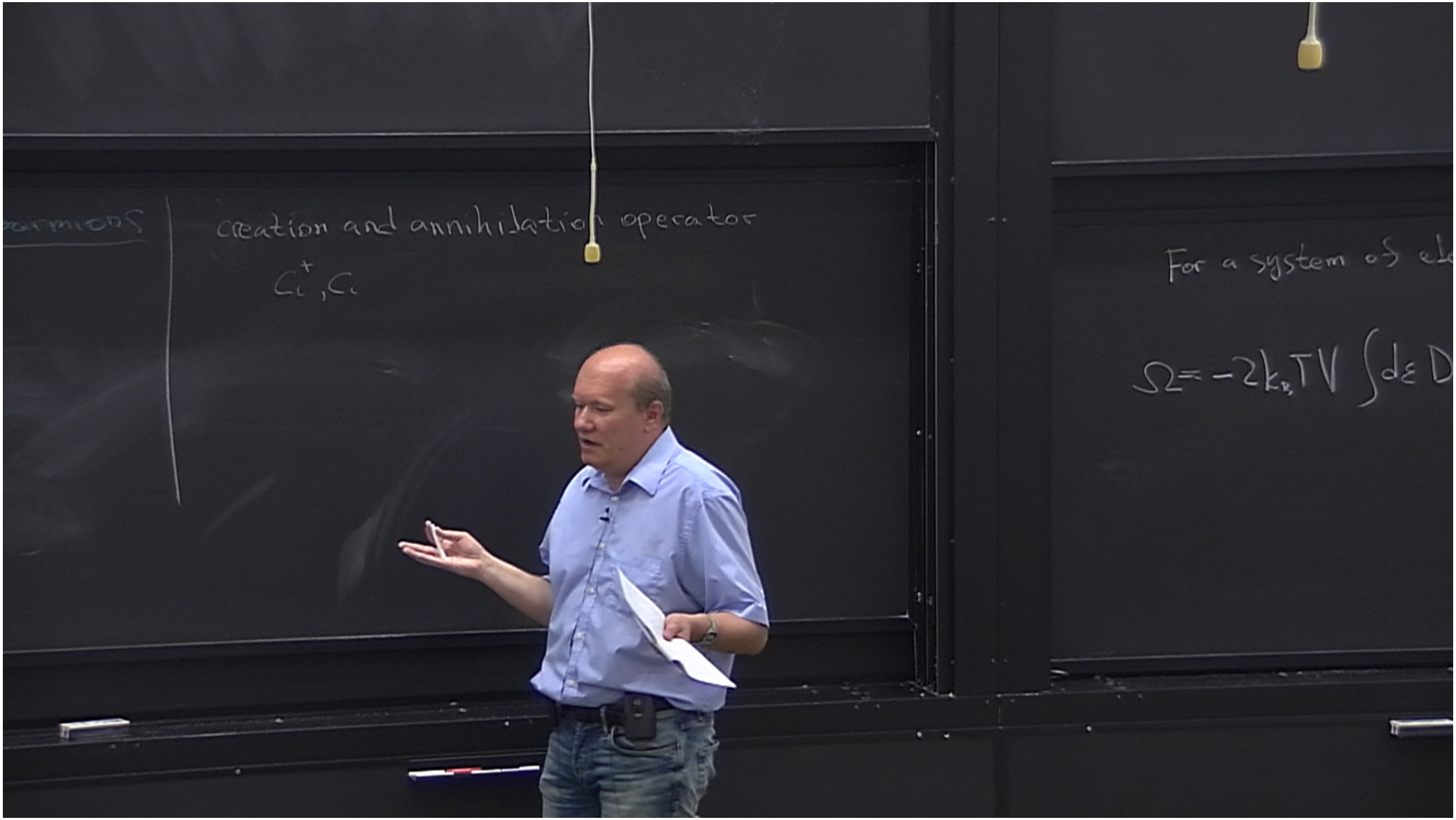

$D(\varepsilon) = \frac{m}{2\pi^2\hbar^3}\sqrt{2m\varepsilon}$
$\Longrightarrow n = 2\int_0^{\varepsilon_F} d\varepsilon \frac{m}{2\pi^2\hbar^3}\sqrt{2m\varepsilon} = \frac{2}{3}\frac{m}{\pi^2\hbar^3}(2m)^{1/2}\varepsilon_F^{3/2}$
$\frac{E}{V} = 2\int_0^{\varepsilon_F} d\varepsilon\, D(\varepsilon)\,\varepsilon = \int_0^{\varepsilon_F} d\varepsilon \frac{m}{\pi^2\hbar^3}\sqrt{2m}\,\varepsilon^{3/2}$

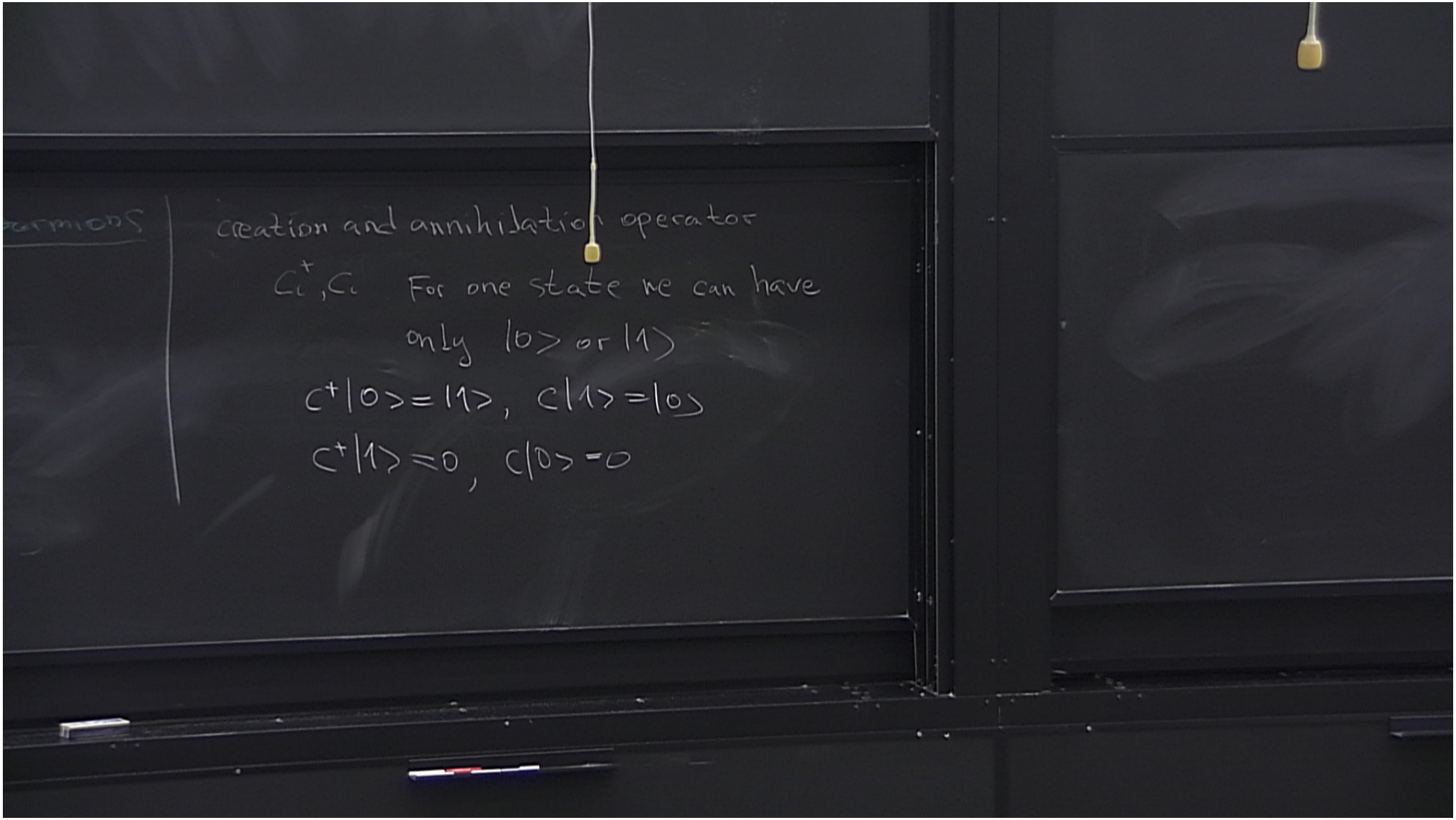

k_x
$D(\varepsilon) = \frac{m}{2\pi^2\hbar^3}\sqrt{2m\varepsilon}$
$\Longrightarrow n = 2\int_0^{\varepsilon_F} d\varepsilon \frac{m}{2\pi^2\hbar^3}\sqrt{2m\varepsilon} = \frac{2}{3}\frac{m}{\pi^2\hbar^3}(2m)^{1/2}\varepsilon_F^{3/2} \Longrightarrow$
$\frac{E}{V} = 2\int_0^{\varepsilon_F} d\varepsilon\, D(\varepsilon)\,\varepsilon = \int_0^{\varepsilon_F} d\varepsilon \frac{m}{\pi^2\hbar^3}\sqrt{2m}\,\varepsilon^{3/2} = \frac{1}{5}\frac{(2m)^{3/2}\varepsilon_F^{5/2}}{\pi^2\hbar^3} = \frac{3}{5}n\varepsilon_F$

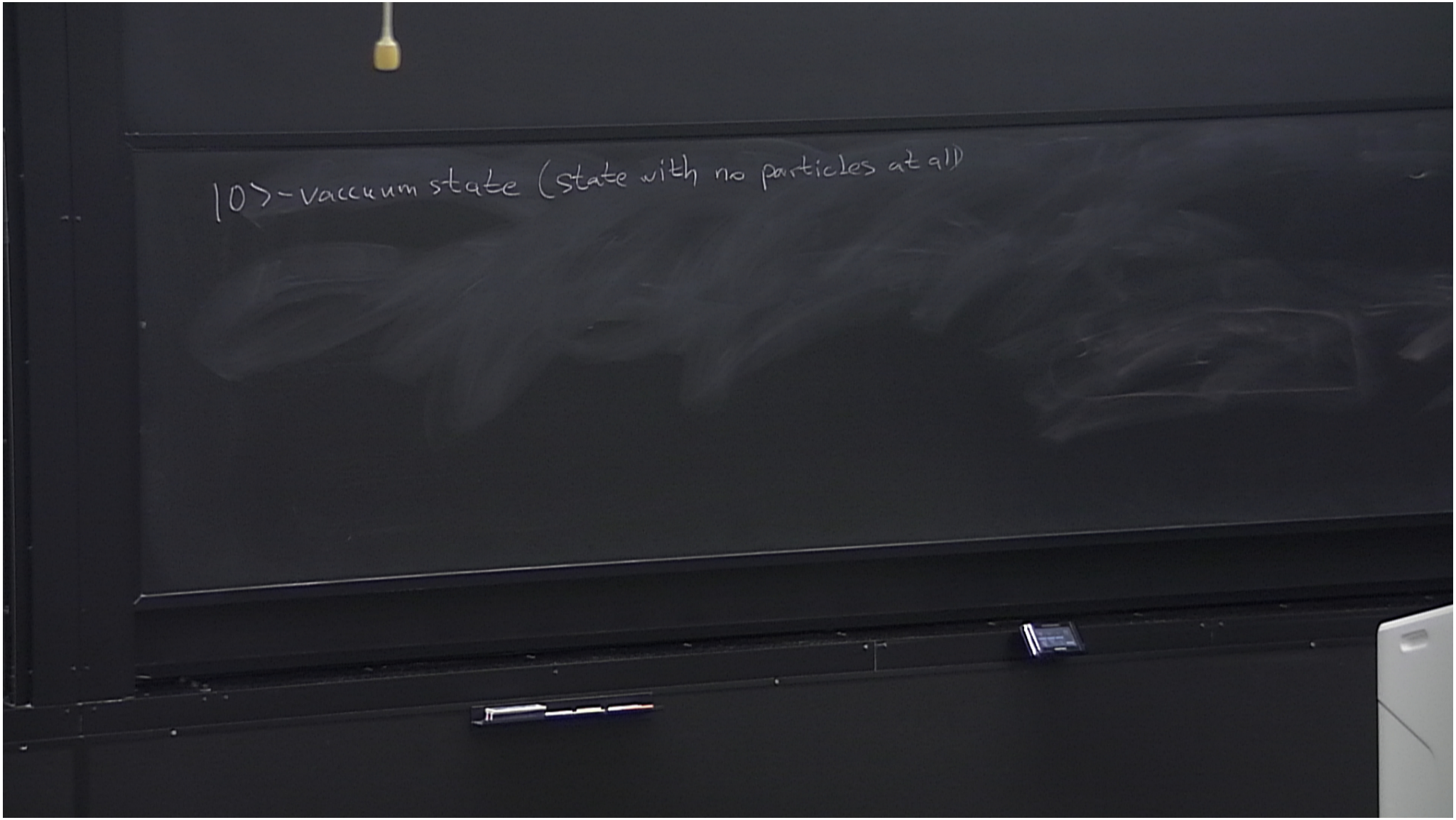

Second quantization for fermions

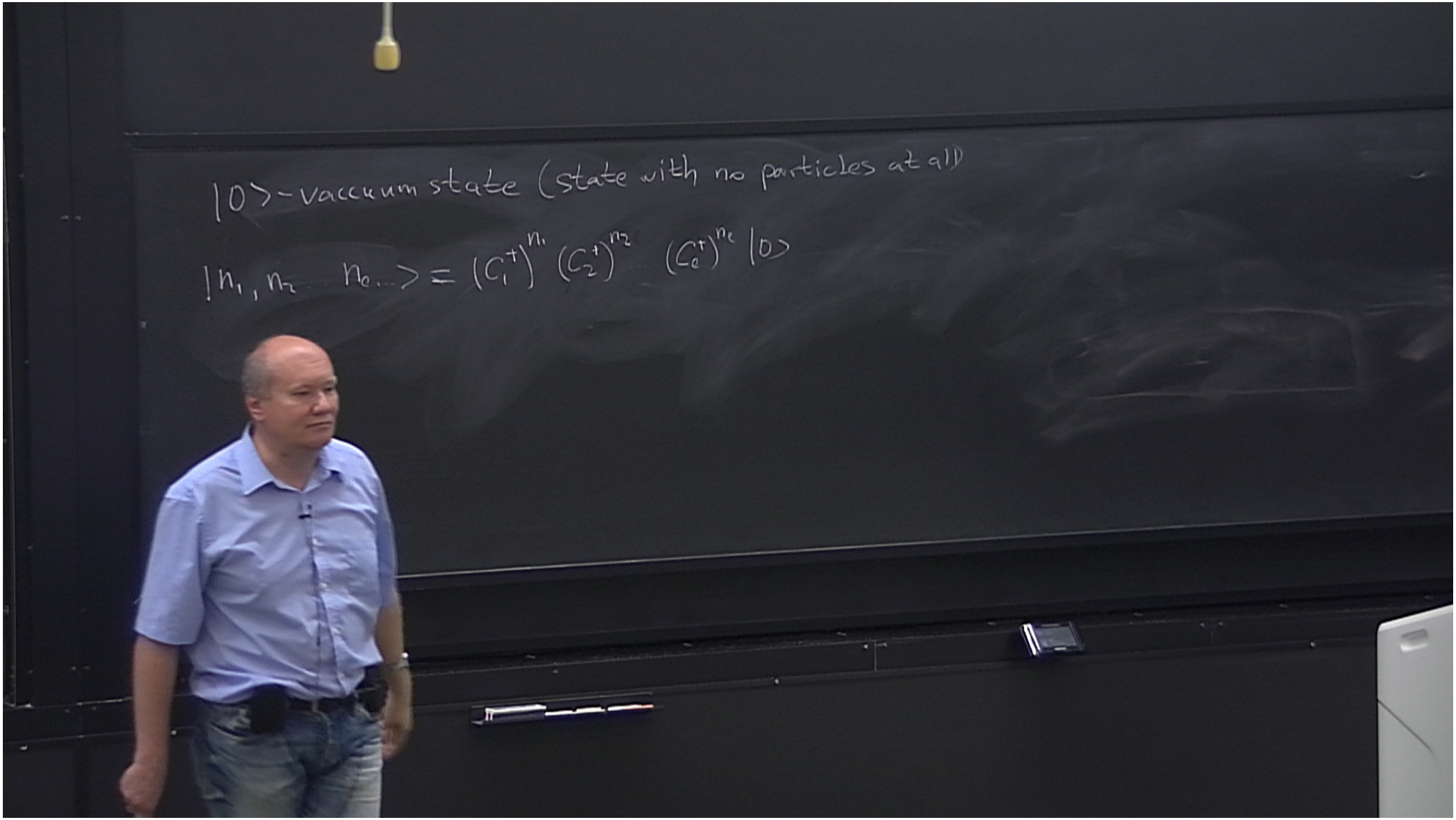

Second quantization for fermions
If we have the states 1, 2, 3, ..., l, l+1, ...
|n1, n2, ..., ne, ...>

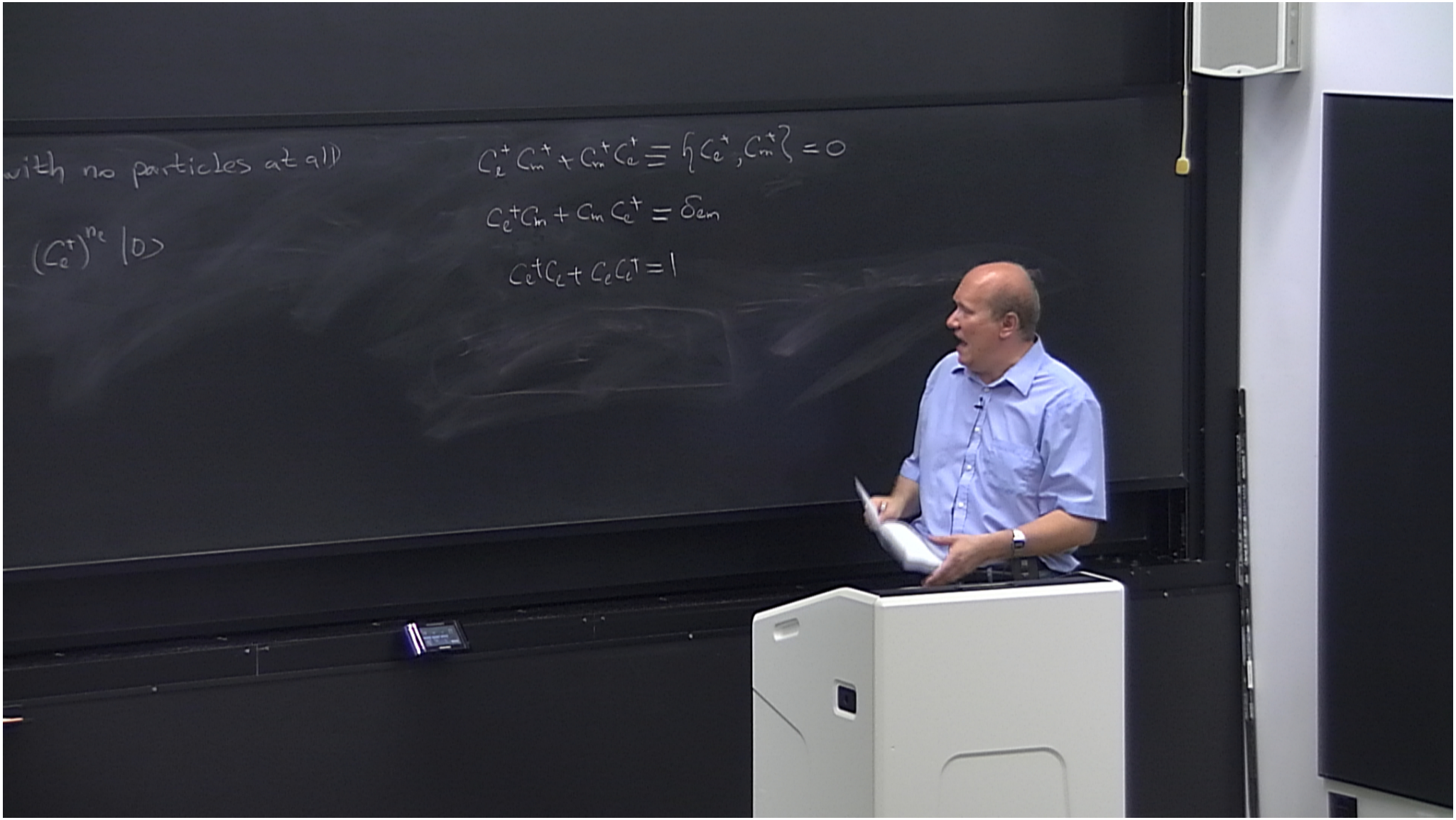

Second quantization for fermions
creation and
If we have the states 1, 2, 3. . . , l, l+1 . . .
$|n_1, n_2, \ldots n_e, \ldots\rangle$ ← $n_i = 0, 1$ for fermions

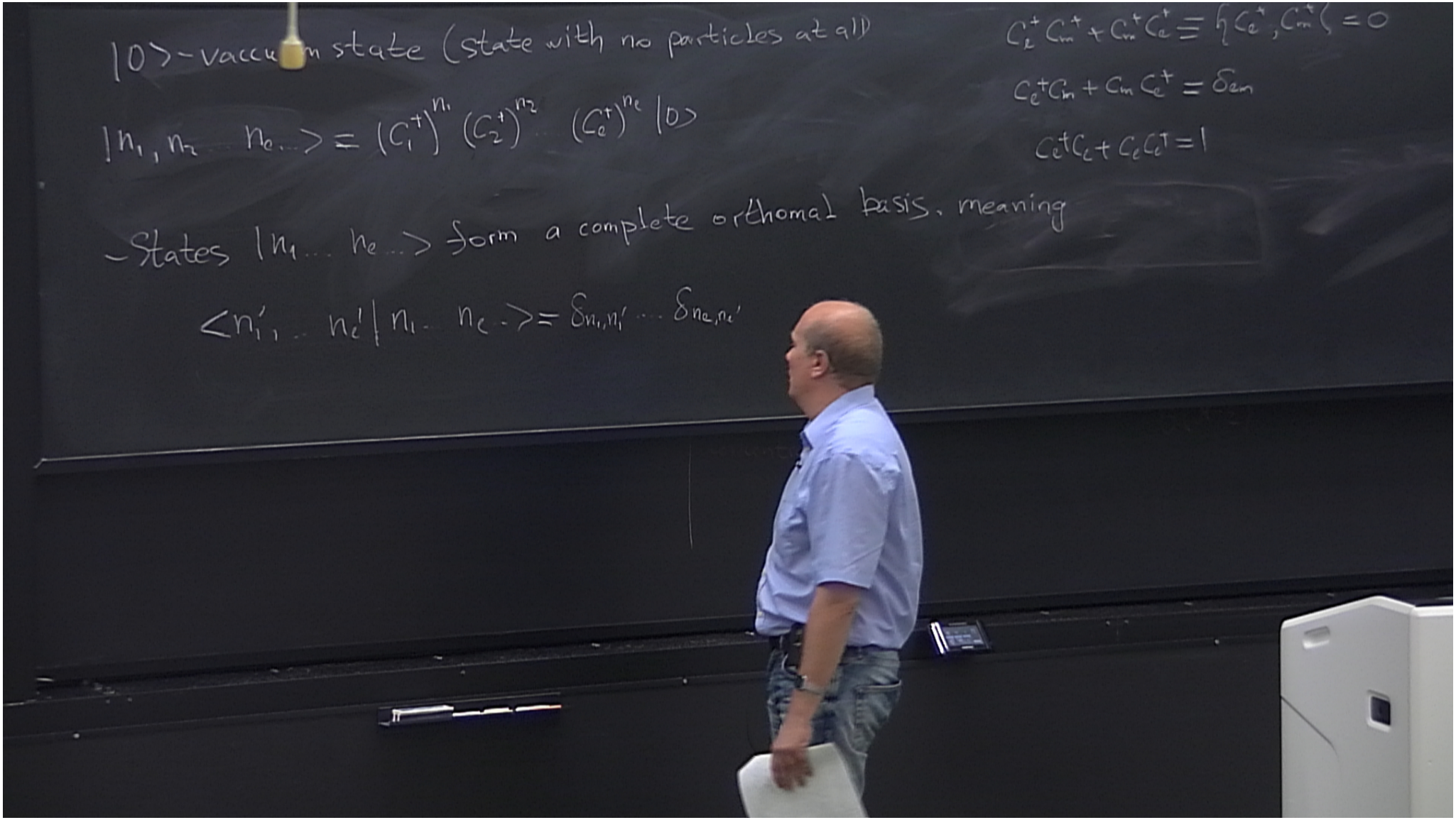

creation and annihilation operator
c_i^+, c_i
For a system of
$\Omega = -2k_B T V \int d\varepsilon$

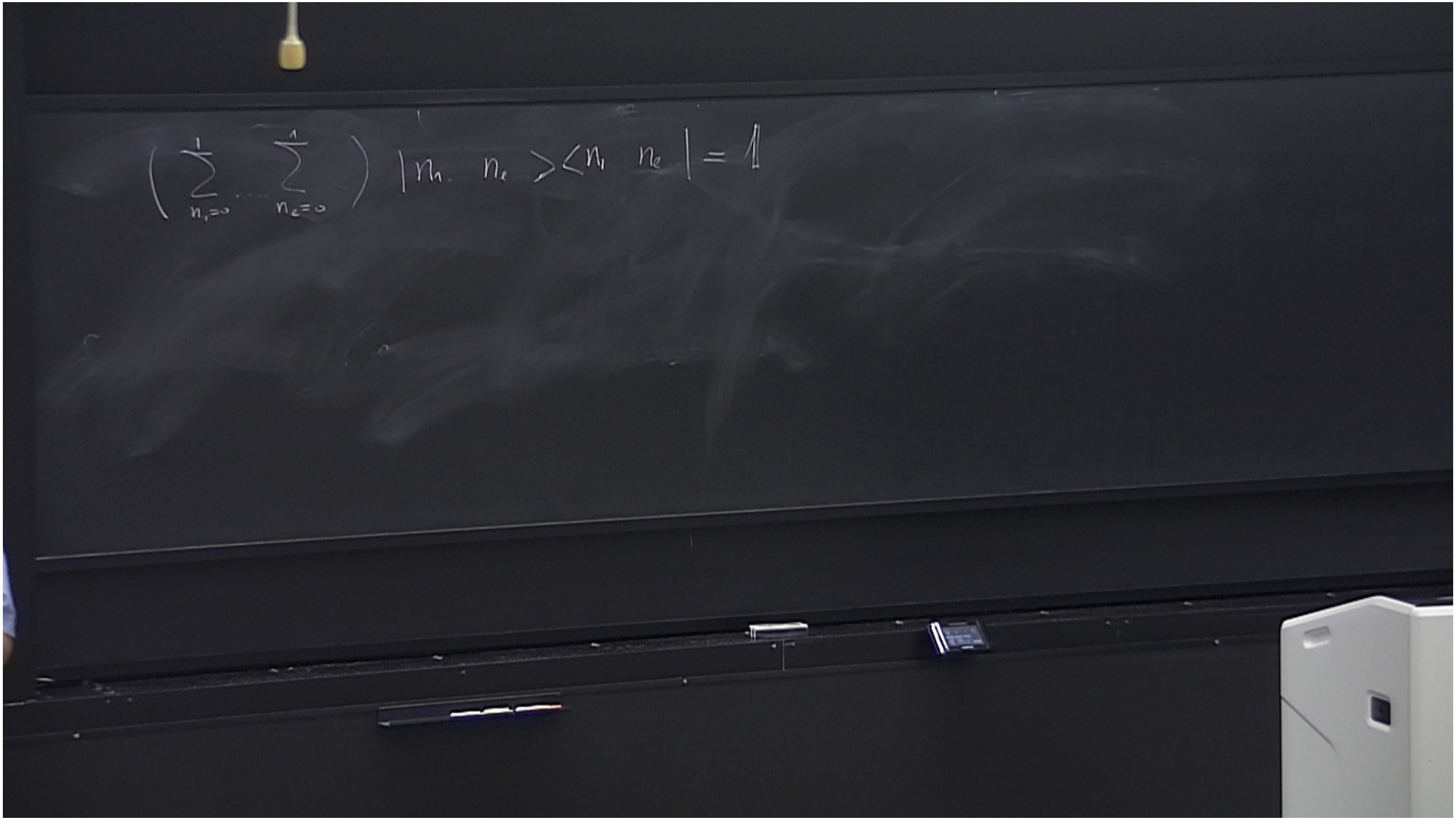

fermions
creation and annihilation operator
c_i^+, c_i For one state we can have only $|0\rangle$ or $|1\rangle$
$c^+|0\rangle = |1\rangle$, $c|1\rangle = |0\rangle$
$c^+|1\rangle = 0$, $c|0\rangle = 0$

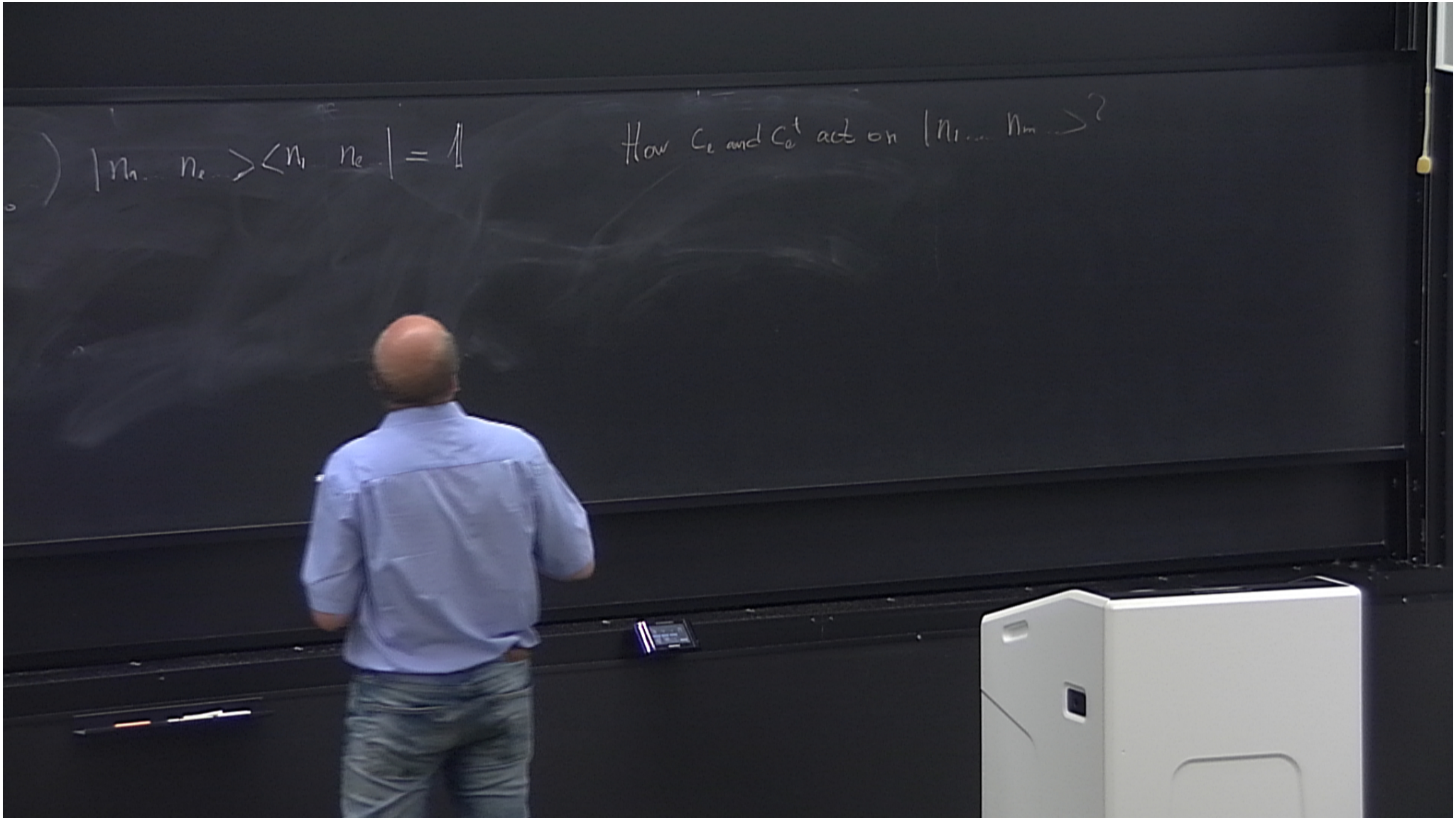

|0> - vacuum state (state with no particles at all)

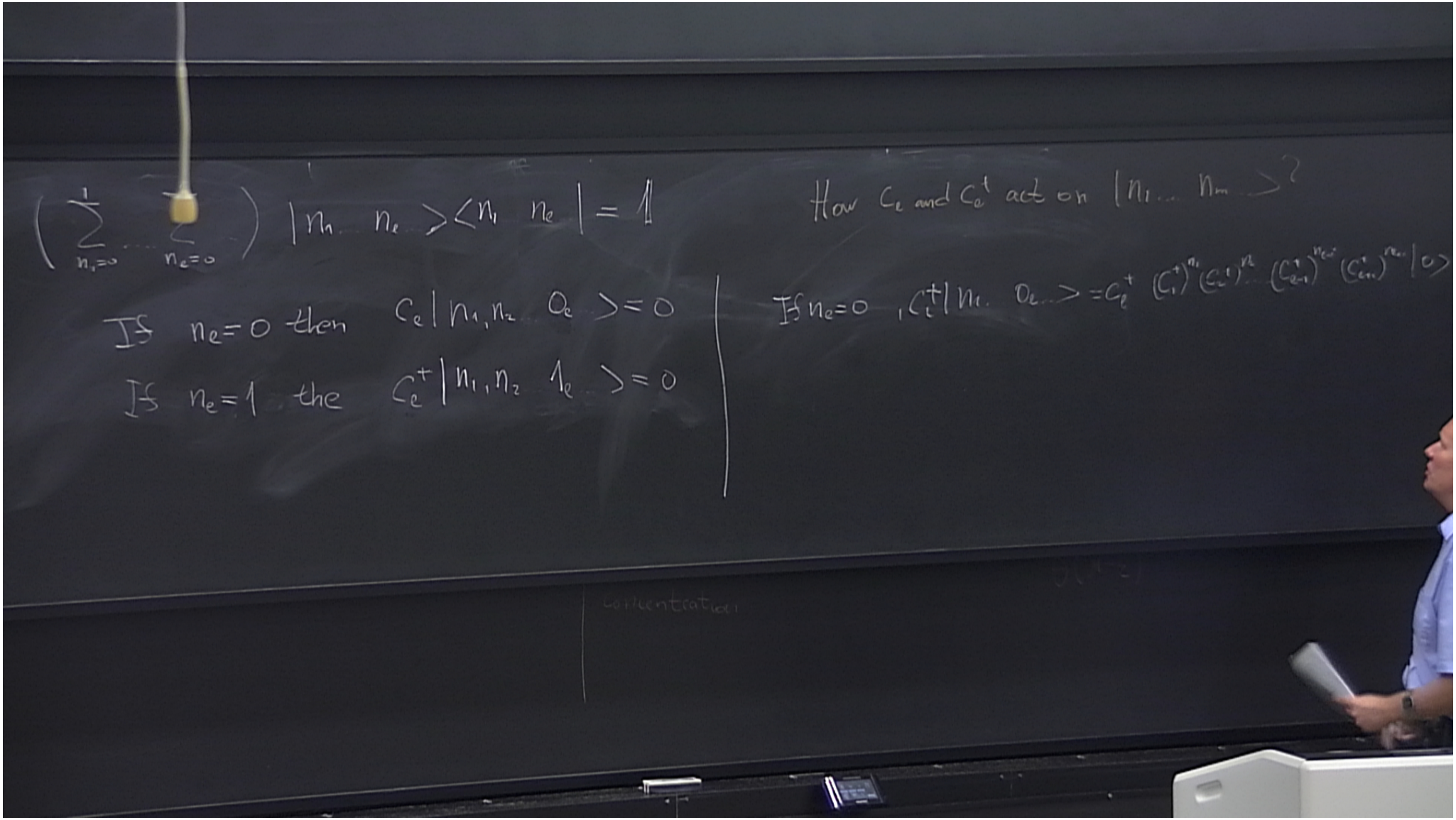

|0> - vacuum state (state with no particles at all)
$|n_1, n_2 \ldots n_\alpha \ldots\rangle = (C_1^+)^{n_1} (C_2^+)^{n_2} \ldots (C_\alpha^+)^{n_\alpha} |0\rangle$

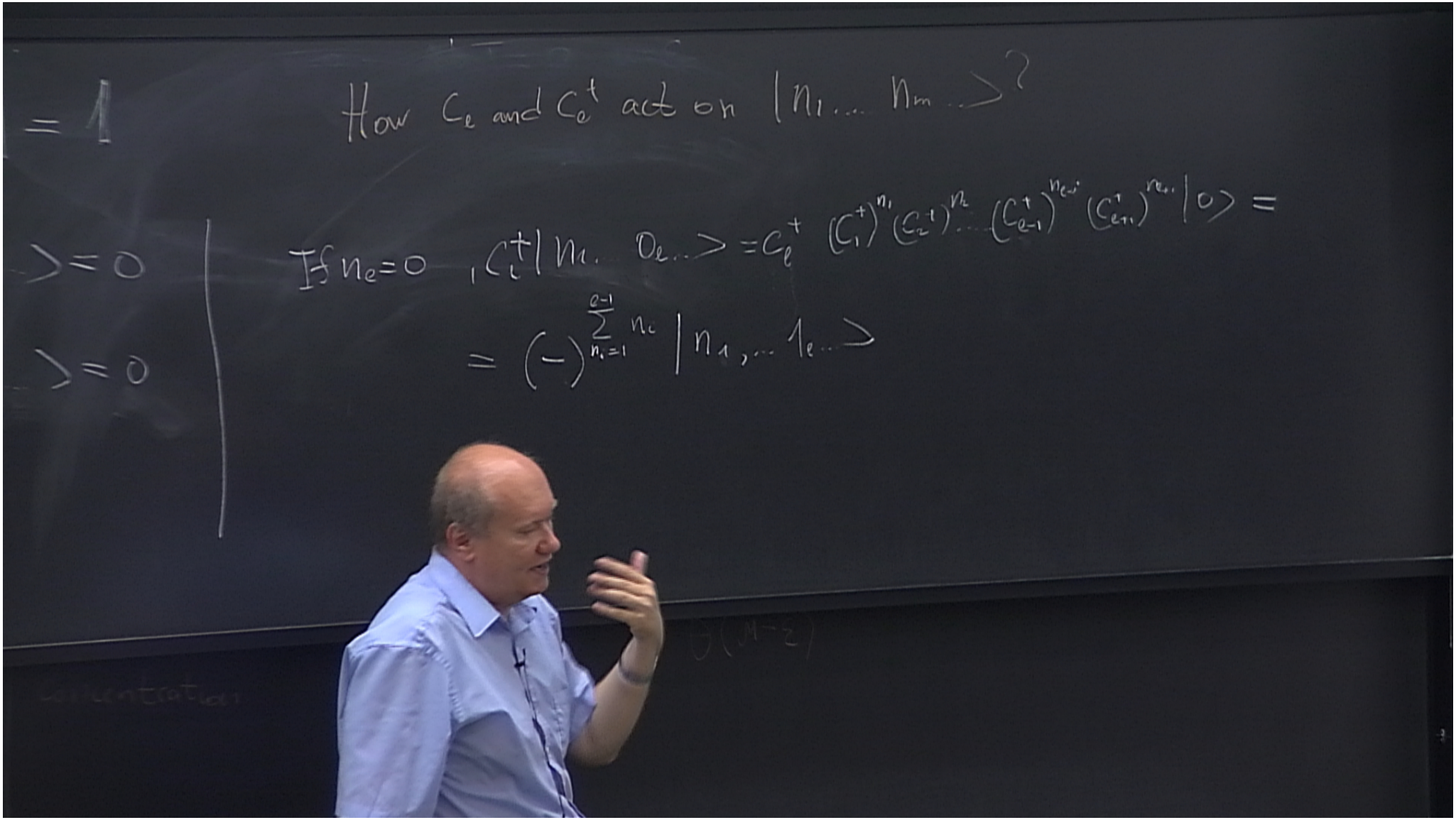

with no particles at all
$(c_e^\dagger)^{n_e}|0\rangle$
$c_e^\dagger c_m^\dagger + c_m^\dagger c_e^\dagger \equiv \{c_e^\dagger, c_m^\dagger\} = 0$
$c_e^\dagger c_m + c_m c_e^\dagger = \delta_{em}$
$c_e^\dagger c_e + c_e c_e^\dagger = 1$


$|0\rangle$ - vacuum state (state with no particles at all)
$|n_1, n_2 \ldots n_e \ldots\rangle = (C_1^\dagger)^{n_1} (C_2^\dagger)^{n_2} \ldots (C_e^\dagger)^{n_e} |0\rangle$
- States $|n_1 \ldots n_e \ldots\rangle$ form a complete orthonormal basis, meaning
$\langle n_1' \ldots n_e' | n_1 \ldots n_e \ldots\rangle = \delta_{n_1,n_1'} \ldots \delta_{n_e,n_e'}$
$C_e^\dagger C_m^\dagger + C_m^\dagger C_e^\dagger \equiv \{C_e^\dagger, C_m^\dagger\} = 0$
$C_e^\dagger C_m + C_m C_e^\dagger = \delta_{em}$
$C_e^\dagger C_e + C_e C_e^\dagger = 1$


$\left(\sum_{n_1=0}^{1} \sum_{n_e=0}^{1}\right) |n_1\ n_e\rangle\langle n_1\ n_e| = \mathbb{1}$


$|n_1 \ldots n_k\rangle\langle n_1 \ldots n_k| = \mathbb{1}$
How c_k and $c_k^\dagger$ act on $|n_1 \ldots n_m\rangle$?


$\left(\sum_{n_1=0}^{1} \cdots \sum_{n_e=0}^{1}\right) |n_1 \ldots n_e\rangle\langle n_1 \ldots n_e| = \mathbb{1}$
How c_e and $c_e^\dagger$ act on $|n_1 \ldots n_m\rangle$?
If $n_e=0$ then $c_e |n_1, n_2 \ldots 0_e \ldots\rangle = 0$
If $n_e=1$ the $c_e^\dagger |n_1, n_2 \ldots 1_e \ldots\rangle = 0$
If $n_e=0$, $c_e^\dagger |n_1 \ldots 0_e \ldots\rangle = c_e^\dagger (c_1^\dagger)^{n_1} (c_2^\dagger)^{n_2} \ldots (c_{e-1}^\dagger)^{n_{e-1}} (c_{e+1}^\dagger)^{n_{e+1}} \ldots |0\rangle$


How c_ℓ and $c_\ell^\dagger$ act on $|n_1 \dots n_m \dots\rangle$?
$= 1$
$\rangle = 0$
$\rangle = 0$
If $n_\ell = 0$, $c_i^\dagger | n_1 \dots 0_\ell \dots \rangle = c_\ell^\dagger (c_1^\dagger)^{n_1} (c_2^\dagger)^{n_2} \dots (c_{\ell-1}^\dagger)^{n_{\ell-1}} (c_{\ell+1}^\dagger)^{n_{\ell+1}} |0\rangle =$
$= (-)^{\sum_{n_i=1}^{\ell-1} n_i} | n_1, \dots 1_\ell \dots \rangle$

$= 1$

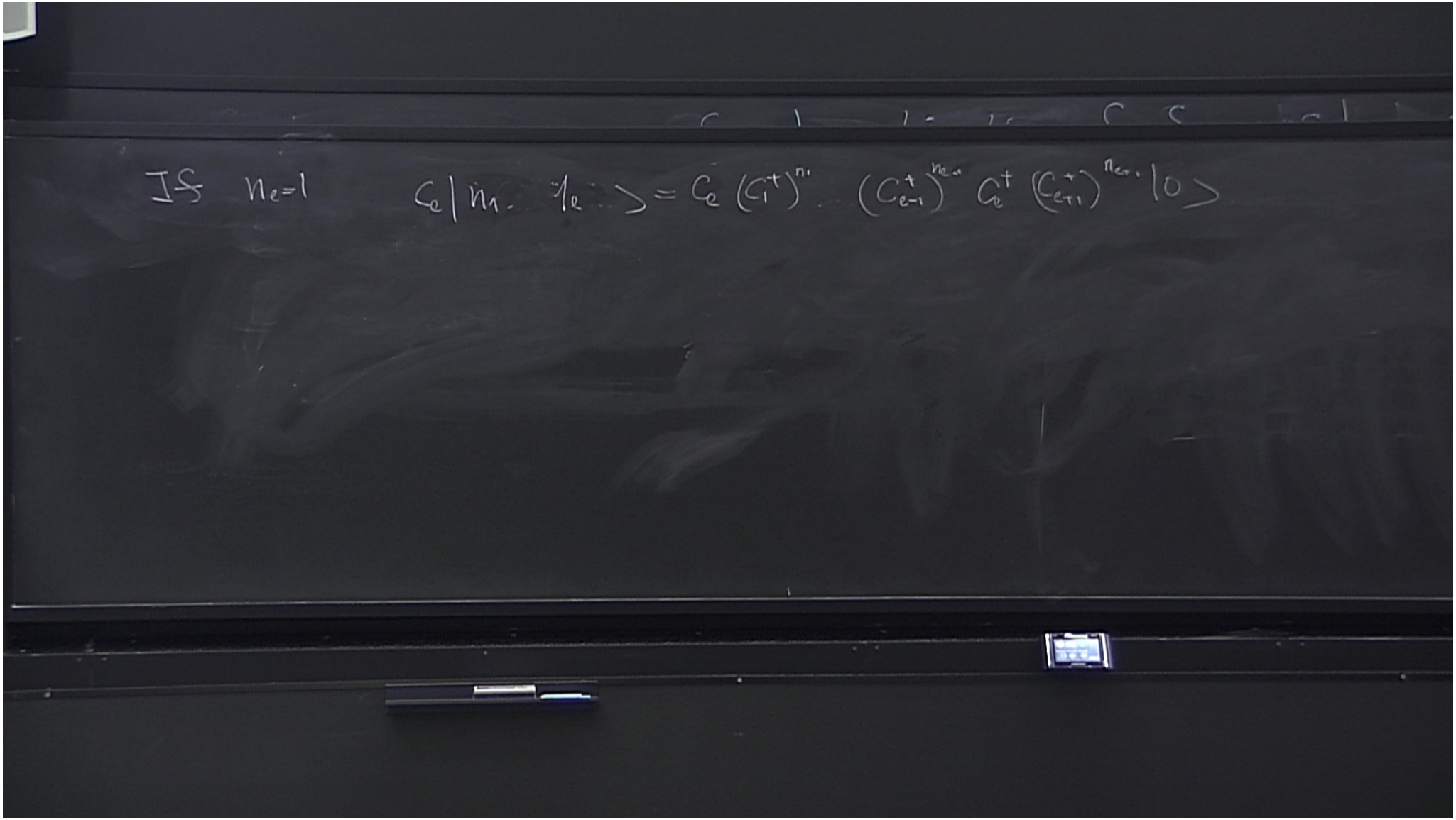
How c_ℓ and $c_\ell^\dagger$ act on $|n_1 \dots n_m \dots\rangle$?

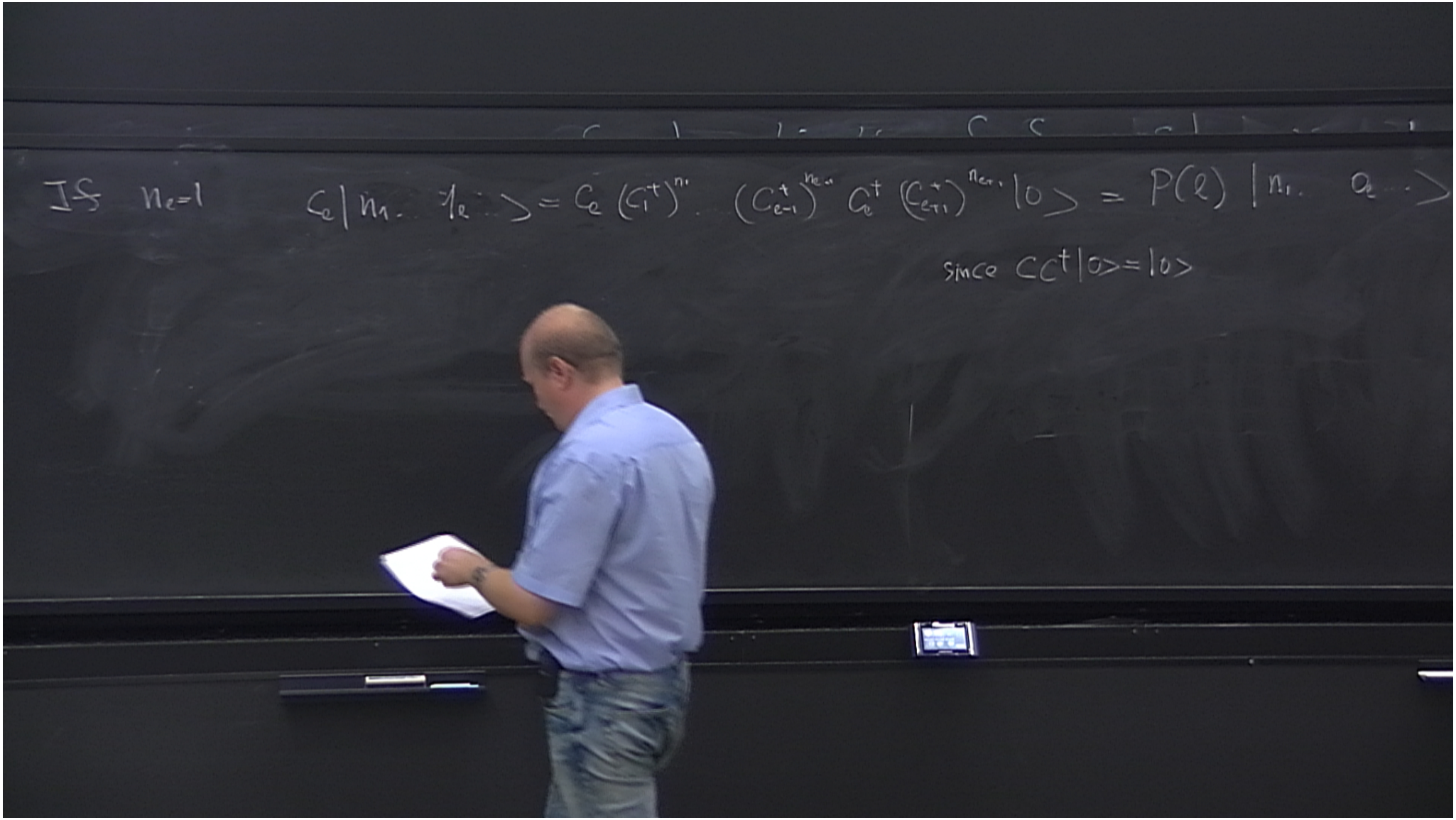
$\rangle = 0$

$\rangle = 0$

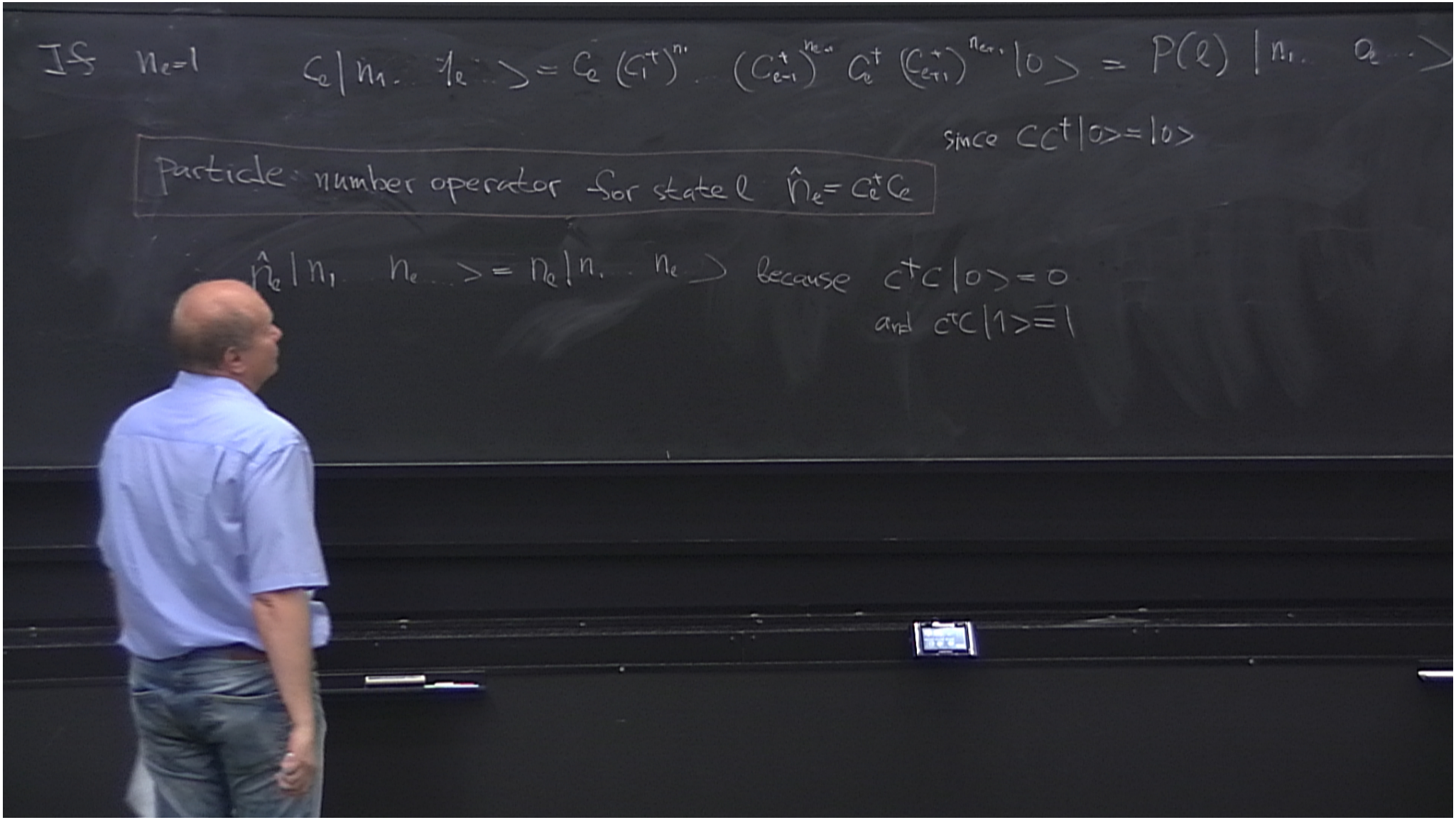
If $n_\ell = 0$, $c_\ell^\dagger |n_1 \dots 0_\ell \dots\rangle = c_\ell^\dagger (c_1^\dagger)^{n_1} (c_2^\dagger)^{n_2} \dots (c_{\ell-1}^\dagger)^{n_{\ell-1}} (c_{\ell+1}^\dagger)^{n_{\ell+1}} |0\rangle =$

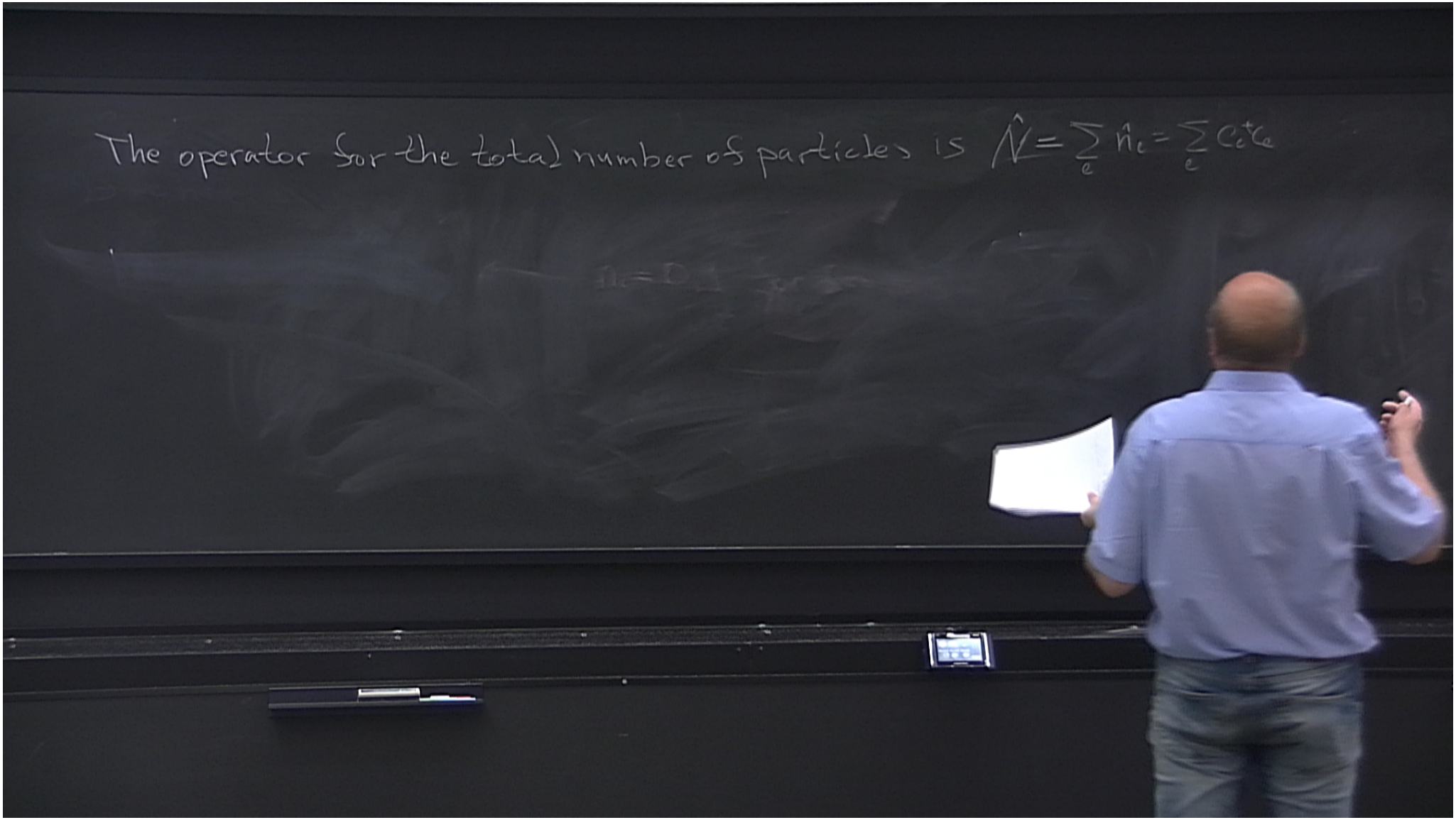
$$= \underbrace{(-)^{\sum_{n_i=1}^{\ell-1} n_i}}_{P(\ell)} |n_1, \dots 1_\ell \dots\rangle$$

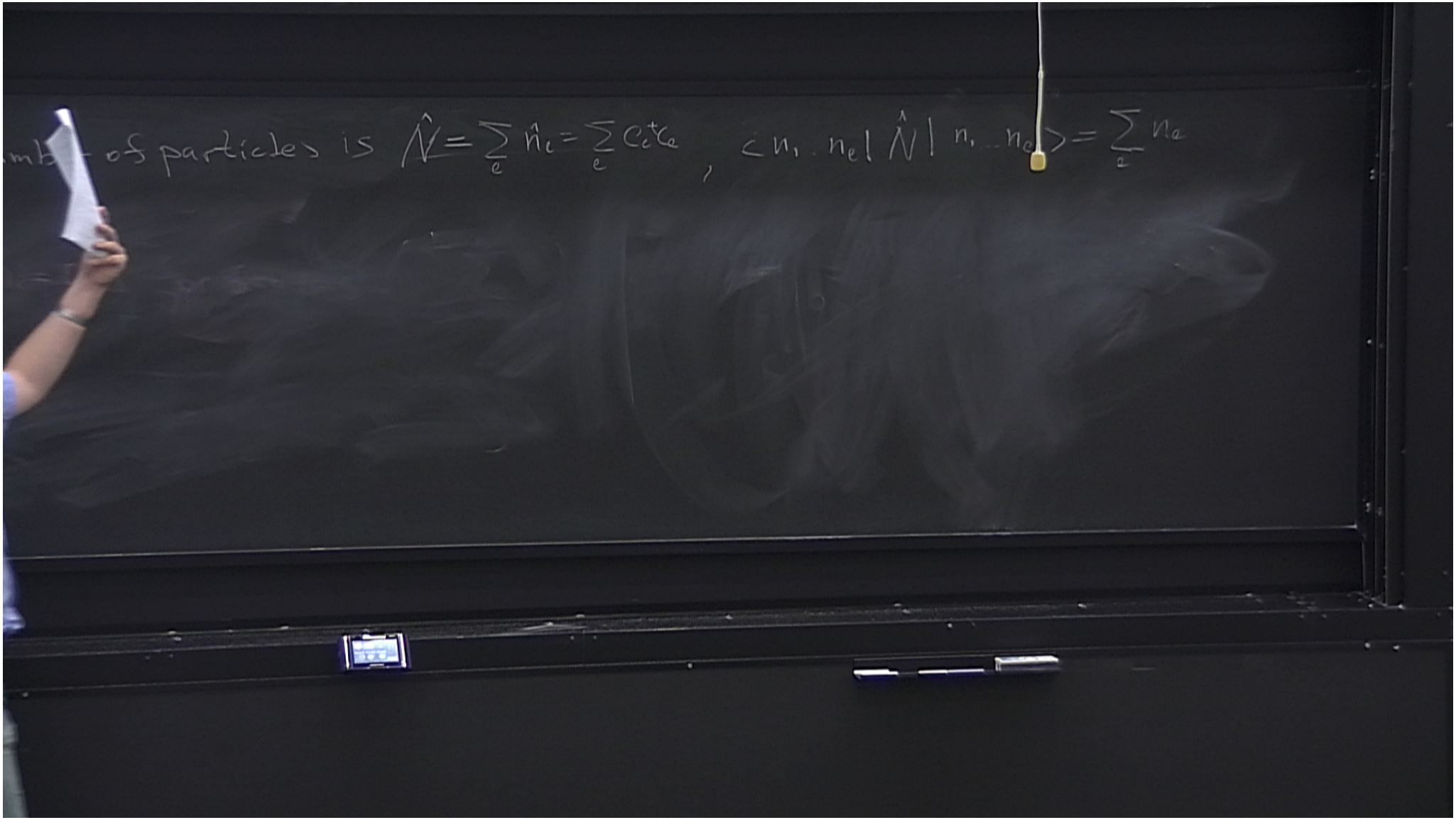

If $n_e=1$ $c_e|n_1 \ldots n_e\rangle = c_e (c_1^\dagger)^{n_1} \ldots (c_{e-1}^\dagger)^{n_{e-1}} c_e^\dagger (c_{e+1}^\dagger)^{n_{e+1}} \ldots |0\rangle$


If $n_\ell = 1$
$C_\ell |n_1 \ldots 1_\ell \ldots\rangle = C_\ell (C_1^\dagger)^{n_1} \ldots (C_{\ell-1}^\dagger)^{n_{\ell-1}} C_\ell^\dagger (C_{\ell+1}^\dagger)^{n_{\ell+1}} \ldots |0\rangle = P(\ell) |n_1 \ldots a_\ell \ldots\rangle$
since $CC^\dagger |0\rangle = |0\rangle$


If $n_\ell = 1$ $c_\ell |n_1 \ldots n_\ell \ldots\rangle = c_\ell (c_1^\dagger)^{n_1} \ldots (c_{\ell-1}^\dagger)^{n_{\ell-1}} c_\ell^\dagger (c_{\ell+1}^\dagger)^{n_{\ell+1}} |0\rangle = P(\ell) |n_1 \ldots n_\ell \ldots\rangle$
since $cc^\dagger|0\rangle = |0\rangle$
particle number operator for state ℓ $\hat{n}_\ell = c_\ell^\dagger c_\ell$
$\hat{n}_\ell |n_1 \ldots n_\ell \ldots\rangle = n_\ell |n_1 \ldots n_\ell \ldots\rangle$


If $n_\ell = 1$ $c_\ell |n_1 \ldots n_\ell \ldots\rangle = c_\ell (c_1^\dagger)^{n_1} \ldots (c_{\ell-1}^\dagger)^{n_{\ell-1}} c_\ell^\dagger (c_{\ell+1}^\dagger)^{n_{\ell+1}} |0\rangle = P(\ell) |n_1 \ldots n_\ell \ldots\rangle$
since $cc^\dagger|0\rangle = |0\rangle$
Particle number operator for state ℓ $\hat{n}_\ell = c_\ell^\dagger c_\ell$
$\hat{n}_\ell |n_1 \ldots n_\ell \ldots\rangle = n_\ell |n_1 \ldots n_\ell \ldots\rangle$ because $c^\dagger c|0\rangle = 0$
and $c^\dagger c|1\rangle = 1$


The operator for the total number of particles is $\hat{N} = \sum_i \hat{n}_i = \sum_i c_i^\dagger c_i$


of particles is $\hat{N} = \sum_i \hat{n}_i = \sum_i c_i^\dagger c_i$, $\langle n_1 \ldots n_i | \hat{N} | n_1 \ldots n_i \rangle = \sum_i n_i$

The operator for the total number of particles is $\hat{N} = \sum_e \hat{n}_e = \sum_e c_e^+ c_e$, $\langle n_1 \ldots n_e | \hat{N}$

$H = \sum_e \varepsilon_e \hat{n}_e = \sum_e \varepsilon_e c_e^+ c_e$ – Hamiltonian and $\langle n_1 \ldots n_e | H | n_1 \ldots n_e \rangle = \sum_e \varepsilon_e n_e$

The operator for the total number of particles is $\hat{N} = \sum_\ell \hat{n}_\ell = \sum_\ell c_\ell^\dagger c_\ell$, $\langle n_1, n_\ell | \hat{N} | n_1 \ldots n_\ell \rangle = \sum_\ell n_\ell$

$H = \sum_\ell \varepsilon_\ell \hat{n}_\ell = \sum_\ell \varepsilon_\ell c_\ell^\dagger c_\ell$ – Hamiltonian and $\langle n_1, n_\ell | H | n_1 \ldots n_\ell \rangle = \sum_\ell \varepsilon_\ell n_\ell$

Often we need $H' = H - \mu N = \sum_\ell (\varepsilon_\ell - \mu) c_\ell^\dagger c_\ell$ that for fermions in a box reduces to $H' = \sum_{k\sigma} \left(\frac{\hbar^2 k^2}{2m} - \mu \right) c_{k\sigma}^\dagger c_{k\sigma}$