Title: Front End - Condensed Matter - 1

Date: Aug 29, 2016 10:30 AM

URL: http://pirsa.org/16080086

Abstract:

Today

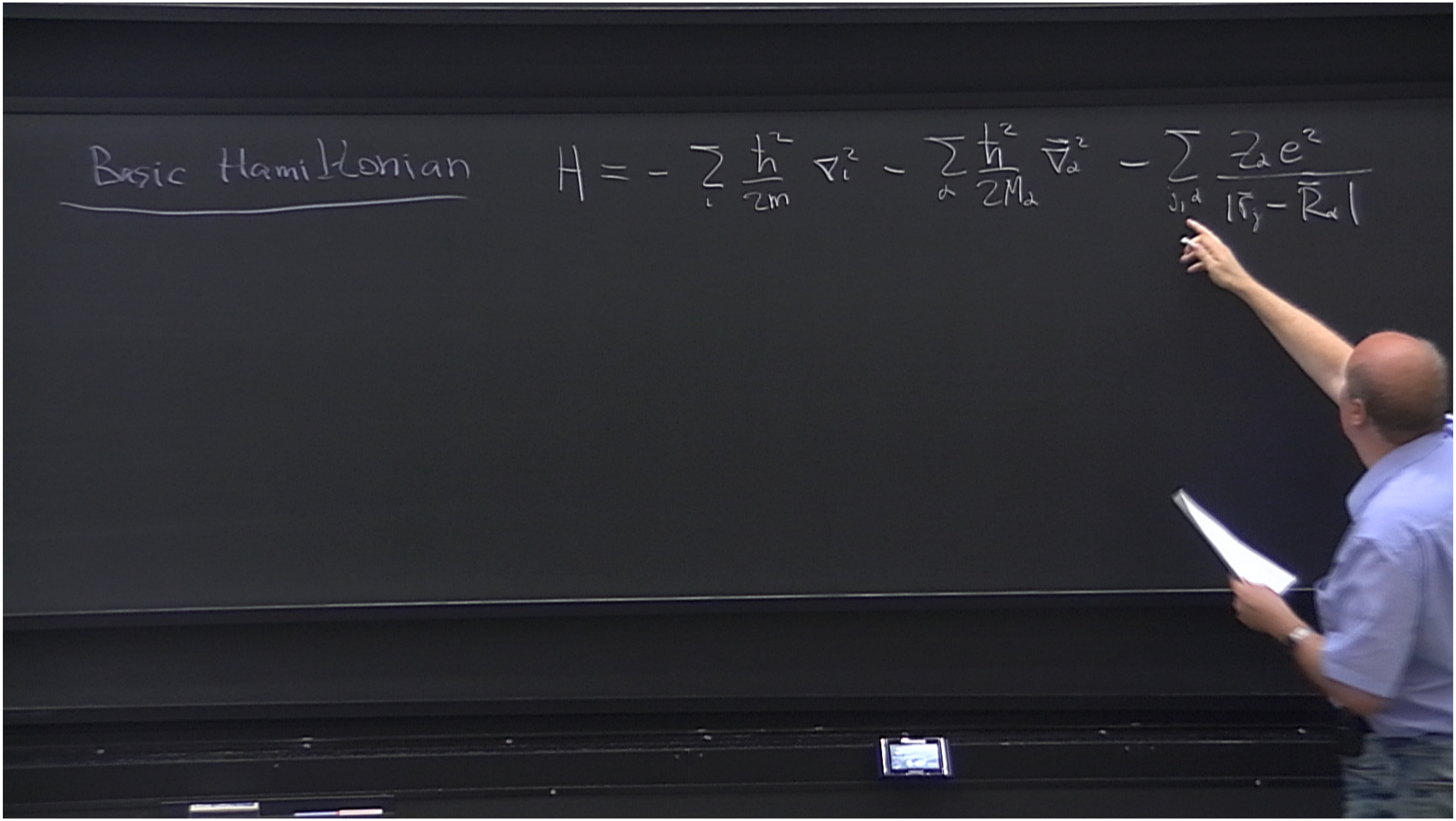
- Basic Hamiltonian and simplified models of condensed ma

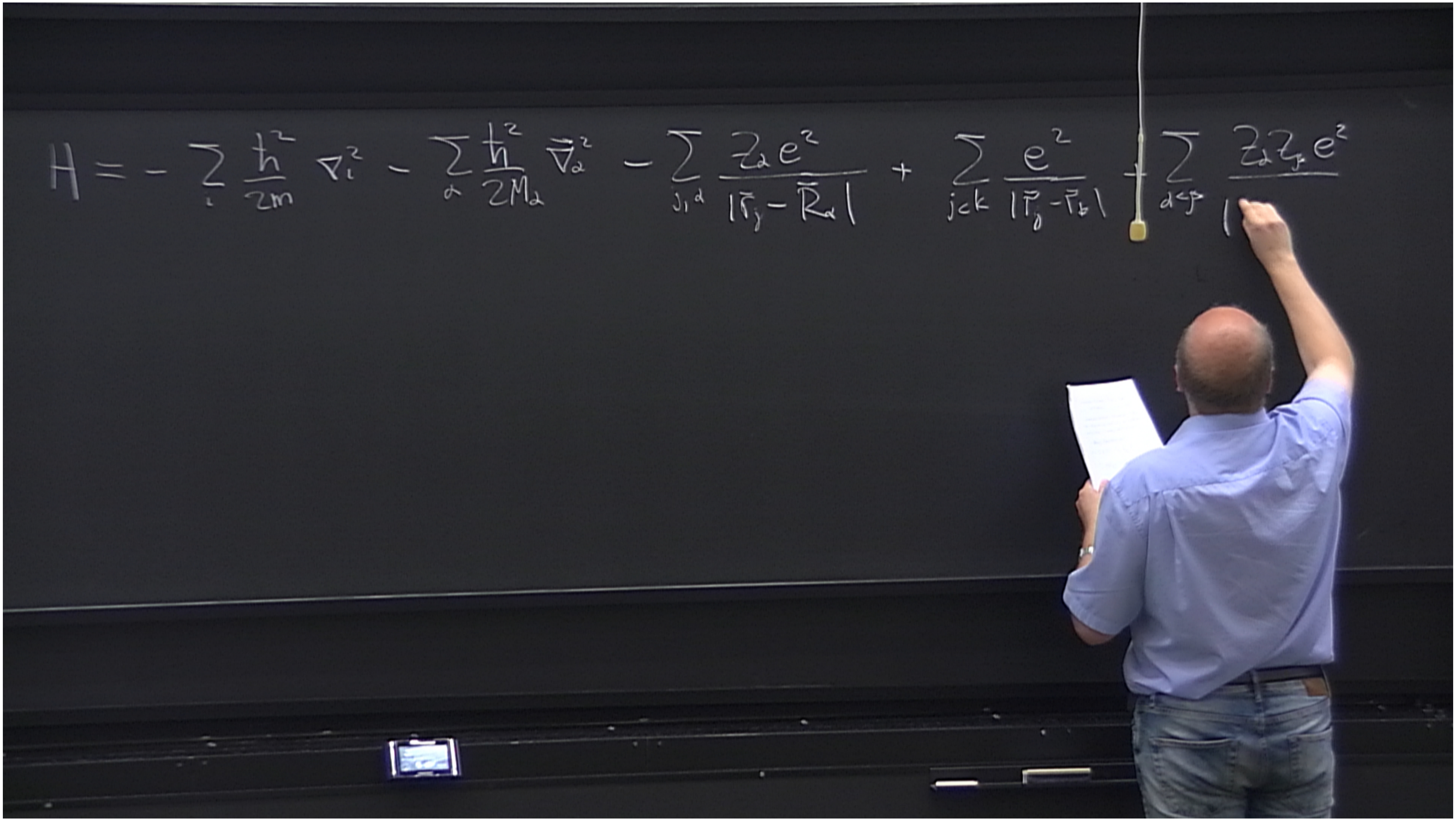
- Thermodynamics (quick recap)

- Free particle in a box and periodic boundary conditions

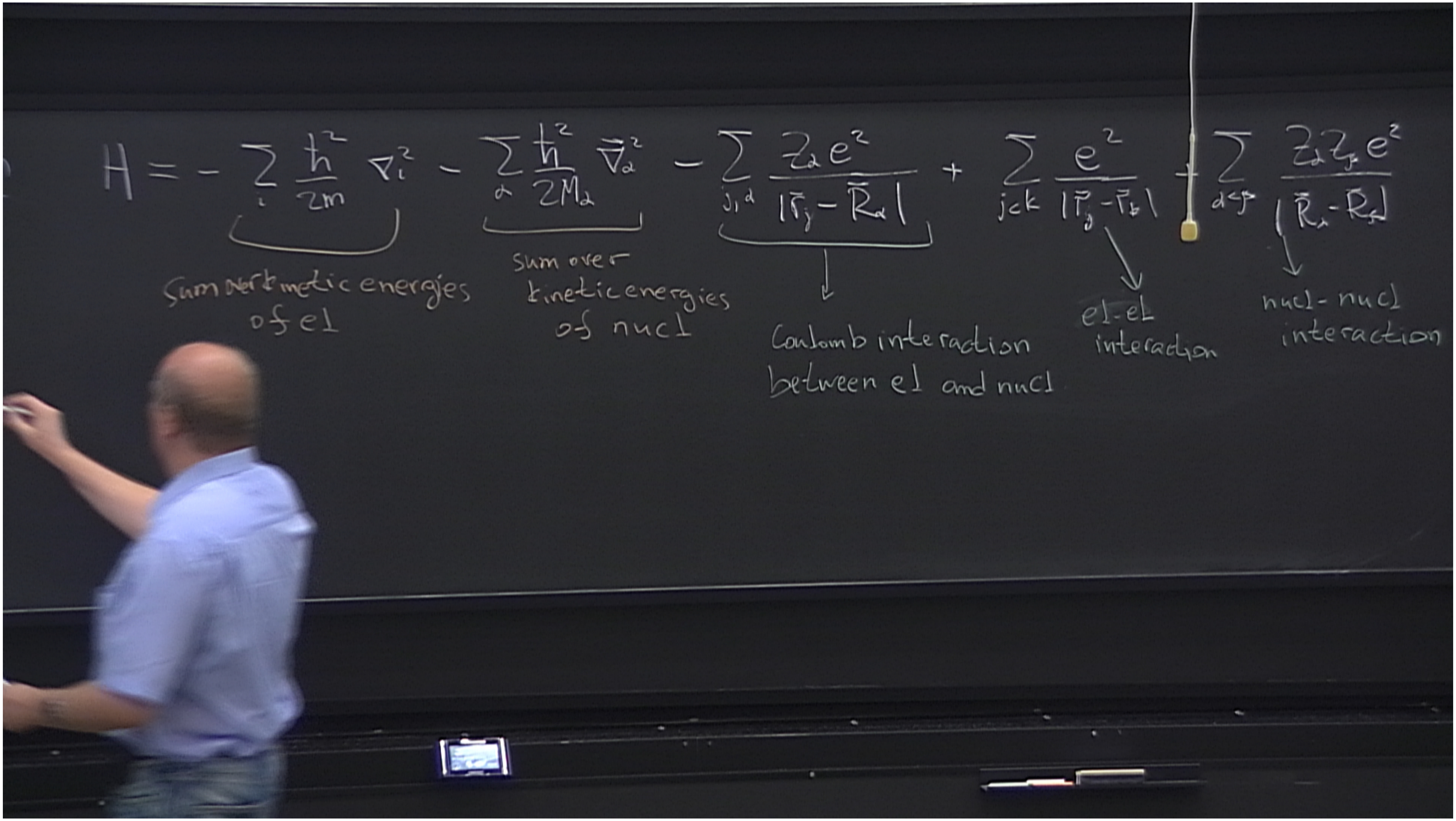
- Thermodynamic limit and density of states

- (start?) Thermodynamics of free electron gas


Basic Hamiltonian
$H = -\sum_i \frac{\hbar^2}{2m}\nabla_i^2 - \sum_\alpha \frac{\hbar^2}{2M_\alpha}\vec{\nabla}_\alpha^2 - \sum_{j,\alpha}\frac{Z_\alpha e^2}{|\vec{r}_j - \vec{R}_\alpha|}$


$H = -\sum_i \frac{\hbar^2}{2m}\nabla_i^2 - \sum_\alpha \frac{\hbar^2}{2M_\alpha}\vec{\nabla}_\alpha^2 - \sum_{j,\alpha} \frac{Z_\alpha e^2}{|\vec{r}_j - \vec{R}_\alpha|} + \sum_{j<k} \frac{e^2}{|\vec{r}_j - \vec{r}_k|} + \sum_{\alpha<\beta} \frac{Z_\alpha Z_\beta e^2}{|}$

$$H = \underbrace{-\sum_i \frac{\hbar^2}{2m}\nabla_i^2}_{\text{sum over kinetic energies of el}} \underbrace{- \sum_\alpha \frac{\hbar^2}{2M_\alpha}\vec{\nabla}_\alpha^2}_{\text{sum over kinetic energies of nucl}} - \sum_{j,\alpha} \frac{Z_\alpha e^2}{|\vec{r}_j - \vec{R}_\alpha|} + \sum_{j<k} \frac{e^2}{|\vec{r}_j - \vec{r}_k|} + \sum_{\alpha<\beta} \frac{Z_\alpha Z_\beta e^2}{|\vec{R}_\alpha - \vec{R}_\beta|}$$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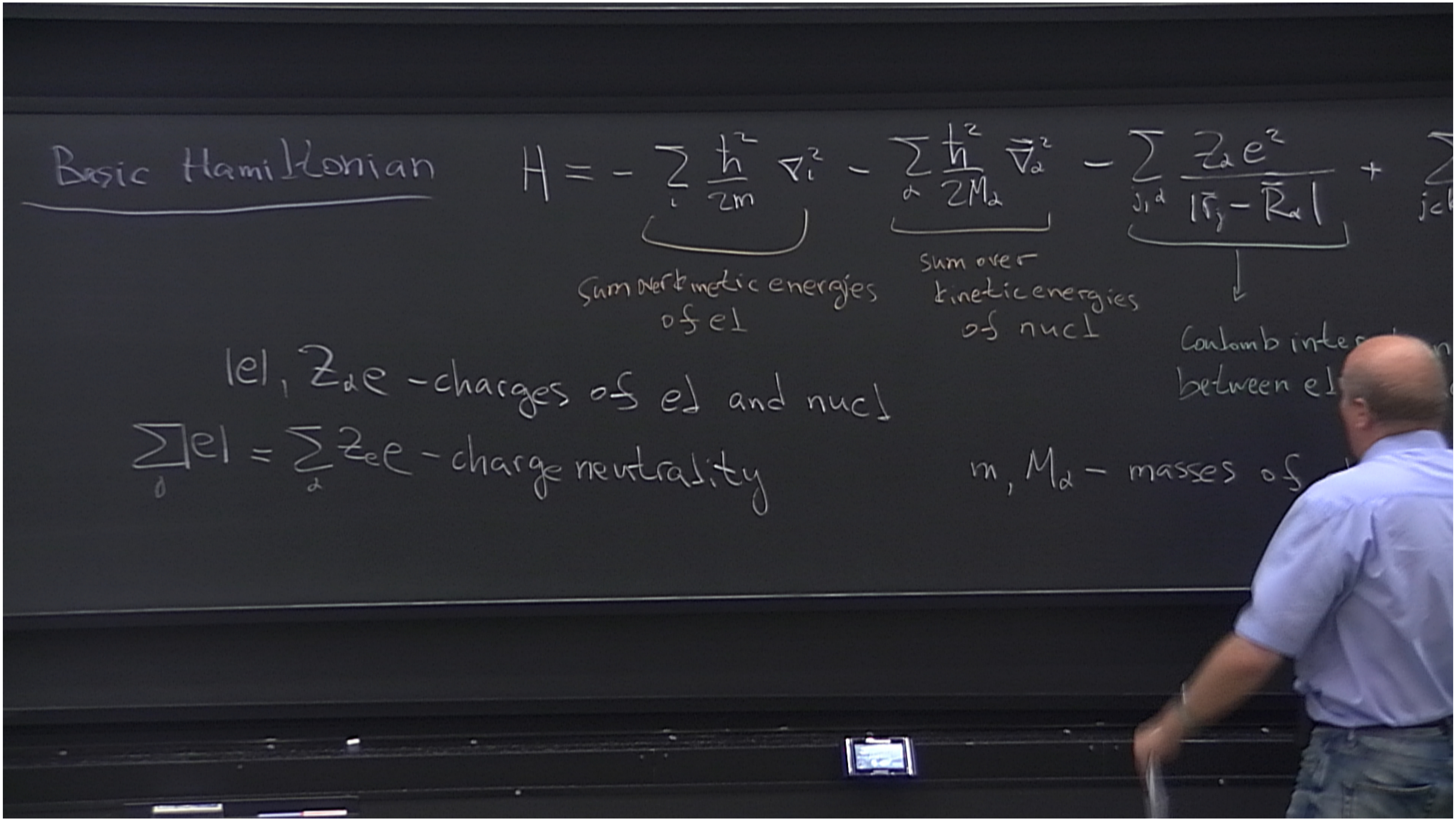
Sum over kinetic energies of el
sum over kinetic energies of nucl
Coulomb interaction between el and nucl
el-el interaction
nucl-nucl interaction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Sum over kinetic energies of el
Sum over kinetic energies of nucl
Coulomb inte
between el
$|e|, Z_\alpha e$ - charges of el and nucl
$\sum_j |e| = \sum_\alpha Z_\alpha e$ - charge neutrality
m, M_α - masses of

$$\underbrace{\sum_i \frac{\ldots}{2m}}_{\text{sum over kinetic energies of el}} \quad \underbrace{\sum_\alpha \frac{\ldots}{2M_\alpha}}_{\text{sum over kinetic energies of nucl}} \quad \underbrace{\sum_{j,\alpha} \frac{\ldots}{|\vec{r}_j - \vec{R}_\alpha|}}_{\text{Coulomb interaction between el and nucl}} \quad \underbrace{\sum_{j<k} \frac{\ldots}{|\vec{r}_j - \vec{r}_k|}}_{\text{el-el interaction}} \quad \underbrace{\sum_{\alpha<\beta} \frac{\ldots}{|\vec{R}_\alpha - \vec{R}_\beta|}}_{\text{nucl-nucl interaction}}$$

- charges of el and nucl
- charge neutrality

m, M_α – masses of el and nucl

$\vec{r}_i$ and $\vec{R}_\alpha$ – coordinates of el and nucl

$\underbrace{2m}$ $\underbrace{2M_\alpha}$ $\underbrace{\sum_{j,\alpha} |\vec{r}_j - \vec{R}_\alpha|}$ $\sum_{j<k} |\vec{r}_j - \vec{r}_k|$ $\sum_{\alpha<\beta} |\vec{R}_\alpha - \vec{R}_\beta|$

sum over kinetic energies of el

sum over kinetic energies of nucl

Coulomb interaction between el and nucl

el-el interaction

nucl-nucl interaction

- charges of el and nucl
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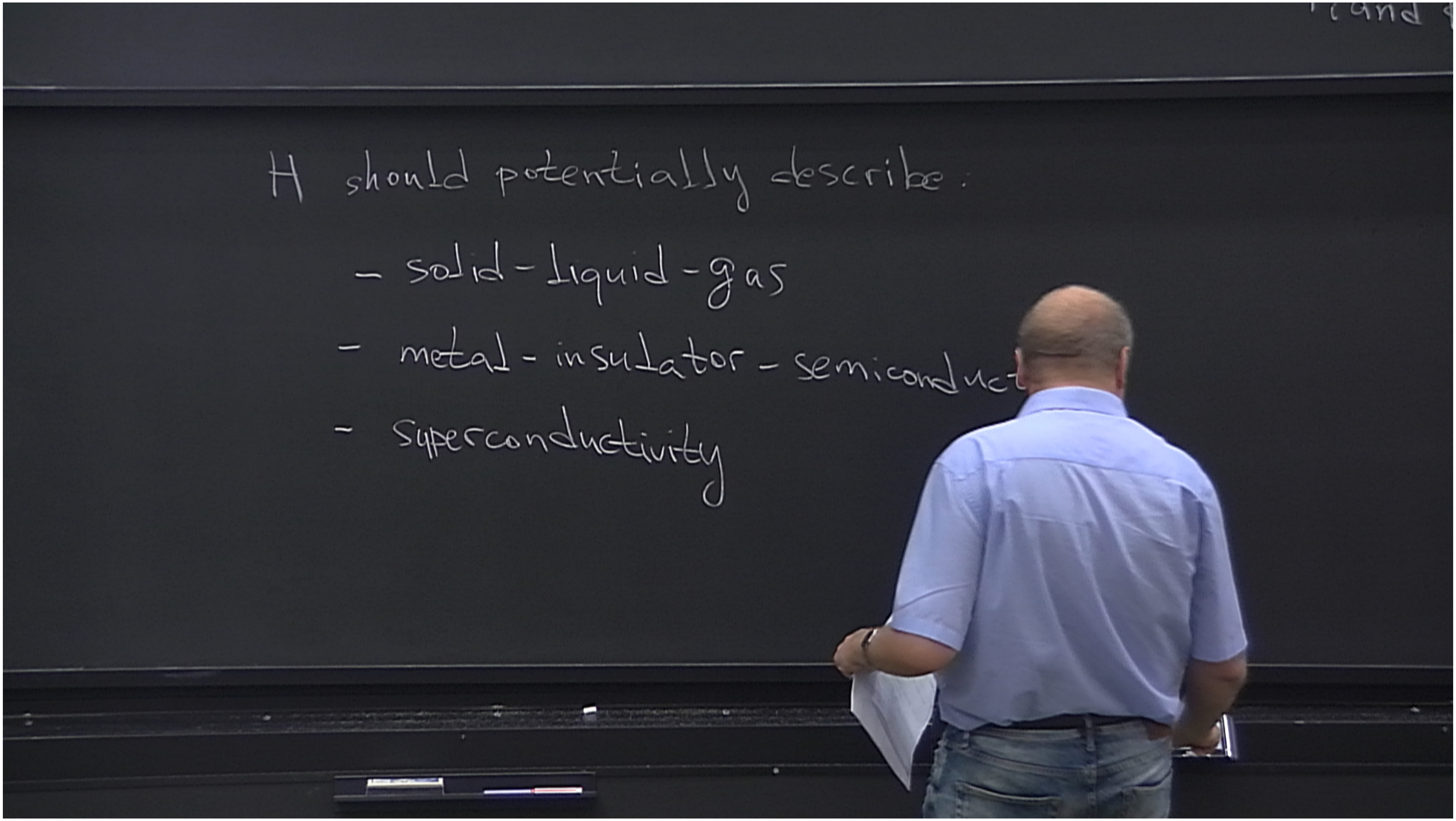
H should potentially describe:
- solid - liquid - gas
- metal - insulator - semiconduct
- superconductivity

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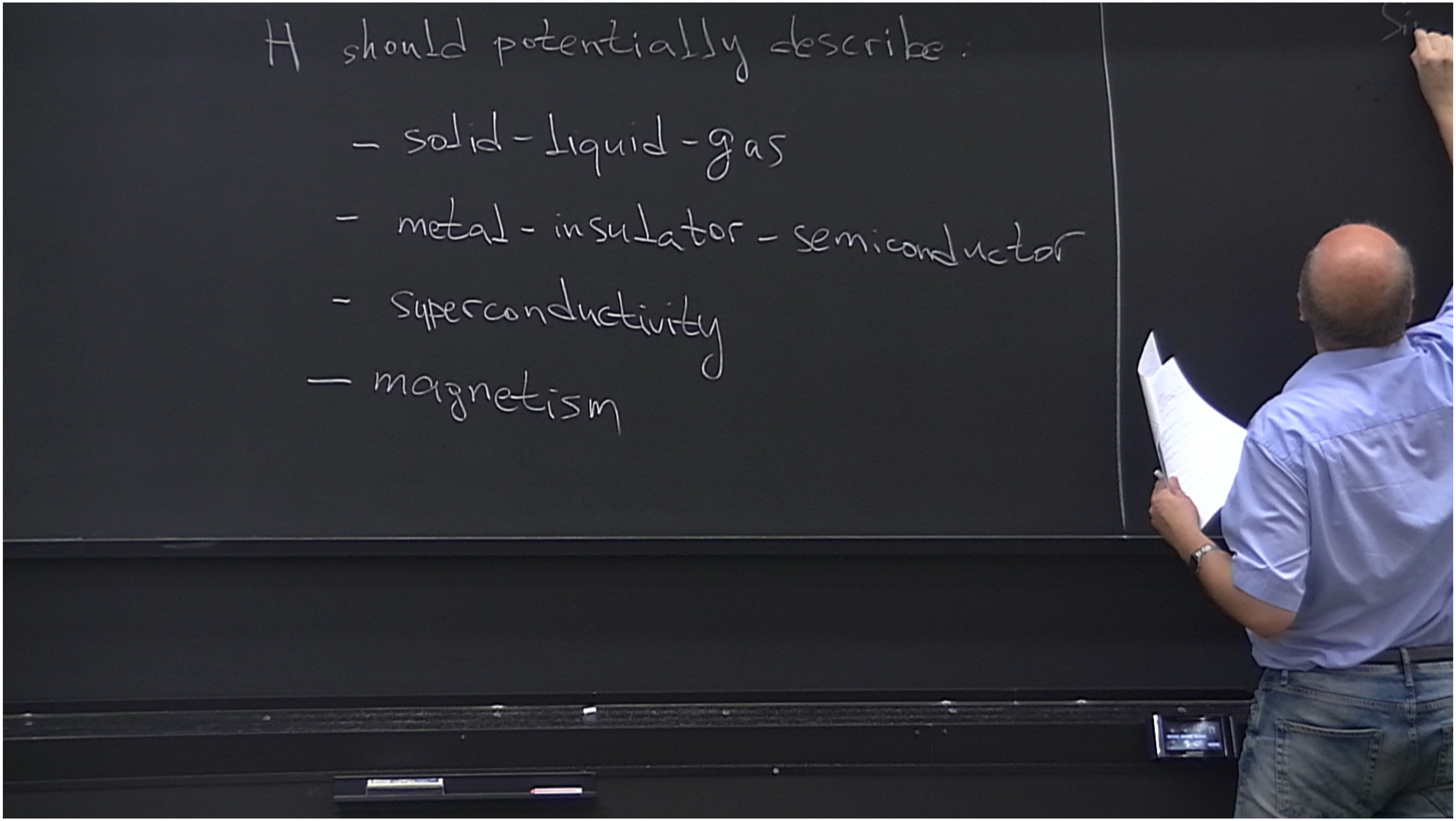
- superconductivity
- magnetism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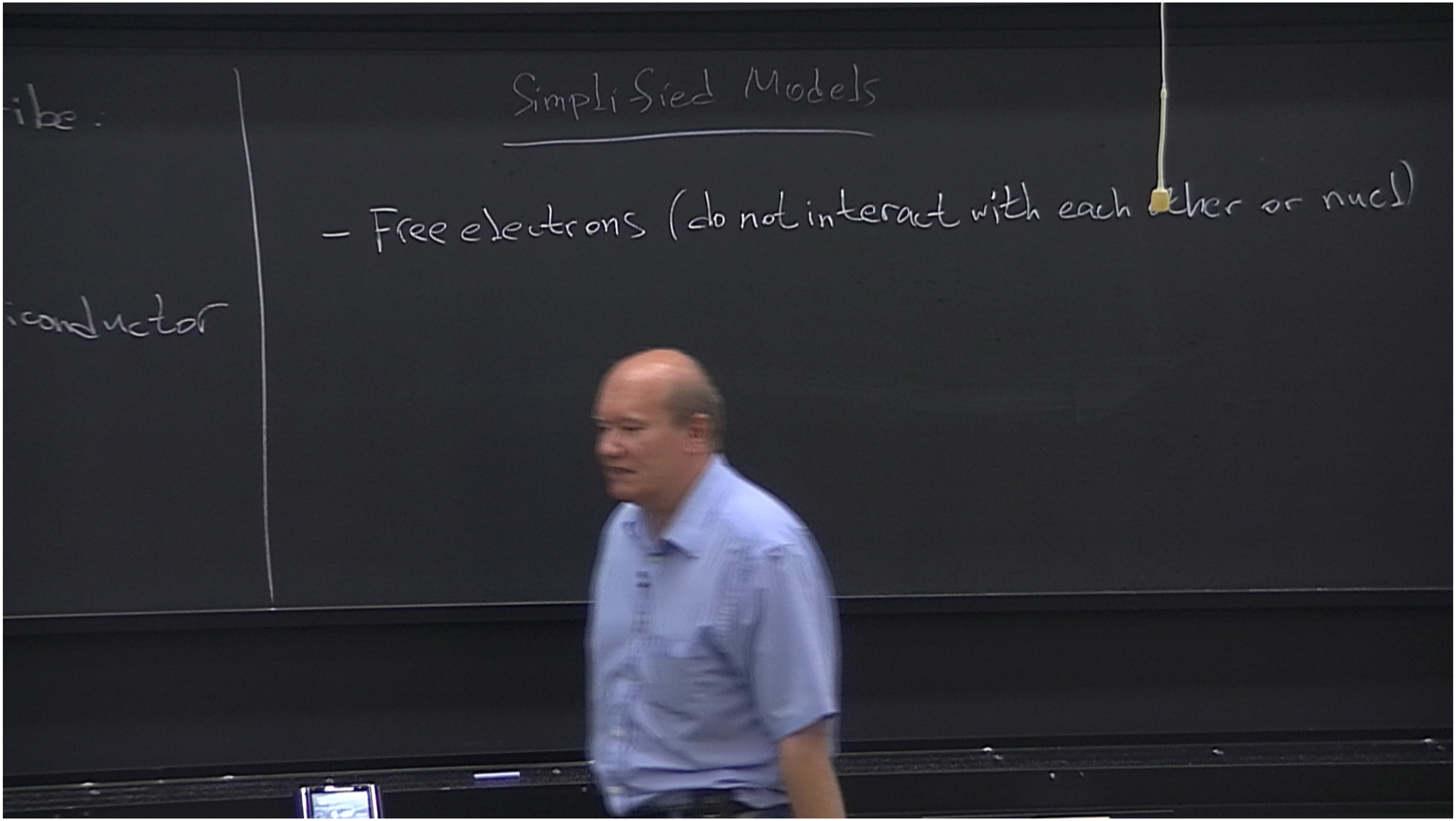

ibe :
iconductor
Simplified Models
- Free electrons (do not interact with each other or nucl)

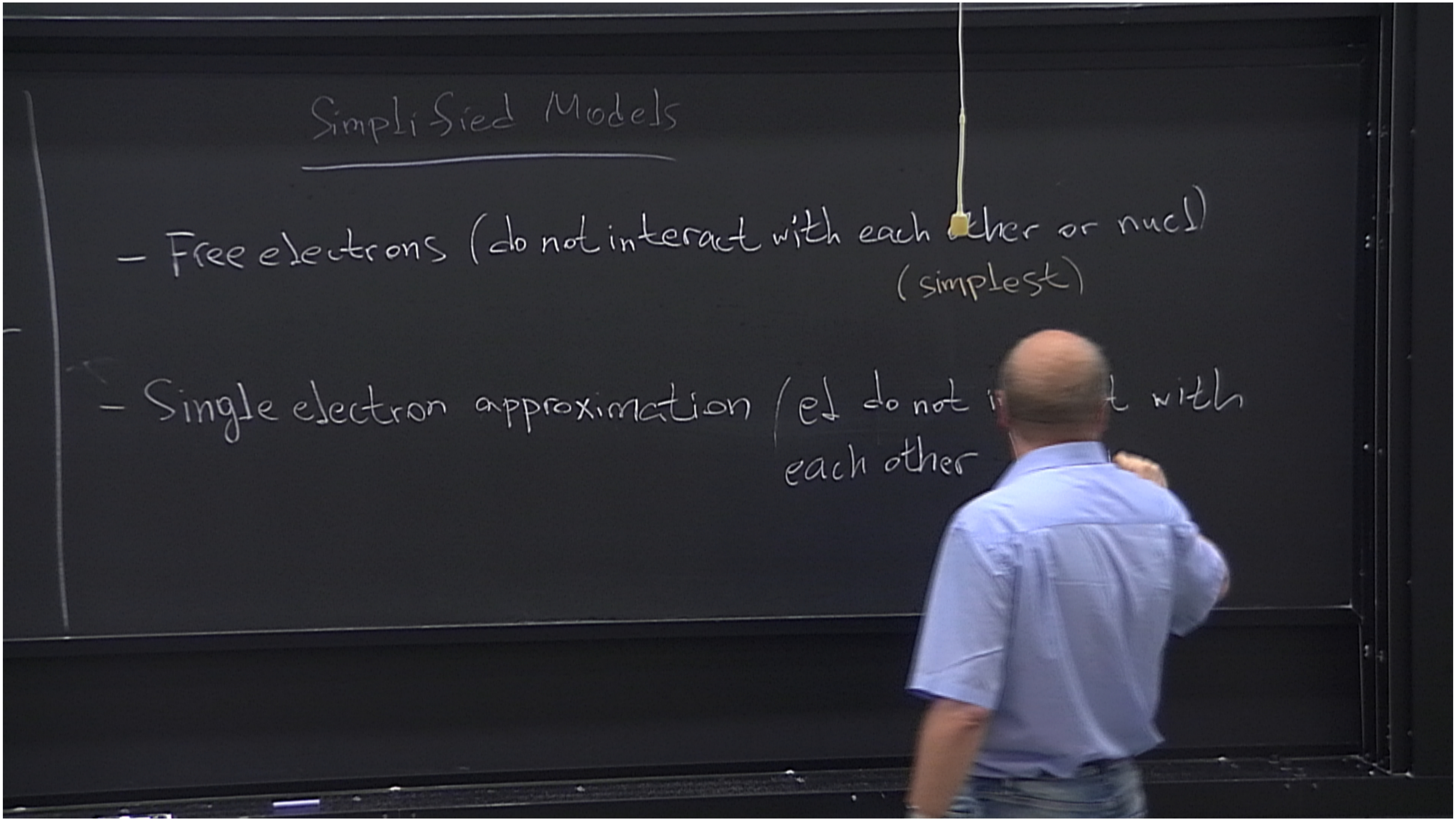
ibe:

iconductor

Simplified Models

- Free electrons (do not interact with each other or nucl)
  (simplest)

- Single electron approximation (


Simplified Models
- Free electrons (do not interact with each other or nucl)
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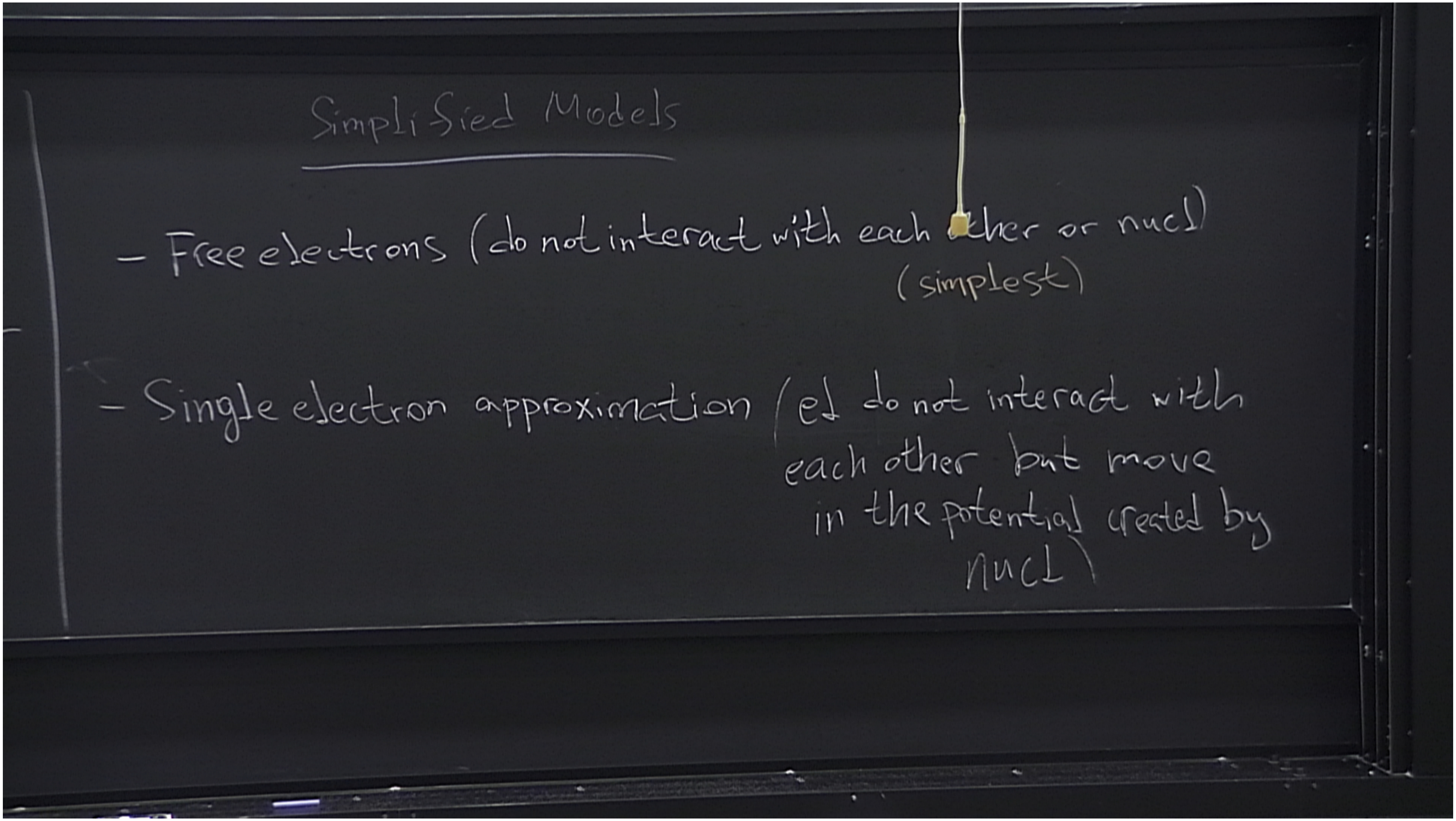
Simplified Models
- Free electrons (do not interact with each other or nucl)
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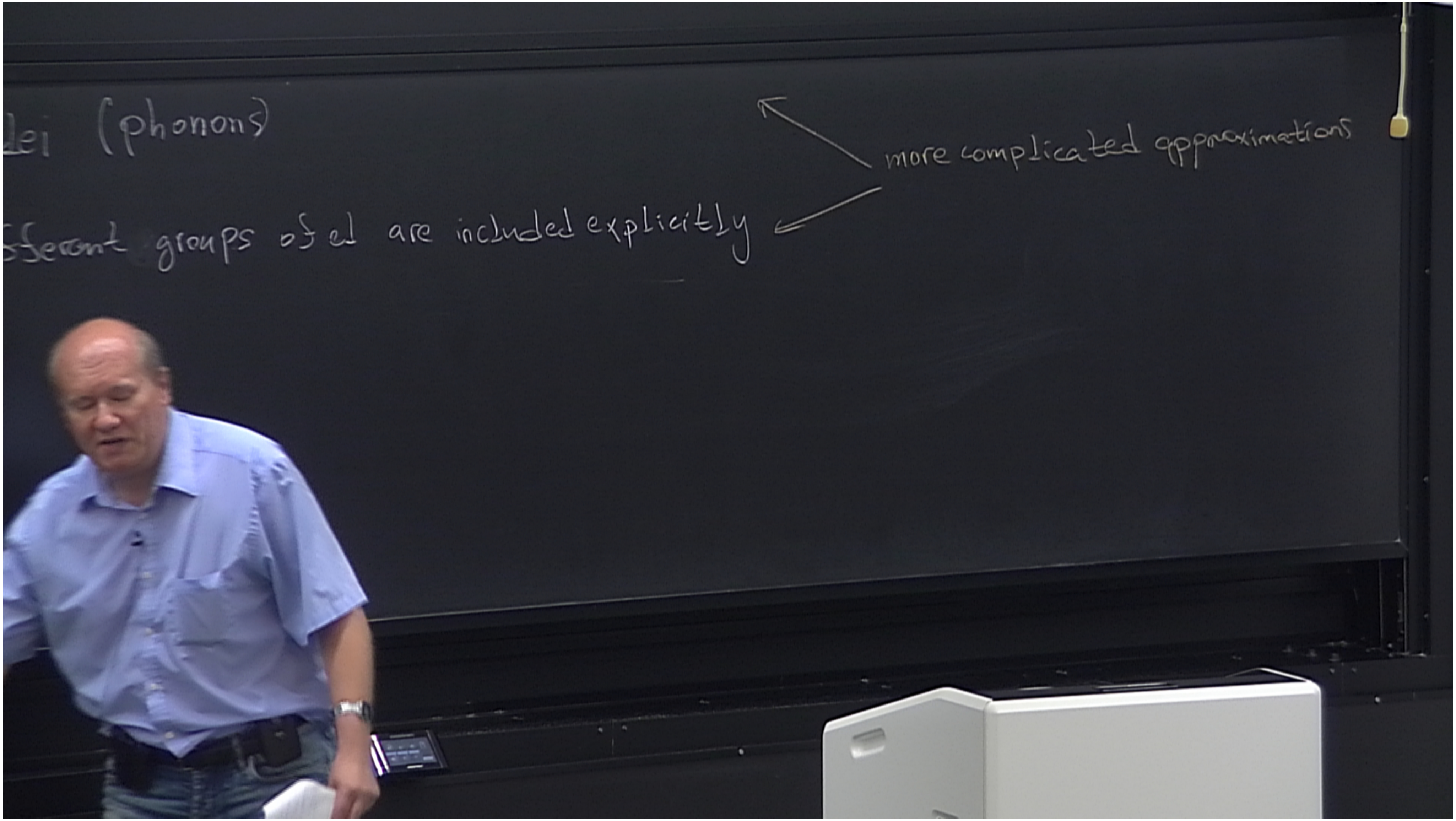
- Single electron approximation (el do not interact with each other but move in the potential created by nucl)

Simplified Models

- Free electrons (do not interact with each other or nucl)
  (simplest)

- Single electron approximation (el do not interact with each other but move in the potential created by nucl)
  (more complicated

- Approximation with moving nuclei (phonons)
- el-el interactions between different groups of el are inc


(phonons)
more complicated approximations
fferent groups of el are included explicitly

- Volume V (pressure P)
- chemical potential μ (number of particles N)

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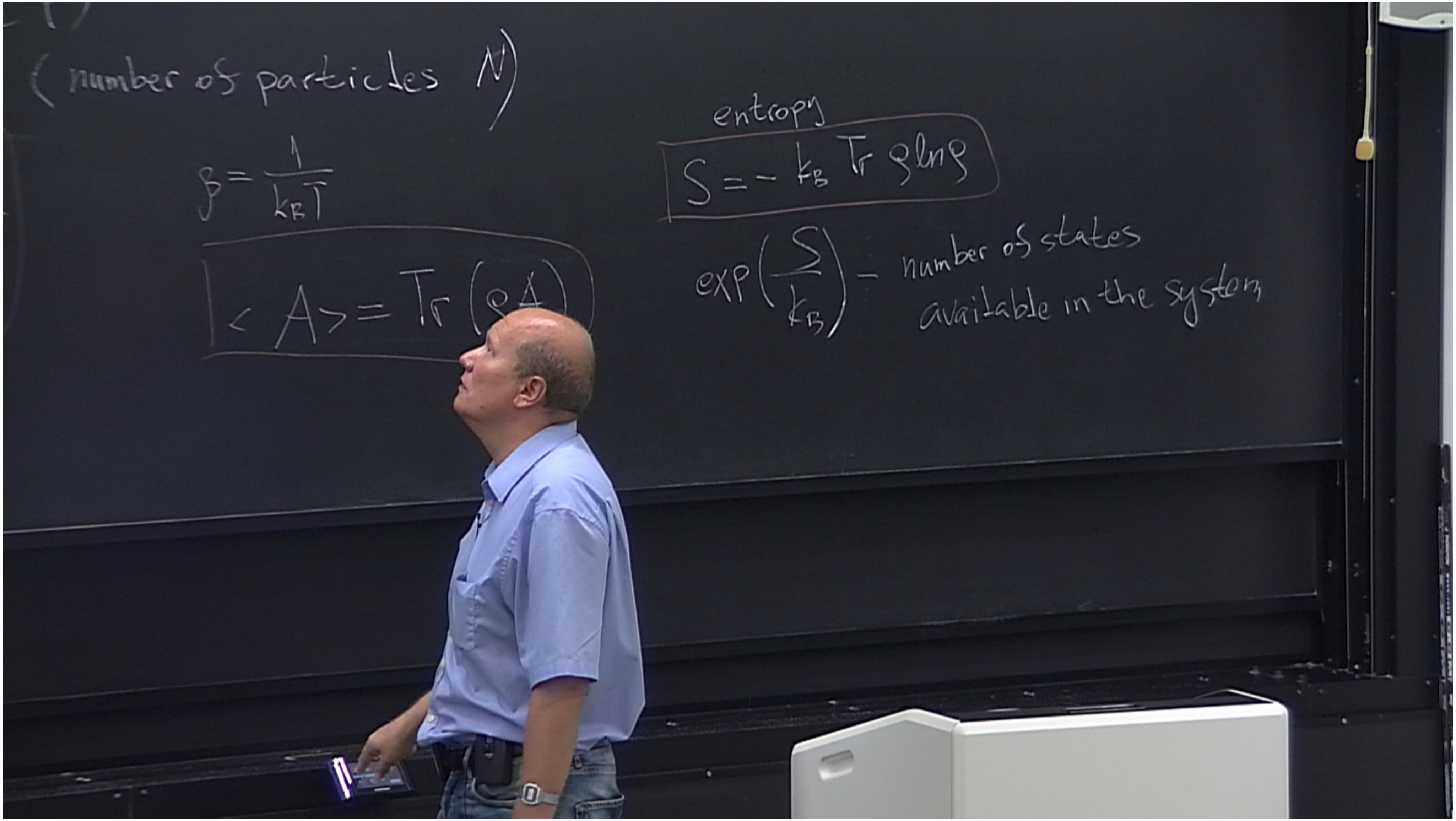
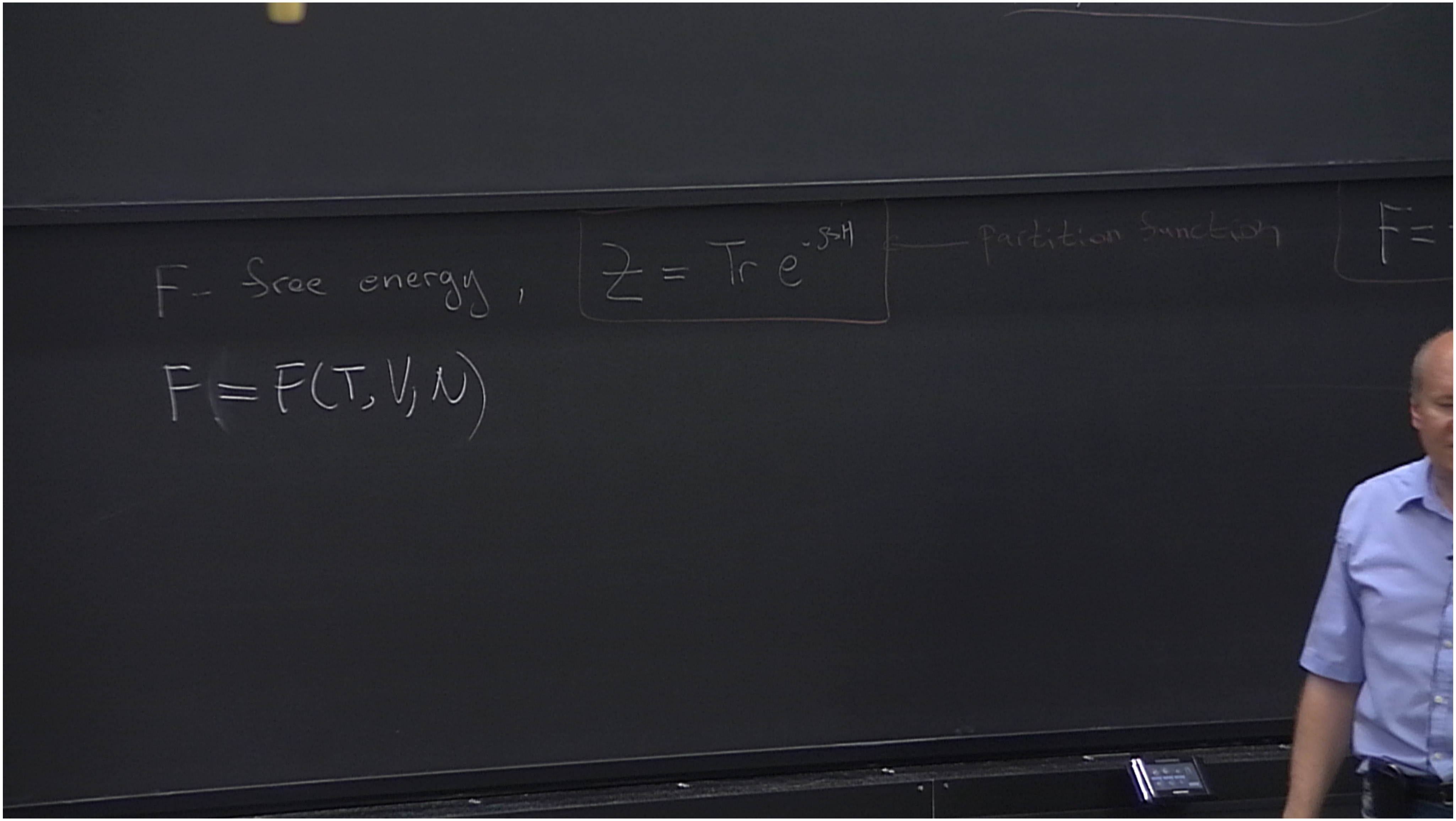
Density matrix $\rho = \dfrac{e^{-\beta H}}{\mathrm{Tr}\, e^{-\beta H}}$ $\qquad \beta = \dfrac{1}{k_B T}$


(number of particles N)
entropy
$S = -k_B \, \mathrm{Tr}\, \rho \ln \rho$
$\beta = \frac{1}{k_B T}$
$\langle A \rangle = \mathrm{Tr}(\rho A)$
$\exp\left(\frac{S}{k_B}\right)$ – number of states available in the system

F – free energy, $\boxed{Z = \mathrm{Tr}\, e^{-\beta H}}$ ⟵ partition function

$F = -$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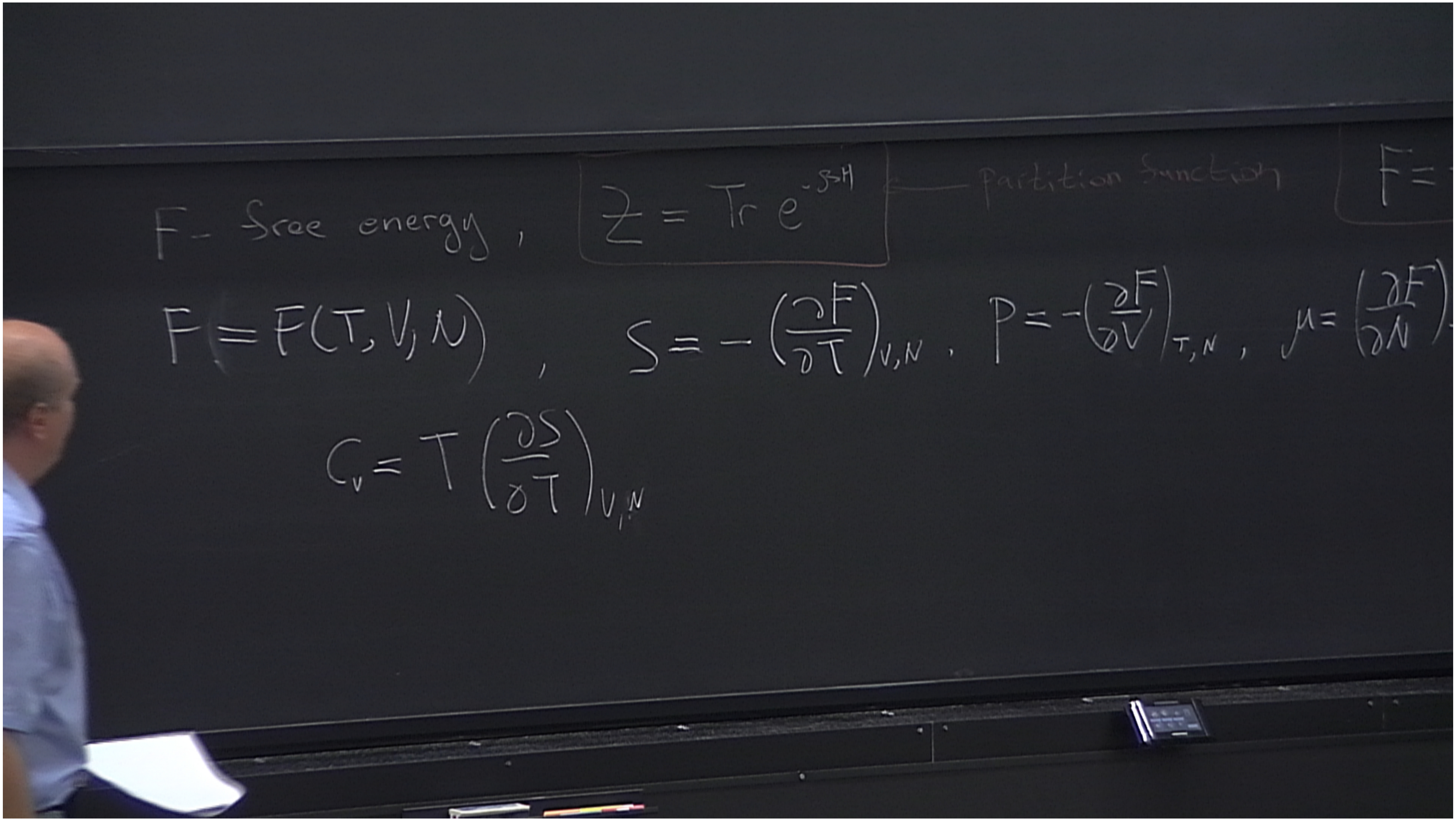
F =
$F = F(T, V, N)$

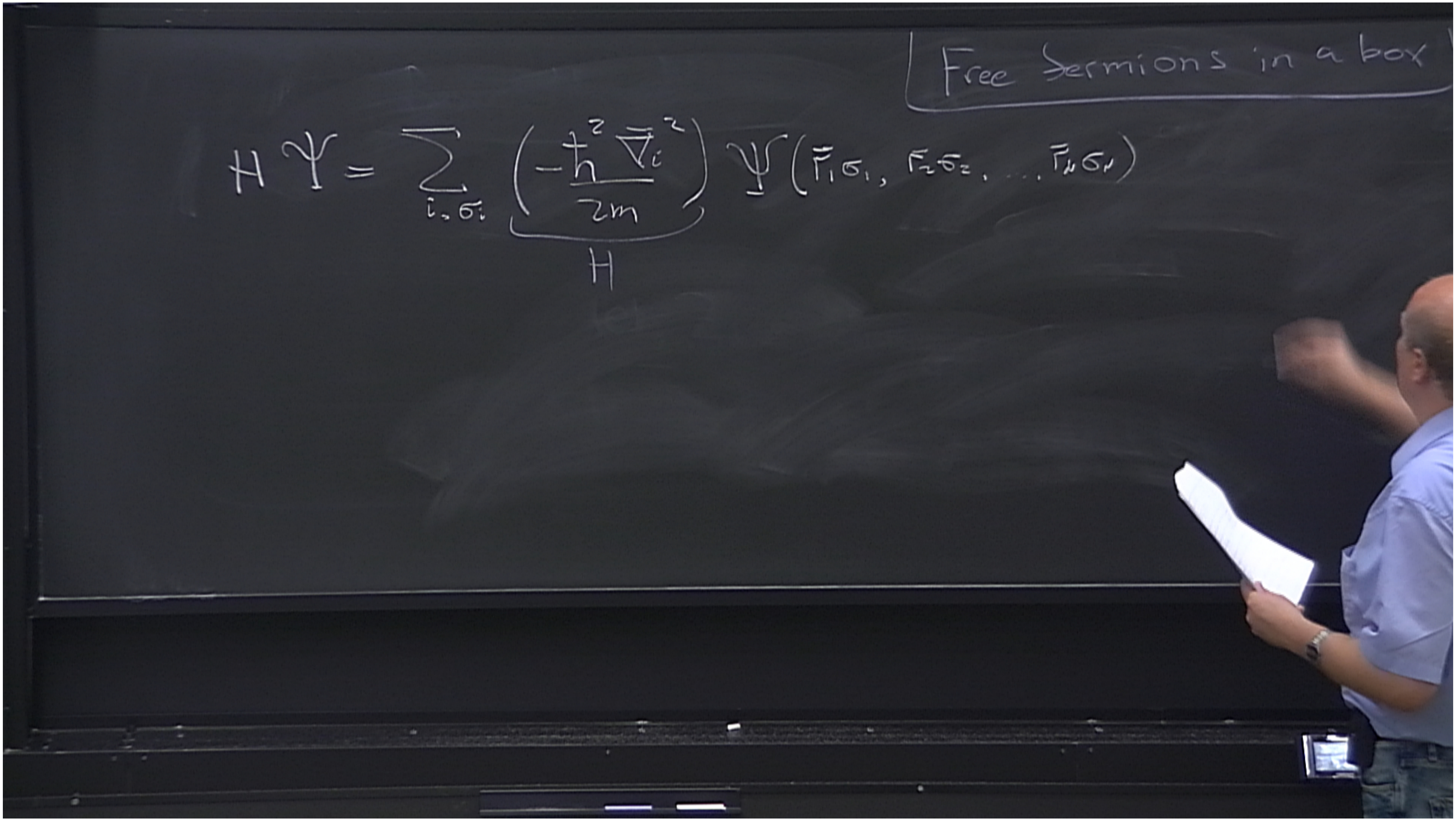
F - free energy, $\boxed{Z = \mathrm{Tr}\, e^{-\beta H}}$ ← partition function $\boxed{F = \ldots}$

$F = F(T, V, N)$, $S = -\left(\frac{\partial F}{\partial T}\right)_{V,N}$, $P = -\left(\frac{\partial F}{\partial V}\right)_{T,N}$, $\mu = \frac{\partial F}{\partial}$


F – free energy, $\boxed{Z = \mathrm{Tr}\, e^{-\beta H}}$ ← partition function
$F = F(T, V, N)$, $S = -\left(\frac{\partial F}{\partial T}\right)_{V,N}$, $P = -\left(\frac{\partial F}{\partial V}\right)_{T,N}$, $\mu = \left(\frac{\partial F}{\partial N}\right)$
$C_V = T\left(\frac{\partial S}{\partial T}\right)_{V,N}$

Free fermions in a box

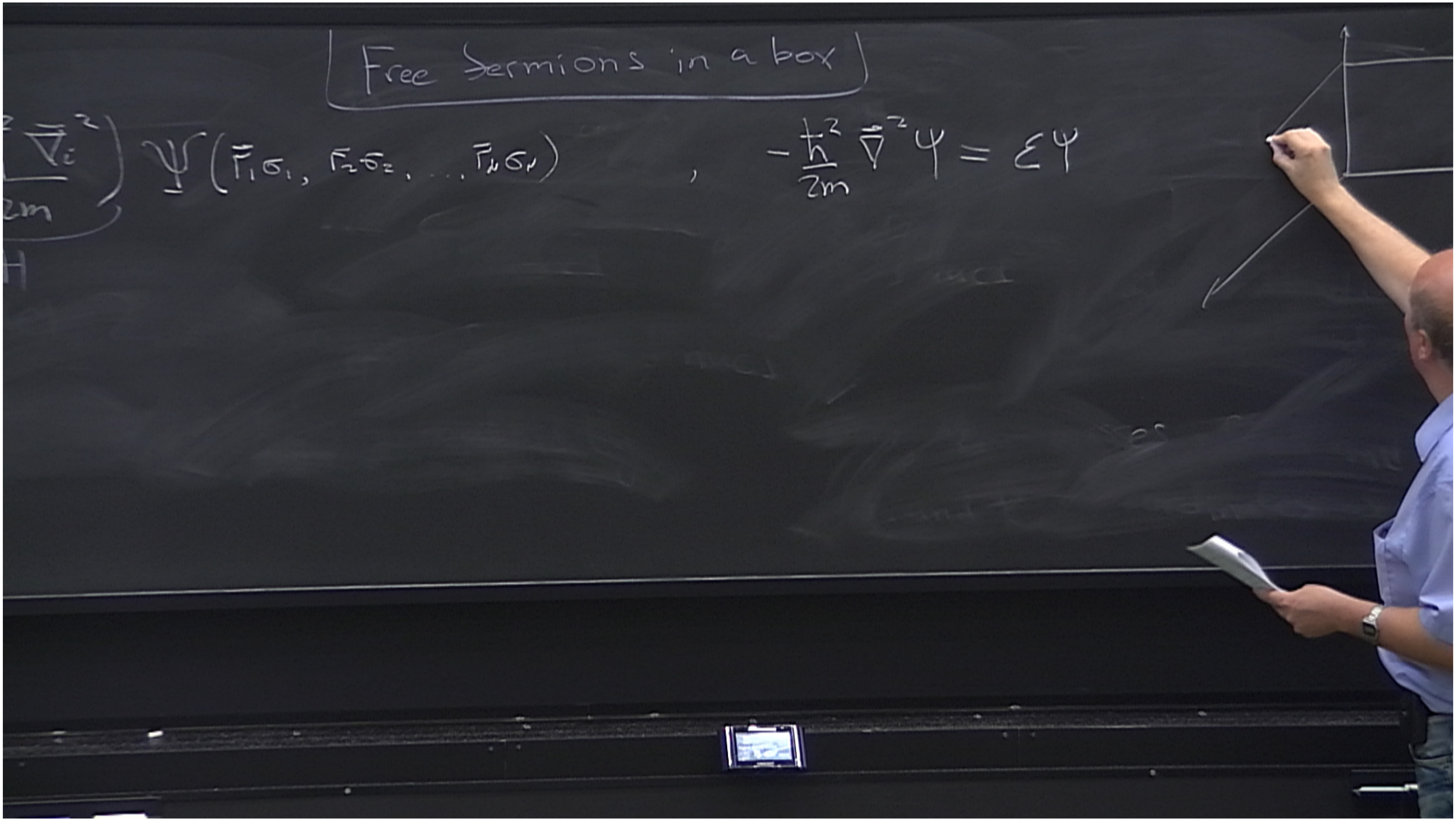
$$H\Psi = \sum_{i,\sigma_i} \underbrace{\left(-\frac{\hbar^2 \vec{\nabla}_i^2}{2m}\right)}_{H} \Psi(\vec{r}_1\sigma_1, \vec{r}_2\sigma_2, \ldots, \vec{r}_N\sigma_N)$$


Free fermions in a box
$H\Psi = \sum_{i,\sigma_i} \underbrace{\left(-\frac{\hbar^2 \nabla_i^2}{2m}\right)}_{H} \Psi(\vec{r}_1\sigma_1, \vec{r}_2\sigma_2, \ldots, \vec{r}_N\sigma_N)$

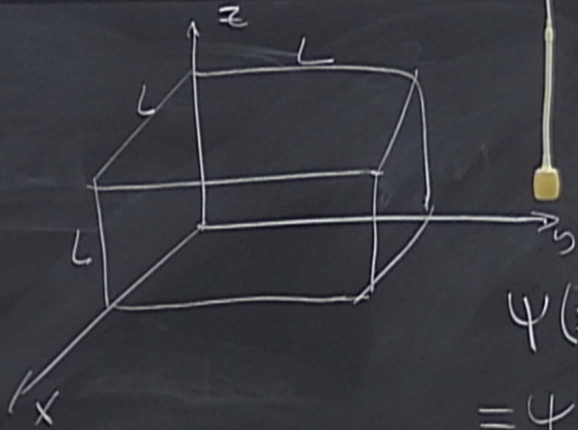
Free fermions in a box

$$\left(\frac{\hbar^2 \vec{\nabla}_i^{\,2}}{2m} \right) \Psi(\vec{r}_1\sigma_1, \vec{r}_2\sigma_2, \ldots, \vec{r}_N\sigma_N) \quad , \quad -\frac{\hbar^2}{2m}\vec{\nabla}^2\psi = \varepsilon\psi$$

H


Free fermions in a box
$\Psi(\vec{r}_1\sigma_1, \vec{r}_2\sigma_2, \ldots, \vec{r}_N\sigma_N)$
$-\frac{\hbar^2}{2m}\vec{\nabla}^2\psi = \varepsilon\psi$

$\nabla^2 \Psi = \varepsilon \Psi$



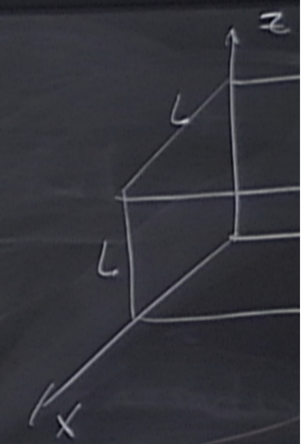
impose periodic boundary conditions (PBC)

$$\Psi(x+L, y, z) = \Psi(x, y, z)$$
$$= \Psi(x, y+L, z) =$$
$$= \Psi(x, y, z+L)$$

Simplified Models

Free fermions in a box

$$\underbrace{\left(-\frac{\hbar^2\vec{\nabla}_i^2}{2m}\right)}_{H}\Psi(\vec{r}_1\sigma_1, \vec{r}_2\sigma_2, \ldots, \vec{r}_N\sigma_N) \quad , \quad -\frac{\hbar^2}{2m}\vec{\nabla}^2\psi_k = \varepsilon_k\psi_k$$



$$\psi_k = \frac{1}{\sqrt{V}}e^{i\vec{k}\cdot\vec{r}}$$

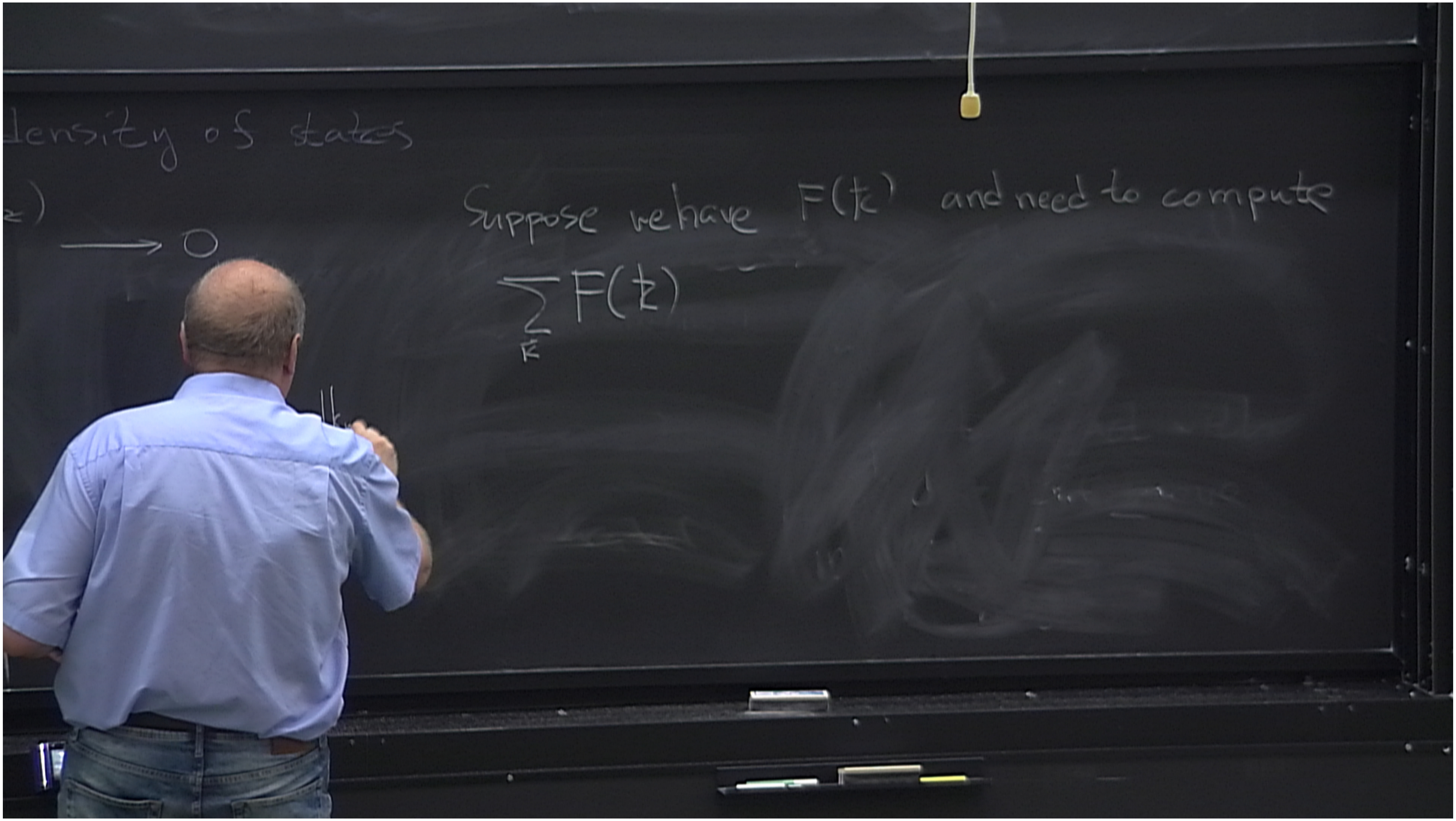
$$\varepsilon_k = \frac{\hbar^2k^2}{2m}$$

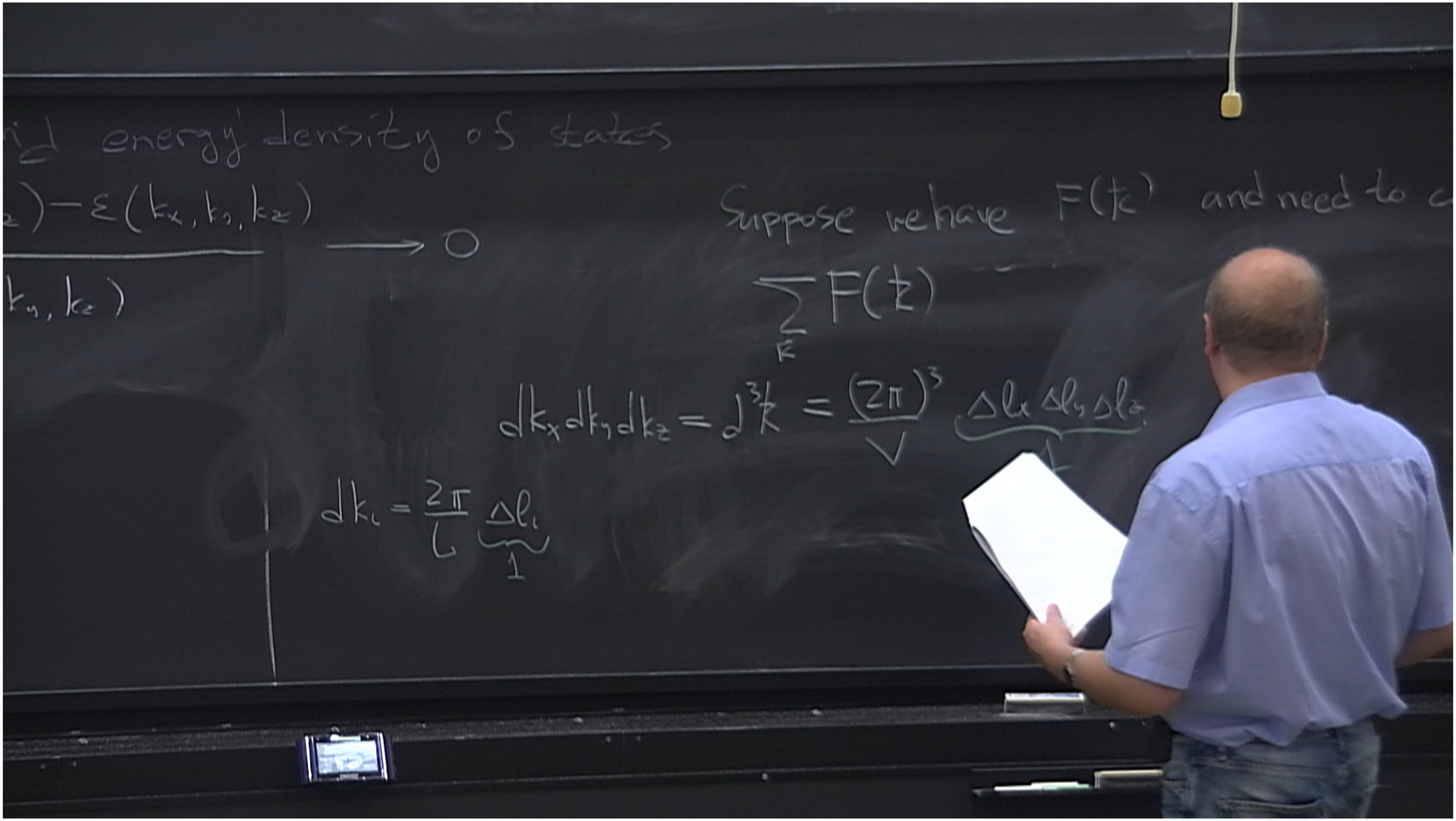
$$\vec{k} = \frac{2\pi}{L}(l_x, l_y, l_z)$$

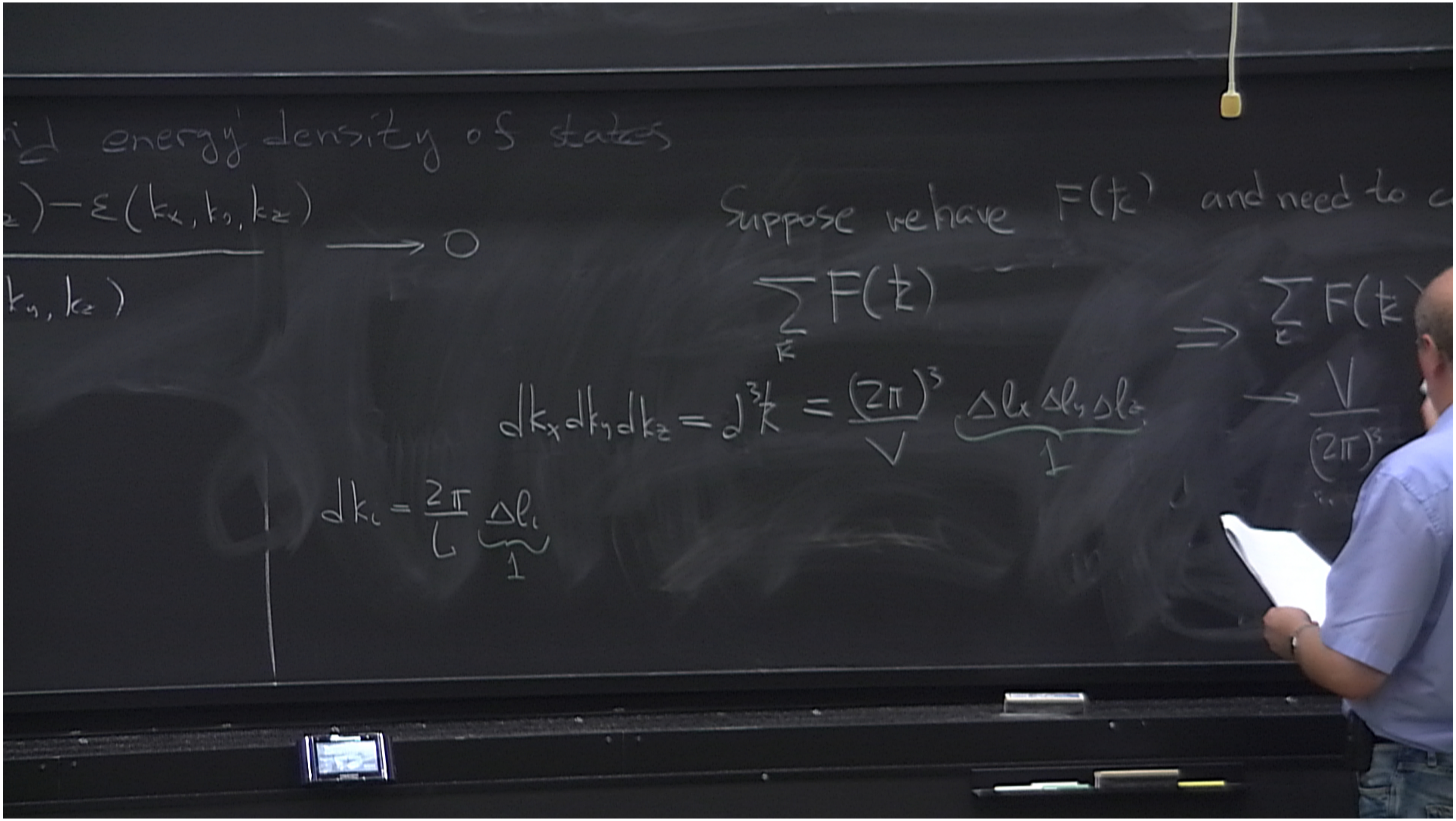
$$l_x, l_y, l_z \in \mathbb{Z}$$

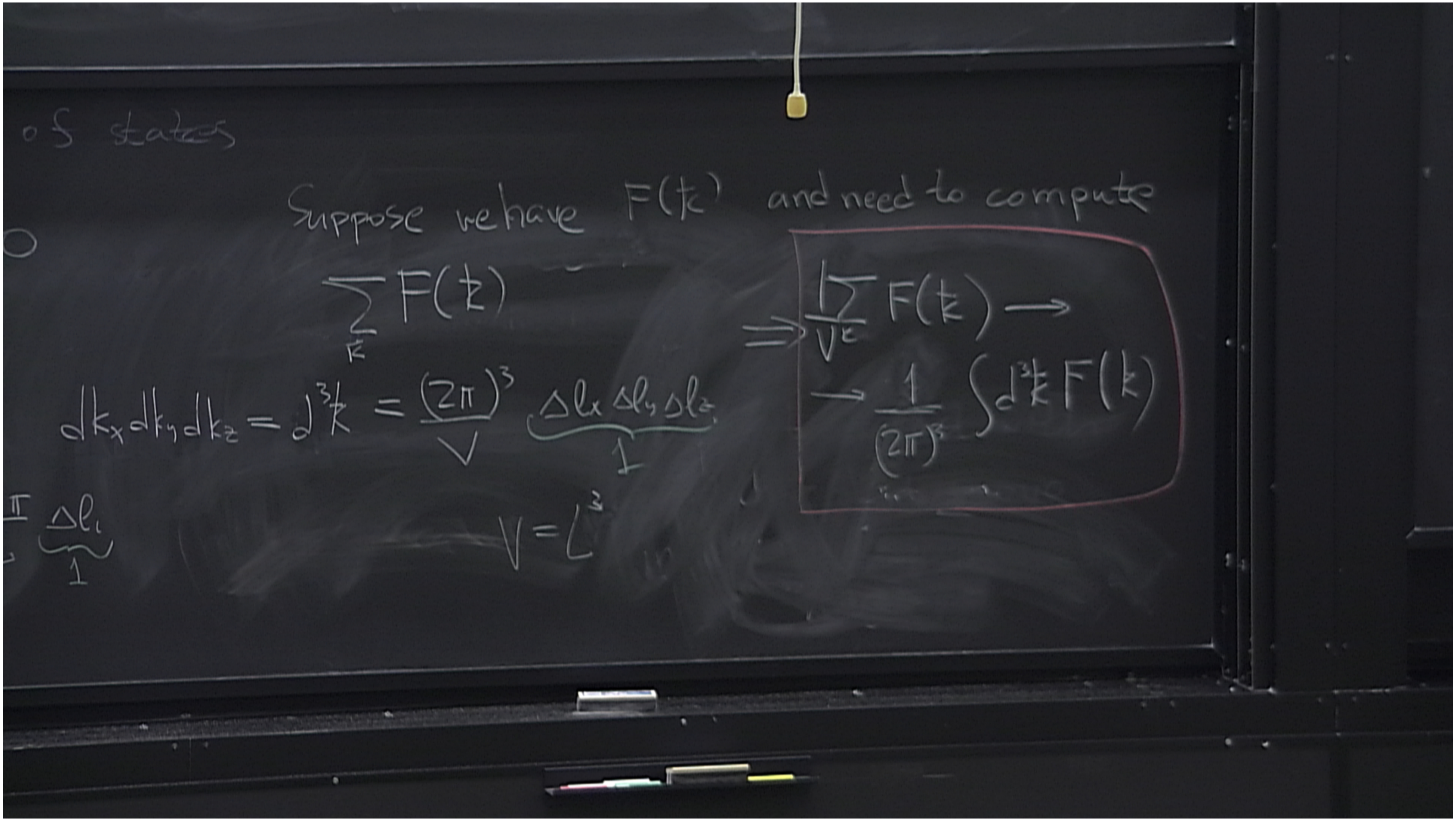
Thermodynamic limit and energy density of states

If $L \to \infty$, $$\frac{\varepsilon\left(k_x + \frac{2\pi}{L} l_x, k_y, k_z\right) - \varepsilon(k_x, k_y, k_z)}{\varepsilon(k_x, k_y, k_z)} \longrightarrow 0$$


density of states
Suppose we have $F(k)$ and need to compute
$\sum_k F(k)$

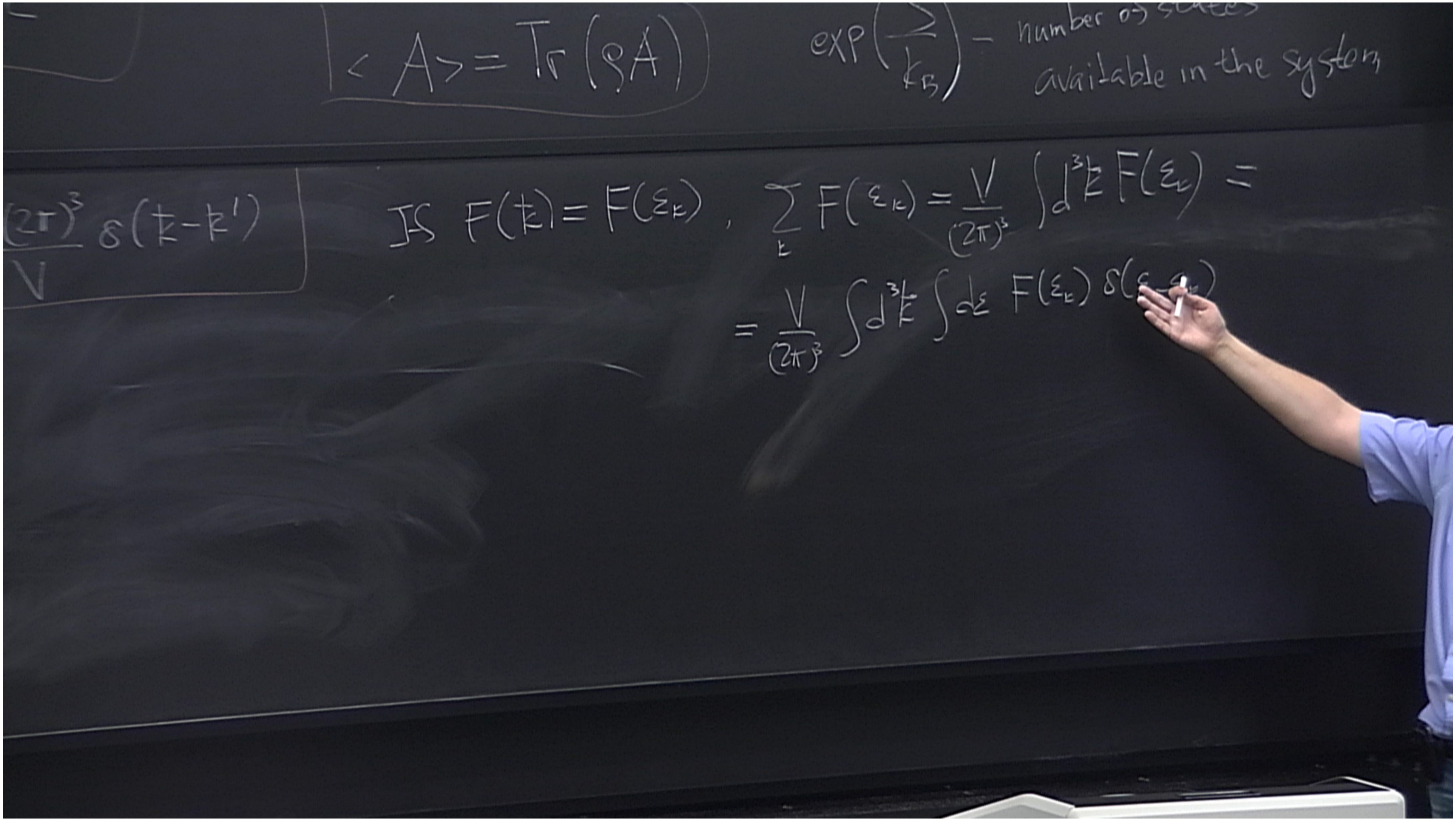

energy density of states
Suppose we have F(k) and need to
∑ F(k)
dk_x dk_y dk_z = d^3k = (2π)^3/V Δl_x Δl_y Δl_z
dk_i = 2π/L Δl_i
1


energy density of states
$)-\varepsilon(k_x, k_y, k_z)$
$\longrightarrow 0$
$k_y, k_z)$
Suppose we have $F(\underline{k})$ and need to c
$\sum_{\underline{k}} F(\underline{k})$
$\Longrightarrow \sum_{k} F(\underline{k}$
$\longrightarrow \frac{V}{(2\pi)^3}$
$dk_x dk_y dk_z = d^3k = \frac{(2\pi)^3}{V} \underbrace{\Delta l_x \Delta l_y \Delta l_z}_{1}$
$dk_i = \frac{2\pi}{L} \underbrace{\Delta l_i}_{1}$


of states
Suppose we have $F(\underline{k})$ and need to compute
$\sum_{\underline{k}} F(\underline{k})$
$\Rightarrow \frac{1}{V} \sum_{\underline{k}} F(\underline{k}) \longrightarrow$
$\longrightarrow \frac{1}{(2\pi)^3} \int d^3\underline{k}\, F(\underline{k})$
$dk_x dk_y dk_z = d^3\underline{k} = \frac{(2\pi)^3}{V} \underbrace{\Delta l_x \Delta l_y \Delta l_z}_{1}$
$\underbrace{\Delta l_i}_{1}$
$V = L^3$

$$\boxed{\delta_{\mathbf{k},\mathbf{k}'} \equiv \delta_{l_x,l_x'}\,\delta_{l_y,l_y'}\,\delta_{l_z,l_z'} \xrightarrow[L\to\infty]{} \frac{(2\pi)^3}{V}\,\delta(\mathbf{k}-\mathbf{k}')}$$

IS $F(\mathbf{k}) = F(\varepsilon_k)$,



< A > = Tr (ρA)
exp(- Σ / k_B) - number of states available in the system
(2π)^3 / V δ(k - k')
If F(k) = F(ε_k) , Σ_k F(ε_k) = V/(2π)^3 ∫d^3k F(ε_k) =
= V/(2π)^3 ∫d^3k ∫dε F(ε_k) δ(ε - ε_k)

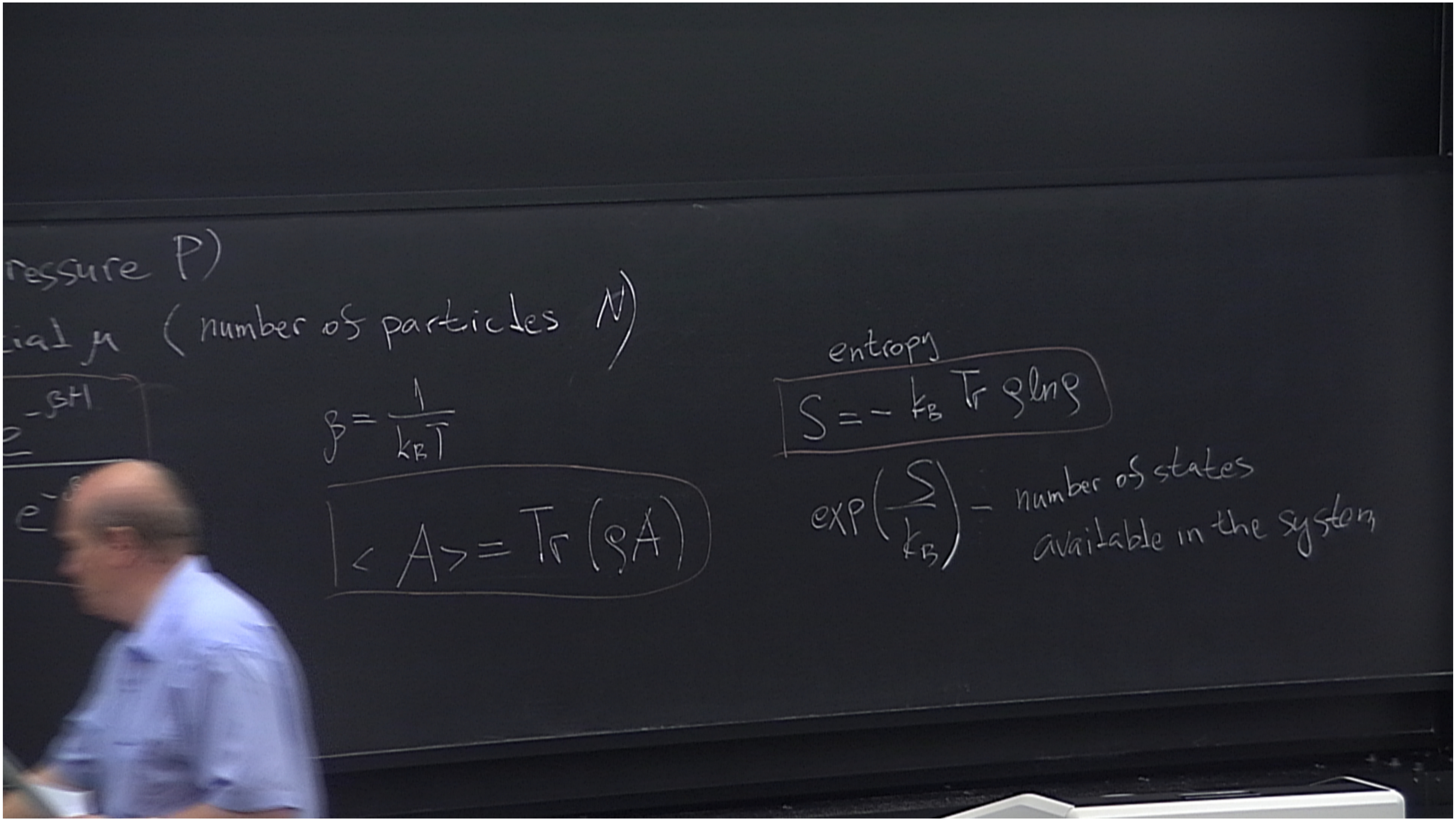
$\frac{(2\pi)^3}{V}\delta(\mathbf{k}-\mathbf{k}')$

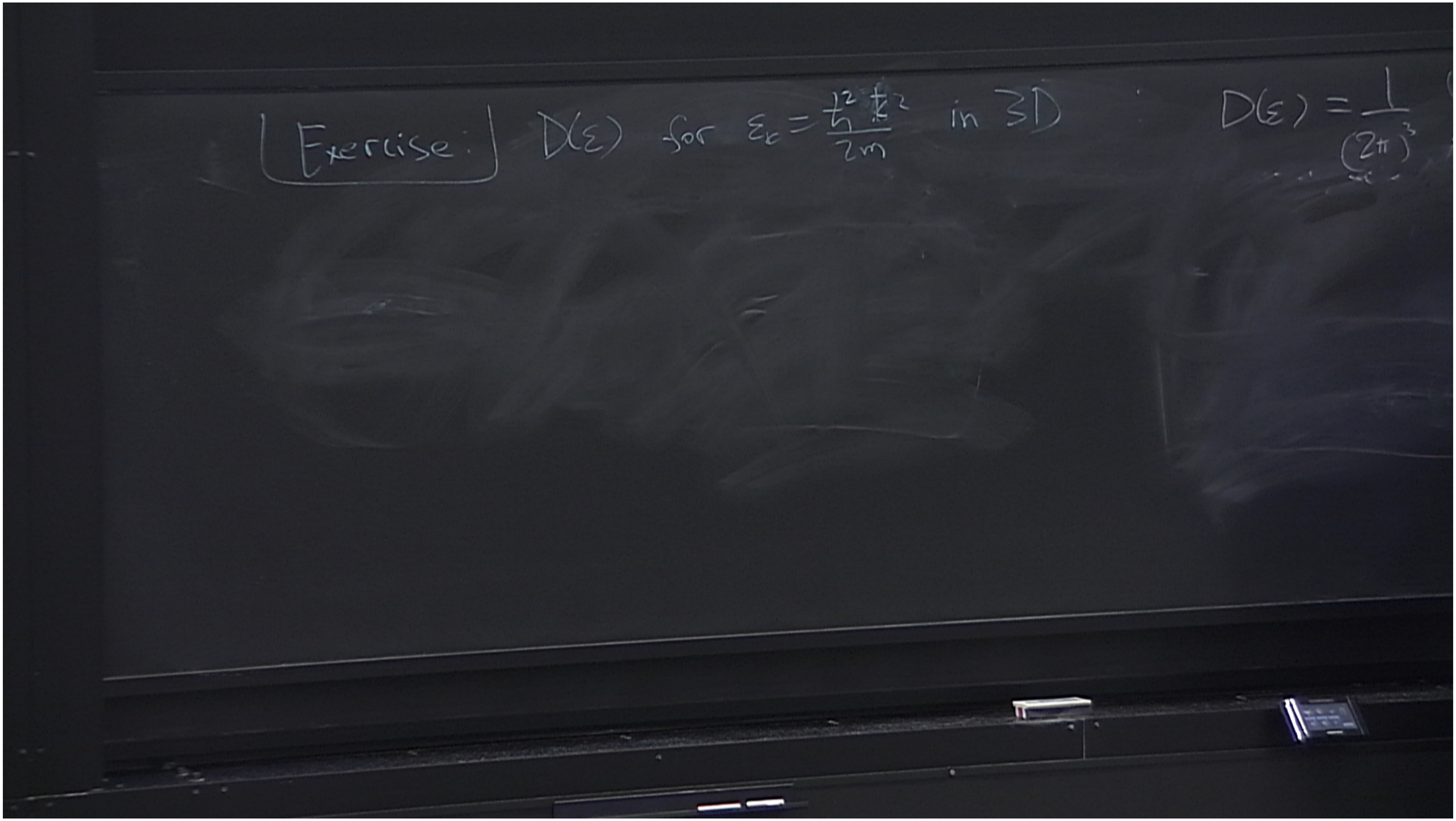
IS $F(\mathbf{k}) = F(\varepsilon_k)$, $\sum_k F(\varepsilon_k) = \frac{V}{(2\pi)^3}\int d^3k\, F(\varepsilon_k)$

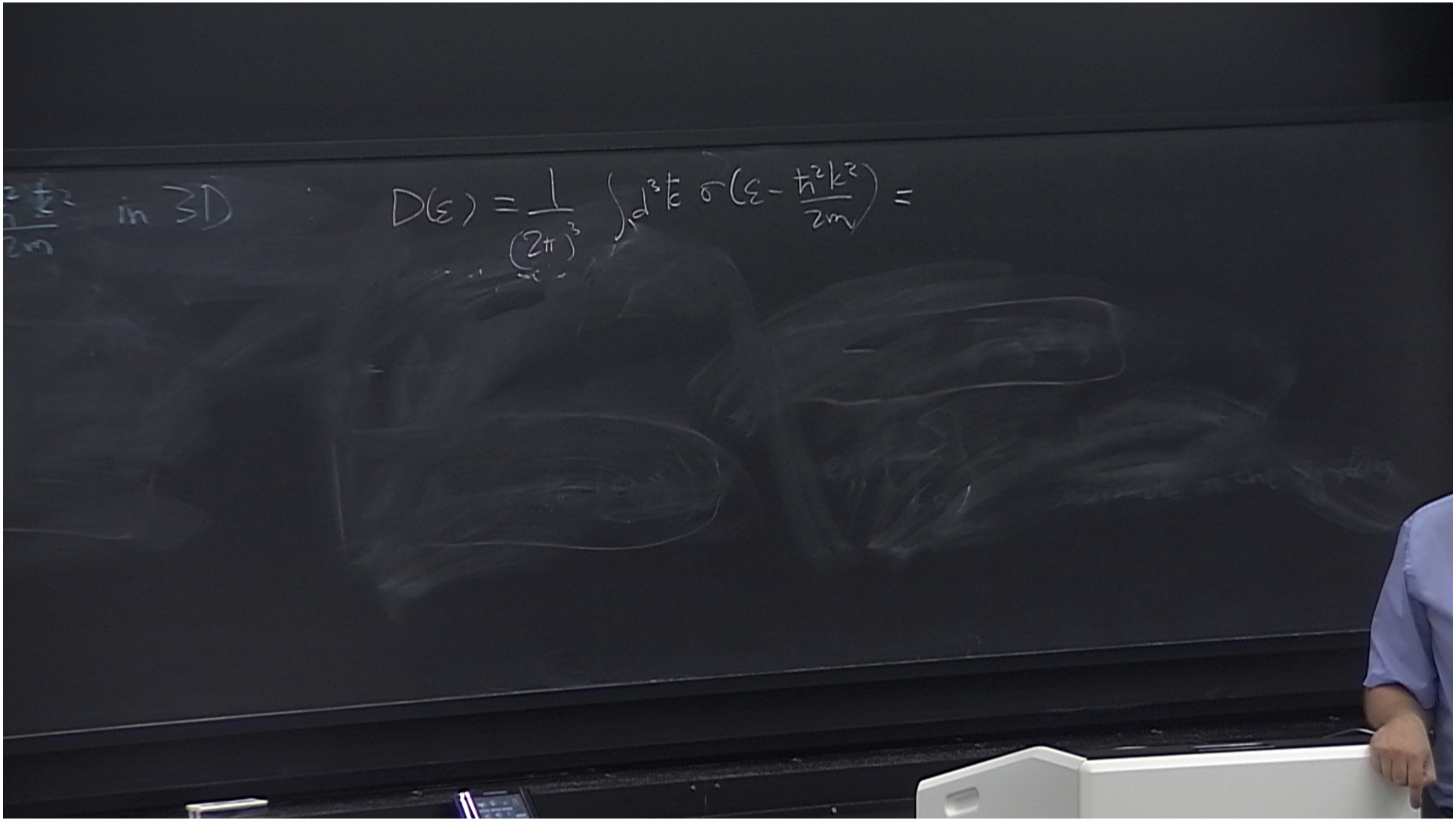
$$= \frac{V}{(2\pi)^3}\int d^3k \int d\varepsilon\, F(\varepsilon_k)\,\delta(\varepsilon-\varepsilon_k) =$$

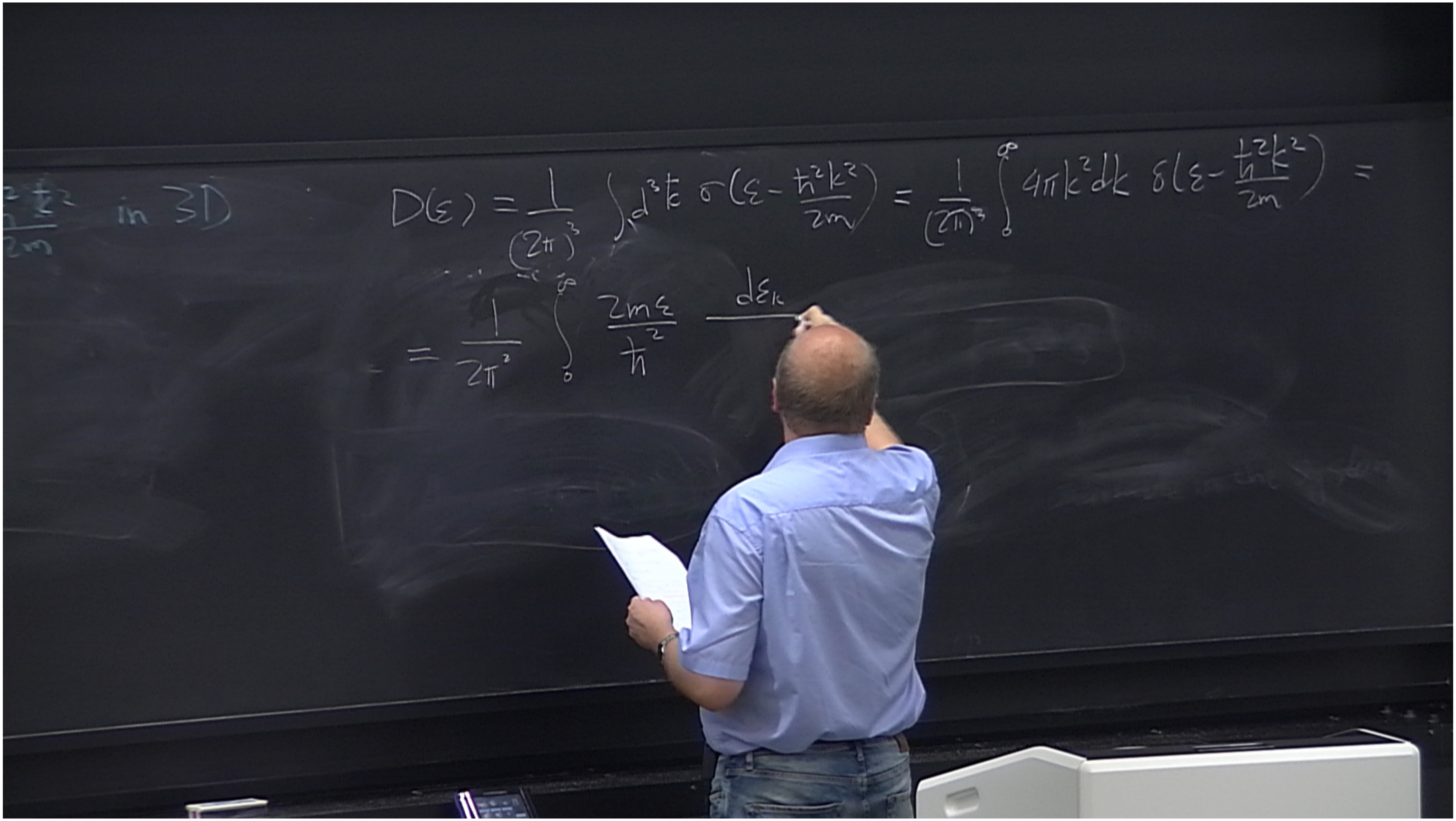
$$= V\int d\varepsilon\, F(\varepsilon)\, D(\varepsilon)$$

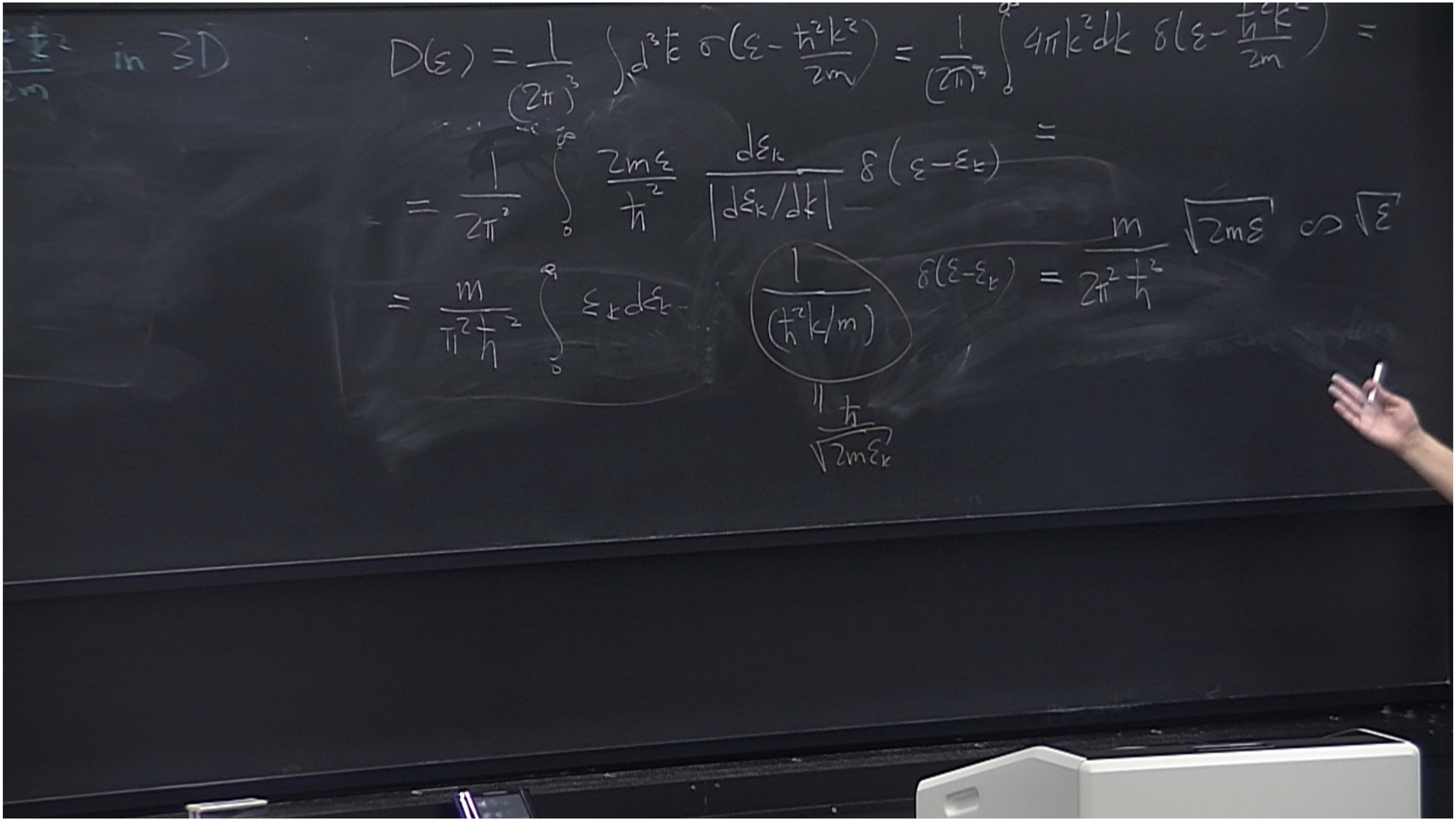
$$\boxed{D(\varepsilon) = \frac{1}{(2\pi)^3}\int d^3k\, \delta(\varepsilon-\varepsilon_k)} \leftarrow \text{density of states}$$


ressure P)
ial μ (number of particles N)
β = 1/(k_B T)
< A > = Tr (ϱA)
entropy
S = - k_B Tr ϱ ln ϱ
exp(S/k_B) - number of states available in the system


Exercise: $D(\varepsilon)$ for $\varepsilon_k = \frac{\hbar^2 k^2}{2m}$ in 3D
$D(\varepsilon) = \frac{1}{(2\pi)^3}$


$\frac{\hbar^2 k^2}{2m}$ in 3D
$D(\varepsilon) = \frac{1}{(2\pi)^3} \int d^3k \, \delta\left(\varepsilon - \frac{\hbar^2 k^2}{2m}\right) =$


in 3D
$D(\varepsilon) = \frac{1}{(2\pi)^3} \int d^3k \, \delta\left(\varepsilon - \frac{\hbar^2 k^2}{2m}\right) = \frac{1}{(2\pi)^3} \int_0^\infty 4\pi k^2 dk \, \delta\left(\varepsilon - \frac{\hbar^2 k^2}{2m}\right) =$
$= \frac{1}{2\pi^2} \int_0^\infty \frac{2m\varepsilon}{\hbar^2} \frac{d\varepsilon_k}{}$



$\frac{\hbar^2 k^2}{2m}$ in 3D
$D(\varepsilon) = \frac{1}{(2\pi)^3} \int d^3k \, \delta\left(\varepsilon - \frac{\hbar^2 k^2}{2m}\right) = \frac{1}{(2\pi)^3} \int_0^\infty 4\pi k^2 dk \, \delta\left(\varepsilon - \frac{\hbar^2 k^2}{2m}\right) =$
$= \frac{1}{2\pi^2} \int_0^\infty \frac{2m\varepsilon}{\hbar^2} \frac{d\varepsilon_k}{|d\varepsilon_k / dk|} \delta(\varepsilon - \varepsilon_k) =$
$= \frac{m}{\pi^2 \hbar^2} \int_0^\infty \varepsilon_k d\varepsilon_k \frac{1}{(\hbar^2 k / m)} \delta(\varepsilon - \varepsilon_k) = \frac{m}{2\pi^2 \hbar^2} \sqrt{2m\varepsilon} \propto \sqrt{\varepsilon}$
$= \frac{\hbar}{\sqrt{2m\varepsilon_k}}$