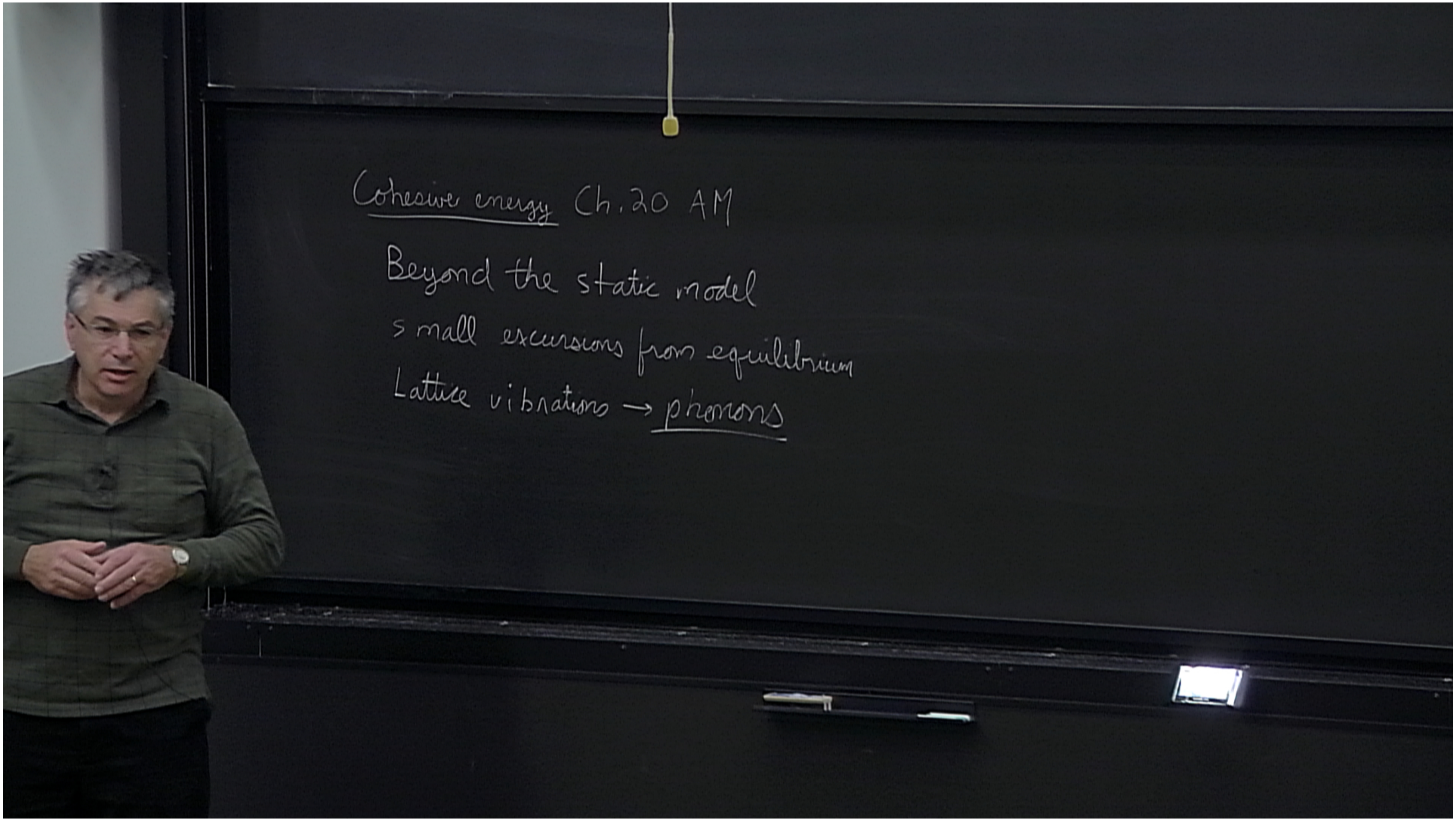
Title: PSI 2016/2017 Condensed Matter - Lecture 6

Date: Nov 14, 2016 10:45 AM

URL: http://pirsa.org/16110057

Abstract:


Cohesive energy Ch. 20 AM
Beyond the static model
small excursions from equilibrium
Lattice vibrations → phonons

y

del

equilibrium

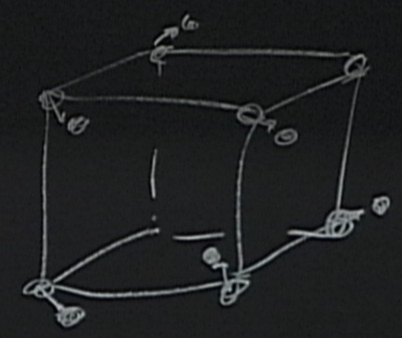
nons

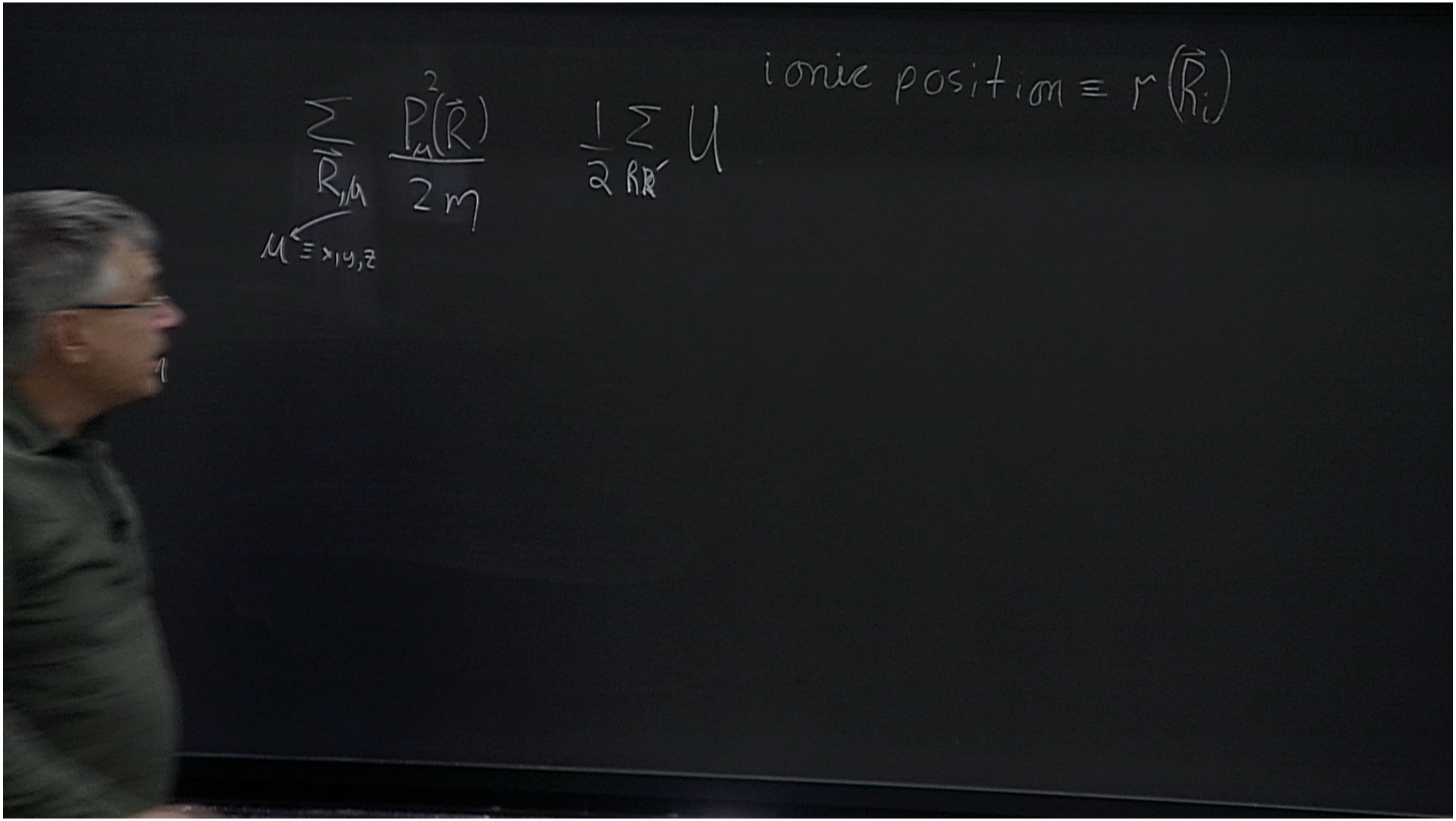
$$\sum_{\vec{R},\mu} \frac{P_\mu^2(\vec{R})}{2m}$$

$\mu \equiv x,y,z$

U

ionic position $\equiv r(\vec{R}_i)$




$\sum_{\vec{R},\mu} \frac{P_\mu^2(\vec{R})}{2m}$
$\mu \equiv x,y,z$
$\frac{1}{2}\sum_{RR'} U$
ionic position $\equiv r(\vec{R}_i)$

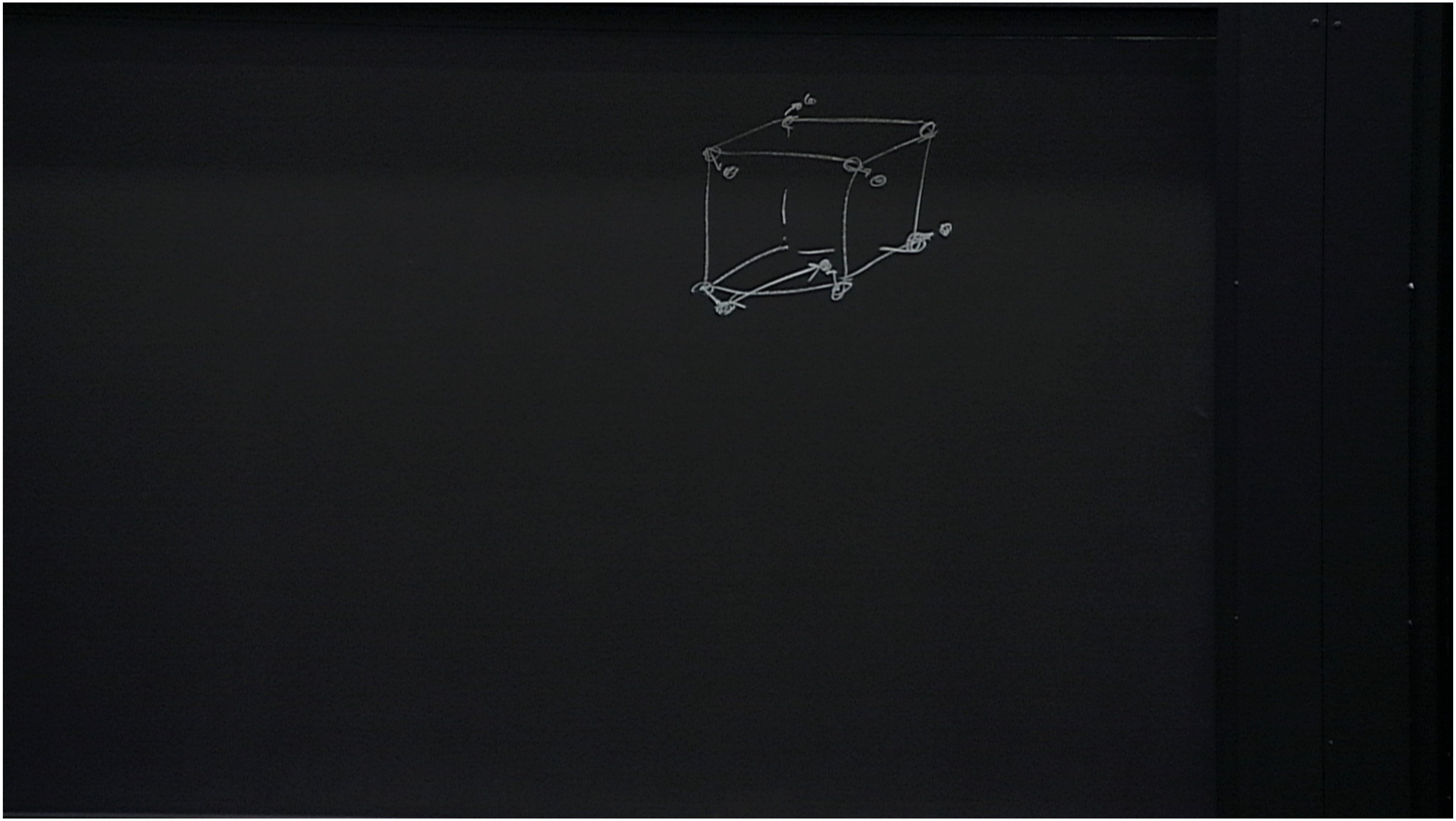
ionic position $\equiv r(\vec{R}_i)$

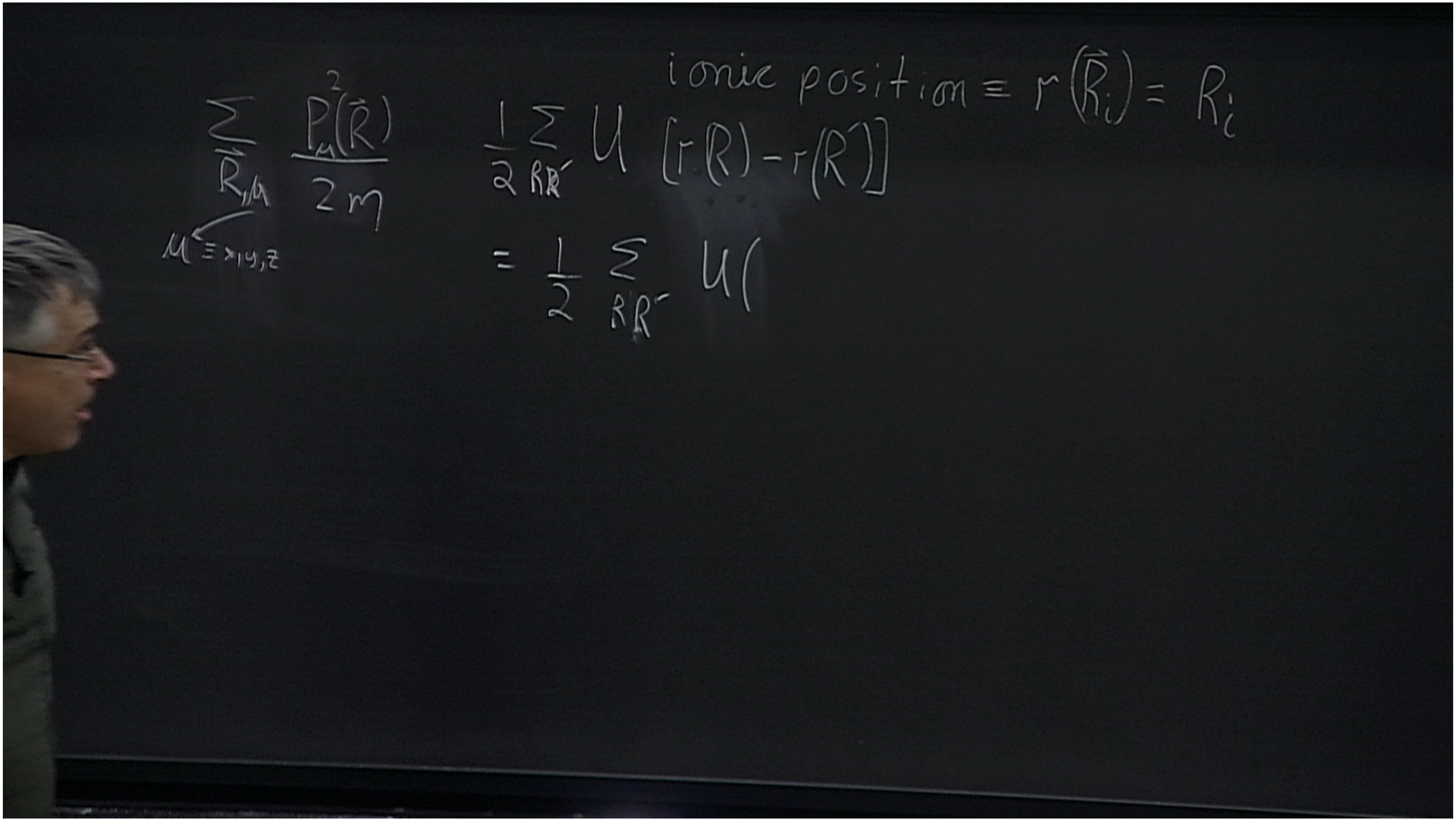
$$\sum_{\vec{R},\mu} \frac{P_\mu^2(\vec{R})}{2m} \quad \frac{1}{2}\sum_{RR'} U\left[r(R) - r(R')\right]$$

$\mu \equiv x, y, z$

uilibrium

ns




ionic position $\equiv r(\vec{R}_i) = R_i$
$\sum_{\vec{R},\mu} \frac{P_\mu^2(\vec{R})}{2m}$
$\mu \equiv x,y,z$
$\frac{1}{2} \sum_{RR'} U\left[r(R) - r(R')\right]$
$= \frac{1}{2} \sum_{RR'} U($

$$\sum_{\vec{R},\mu} \frac{P_\mu^2(\vec{R})}{2m}$$

$\mu \equiv x, y, z$

ionic position $\equiv r(\vec{R}) = R + u(\vec{R})$

$$\frac{1}{2} \sum_{RR'} U\left[\vec{r}(\vec{R}) - \vec{r}(\vec{R}')\right]$$

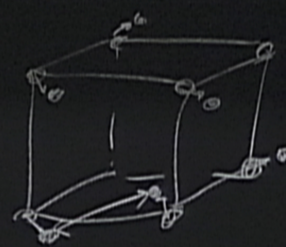
$$= \frac{1}{2} \sum_{RR'} U\left(\vec{R} - \vec{R}' + \vec{u}(\vec{R}) - \vec{u}(\vec{R}')\right)$$

ionic position $= r(\vec{R}) = R + u(\vec{R})$

$$\frac{1}{2}\sum_{RR'} U\,[r(\vec{R}) - r(\vec{R}')]$$

$$= \frac{1}{2}\sum_{RR'} U(\vec{R} - \vec{R}' + \vec{u}(\vec{R}) - \vec{u}(\vec{R}'))$$

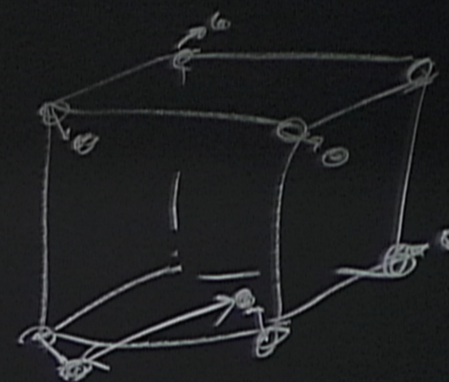
$$= \frac{1}{2}\sum_{RR'} U(\vec{R}-\vec{R}') + \frac{1}{2}\sum_{RR'} [\vec{u}(\vec{R}) - \vec{u}(\vec{R}')]\cdot\vec{\nabla}\, U(\vec{R}-\vec{R}') + \frac{1}{4}\sum_{RR'} \left([\vec{u}(\vec{R}) - \vec{u}(\vec{R}')]\cdot\vec{\nabla}\right)^2 U(\vec{R}-\vec{R}') + O(u^3)$$



$(\vec{R}) = R + u(\vec{R})$

$$\vec{r}_j = \vec{R} + d_j + \vec{u}_j(\vec{R})$$

$j = 1, \ldots N_{basis}$



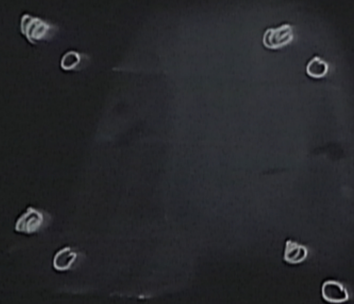
$\vec{R}))$

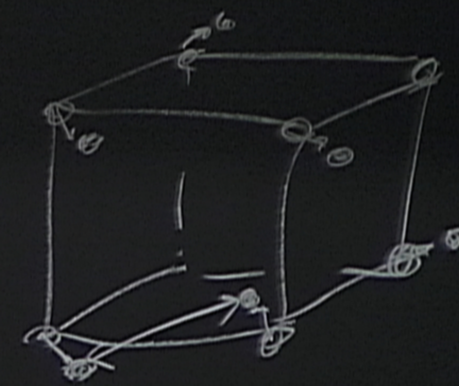
$$[\vec{u}(\vec{R}) - \vec{u}(\vec{R}')] \cdot \vec{\nabla} U(\vec{R} - \vec{R}') + \frac{1}{4} \sum_{RR'} \left([\vec{u}(\vec{R}) - \vec{u}(\vec{R}')] \cdot \vec{\nabla} \right)^2 U(\vec{R} - \vec{R}') + O$$

$(\vec{R}) = R + u(\vec{R})$

$\vec{r}_j = \vec{R} + d_j + \vec{u}_j(\vec{R})$

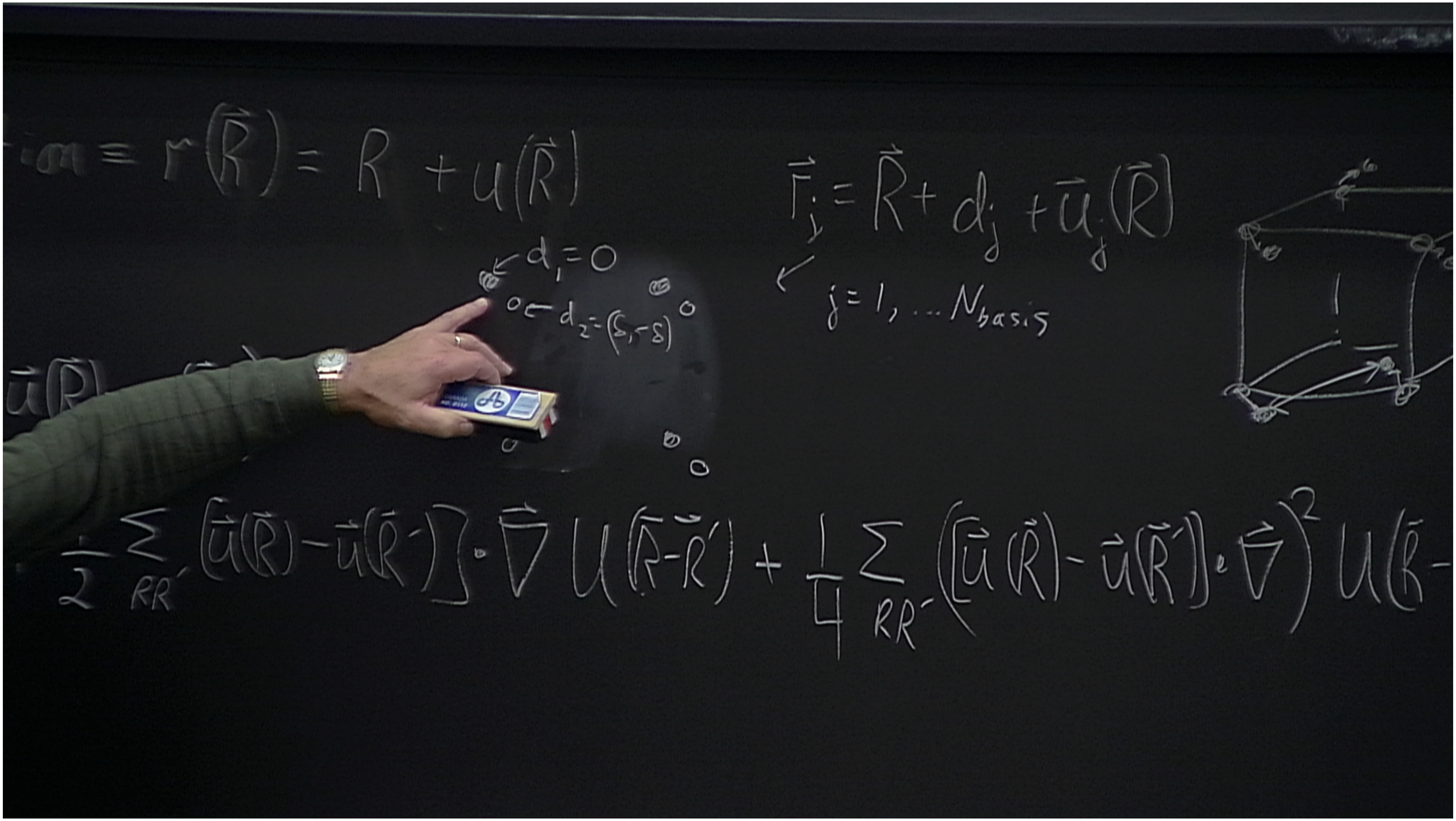
$j = 1, \ldots N_{basis}$

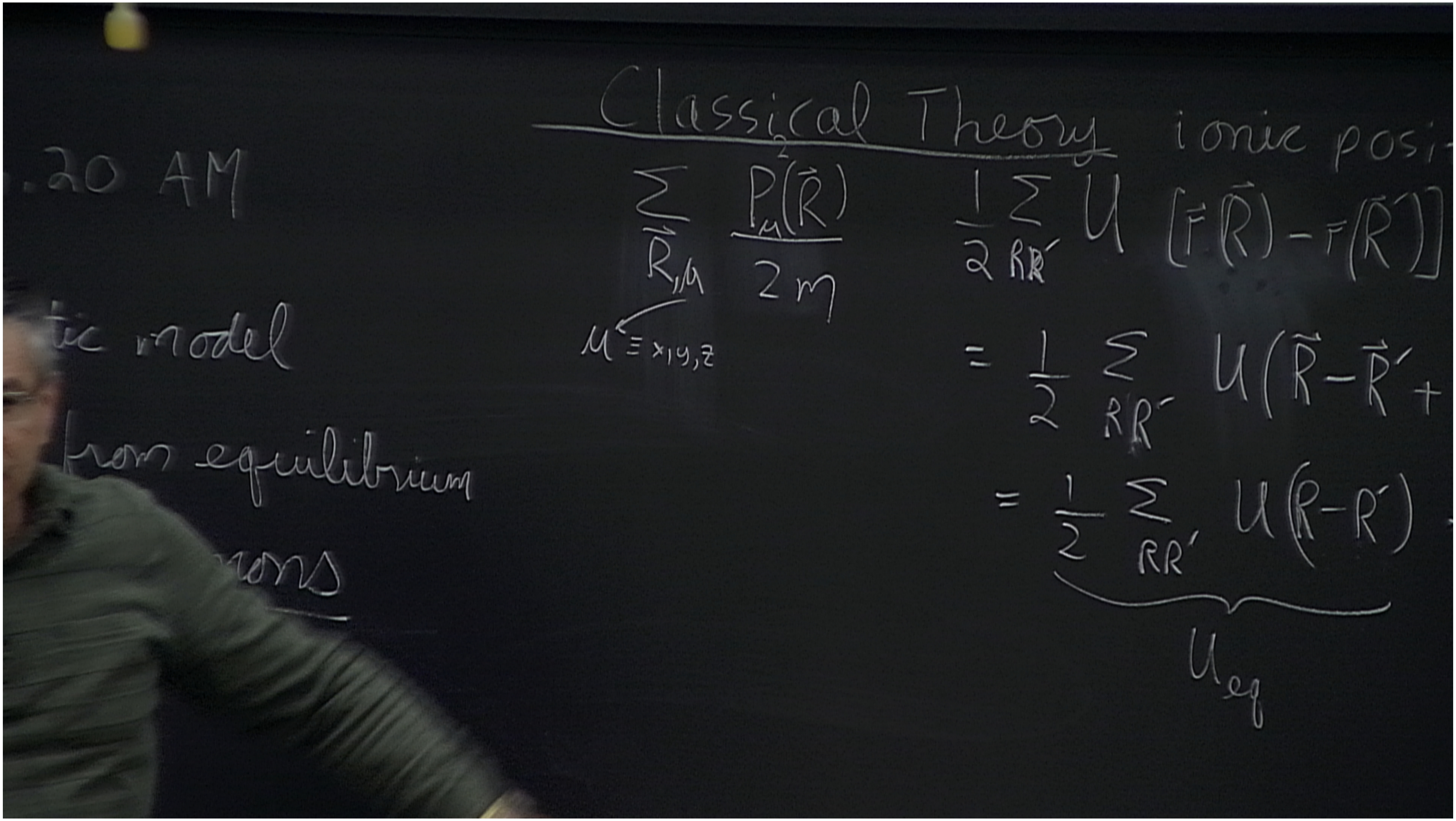




$\vec{R}))$

$[\vec{u}(\vec{R}) - \vec{u}(\vec{R}')] \cdot \vec{\nabla} U(\vec{R} - \vec{R}') + \frac{1}{4} \sum_{RR'} \left([\vec{u}(\vec{R}) - \vec{u}(\vec{R}')] \cdot \vec{\nabla} \right)^2 U(\vec{R} - \vec{R}') + O$


r(R) = R + u(R)
r_j = R + d_j + u_j(R)
j = 1, ... N_basis
d_1 = 0
d_2 = (δ, -δ)
1/2 Σ_RR' [u(R) - u(R')] · ∇ U(R - R') + 1/4 Σ_RR' ([u(R) - u(R')] · ∇)^2 U(R -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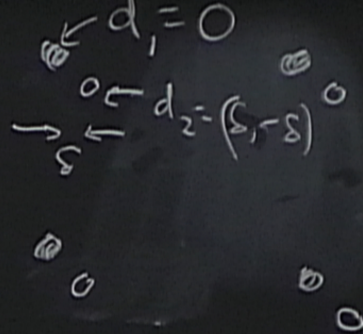
Classical Theory
ionic posi-
tic model
from equilibrium
nons
$\sum_{\vec{R},\mu} \frac{P_\mu^2(\vec{R})}{2m}$
$\mu \equiv x, y, z$
$\frac{1}{2}\sum_{RR'} U\,[\vec{r}(\vec{R}) - \vec{r}(\vec{R}')]$
$= \frac{1}{2}\sum_{RR'} U(\vec{R} - \vec{R}' +$
$= \frac{1}{2}\sum_{RR'} U(R - R')$
U_{eq}

...omic position $\equiv r(\vec{R}) = \vec{R} + u(\vec{R})$

$\vec{r}_j = \vec{R} + d_j + \ldots$

$U\,[\vec{r}(\vec{R}) - \vec{r}(\vec{R}')]$



$j = 1, \ldots N_{basis}$

$$\sum_{RR'} U(\vec{R} - \vec{R}' + \vec{u}(\vec{R}) - \vec{u}(\vec{R}'))$$

$$= \underbrace{\sum_{RR'} U(\vec{R} - \vec{R}')}_{U_{eq}} + \frac{1}{2}\sum_{RR'} [\vec{u}(\vec{R}) - \vec{u}(\vec{R}')] \cdot \vec{\nabla} U(\vec{R} - \vec{R}') + \frac{1}{4}\sum_{RR'} ([\vec{u}(\vec{R}) - \ldots$$

$$-\sum_{R'} \vec{\nabla} U(\vec{R} - \vec{R}')$$

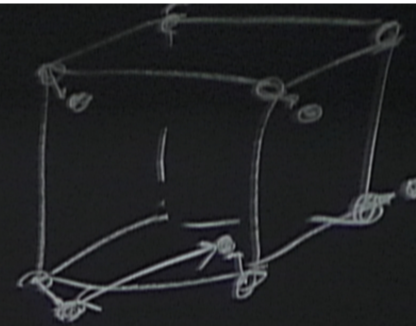
$\ldots \vec{u}(\vec{R})$

$$\vec{r}_j = \vec{R} + \vec{d}_j + \vec{u}_j(\vec{R})$$

$d_1 = 0$

$d_2 = (\delta_1 - \delta)$

$j = 1, \ldots N_{basis}$



$\ldots(\vec{R}))$

$$\ldots [\vec{u}(\vec{R}) - \vec{u}(\vec{R}')] \cdot \vec{\nabla}\, U(\vec{R} - \vec{R}') + \frac{1}{4} \sum_{RR'} \left([\vec{u}(\vec{R}) - \vec{u}(\vec{R}')] \cdot \vec{\nabla} \right)^2 U(\vec{R} - \vec{R}') + O(u^3)$$

$-\sum_{R'} \vec{\nabla} U(\vec{R} - \vec{R}') \equiv$ force exerted on the ion at $\vec{R}$ by all the other ions in the lattice

$$(\vec R) = R + u(\vec R)$$

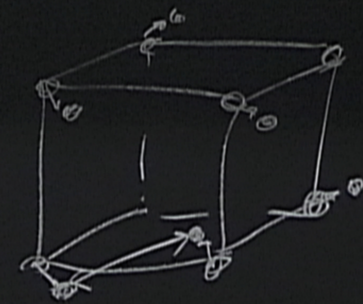
$$\vec r_j = \vec R + d_j + \vec u_j(\vec R)$$

$j = 1, \ldots N_{basis}$

$d_1 = 0$

$d_2 = (\delta, -\delta)$

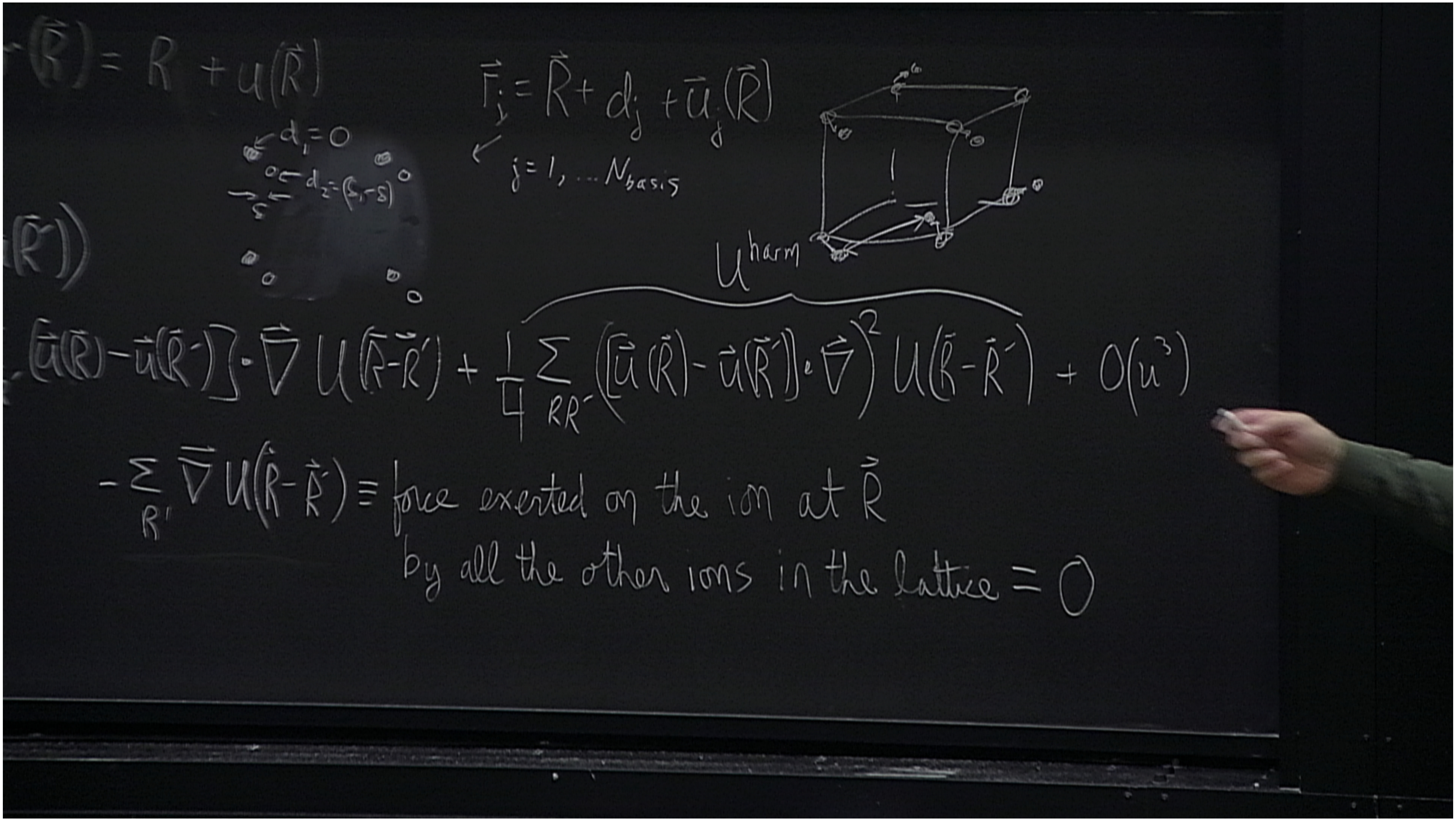
$\vec\delta$



$$(\vec R))$$

$$[\vec u(\vec R) - \vec u(\vec R')] \cdot \vec\nabla\, U(\vec R - \vec R') + \frac{1}{4}\sum_{RR'} \left([\vec u(\vec R) - \vec u(\vec R')] \cdot \vec\nabla \right)^2 U(\vec R - \vec R') + O(u^3)$$

$$-\sum_{R'} \vec\nabla\, U(\vec R - \vec R') \equiv \text{force exerted on the ion at } \vec R \text{ by all the other ions in the lattice} = 0$$



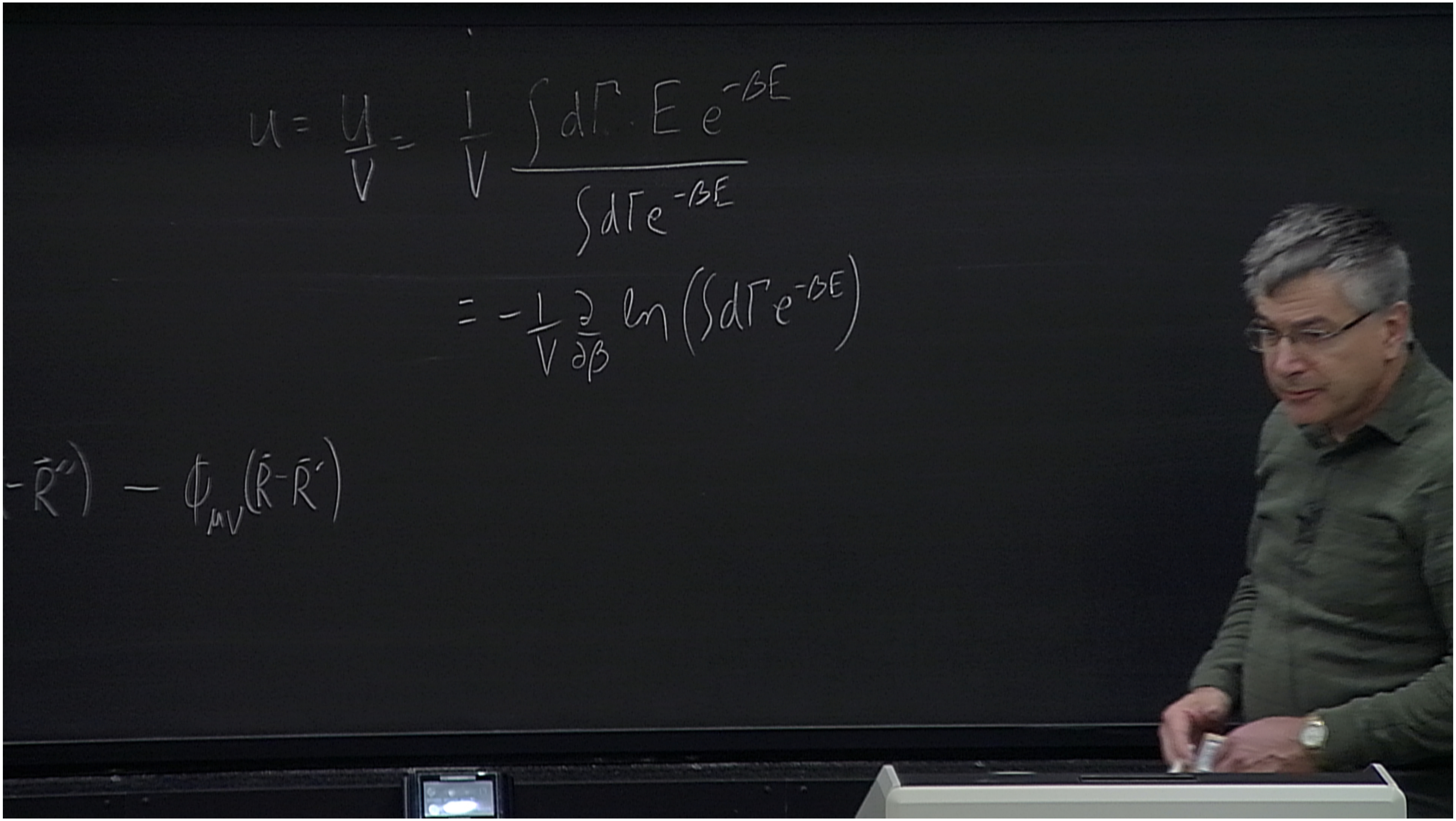
r_j = R + d_j + u_j(R)
j = 1, … N_basis
d_1 = 0
U^harm
+ 1/4 Σ_RR' ([u(R) − u(R')] · ∇)^2 U(R − R') + O(u^3)
− Σ_R' ∇ U(R − R') ≡ force exerted on the ion at R
by all the other ions in the lattice = 0

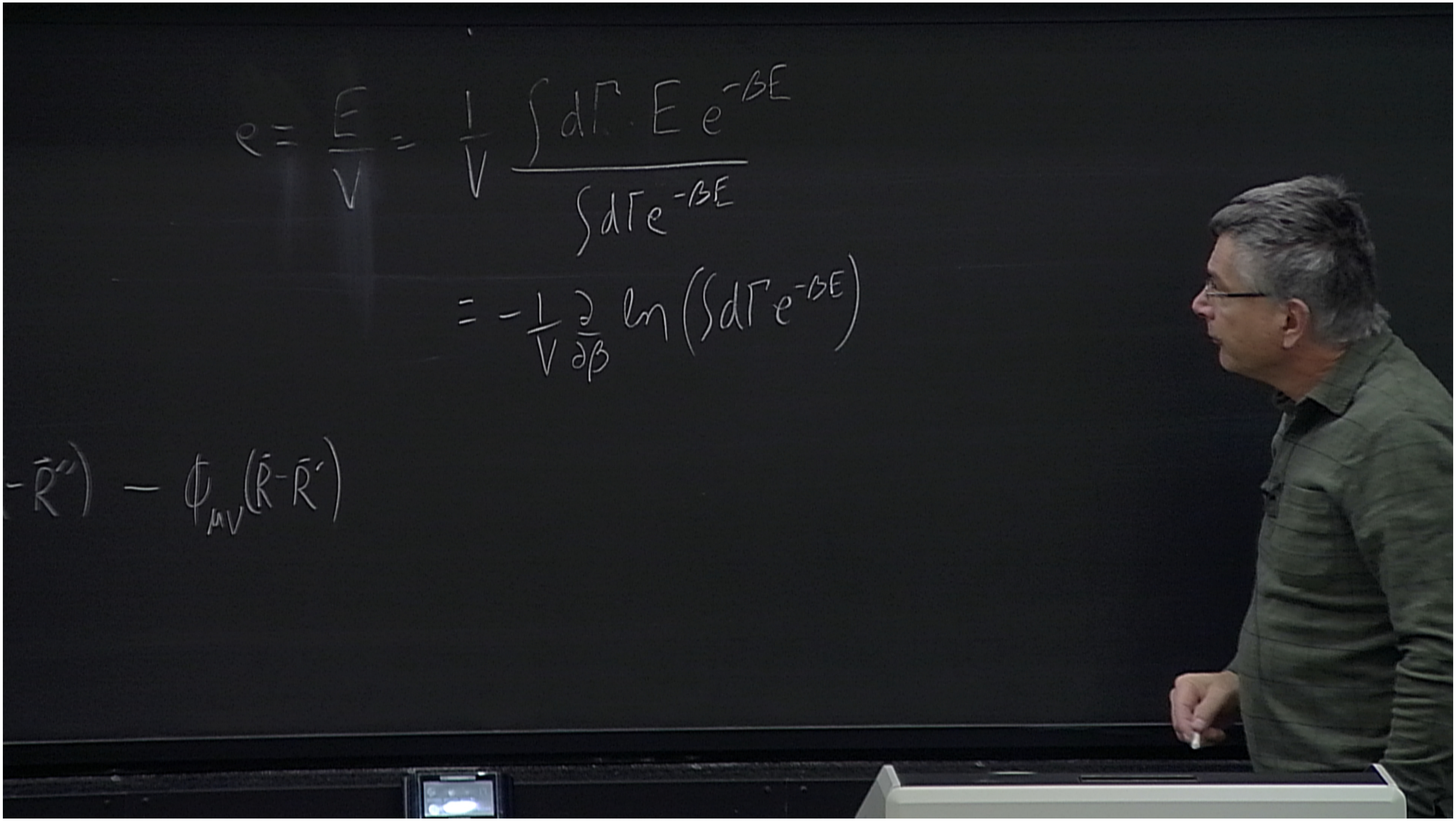
$$U^{harm} = \frac{1}{4} \sum_{\substack{RR' \\ \mu,\nu = x,y,z}} \left[u_\mu(\vec{R}) - u_\mu(\vec{R}')\right] \phi_{\mu\nu}(\vec{R}-\vec{R}') \left[u_\nu(\vec{R}) - u_\nu(\vec{R}')\right]$$

$$\phi_{\mu\nu}(\vec{R}-\vec{R}') \equiv \frac{\partial^2 U(r)}{\partial r_\mu \partial r_\nu}$$

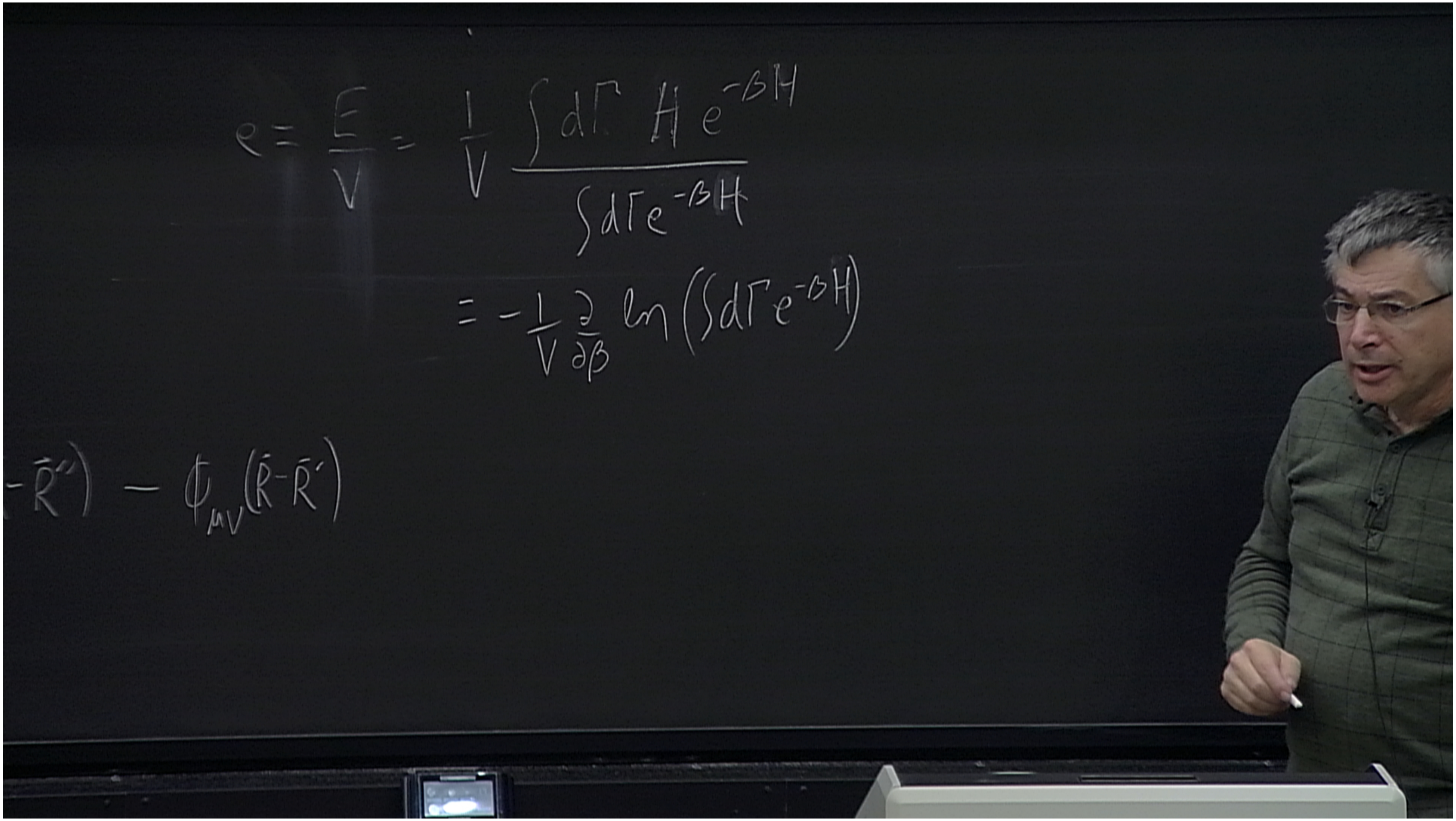
$$= \frac{1}{2} \sum_{RR'} u_\mu(\vec{R}) D_{\mu\nu}(\vec{R}-\vec{R}') u_\nu(\vec{R}')$$

where $D_{\mu\nu}(\vec{R}-\vec{R}') = \delta_{\vec{R}\vec{R}'} \sum_{R''} \phi_{\mu\nu}(\vec{R}-\vec{R}'') - \phi_{\mu\nu}(\vec{R}-\vec{R}')$


$u = \frac{U}{V} = \frac{1}{V}\frac{\int d\Gamma \cdot E\, e^{-\beta E}}{\int d\Gamma\, e^{-\beta E}}$
$= -\frac{1}{V}\frac{\partial}{\partial\beta}\ln\left(\int d\Gamma\, e^{-\beta E}\right)$
$-\vec{R}'') - \phi_{\mu\nu}(\vec{R}-\vec{R}')$



$e = \frac{E}{V} = \frac{1}{V}\frac{\int d\Gamma \cdot E\, e^{-\beta E}}{\int d\Gamma\, e^{-\beta E}}$
$= -\frac{1}{V}\frac{\partial}{\partial\beta}\ln\left(\int d\Gamma\, e^{-\beta E}\right)$
$-\vec{R}'') - \phi_{\mu\nu}(\vec{R}-\vec{R}')$


$e = \frac{E}{V} = \frac{1}{V} \frac{\int d\Gamma\, H\, e^{-\beta H}}{\int d\Gamma\, e^{-\beta H}}$
$= -\frac{1}{V} \frac{\partial}{\partial\beta} \ln\left(\int d\Gamma\, e^{-\beta H}\right)$
$-\vec{R}'') - \phi_{\mu\nu}(\vec{R}-\vec{R}')$

$$e = \frac{E}{V} = \frac{1}{V}\frac{\int d\Gamma\, H e^{-\beta H}}{\int d\Gamma\, e^{-\beta H}}$$

$$H \sim \sum p^2 + \sum u^2$$

$$= -\frac{1}{V}\frac{\partial}{\partial\beta}\ln\left(\int d\Gamma\, e^{-\beta H}\right)$$

$$- \phi_{\mu\nu}(\bar{R}-\bar{R}')$$

$$- u_\nu(\vec{R}')]$$

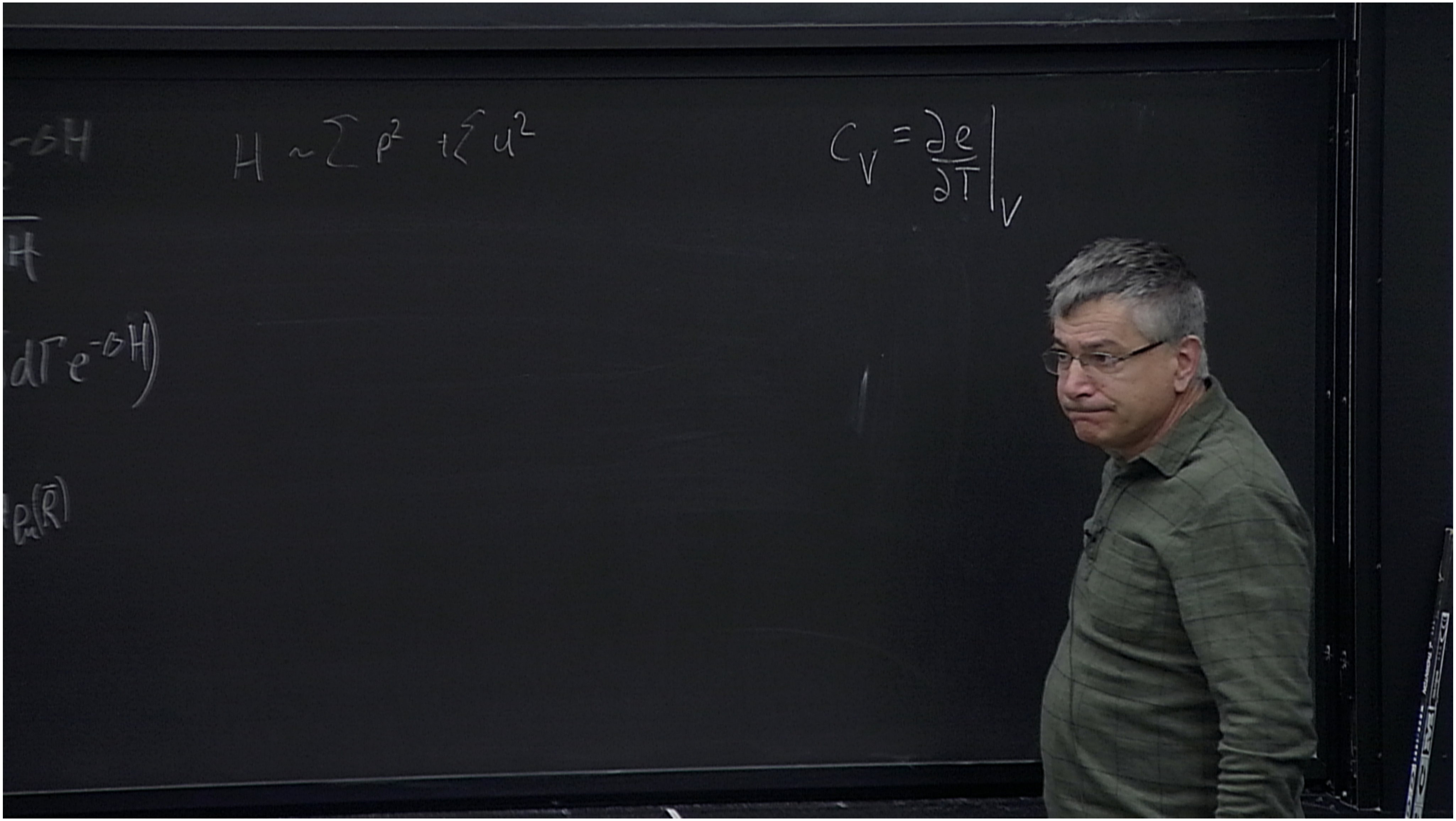
$$e = \frac{E}{V} = \frac{1}{V} \frac{\int d\Gamma\, H\, e^{-\beta H}}{\int d\Gamma\, e^{-\beta H}}$$

$$H \sim \sum p^2 + \sum u^2$$

$$= -\frac{1}{V}\frac{\partial}{\partial\beta} \ln\left(\int d\Gamma\, e^{-\beta H}\right)$$

$$\sum_{\vec{R}''} \phi_{\mu\nu}(\vec{R}-\vec{R}'') - \phi_{\mu\nu}(\vec{R}-\vec{R}')$$

$$d\Gamma = \prod_{\substack{\vec{R} \\ \mu}} du_\mu(\vec{R})\, dp_\mu(\vec{R})$$


$H \sim \sum p^2 + \sum u^2$
$C_V = \frac{\partial e}{\partial T}\Big|_V$

$$= \frac{1}{V}\frac{\int d\Gamma\, H e^{-\beta H}}{\int d\Gamma\, e^{-\beta H}}$$

$$= -\frac{1}{V}\frac{\partial}{\partial\beta}\ln\left(\int d\Gamma\, e^{-\beta H}\right)$$

$$H \sim \sum p^2 + \sum u^2$$

$$\beta \equiv \frac{1}{k_B T}$$

$$\left.\begin{aligned} \tilde{p}_\mu(\vec{R}) &\equiv \sqrt{\beta}\, p_\mu(\vec{R}) \\ \tilde{u}_\mu(\vec{R}) &\equiv \sqrt{\beta}\, u_\mu(\vec{R}) \end{aligned}\right\}$$

$$C_V = \left.\frac{\partial e}{\partial T}\right|_V$$

$$\int d\Gamma\, e^{-\beta H} \to \beta^{-3N} \text{const.}$$

$$d\Gamma = \prod_{\substack{\vec{R} \\ \mu}} du_\mu(\vec{R})\, dp_\mu(\vec{R}) \to \frac{1}{\beta^{3N}} \prod_{\substack{\vec{R} \\ \mu}} d\tilde{u}_\mu(\vec{R})\, d\tilde{p}_\mu(\vec{R})$$

$$= \frac{1}{V}\frac{\int d\Gamma\, H e^{-\beta H}}{\int d\Gamma e^{-\beta H}}$$

$$H \sim \sum p^2 + \sum u^2$$

$$C_V = \frac{\partial e}{\partial T}\bigg|_V$$

$$\beta \equiv \frac{1}{k_B T}$$

$$= -\frac{1}{V}\frac{\partial}{\partial \beta} \ln\left(\int d\Gamma e^{-\beta H}\right)$$

$$\left.\begin{aligned} \tilde{p}_\mu(\vec{R}) &\equiv \sqrt{\beta}\, p_\mu(\vec{R}) \\ \tilde{u}_\mu(\vec{R}) &\equiv \sqrt{\beta}\, u_\mu(\vec{R}) \end{aligned}\right\}$$

$$\int d\Gamma e^{-\beta H} \to \beta^{-3N} \text{ const.}$$

$$e \equiv \frac{E}{V} = -\frac{1}{V}\frac{\partial}{\partial \beta} \ln \beta^{-3N} \text{const}$$

$$d\Gamma = \prod_{\substack{\vec{R} \\ \mu}} du_\mu(\vec{R})\, dp_\mu(\vec{R}) \rightarrow \frac{1}{\beta^{3N}} \prod_{\substack{\vec{R} \\ \mu}} d\tilde{u}_\mu(\vec{R})\, d\tilde{p}_\mu(\vec{R})$$

$$H e^{-\beta H}$$

$$\overline{\Gamma e^{-\beta H}}$$

$$\ln\left(\int d\Gamma e^{-\beta H}\right)$$

$$du_\mu(\vec{R})\, dp_\mu(\vec{R}) \rightsquigarrow \frac{1}{\beta^{3N}} \prod_{\vec{R}, \mu} d\tilde{u}_\mu(\vec{R})\, d\tilde{p}_\mu(\vec{R})$$

$$H \sim \sum p^2 + \sum u^2$$

$$\beta \equiv \frac{1}{k_B T}$$

$$\left.\begin{aligned} \tilde{p}_\mu(\vec{R}) &\equiv \sqrt{\beta}\, p_\mu(\vec{R}) \\ \tilde{u}_\mu(\vec{R}) &\equiv \sqrt{\beta}\, u_\mu(\vec{R}) \end{aligned}\right\}$$

$$C_V = \left.\frac{\partial e}{\partial T}\right|_V$$

$$\int d\Gamma e^{-\beta H} \to \beta^{-3N} \text{ const.}$$

$$e \equiv \frac{E}{V} = -\frac{1}{V}\frac{\partial}{\partial \beta} \ln\left[\beta^{-3N} \text{ const}\right) + \frac{U_{eq}}{V}$$

$$e^{-\beta H}$$

$$\overline{\quad -\beta H}$$

$$\left(\int d\Gamma\, e^{-\beta H}\right)$$

$$H \sim \sum p^2 + \sum u^2$$

$$\beta \equiv \frac{1}{k_B T}$$

$$\tilde{p}_\mu(\vec{R}) \equiv \sqrt{\beta}\, p_\mu(\vec{R})$$

$$\tilde{u}_\mu(\vec{R}) \equiv \sqrt{\beta}\, u_\mu(\vec{R})$$

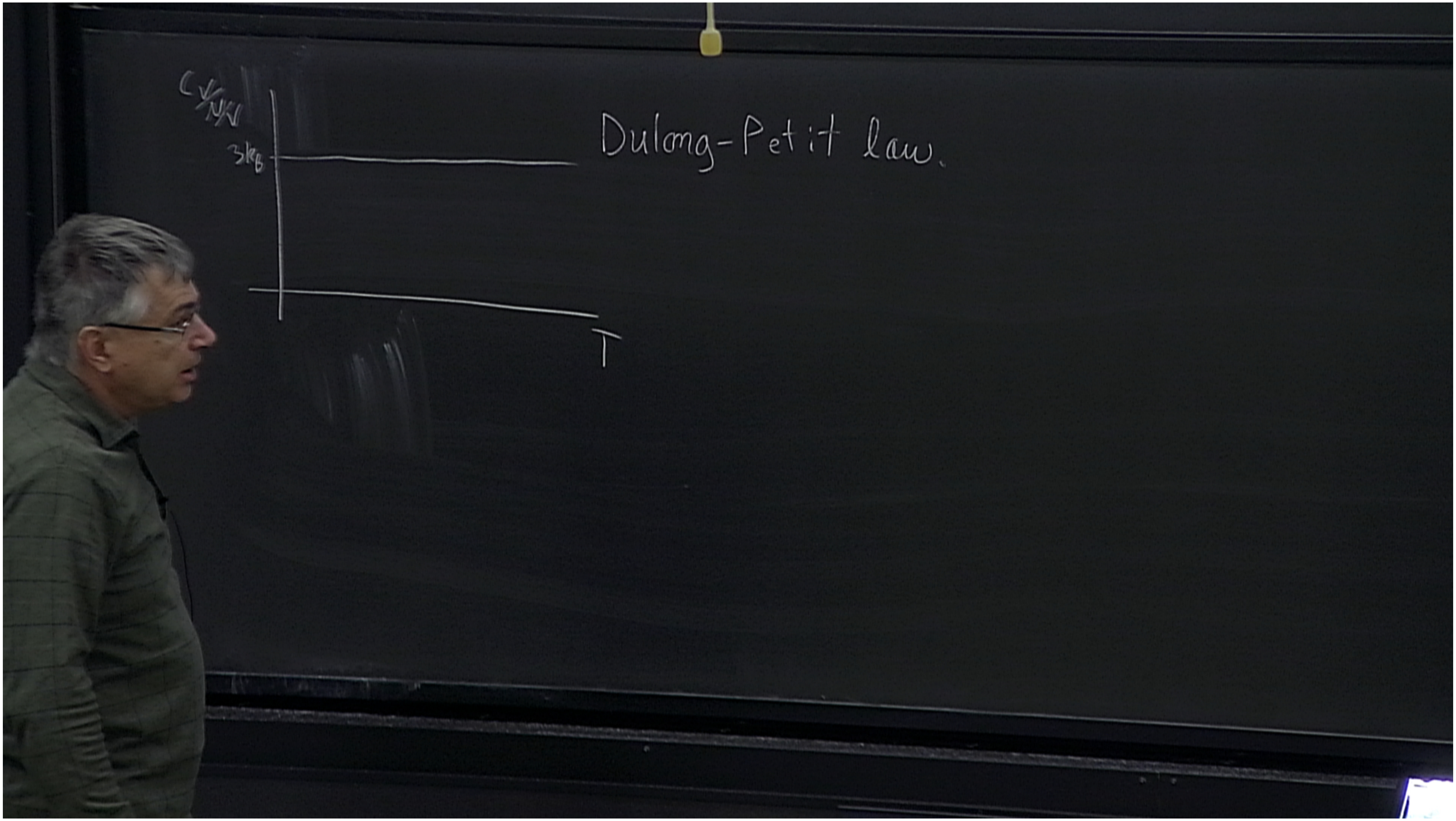
$$\ldots d p_\mu(\vec{R}) \rightarrow \frac{1}{\beta^{3N}} \prod_{\vec{R},\mu} d\tilde{u}_\mu(\vec{R})\, d\tilde{p}_\mu(\vec{R})$$

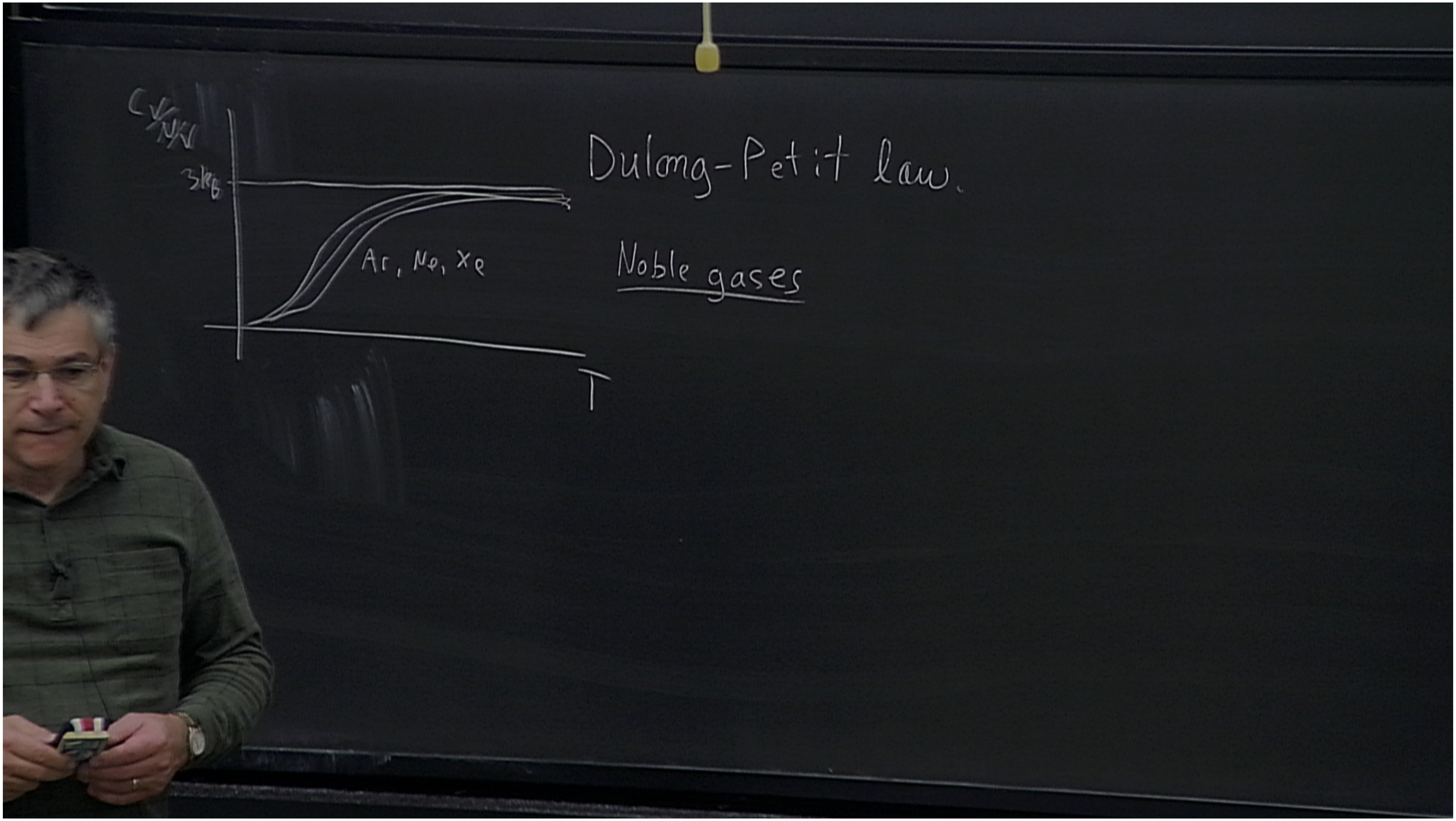
$$C_V = \left.\frac{\partial e}{\partial T}\right|_V$$

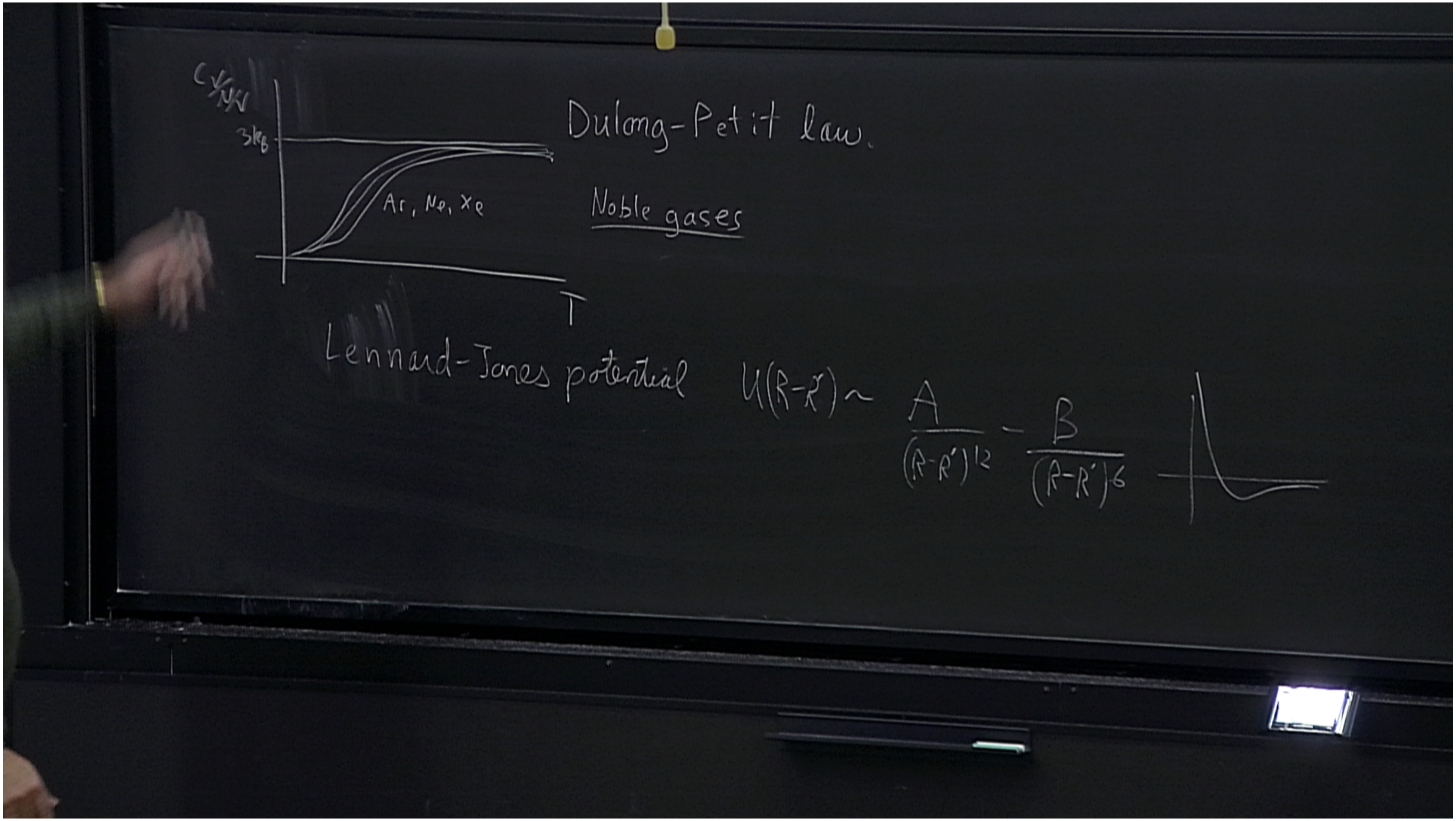
$$\int d\Gamma\, e^{-\beta H} \rightarrow \beta^{-3N} \text{const.}$$

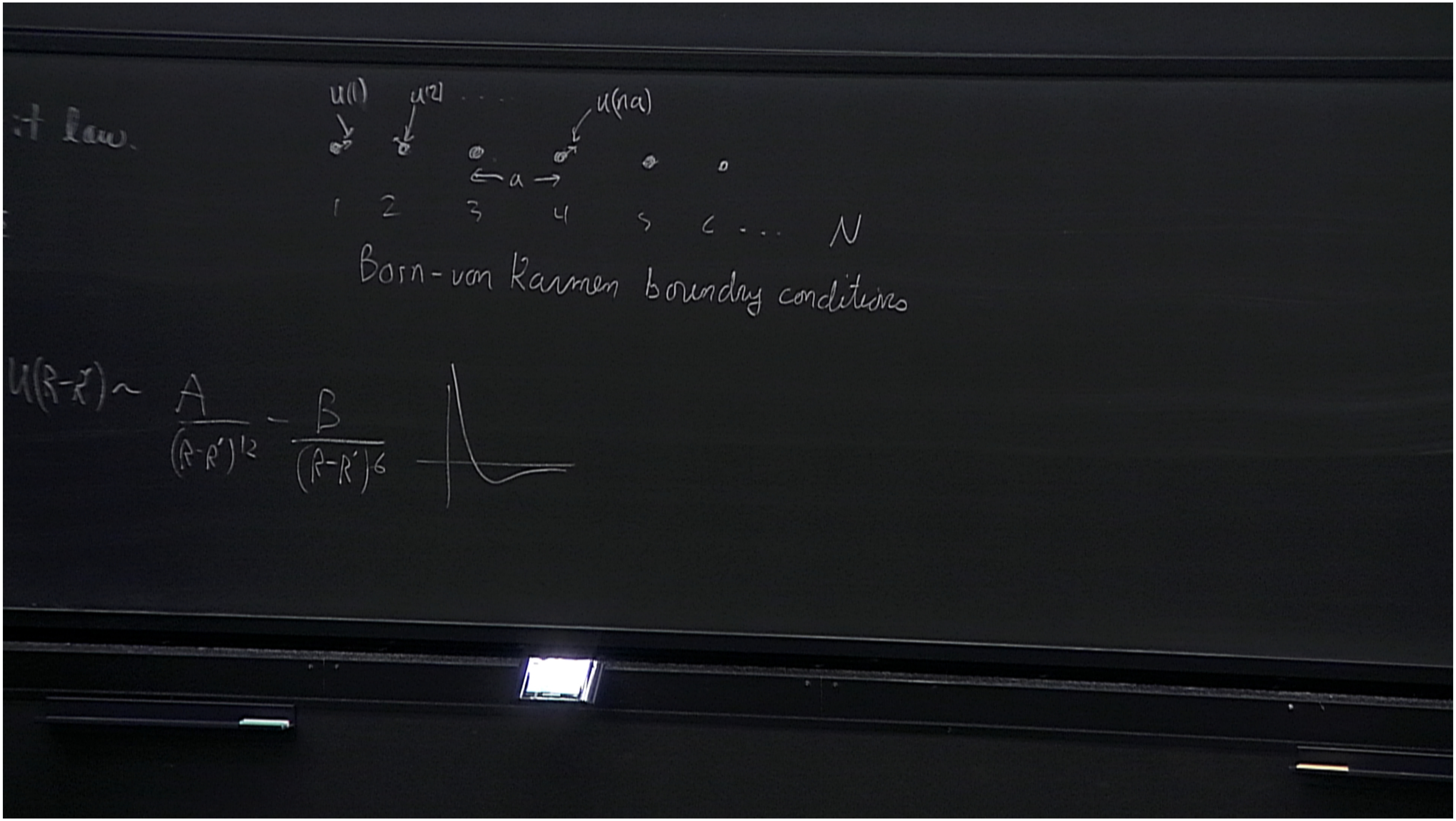
$$e \equiv \frac{E}{V} = -\frac{1}{V}\frac{\partial}{\partial \beta} \ln\left[\beta^{-3N} \text{const}\right] + \frac{U_{eq}}{V}$$

$$e = \frac{E}{V} = 3\frac{N}{V} k_B T \Rightarrow C_V = 3\frac{N}{V} k_B$$

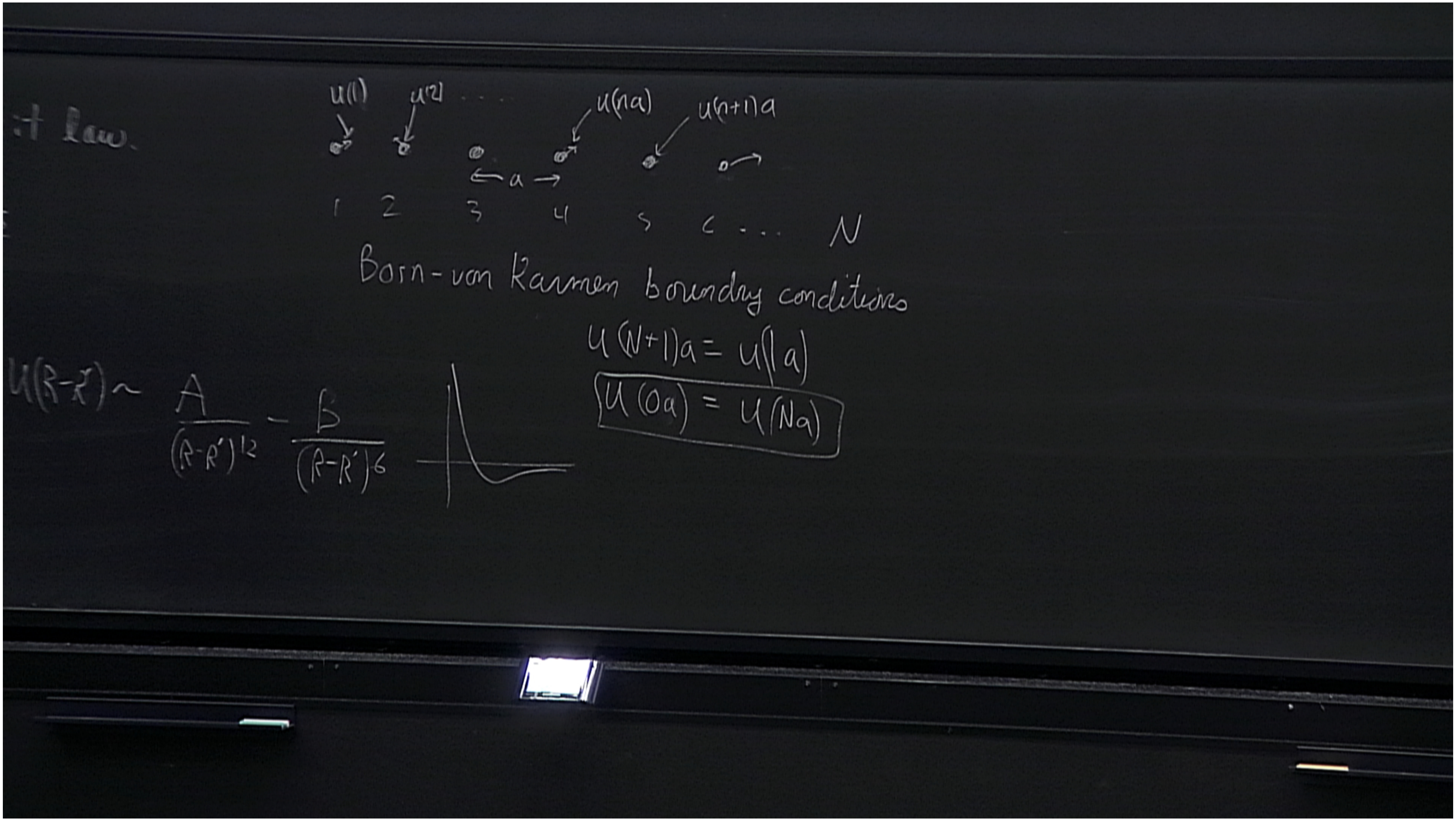

Dulong-Petit law.
3k_B
T

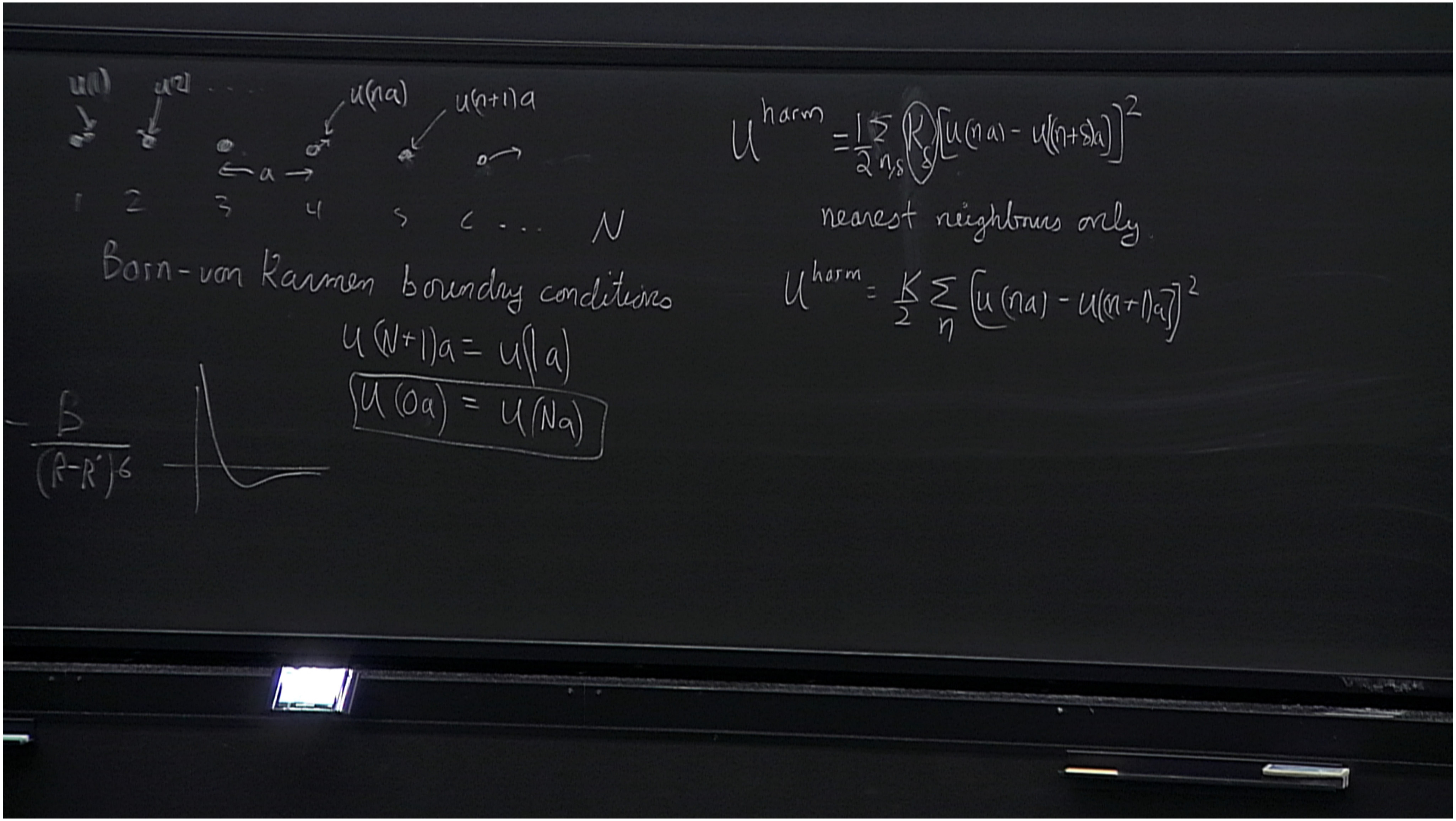

Dulong-Petit law.
Noble gases
Ar, Ne, Xe
T


Dulong-Petit law.
Noble gases
$3k_B$
Ar, Ne, Xe
T
Lennard-Jones potential
$U(R-R') \sim \frac{A}{(R-R')^{12}} - \frac{B}{(R-R')^{6}}$



t law.
u(1)
u(2)
u(na)
a
1 2 3 4 5 6 ... N
Born-von Karmen boundary conditions
$U(R-R') \sim \frac{A}{(R-R')^{12}} - \frac{B}{(R-R')^{6}}$


t law.
u(1)
u(2)
u(na)
u(n+1)a
a
1 2 3 4 5 6 ... N
Born-von Karmen boundary conditions
u((N+1)a) = u(1a)
u(0a) = u(Na)
U(R-R') ~ A/(R-R')^12 - B/(R-R')^6


u(1) u(2) . . . u(na) u(n+1)a
1 2 3 4 5 6 . . . N
Born-von Karmen boundary conditions
u(N+1)a = u(1a)
u(0a) = u(Na)
$-\frac{B}{(R-R')^6}$
$U^{harm} = \frac{1}{2}\sum_{n,s} K_s [u(na) - u((n+s)a)]^2$
nearest neighbours only
$U^{harm} = \frac{K}{2}\sum_{n} [u(na) - u((n+1)a)]^2$

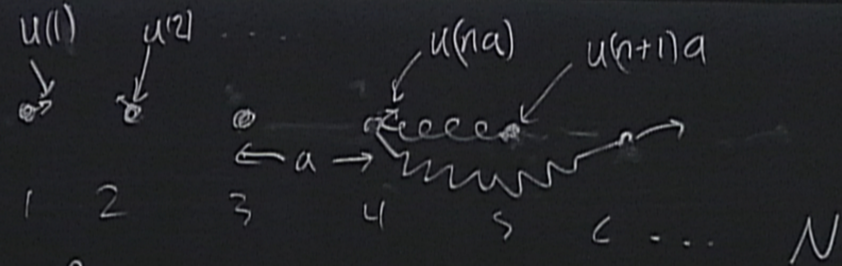
$$U^{harm} = \frac{1}{2}\sum_{n,s} K_s \left[u(na) - u((n+s)a)\right]^2$$

nearest neighbours only

$$U^{harm} = \frac{K}{2}\sum_{n} \left[u(na) - u((n+1)a)\right]^2$$

...etit law.

...es

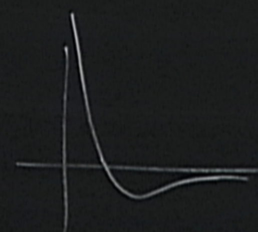


Born-von Karmen boundary conditions

$u(N+1)a = u(1a)$

$$\boxed{u(0a) = u(Na)}$$

$$U(R-R') \sim \frac{A}{(R-R')^{12}} - \frac{B}{(R-R')^{6}}$$



$$U^{harm} = \frac{1}{2}\sum_{n,s} K_s \left[u(na) - u(\ldots\right.$$

nearest neighbours

$$U^{harm} = \frac{K}{2}\sum_{n} \left(u(na) \ldots\right.$$

$$m\frac{d^2 u(na)}{dt^2} = -\frac{K}{2} \ldots$$

N

ditions

$$U^{harm} = \frac{1}{2}\sum_{n,s} K_s \left[u(na) - u((n+s)a)\right]^2$$

nearest neighbours only

$$U^{harm} = \frac{K}{2}\sum_{n} \left[u(na) - u((n+1)a)\right]^2$$

$$m\frac{d^2 u(na)}{dt^2} = -\frac{K}{2}\left\{2\left[u(na) - u(n+1)\right] - 2\left[u((n-1)a) - u(na)\right]\right\}$$

$$= K\left[2u(na) - \left[u(n+1) + u(n-1)\right]\right]$$

$$u(na) = \sum_k u_k e^{i(kna - \omega t)}$$

$$-m \sum_k \omega_k^2 u_k e^{i(kna - \omega t)} = K \sum_k u_k \left[2 - \left(e^{ika} + e^{-ika}\right)\right] e^{i(kna - \omega t)}$$

$$u(na) = \sum_k u_k e^{i(kna-\omega t)}$$

$$-m\sum_k \omega_k^2 u_k e^{i(kna-\omega t)} = -K\sum_k u_k\left[2-\left(e^{ika}+e^{-ika}\right)\right]e^{i(kna-\omega t)}$$

$$e^{-i(pna-\omega t)} \quad \Rightarrow \omega_k^2 = +\frac{2K}{m}(1-\cos ka)$$

$\cos ka = 1-2\sin^2\frac{ka}{2}$

$$= \frac{4K}{m}\sin^2\left(\frac{ka}{2}\right)$$

$$\Rightarrow \omega_k = 2\sqrt{\frac{K}{m}}\left|\sin\frac{ka}{2}\right|$$

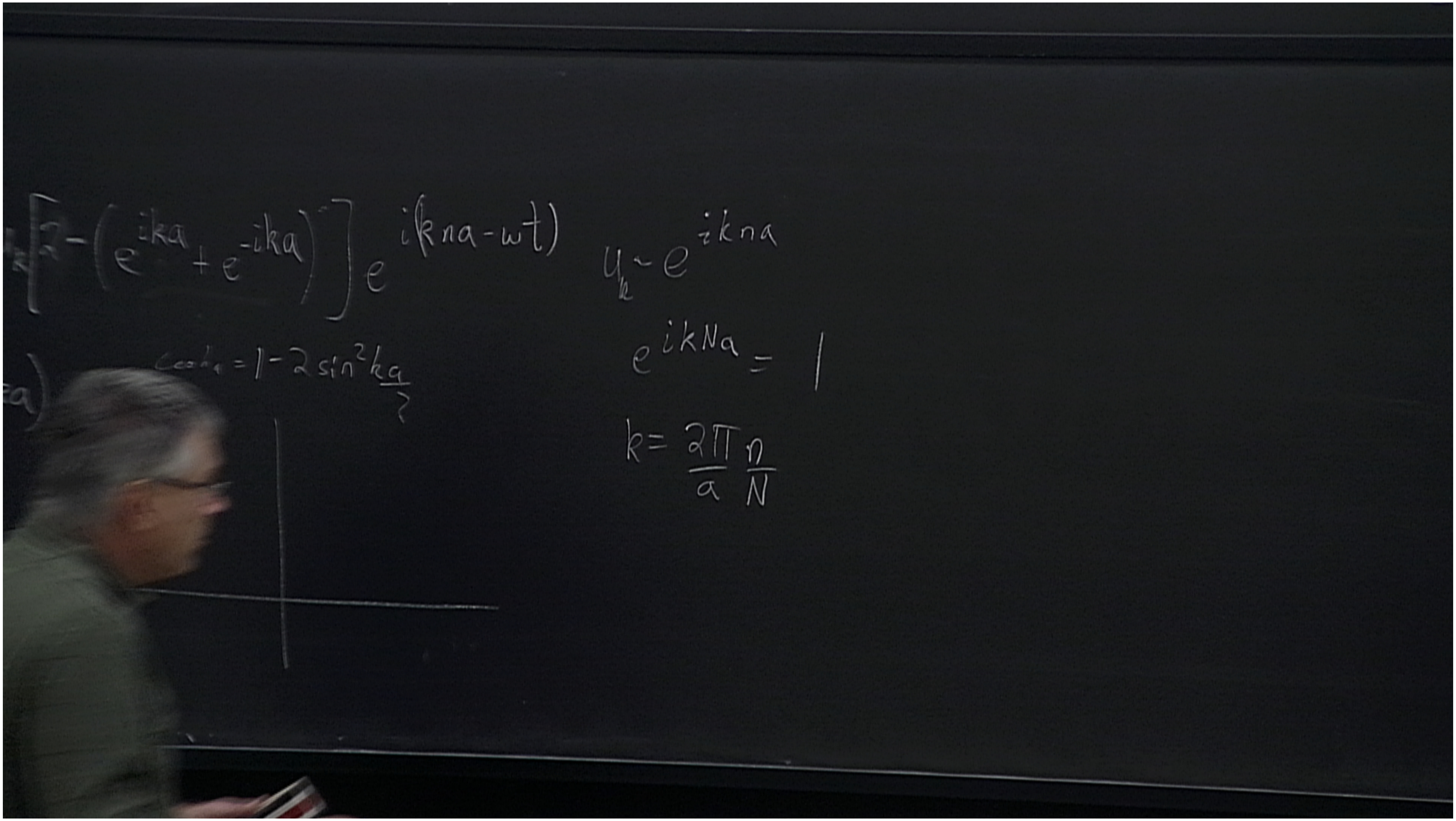
$$U^{harm} = \frac{1}{4} \sum_{\substack{RR' \\ \mu,\nu = x,y,z}} \left[u_\mu(\vec{R}) - u_\mu(\vec{R}')\right] \phi_{\mu\nu}(\vec{R}-\vec{R}') \left[u_\nu(\vec{R}) - u_\nu(\vec{R}')\right] \qquad e =$$

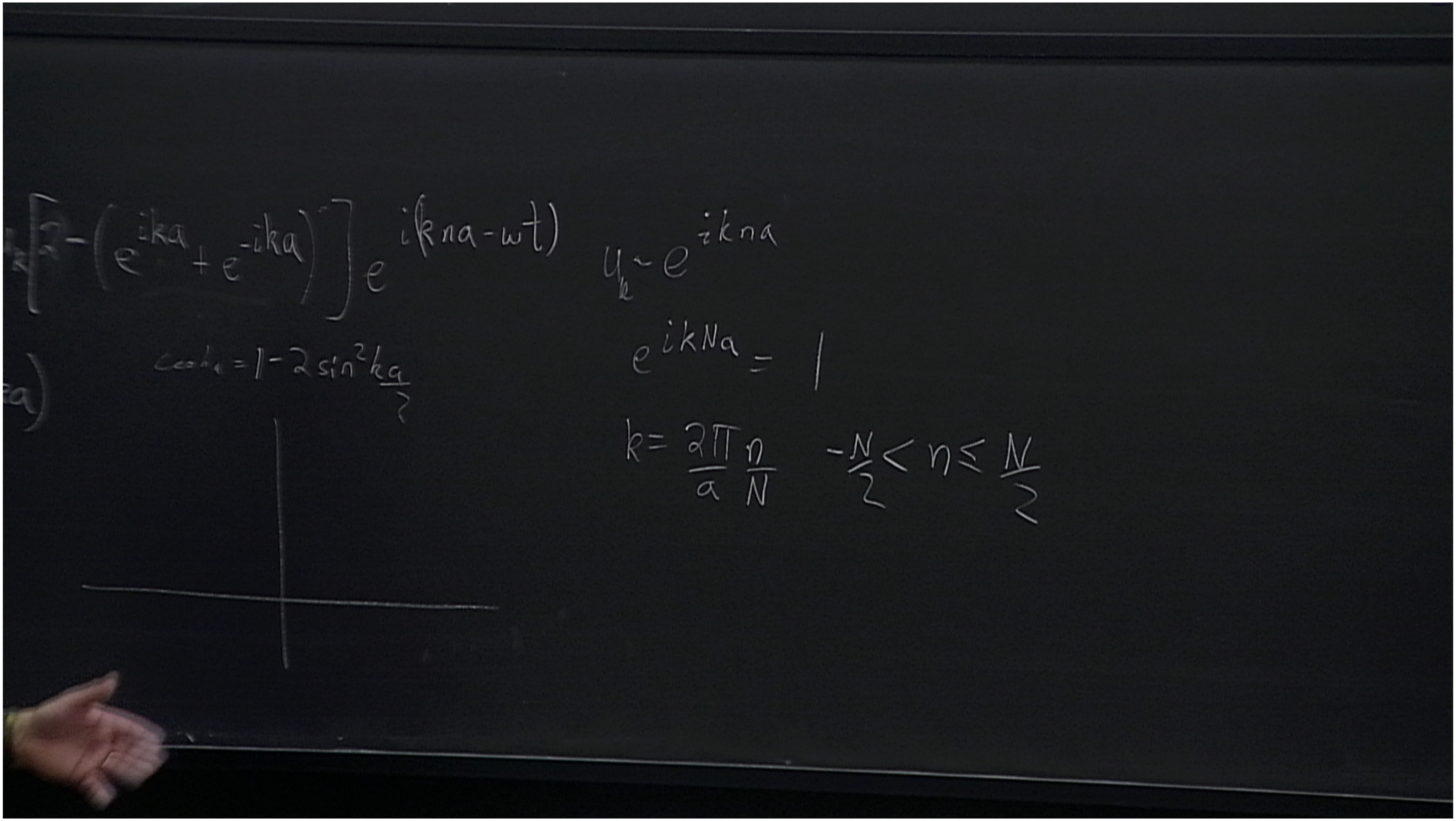
$$\phi_{\mu\nu}(\vec{R}-\vec{R}') \equiv \frac{\partial^2 U(r)}{\partial r_\mu \partial r_\nu}$$

$$= \frac{1}{2} \sum_{\substack{RR' \\ \mu\nu}} u_\mu(\vec{R}) D_{\mu\nu}(\vec{R}-\vec{R}') u_\nu(\vec{R}')$$

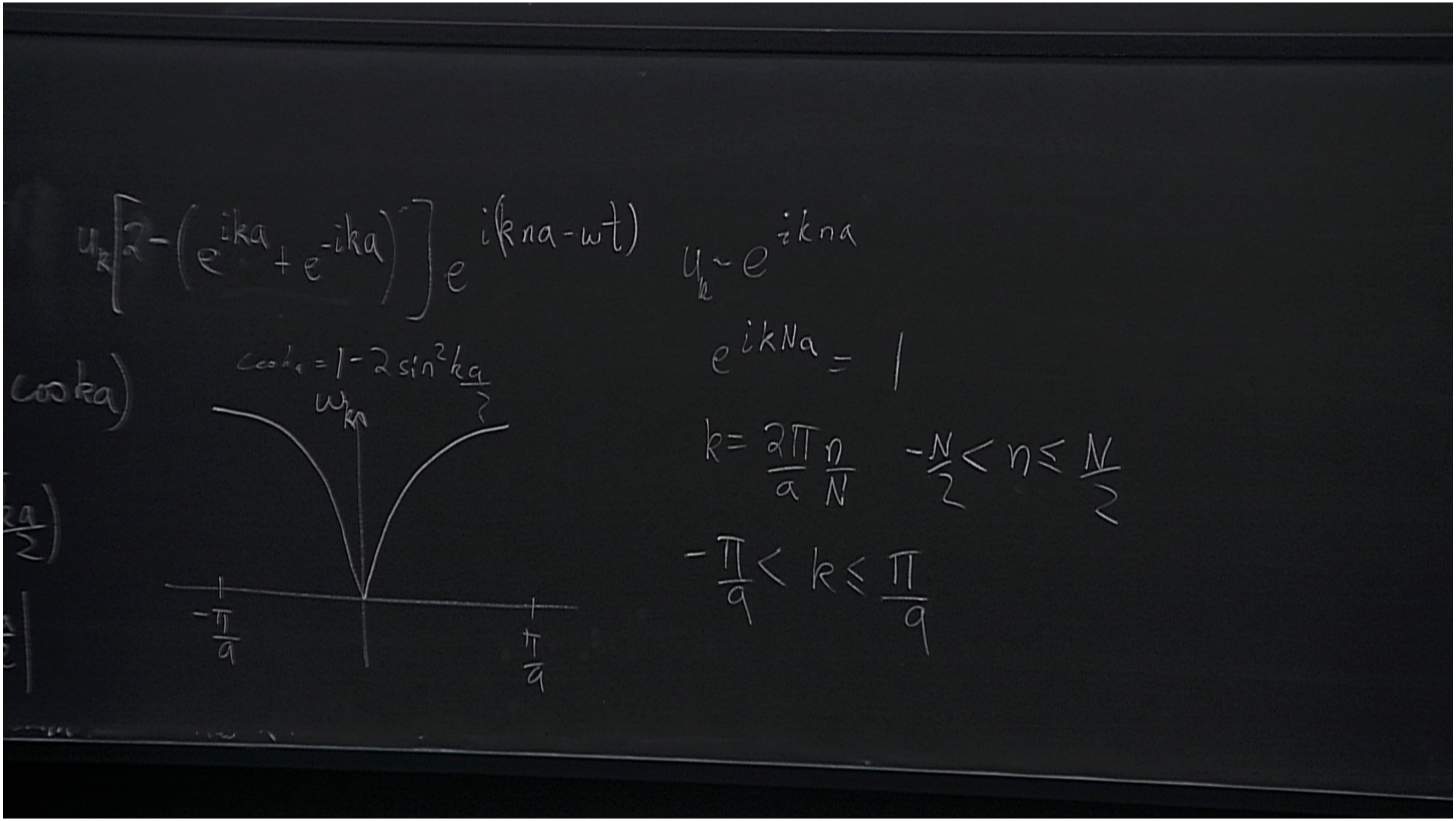
Dynamical matrix

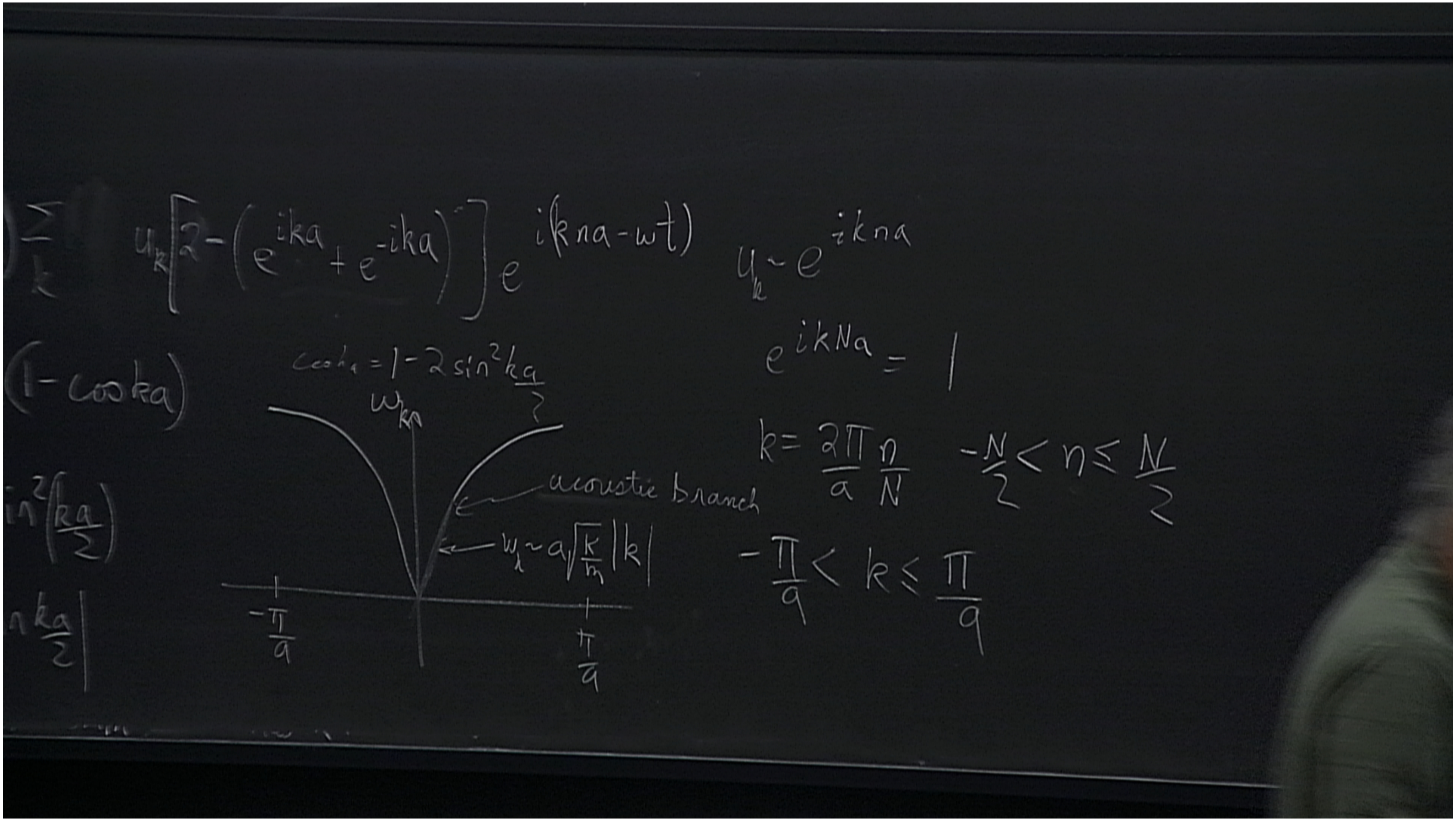
where $D_{\mu\nu}(\vec{R}-\vec{R}') = \delta_{RR'} \sum_{R''} \phi_{\mu\nu}(\vec{R}-\vec{R}'') - \phi_{\mu\nu}(\vec{R}-\vec{R}')$


$e^{i(kna-\omega t)}$
$u_k \sim e^{ikna}$
$\cos ka = 1 - 2\sin^2 \frac{ka}{2}$
$e^{ikNa} = 1$
$k = \frac{2\pi}{a} \frac{n}{N}$



$\left[2-\left(e^{ika}+e^{-ika}\right)\right]e^{i(kna-\omega t)}$
$\cos ka = 1-2\sin^2\frac{ka}{2}$
$u_k \sim e^{ikna}$
$e^{ikNa}=1$
$k=\frac{2\pi}{a}\frac{n}{N}$
$-\frac{N}{2}<n\leq\frac{N}{2}$


$u_k\left[2-\left(e^{ika}+e^{-ika}\right)\right]e^{i(kna-\omega t)}$
$u_k \sim e^{ikna}$
$\cos ka = 1-2\sin^2\frac{ka}{2}$
$e^{ikNa}=1$
$k=\frac{2\pi}{a}\frac{n}{N}$
$-\frac{N}{2}<n\leq\frac{N}{2}$
$-\frac{\pi}{a}<k\leq\frac{\pi}{a}$
ω_{ka}
$-\frac{\pi}{a}$
$\frac{\pi}{a}$


$u_k \left[2 - \left(e^{ika} + e^{-ika}\right)\right] e^{i(kna - \omega t)}$
$u_k \sim e^{ikna}$
$(1 - \cos ka)$
$\cos ka = 1 - 2\sin^2 \frac{ka}{2}$
$e^{ikNa} = 1$
ω_{ka}
$k = \frac{2\pi}{a}\frac{n}{N}$
$-\frac{N}{2} < n \le \frac{N}{2}$
acoustic branch
$\omega_k \sim a\sqrt{\frac{K}{m}}|k|$
$-\frac{\pi}{a} < k \le \frac{\pi}{a}$
$-\frac{\pi}{a}$
$\frac{\pi}{a}$

$$D_{\mu\nu}(\vec{R}) = D_{\mu\nu}(-\vec{R})$$

$$D_{\mu\nu}(\vec{R}) = -D_{\nu\mu}(-\vec{R})$$

$$\sum_{R} D_{\mu\nu}(\vec{R}) = 0$$

$$< n \leq \frac{N}{2}$$

$$M \frac{d^2 \vec{u}}{dt^2} = - \sum_{\vec{R}'} D(\vec{R} - \vec{R}') \, \vec{u}(\vec{R}')$$

$$\vec{u}(\vec{R}, t) = \vec{\epsilon} \, e^{i(\vec{k} \cdot \vec{R} - \omega t)}$$

polarization vector

$$M \frac{d^2 \vec{u}}{dt^2} = - \sum_{\vec{R}'} D(\vec{R} - \vec{R}')\, \vec{u}(\vec{R}')$$

$$\vec{u}(\vec{R}, t) = \vec{\epsilon}\, e^{i(\vec{k}\cdot\vec{R} - \omega t)}$$

polarization vector

$\vec{k} = \frac{n_1}{N_1}\vec{b}_1 + \frac{n_2}{N_2}\vec{b}_2 + \frac{n_3}{N_3}\vec{b}_3$ where $\vec{b}_i$ are reciprocal lattice vectors

$$N \equiv N_1 \cdot N_2 \cdot N_3$$

$$M\omega^2 \bar{\epsilon} = D(\vec{k})\,\bar{\epsilon}$$

$$D(\vec{k}) = \sum_{R} D(\vec{R})\, e^{-i\vec{k}\cdot\vec{R}}$$

$$D(\vec{k}) = -2 \sum_{\vec{R}} D(\vec{R}) \sin^2 \frac{\vec{k}\cdot\vec{R}}{2}$$

3 solns for each of N modes (labelled by k)

iprocal

ctors

$$D(\vec{k}) = -2 \sum_{\vec{R}} D(\vec{R}) \sin^2 \frac{\vec{k}\cdot\vec{R}}{2} \qquad \vec{\epsilon}_s(k)\cdot\epsilon_{s'}(\vec{k}) = \delta_{ss'}$$

real, symmetric

$\Rightarrow$ real eigenvalues

es (labelled by k)

$$\bar{\bar{D}}(\bar{k})\,\bar{\epsilon}_s(\bar{k}) = \lambda_s(\bar{k})\,\bar{\epsilon}_s(\bar{k})$$

$$s = 1,2,3 \qquad \lambda_s(\bar{k}) \equiv M\omega_s^2(\bar{k})$$

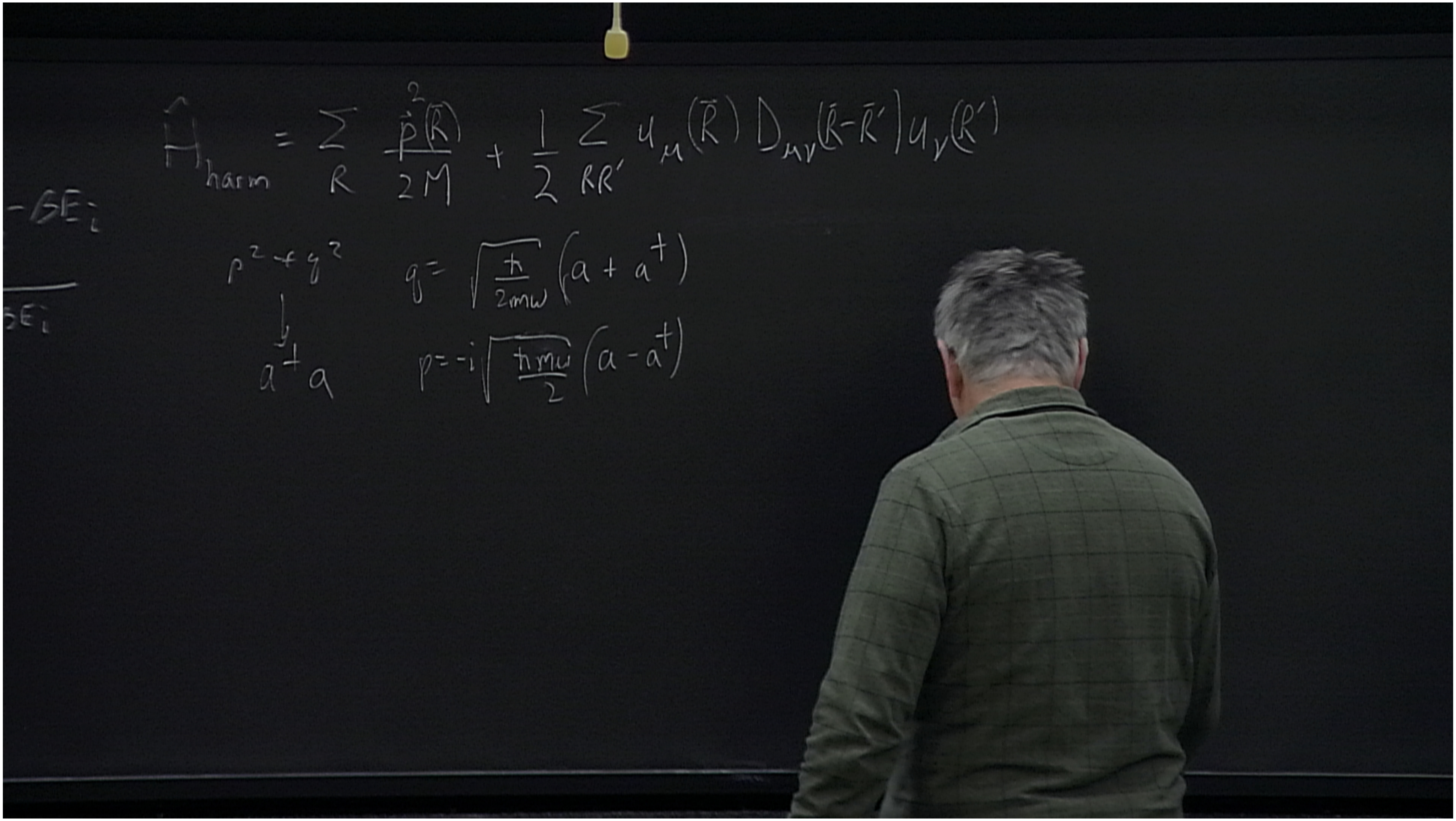
Quantum Mechanics

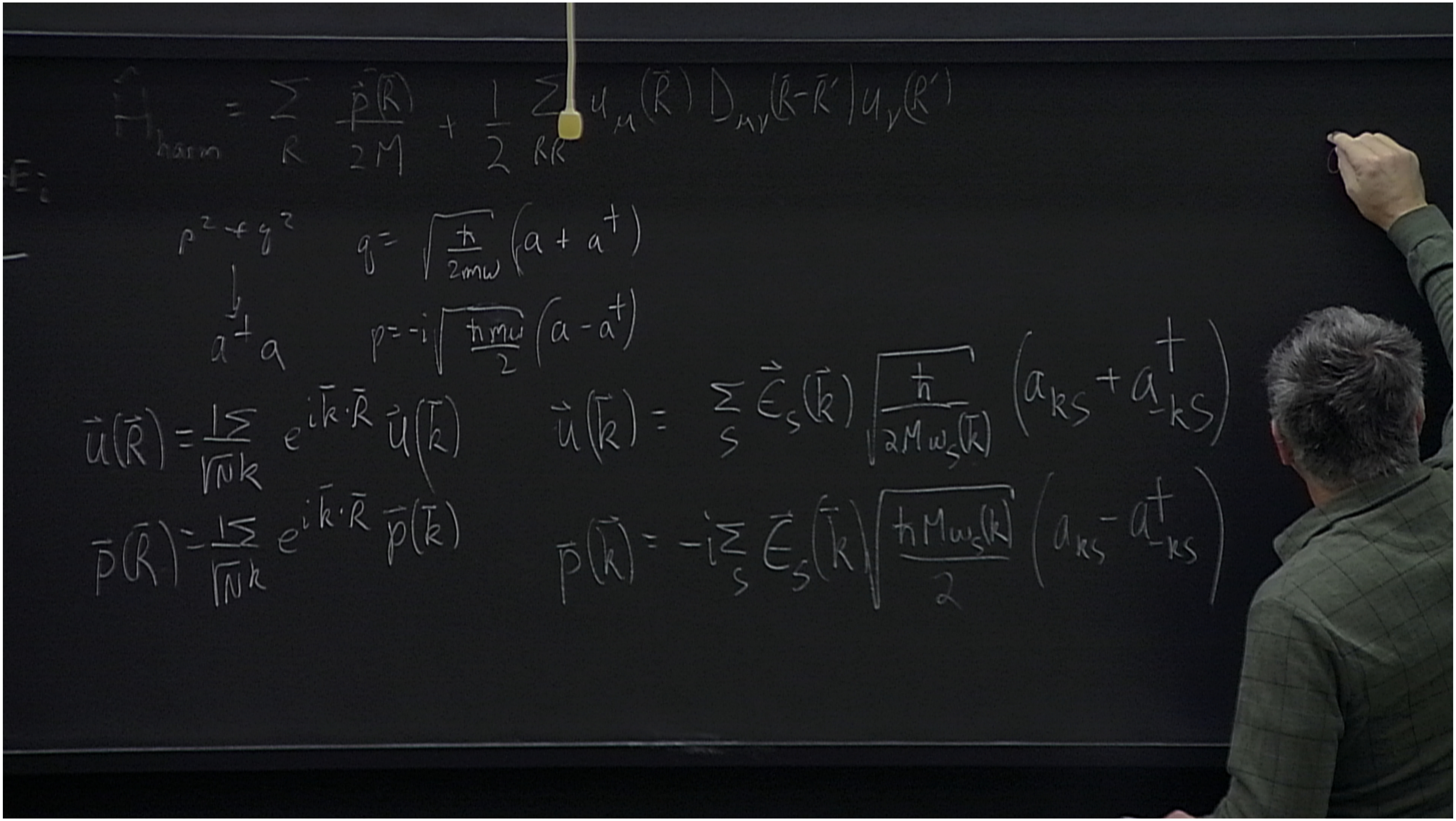
$$\hat{H}_{harm} = \sum_{R} \frac{\vec{p}^{\,2}(\vec{R})}{2M} + \frac{1}{2} \sum_{RR'} u_{\mu}(\vec{R})\, D_{\mu\nu}(\vec{R}-\vec{R}')\, u_{\nu}(\vec{R}')$$

$$e = \frac{E}{V} = \frac{1}{V} \frac{\sum_i E_i e^{-\beta E_i}}{\sum_i e^{-\beta E_i}}$$

$$= -\frac{1}{V} \frac{\partial}{\partial \beta} \ln Z$$

$$Z = \sum_i e^{-\beta E_i}$$


$\hat{H}_{harm} = \sum_R \frac{\vec{p}^2(\vec{R})}{2M} + \frac{1}{2}\sum_{RR'} u_\mu(\vec{R}) D_{\mu\nu}(\vec{R}-\vec{R}') u_\nu(\vec{R}')$
$p^2 + q^2$
$a^\dagger a$
$q = \sqrt{\frac{\hbar}{2m\omega}}(a + a^\dagger)$
$p = -i\sqrt{\frac{\hbar m\omega}{2}}(a - a^\dagger)$


$\hat{H}_{harm} = \sum_R \frac{\vec{p}(R)}{2M} + \frac{1}{2}\sum_{RR'} u_\mu(\vec{R}) D_{\mu\nu}(\vec{R}-\vec{R}') u_\nu(\vec{R}')$
$p^2 + q^2$
$a^\dagger a$
$q = \sqrt{\frac{\hbar}{2m\omega}}(a + a^\dagger)$
$p = -i\sqrt{\frac{\hbar m\omega}{2}}(a - a^\dagger)$
$\vec{u}(\vec{R}) = \frac{1}{\sqrt{N}}\sum_k e^{i\vec{k}\cdot\vec{R}}\,\vec{u}(\vec{k})$
$\vec{p}(\vec{R}) = \frac{1}{\sqrt{N}}\sum_k e^{i\vec{k}\cdot\vec{R}}\,\vec{p}(\vec{k})$
$\vec{u}(\vec{k}) = \sum_s \vec{\epsilon}_s(\vec{k})\sqrt{\frac{\hbar}{2M\omega_s(\vec{k})}}\left(a_{ks} + a^\dagger_{-ks}\right)$
$\vec{p}(\vec{k}) = -i\sum_s \vec{\epsilon}_s(\vec{k})\sqrt{\frac{\hbar M\omega_s(\vec{k})}{2}}\left(a_{ks} - a^\dagger_{-ks}\right)$

$$\hat{a}_{ks} = \frac{1}{\sqrt{N}} \sum_{R} e^{-i\vec{k}\cdot\vec{R}}\, \vec{\epsilon}_s(\vec{k}) \left[\sqrt{\frac{M\omega_s(k)}{2\hbar}}\, \vec{u}(\vec{R}) + i\sqrt{\frac{1}{2M\hbar\omega_s(k)}}\, \vec{p}(\vec{R}) \right]$$

$$\hat{a}^{\dagger}_{ks} = \frac{1}{\sqrt{N}} \sum_{R} e^{i\vec{k}\cdot\vec{R}}\, \vec{\epsilon}_s(\vec{k}) \left[\sqrt{}\, \vec{u}(\vec{R}) - i\sqrt{}\, \vec{p}(\vec{R}) \right]$$

$$\left[a_{ks},\, a^{\dagger}_{k's'}\right] = \delta_{kk'}\,\delta_{ss'}$$

$\dagger$

$_{-ks}$)

$\dagger$

$_{-ks}$)