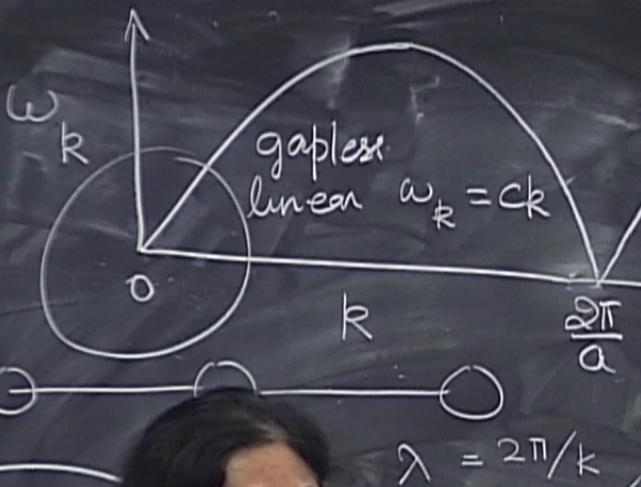
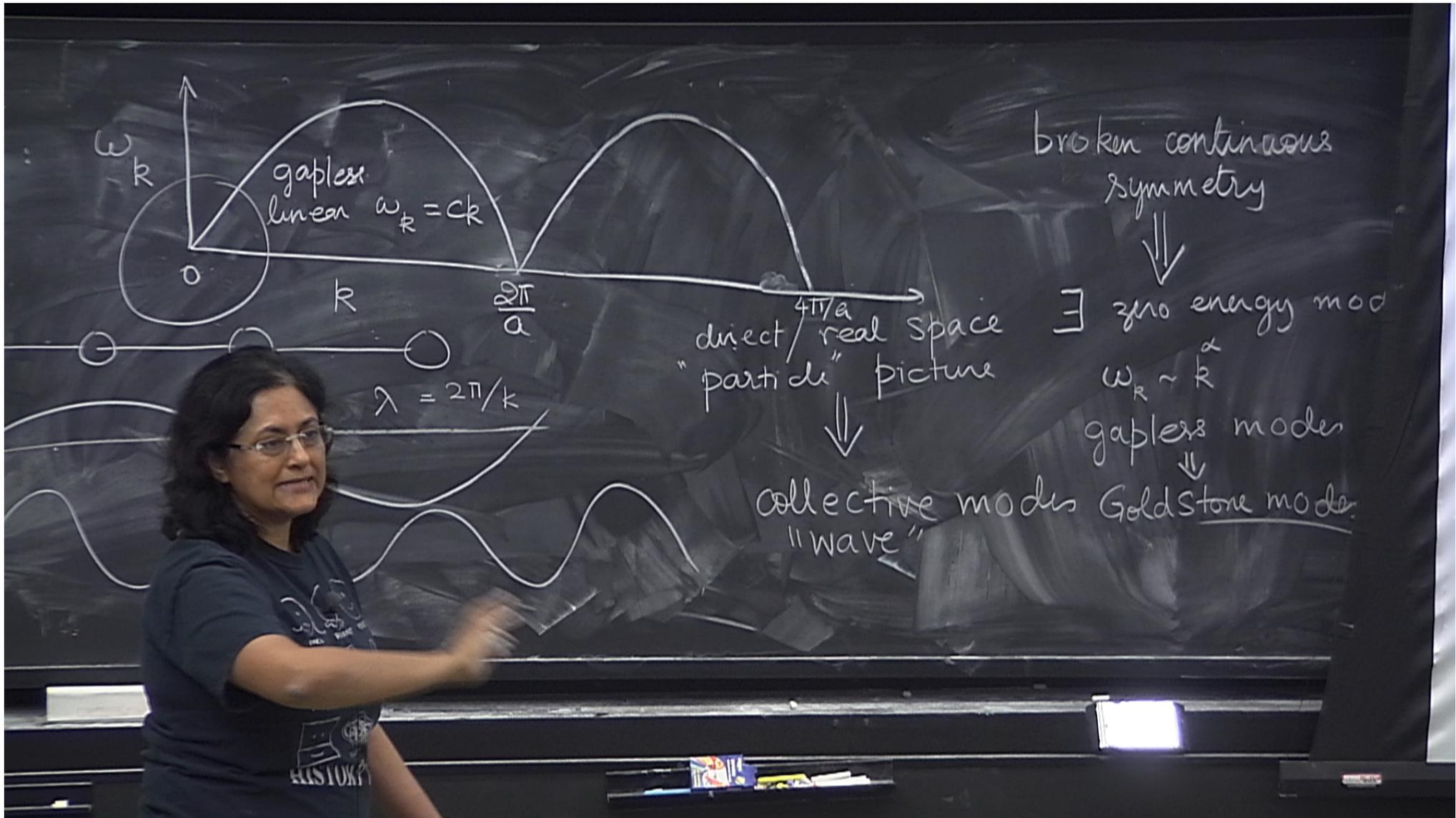


Title: Condensed Matter - Lecture 3

Date: Nov 02, 2011 10:30 AM

URL: <http://pirsa.org/11110023>

Abstract:



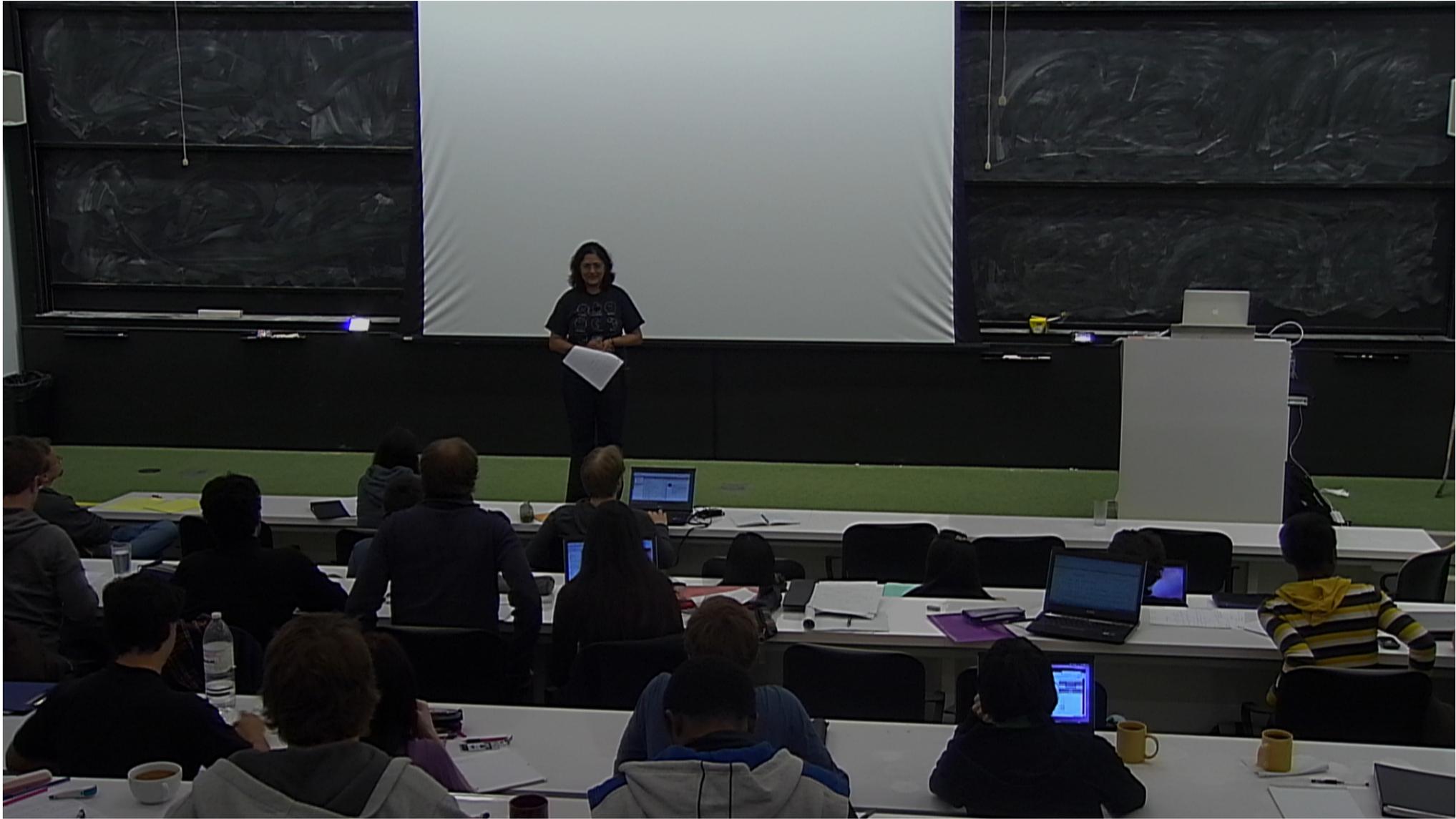
direct/real space
 "particle" picture

collective modes
 "wave"

broken continuous
 symmetry

\exists zero energy mod

$\omega_k \sim k^\alpha$
 gapless modes
 Goldstone mode



$$H = H_e + H_{ion} + H_{e-ion}$$

Condensed
matter system

$$H = H_e + H_{ion} + H_{e-ion}$$

Condensed
matter system

$$H_e = \sum_i \frac{\vec{p}_i^2}{2m} + \frac{1}{2} \sum'_{i,j} V_{ee}(\vec{r}_i - \vec{r}_j) \quad \{\vec{r}_i\} \text{ electronic coordinates}$$

$$H_{ion} = \sum_I \frac{\vec{P}_I^2}{2M} + \frac{1}{2} \sum'_{I,J} V_{II'}(\vec{R}_I - \vec{R}_{I'})$$

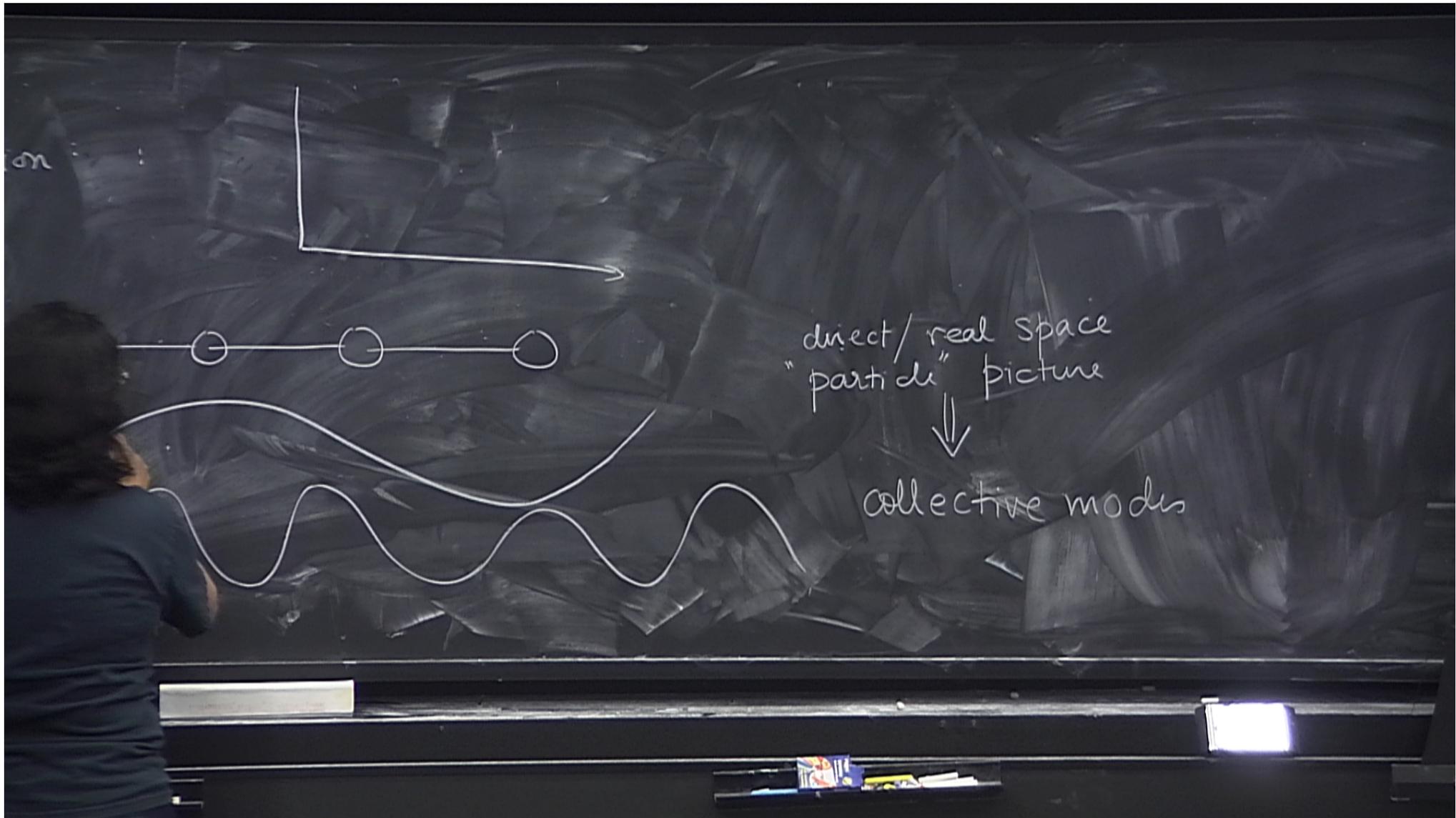
$$H = H_e + H_{ion} + H_{e-ion}$$

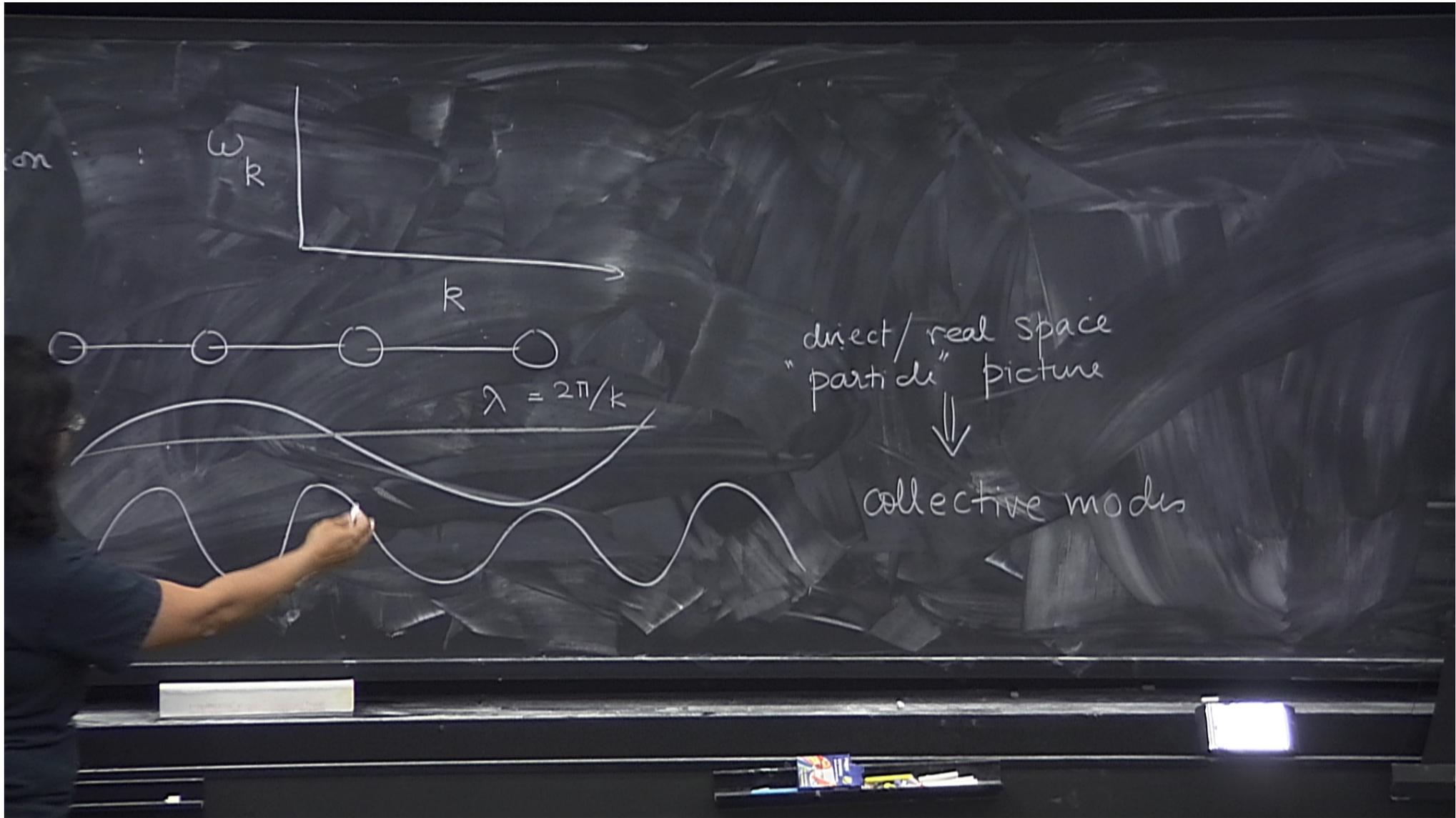
Condensed
matter system

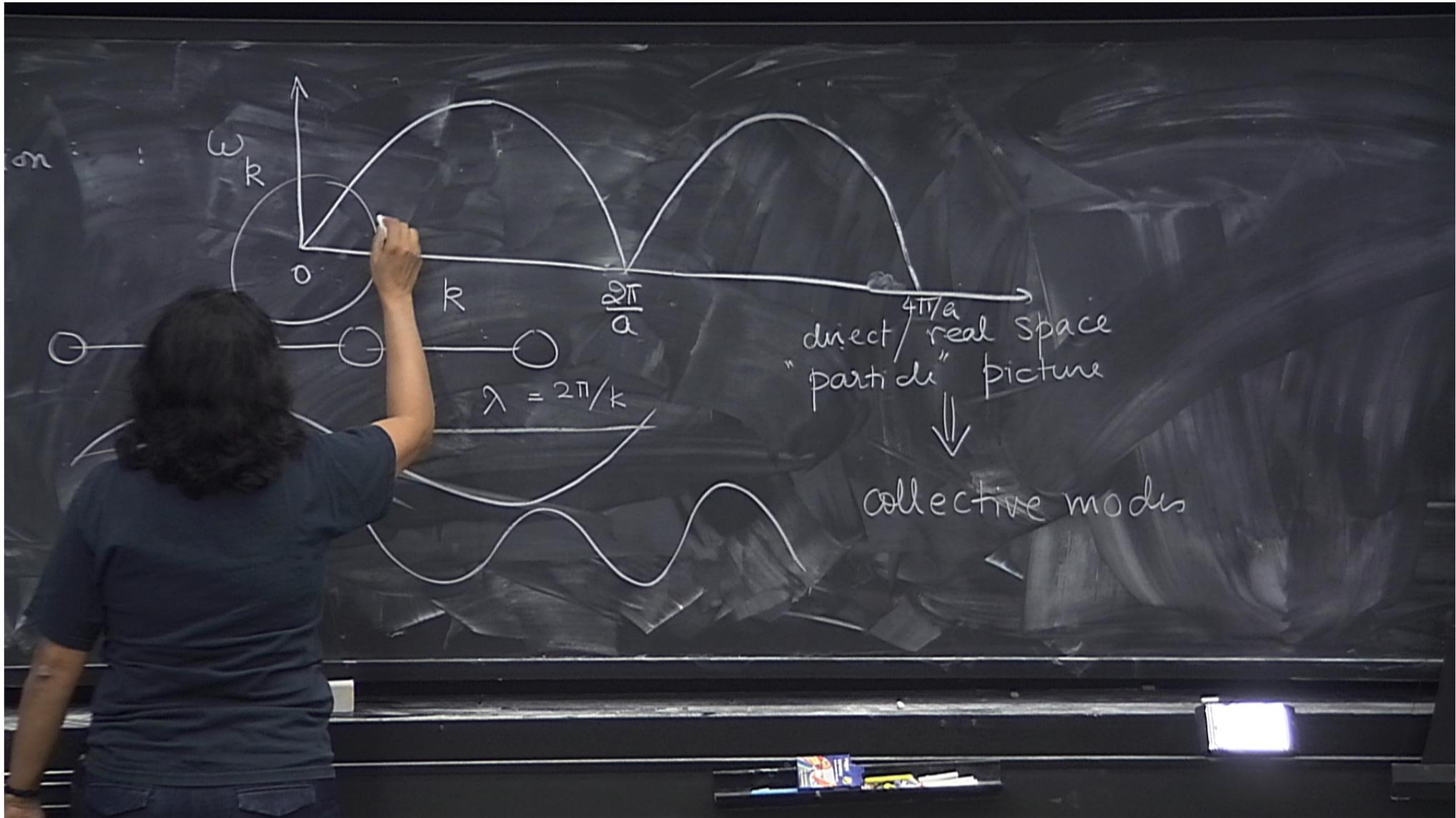
$$H_e = \sum_i \frac{\vec{p}_i^2}{2m} + \frac{1}{2} \sum'_{i,j} V_{ee}(\vec{r}_i - \vec{r}_j) \quad \{\vec{r}_i\} \text{ electronic coordinates}$$

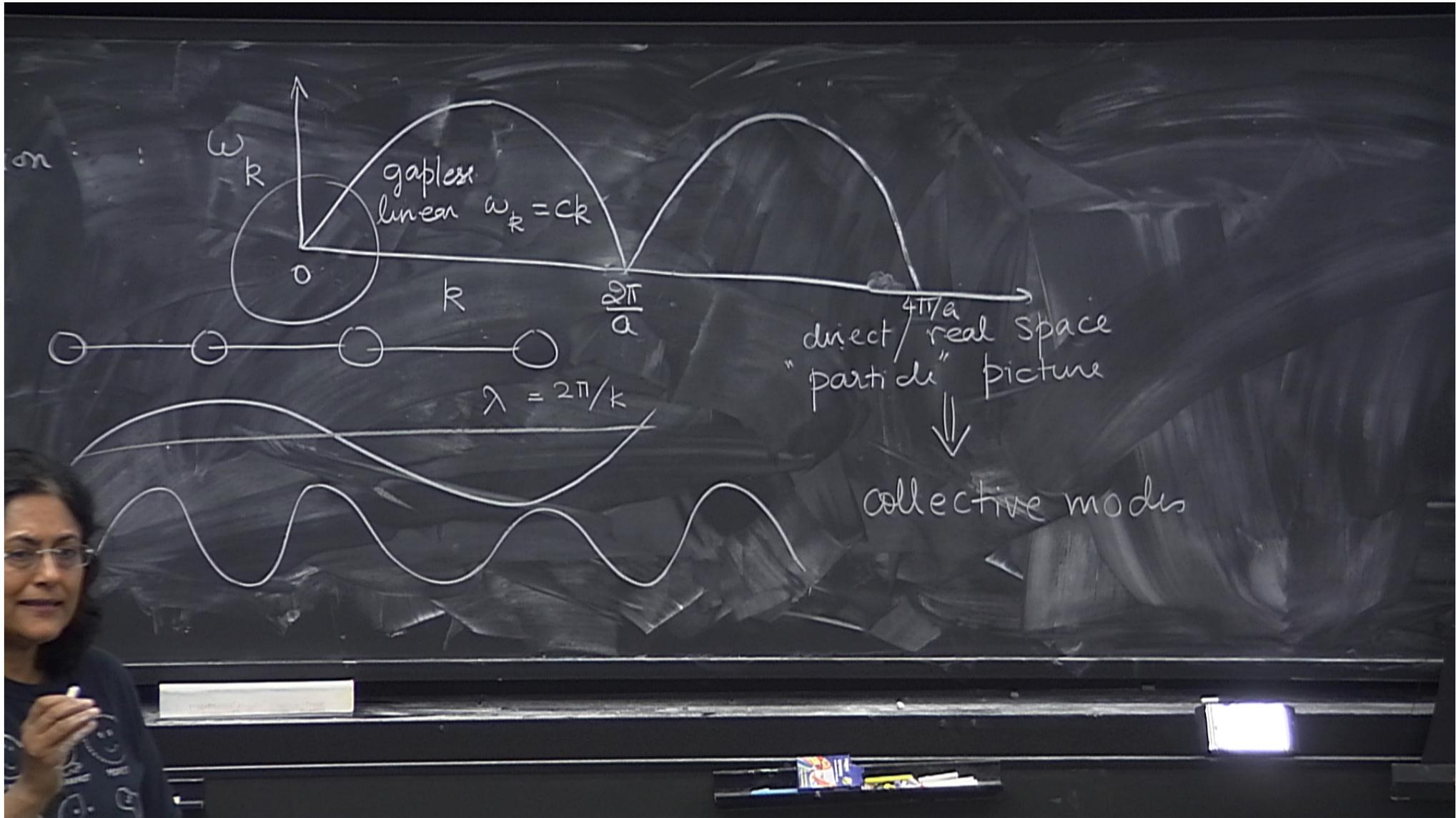
$$H_{ion} = \sum_I \frac{\vec{P}_I^2}{2M} + \frac{1}{2} \sum'_{I,J} V_{ion-ion}(\vec{R}_I - \vec{R}_J) \quad \{\vec{R}_I\} \text{ ionic coordinates}$$

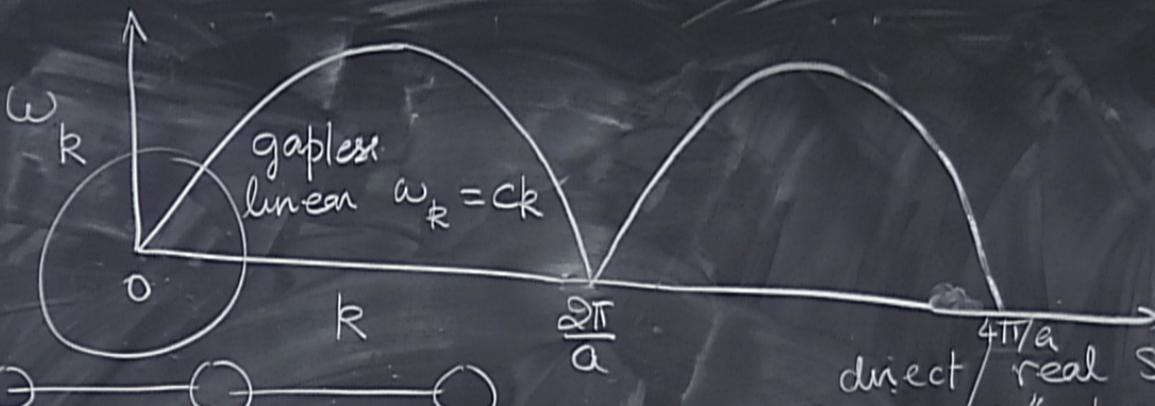
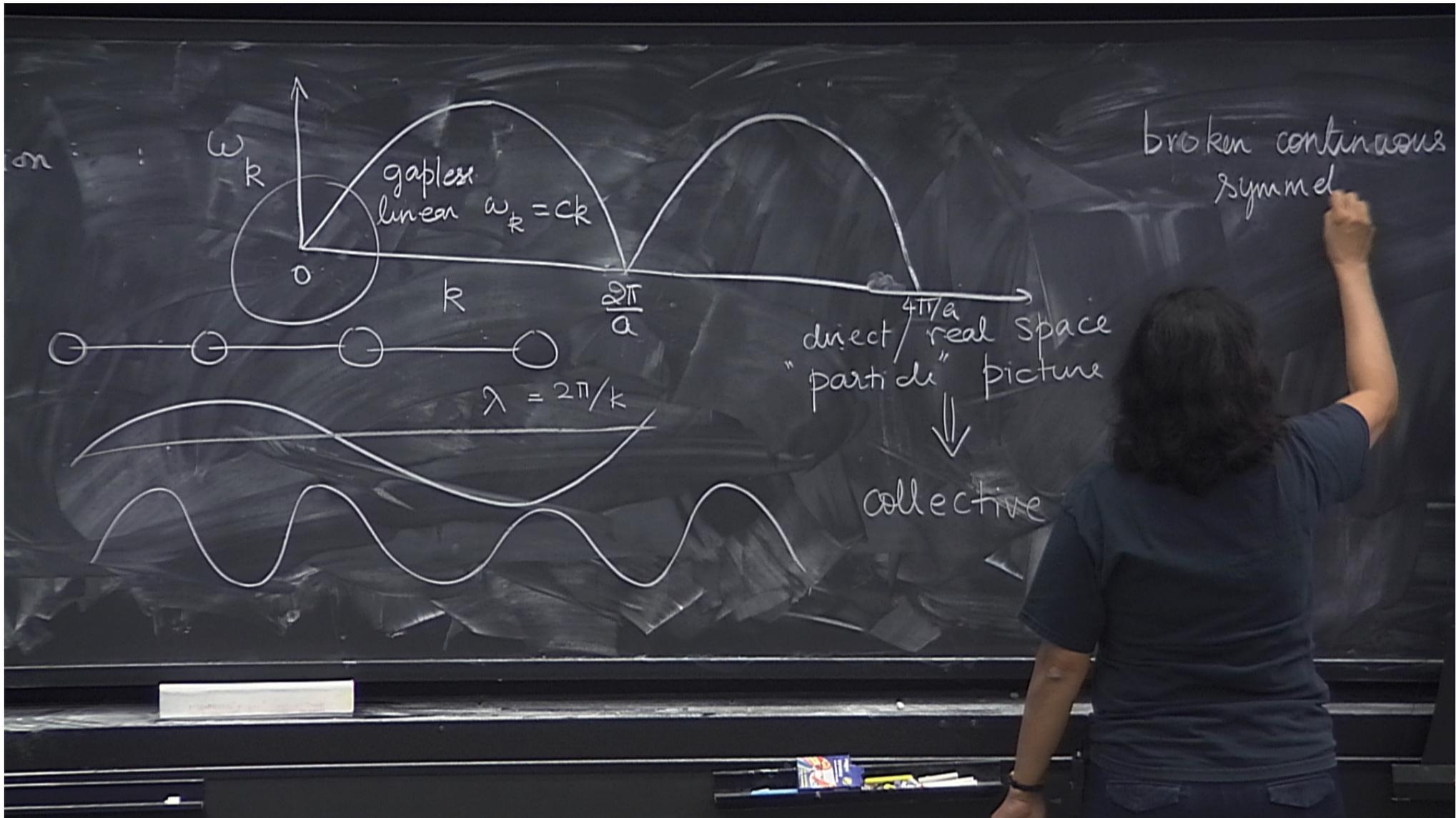
$$H_{e-ion} = \sum_{i,I} V_{e-i}(\vec{r}_i - \vec{R}_I)$$









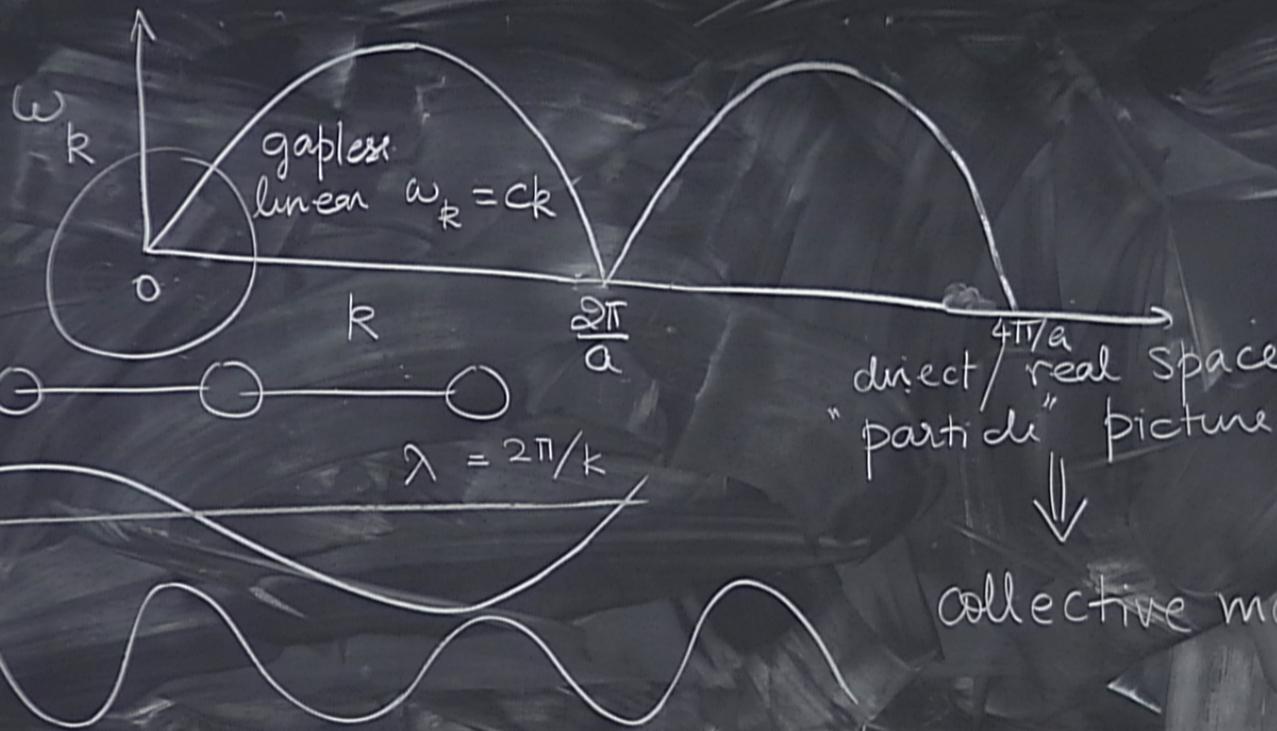


broken continuous symmet



direct/real space "particle" picture

collective



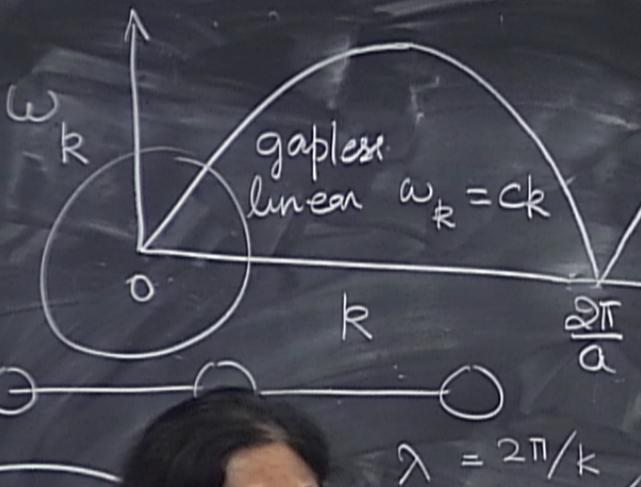
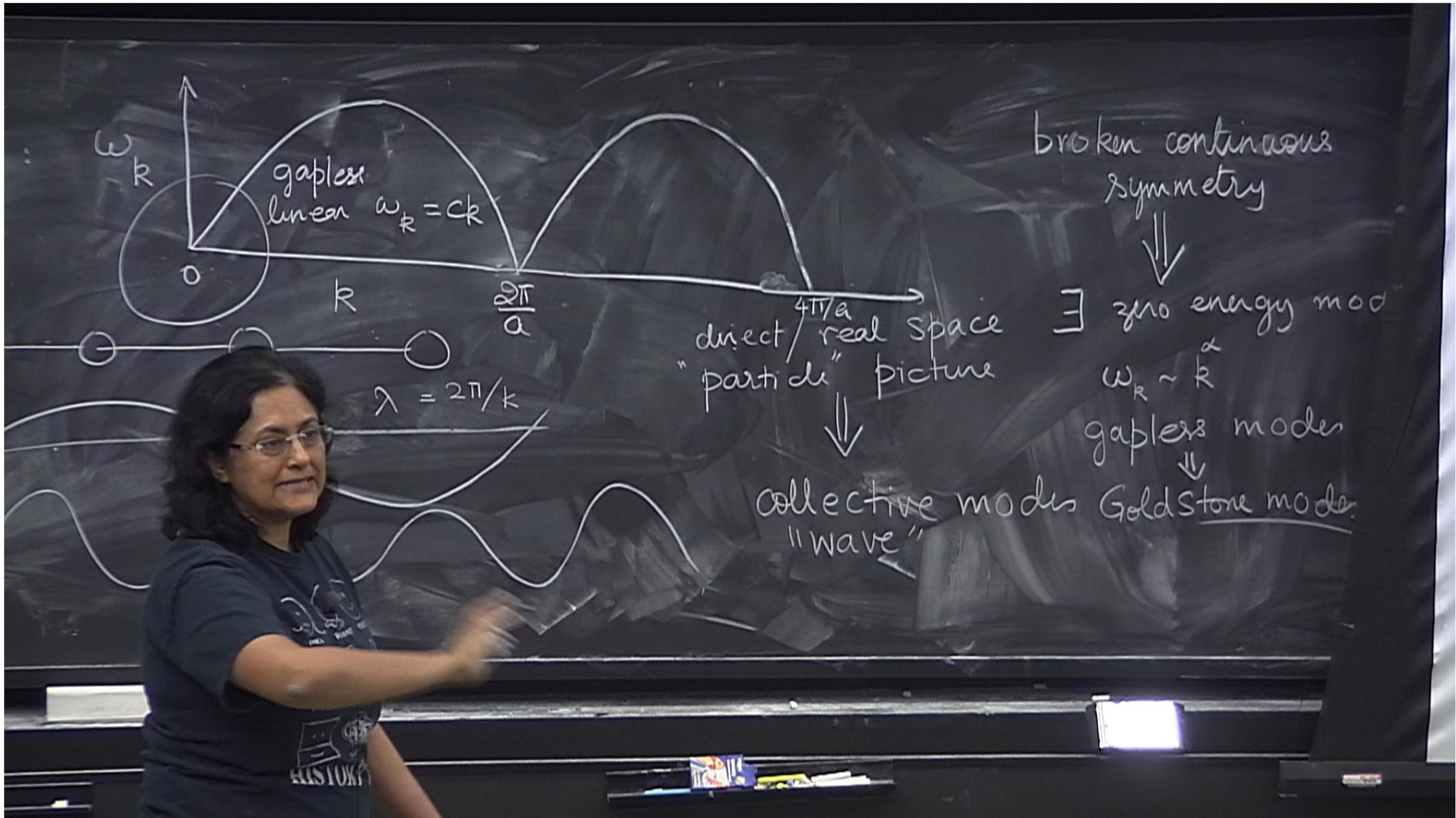
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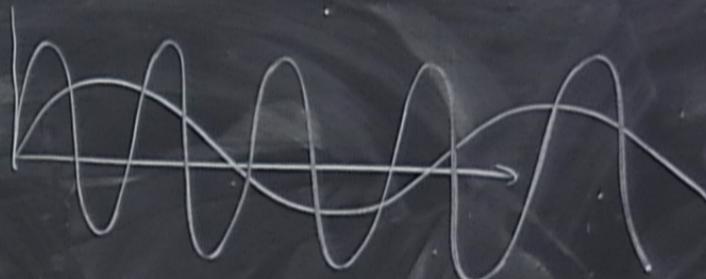
$\omega_k \sim k^\alpha$
 gapless modes
 Goldstone mode

Field theory connection:



Field theory connection:

Xtal \Rightarrow

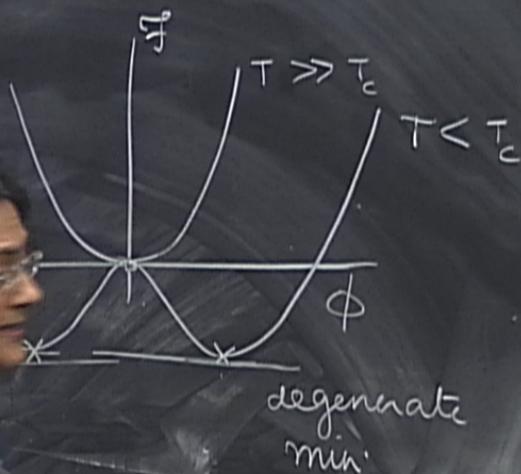
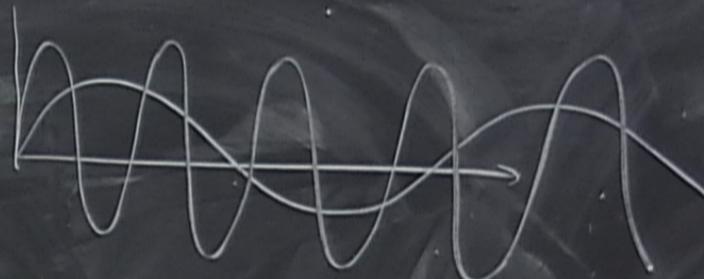


$$\vec{r}_i(t) = \vec{R}_i + \underbrace{u_i(t)}_{\text{BL deviation}}$$

↑
instantaneous
position of atom

BL deviation

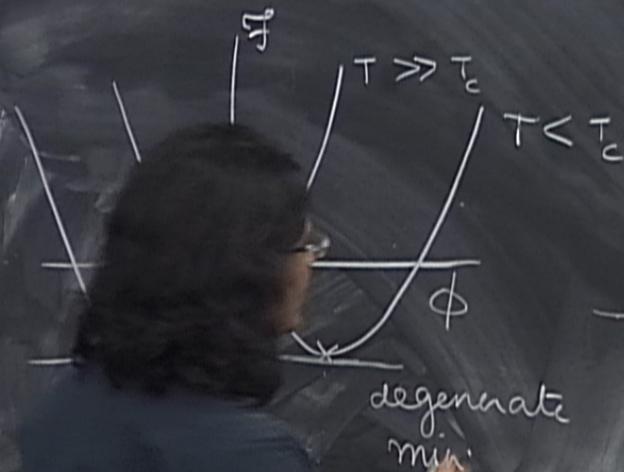
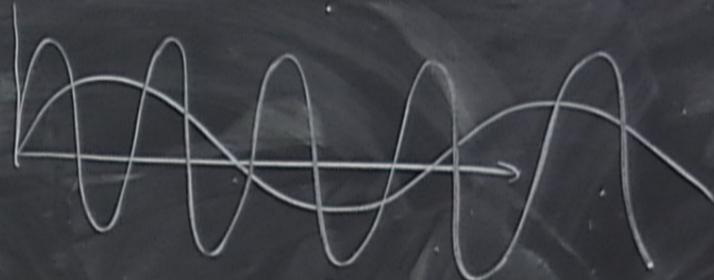
Field theory connection: Xtal \Rightarrow



$$\vec{r}_i(t) = \vec{R}_i + \underbrace{u_i(t)}_{\text{BL deviation}}$$

↑
instantaneous position of atom

Field theory connection: $X_{\text{tal}} \Rightarrow$

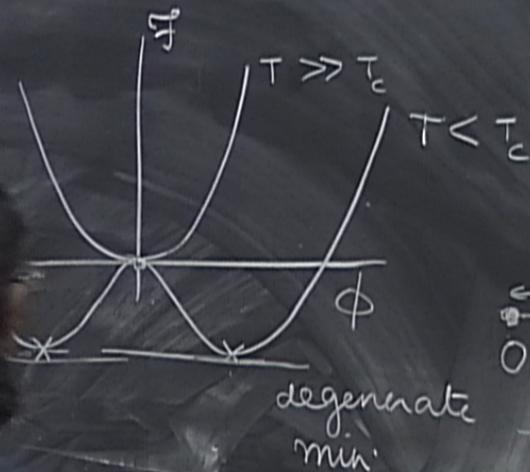
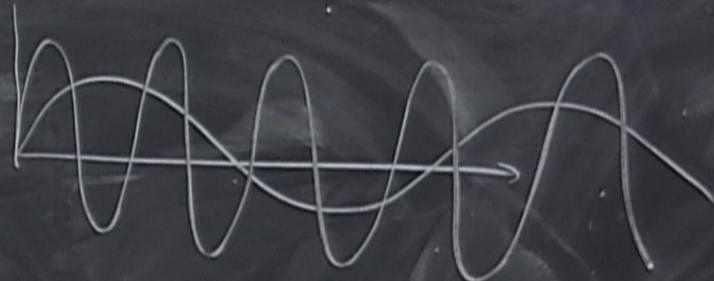


$$\vec{r}_i(t) = \vec{R}_i + \underbrace{u_i(t)}_{\text{BL deviation}}$$

↑
instantaneous
position of atom

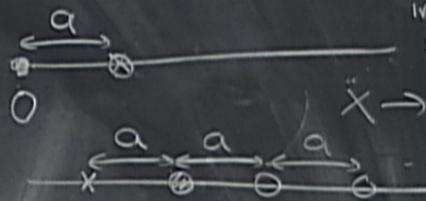
Field theory connection:

Xtal \Rightarrow



$$\vec{r}_i(t) = \vec{R}_i + \underbrace{u_i(t)}_{\text{BL deviation}}$$

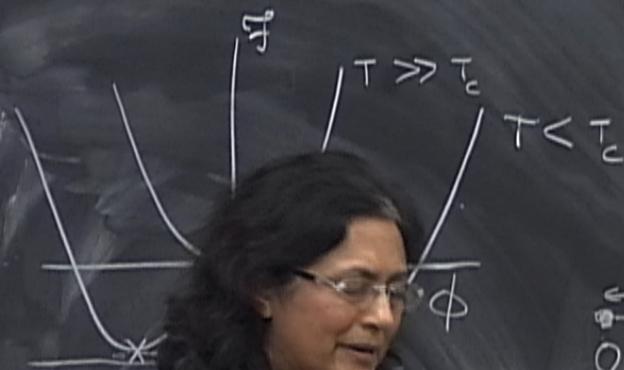
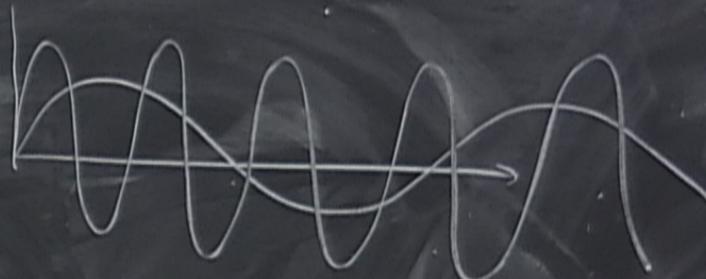
↑
instantaneous position of atom



Long-range positional order

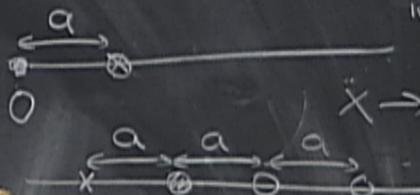
Field theory connection:

Xtal \Rightarrow



$$\vec{r}_i(t) = \vec{R}_i + \underbrace{u_i(t)}_{\text{BL deviation}}$$

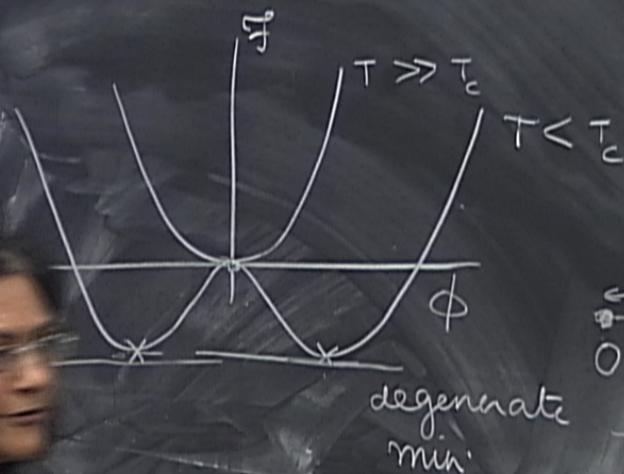
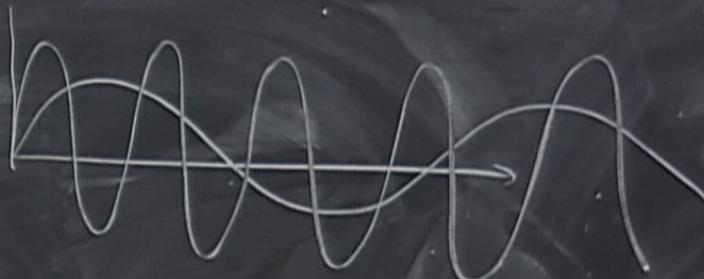
instantaneous position of atom



Long-range positional order

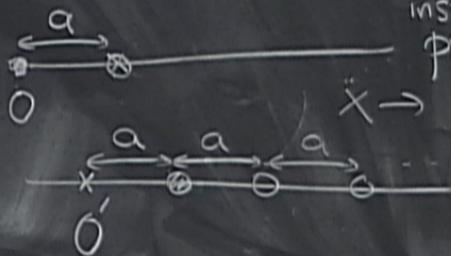
Field theory connection:

Xtal \Rightarrow

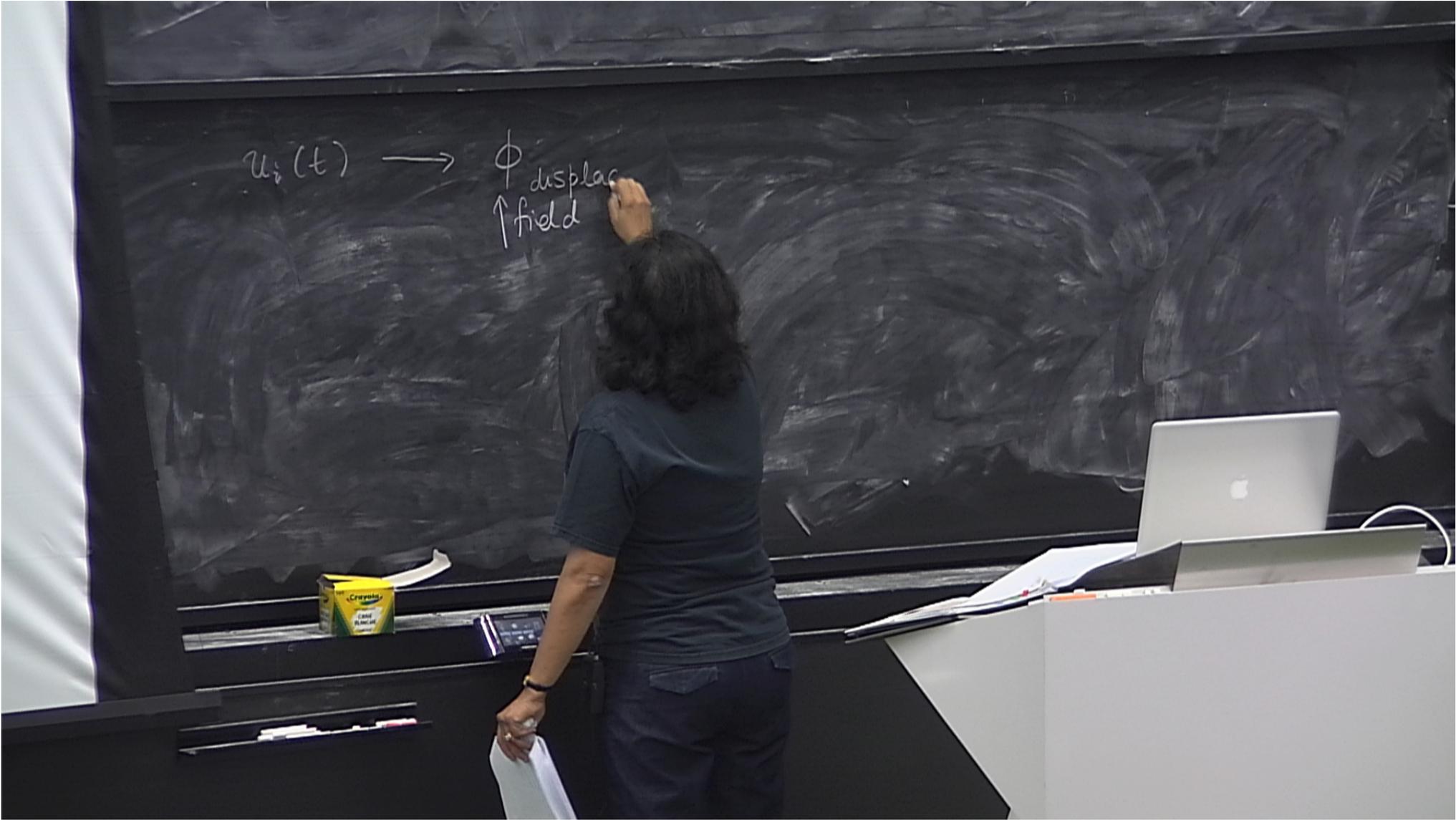


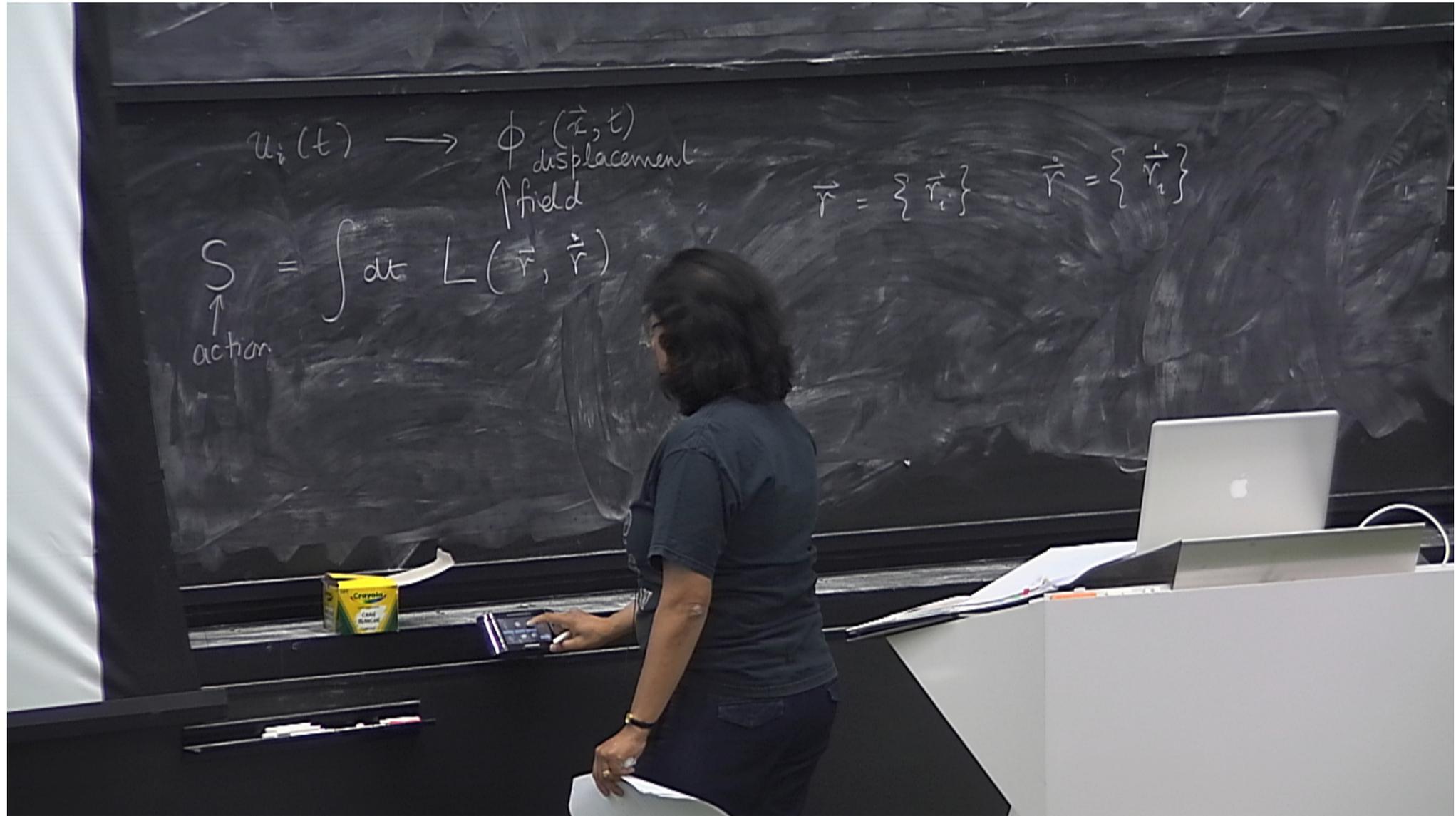
$$\vec{r}_i(t) = \vec{R}_i + \underbrace{u_i(t)}_{\text{BL deviation}}$$

↑
instantaneous position of atom



Long-range positional order





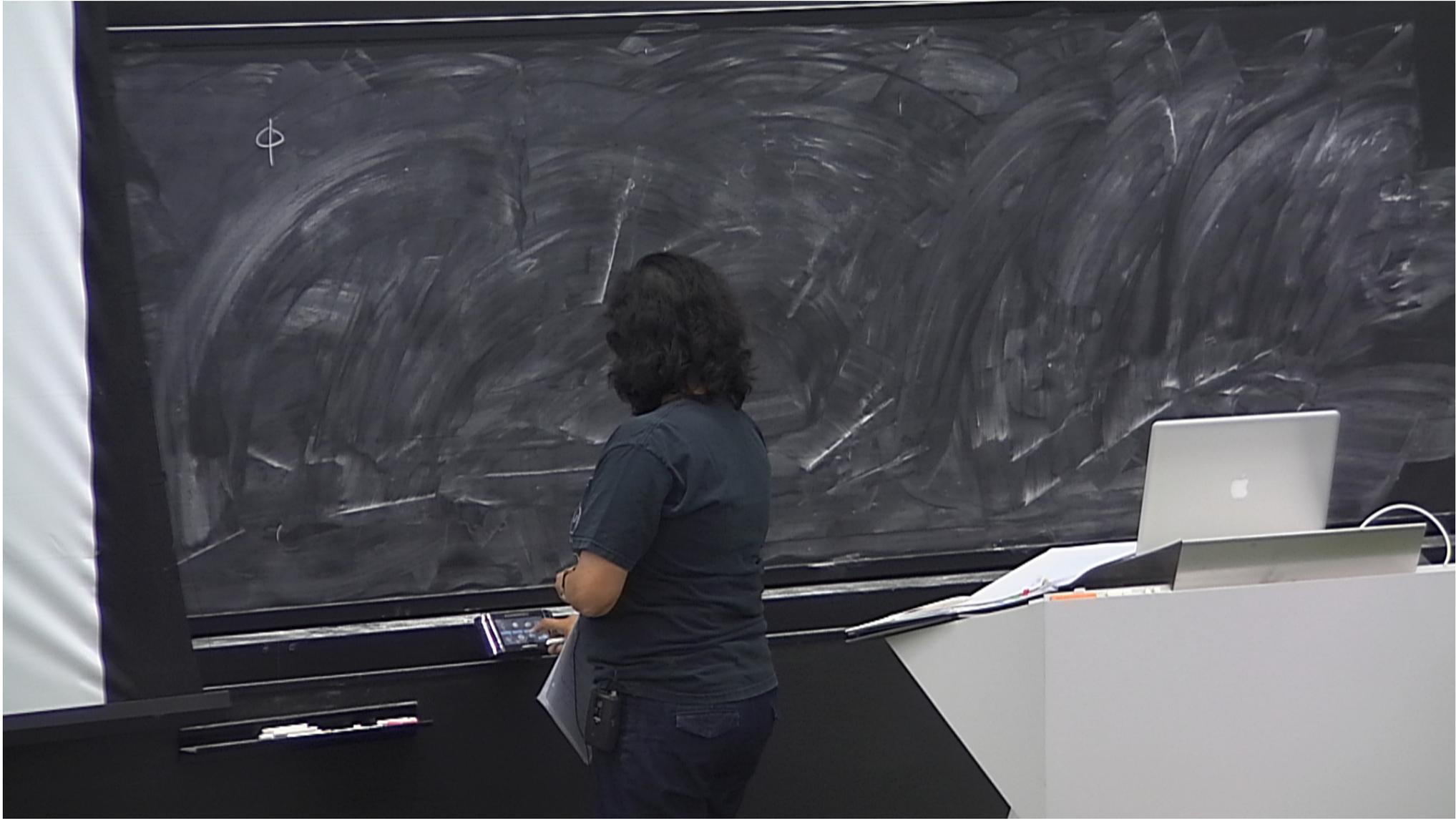
$$u_i(t) \longrightarrow \phi(\vec{r}, t)$$

↑ displacement
↑ field

$$S = \int dt L(\vec{r}, \dot{\vec{r}})$$

↑ action

$$\vec{r} = \{ \vec{r}_i \} \quad \dot{\vec{r}} = \{ \dot{\vec{r}}_i \}$$



$$u_i(t) \rightarrow \phi(\vec{z}, t)$$

↑ displacement
↑ field

$$S = \int dt L(\vec{r}, \dot{\vec{r}})$$

↑ action

$$\vec{r} = \{ \vec{r}_i \} \quad \dot{\vec{r}} = \{ \dot{\vec{r}}_i \}$$

$$L = T - U = \sum_{i=1}^N \frac{M \dot{\vec{r}}_i^2}{2} - \frac{k}{2} (\vec{r}_{i+1} - \vec{r}_i - a)$$

$$\phi_1 \rightarrow \sqrt{a} \phi(x)$$

$$[\phi] = \sqrt{\text{length}}$$

$$\phi_i \rightarrow \sqrt{a} \phi(x)$$

$$[\phi] = \sqrt{\text{length}}$$

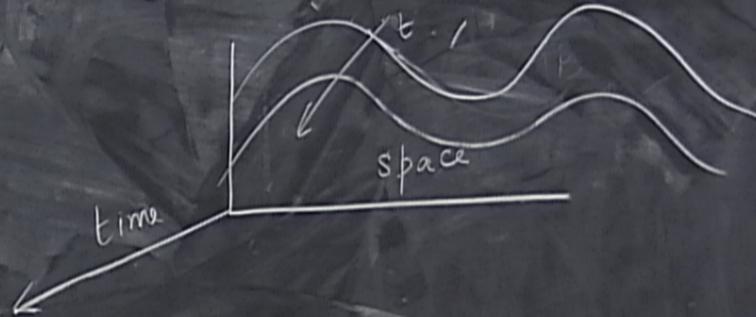
$$\phi_{i+1} - \phi_i = a^{3/2} \partial_x \phi(x)$$

$$\mathcal{L}[\phi] = \int dx \mathcal{L}(\phi, \dot{\phi}) = \int dx \left[\frac{1}{2} m \dot{\phi}^2 - \frac{1}{2} k a^2 (\partial_x \phi)^2 \right]$$

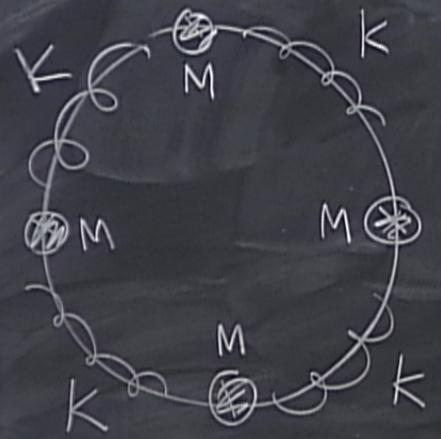
Action. $S = \int dt \int dx \mathcal{L}(\phi, \partial_x \phi, \dot{\phi})$

time

Action. $S = \int dt \int dx \mathcal{L}(\phi, \partial_x \phi, \dot{\phi})$



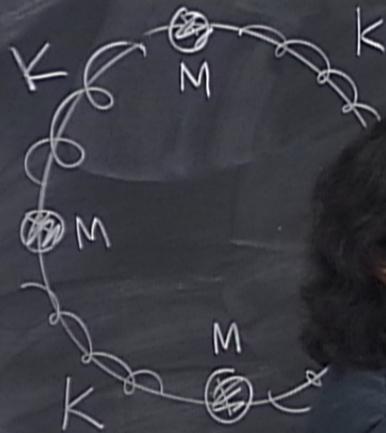
1d string of atoms with a defect



$$D =$$



1d string of atoms with a defect



D

$$= \begin{pmatrix} \langle 1 | \\ \langle 2 | \\ \langle 3 | \\ \langle 4 | \end{pmatrix}$$

site labels

$|1\rangle$

$|2\rangle$

$|3\rangle$

$|4\rangle$

1d string of atoms with a defect



$$D =$$

$$\sum_j D_{ij} = 0 \neq i$$

site labels

	$ 1\rangle$	$ 2\rangle$	$ 3\rangle$	$ 4\rangle$
$\langle 1 $	$2K$	$-K$		$-K$ ← PBC
$\langle 2 $	$-K$		$-K$	
$\langle 3 $				
$\langle 4 $				

translation invariance : e-values can be indexed by a \mathbf{k}
↑
wave vector

re
|| wave

translation invariance

e-values can be indexed by a \vec{k}

\vec{k}
↑
wave vector

$$|i\rangle = \frac{1}{N} \sum_{\vec{k}} e^{i\vec{k} \cdot \vec{r}_i} |k\rangle$$

$$\langle k' | D | k \rangle = \sum_{ij} e^{i(k' r_i - k r_j)} \langle j | D | i \rangle = 2NK \delta_{k'k}$$

translation invariance

e-values can be indexed by a \mathbf{k}

\uparrow
wave vector

$$|i\rangle = \frac{1}{N} \sum_{\mathbf{k}} e^{i\mathbf{k} \cdot \mathbf{r}_i} |\mathbf{k}\rangle$$

$$\langle i | j \rangle = \sum_{\mathbf{k}, \mathbf{k}'} e^{i(\mathbf{k}' \cdot \mathbf{r}_i - \mathbf{k} \cdot \mathbf{r}_i)} \langle \mathbf{k} | \mathbf{k}' \rangle = 2NK \delta_{\mathbf{k}\mathbf{k}'} - KN \delta_{\mathbf{k}\mathbf{k}'} \cos ka$$

translation invariance: e-values can be indexed by a \vec{k}

$$|i\rangle = \frac{1}{N} \sum_{\vec{k}} e^{i\vec{k} \cdot \vec{r}_i} |k\rangle$$

\vec{k}
↑
wave vector

$$|D|k\rangle = \sum_{i,j} e^{i(k' r_i - k r_j)} \langle j|D|i\rangle = 2NK \delta_{\vec{k}\vec{k}'}$$

$$- KNS_{\vec{k}\vec{k}'} \cos ka$$

$$D_{\vec{k}\vec{k}'} = N \delta_{\vec{k}\vec{k}'} 4K \sin^2\left(\frac{ka}{2}\right)$$

translation invariance: e-values can be indexed by a \vec{k}

\vec{k}
↑
wave vector

$$|i\rangle = \frac{1}{N} \sum_{\vec{k}} e^{i\vec{k} \cdot \vec{r}_i} |k\rangle$$

$$\langle k' | D | k \rangle = \sum_{i,j} e^{i(k' \cdot r_i - k \cdot r_j)} \langle j | D | i \rangle = 2NK \delta_{\vec{k}\vec{k}'}$$

$$-KN \delta_{\vec{k}\vec{k}'} \cos ka$$

$$D_{\vec{k}\vec{k}'} = N \delta_{\vec{k}\vec{k}'} \left[4K \sin^2\left(\frac{ka}{2}\right) - KN \cos ka \right]$$

↑
diagonal

Translation invariance: e-values can be indexed by a \vec{k}

\vec{k}
↑
wave vector

$$|i\rangle = \frac{1}{N} \sum_{\vec{k}} e^{i\vec{k} \cdot \vec{r}_i} |k\rangle$$

$$\langle k' | D | i \rangle = \sum_{i_1} e^{i(k' r_{i_1} - k r_{i_1})} \langle 0 | D | i \rangle = 2NK \delta_{\vec{k}\vec{k}'}$$

$$-KN \delta_{\vec{k}\vec{k}'} 2 \cos ka$$

$$= N \delta_{\vec{k}\vec{k}'} 4K \sin^2\left(\frac{ka}{2}\right)$$

↑
diagonal

translation invariance

e-values can be indexed by a

\vec{k}
↑
wave vector

$$|i\rangle = \frac{1}{N} \sum_{\vec{k}} e^{i\vec{k} \cdot \vec{r}_i} |k\rangle$$

$$\langle k' | D | k \rangle = \sum_{i,j} e^{i(k' \cdot r_i - k \cdot r_j)} \langle j | D | i \rangle = 2NK \delta_{kk'} - KNS_{kk'} \cos ka$$

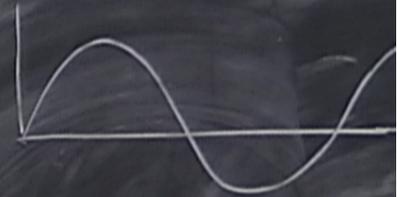
$$D_{kk'} = N \delta_{kk'} \quad \text{diagonal}$$
$$4K \sin^2\left(\frac{ka}{2}\right)$$

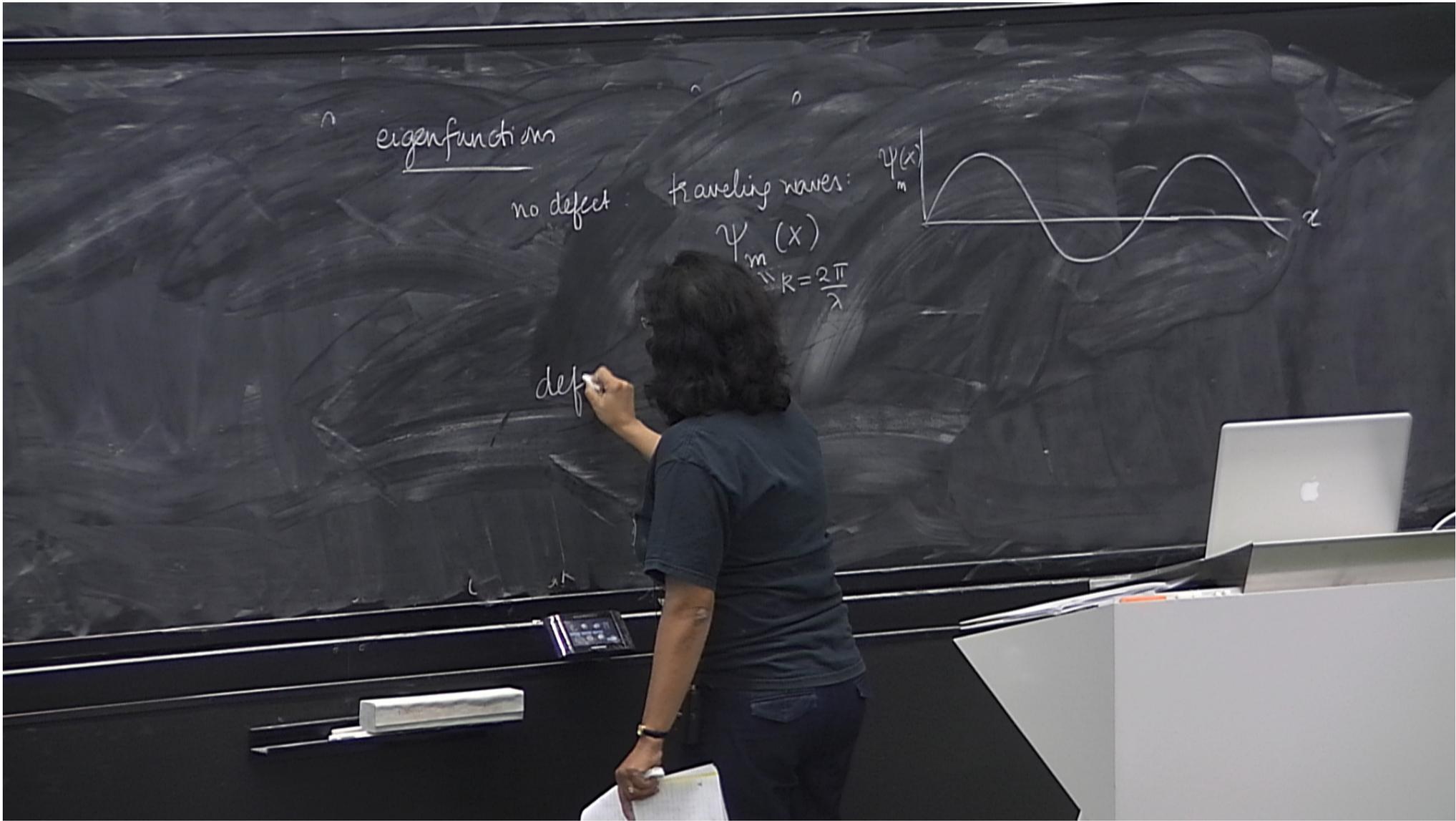
eigenfunction

no defect

traveling waves:

$$\psi_m(x)$$





eigenfunctions

no defect

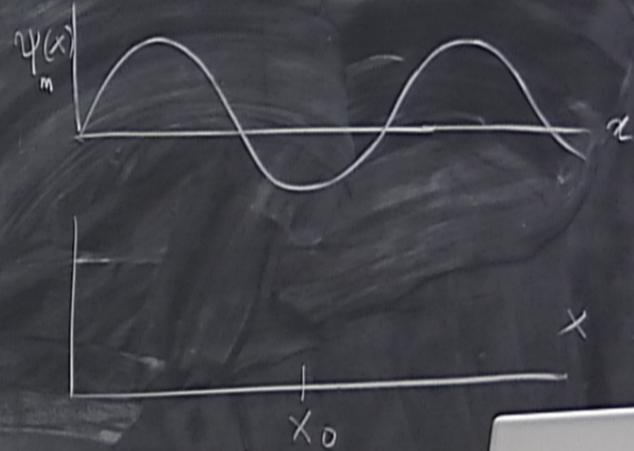
traveling waves:

$$\psi_m(x)$$

$$\Rightarrow k = \frac{2\pi}{\lambda}$$

defect

1 spring $k' \neq k$



eigenfunctions

no defect

traveling waves:

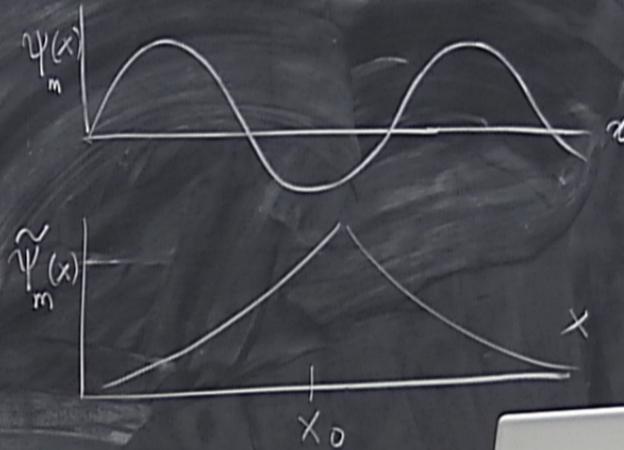
$$\psi_m(x)$$

$$\Rightarrow k = \frac{2\pi}{\lambda}$$

defect

1 spring

$$k' \neq k$$



eigenfunctions

no defect

traveling waves:

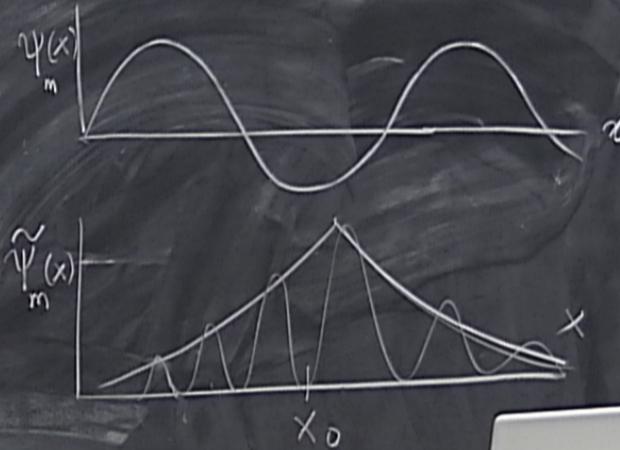
$$\psi_m(x)$$

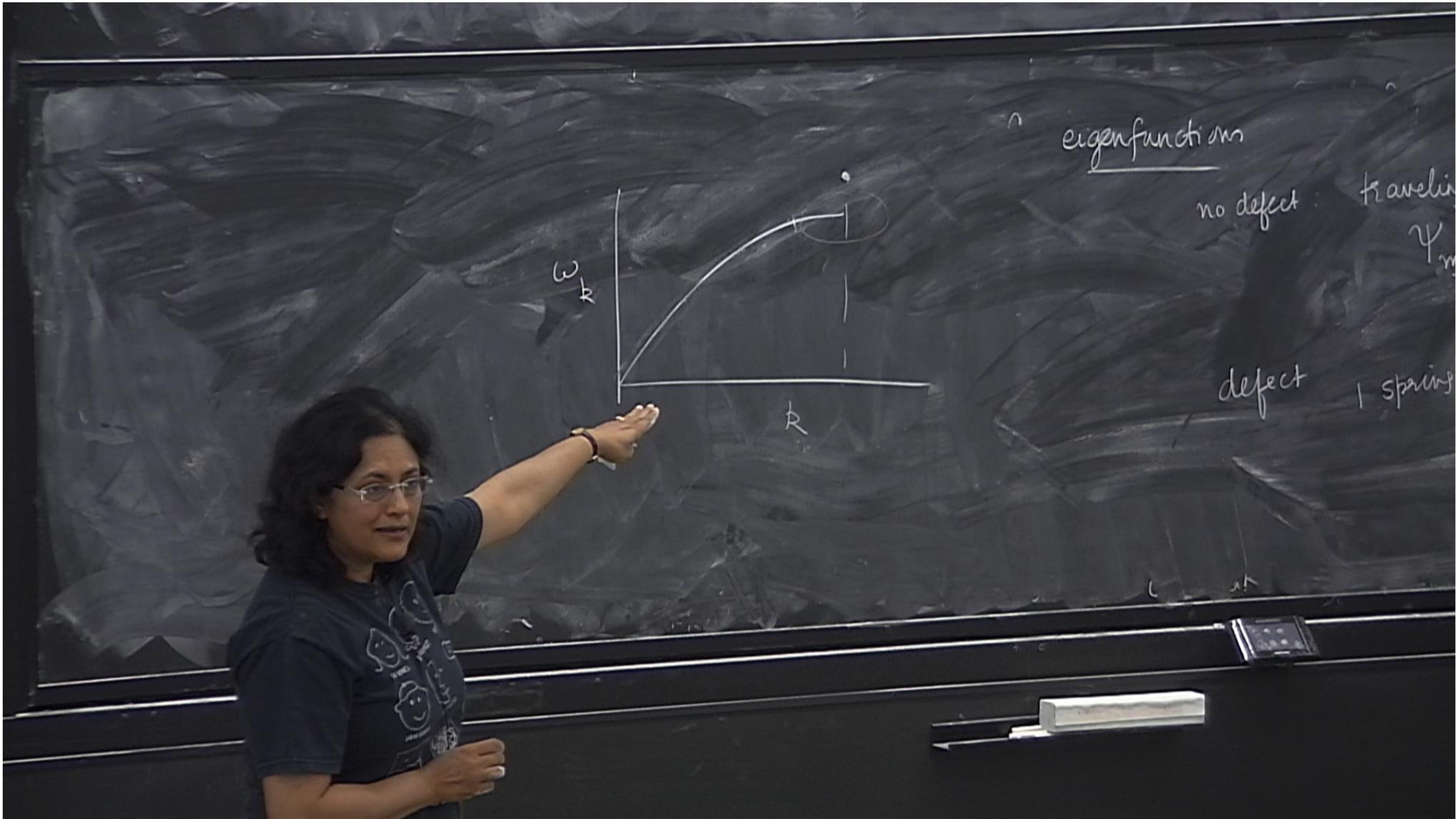
$$\Rightarrow k = \frac{2\pi}{\lambda}$$

defect

1 spring

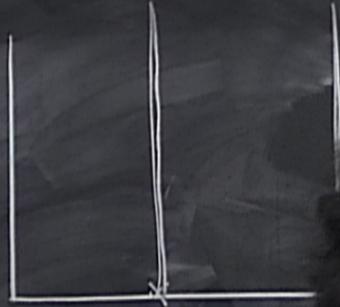
$$k' \neq k$$





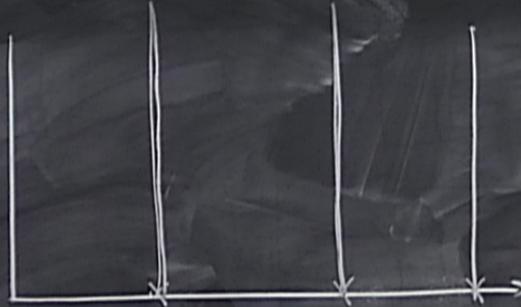
Xtal at $T \neq 0$

$S(q)$
↑
structure
factor



Xtal at $T \neq 0$

$S(q)$
↑
structure
factor



$$S(q) = N \delta_{q,G} \quad \underline{T=0}$$

Xtal at $T \neq 0$

$S(q)$
↑
structure
factor

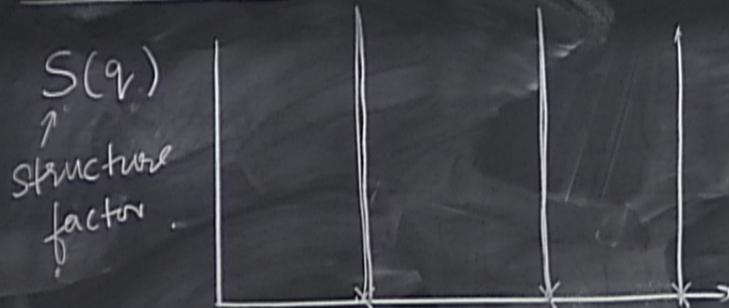


$$S(q) = N \delta_{\vec{q}, \vec{G}} \quad T = \bar{0}$$

$$S(\vec{q}) =$$

$$T \neq 0$$

Xtal at $T \neq 0$

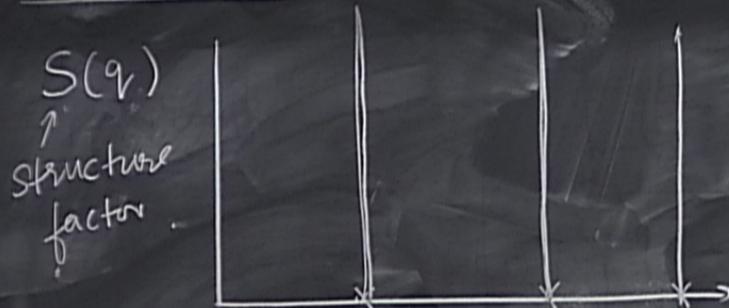


$$S(q) = N \delta_{\vec{q}, \vec{G}} \quad T=0$$

$$S(\vec{q}) = e^{-2W} N \delta_{\vec{q}, \vec{G}} \quad T \neq 0$$

Debye Waller factor

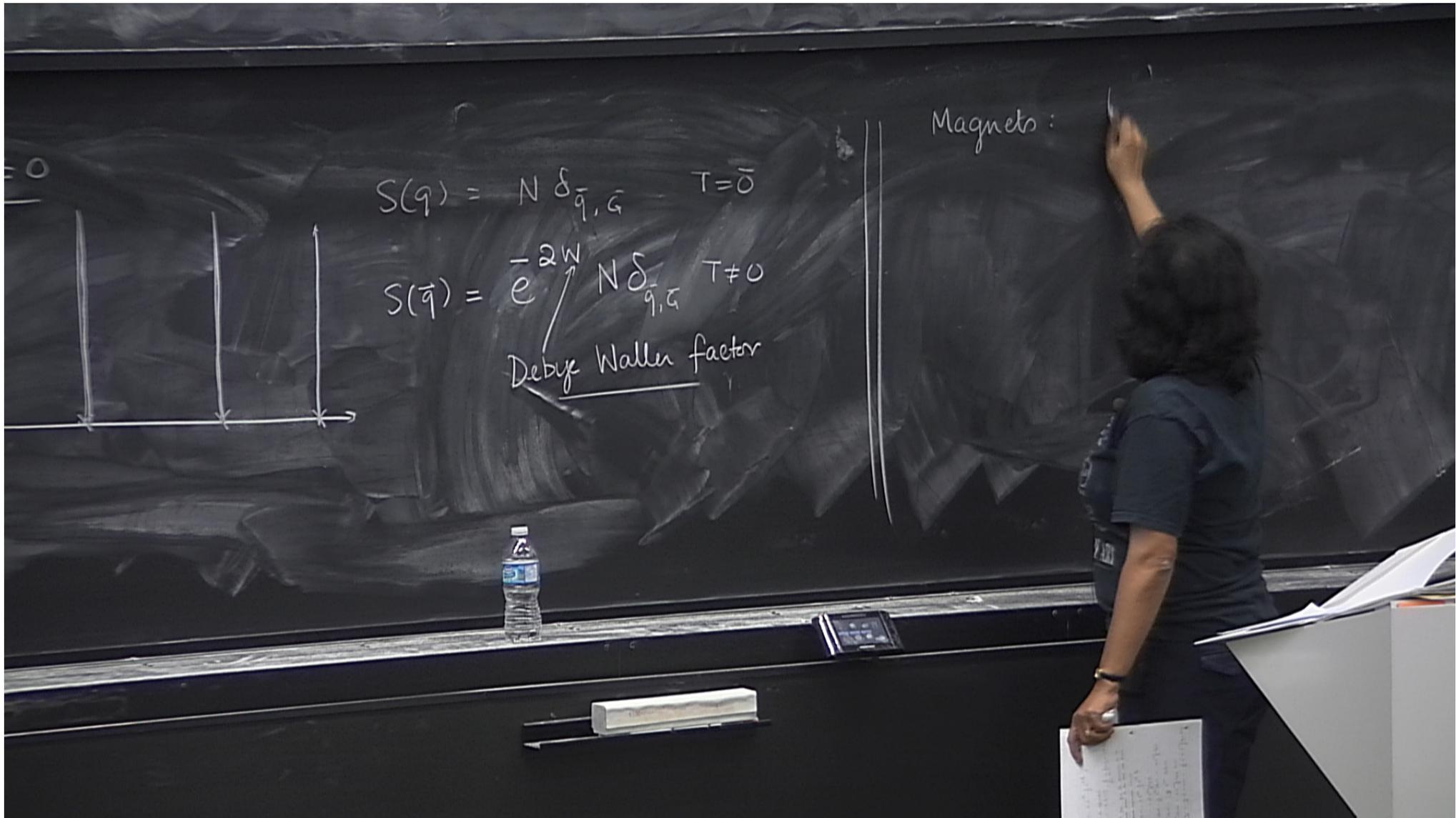
Xtal at $T \neq 0$



$$S(q) = N \delta_{q, G} \quad T=0$$

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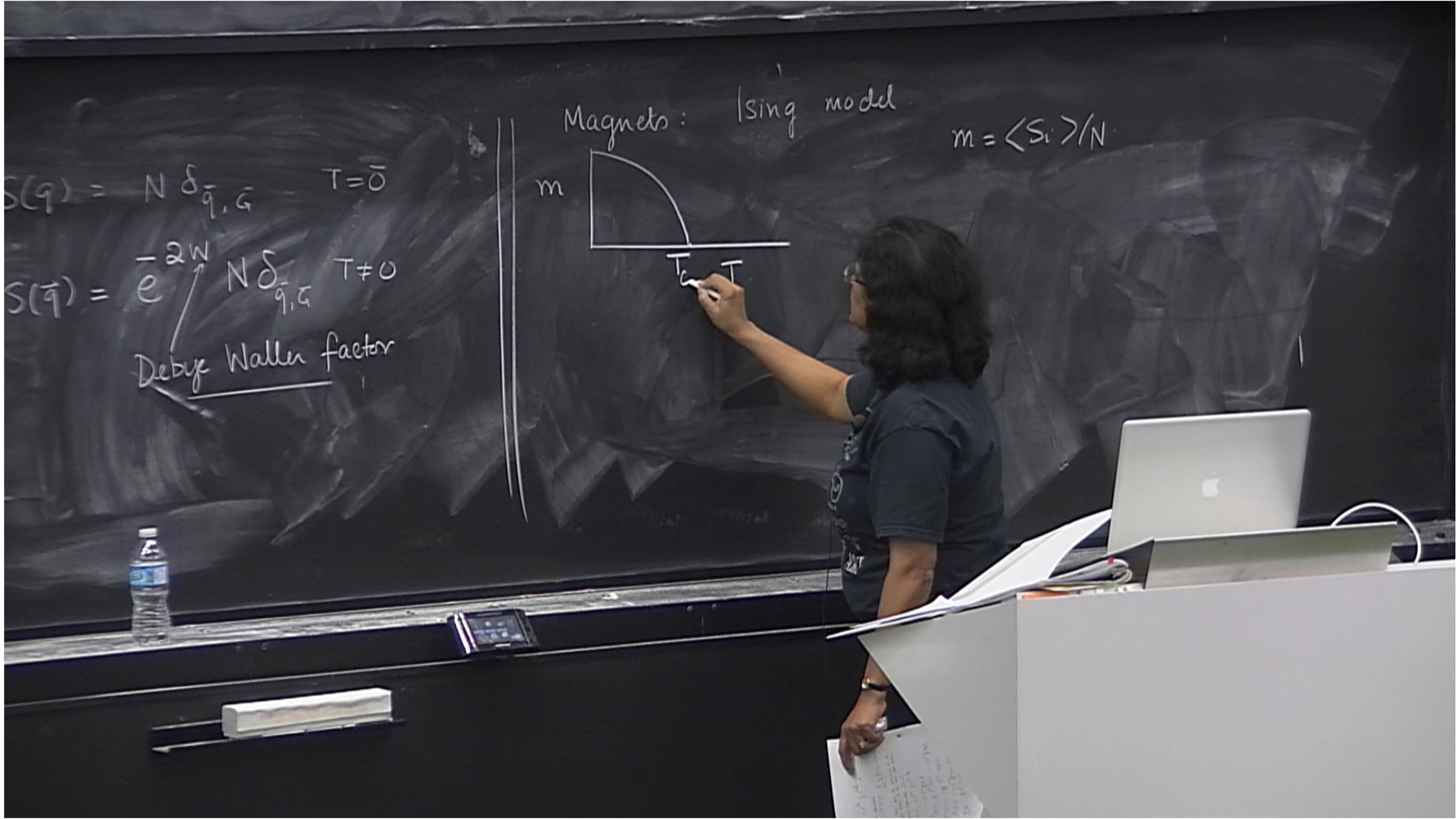


$$S(\vec{q}) = N \delta_{\vec{q}, \vec{G}} \quad T=0$$

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Debye Waller factor

Magnets:

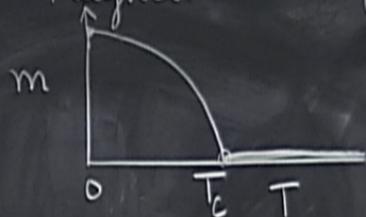


$$S(\vec{q}) = N \delta_{\vec{q}, \vec{G}} \quad T=0$$

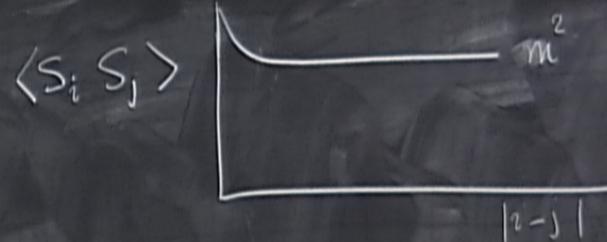
$$S(\vec{q}) = e^{-2W} N \delta_{\vec{q}, \vec{G}} \quad T \neq 0$$

Debye Waller factor

Magnets: Ising model



$$m = \langle S_i \rangle / N$$

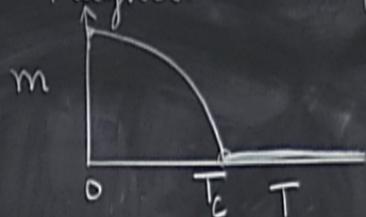


$$S(\vec{q}) = N \delta_{\vec{q}, \vec{G}} \quad T=0$$

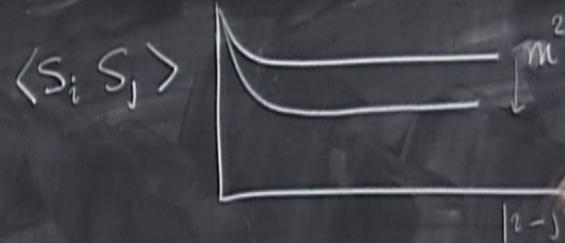
$$S(\vec{q}) = e^{-2W} N \delta_{\vec{q}, \vec{G}} \quad T \neq 0$$

Debye Waller factor

Magnets: Ising model



$$m = \langle S_i \rangle / N$$

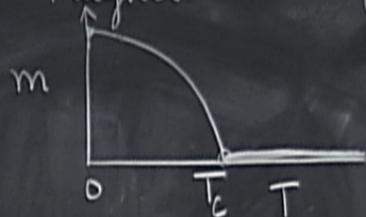


$$S(\vec{q}) = N \delta_{\vec{q}, \vec{G}} \quad T=0$$

$$S(\vec{q}) = e^{-2W} N \delta_{\vec{q}, \vec{G}} \quad T \neq 0$$

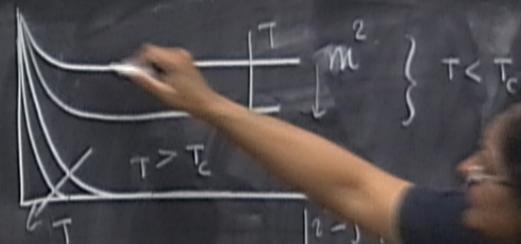
Debye Waller factor

Magnets: Ising model



$$m = \langle S_i \rangle / N$$

$$\langle S_i S_j \rangle$$

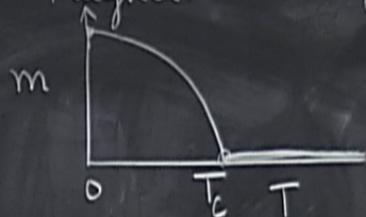


$$S(\vec{q}) = N \delta_{\vec{q}, \vec{G}} \quad T=0$$

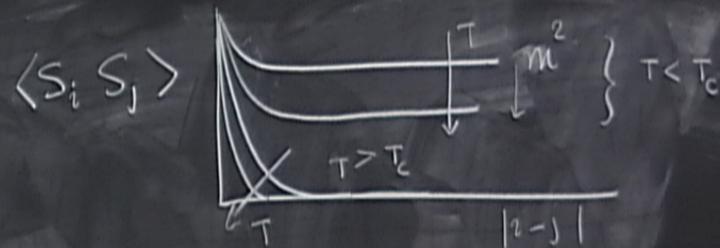
$$S(\vec{q}) = e^{-2W} N \delta_{\vec{q}, \vec{G}} \quad T \neq 0$$

Debye Waller factor

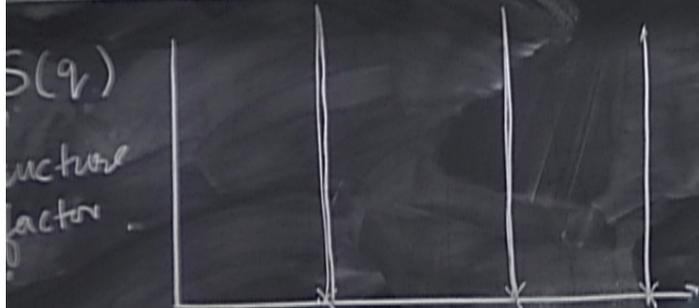
Magnets: Ising model



$$m = \langle S_i \rangle / N$$



at $T \neq 0$



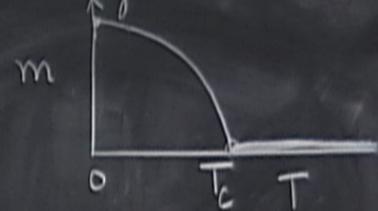
$$S(q) = N \delta_{\vec{q}, \vec{G}} \quad T=0$$

$$S(q) = \frac{-2W}{N} \delta_{\vec{q}, \vec{G}} \quad T \neq 0$$

Waller factor

LRO

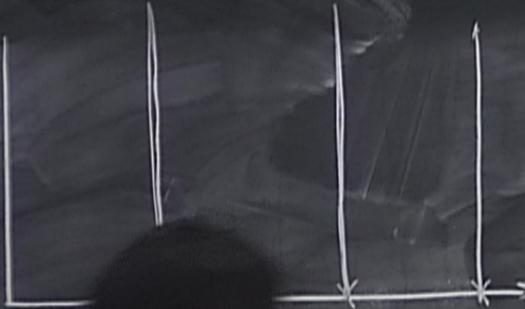
Magnets: Ising model



$\langle S_i S_j \rangle$

at $T \neq 0$

$S(q)$
structure factor



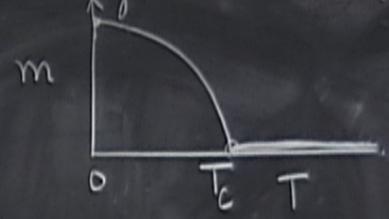
$$S(q) = N \delta_{q, G} \quad T=0$$

$$S(q) = e^{-2W} N \delta_{q, G} \quad T \neq 0$$

Debye Waller factor

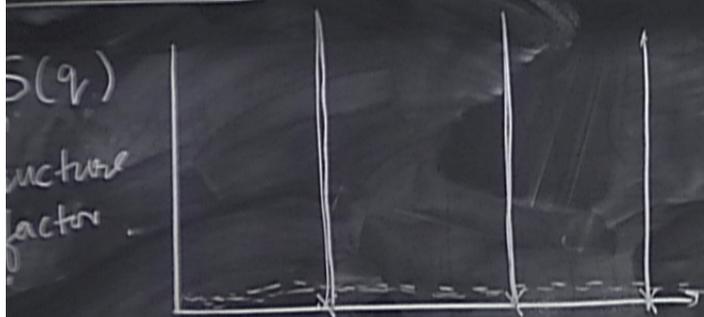
δ -fn \Rightarrow F of LRO

Magnets: Ising model



$\langle S_i S_j \rangle$

at $T \neq 0$



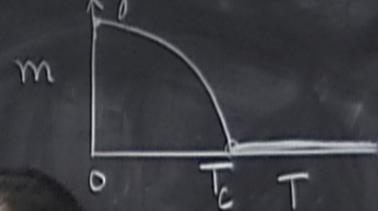
$$S(q) = N \delta_{q,0} \quad T=0$$

$$S(q) = e^{-2W} N \delta_{q,0} \quad T \neq 0$$

Debye Waller factor

δ -fn \Rightarrow F of LRO

Magnets: Ising model



$\langle S_i S_j \rangle$

Single Harmonic oscillator:

Single Harmonic oscillator: root mean square fluctuation

$$\langle x^2 \rangle$$

Single Harmonic oscillator: root mean square fluctuation

$$\hat{x} =$$

Single Harmonic oscillator: root mean square fluctuation

$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega}} (a + a^\dagger)$$

x^2

Single Harmonic oscillator: root mean square fluctuation

$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega}} (a + a^\dagger)$$

$$\langle n | x^2 | n \rangle = \frac{\hbar}{2m} \omega (1 + 2n)$$

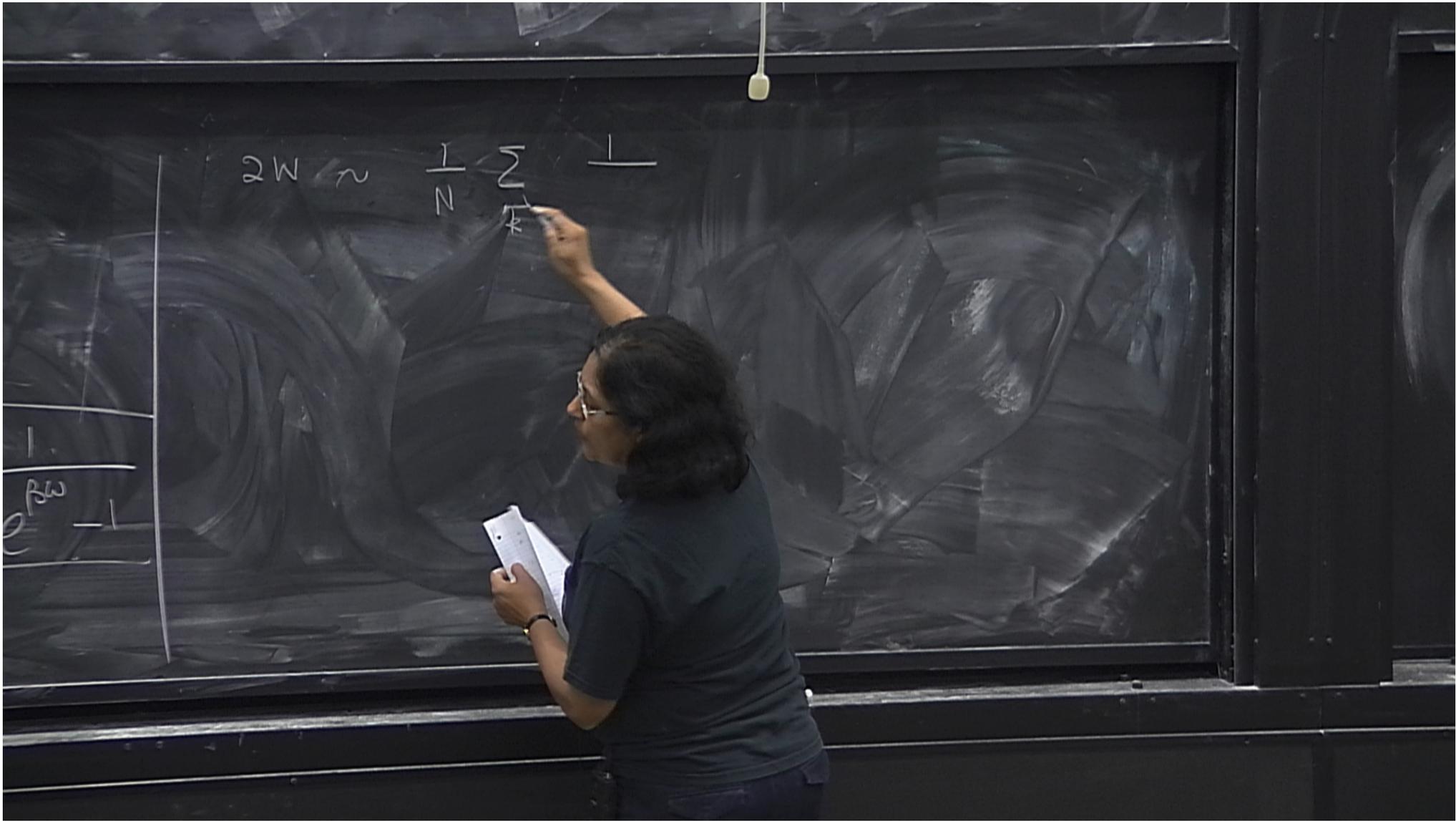
$$\overbrace{\langle n | x^2 | n \rangle}^{\text{thermal average}} = \frac{\hbar}{2m\omega} (1 + 2\langle n \rangle)$$

single Harmonic oscillator: root mean square fluctuation

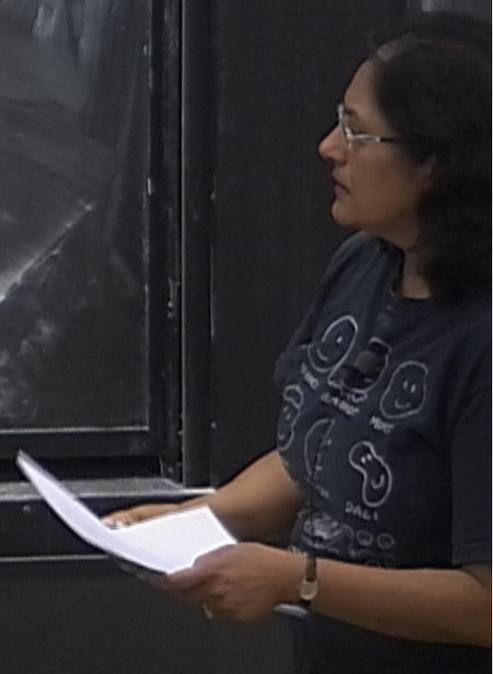
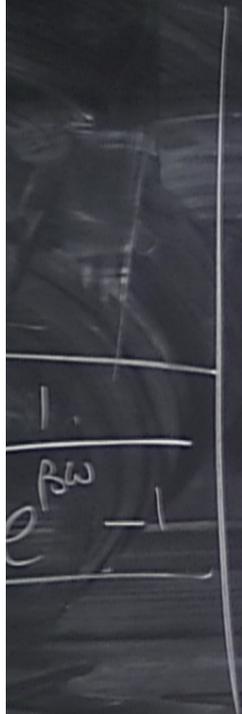
$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega}} (a + a^\dagger)$$

$$\langle n | x^2 | n \rangle = \frac{\hbar}{2m} \omega (1 + 2n)$$

$$\underbrace{\langle n | x^2 | n \rangle}_{\text{thermal average}} = \frac{\hbar}{2m\omega} (1 + 2\langle n \rangle) = \frac{\hbar}{2m\omega} \coth\left(\frac{\theta}{2}\right); \quad \langle n \rangle = \frac{1}{e^{\beta\hbar\omega} + 1}$$



$$2W \sim \frac{1}{N} \sum_{\mathbf{k}} \frac{1}{\hbar \omega_{\mathbf{k}}} \coth\left(\frac{\hbar \omega_{\mathbf{k}}}{2k_B T}\right)$$



Single Harmonic oscillator: root mean square fluctuation

$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega}} (a + a^\dagger)$$

$$\langle n | x^2 | n \rangle = \frac{\hbar}{2m\omega} (1 + 2n)$$

$$\overbrace{\langle n | x^2 | n \rangle}^{\text{thermal average}} = \frac{\hbar}{2m\omega} (1 + 2\langle n \rangle) = \frac{\hbar}{2m\omega} \coth\left(\frac{\beta\hbar\omega}{2}\right); \quad \langle n \rangle$$

fluctuation

$$\frac{\hbar}{2m\omega} \coth\left(\frac{\hbar\omega}{2}\right) ;$$

$$\langle n \rangle = \frac{1}{e^{\beta\hbar\omega} - 1}$$

$$2W \sim \frac{1}{N} \sum_k \frac{1}{\hbar\omega_k} \coth\left(\frac{\hbar\omega_k}{2k_B T}\right)$$

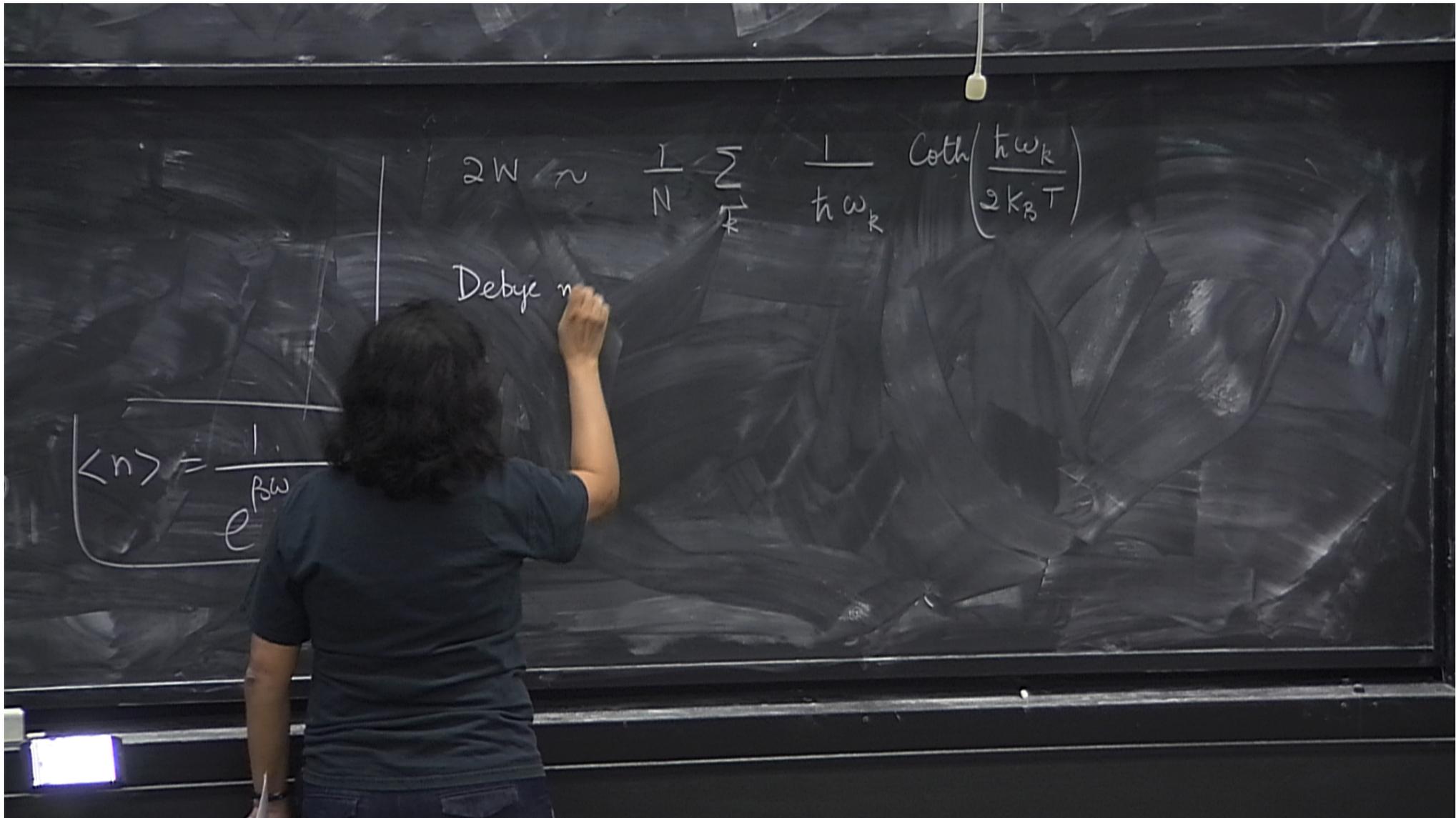
fluctuation

$$\frac{\hbar}{2m\omega} \coth\left(\frac{\beta\hbar\omega}{2}\right);$$

$$\langle n \rangle = \frac{1}{e^{\beta\hbar\omega} - 1}$$

$$2W \sim \frac{1}{N} \sum_k \frac{1}{\hbar\omega_k} \coth\left(\frac{\hbar\omega_k}{2k_B T}\right)$$

$$2W \sim \frac{1}{N} \sum_{\vec{k}} \frac{1}{\hbar \omega_{\vec{k}}} \coth\left(\frac{\hbar \omega_{\vec{k}}}{2k_B T}\right)$$



$$2W \sim \frac{1}{N} \sum_{\vec{k}} \frac{1}{\hbar \omega_{\vec{k}}} \text{Coth}\left(\frac{\hbar \omega_{\vec{k}}}{2k_B T}\right)$$

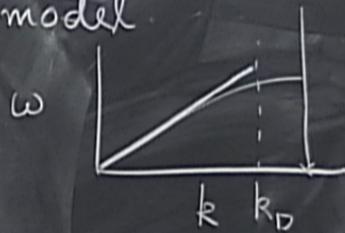
Debye n

$$\langle n \rangle = \frac{1}{e^{\beta \hbar \omega}}$$

$$\langle n \rangle = \frac{1}{e^{\beta \hbar \omega} - 1}$$

$$2W \sim \frac{1}{N} \sum_{\vec{k}} \frac{1}{\hbar \omega_{\vec{k}}} \coth\left(\frac{\hbar \omega_{\vec{k}}}{2k_B T}\right)$$

Debye model



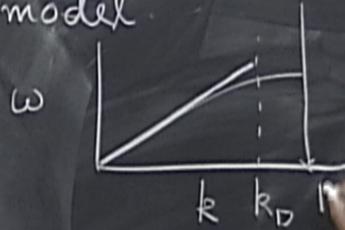
k_D cut off determined by

$$\frac{1}{V} \sum$$

$$2W \sim \frac{1}{N} \sum_{\vec{k}} \frac{1}{\hbar \omega_{\vec{k}}} \coth\left(\frac{\hbar \omega_{\vec{k}}}{2k_B T}\right)$$

Debye model

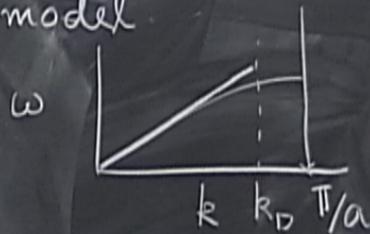
k_D cut off determined by



$$\langle n \rangle = \frac{1}{e^{\beta \hbar \omega} - 1}$$

$$2W \sim \frac{1}{N} \sum_{\mathbf{k}} \frac{1}{\hbar \omega_{\mathbf{k}}} \coth\left(\frac{\hbar \omega_{\mathbf{k}}}{2k_B T}\right)$$

Debye model



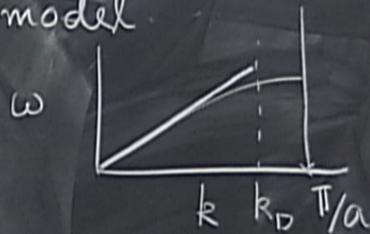
k_D cut off determined by

$$k_D \approx \pi/a$$

$$\langle n \rangle = \frac{1}{e^{\beta \hbar \omega} - 1}$$

$$2W \sim \frac{1}{N} \sum_{\vec{k}} \frac{1}{\hbar \omega_{\vec{k}}} \coth\left(\frac{\hbar \omega_{\vec{k}}}{2k_B T}\right)$$

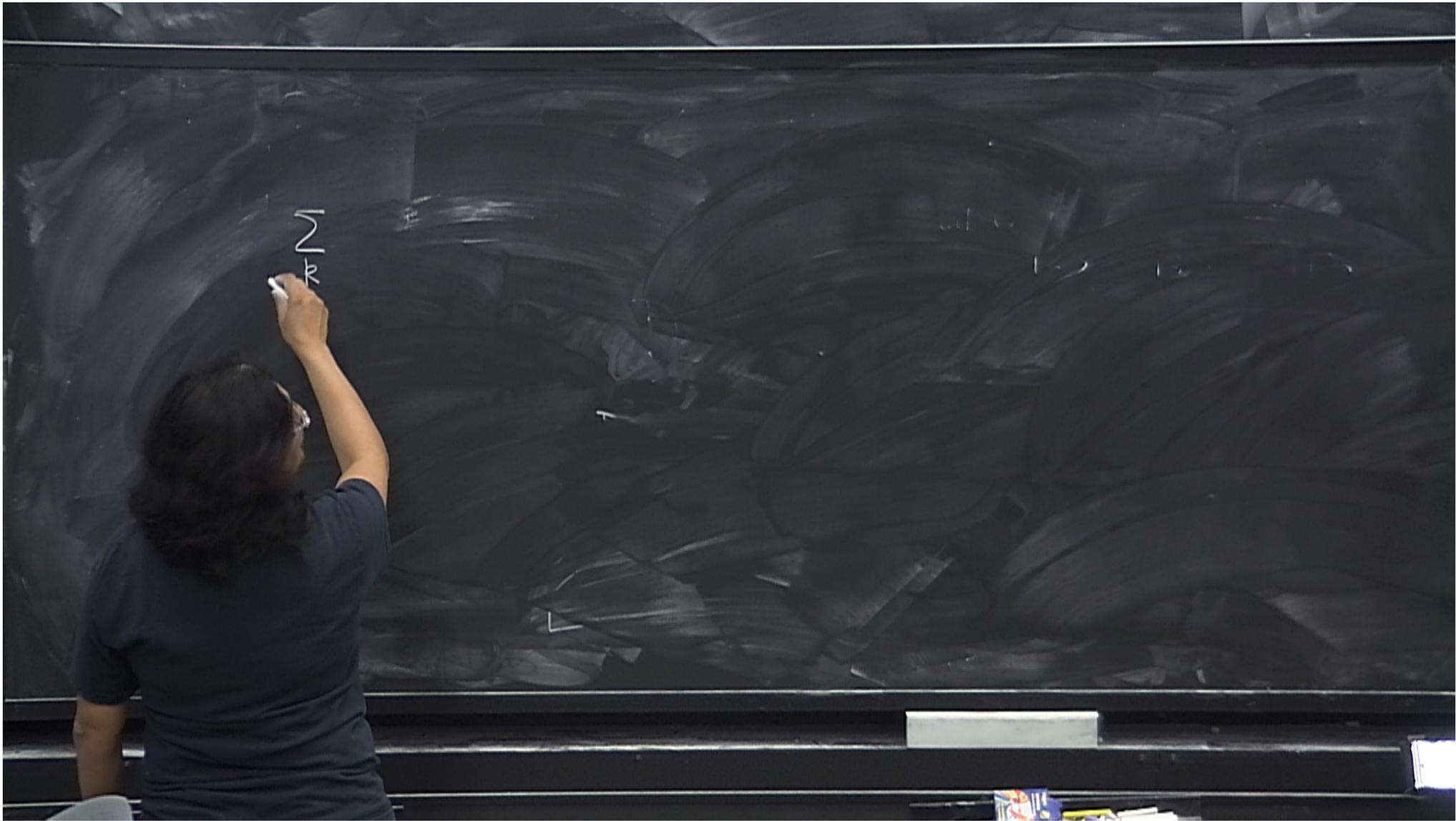
Debye model



k_D cut off determined by adding up all modes

$$k_D \approx \pi/a$$

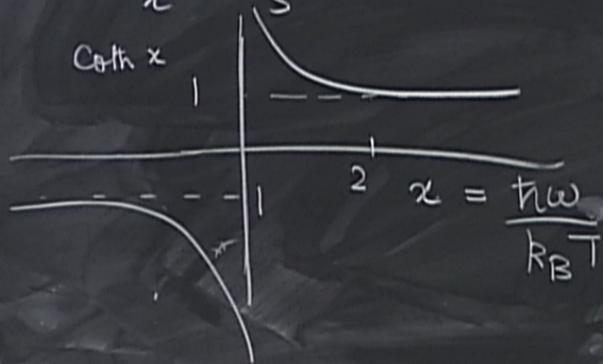
$$\langle n \rangle = \frac{1}{e^{\beta \hbar \omega} - 1}$$



$$\frac{1}{N} \sum_R \frac{1}{\hbar \omega_k} \coth \left(\frac{\hbar \omega_k}{2 k_B T} \right)$$

$$\frac{1}{N} \sum_R \frac{1}{\hbar \omega_k} \coth \left(\frac{\hbar \omega_k}{2 k_B T} \right)$$

$$\coth z = \frac{1}{z} + \frac{z}{3} \dots$$

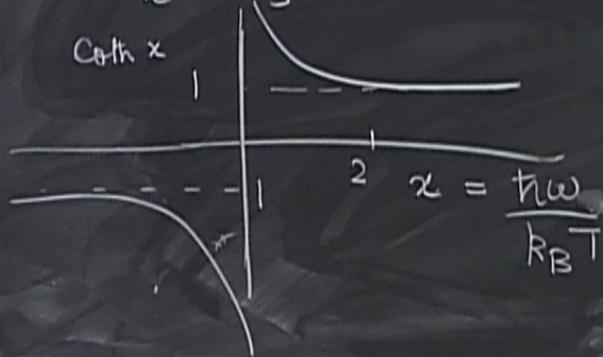


$$\frac{1}{N} \sum_{\mathbf{k}} \frac{1}{\hbar \omega_{\mathbf{k}}} \coth \left(\frac{\hbar \omega_{\mathbf{k}}}{2 k_B T} \right)$$

$$\longrightarrow \int d^d k \frac{1}{k}$$

$$\coth z = \frac{1}{z} + \frac{z}{3} \dots$$

$$\omega_{\mathbf{k}} = c k$$



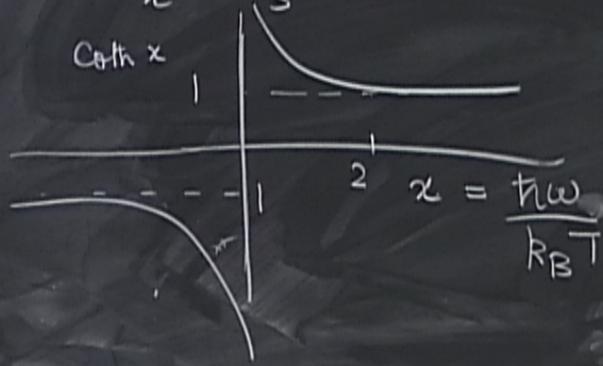
$$\frac{1}{N} \sum_{\mathbf{k}} \frac{1}{\hbar \omega_{\mathbf{k}}} \coth \left(\frac{\hbar \omega_{\mathbf{k}}}{2 k_B T} \right)$$

$$\longrightarrow \int d^d k \frac{1}{k} \frac{1}{k}$$

$$\coth z = \frac{1}{z} + \frac{z}{3} \dots$$

$$\omega_{\mathbf{k}} = c k$$

$$\coth x \sim \frac{1}{x} \text{ for small } x$$



$$\rightarrow \int d^d k \frac{1}{k} \frac{1}{k} = \int \frac{k^{d-1} dk}{k^2}$$

$$\omega_k = ck$$

$$\ln x \sim \frac{1}{x} \text{ for small } x$$

$$\rightarrow \int d^d k \frac{1}{k} \frac{1}{k} = \int_0^{k_D} \frac{k^{d-1} dk}{k^2}$$

$$\omega_k = ck$$

$$\ln x \sim \frac{1}{x} \text{ for small } x$$

$$\int d^d k \frac{1}{k} \frac{1}{k} = \int_0^{k_D} \frac{k^{d-1} dk}{k^2}$$

3D

$$2W = \frac{\omega_0}{\omega_D}$$

$$\omega_k = ck$$

then $x \sim \frac{1}{x}$ for small x

$$= \int_0^{k_D} \frac{k^{d-1} dk}{k^2}$$

3D

$$2W = \frac{\omega_0}{\omega_D}$$

$$T \ll \Theta_D$$

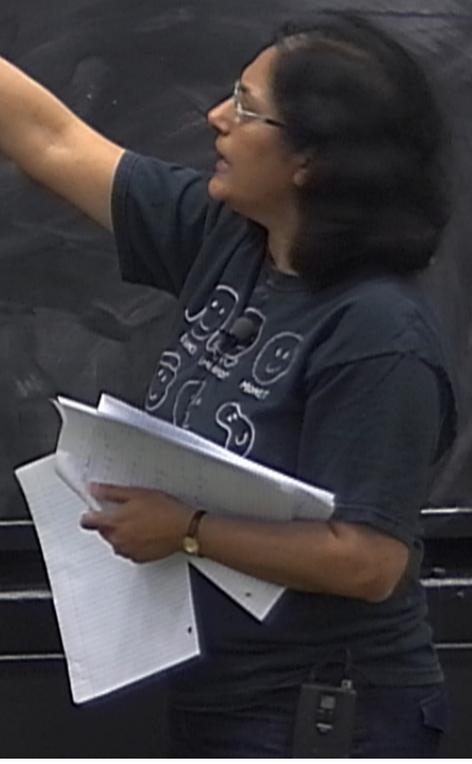
$$\hbar \omega_D = k_B \Theta_D$$

$$= \int_0^{k_D} \frac{k^{d-1} dk}{k^2}$$

3D

$$2W = \begin{cases} \frac{\omega_0}{\omega_D} & T \ll \Theta_D \\ \frac{\omega_0}{\omega_D} \left(\frac{T}{\Theta_D} \right) & T \gg \Theta_D \end{cases}$$

$$\hbar \omega_D = k_B \Theta_D$$



$$= \int_0^{k_D} \frac{k^{d-1} dk}{k^2}$$

→ 3D

→ 2D

$$2W = \begin{cases} \frac{\omega_0}{\omega_D} & T \ll \Theta_D \\ \frac{\omega_0}{\omega_D} \left(\frac{T}{\Theta_D} \right) & T \gg \Theta_D \end{cases}$$

$$\hbar \omega_D = k_B \Theta_D$$

$$2W \sim \sum_k \ln k \rightarrow \text{inf}$$

$$= \int_0^{k_D} \frac{k^{d-1} dk}{k^2}$$

3D

2D

$$2W = \begin{cases} \frac{\omega_0}{\omega_D} & T \ll \Theta_D \\ \frac{\omega_0}{\omega_D} \left(\frac{T}{\Theta_D} \right) & T \gg \Theta_D \end{cases}$$

$$\hbar \omega_D = k_B \Theta_D$$

$$2W \sim \sum_k \ln k \rightarrow \text{infrared divergence}$$

$$C(\vec{r}, t; \vec{r}', t') = \langle \hat{n}(\vec{r}, t) \hat{n}(\vec{r}', t') \rangle$$

$$C(\vec{r}, t; \vec{r}', t') = \langle \hat{n}(\vec{r}, t) \hat{n}(\vec{r}', t') \rangle$$

$$\downarrow \hat{n}(\vec{r}, t) = \sum_i \delta(\vec{r} - \vec{r}_i(t))$$

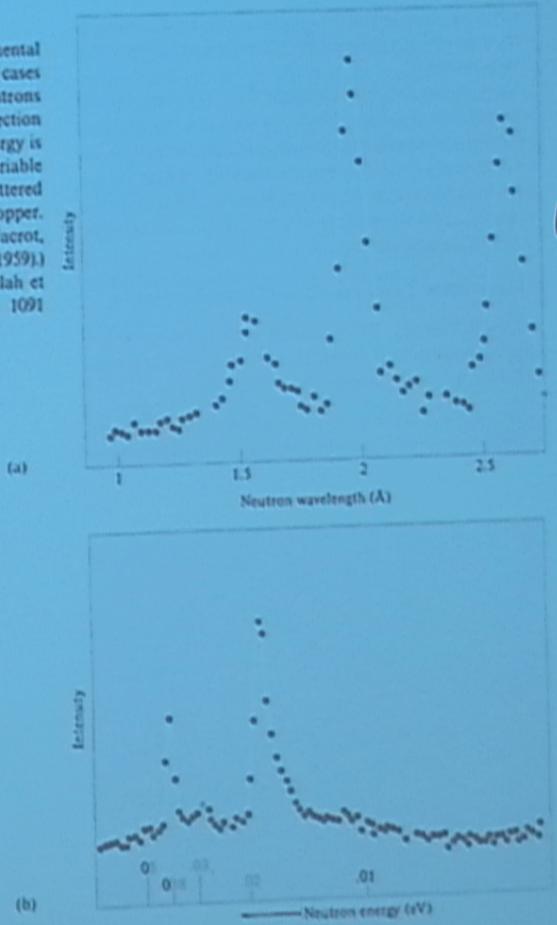
$$C(\vec{q}, \omega)$$

$$C(\vec{r}, t; \vec{r}', t') = \langle \hat{n}(\vec{r}, t) \hat{n}(\vec{r}', t') \rangle$$

$$\downarrow \hat{n}(\vec{r}, t) = \sum_i \delta(\vec{r} - \vec{r}_i(t))$$

$$C(\vec{q}, \omega) = N \underbrace{S(\vec{q}, \omega)}_{\text{dynamical structure factor}}$$

Figure 24.4
Some typical experimental neutron groups. In all cases the number of neutrons emerging in a fixed direction for a fixed incident energy is plotted against a variable that distinguishes scattered neutron energies. (a) Copper. (G. Gobert and B. Jacrot, *J. Phys. Radium* 19 (1959).) (b) Germanium. (I. Pelah et al., *Phys. Rev.* 108, 1091 (1957).)



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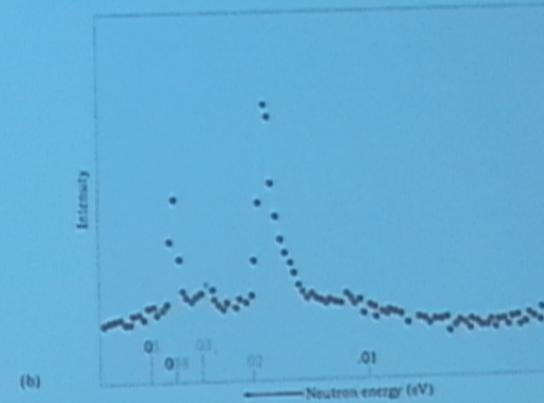
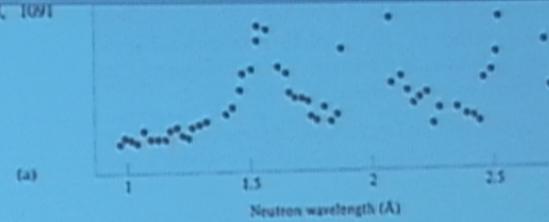
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to the phonons finite lifetimes, reflecting the eventual decay of the approximate harmonic stationary state. Associated with a phonon of lifetime τ , there will be an uncertainty \hbar/τ in the phonon energy. The energy conservation law determining the one-phonon peaks will then be correspondingly weakened.

These points will be taken up in more detail in Chapter 25. Here we merely note that the one-phonon peaks, though broadened, are still clearly identifiable. The fact that they are indeed due to one-phonon processes is strikingly confirmed by the consistency of the $\omega_s(k)$ curves inferred from their positions, for there is considerable redundancy in the data furnished by the one-phonon peaks. One can extract infor-

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Normal Modes of a Monatomic Three-Dimensional Bravais Lattice 441

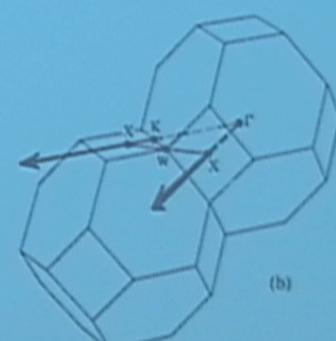
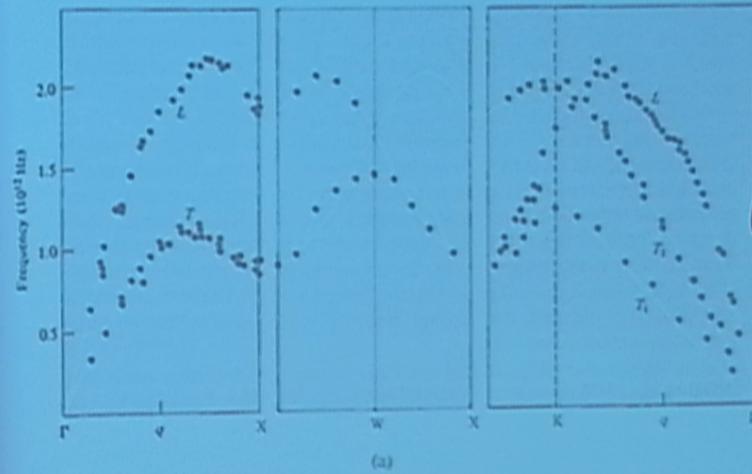


Figure 22.13

(a) Typical dispersion curves for the normal-mode frequencies in a monatomic Bravais lattice. The curves are for lead (face-centered cubic) and are plotted in a repeated-zone scheme along the edges of the shaded triangle shown in (b). Note that the two transverse branches are degenerate in the $[100]$ direction. (After Brockhouse et al., *Phys. Rev.* **128**, 1699 (1962).)

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Normal Modes of a Monatomic Three-Dimensional Bravais Lattice 441

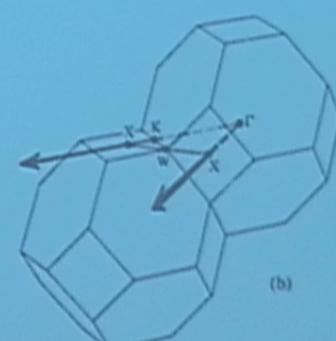
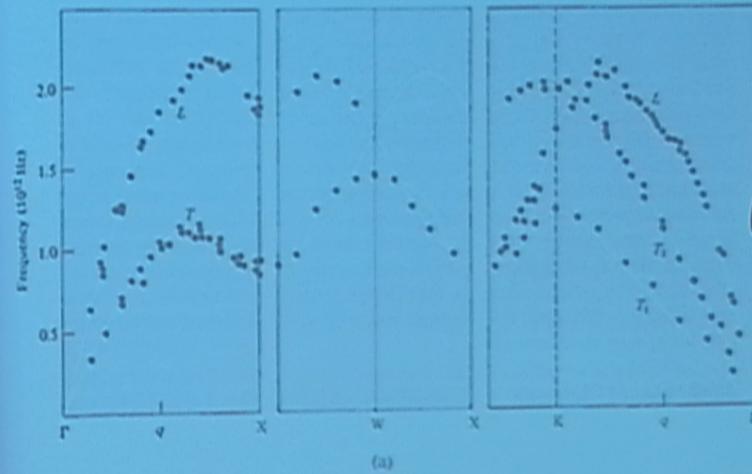


Figure 22.13

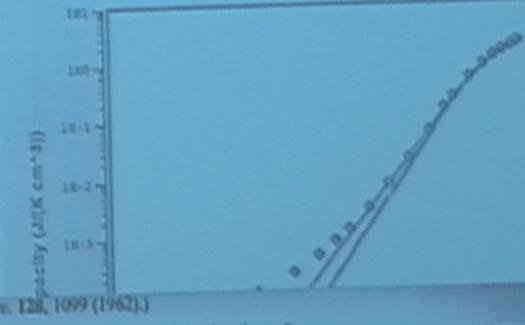
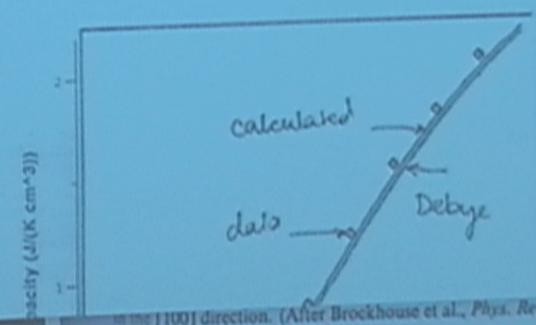
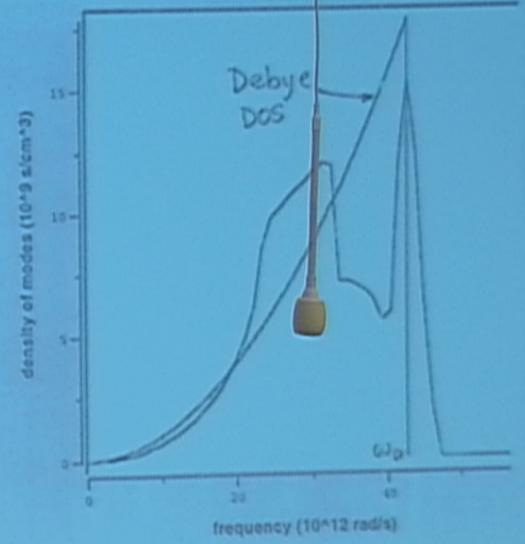
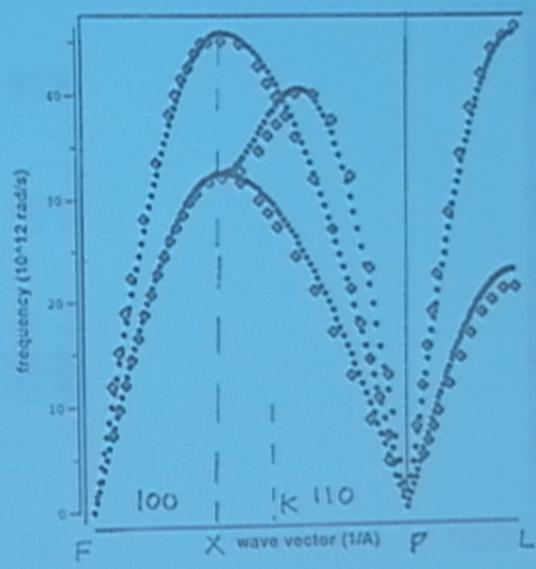
(a) Typical dispersion curves for the normal-mode frequencies in a monatomic Bravais lattice. The curves are for lead (face-centered cubic) and are plotted in a repeated-zone scheme along the edges of the shaded triangle shown in (b). Note that the two transverse branches are degenerate in the [100] direction. (After Brockhouse et al., *Phys. Rev.* **128**, 1099 (1962).)

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In the three-dimensional case it is important to consider not only the behavior of

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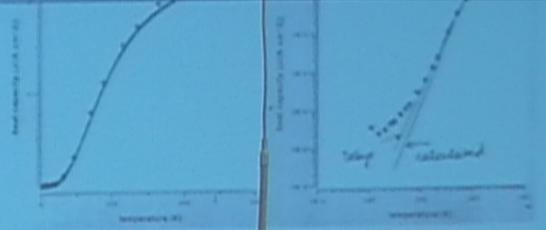
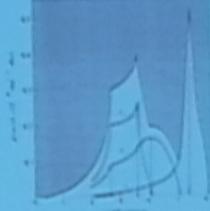
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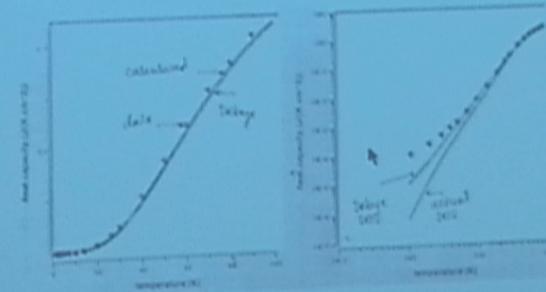
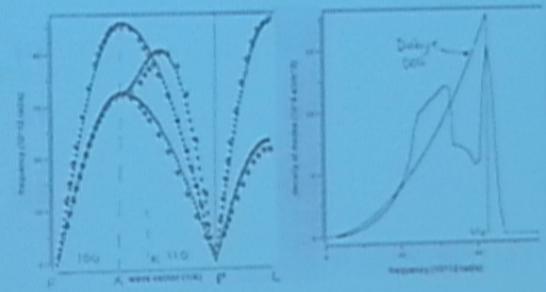
are known as Rayleigh waves. A typical density of states displaying these singularities is shown in Figure 114, and a concrete illustration of how the singularities arise in the linear chain is given in Problem 1.

Figure 114

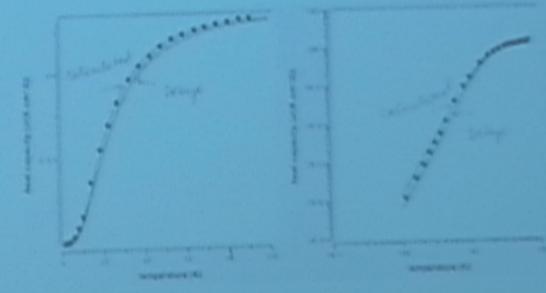
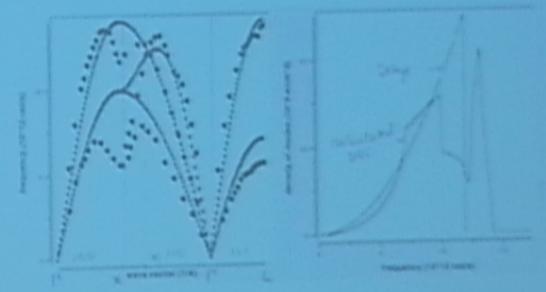
Phonon density of states in aluminum, as defined from neutron scattering data (Figure 11). The lighter curve is the full density of states. Separate calculations for the three branches are also shown. (After R. Brattain, I. Anusca, and G. Nisenz, Phys. Rev. 102, 106 (1953).)



Problem 67 DEBYE Cu: $B=55.5 \text{ N/m}$, $\rho=8.93 \times 10^3 \text{ cm}^3/\text{m}^3$, $a=3.61 \text{ \AA}$



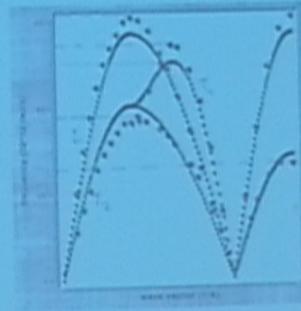
Problem 62 DEBYE Pb: $B=17 \text{ N/m}$, $\rho=11.35 \times 10^3 \text{ cm}^3/\text{m}^3$, $a=4.95 \text{ \AA}$



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Density of Normal Modes (Phonon Level Density) 405

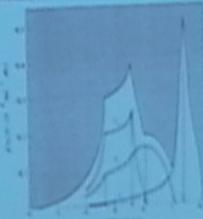
electron density of levels, one can represent the phonon density of levels in the alternative form

$$g(\omega) = \sum_k \frac{d\omega}{d\omega_k} \frac{1}{\omega_k} \quad (18.36)$$

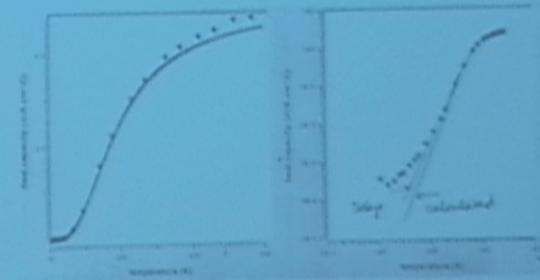
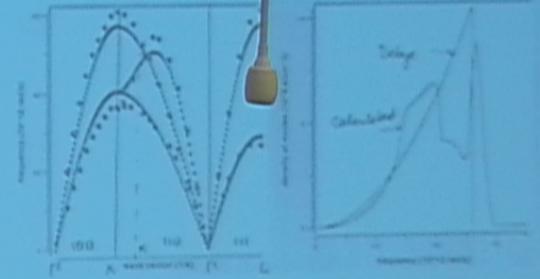
where the integral is over that surface in the first Brillouin zone which $\omega_k(\mathbf{k}) = \omega$. Just as in the electronic case, because $\omega_k(\mathbf{k})$ is periodic there will be a situation of degeneracies in \mathbf{k} space, reflecting the fact that the group velocity appearing in the denominator of (18.36) need vanish at some frequencies. As in the electronic case, the singularities will occur at very sharp singularities¹⁸. A typical density of levels displaying these singularities is shown in Figure 23.6, and a somewhat quantitative view of how the singularities arise in the lattice chain is given in Problem 5.

Figure 23.6

Phonon density of levels in a diatomic lattice, as defined from equation (18.36), showing the singularities. The upper curve is the full density of states, separated and labeled for the three branches and also shown (after R. Fiesh, J. Appl. Phys. 42, 1971, 1972).



Problem 18 DEBYE Al: $B=36.5N/m$; $v_s = 0.34 \times 10^8$ cm/s; $n=4.95$ Å



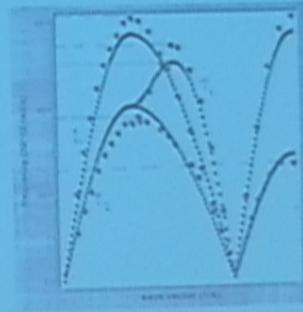
Problem 12 DEBYE P: $B=17$ N/m; $v_s = 0.13 \times 10^8$ cm/s; $n=4.95$ Å

Problem 17 DEBYE Cu: $B=55.5N/m$; $v_s = 0.25 \times 10^8$ cm/s; $n=3.61$ Å

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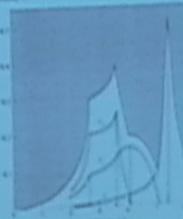
Density of Normal Modes (Phonon-Level Density)

electron density of levels, one can represent the phonon density of levels in the alternative form:

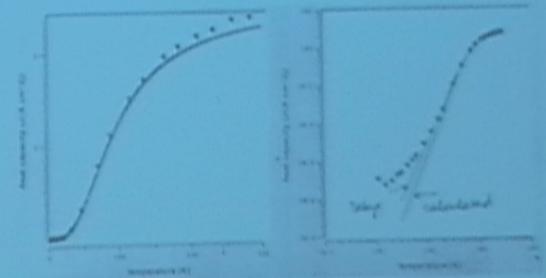
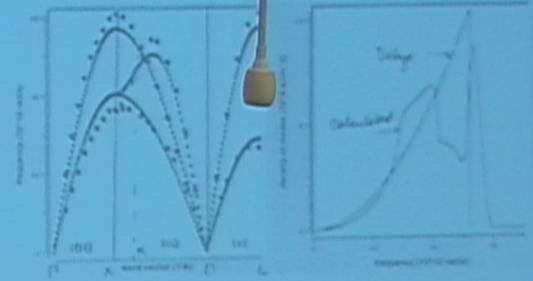
$$g(\omega) = \sum_k \frac{d\Omega}{d\omega} \frac{1}{N \omega_k^2} \quad (23.30)$$

where the integral is over that surface in the first zone on which $\omega(k) = \omega$. Just as in the electronic case, because $\omega(k)$ is periodic there will be a structure of singularities in $g(\omega)$, reflecting the fact that the group velocity appearing in the denominator of (23.30) must vanish at other frequencies. As in the electronic case, the singularities are known as van Hove singularities.¹³ A typical density of levels displaying these singularities is shown in Figure 23.6, and a concrete illustration of how the singularities show up in the lowest chart is given in Problem 5.

Figure 23.6
Phonon density of levels in aluminum, as deduced from neutron scattering data (Figure 20). The figure shows the full density of levels, because level densities for the three branches are also shown (after R. Taylor, J. Appl. Phys. 42, 1967).



Plot of ω DEBYE Al: $B=36.5N/m$, $v_s = 0.34 \times 10^8$ cm/s, $n=4.05 \text{ \AA}$



Plot of ω DEBYE Cu: $B=55.5N/m$, $v_s = 0.25 \times 10^8$ cm/s, $n=3.61 \text{ \AA}$

Plot of ω DEBYE Pb: $B=17 N/m$, $v_s = 0.13 \times 10^8$ cm/s, $n=4.55 \text{ \AA}$