KARAKTERISTIK FONON
(PHONON CHARACTERISTICS)

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Assume waves with a spread of k of $\frac{\pi}{10a}$; so this wavepacket will be localized within 10 unit cells.

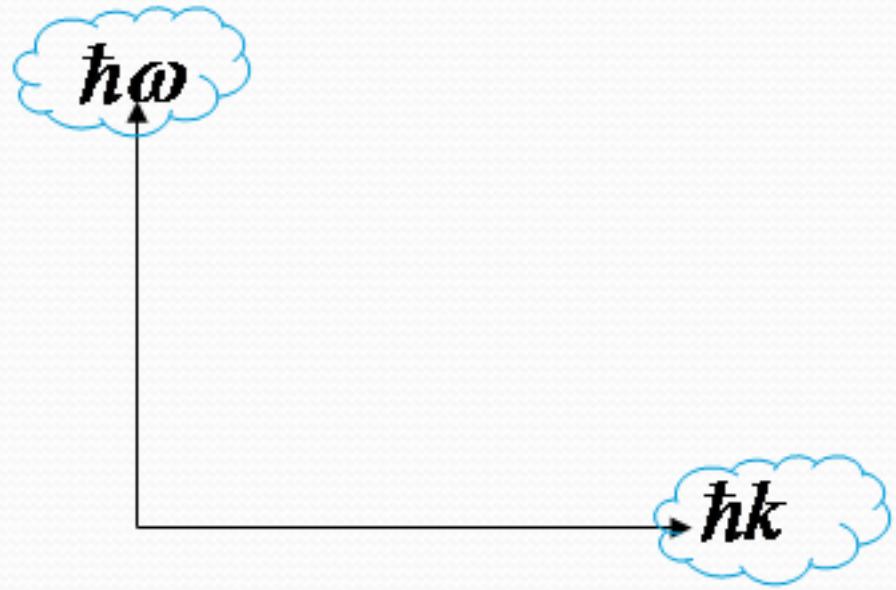
This wavepacket will represent a fairly localized phonon moving with group velocity $\frac{d\omega}{dk}$

Phonons can be treated as *localized particles* within some limits.

1D crystals

Multiply by $\hbar$

Energy of phonons



Crystal momentum

- Phonons are not conserved
- They can be created and destroyed during collisions .

Energy and heat capacity of a harmonic oscillator, Einstein Model

$$\bar{\varepsilon} = \sum_n P_n \varepsilon_n$$

Avarage energy of a harmonic oscillator and hence of a lattice mode of angular frequency at temperature T

Energy of oscillator

$$\varepsilon_n = \left(n + \frac{1}{2}\right)\hbar\omega$$

The probability of the oscillator being in this level as given by the Boltzman factor

$$\exp(-\varepsilon_n / k_B T)$$

$$\bar{\varepsilon} = \sum_n P_n \varepsilon_n$$

$$\bar{\varepsilon} = \frac{\sum_{n=0}^{\infty} \left(n+\frac{1}{2}\right)\hbar\omega \exp\left[-\left(n+\frac{1}{2}\right)\hbar\omega / k_B T\right]}{\sum_{n=0}^{\infty} \exp\left[-\left(n+\frac{1}{2}\right)\hbar\omega / k_B T\right]} \qquad (*)$$

$$Z = \sum_{n=0}^{\infty} \exp[-(n+\frac{1}{2})\frac{\hbar\omega}{k_B T}]$$

$$Z = e^{-\hbar\omega/2k_B T} + e^{-3\hbar\omega/2k_B T} + e^{-5\hbar\omega/2k_B T} + ...$$

$$Z = e^{-\hbar\omega/2k_B T}(1 + e^{-\hbar\omega/k_B T} + e^{-2\hbar\omega/k_B T} + ...$$

$$Z = e^{-\hbar\omega/2k_B T}(1 - e^{-\hbar\omega/k_B T})^{-1}$$

According to the Binomial expansion for x«1 where $x = -\hbar\omega / k_B T$

Eqn (*) can be written

$$\bar{\varepsilon} = k_B T^2 \frac{1}{z}\frac{\partial z}{\partial T} = k_B T^2 \frac{\partial}{\partial T}(\ln z)$$

$$\bar{\varepsilon} = k_B T^2 \frac{\partial}{\partial T}\ln\left(\frac{e^{-\hbar\omega/2k_BT}}{1-e^{-\hbar\omega/k_BT}}\right)$$

$$\bar{\varepsilon} = k_B T^2 \frac{\partial}{\partial T}\left[\ln e^{-\hbar\omega/2k_BT} - \ln\left(1-e^{-\hbar\omega/k_BT}\right)\right]$$

$$\bar{\varepsilon} = k_B T^2 \left[\frac{\partial}{\partial T}\left(-\frac{\hbar\omega}{2k_BT}\right) - \frac{\partial}{\partial T}\ln\left(1-e^{-\hbar\omega/k_BT}\right)\right]$$

$$\frac{\partial}{\partial x}(\ln x) = \frac{x'}{x}$$

$$\bar{\varepsilon} = k_B T^2 \left[\frac{2k_B\hbar\omega}{4k_B^2T^2} + \frac{\frac{\hbar\omega k_B}{k_B^2T^2}e^{-\hbar\omega/k_BT}}{\left(1-e^{-\hbar\omega/k_BT}\right)}\right] = \frac{1}{2}\hbar\omega + \frac{\hbar\omega e^{-\hbar\omega/k_BT}}{\left(1-e^{-\hbar\omega/k_BT}\right)}$$

$$\bar{\varepsilon} = \frac{1}{2}\hbar\omega + \frac{\hbar\omega}{e^{\hbar\omega/k_BT}-1}$$

$$\bar{\varepsilon} = \frac{1}{2}\hbar\omega + \frac{\hbar\omega}{e^{\hbar\omega/k_B T} - 1}$$

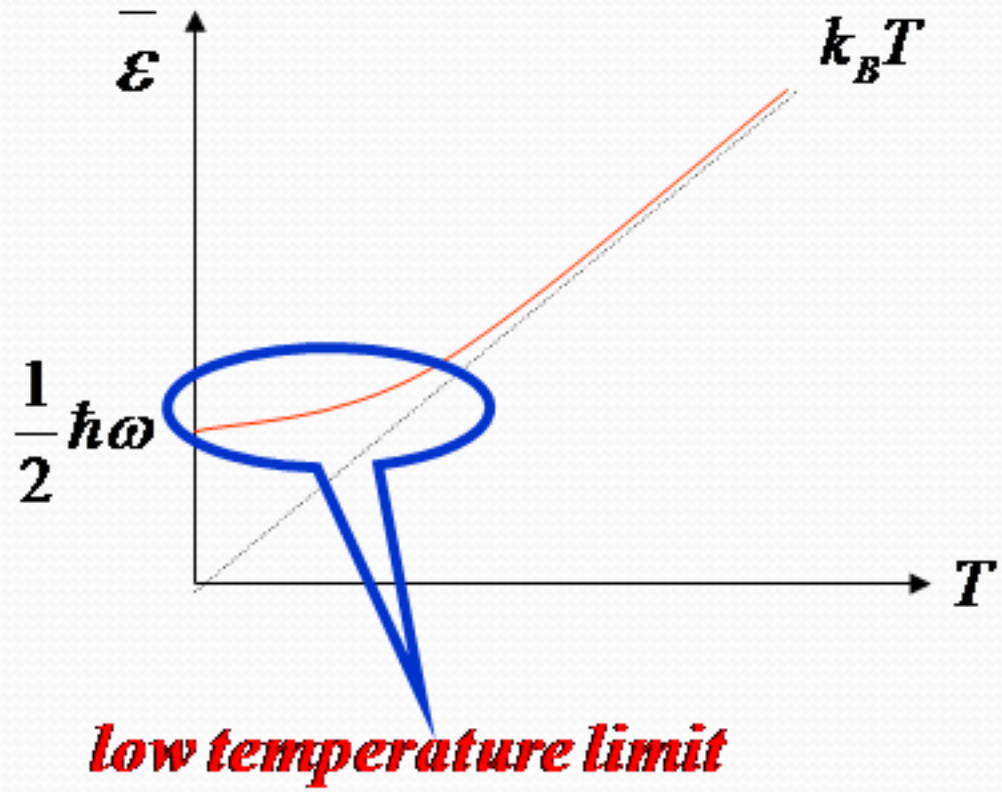
This is the mean energy of phonons.The first term in the above equation is the zero-point energy. As we have mentioned before even at 0°K atoms vibrate in the crystal and have zero-point energy. This is the minimum energy of the system.

The avarage number of phonons is given by Bose-Einstein distribution as

(number of phonons) x (energy of phonon)=(second term in $\bar{\varepsilon}$)

$$n(\omega) = \frac{1}{e^{\hbar\omega/k_B T} - 1}$$

The second term in the mean energy is the contribution of phonons to the energy.



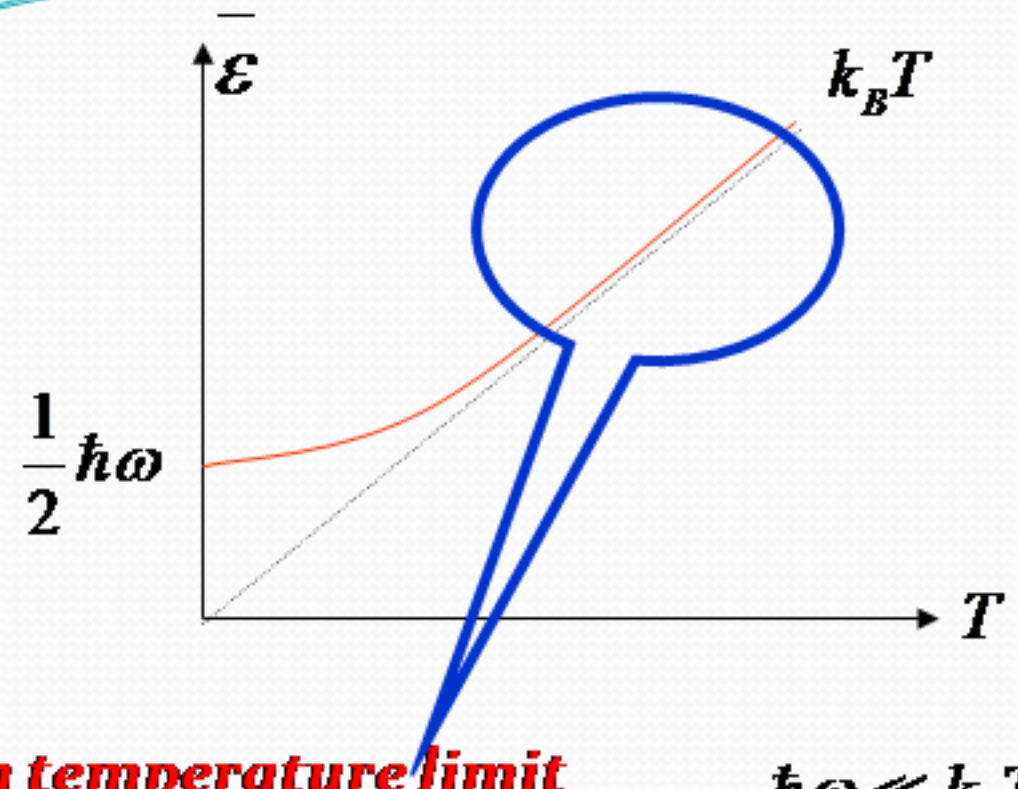
Mean energy of a harmonic oscillator as a function of T

$$\hbar\omega \succ\succ k_B T$$

$$\bar{\varepsilon} = \frac{1}{2}\hbar\omega + \frac{\hbar\omega}{e^{\hbar\omega/k_B T} - 1}$$

Since exponential term gets bigger

$$\Rightarrow \quad \bar{\varepsilon} = \frac{1}{2}\hbar\omega$$ ***Zero point energy***



high temperature limit

$$\hbar\omega \ll k_BT$$

- $\bar{\varepsilon}$ is independent of frequency of oscillation.
- This is the classical limit because the energy steps are now small compared with the energy of the harmonic oscillator.
- So that is the thermal energy of the classical 1D harmonic oscillator.

Mean energy of a harmonic oscillator as a function of T

$$e^x = 1 + x + \frac{x^2}{2!} + \ldots\ldots\ldots$$

$$e^{\hbar\omega/k_BT} = 1 + \frac{\hbar\omega}{k_BT}$$

$$\bar{\varepsilon} = \frac{1}{2}\hbar\omega + \frac{\hbar\omega}{1 + \frac{\hbar\omega}{k_BT} - 1}$$

$$\bar{\varepsilon} = \frac{1}{2}\hbar\omega + k_BT$$

$$\bar{\varepsilon} \approx k_BT$$

Model Einstein

- Dalam model ini, atom dianggap sebagai osilator bebas, dan energinya ditentukan lewat mekanika kuantum
- Energi sebuah osilator terisolasi secara kuantum bernilai $\varepsilon = n\hbar\omega$ *dengan* $n = 0, 1, 2, 3, \ldots$ dan ω adalah frekuensi osilator
- Pada bahan, osilator tidak terisolasi, namun saling berinteraksi, bertukar energi dengan reservoir panas dari bahan, sehingga selalu berubah

Energi rerata dari osilator pada bahan adalah:

$$\bar{\epsilon} = \frac{\sum_{n=0}^{\infty} \epsilon_n e^{-\epsilon_n / k_B T}}{\sum_{n=0}^{\infty} e^{-\epsilon_n / k_B T}}$$

Persamaan tersebut menghasilkan:

$$\bar{\epsilon} = \frac{\hbar \omega}{e^{\hbar \omega / k_B T} - 1}$$

pada suhu tinggi $\varepsilon \rightarrow kBT$, sesuai kajian klasik,
saat *T berkurang*, nilai ε berkurang,
hingga lenyap saat $T = o\ K$

Fonon?

- Pada model Debye, energi setiap model terkuantisasi dengan satuan energi kuantumnya $\hbar\omega$
- Karena modenya adalah gelombang elastik, maka yang terkuantisasi adalah energi gelombang suara, dan quasi-partikel yang membawa kuantisasi energi ini disebut sebagai **fonon**, membawa energi sebesar $\hbar\omega$
- Fonon juga merepresentasikan gelombang berjalan dengan momentum $\boldsymbol{p} = \hbar\boldsymbol{k}$
- Maka gelombang suara elastik dapat dilihat sebagai aliran fonon yang bergerak dengan kecepatan suara dalam bahan

Dalam bahan, setiap atom mewakili 3 osilator, sehingga total terdapat $3N_A$ *osilator,* *jadi energi* totalnya:

$$\bar{\epsilon} = 3\,N_A \frac{\hbar\omega_E}{e^{\hbar\omega_E/k_BT} - 1}$$

dengan ω_E *adalah frekuensi Einstein*

Model Debye

- Atom pada model Einstein diasumsikan berosilasi bebas, sedangkan pada kenyataannya atom-atom saling berinteraksi, sehingga osilasi satu atom akan mempengaruhi atom lainnya
- Gerak yang ditinjau adalah gerak kisi secara keseluruhan, bukan gerak atom secara individu, sehingga ditinjau mode kisi kolektif
- Contoh umum dari mode kolektif ini adalah gelombang suara pada bahan

Debye mengasumsikan bahwa mode kisi menyerupai sifat gelombang suara yang memiliki relasi dispersi: $\omega = v_s k$

Nilai ω pada model Einstein adalah tunggal, yaitu ω_E, *sedangkan pada model Debye nilai ω* bervariasi dari o hingga nilai ω maksimum

Total energi getaran seluruh kisi adalah:

$$E = \int \bar{\epsilon}(\omega)\, g(\omega)\, d\omega$$

dengan *g(ω) adalah rapat keadaan (density of states)*

Energi rerata dinyatakan oleh:

$$\bar{\epsilon} = \frac{\hbar \omega_E}{e^{\hbar \omega_E / k_B T} - 1}$$

Bentuk integral tersebut harus memiliki batas integrasi, yaitu ujung bawah dan atas spektrum frekuensi

Batas bawah spektrum frekuensi adalah $\omega = 0$ sedangkan batas atas ditentukan sedemikian sehingga banyaknya mode harus sama dengan banyaknya derajat kebebasan atom diseluruh bahan, yaitu $3N_A$

Untuk menentukan banyaknya mode, digunakan DOS medium kontinyu, karena Debye mengasumsikan bentuk relasi dispersi yang sama dengan gelombang suara pada bahan :

$$g(\omega)=\frac{3V}{2\pi^2}\frac{\omega^2}{v_s^3}$$

Frekuensi Debye yang merupakan frekuensi batas (*cutoff frequency) pada getaran kekisi ini ditentukan melalui :* $\int_0^{\omega_D} g(\omega)\,d\omega=3N_A$

sehingga diperoleh: $\omega_D=v_s(6\pi^2 n)^{1/3}$

dengan $n = N_A/V$

Energi total getaran kekisinya adalah:

$$E = \frac{3V}{2\pi^2 v_s^3} \int_0^{\omega_D} \frac{\hbar \omega^3}{e^{\hbar \omega / k_B T} - 1} d\omega$$

Density of State 1D

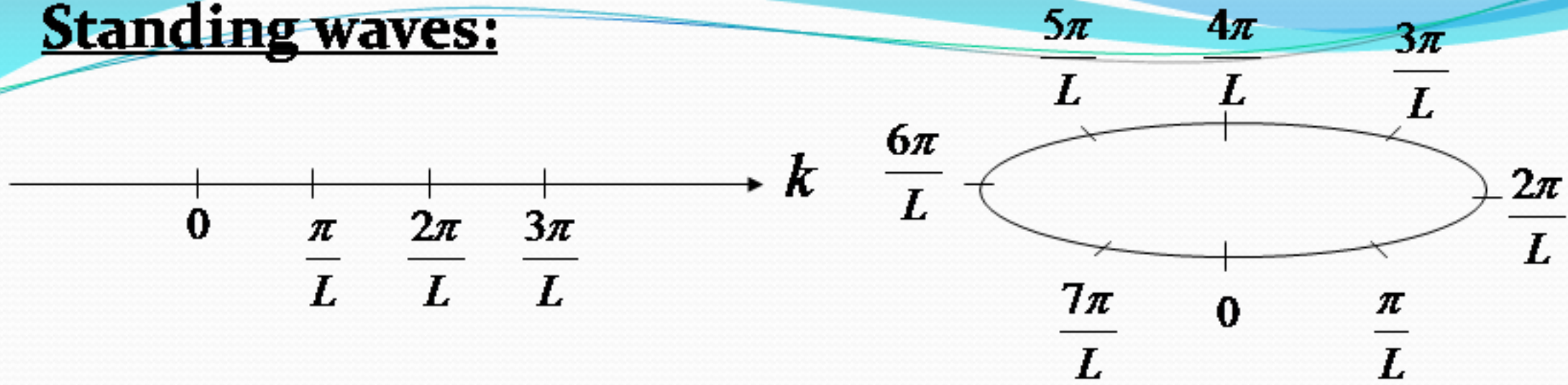
- Ditinjau gelombang elastik pada batang panjang dimana gelombang merambat dalam 1-D
- Solusinya (bagian waktu diabaikan) :

  $u(x) = Aeikx$

- Jika jumlah ion/atom sangat banyak, dapat diterapkan syarat batas periodik pada solusi gelombang elastik

  (→ ujung kanan batang selalu memiliki state osilasi yang sama dengan ujung kiri)
- Seolah-olah batang diubah ke bentuk lingkaran sehingga ujung kiri dan kanan bergabung

Standing waves:



In some cases it is more suitable to use standing waves,i.e. chain with fixed ends. Therefore we will have an integral number of half wavelengths in the chain;

$$L=\frac{n\lambda}{2};k=\frac{2\pi}{\lambda}\Rightarrow k=\frac{2\pi n}{2L}\Rightarrow k=\frac{n\pi}{L}$$

These are the allowed wavenumbers for standing waves; only positive values are allowed.

$$k=\frac{2\pi}{L}p\longrightarrow \text{for running waves} \qquad k=\frac{\pi}{L}p\longrightarrow \text{for standing waves}$$

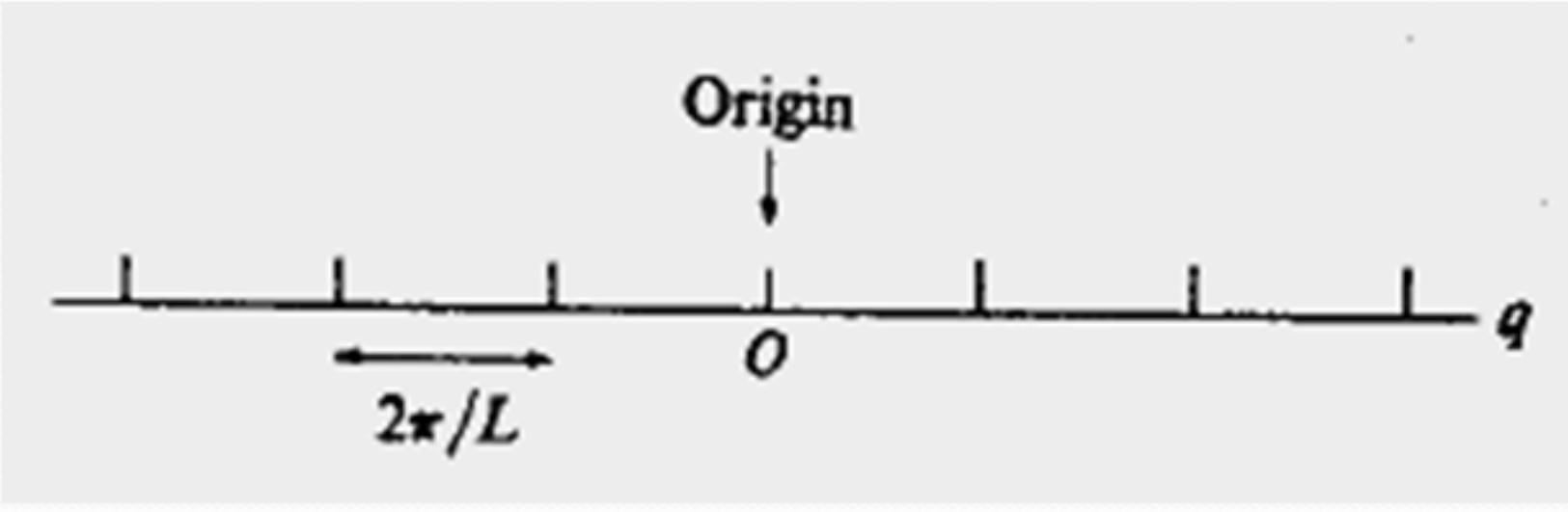
Jika panjang batang adalah $L = Na$
(N adalah banyaknya ion, *a adalah jarak antar atom), maka :*

$u(x = 0) = u(x = L)$

Sehingga $e^{ikl} = 1$, *dipenuhi ketika* $k = n\ 2\pi/L$

dengan $n = 0, \pm 1, \pm 2, \pm 3, \ldots$

Jarak antar dua nilai *k yang bersebelahan adalah* $2\pi/L$



Ketika L besar, jarak pi sah menjadi kecil dan titik-titik membentuk garis kuasi-kontinyu
Tiap nilai-k *(tiap titik) mewakili sebuah mode* getaran
Misal dk adalah interval pada ruang-k, banyaknya mode yang nilai k-nya terletak pada interval ini adalah:

$$\frac{dq}{2\pi/L} = \frac{L}{2\pi} dq$$

Namun k *dan* ω terkait melalui hubungan dispersi, sehingga banyaknya mode juga dapat ditentukan pada interval frekuensi $d\omega$ yang terletak antara ω dan $\omega+d\omega$

- These **quantized normal modes** of vibration are called ***PHONONS***
- **PHONONS** are massless quantum mechanical particles which have ***no classical analogue.***
  - They behave like particles in momentum space or **k space**.
- Phonons are one example of many like this in many areas of physics. Such quantum mechanical particles are often called ***"Quasiparticles"***

Examples of other Quasiparticles:

Photons: Quantized Normal Modes of electromagnetic waves.

Rotons: Quantized Normal Modes of molecular rotational excitations.

Magnons: Quantized Normal Modes of magnetic excitations in magnetic solids

Excitons: Quantized Normal Modes of electron-hole pairs

Polaritons: Quantized Normal Modes of electric polarization excitations in solids

+ Many Others!!!

Rapat keadaan (***density of states***) $g(\omega)$
didefinisikan sedemikian sehingga $g(\omega)d\omega$
memberikan banyaknya mode

Maka $g(\omega)d\omega = (L/2\pi)\, dk$
atau $g(\omega) = (L/2\pi) \,/\, (d\omega/dk)$

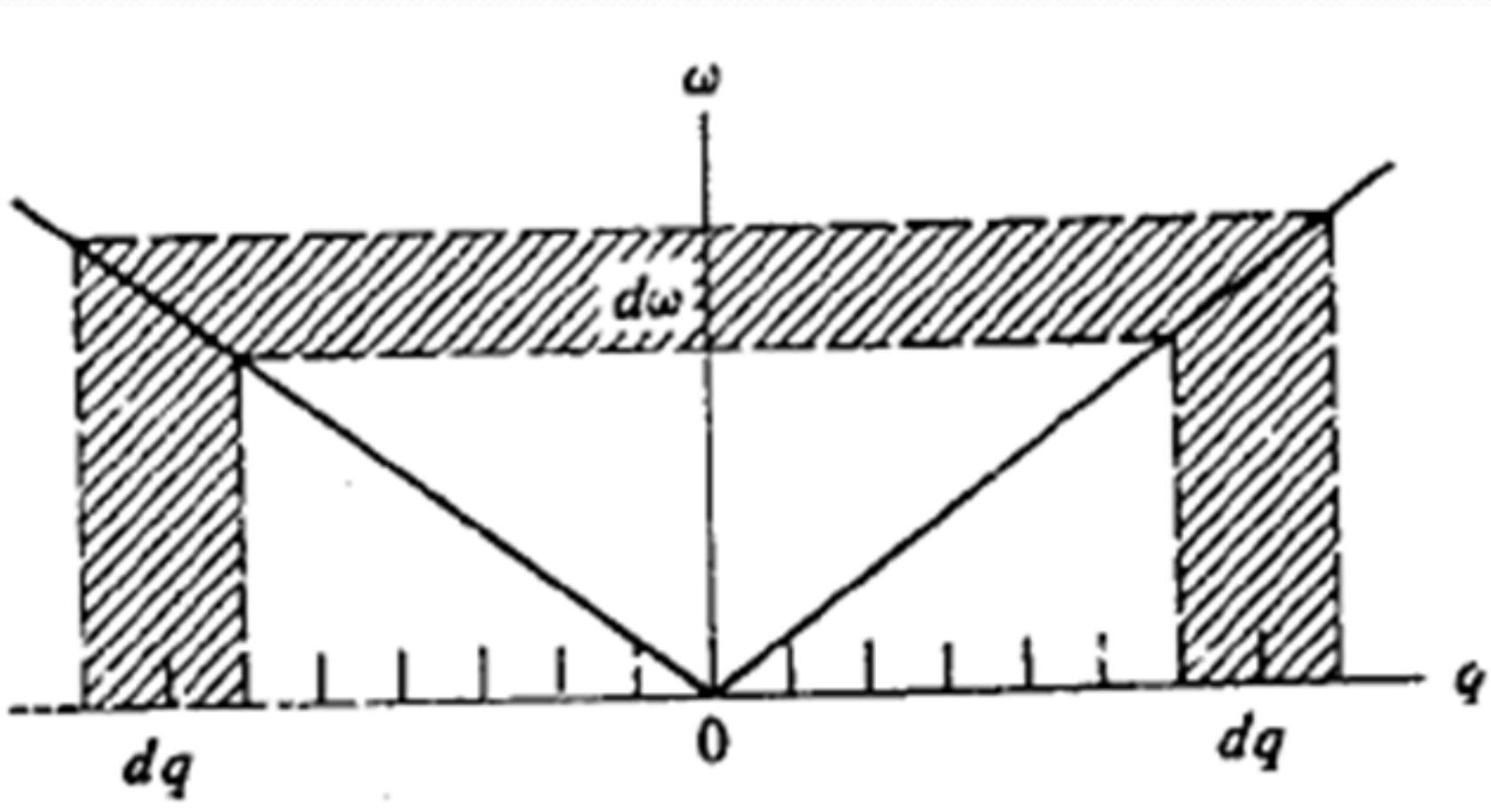
Karena daerah k negatif juga harus disertakan (mewakili gelombang yang berjalan ke kiri), $g(\omega)$ dikalikan dua, sehingga:

$$g(\omega) = \frac{L}{\pi} \frac{1}{d\,\omega / dk}$$

Karena $d\omega/dk = v_s$, maka :

$$g(\omega) = \frac{L}{\pi}\frac{1}{v_s}$$

yang merupakan tetapan tak gayut ω



Density of State 2D

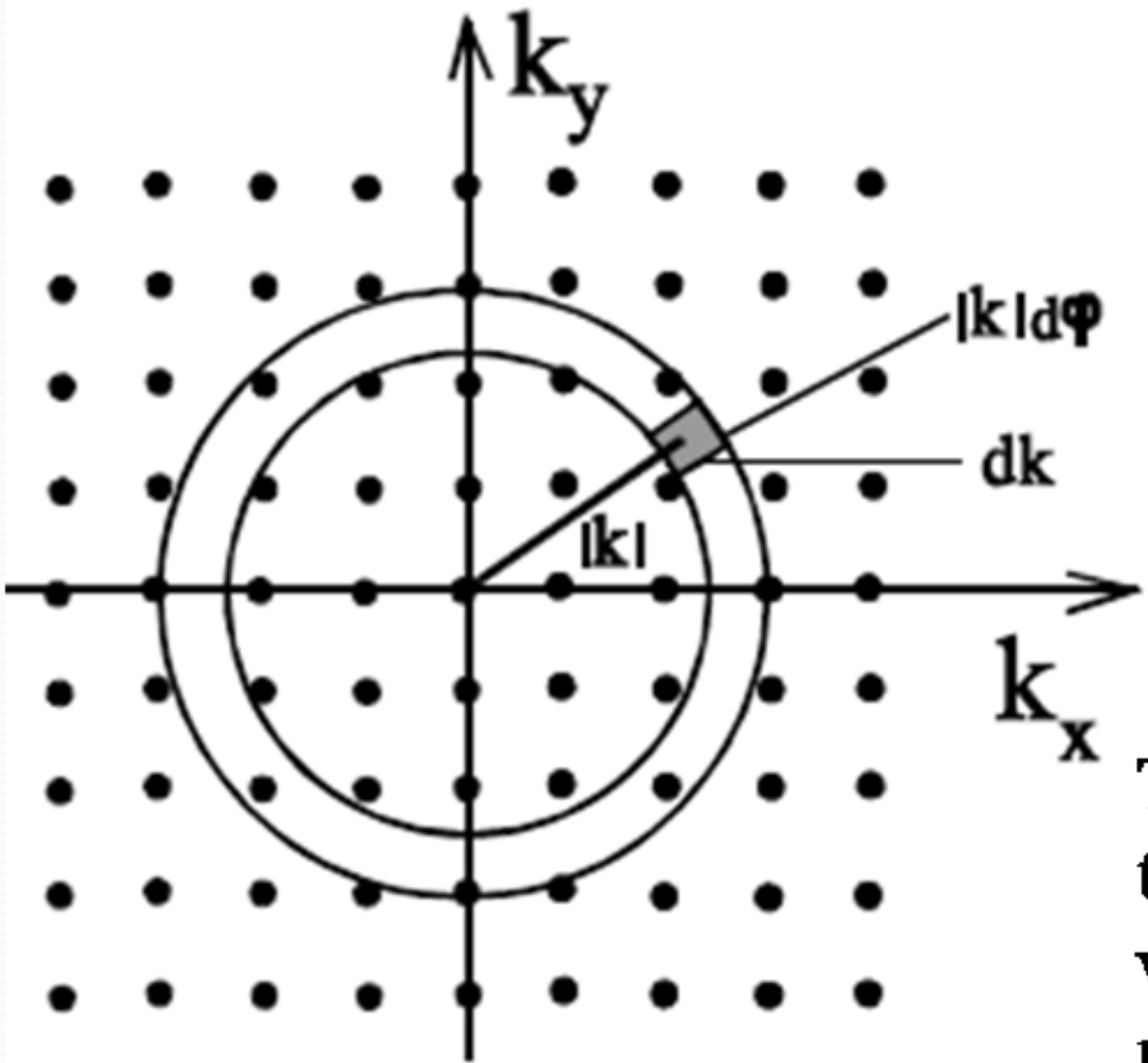
Density of States for a 2-D Crystal near k=0 for the Acoustic Branch

The density of states g(ω) can be calculated for the 2-D monatomic crystal using the **k**-state density

We limit the range of **k** to small values, so that the medium can be considered to be non-dispersive in that the angular frequency can be related to the magnitude of the wave vector $\mathbf{k} = |\mathbf{k}|$ through the speed *v* as :

$$\omega = v\left|\vec{k}\right| = vk$$

The group velocity has the same value as the phase speed in this case ➔ small **k** values



The frequency depends on the magnitude of the wave vector k, which also provides the approximate radius of the outer circle.

The total number of states within the area of a circle of radius k can be written as :

$$\text{total number} = \sum \frac{\text{number}}{\text{k}-\text{area}}\ \Delta(\text{k}-\text{area}) = \sum g_{\vec{k}}^{(2D)}\ \left(dk\ |k|\ d\varphi\right)$$

$$N_T = \int_0^k g_{\vec{k}}^{(2D)}\, k' dk' d\varphi = \int_0^k \frac{A_{xal}}{4\pi^2} k' dk' d\varphi$$

$$A_{xal} = L^2$$

The last integral can also be written for the total number per unit crystal area as :

$$N_A = \frac{N_T}{A_{xal}} = \int_0^k \frac{1}{4\pi^2} k' dk' d\varphi$$

Integrating over the angle :

$$N_T = \frac{A_{xal}}{2\pi}\int_0^k k' dk'$$

The density of states per unit |**k**| (i.e., the magnitude) comes from the last equation by differentiating :

$$g_k^{(2D)} = \frac{\partial N_T}{\partial k} = \frac{A_{xal}\, k}{2\pi}$$

We can find the density of modes for ω-space by substituting $\omega = v\,k$:

$$N_T = \frac{A_{xal}}{\pi v^2}\int_0^{\omega} \omega' d\omega'$$

$$N_T = \frac{A_{xal}\omega^2}{2\pi\ v^2}$$

the number of states per unit angular frequency is given by :

$$g_{\omega}^{(2D)} = \frac{\partial N_T}{\partial \omega} = \frac{A_{xal}\omega}{\pi\ v^2}$$

PHONONS

- Quanta of lattice vibrations
- Energies of phonons are quantized

PHOTONS

- Quanta of electromagnetic radiation
- Energies of photons are quantized as well

$$E_{phonon} = \frac{h\nu_s}{\lambda}$$

$\lambda \sim a_o = 10^{-10}\text{m}$

$$E_{photon} = \frac{hc}{\lambda}$$

$\lambda \sim 10^{-6}\text{m}$

$$p_{phonon} = \frac{h}{\lambda}$$

$$p_{photon} = \frac{h}{\lambda}$$

Bagaimana fonon terbentuk?

➢Banyaknya fonon pada suatu mode pada suhu tertentu dinyatakan sebagai:

$$\bar{n} = \frac{1}{e^{\hbar\omega / k_B T} - 1}$$

yang bergantung pada suhu, dengan $n = o$ *saat* $T = o$ *dan membesar ketika suhunya juga naik*

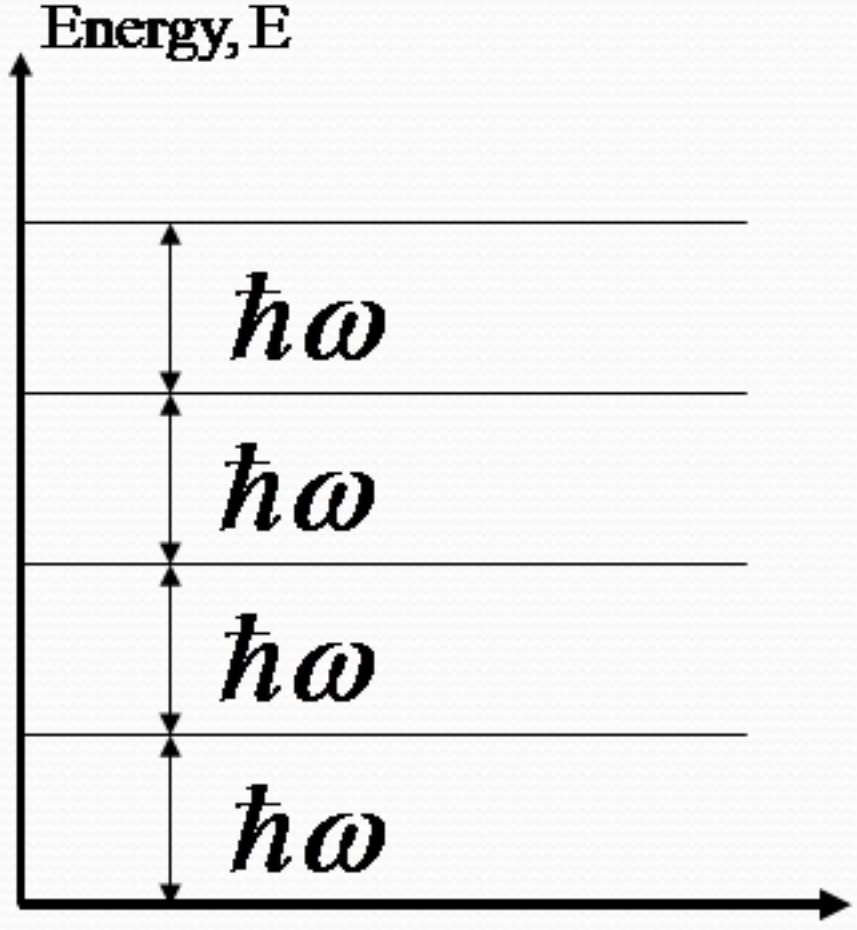
➢Maka fonon 'diciptakan' dengan menaikkan suhu bahan kristal dan cacahnya tidak tetap (berbeda dengan partikel biasa yang cacahnya selalu tetap)

Energy of harmonic oscillator

Obtained by in a classical way of considering the normal modes that we have found are independent and harmonic.

$$\varepsilon_n = \left(n + \frac{1}{2}\right)\hbar\omega$$

- **Make a transition to Q.M.**



- **Represents equally spaced energy levels**

Energy levels of atoms vibrating at a single frequency ω

Often, we consider E_n as being constructed by adding **n** excitation quanta of energy $\hbar\omega$ to the ground state.

$$E_0 = \frac{1}{2}\hbar\omega$$

← ***Ground state energy of the oscillator.***

If the system makes a transition from a lower energy level to a higher energy level, it is always true that the change in energy is an integer multiple of $\hbar\omega$

It is possible to consider ε_n as constructed by adding n excitation quanta each of energy $\hbar\omega$ to the ground state.

$$\varepsilon_0 = \frac{1}{2}\hbar\omega$$

A transition from a lower energy level to a higher energy level.

$$\Delta\varepsilon = \left(n_2 + \frac{1}{2}\right)\hbar\omega - \left(n_1 + \frac{1}{2}\right)\hbar\omega$$

$$\Delta\varepsilon = \underbrace{\left(n_2 - n_1\right)}_{unity}\hbar\omega \Rightarrow \Delta\varepsilon = \hbar\omega$$

absorption of phonon

- The converse transition results an emission of phonon with an energy $\hbar\omega$.
- Phonons are quanta of lattice vibrations with an angular frequency of ω
- Phonons are not localized particles.
- Its momentum is exact, but position can not be determined because of the uncertainity principle.
- However, a slightly localized wavepacket can be considered by combining modes of slightly different λ and ω .