## ***Question asked in the discussion forum:***

In Einstein's formula for specific heat, there is frequency term, what frequency is that?

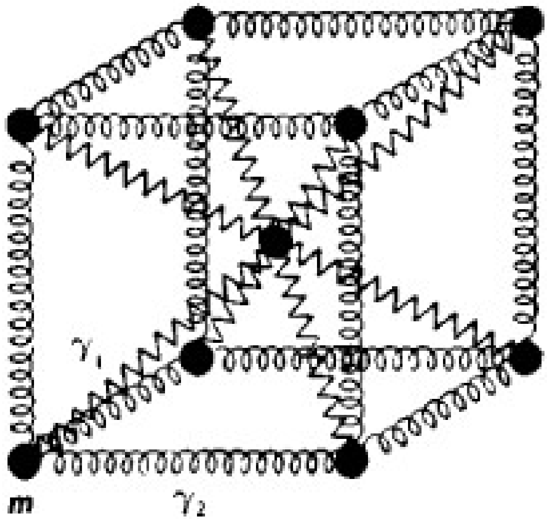
Is it the natural frequency of the solid?

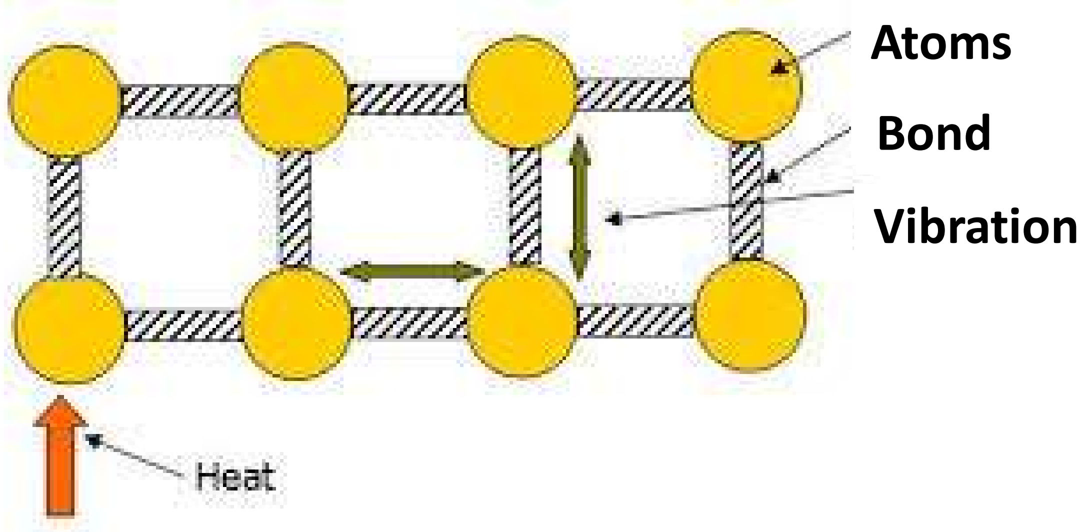
We are assuming that all $3N_A$ vibrations are happening at that frequency f?

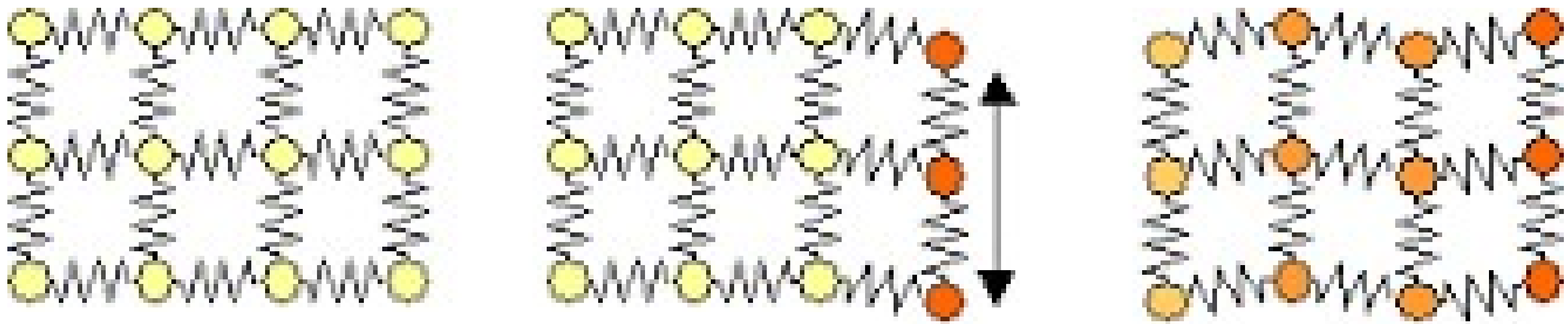
In black body radiation, we considered oscillators of frequency f to be responsible for radiation of frequency f. Since all frequencies are present in the spectrum, oscillators of all frequencies must be there in the body.

But in case of specific heats, we consider all oscillator oscillating at a single frequency. Why???

# Atomic Vibrations in Solids



**Atoms vibrating about their equilibrium positions:**

**Lattice vibrations**

**Typical value of vibration frequency is very small**

**~ acoustic frequency**

**Smaller than the typical vibration frequencies of gas molecules**

For a solid containing N atoms, there are N lattice vibration frequencies.

Quanta of lattice vibrations are called '**Phonons**'

## The lattice vibrations have different frequencies

However, Einstein assumed that all lattice vibrations have same frequency, ν

$$\varepsilon = 3N_A \frac{h\nu}{e^{h\nu/kT} - 1}$$

$$\langle E \rangle = \frac{\sum_{n=0}^{\infty} nh\nu \, e^{-(nh\nu/kT)}}{\sum_{n=0}^{\infty} e^{-(nh\nu/kT)}} = \frac{h\nu}{e^{h\nu/kT} - 1}$$

$$C_V = 3R \frac{x^2 e^x}{(e^x - 1)^2}$$

$$x = \frac{h\nu}{kT} = \frac{\theta_E}{T}$$

$$C_V = 3R\frac{x^2 e^x}{(e^x - 1)^2} \qquad x = \frac{h\nu}{kT} = \frac{\theta_E}{T}$$

**High temperature limit:**

$$T >> \theta_E \Rightarrow x << 1 \Rightarrow e^x - 1 \approx x \Rightarrow C_V \to 3R$$

**Low temperature limit:**

$$T << \theta_E \Rightarrow x >> 1 \Rightarrow e^x - 1 \approx e^x \qquad T \to 0,\ C_V \to 0$$

**However, the following observation can not be explained:**

• $C_v$ decrease in a nonlinear manner with decreasing temperature; at low temperature, **$C_v = aT^3$**

***This is due the assumption that all lattice vibration frequencies are identical.***

# Lattice vibrations

A particular vibrational mode (of frequency ν) will contribute to $C_v$ if $h\nu \sim kT$

## High frequency

*On reduction in temperature, these modes of vibration start freezing, their contribution to specific heat decreases*

## Low frequency

Separation between modes is small

*On reduction in temperature, these modes freeze very slowly, and continue to contribute to specific heat, eventually freezing out completely at T=0.*

Einstein's theory therefore does not predict correctly the $T^3$ behaviour at low temperatures

**More realistic model is by Debye.**

# Fourier Transform

Understanding the Fourier Transform and its general usages

*Do not get frightened by the complicated integrals. They are going to be there, you can not avoid them. But see the usefulness of the concept, which is useful to all engineers and scientists.*

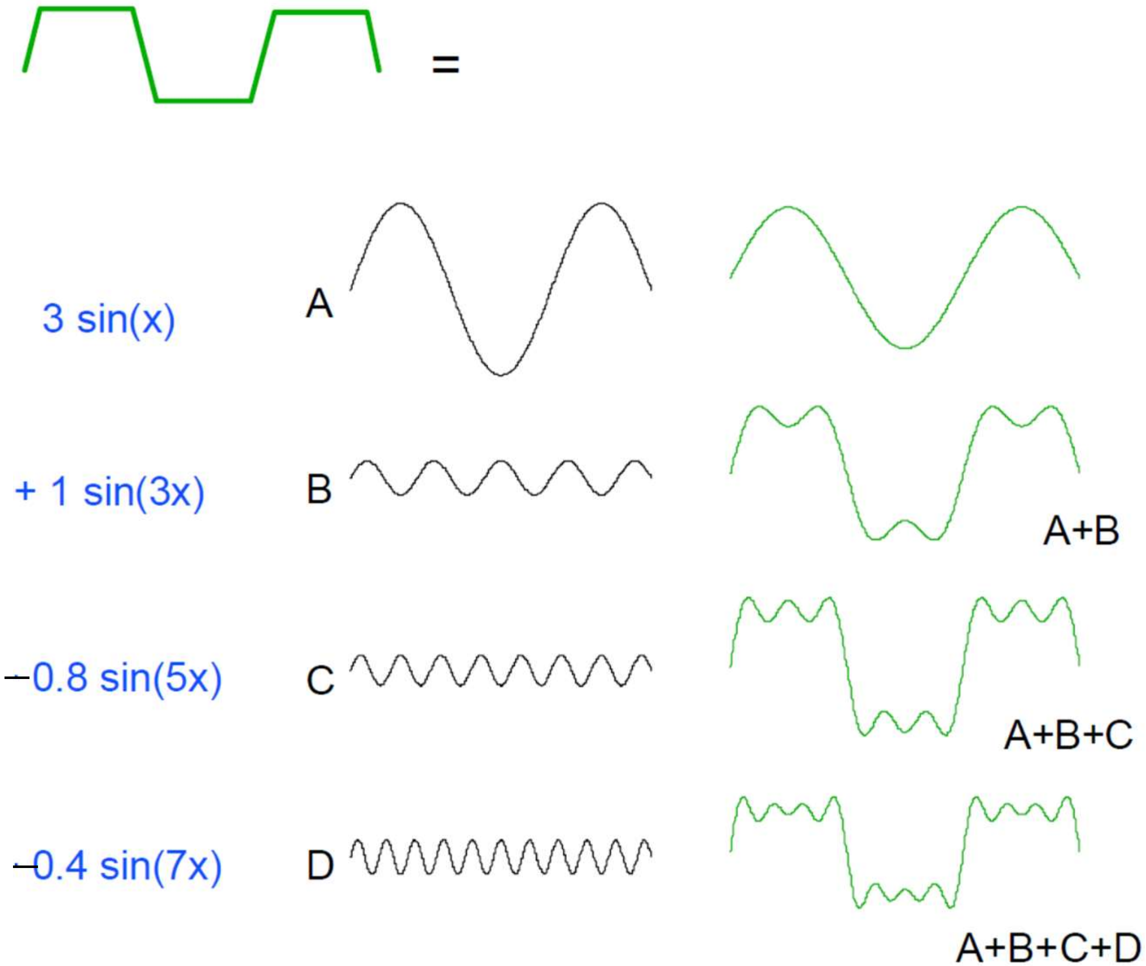
*In earlier lectures, we used Fourier transform for constructing wave packets and for arriving at the uncertainty relation. Here is a brief 'primer' on Fourier transform.*

Jean Baptiste Joseph Fourier

1768-1830

**Discovered Fourier Transform in 1822.**

## Every function can be expressed as a sum of sines and cosines




$$f(x) = \sum_n a_n \sin nx$$

$$f(x) = \sum_n a_n \cos nx$$

$$\textit{In general} \quad f(x) = \sum_n a_n \sin nx + \sum_n b_n \cos nx$$

## Generalization

$$f(x) = \sum_n a_n \sin nx + \sum_n b_n \cos nx$$

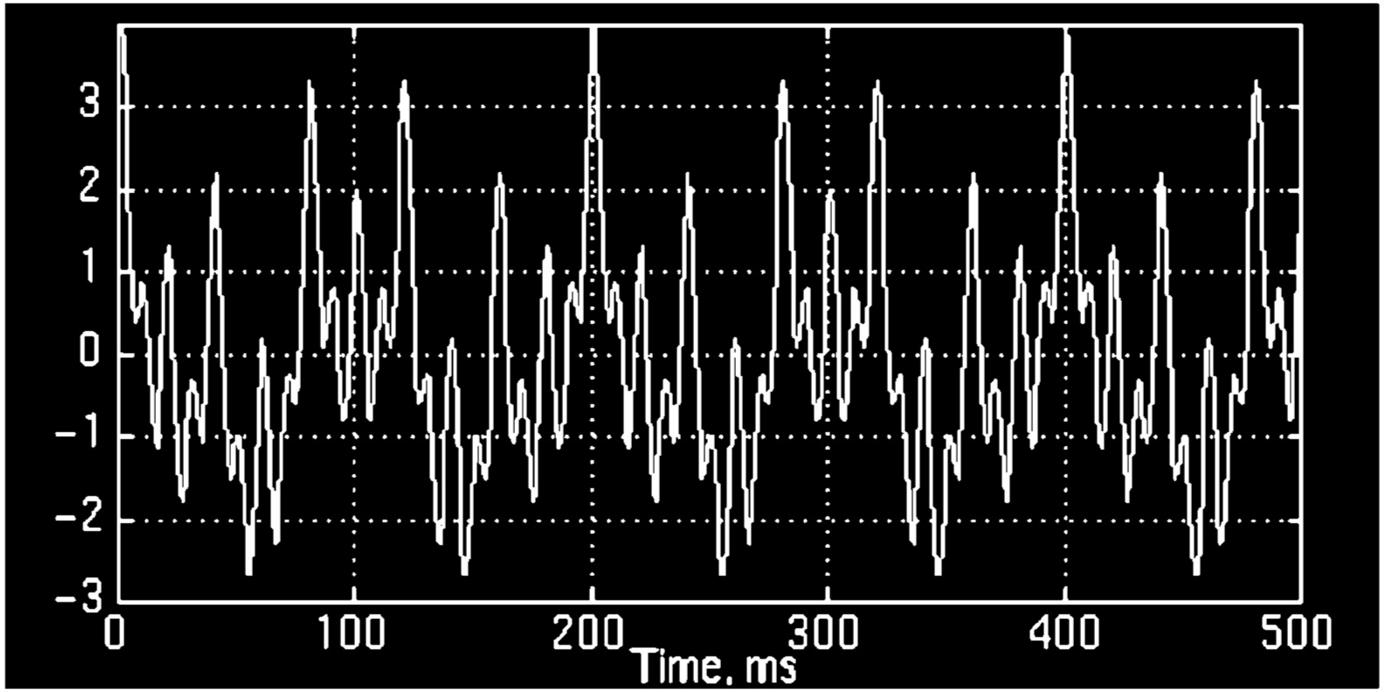
$$f(t) = \int_{-\infty}^{\infty} g(\omega) e^{i\omega t} d\omega$$

Expressing *f(t)* as an infinite '**sum**' of sine and cosine functions

$$g(\omega) = \int_{-\infty}^{\infty} f(t) e^{-i\omega t} dt$$

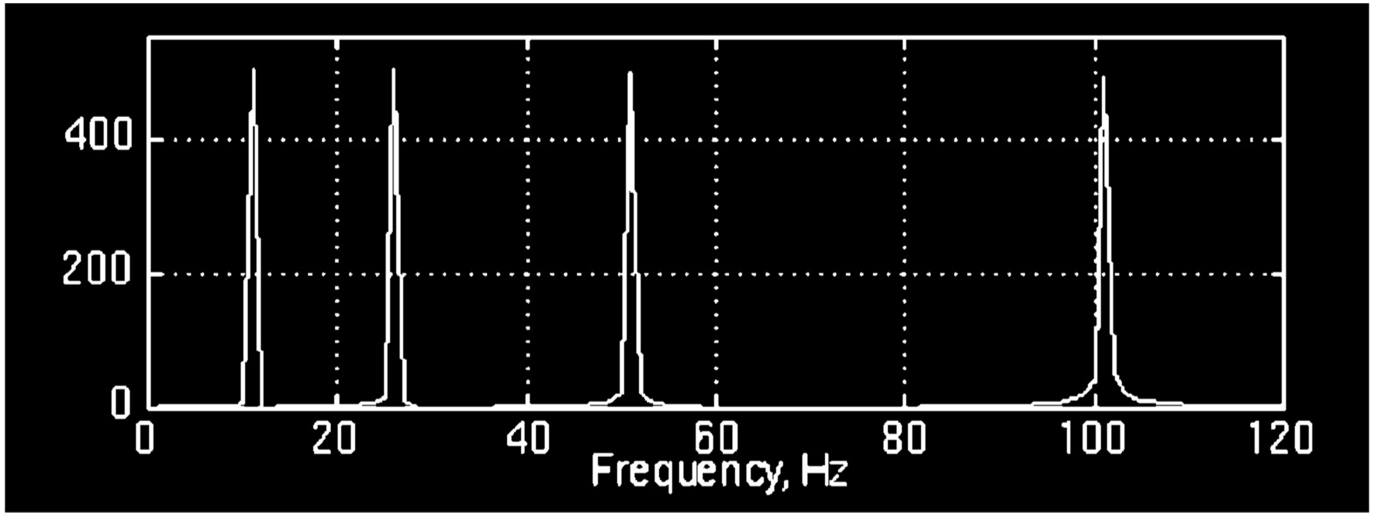
g(ω) is the coefficient of the term of 'frequency' ω

Fourier transform is a change of '**representation**', from **t-space** to **ω-space**. All information is intact!




**Periodic signal f(t)**

*This could be a signal of vibrating floor or an ECG*




**Fourier Transform $g(\omega)$ of f(t)**

**(Spectrum)**

*By taking Fourier transform, we have identified the frequencies and their 'weights' in the signal.*

# General periodic function

$$f(t) = \sum_n c_n e^{i\omega_n t}$$

$$g(\omega) = \int_{-\infty}^{\infty} f(t) e^{-i\omega t} dt = \sum_n c_n \int_{-\infty}^{\infty} e^{-i(\omega - \omega_n)t} dt$$

$$= \sum_n c_n \delta(\omega - \omega_n)$$

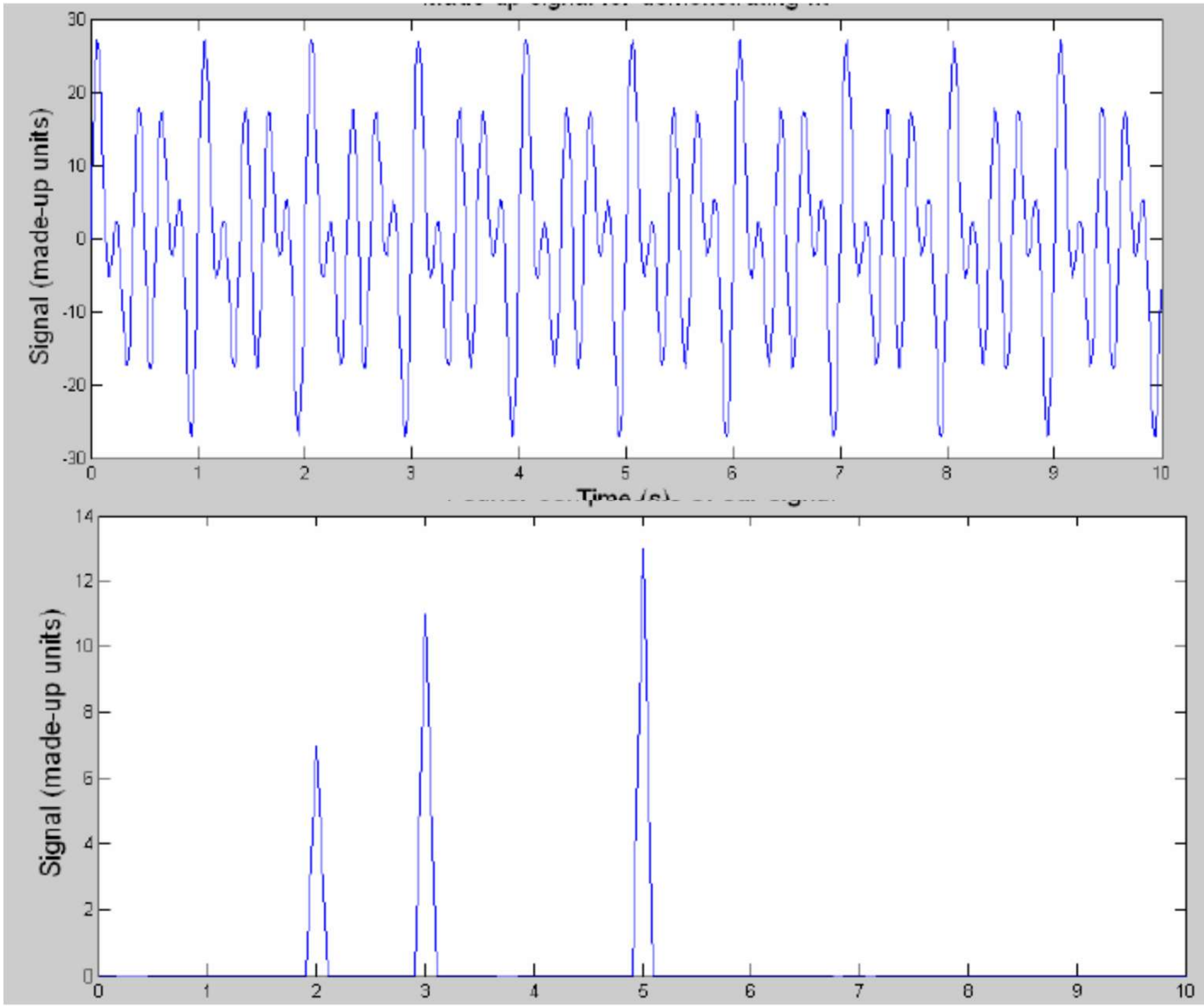
***We recover all frequency components of the signal with appropriate weightages.***

*The operation of Fourier transform has merely* ***transformed*** *f(t) into g($\omega$). No information is lost. From g($\omega$) we can* ***recover*** *f(t) by inverse Fourier transform.*

$$f(t) = 7\sin(2\pi \bullet 2t) + 11\sin(2\pi \bullet 3t) + 13\sin(2\pi \bullet 5t)$$

$f(t)$

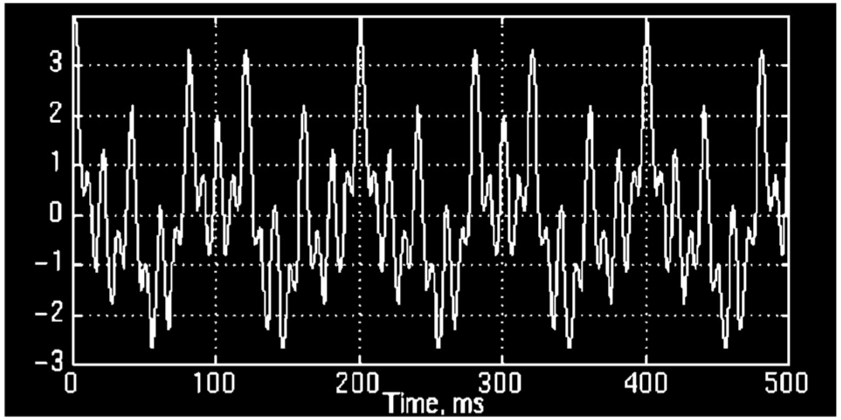
$g(\omega)$

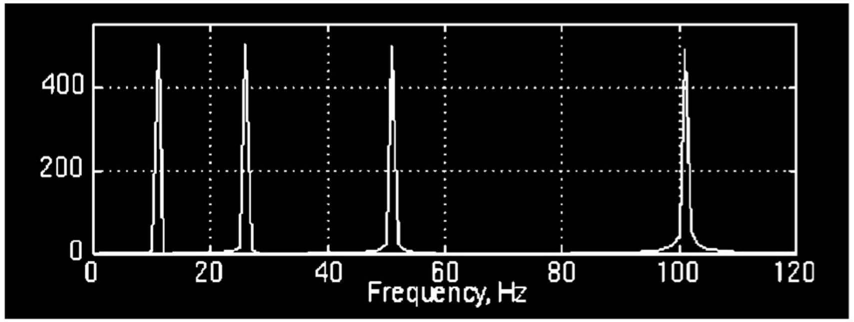


## Advantage#1

***Efficient data representation, interpretation, communication and reconstruction***

*It is easier to describe a given signal in terms of finite frequencies rather than point to point original data.*




*The frequencies carry the all and essential information.*

## Generalization

## Extended to non-periodic functions

$$f(x) \qquad FT[f(x)] = a(k)$$

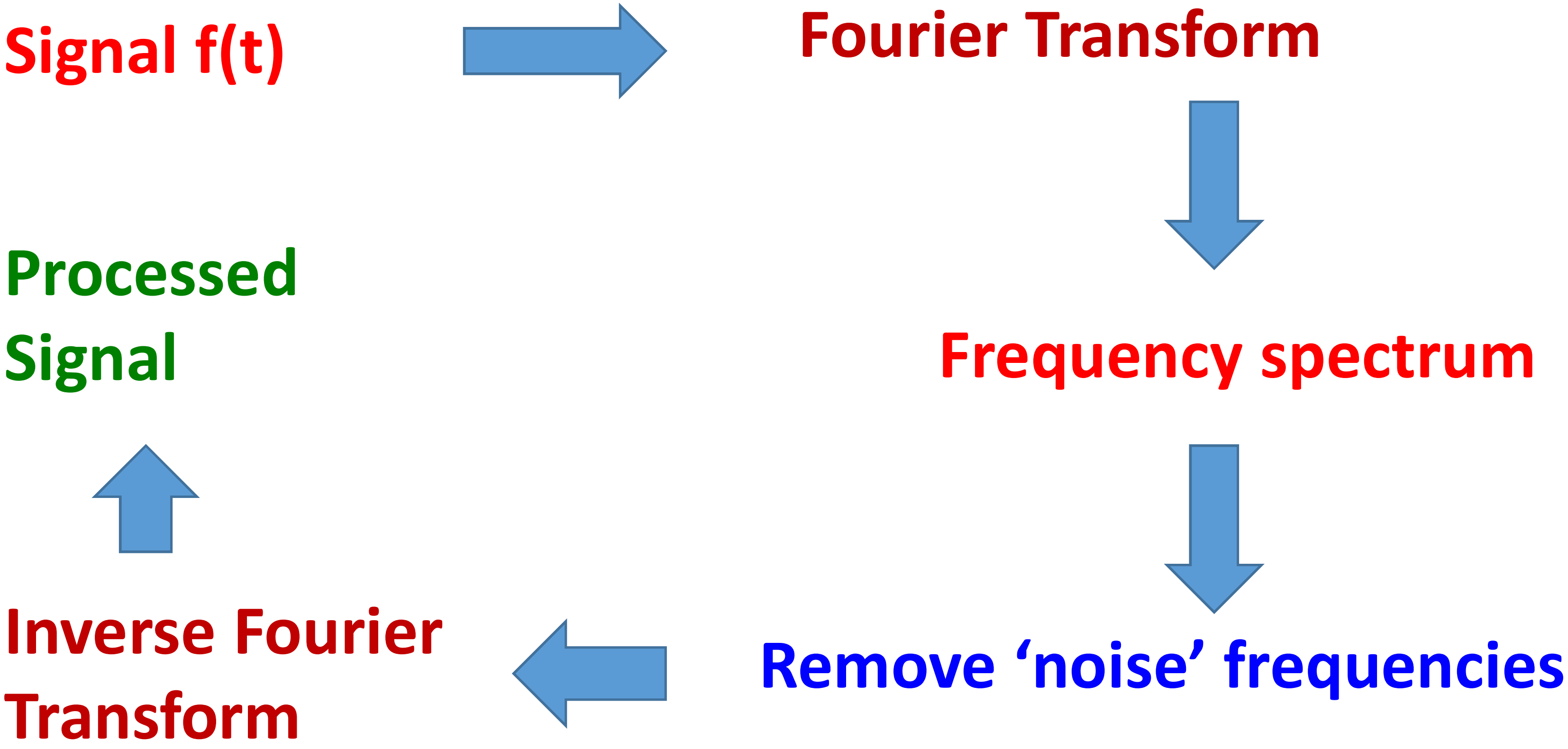
$$FT^{-1}[a(k)] = f(x)$$

***a(k) can also be called as the spectrum of f(x)***

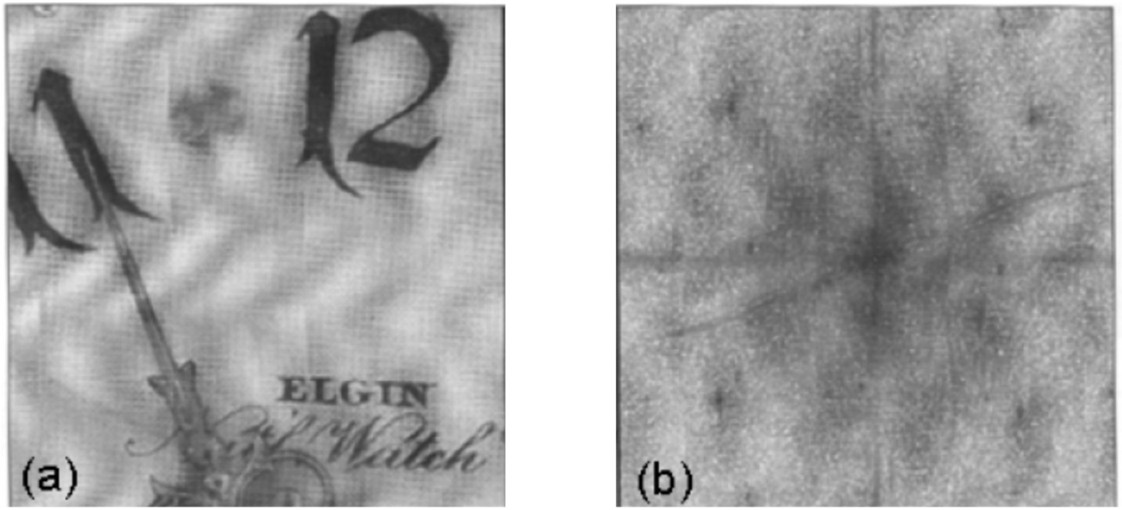
***In Quantum Physics: f(x) is a wave function in coordinate space, a(k) is a wave function in momentum (k) space.***

# Advantage#2

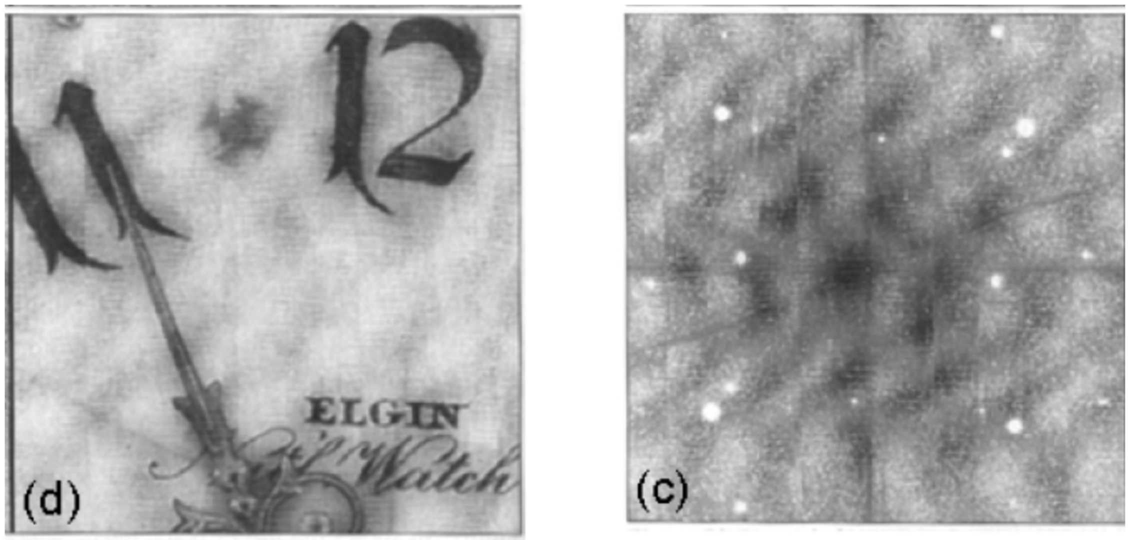
## Signal processing



**Dirty looking photocopied image**



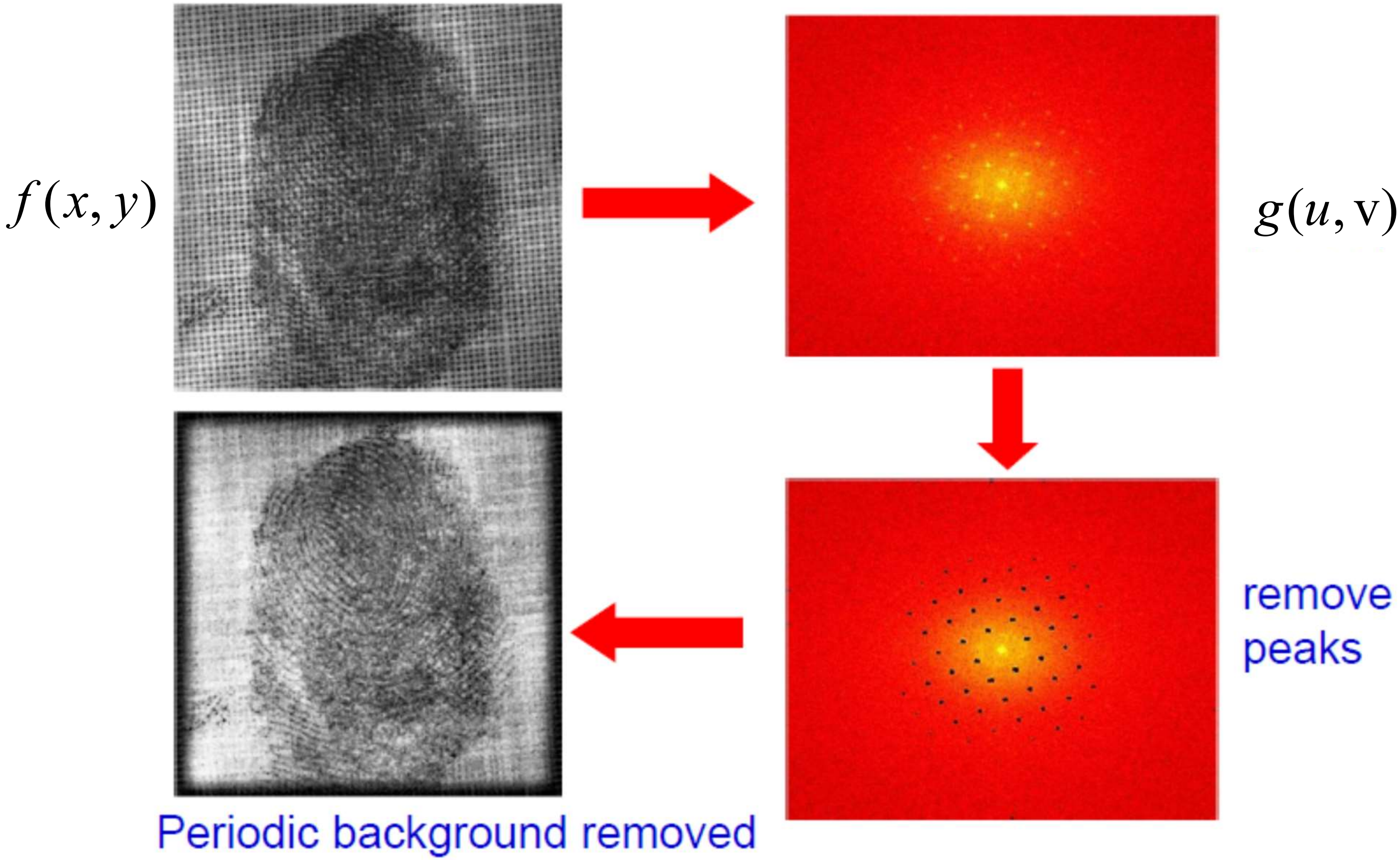

**Fourier transform**



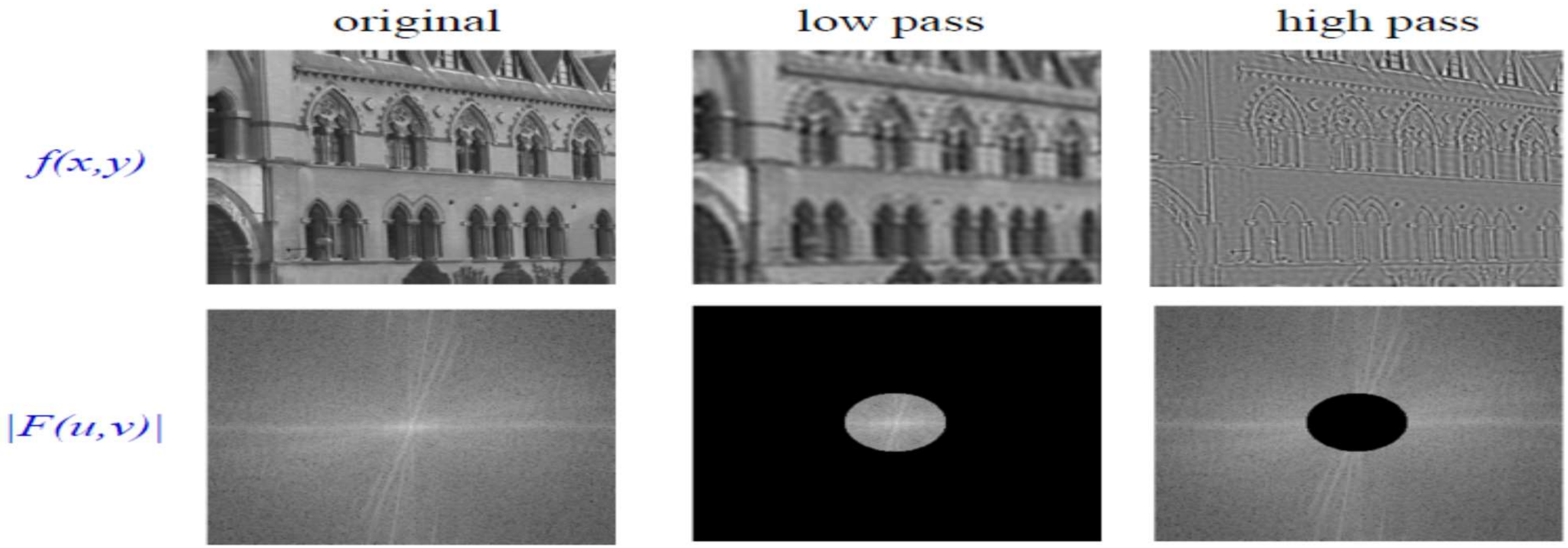

**Remove ‘stars’ and take inverse Fourier transform**

**Dirty spots on the image gone.**

# Example – Forensic application



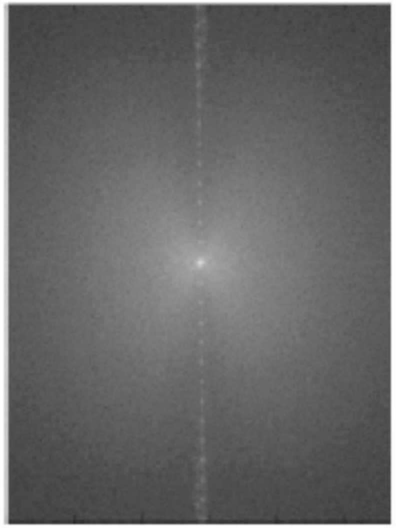
Example: action of filters on a real image



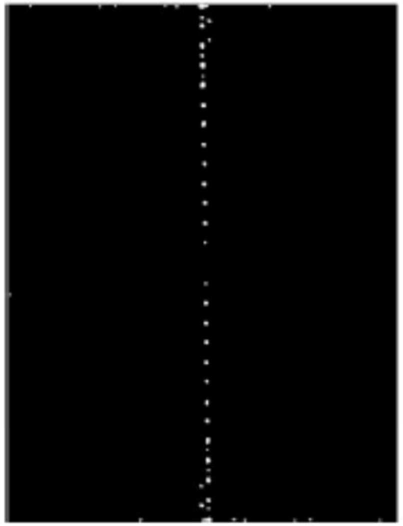

FT [*f(x,y)*] → *g(u,v)* → Remove low/high frequencies → *g'(u,v)* → Inverse FT → **Reconstructed Image**

# Example – Image processing

Lunar orbital image (1966)



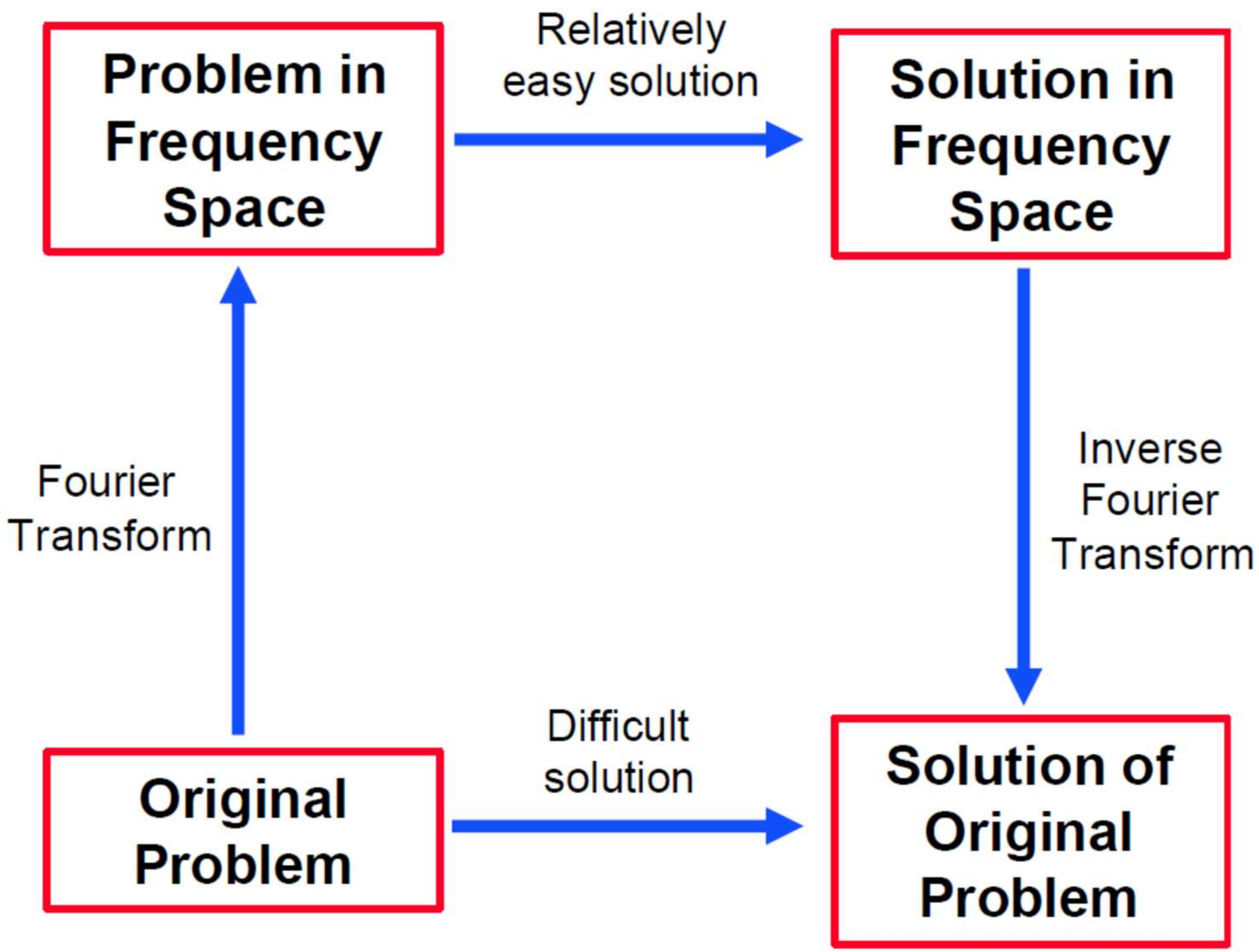
$|F(u,v)|$



remove peaks

join lines removed

# Advantage#3


Problem in Frequency Space
Relatively easy solution
Solution in Frequency Space
Fourier Transform
Inverse Fourier Transform
Original Problem
Difficult solution
Solution of Original Problem

# Solve differential equation

$$\frac{d^2x(t)}{dt^2} - x(t) = -g(t)$$

$$FT\left(\frac{d^2x(t)}{dt^2}\right) - FT[x(t)] = FT[-g(t)]$$

$$X(\omega) = FT[x(t)]$$

$$FT\left(\frac{d^2x(t)}{dt^2}\right) = (i\omega)^2 X(\omega)$$

$$(i\omega)^2 X(\omega) - X(\omega) = -G(\omega)$$

$$X(\omega) = \frac{-G(\omega)}{(i\omega)^2 - 1} = \frac{G(\omega)}{\omega^2 + 1}$$

Solution

$$x(t) = FT^{-1}\left(\frac{G(\omega)}{\omega^2 + 1}\right)$$

**What is important for our course on Quantum Physics**

$$\psi(x) = \int_{-\infty}^{\infty} a(k) e^{ikx} dk$$

***$\psi(x)$ is a wave function in coordinate space, $a(k)$ is a wave function in momentum (k) space.***

***If $a(k)$ is chosen as Gaussian function of width $\sigma_k$ then $\psi(x)$ is a Gaussian function of width $\sigma_x=1/\sigma_k$ .***

$$\sigma_x \sigma_k = 1 \quad \Rightarrow \quad \Delta x \Delta p_x = \hbar$$

***Uncertainty in the wave packet***

***When we calculate uncertainties in $x$ and $p_x$ using $\psi(x)$ and $a(k)$,*** $\Delta x \Delta p_x = \frac{\hbar}{2}$

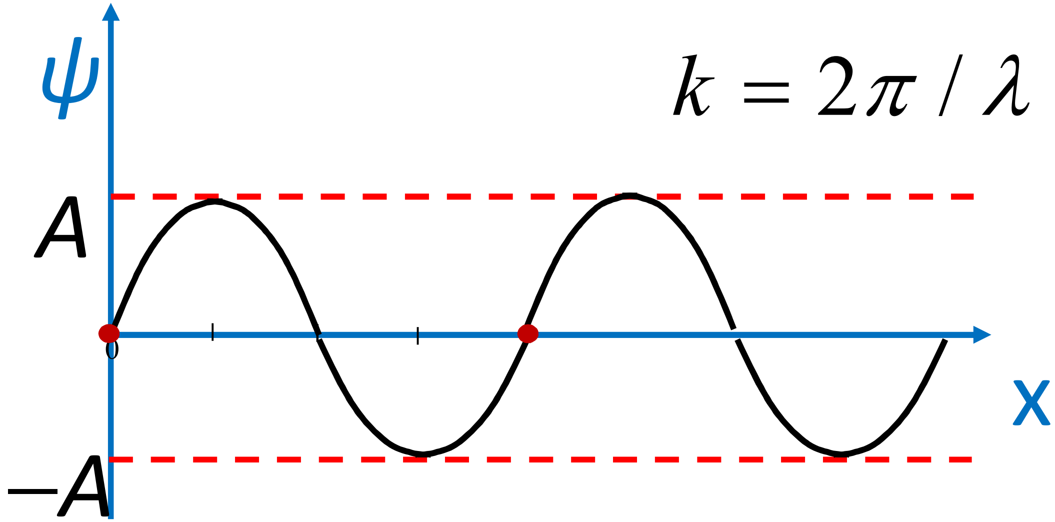
***Heisenberg uncertainty relation***

# Phase Velocity and Group Velocity

We have covered these topics in the class. However, there appear to be some difficulty to some students. Here we sketch the development of the concept. It is a repetition. We re-discuss the concepts. For details refer to the lecture 6,7,8,9.

# Phase Velocity

Consider an ideal wave $\psi = A\sin(kx - \omega t)$




$$k = 2\pi / \lambda$$

$$\omega = 2\pi\nu$$

*k measured in wavenumber*

***Take a point at t = 0 for which ψ = 0. Let time increase to Δt. What would be Δx to maintain ψ = 0.***

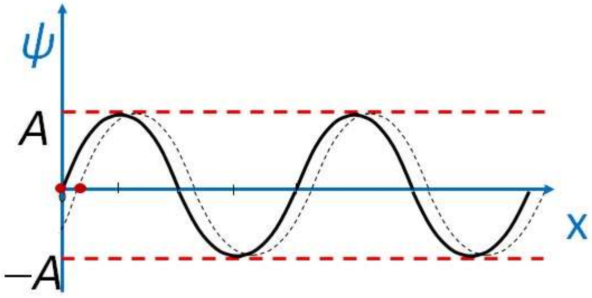
$$k\Delta x - \omega \Delta t = 0$$

$$v_p = \frac{\Delta x}{\Delta t} = \frac{\omega}{k}$$

**Phase Velocity**

***Phase velocity is the velocity of a point of constant phase on the wave.***

# Now consider superposition of two waves

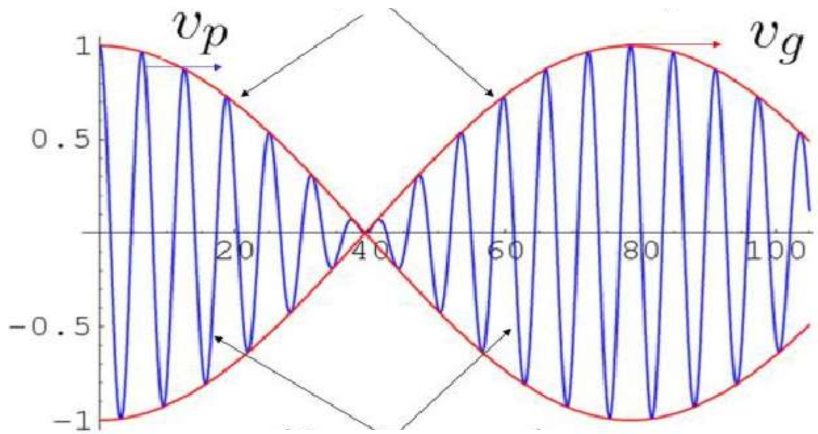



$$\psi_1 = A\sin(kx - \omega t)$$

$$\psi_2 = A\sin[(k + \Delta k)x - (\omega + \Delta\omega)t]$$

$$\psi = \psi_1 + \psi_2 = 2A\sin(kx - \omega t)\cos\left(\frac{\Delta kx}{2} - \frac{\Delta\omega t}{2}\right)$$

$$\cos\left(\frac{\Delta kx}{2} - \frac{\Delta\omega t}{2}\right)$$




$$\sin(kx - \omega t)$$

**Group velocity is the velocity with which the envelope of the wave packet moves.**

$$v_g = \frac{\Delta\omega}{\Delta k} = \frac{d\omega}{dk}$$

**$v_g$ is the velocity with which the wave packet moves.**

***Useful Relations*** $p = \hbar k$ $m = \dfrac{m_0}{\sqrt{1 - \mathrm{v}^2 / c^2}} = \gamma m_0$

$$E = mc^2 = \frac{m_0 c^2}{\sqrt{1 - \mathrm{v}^2 / c^2}} = \gamma m_0 c^2 = \sqrt{p^2 c^2 + m_0^2 c^4}$$

## For a de Broglie wave

### *Wavelength*

$$\lambda = h / p = h / m\mathrm{v}$$

### *Frequency*

$$\nu = E / h = mc^2 / h = \frac{m_0 c^2}{h\sqrt{1 - \mathrm{v}^2 / c^2}} = \frac{\sqrt{p^2 c^2 + m_0^2 c^4}}{h}$$

## Phase velocity

$$v_p = \frac{\omega}{k} = \frac{2\pi\nu}{2\pi/\lambda} = \lambda\nu$$

$$\lambda = h/p = h/m\text{v}$$

$$\nu = E/h = mc^2/h$$

$$v_p = \frac{h}{m\text{v}}\frac{mc^2}{h} = \frac{c^2}{\text{v}}$$

$$\lambda = h/p \qquad p = \hbar k$$

$$\nu = E/h = \frac{\sqrt{p^2c^2 + m_0^2c^4}}{h}$$

$$v_p = \frac{\sqrt{p^2c^2 + m_0^2c^4}}{p} = c\sqrt{1 + \left(\frac{m_0c}{\hbar k}\right)^2}$$

$$v_p = c\sqrt{1 + \left(\frac{m_0c}{\hbar k}\right)^2} = c\sqrt{\frac{p^2 + m_0^2c^2}{p^2}}$$

$$v_p = c\sqrt{\frac{\gamma^2 m_0^2 \text{v}^2 + m_0^2c^2}{\gamma^2 m_0^2 c^2}} = \frac{c^2}{\text{v}}$$

The two formulae for $v_p$ are one and the same. Second formula is useful to see *k* dependence of $v_p$ and therefore dispersion properties of de Broglie waves.

$$v_p = \frac{c^2}{v} \Rightarrow v \neq v_p$$

***The de Broglie wave associated with the particle would leave the particle behind. This is against the wave concept of the particle.***

**Is $v = v_g$?**

$$v_g = \frac{\partial \omega}{\partial k}$$

*Since the wave group is associated with several k*

$$v_g = \frac{d\omega}{dk} \Rightarrow v_g = \left.\frac{d\omega}{dk}\right|_{k_0}$$

***where the derivative is to be evaluated at the central $k_0$.***

## ***Group velocity***

$$\mathrm{v}_p = \frac{\omega}{k}, \quad \mathrm{v}_\mathrm{g} = \frac{d\omega}{dk} \quad \Rightarrow \quad \mathrm{v}_\mathrm{g} = \frac{d}{dk}(k\mathrm{v}_\mathrm{p}) = \left[ \mathrm{v}_\mathrm{p} + k\frac{d\mathrm{v}_\mathrm{p}}{dk} \right]_{k_0}$$

$$\text{since} \;\; \mathrm{v}_\mathrm{p} = c\sqrt{1 + \left(\frac{m_0 c}{\hbar k}\right)^2} \qquad \mathrm{v}_\mathrm{g} = c\left[1 + \left(\frac{mc}{\hbar k_0}\right)^2\right]^{-1/2} = \frac{c^2}{\mathrm{v}_\mathrm{p}\big|_{k_0}}$$

Since $\mathrm{v}_\mathrm{p} = c^2 / \mathrm{v}$ $\qquad \mathrm{v}_\mathrm{g} = \mathrm{v}$

***de Broglie wave group associated with a moving body travels with the same velocity as the body!***

# Dispersion Relations (A general wave group)

**Relation between $\omega$ and *k* is known as dispersion relation.**

**Plot of $\omega$ vs *k* is called the dispersion curve.**

$$\mathrm{v_g} = \frac{d}{dk}(k\mathrm{v_p}) = \left[\mathrm{v_p} + k\frac{d\mathrm{v_p}}{dk}\right]_{k_0} = \left[\mathrm{v_p} - \lambda\frac{d\mathrm{v_p}}{d\lambda}\right]_{\lambda_0}$$

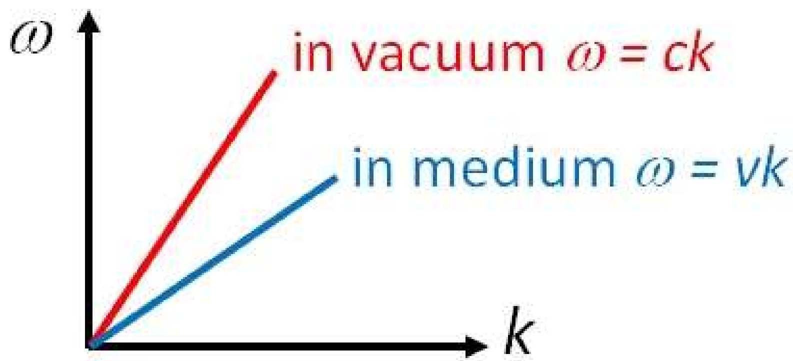
## Non-dispersive medium:

$$d\mathrm{v_p}/dk = 0 \Rightarrow \mathrm{v_g} = \mathrm{v_p}$$

Since $\mathrm{v}_p = \omega / k$,

$$\omega = k\mathrm{v_g} \Rightarrow \omega = k\mathrm{v}$$

## Example: propagation of light in a medium




$$\frac{\omega}{k} = \mathrm{v} = \frac{c}{n_r} = \mathrm{v_p}$$

*$n_r$= Refractive index*

# Dispersion Relations

$$\mathrm{v_g} = \left[ \mathrm{v_p} + k\frac{d\mathrm{v_p}}{dk} \right]_{k_0} = \left[ \mathrm{v_p} - \lambda\frac{d\mathrm{v_p}}{d\lambda} \right]_{\lambda_0}$$

**Non-dispersive medium:**

$$d\mathrm{v_p} / dk = 0 \qquad \mathrm{v_g} = \mathrm{v_p}$$

**Dispersive medium:** $$d\mathrm{v_p} / dk \neq 0 \qquad \mathrm{v_g} \neq \mathrm{v_p}$$

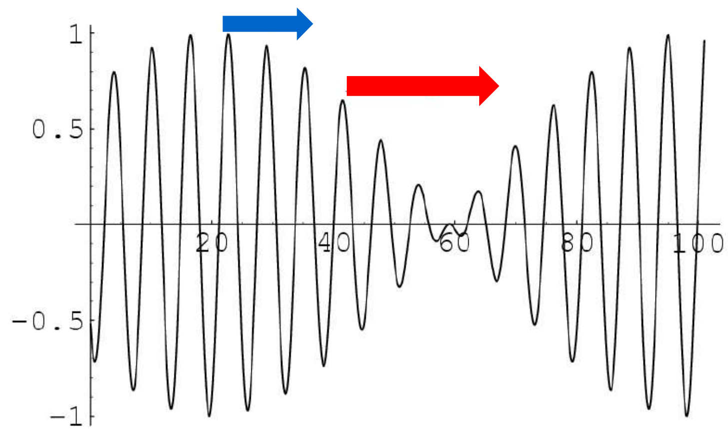
*Dispersive occurs when phase velocity depends on k (or $\lambda$):* $\mathrm{v_p} = c / n_r(\lambda)$

**Normal dispersion**

$$d\mathrm{v_p} / d\lambda > 0$$

$$n_r(red) < n_r(blue), \quad dn_r / d\lambda < 0,$$

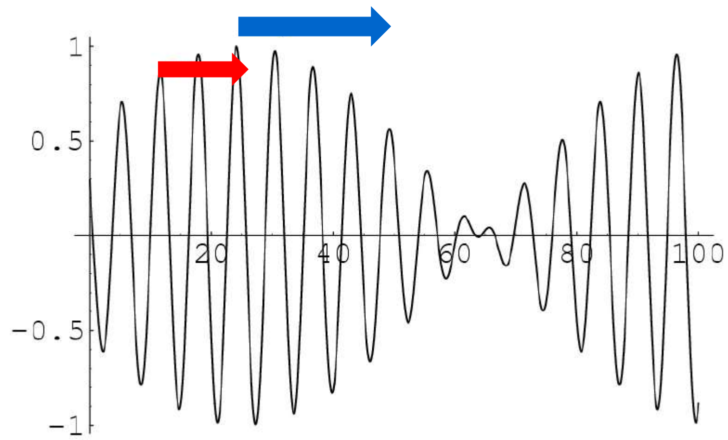
$$\mathrm{v_g} < \mathrm{v_p}$$




**Anomalous dispersion**

$$d\mathrm{v_p} / d\lambda < 0$$

$$\mathrm{v_g} > \mathrm{v_p}$$



## What is the dispersion relation for de Broglie Waves?

$$\mathrm{v_p} = c\sqrt{1+\left(\frac{m_0 c}{\hbar k}\right)^2}$$

$$d\mathrm{v_p}/dk \neq 0 \qquad \frac{\partial \mathrm{v_p}}{\partial k} = -\frac{c}{k}\frac{(m_0 c/\hbar k)^2}{\left[1+(m_0 c/\hbar k)^2\right]}$$

***All media are dispersive for de Broglie wave***

***Is it normal dispersion or anomalous dispersion?***

*Just have a look at the above formula for dv$_p$/dt and decide!*

# De Broglie Wave: Dispersion relation

## ω Vs k relation

$$\mathrm{v}_\mathrm{p} = c\sqrt{1+\left(\frac{m_0 c}{\hbar k}\right)^2} = \frac{\omega}{k}$$

$$\omega = c\sqrt{k^2+\left(\frac{m_0 c}{\hbar}\right)^2}$$

**Nonrelativistic particle**

$$E = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m} = \hbar\omega$$