The physics of Quantum materials

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Office hours: by appointment

Lectures: Tuesday, Thursday 3:50 - 5:10 p.m.
Synchronous on-line lectures via Zoom
Meeting ID: 99841802916
Password: 030852

Course website: http://www.physics.rutgers.edu/ugrad/406
User name: SS406 Password: graphene

- Lecture notes
- Links to textbooks and supplementary material
- Homework assignments and solutions
- Project suggestions

The physics of Quantum materials

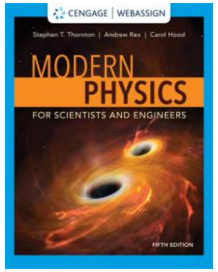
- ***Suggested Textbooks:***
  - C. Kittel, Introduction to Solid State Physics, 8th edition (John Wiley & Sons 2005).
  - S.H. Simon, The Oxford Solid State Basics (Oxford University Press 2013).
  - H. Ibach and H. Luth. Solid-State Physics. 4th edition (Springer 2009)
  - Ashcroft and Mermin, Solid State Physics

- ***Pre-requisites:***

Familiarity with basic principles of quantum mechanics (Schrödinger equation, energy quantization, tunneling, spin, operators). Knowledge of basics of statistical physics (classical statistics, Bose-Einstein and Fermi-Dirac statistics).

- ***Suggested Textbook for reviewing background material***

Modern Physics for Scientists and Engineers 5th Edition, by Thornton, Rex and Hood



The physics of Quantum materials

- ***Grading:***

  30% Homework -Assignments will be due weekly at the beginning of class

  10% In class participation

  10% Projects - A reading project on a selected topic of contemporary solid state physics. An oral presentation(~10slides).

  20%, 30% Exams midterm and a final.

What I do – when not teaching 406

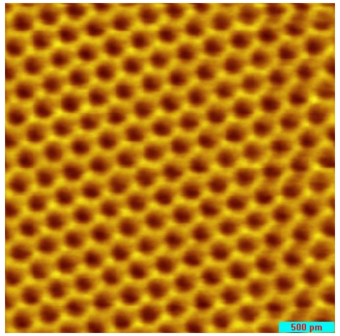
Experimental research in condensed matter physics

http://www.physics.rutgers.edu/~eandrei/

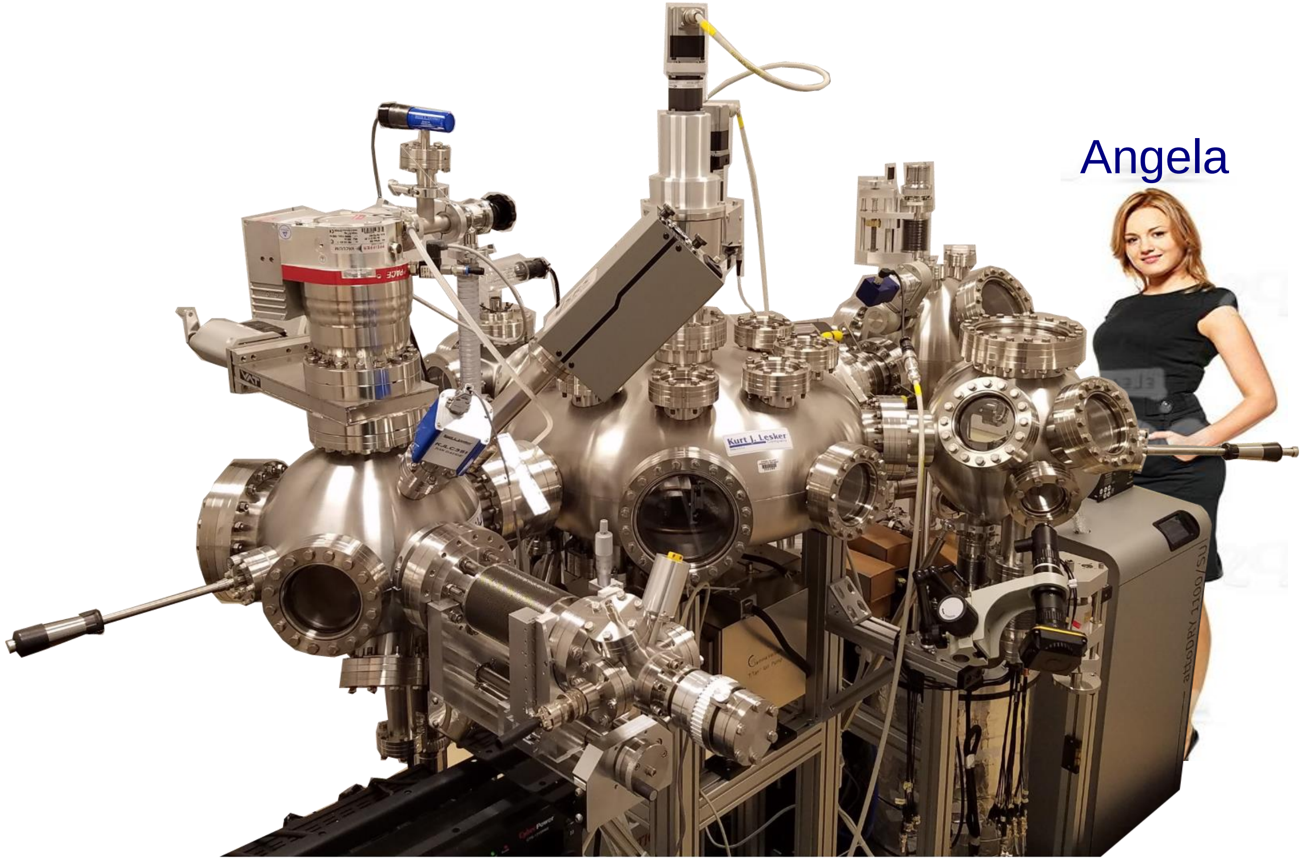
- Scanning tunneling microscope – visualize atoms and electronic wavefunctions in materials

Microscope

Graphene



Angela

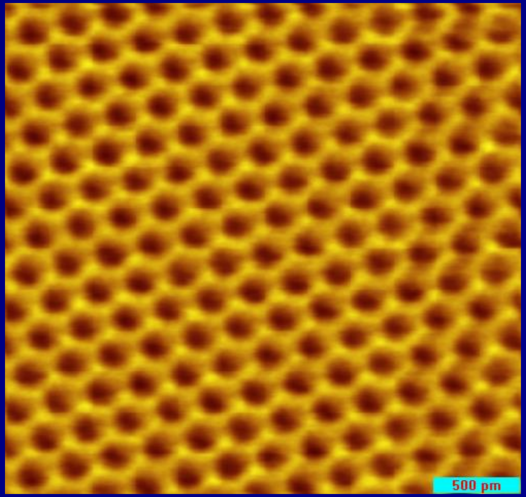


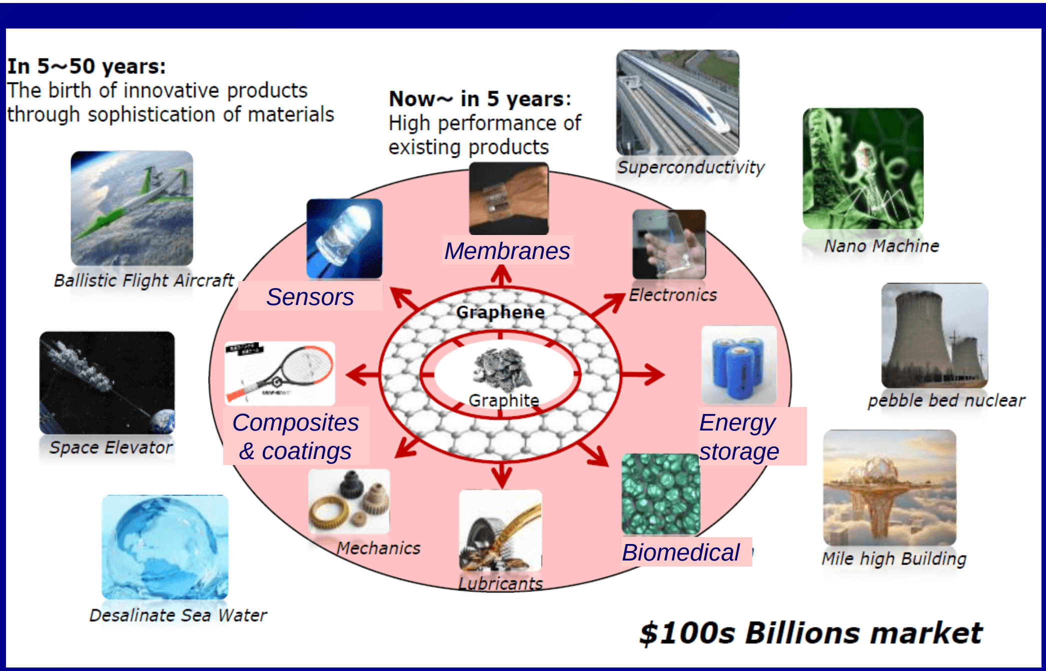
My Research

- Graphene :
- One atom thick crystal
- Carbon atoms arranged in honeycomb structure
- electrons behave like ultra-relativistic massless particles

GRAPHENE SUPERLATIVES

- Strongest material ever measured (200X Stronger than steel)
- Stiffest known material (stiffer than diamond)
- Most stretchable crystal (up to 25% elastically)
- Completely impermeable (even He atoms cannot squeeze through)
- Record thermal conductivity (outperforms diamond)
- Highest current density at room temp (million times that of copper)
- Highest intrinsic mobility (100 times more than in Si)
- Conducts electricity in the limit of no electrons





Students 406-2022


BOERSTOEL, PAUL


SUNG, SEUNG HEE


UGOLOTTI, JOHN


ZHU, YUNHAO

My tasks and yours

My tasks:

- ✓ Provide an introduction to the physics of quantum materials
- ✓ Provide a solid grounding for more advanced courses on the behavior of condensed matter
- ✓ Demonstrate the links with Quantum Mechanics, Thermal and Statistical Physics.
- ✓ Provide the background and tools to understand publications and research articles in this field
- ✓ Inspire you to delve deeper into the subject

Your tasks

- ✓ To learn about the subject.
- ✓ To maximize your performance on homework exams and projects!

How to succeed in this course

- ✓ Attend lectures
  - Ask questions
  - Participate
  - Take notes
- ✓ Outside of class
  - Go over material, asses your understanding
  - Complement class learning with material from on-line resources – textbooks, articles, lectures, etc
  - Think about challenge questions posed in class
  - Solve weekly homework problems
- ✓ Pick your project topic early
  - Scour the literature for background information
  - Pick your favorite article(s) to present
  - Use class learning to shed light on your topic

Condensed Matter Physics (1960-

What is it?

Wikipedia:
Condensed matter physics is the field of physics that deals with the macroscopic and microscopic physical properties of matter, especially the solid and liquid phases which arise from electromagnetic forces between atoms.

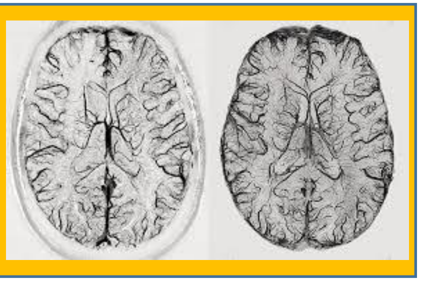
Why study it?

- Because it is the world around us




- Because it is useful

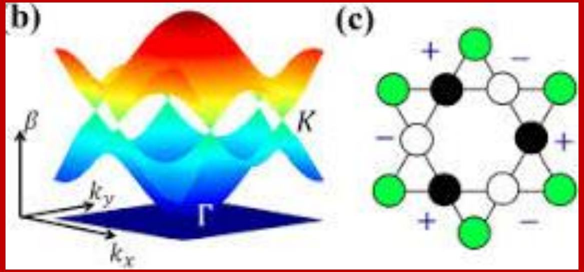


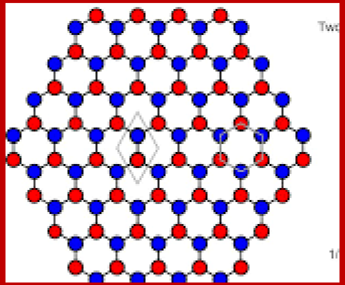



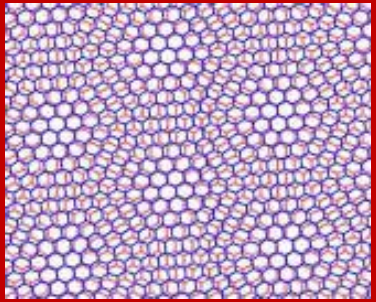
Condensed Matter Physics (1960-

- Because it is Deep and beautiful

Simple principles: Symmetry, topology, geometry
↦ phases of matter – superconductivity, magnetism, superfluidity
↦ fractionally charged, chiral, ultra-relativistic quasi-particles

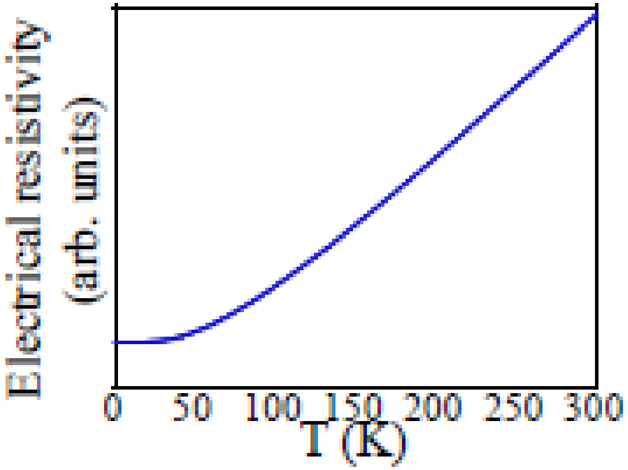




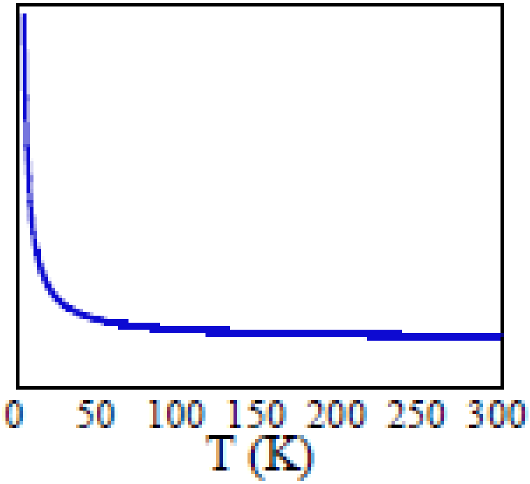


- Because it is a laboratory for realizing and studying quantum mechanics and statistical physics

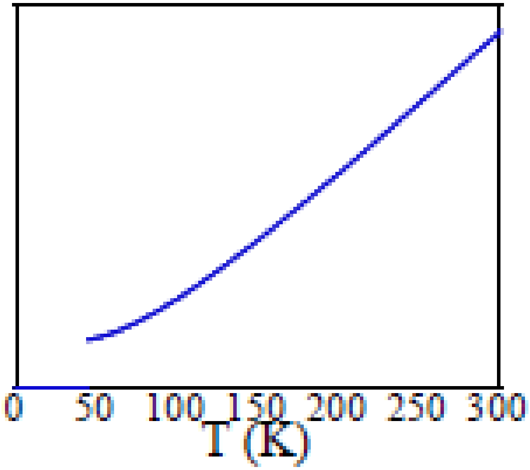
Three states of solid matter as defined by electrical resistivity in the low temperature limit



Metal

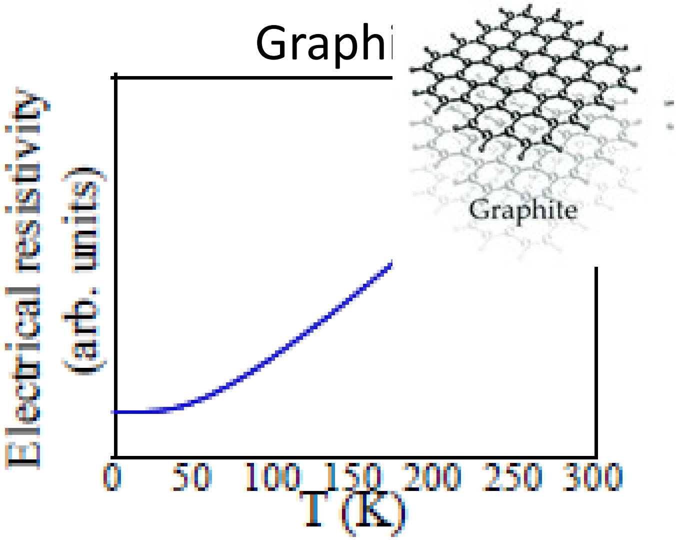


Insulator

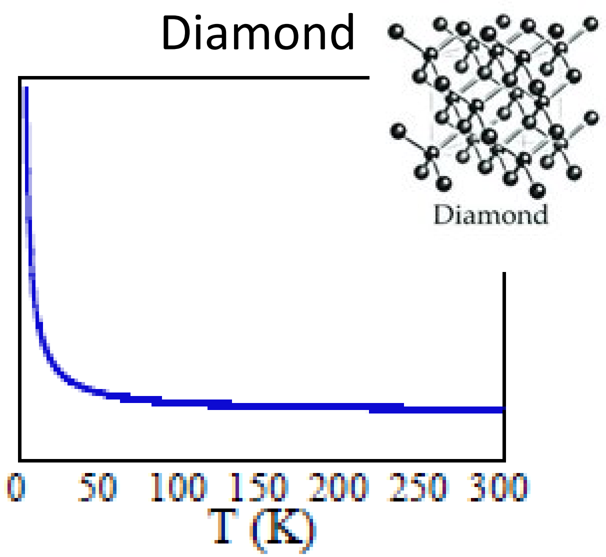


Superconductor

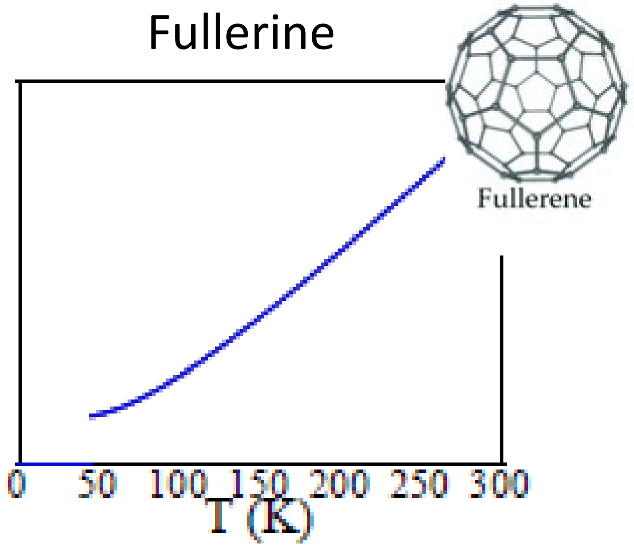
Three states of solid matter as defined by electrical resistivity in the low temperature limit



Metal



Insulator



Superconductor

- Graphite is a metal, diamond an insulator and buckminster-fullerene is a superconductor
- How can this be? After all, they each contain a system of atoms and especially electrons of similar density.
- And the plot thickens: They are all just carbon – arranged in different ways!

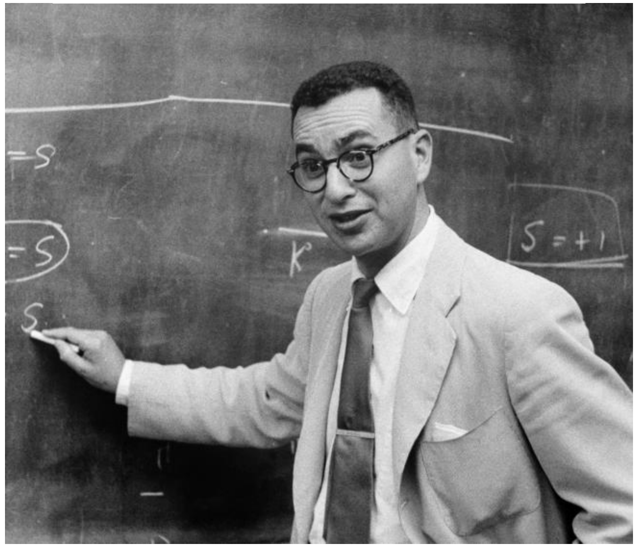
Condensed Matter Physics (1960-

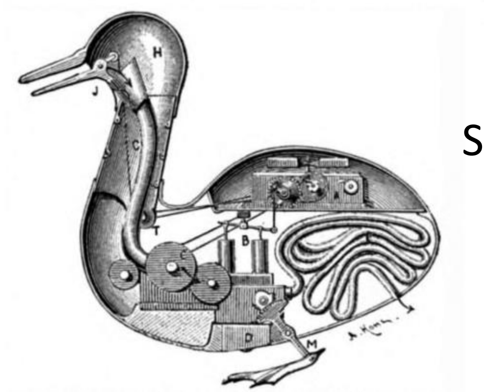
- Because reductionism does not work

water ↦ molecules ↦ atoms
electrons and protons ↦ quarks
quarks ↦ ????.
How does this help me windsurf??

Reductionism vs Emergence

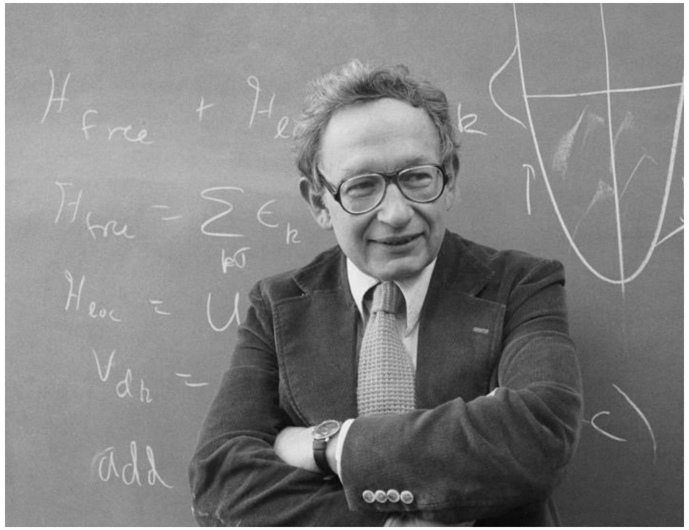
"Squalid state physics"
Murray Gell-Mann
discoverer of the quark
Nobel prize 1969





INTERIOR OF VAUCANSON'S AUTOMATIC DUCK.
A, clockwork; *B*, pump; *C*, mill for grinding grain; *F*, intestinal tube; *J*, bill; *H*, head; *M*, feet.

"More is different"
Philip W. Anderson
Symmetry breaking and 'Anderson-Higgs' mechanism
Nobel prize 1977

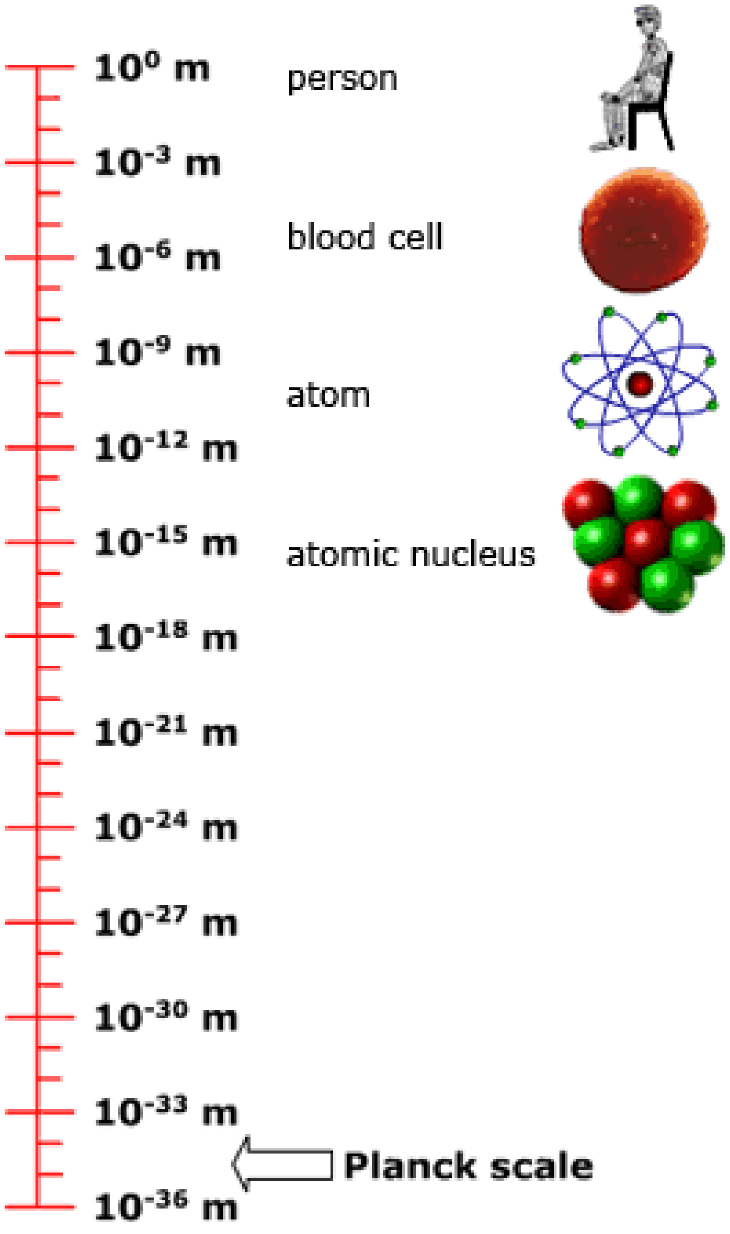


Everything is made of sub-atomic particles. Once you understand the constituent particles and the forces between them
- ➢ the rest is just engineering

Large systems of smaller entities interacting through simple rules can exhibit surprising
- ➢ emergent, collective properties

obeying "higher organizing principles" that cannot be further simplified.

Basic scales



$$k_B T \leftrightarrow eV \leftrightarrow \hbar\omega$$

$$k_B \approx 1.38 \cdot 10^{-23} J/K$$

$$e \approx 1.6 \cdot 10^{-19} C$$

$$\hbar \approx 1.05 \cdot 10^{-34} Js$$

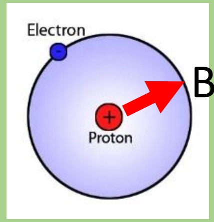
$$1eV \cong 11{,}600K \approx 10^4 K$$

$$1K \sim 0.1meV \sim 20GHz$$

EM interactions are characterized by the fine structure constant:

$$\alpha = e^2/\hbar c = 1/137.$$

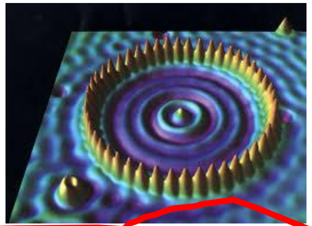
ε_0	Permitivity of free space	8.9x10^{-12} C^2/ N m^2
μ_0	Permeability of free space	4π×10^{-7} H/m
$c = \frac{1}{\sqrt{\varepsilon_0 \mu_0}}$	Speed of light	~3x10^8m/s

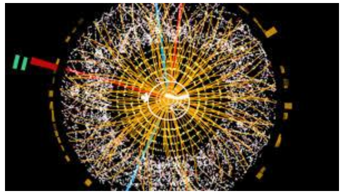


Bohr radius

Bohr radius	$a_B = \frac{\hbar^2}{me^2} \approx 0.5 \cdot 10^{-10} m$
Hartree energy	$\frac{e^2}{a_B} = mc^2\alpha^2 \approx 27eV = 2Ry$

Energy scales






solid state physics

Atomic

Nuclear

high-energy physics
astrophysics and cosmology

10 meV

10 eV

1 MeV

10^{19} GeV

metals
semiconductors
magnets
superconductors
ferroelectrics
……

electrons, cores

atom

phenomenological
particle physics

standard model

GUT

string theory

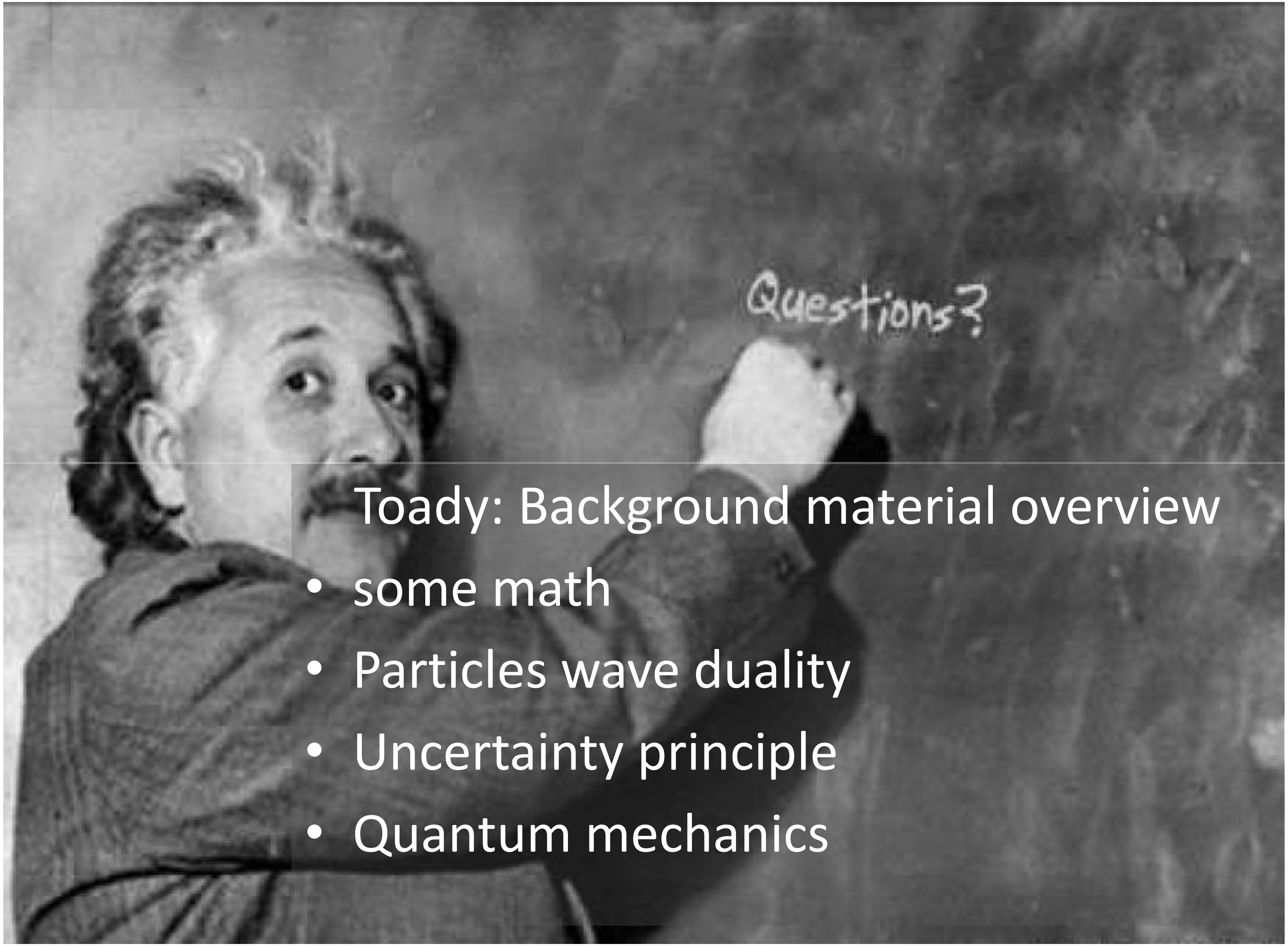
M-theory

effective
models

most fundamental
theory

$$E_{\text{Planck}} = c^2\sqrt{\frac{\hbar c}{G}} \sim 10^{19}\text{GeV}, \qquad l_{\text{Planck}} = \sqrt{\frac{\hbar G}{c^3}} \sim 1.6 \times 10^{-35}\text{m}$$

$G = 6.673 \times 10^{-11}\text{m}^3\text{kg}^{-1}\text{s}^{-2}$ is the gravitational constant



Toady: Background material overview

- some math
- Particles wave duality
- Uncertainty principle
- Quantum mechanics

Math you will need

You should be comfortable with

- exponential notation
- Basic calculus: derivatives, integrals
- Trigonometry
- Complex numbers
- Simple differential equations

Complex numbers

$i \equiv \sqrt{-1}$ $i^2 = -1$

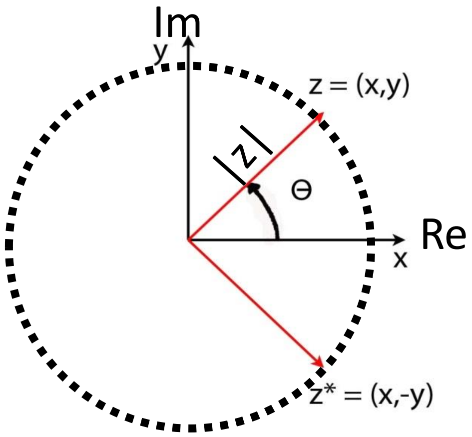
$z = x + i\,y$ (x is **real** *part*; y is **imaginary** *part*)

$z^* = x - i\,y$ *complex conjugate*; replace "i" with "-i"

Magnitude of z:

$$|z|^2 = z^*z$$

$$= (x - iy)(x + iy) = x^2 + ixy - ixy + y^2 = x^2 + y^2$$



$$\mathrm{Re}\,Z = |Z|\cos\theta$$

$$\mathrm{Im}\,Z = |Z|\sin\theta$$

Euler’s Equation

$$\exp(i\theta) = \cos(\theta) + i\sin(\theta)$$

A) I know exactly what this equation means.
B) I think I know what this equation means.
C) I’ve seen it before but am not sure what it means.
D) I’ve never seen this equation before.

Follows from Taylor expansion

$$e^x = \sum_{n=0}^{\infty} \frac{x^n}{n!}$$

$$\cos(x) = \sum_{n=0}^{\infty} (-1)^n \frac{x^{2n}}{(2n)!}$$

$$\sin(x) = \sum_{n=0}^{\infty} (-1)^{2n+1} \frac{x^{2n+1}}{(2n+1)!}$$

$$e^x = 1 + \frac{x}{1!} + \frac{x^2}{2!} + \frac{x^3}{3!} + \cdots$$

$$\cos x = 1 - \frac{x^2}{2!} + \frac{x^4}{4!} - \frac{x^6}{6!} + \ldots$$

$$\sin x = x - \frac{x^3}{3!} + \frac{x^5}{5!} - \frac{x^7}{7!} + \ldots$$

Gradient divergence and curl

$$\boldsymbol{F} = F_1\,\boldsymbol{i} + F_2\,\boldsymbol{j} + F_3\,\boldsymbol{k} = \left\langle F_1, F_2, F_3 \right\rangle$$ Vector

Gradient: $$\nabla = \frac{\partial}{\partial x}\boldsymbol{i} + \frac{\partial}{\partial y}\boldsymbol{j} + \frac{\partial}{\partial z}\boldsymbol{k} = \left\langle \frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z} \right\rangle$$ Vector

Divergence: $$\mathrm{Div} = \nabla \cdot \boldsymbol{F} = \frac{\partial F_1}{\partial x} + \frac{\partial F_2}{\partial y} + \frac{\partial F_3}{\partial z}$$ scalar

$$\mathrm{Curl} = \nabla \times \boldsymbol{F} = \begin{vmatrix} \boldsymbol{i} & \boldsymbol{j} & \boldsymbol{k} \\ \frac{\partial}{\partial x} & \frac{\partial}{\partial y} & \frac{\partial}{\partial z} \\ F_1 & F_2 & F_3 \end{vmatrix}$$ Vector

Differential equations

What is the most general solution to the differential equation:

$$y''(x) = -k^2 \cdot y(x)$$

A) $y(x) = A\cos(kx) + B\sin(kx)$
B) $y(x) = A\exp(ikx) + B\exp(-ikx)$
C) $y(x) = A\exp(kx) + B\exp(-kx)$
D) A & B
E) A & B & C

Important integrals and derivatives

Gaussian integral :

$$\int_{-\infty}^{\infty} e^{-x^2}\,dx = \quad ?$$

Dirac delta:

$$\int_{-\infty}^{\infty} f(x)\delta(x)\,dx = \quad ?$$

What function is equal to its derivative?

- e^x is the only function whose derivative is equal to itself:

$$\frac{d}{dx}y(x) = y(x) \quad \Leftrightarrow \quad y(x) = Ae^x$$

Vector Identities

$$\boxed{\mathbf{a} \times (\mathbf{b} \times \mathbf{c}) = \mathbf{b}(\mathbf{a} \cdot \mathbf{c}) - \mathbf{c}(\mathbf{a} \cdot \mathbf{b})}$$

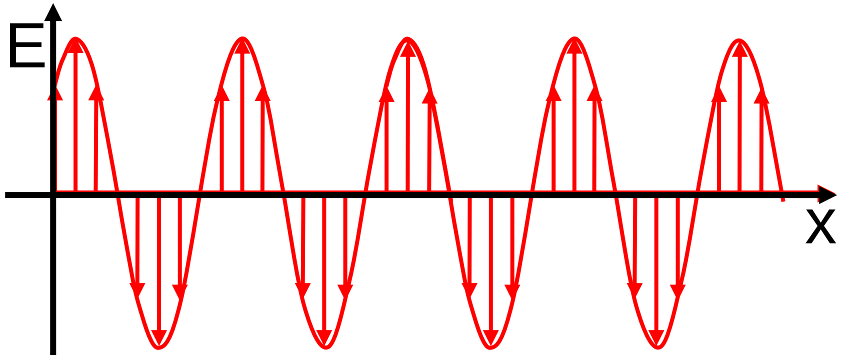
$$\boxed{\nabla \cdot (\nabla \times \mathbf{A}) = 0}$$

$$\boxed{\nabla \times \left(\nabla \cdot \mathbf{A}\right) = 0}$$

https://en.wikipedia.org/wiki/Vector_calculus_identities

Wave equations

Electromagnetic waves:



$$\boxed{\frac{\partial^2 E}{\partial x^2} = \frac{1}{c^2}\frac{\partial^2 E}{\partial t^2}}$$

c=speed of light

Solutions: E(x,t)

Magnitude is non-spatial:
= Strength of electric field

This Differential equation
- Linear
- Homogeneous
- Second order

Wave equations

Solution to the wave equation:

$$\frac{\partial^2 f}{\partial x^2} = \frac{1}{\mathrm{v}^2}\frac{\partial^2 f}{\partial t^2}$$

$$\boxed{\begin{aligned} &f(x,t) = f[\frac{2\pi}{\lambda}(x - vt)] = f[k(x - vt)] \\ &= f(kx - \omega t) = f(kx - 2\pi\nu t) \end{aligned}}$$

$f(x,t) = \text{displacement from equilibrium}$

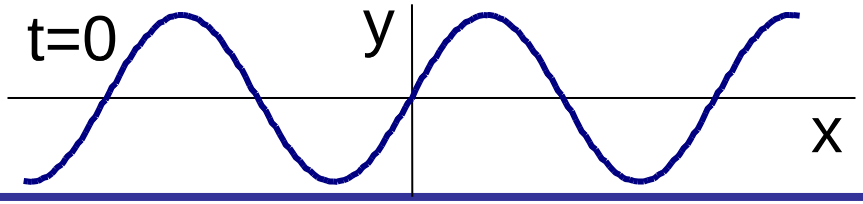
$\mathrm{v} = \text{speed}$

$\lambda = \text{wavelength}; \quad \mathrm{k} = \frac{2\pi}{\lambda} = \text{wavenumber}$

$\nu = \text{frequency}; \quad \omega = 2\pi\nu = \text{angular frequency}$

$$\boxed{\frac{\partial^2 y}{\partial x^2} = \frac{1}{v^2}\frac{\partial^2 y}{\partial t^2}}$$

y(x,t)=Csin(kx-ωt)



What is the wavelength of this wave? Ask yourself …

→How much does x need to increase to increase kx-ωt by 2π?

$\sin(k(x+\lambda) - \omega t) = \sin(kx - \omega t + 2\pi)$

$k(x+\lambda)=kx+2\pi$

$k\lambda=2\pi$ ➔ $k=\underline{2\pi/\lambda}$

k=wave number (radians-m^{-1})

What is the period of this wave? Ask yourself …

→How much does t need to increase to increase kx-ωt by 2π?

$\sin(kx-\omega(t+T)) = \sin(kx - \omega t + 2\pi)$

$\omega T=2\pi$ ➔ $\omega=2\pi/T$

$= 2\pi\nu$

ω= angular frequency

Speed

$$\boxed{v = \frac{\lambda}{T} = \frac{\omega}{k}}$$

Differential equations

What is the most general solution to the wave equation:

$$\boxed{\frac{\partial^2 y}{\partial x^2} = \frac{1}{v^2}\frac{\partial^2 y}{\partial t^2}}$$

A) $y(x,t) = A\cos(kx)\sin\left(\omega t\right) + B\sin(kx)\cos\left(\omega t\right)$

B) $y(x,t) = Ae^{-k(x-vt)} + Be^{-k(x+vt)}$

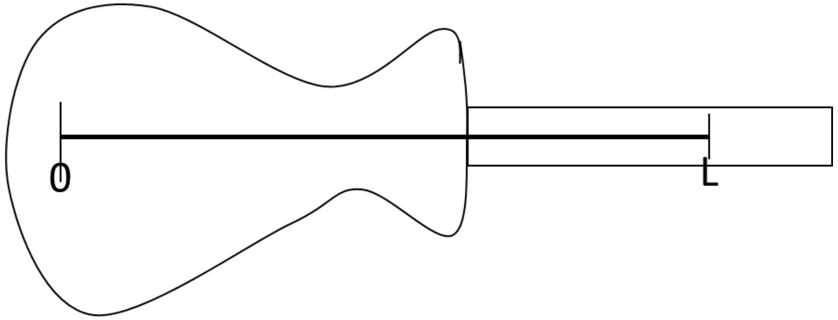
C) $y(x,t) = A\cos k(x-vt) + B\sin k(x-vt)$

D) $y(x,t) = Ae^{-ik(x-vt)} + Be^{-ik(x+vt)}$

E) A, B, C & D

Boundary conditions

$$\boxed{\frac{\partial^2 y}{\partial x^2} = \frac{1}{v^2}\frac{\partial^2 y}{\partial t^2}}$$



Which boundary conditions need to be satisfied?

I. y(x,t) = 0 at x=0 and x=L

y(x,t) = Asin(kx)cos(ωt) +Bcos(kx)sin(ωt)

At x=0:

y = Bsin(ωt) = 0

→ B=0

At x=L:

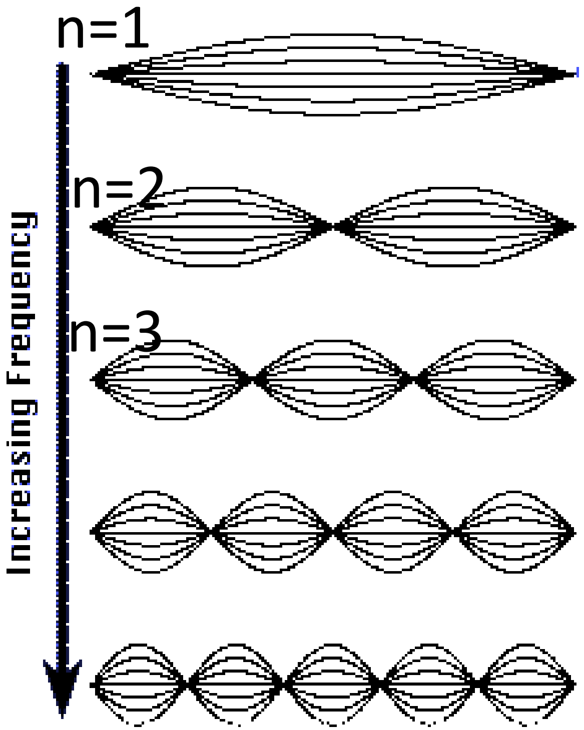
y= Asin(kL)cos(ωt)= 0

→ sin(kL)=0

→ kL = nπ (n=1,2,3, …)

→ k=nπ/L

$$\boxed{y(x,t) = A\sin(n\pi x/L)\cos(\omega t)}$$



Plane Waves

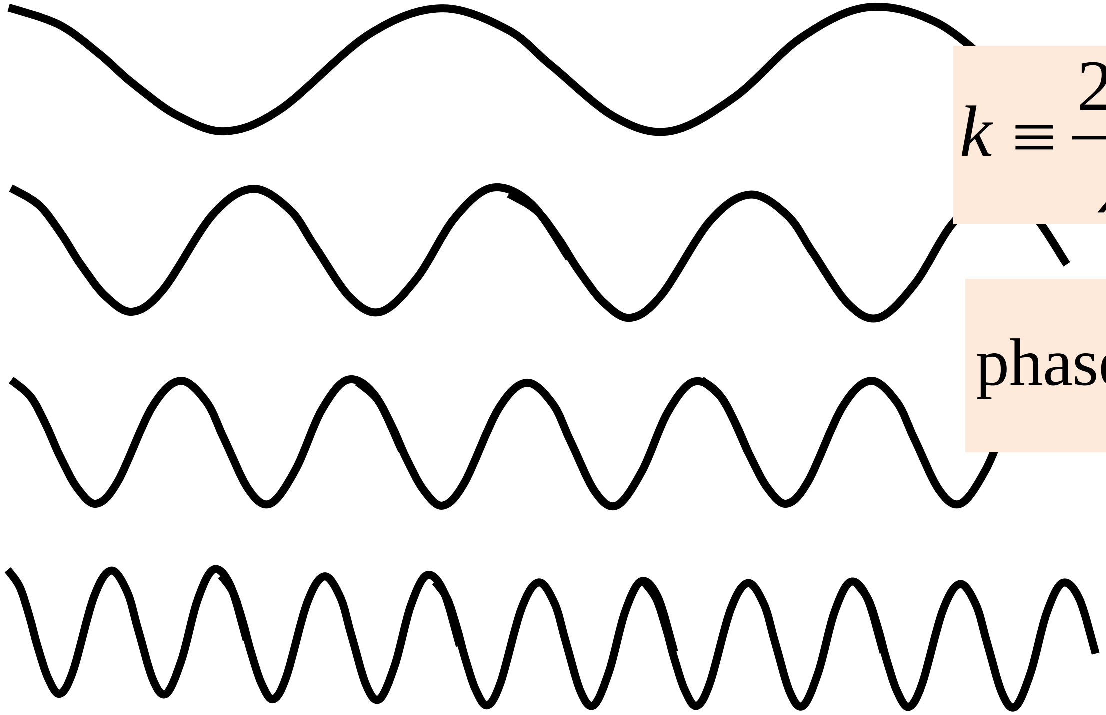
Plane waves (sines, cosines, complex exponentials) extend forever in space:

$$\Psi_1(x,t) = \exp\left[i\left(k_1 x - \omega_1 t\right)\right]$$

$$\Psi_2(x,t) = \exp\left[i\left(k_2 x - \omega_2 t\right)\right]$$

$$\Psi_3(x,t) = \exp\left[i\left(k_3 x - \omega_3 t\right)\right]$$

$$\Psi_4(x,t) = \exp\left[i\left(k_4 x - \omega_4 t\right)\right]$$



$$k \equiv \frac{2\pi}{\lambda} \quad \text{and} \quad \omega = \frac{2\pi}{T}$$

$$\text{phase velocity } \mathrm{v}_{\text{phase}} = \frac{\omega}{k}$$

Principle of Superposition

- If Ψ_1 , $\Psi_2 \ldots \Psi_n$ are solutions of the wave equation (or any homogeneous linear differential equation) then any linear combination $\Psi = \Sigma A_i \Psi_i$ is also a solution.
- When two or more waves traverse the same region, they act independently of each other.
  - Combining two waves yields:

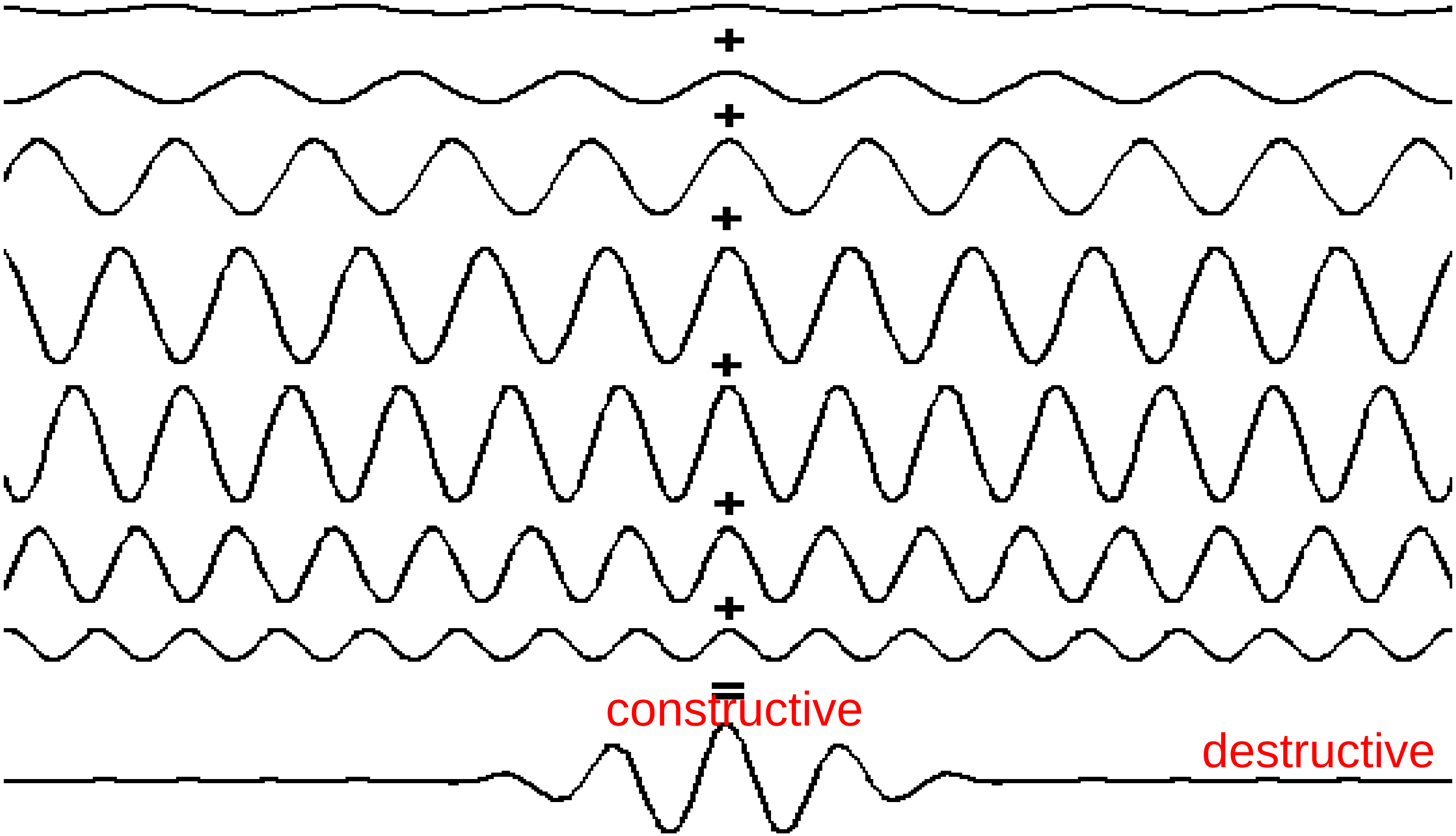
$$\Psi(x,t) = \Psi_1(x,t) + \Psi_2(x,t) = 2A\cos\left(\frac{\Delta k}{2}x - \frac{\Delta\omega}{2}t\right)\cos\left(k_{av}x - \omega_{av}t\right)$$

- We can construct a **"<u>wave packet</u>"** by combining many plane waves of different ω and k's.

$$\Psi(x,t) = \sum_n A_n \exp\left[i\left(k_n x - \omega_n t\right)\right]$$

Wave Packets

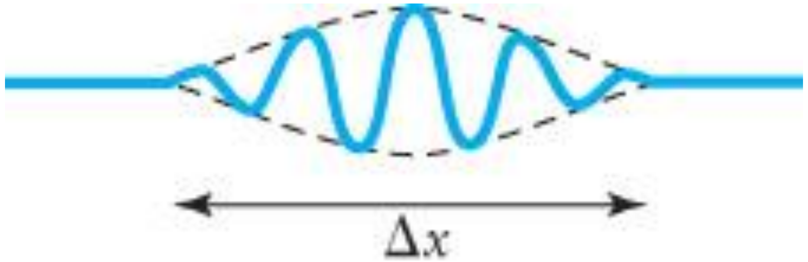
$$\Psi(x,t)=\sum_n A_n \exp\left[i\left(k_n x-\omega_n t\right)\right]$$



constructive

destructive

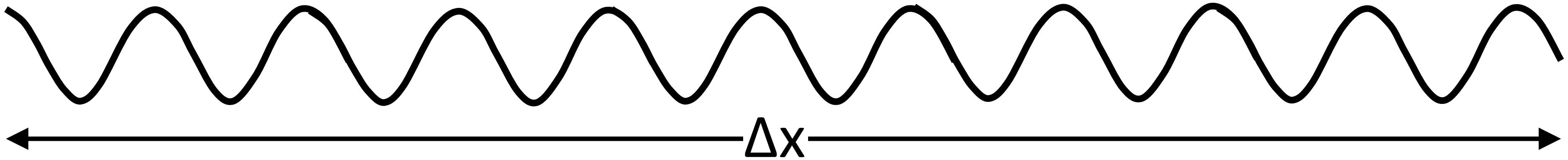
Wave Packet



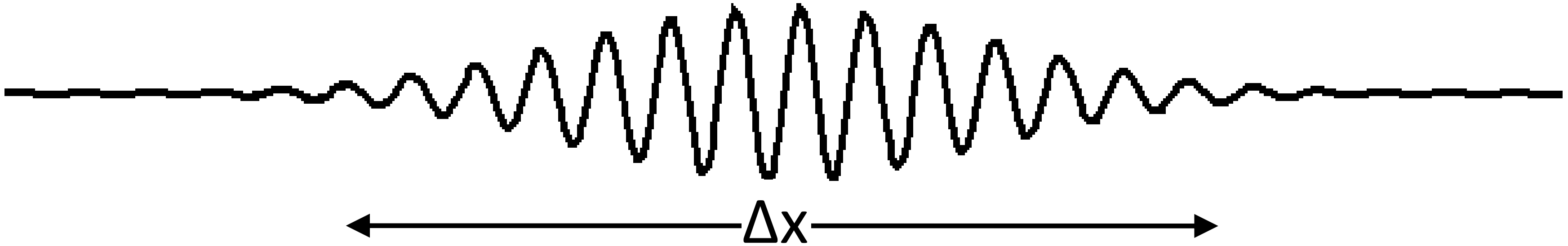
- The combined wave oscillates within an envelope that denotes the maximum displacement of the combined waves.
- The **wave packet** moves at a **group velocity**:

$$u_{\mathrm{gr}} = \frac{\Delta\omega}{\Delta k}$$

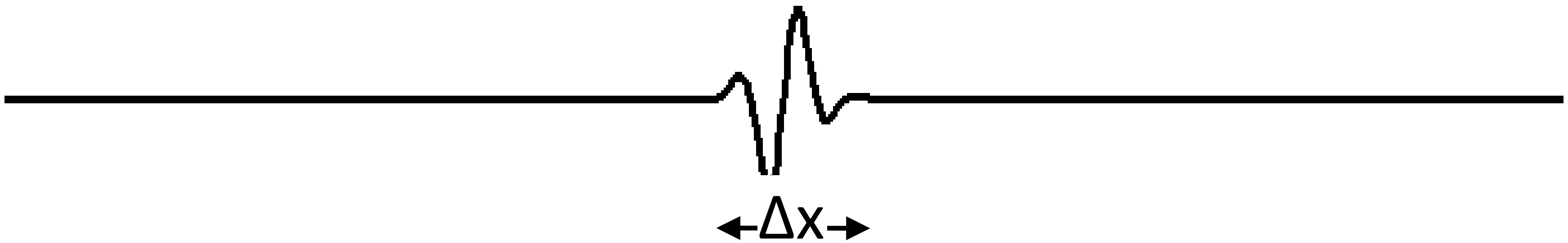
Waves: Uncertainty Principle



small Δk – only one wavelength



medium Δk – wave packet made of several waves



large Δk – wave packet made of lots of waves – small Δx :narrow packet

$$\Delta x \Delta k \geq 1/2$$

Fourier series

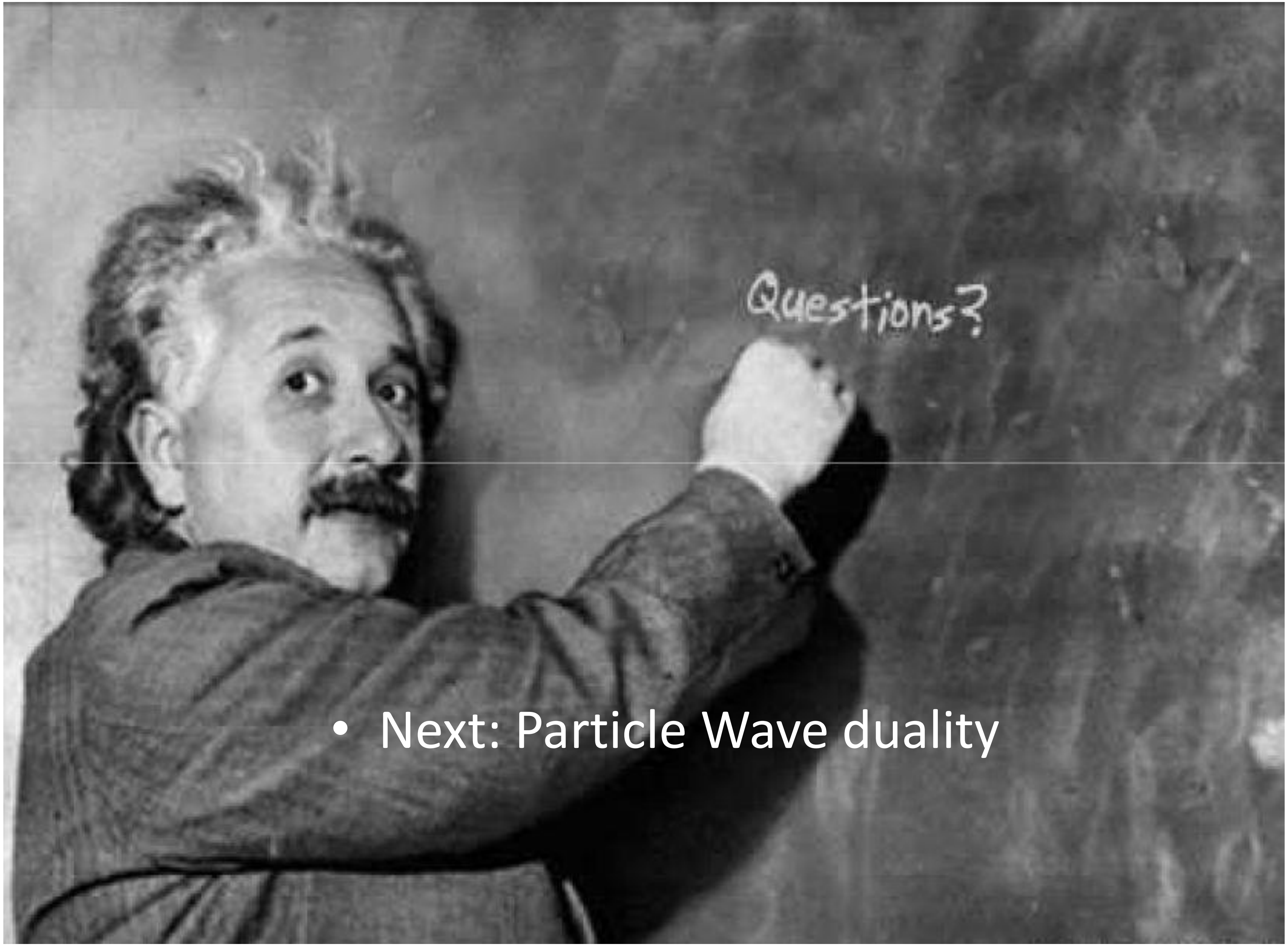
- The sum of many waves that form a wave packet is called a **Fourier series:**

$$\Psi\left(x,t\right)=\sum_{i}A_i\cos\left(k_ix-\omega_it\right)$$

- If k is a continuous variable, then summing the waves gives the Fourier integral:

$$\Psi(x,t)=\int A(k)\cos(kx-\omega t)\,dk$$

More later in the course



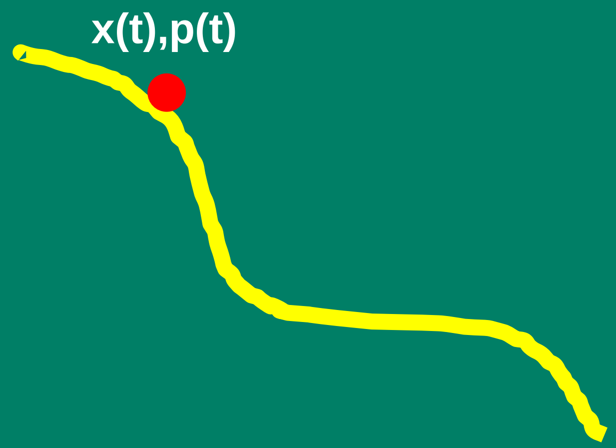
- Next: Particle Wave duality

Waves and Particles

In classical mechanics wave and particle behavior is mutually exclusive.

Particles

- Well defined momentum and position **x(t),p(t)**
- Motion determined by Newton’s laws

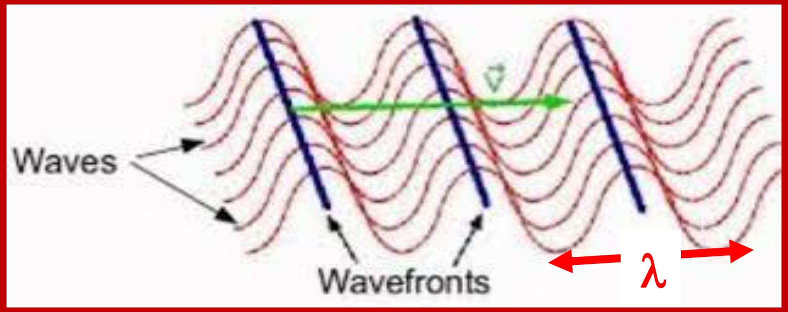


Waves

- Described by a function of position and time f(x,t)
- Motion determined by wave equation

$$\frac{\partial^2 f}{\partial x^2} = \frac{1}{\mathrm{v}^2}\frac{\partial^2 f}{\partial t^2}$$

$$f(x,t) = f(kx - \omega t)$$



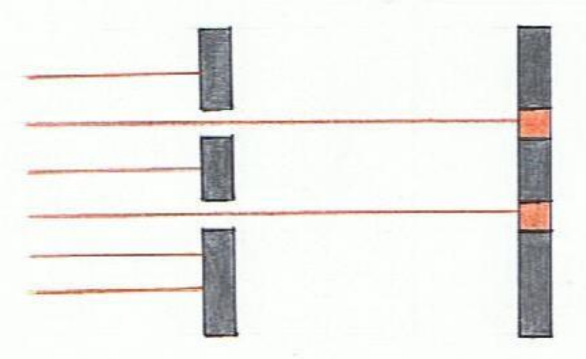
$$\Delta x \Delta k \geq 1/2$$

Waves and Particles

Example: Double slit experiment.

Particles

- Well defined momentum and position **x(t),p(t)**
- Motion determined by Newton’s laws

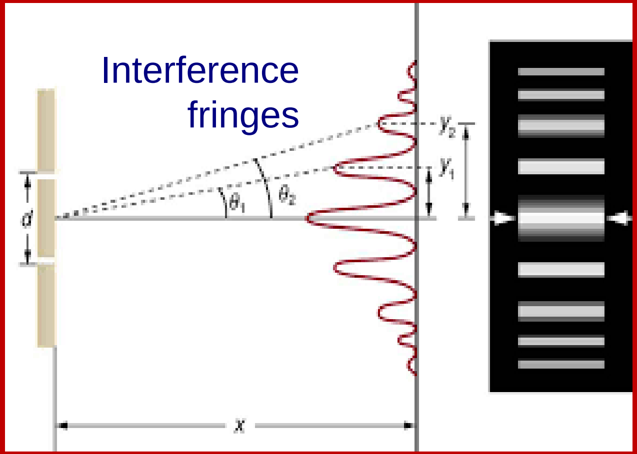


A stream of particles (small balls) is incident on a screen with two slits.

The particles will hit the wall directly behind the holes in the screen.

Waves

- Described by a function of position and time f(x,t)
- Motion determined by wave equation



A monochromatic wave with wavelength λ is incident on two narrow slits.

Bright and dark bands (fringes), form by constructive and destructive interference of the wave passing through the two slits.

Superposition principle.

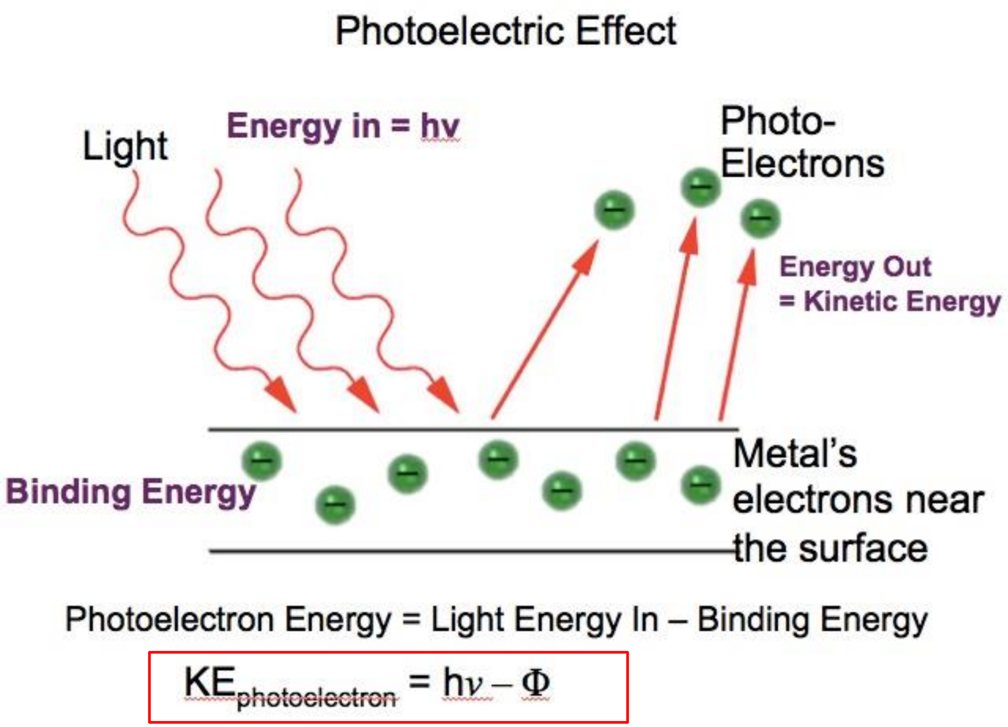
Bright :

$$d\sin\theta = n\lambda \quad n = 0,\pm1,\pm2..$$

PHOTON: Particle manifestation of electromagnetic wave

At the atomic scale both wave and particle behavior are possible for the same object.

Light “Particles”



Photoelectron Energy = Light Energy In – Binding Energy

$KE_{photoelectron} = h\nu - \Phi$

Planck Constant
$h = 6.626 \times 10^{-34}$ J-s

Matter Waves

- The **wave nature** of light is revealed by interference
- **The particle nature** by the fact that light is detected as quanta: “photons”.

Photon energy and momentum :

$$\boxed{E = h\nu \quad \text{and} \quad p = h/\lambda}$$

Louis de Broglie (1923) proposed that **particles also behave as waves**;

with frequency and wavelength given by :

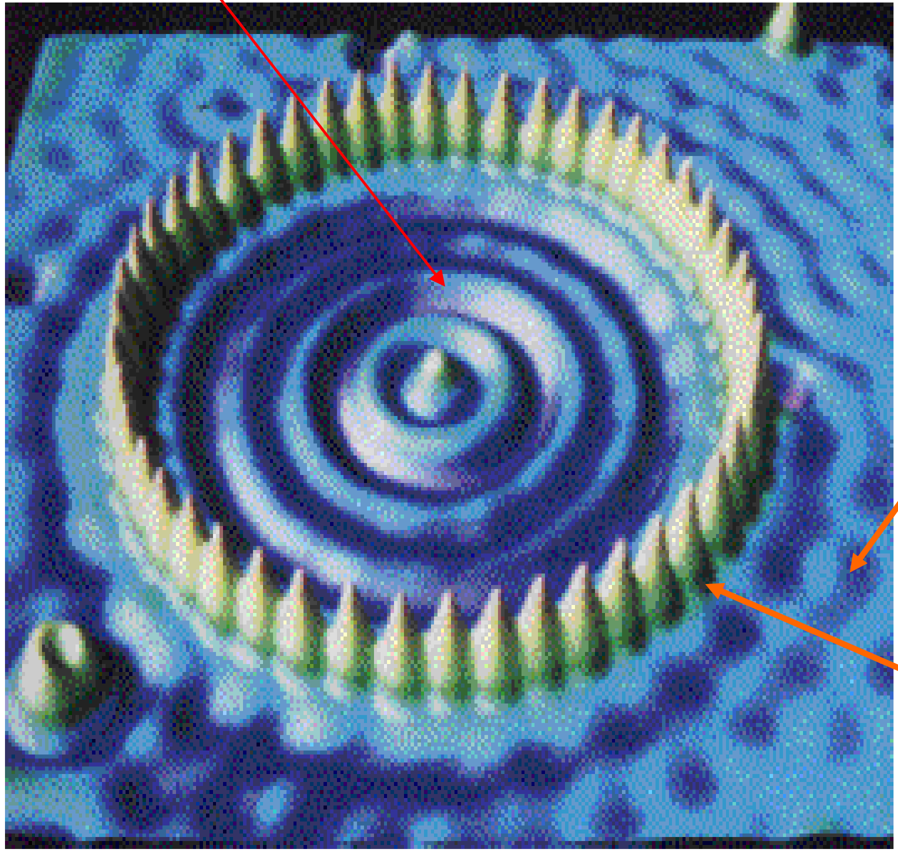
$$\boxed{\begin{array}{l} \nu = E/h \\ \lambda = h/p \end{array}}$$

De Broglie wavelength

Observation of an electron wave "in a box"

Image taken with a scanning tunneling microscope (more later)
(Note: the color is not real! – it is a representation of the electrical current observed in the experiment)

Real <u>standing waves</u> of electron density in a "quantum corral"



Cu

Single atoms (Fe)

IBM Almaden

Convenient Units for Quantum Mechanics

Because most of the applications we will consider involve atoms,
it is useful to use units appropriate to those objects.

We will express wavelength in nanometers (nm).

energy in electron volts (eV).

1 eV = energy an electron gains moving across a one volt potential difference:

1 eV = (1.6 x 10^{-19} Coulomb)(1 volt) = 1.6 x 10^{-19} Joules.

→ h = 4.14 x 10^{-15} eV-s,
hc = 1240 eV-nm.

$$\boxed{E_{photon} = \frac{hc}{\lambda} = \frac{1240}{\lambda} eV}$$

E_{photon} in electron volts

λ in nanometers

Example: A red photon with λ = 620 nm has E =?

Exercise: Wavelengths of Various Particles

Which of these “particles” have the shortest wavelength:

a. an electron that has been accelerated from rest across a 3-Volt potential difference ($m_e = 9.11 \times 10^{-31}$ kg).

b. A proton with the same energy ($m_p = 1.67 \times 10^{-27}$ kg).

[✓ c.] A ball with the same energy ($m_{baseball} = 0.15$ kg).

$$p = \sqrt{2mE} \Rightarrow \lambda = \frac{h}{\sqrt{2mE}}$$

E is the same.

Mass is bigger ⇒ λ smaller.

Solution: Wavelengths of Various Particles

Which of these “particles” have the shortest wavelength

a. an electron that has been accelerated from rest

across a 3-Volt potential difference ($m_e = 9.11\times10^{-31}$ kg).

b. A proton with the same energy ($m_p = 1.67\times10^{-27}$ kg).

c. A ball with the same energy ($m_{baseball} = 0.15$ kg).

$$p = \sqrt{2mE} \Rightarrow \lambda = \frac{h}{\sqrt{2mE}}$$

E is the same.

Mass is bigger $\Rightarrow \lambda$ smaller.

a. $E = e\cdot V = 4.8\times10^{-19}$ J

$p = \sqrt{(2m_eE)} = 9.35\times10^{-25}$ kg m/s $\quad \lambda = h/p = 7.1\times10^{-10}$ m = 0.7nm

b. $p = \sqrt{(2m_pE)} = 4.00\times10^{-23}$ kg m/s $\quad \lambda = h/p = 1.7\times10^{-2}$ nm

c. $p = mv = 3.9\times10^{-9}$ kg m/s $\quad \lambda = h/p = 1.5\times10^{-16}$ nm

QM wave effects are negligible in the motion of macroscopic objects. 10^{-16} nm is smaller than the size of a nucleus

Energy momentum relation

Everything

$E = h\nu = \hbar\omega$

$p = h/\lambda$

Reduced planck constant $\hbar \equiv \dfrac{h}{2\pi} \sim 10^{-34}\, J \cdot s$

Why do we use different formulas for energy-momentum relation?

Photons (v=c)

$E = pc$

Slow Matter (v << c)

$KE = p^2/2m$

Remember Special Relativity

Theory of Relativity

A stationary particle (p=0) has rest energy

$$E = mc^2$$

A particle in motion is described by the relativistic dispersion relation:

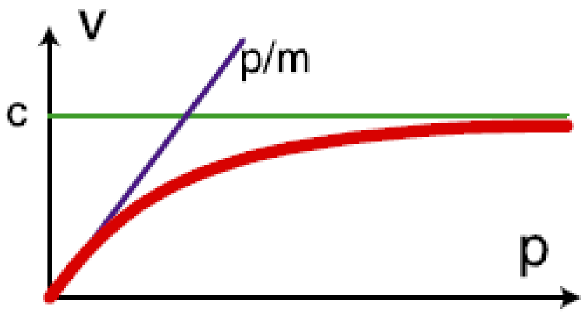
Total energy $$E = \sqrt{(mc^2)^2 + (cp)^2}$$

Albert Einstein 1879-1955

Velocity momentum relation

Velocity:

$$v = \frac{\partial E}{\partial p} = c\frac{cp}{\sqrt{(mc^2)^2 + (cp)^2}}$$



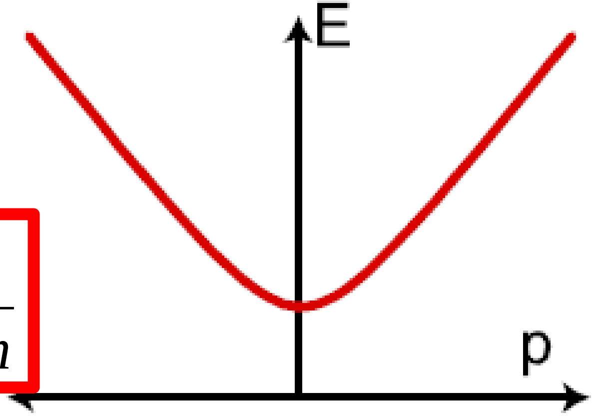
Remember Special Relativity

Massive Particle (e.g. electron)

$$E = \sqrt{(mc^2)^2 + (cp)^2}$$

Nonrelativistic limit (v<<c)

$$E \approx mc^2 + \frac{p^2}{2m} + \ldots \quad \boxed{\Rightarrow KE \sim \frac{p^2}{2m}}$$

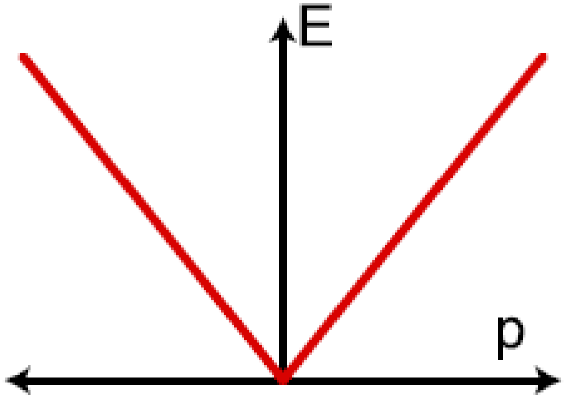


Massless Particle (e.g. photon)

$$m = 0$$

$$E = c\,|\,p\,|$$

$$\mathrm{v} = c$$



Summary of L1

- Math background
- Particle-wave duality

Next time

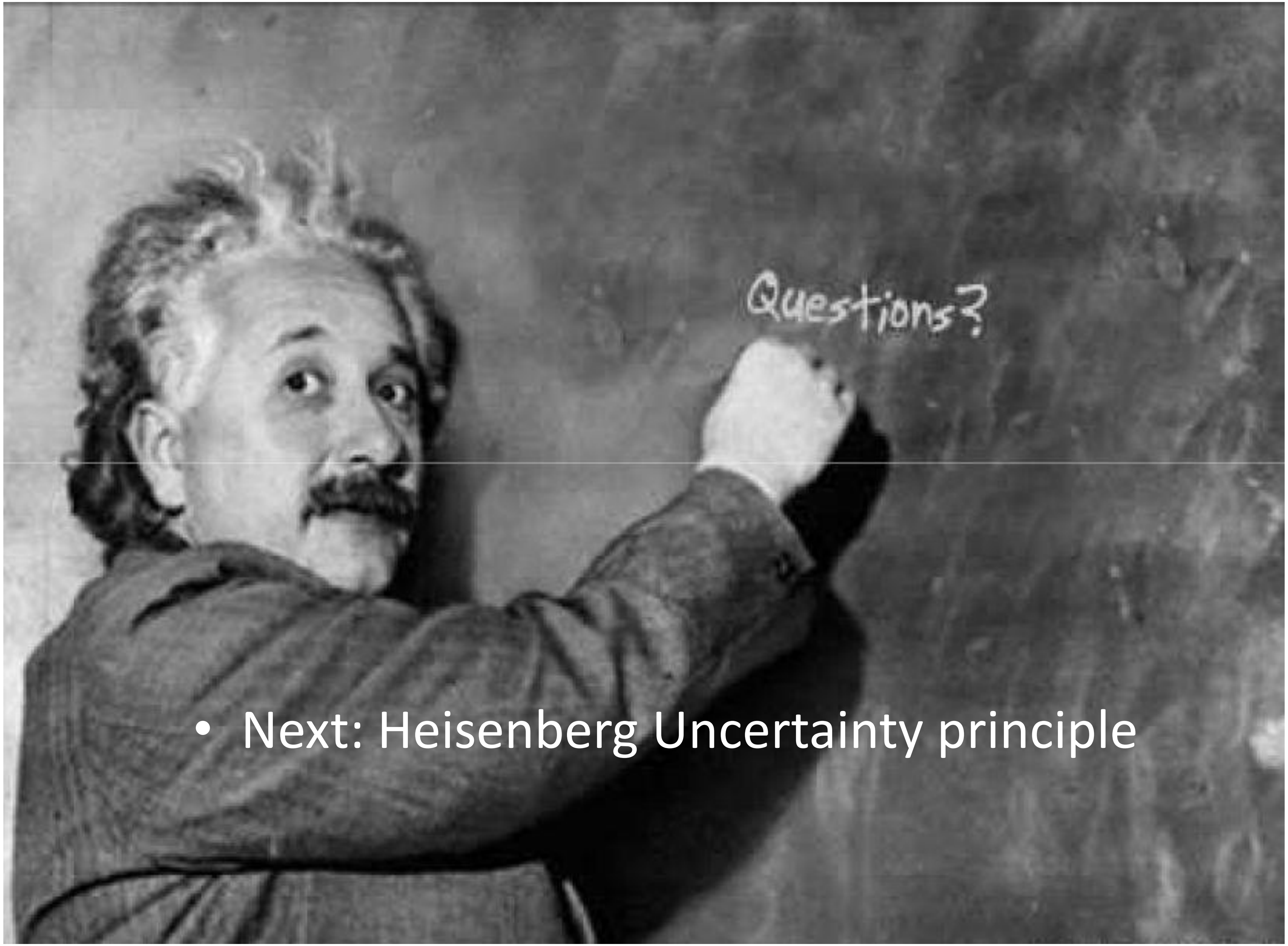
- Uncertainty principle
- Quantum mechanics
- Schrodinger equation
- 3 solved problems: Particle in a well, Harmonic oscillator, hydrogen atom
- Classical statistics
- Quantum statistics

Reading assignment

- QM refresher (Thornton Ch 6, 7 or equivalent, or Ch 1.9 and 3 from website)
- Simon Ch 1, Ch 2

Homework 1 posted

Math diagnostics (course website)



- Next: Heisenberg Uncertainty principle

Plane Waves

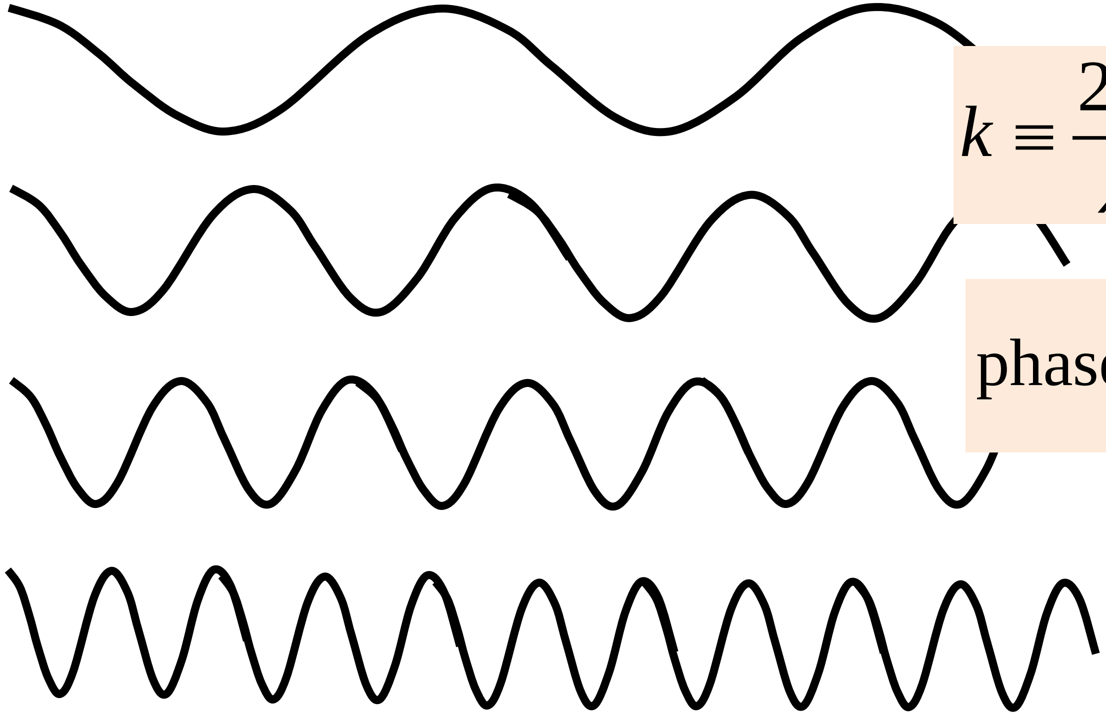
Plane waves (sines, cosines, complex exponentials) extend forever in space:

$$\Psi_1(x,t) = \exp\left[i\left(k_1 x - \omega_1 t\right)\right]$$

$$\Psi_2(x,t) = \exp\left[i\left(k_2 x - \omega_2 t\right)\right]$$

$$\Psi_3(x,t) = \exp\left[i\left(k_3 x - \omega_3 t\right)\right]$$

$$\Psi_4(x,t) = \exp\left[i\left(k_4 x - \omega_4 t\right)\right]$$



$$k \equiv \frac{2\pi}{\lambda} \quad \text{and} \quad \omega = \frac{2\pi}{T}$$

$$\text{phase velocity } \mathrm{v}_{\text{phase}} = \frac{\omega}{k}$$

Different *k*’s correspond to different momenta

$$p = \hbar k$$

Different ω’s correspond to different energies

$$E = \hbar\omega$$

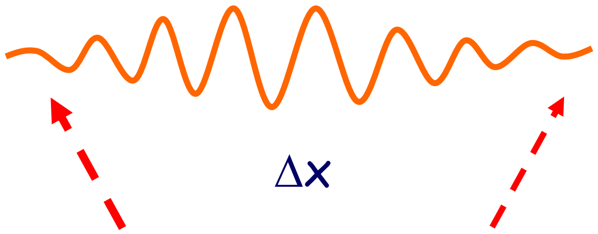
Heisenberg Uncertainty Principle

Mathematical property of waves: $\Delta k \cdot \Delta x \geq 1$

:

- A definite wavelength must extend forever.

- Finite wave packet:
  A wave packet requires a spread Δk of wavelengths.



We need a spread of wavelengths in order to get destructive interference.

Using $p = h/\lambda = \hbar k$, we have:

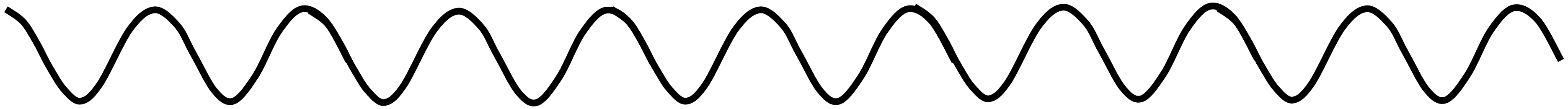
$$\hbar\,(\Delta k \cdot \Delta x \geq 1) \Rightarrow (\hbar \Delta k) \cdot \Delta x \geq \hbar \Rightarrow \boxed{\Delta p \cdot \Delta x \geq \hbar}$$

The Heisenberg Uncertainty Principle limits the accuracy with which we can know the position and momentum of objects.

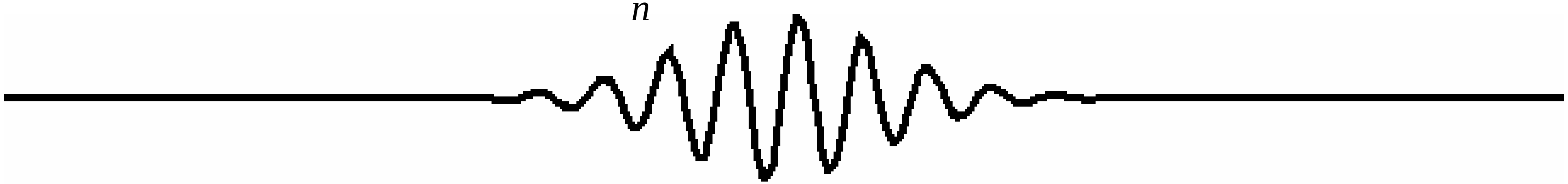
ICLICKER

Plane Waves vs. Wave Packets

$$\Psi(x,t) = A\exp\left[i\left(kx-\omega t\right)\right]$$



$$\Psi(x,t) = \sum_n A_n \exp\left[i\left(k_n x-\omega_n t\right)\right]$$

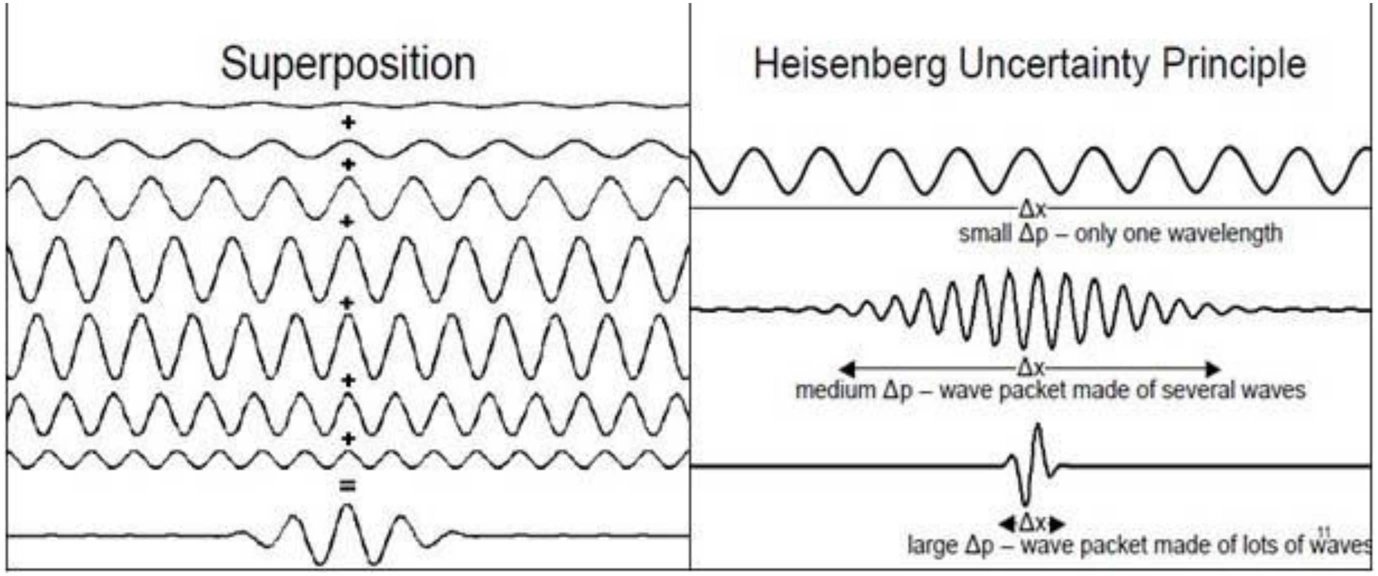


For which type of wave are the position (x) and momentum (p) most well-defined?

A) x most well-defined for plane wave, p most well-defined for wave packet.
B) p most well-defined for plane wave, x most well-defined for wave packet.
C) p most well-defined for plane wave, x equally well-defined for both.
D) x most well-defined for wave packet, p equally well-defined for both.
E) p and x are equally well-defined for both.

Uncertainty Principle

A <u>Wave</u> Interpretation:



- Wave packets are constructed from a series of plane waves.
- The more spatially localized the wave packet, the less uncertainty in position.
- With less uncertainty in position comes a greater uncertainty in momentum.

Energy-Time Uncertainty Principle

If we are to make a wave packet in time– ie a pulse that last for a time Δt (instead of over an infinite time as for a single wave), we must include the frequencies of many waves to have them cancel everywhere but over the time interval Δt

$$\Psi(x,t) = \sum_n A_n \exp\left[i\left(k_n x - \omega_n t\right)\right]$$

$$\Delta\omega\Delta t \geq 1/2$$

combined with the energy frequency relation

$$E = hf = \hbar\omega \Rightarrow \Delta E = \hbar\Delta\omega$$

Heisenberg uncertainty principle for energy and time

$$\Rightarrow \quad \boxed{\Delta E \cdot \Delta t \geq \frac{\hbar}{2}}$$

The energy and lifetime of a particle cannot **both** be determined with complete precision.

Implication of uncertainty principle

Consider a particle for which the location is known within a width of $\Delta\ell$ along the axis. We then know the position of the particle to within a distance

$$\Delta x \leq l / 2$$

The uncertainty principle specifies that Δp is limited by

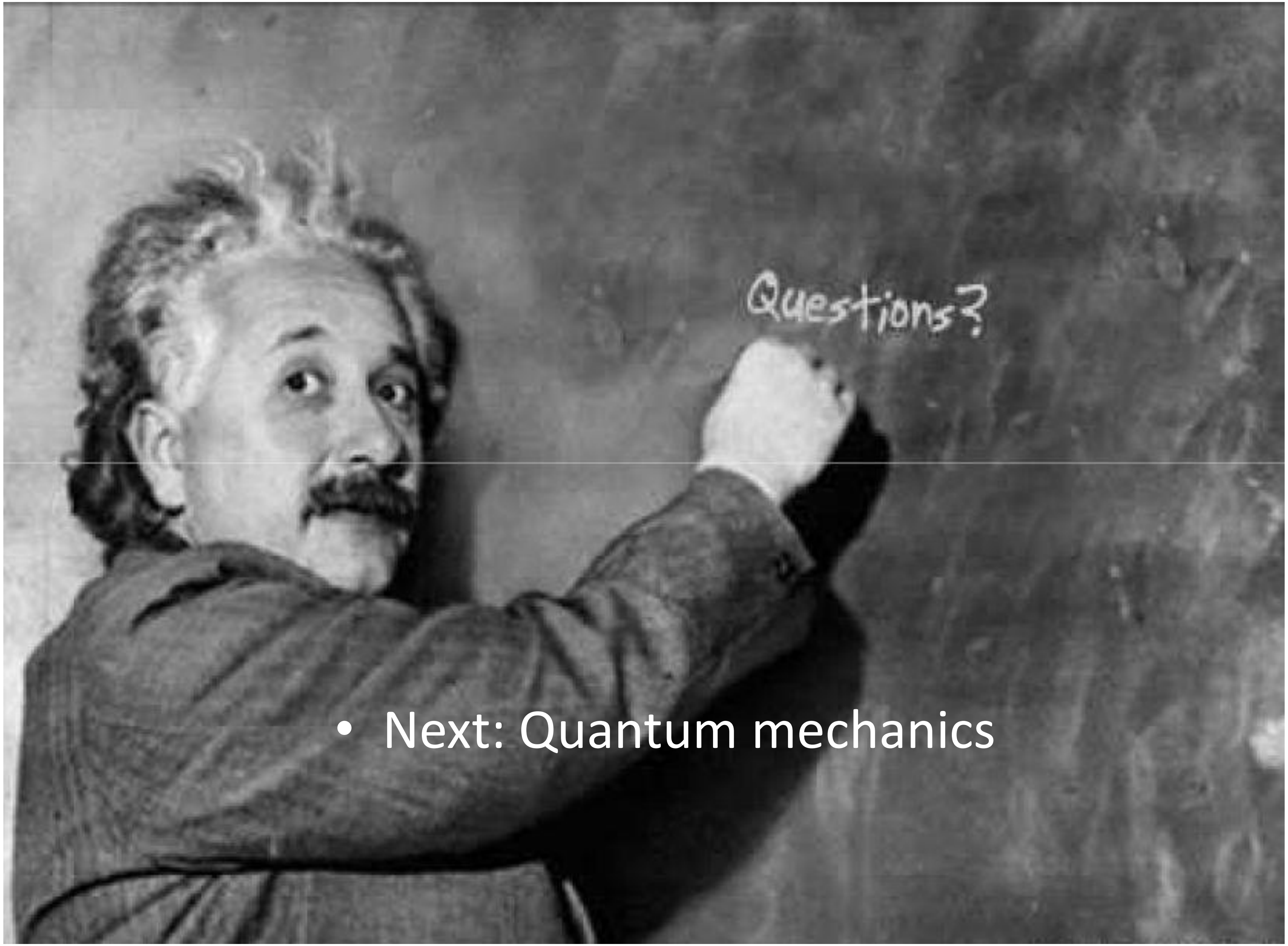
$$\Delta p \geq \frac{\hbar}{2\Delta x} \geq \frac{\hbar}{l}$$

The kinetic energy (non-relativistic)

$$\boxed{K_{\min} = \frac{p_{\min}^2}{2m} \geq \frac{(\Delta p)^2}{2m} \geq \frac{\hbar^2}{2m\ell^2}}$$

Zero point energy

$\mapsto$ if a particle is confined to a region of finite size, the particle’s kinetic energy must be non-zero!!!



- Next: Quantum mechanics

Quantum Mechanics: Law 1

Law 1. The state of a quantum mechanical system is completely specified by a function Ψ(r, t) that depends on the coordinates of the particle(s) and on time.

$\psi(\mathbf{r},t)$ ***Wave function***

$$|\psi(\mathrm{r},t)|^2 = \psi(\mathrm{r},t)^* \cdot \psi(\mathrm{r},t)$$

Probability to find particle at position r at time t.

$$\int_{-\infty}^{+\infty} |\psi(\mathbf{r},t)|^2 dr = 1$$

Normalization.

$$\text{if } \psi_1 \text{ and } \psi_2 \text{ are states then :}$$

$$\mathrm{c}_1\psi_1 + \mathrm{c}_2\psi_2 \equiv \psi_3 \text{ is also a state}$$

Superposition principle

Schrödinger equation in 1D

the Schrödinger equation for an electron wave in one-dimension Ψ(x,t)

$$\boxed{-\frac{\hbar^2}{2m}\frac{\partial^2\Psi(x,t)}{\partial x^2}+V(x,t)\Psi(x,t)=i\hbar\frac{\partial\Psi(x,t)}{\partial t}}$$

Of course for any real system, need 3 dimensions,
just add partial derivatives of y and z, and V(x,y,z) etc.

Schrödinger wrote it down, solved for hydrogen,
got solutions that gave exactly the same electron energy levels as Bohr.

Time independent Schrödinger equation in 1D

$$\boxed{-\frac{\hbar^2}{2m}\frac{\partial^2\Psi(x,t)}{\partial x^2}+V(x,t)\Psi(x,t)=i\hbar\frac{\partial\Psi(x,t)}{\partial t}}$$

Most physical situations, like H atom, no time dependence in V!

Simplification #1:V = V(x) only.

(Important, will use in all Shrödinger equation problems!!)

Ψ(x,t) separates into position dependent part ψ(x)
and time dependent part φ(t) =exp(-iEt/ħ). Ψ(x,t)= ψ(x)φ(t)

Plug in, get equation for ψ(x)

Plug in, get equation for ϕ(x)

$$\boxed{-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2}+V(x)\psi(x)=E\psi(x)}$$

$$\boxed{\phi(t)=e^{-iEt/\hbar}}$$

"time independent Schrodinger equation"

Stationary states

the wave function can be written as:

$$\Psi(x,t)=\psi(x)e^{-i\omega t}$$

$$\boxed{\text{with}:\omega=E/\hbar}$$

- The probability density becomes:

$$\Psi^*\Psi=\psi^2(x)\left(e^{i\omega t}e^{-i\omega t}\right)$$

$$\Psi^*\Psi=\psi^2(x)$$

- The probability distributions are constant in time. This is a standing wave phenomenon that is called the stationary state.

Properties of Valid Wave Functions

1) To avoid infinite probabilities, the wave function must be finite everywhere.
2) to avoid multiple values of the probability, the wave function must be single valued.
3) For finite potentials, the wave function and its derivative must be continuous. This is required because the second-order derivative term in the wave equation must be single valued. (There are exceptions to this rule when V is infinite.)
4) to normalize the wave functions, they must approach zero as x approaches infinity.

$$\int_{-\infty}^{\infty} |\psi(x)|^2 dx = 1$$

Solving Schrodinger Equation for free particle

$$\boxed{-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2}+V(x)\psi(x)=E\psi(x)}$$

Electron in free space, no electric fields or gravity around.

1. Where does it want to be?	1. No preference- all x the same.
2. What is V(x)?	2. Constant.
3. What are boundary conditions on ψ(x)?	3. None, could be anywhere.

Smart choice of constant, V(x) = 0!

$$\boxed{-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2}=E\psi(x)}$$

I-Clicker

$$\boxed{-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2} = E\psi(x)}$$

$$\psi(x) = A\cos kx + B\sin kx$$

The total energy of the electron is:

A. Quantized according to E_n = (constant) x n^2, n= 1,2, 3,…
B. Quantized according to E_n = const. x (n)
C. Quantized according to E_n = const. x ($1/n^2$)
D. Quantized according to some other condition but don't know what it is.
E. Not quantized, energy can take on any value.

Ans: E - No boundary, energy can take on any value.

$$\psi(x) = A\cos kx \quad \frac{\hbar^2 k^2}{2m} = E \quad p = \hbar k$$

k (and therefore E) can take on any value.

Almost have a solution, but remember we still have to include time dependence:

$$\Psi(x,t) = \psi(x)\phi(t) \quad \boxed{\phi(t) = e^{-iEt/\hbar}}$$

…bit of algebra, using identity: e^{ix} =cos(x) + i sin(x) and wave propagating in the positive x direction

$$\Psi(x,t) = A\cos(kx - \omega t) + i\,A\sin(kx - \omega t)$$

The wave function is not restricted to being real.

Only the physically measurable quantities must be real: probability, momentum and energy.

Quantum Mechanics: : Law 1

Law1. The state of a quantum mechanical system is completely specified by a function $\Psi(r, t)$.

- Dirac notation

$$\psi(x) \Rightarrow |\psi\rangle \quad ket$$

$$\psi^*(x) \Rightarrow \langle\psi| \quad bra$$

- Principle of superposition. If Ψ_1 and Ψ_2 are possible states of a system then any linear superposition. Ψ is also an allowed state.

$$|\psi\rangle = a_1|\psi_1\rangle + a_2|\psi\rangle_2$$

- Inner product

$$\langle\phi|\psi\rangle = \int \phi^*(r)\psi(r)d\mathbf{r}$$

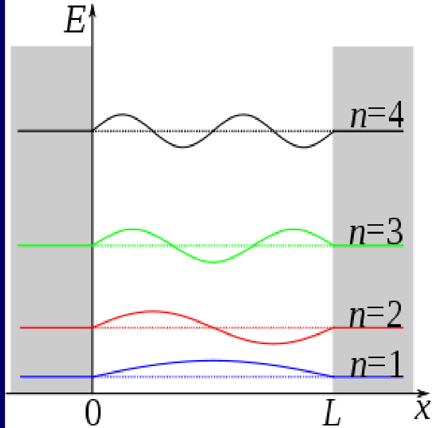
- A wave function $\psi(x)$ corresponds to a state $|\psi\rangle$ in the $\hat{x}$ representation
- A wave function $\psi(p)$ corresponds to a state $|\psi\rangle$ in the p representation

Quantum Mechanics

Only 3 exactly Solved Problems!

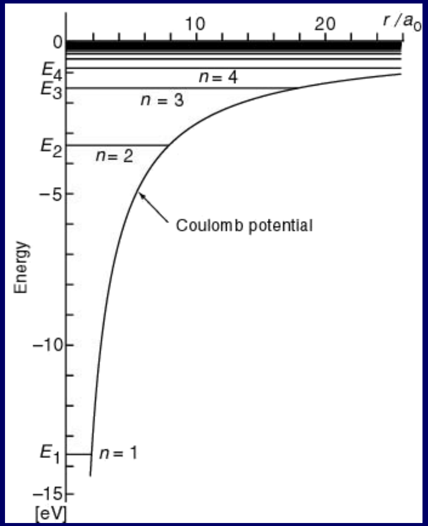
Particle in a box

$$U(x)=\begin{cases}0 & 0<x<L\\ \infty & x<0;\, x>L\end{cases}$$



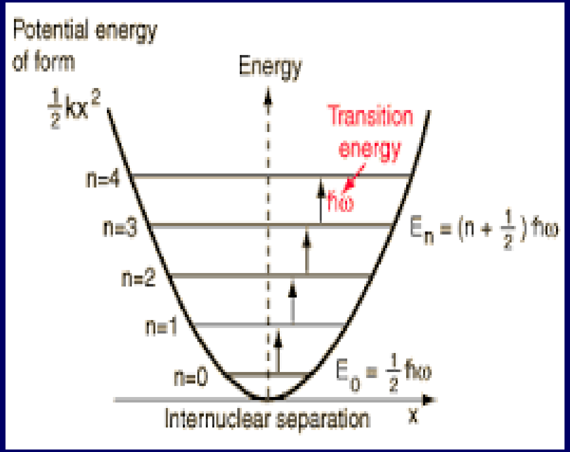
Hydrogen atom

$$U(r)=\frac{1}{4\pi\varepsilon_0}\frac{q}{r}$$



Harmonic oscillator

$$U(r)=\frac{1}{2}m\omega^2x^2$$



Skip examples

Constraints on the Form of $\psi(x)$

$|\psi(x)|^2$ corresponds to a physically meaningful quantity:
the probability density of finding the particle near x.

To avoid unphysical behavior, $\psi(x)$ must satisfy :

- $\psi(x)$ must be single-valued, and finite.
- $\psi(x)$ must be continuous, with finite $d\psi/dx$.
  $d\psi/dx$ is related to the momentum.
- $d^2\psi/dx^2$ must be finite.
- To avoid infinite energies.
  This also means that $d\psi/dx$ must be continuous.
- There is no significance to the overall *sign* of $\psi(x)$.

It goes away when we take the absolute square.

Properties of Valid Wave Functions

<u>To be physically acceptable, a wave function:</u>

1. Must be normalizable! $\int_{-\infty}^{\infty} |\psi(x)|^2 dx = 1$

Wave function must be finite everywhere, and approach zero at infinity.

2. Must be smooth, continuity of the wave function and continuity of its derivative!

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↓

Acts like a 0 wavelength
→ ∞ Momentum and KE

If the Ψ had a discontinuity, its first derivative would be infinite at the point of discontinuity→ non physical!

Lecture 1


Ludwig Boltzma
1844-1906

- Introduction
  - What is condensed matter physics and why do it
- The power of simple models – specific heat of solids
  - Boltzmann
  - Einstein
  - Debye

References:
Simons Chapter 2.1

Supplementary reading
(Course website links)

Anderson
Coleman
Morisson

Elementary particles as vacuum excitations

Stuff is made of particles

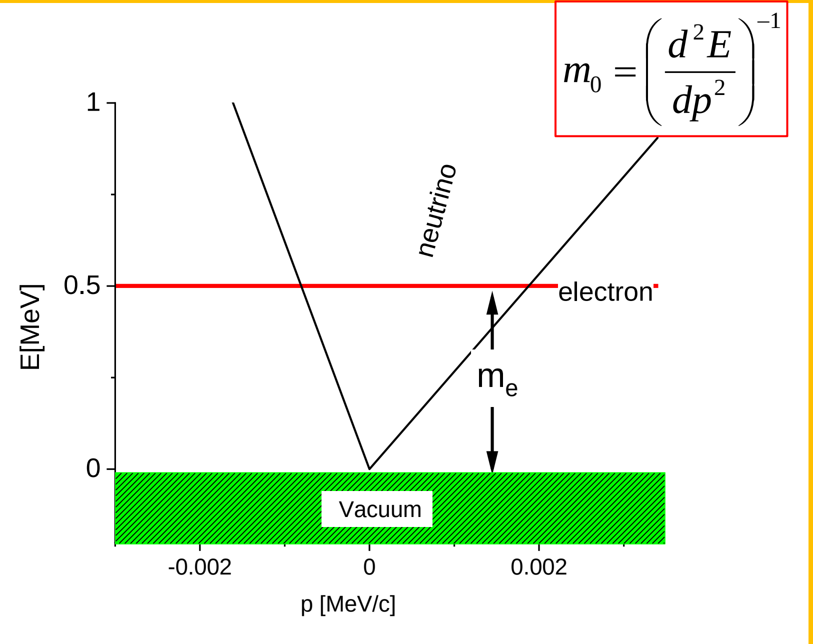
Particle mass determines:	
response to forces	$F = dp/dt$
E(p) - dynamics	$E = \sqrt{c^2 p^2 + m_0^2 c^4}$

$$E(p) \rightarrow \begin{cases} \approx m_0 c^2 + \dfrac{p^2}{2m_0} & p << m_0 c \text{ massive slow particles v} << \text{c} \\ pc & p >> m_0 c \text{ ultra-relativistic (photon, neutrino)} \end{cases}$$

Why Same m_0 ?

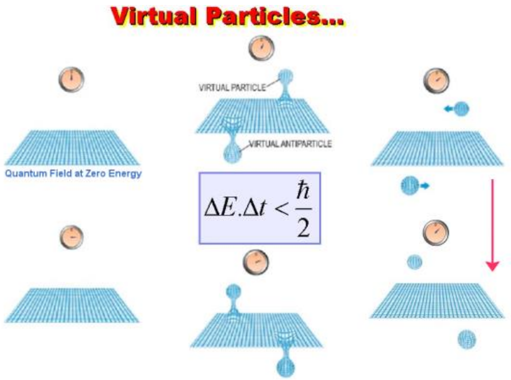
- ➢ Lorentz invariance!
- ➢ Physics laws same in all reference frames

particle	Rest mass m_0c^2 [MeV]
e	0.5
n, p	940
neutrino (ν)	~0



$$m_0 = \left(\frac{d^2E}{dp^2}\right)^{-1}$$

- ➢ Particles are elementary excitation out of our Universe’s ground state (vacuum) E< 0
- ➢ String theory: 10^{500} possible vacuums! We are ‘stuck’ in one.
- ➢ Figure out our vacuum ↦ predict the masses of all elementary particles (standard model)



$$\Delta E.\Delta t < \frac{\hbar}{2}$$

Elementary particles as vacuum excitations

Stuff is made of particles

Particle mass determines:	
response to forces	$F = dp/dt$
E(p) - dynamics	$E = \sqrt{c^2 p^2 + m_0^2 c^4}$

$$E(p) \rightarrow \begin{cases} \approx m_0 c^2 + \dfrac{p^2}{2m_0} & p << m_0 c \ \text{ massive slow particles v} << \text{c} \\ pc & p >> m_0 c \ \text{ultra-relativistic (photon, neutrino)} \end{cases}$$

Condensed matter: No Lorentz invariance

$$E(p) \approx \Delta + \frac{p^2}{2m^*}$$

Spectral gap (Insulators)

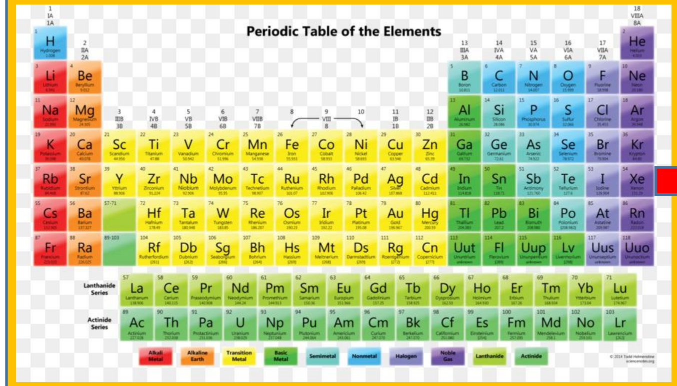
Dispersion curvature independent of Δ

Many other types of dispersions are available or can be engineered

Condensed matter vacuum

- Elementary excitation out of the vacuum – quasi-particles
- The lattice of ions defines a preferred reference frame – no Lorentz invariance
- ~ 100 elements x 20 arrangements x 10 allotropes $\mapsto 10^{40}$ possible vacuums.
- We can engineer and study many of the vacuums. No fundamental restrictions.

Condensed matter vacuum



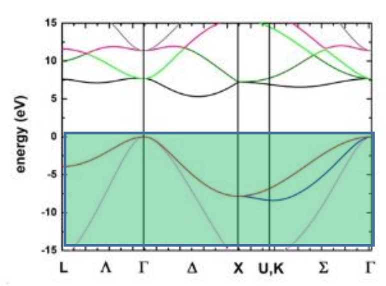
Building blocks: electrons and nuclei

- Electrons moving in a crystal (lattice of atoms)
- E(p) determined by crystal geometry: Energy bands
- Ground state(vacuum) occupied states $E < E_F$ Fermi energy
- Low energy Excitations: ‘dressed electrons’ with effective mass

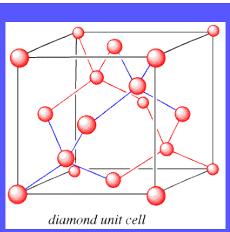
$$m^* = \left(\frac{\partial^2 E}{\partial p^2}\right)^{-1}$$

~10^{50} Ground states

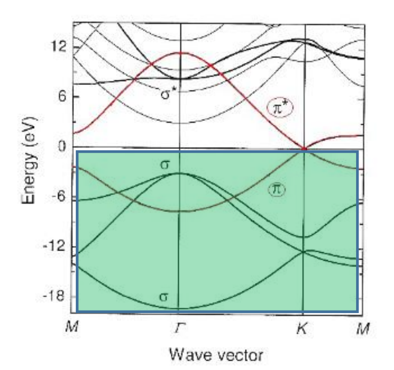
Diamond:
QP mass ~$1.13m_e$

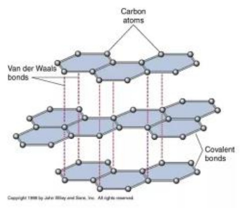


Momentum along crystal directions

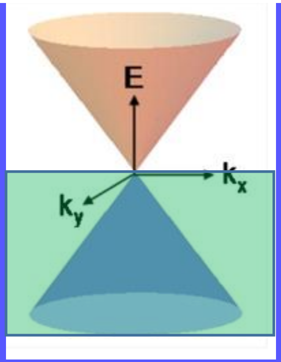


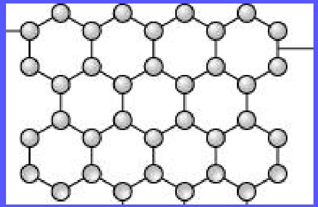
Graphite:
QP masses ~ $0.043m_e$



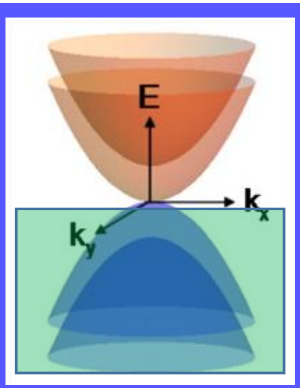


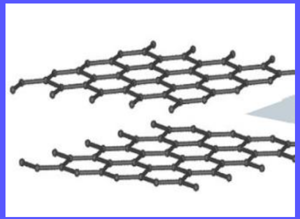
Graphene :
Chiral massless fermions
Ultra-relativistic



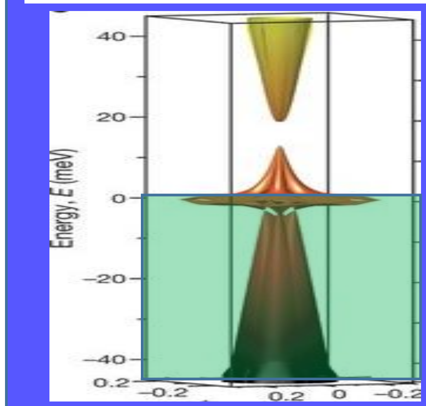


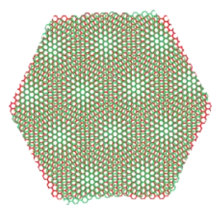
Bilayer graphene:
Chiral massive fermions
m*=0.03me





Twisted Bilayer graphene:
Flat band m* - large
QP velocity - small





Effective Theories

$$\hat{H} = \hat{H}_e + \hat{H}_n + \hat{H}_{n-e},$$

- The Hamiltonian describes the physics of electrons in a potential created by ions (on the energy scale of Hartree),
- We are interested in the measurable low-energy properties.
- Try using reduced effective (phenomenological) theories.

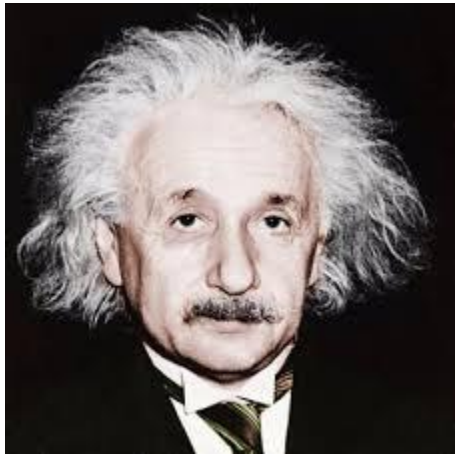
➢ Low energy (long wavelength) excitations around the ground state : *quasiparticles* *(Physics of windsurfing)*

Examples:

- Quasiparticles in Fermi liquids – like free particles but different from electrons (effective mass, E-p relation, charge)
- Phonons in lattices

The power of simple models

Max Planck
1858 -1947



Albert Einstein
1879, -1955,

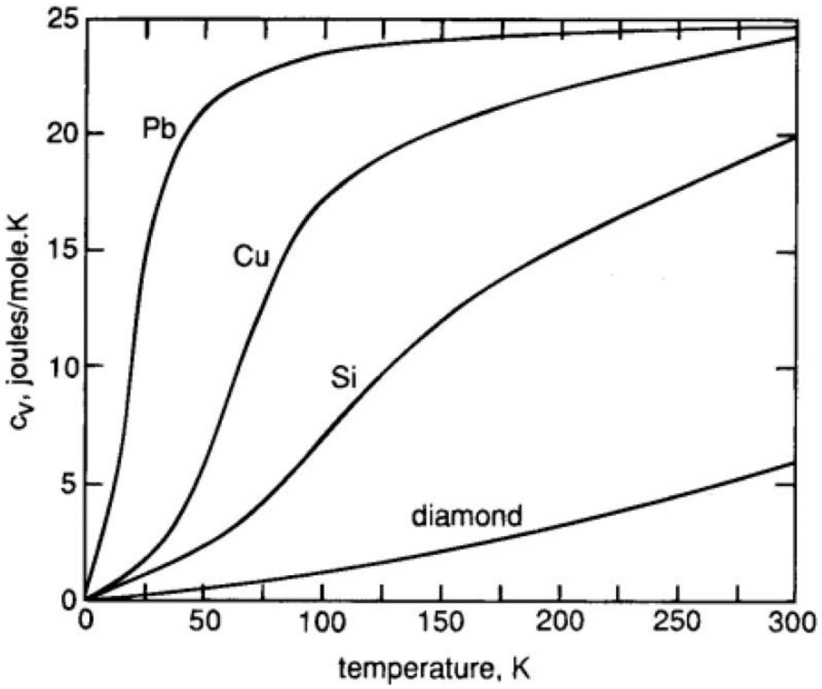
Ludwig Boltzmann
1844-1906

- Introduction
  - What is condensed matter physics and why do it
- The power of simple models

Specific Heat of Solids

1819 - A one hundred year old puzzle

$$C = \frac{\partial Q}{\partial T}$$

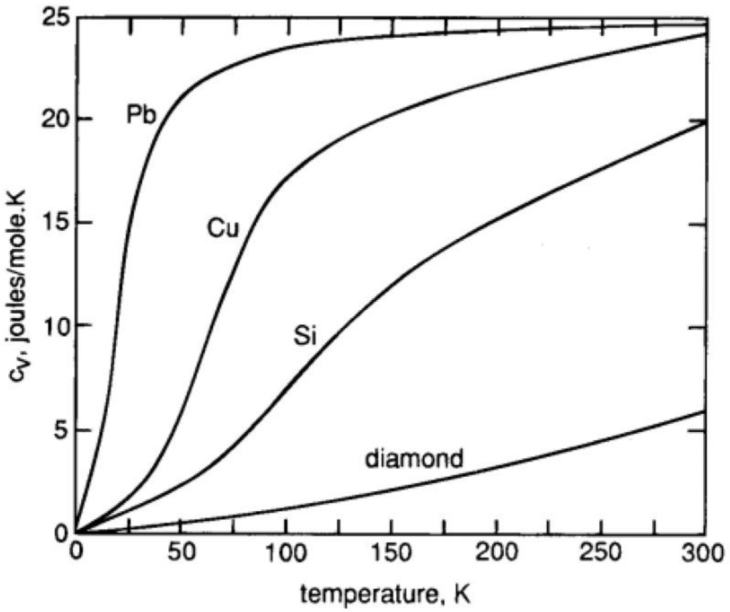


Specific heat of solids

Specific Heat of Solids: Boltzmann, Einstein, and Debye

$$\boxed{C = \frac{\partial Q}{\partial T}}$$

$$\boxed{C(T) \xrightarrow[T \to 0]{} 0}$$



at high T: C~ $3R \approx 25\ J/K$-mol
Unsurprising – like monoatomic gas

- We don't distinguish between C_V and C_P - solids, in contrast to gases, do not expand/contract much with T.

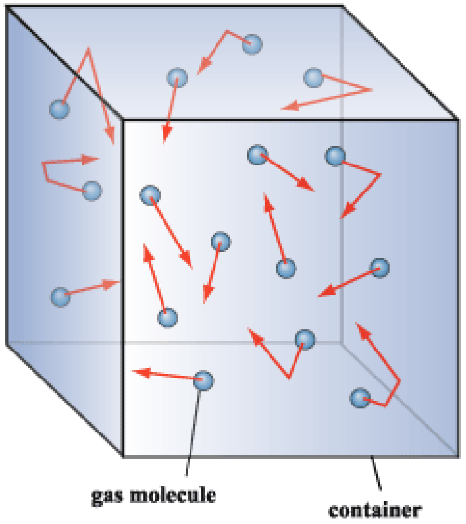
$$\boxed{C_P - C_V = VT\alpha^2 / \beta_T}$$

Coefficient. of thermal expansion

Isothermal compressibility

- The electron contribution to C is typically small at $T \gtrsim 10K$ – we'll discuss this later.

Some background: Kinetic theory of gases



The theory for ideal gases assumptions:

- The average distance between the gas particles is large compared to their size
- The number of particles is so large that statistical treatment can be applied.
- The moving particles collide among themselves and with the walls of the container in perfectly elastic collisions.

Equipartition theorem: each quadratic degree of freedom contributes $\frac{1}{2}k_B T$ to the average energy .

Can you think of examples of quadratic degrees of freedom
i.e the energy is proportional to the square of a variable?

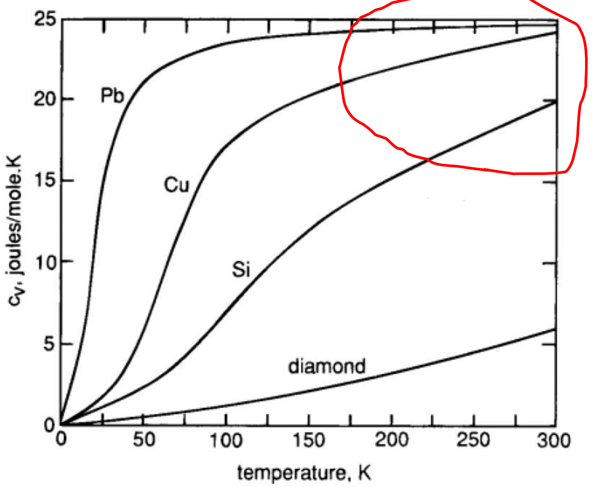
Boltzmann – classical high T limit

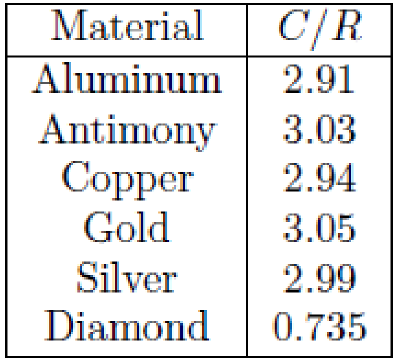
Dulong-Petit Law (1819).

At High T (room temperature)

$$\boxed{C = 3N_A k_B = 3R}$$

Molar heat capacity





Material	C/R
Aluminum	2.91
Antimony	3.03
Copper	2.94
Gold	3.05
Silver	2.99
Diamond	0.735

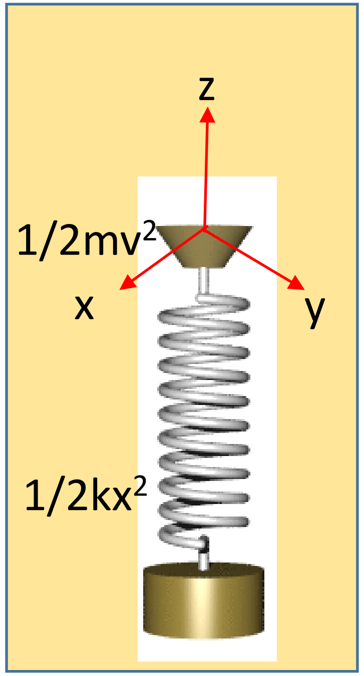
Heat Capacities of Some Solids at Room temperature

Ludwig Boltzmann
1844-1906

Boltzmann (1897)

- N independent atoms trapped in potential wells formed by interactions with other atoms. The atoms/ions are in thermal equilibrium with a thermal bath.
- N atoms have 6N degrees of freedom: 3N for center of mass KE and 3N for the spring potential energy ½ kx^2 , ½ ky^2, ½ kz^2
- According to the equipartition theorem, each quadratic degree of freedom contributes an average energy ½$k_B T$.

$$\boxed{\langle E\rangle = \frac{6}{2}N_A k_B T \Rightarrow C_v = \frac{\partial\langle E\rangle}{\partial T} = 3N_A k_B = 3R}$$

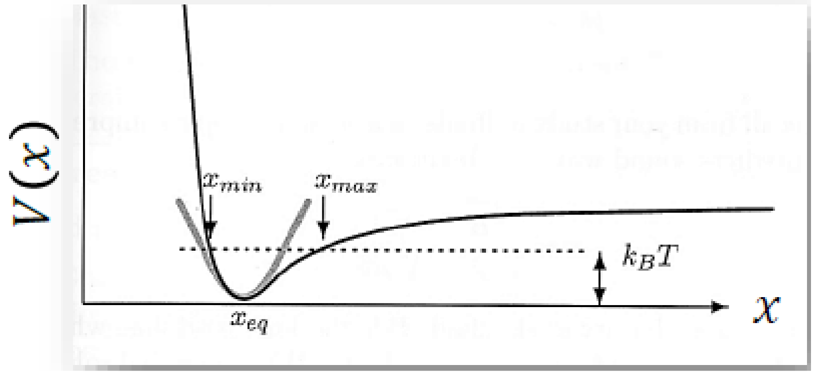


Note: This is a classical result ($k_B T \gg \hbar\omega$). The low-T behavior remained a puzzle.

Einstein – quantum (low T) model

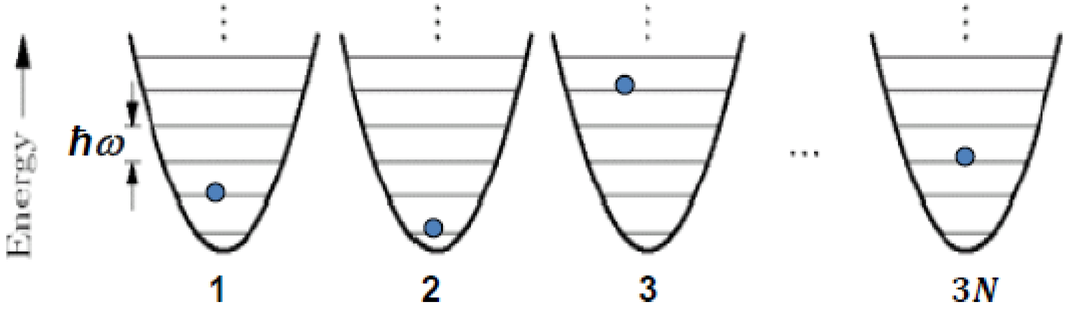
The low-T value of C is quite different from $3R$, it approaches 0 as $T \to 0$.

Einstein (1907) replaced classical oscillators with quantum ones.



In general, interactions between atoms (ions) in crystals are not harmonic. However, at low T (think small amplitude), the harmonic approximation works well.

N atoms ⇒ $3N$ normal modes.



$3N$ identical (the same ω) quantum oscillators

The energy of each quantum oscillator

$$\boxed{E_n = \hbar\omega(n + 1/2) \quad n = 0,1,2..}$$

Number of excited modes of energy $\hbar\omega$

Later in the course we will see that these represent lattice vibrations called - phonons

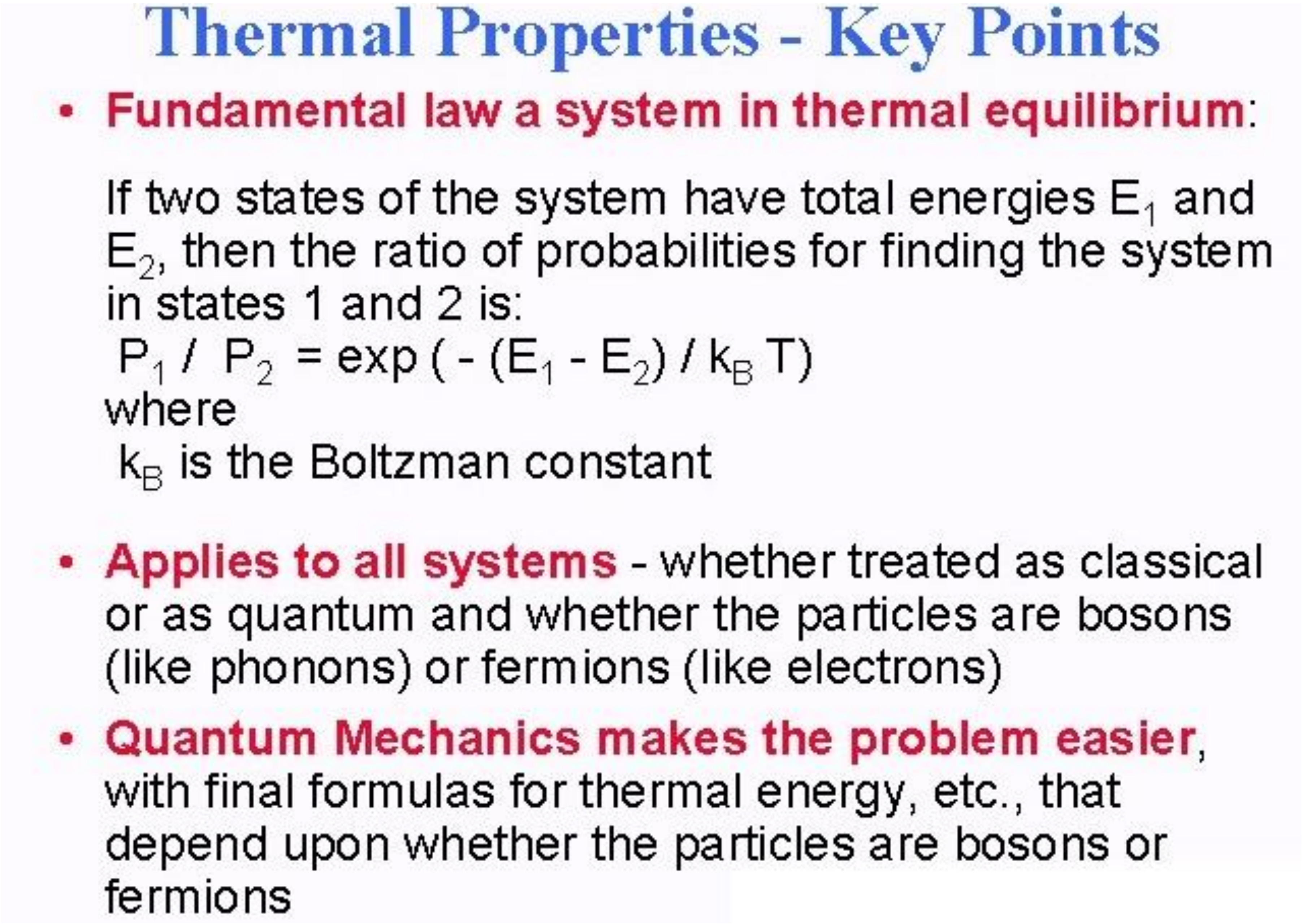
Preliminaries : Bosons and Fermions

- To calculate the average number of excited modes at a given temperature we need to use a few facts about the statistics obeyed by different types of quantum excitations.
- The type of statistics divides particles into two categories:

1. Fermions : particles that cannot be in the same energy level (eg. Electrons – that obey Pauli exclusion exclusion principle.
    - Fermions have ½ integer spin (electrons have s = ½, for example))
    - Their wavefunction is anti-symmetric under exchange of two particles
2. Bosons : particles that can be in the same energy state (eg. Photons, phonons. No exclusion principle.)
    - Bosons have integer spin (photons have S = 0, for example)
    - Their wavefunction is symmetric under exchange of two particles

Therefore one can have more than one photon, or lattice vibration at the same energy. This is not the case for electrons. (later in the course)

Preliminaries : Thermal equilibrium



Thermal Properties - Key Points

- **Fundamental law a system in thermal equilibrium**:

  If two states of the system have total energies E_1 and E_2, then the ratio of probabilities for finding the system in states 1 and 2 is:
  $P_1 / P_2 = \exp(-(E_1 - E_2) / k_B T)$
  where
  k_B is the Boltzman constant

- **Applies to all systems** - whether treated as classical or as quantum and whether the particles are bosons (like phonons) or fermions (like electrons)
- **Quantum Mechanics makes the problem easier**, with final formulas for thermal energy, etc., that depend upon whether the particles are bosons or fermions

Harmonic oscillator thermally excited states

- Excitations of a harmonic oscillator are bosons. They do not obey an exclusion principle
- There can be any number n of excited states in each oscillator, ie the energy of each oscillator can take on any value in the series:

$$\boxed{E_n = \hbar\omega(n+1/2) \quad n = 0,1,2\ldots}$$

$$\frac{P_{n+1}}{P_n} = \exp(-(E_{n+1} - E_n)/k_B T) \Rightarrow P_n = C\exp(-E_n/k_B T)$$

C is a normalizat ion factor independen t of n

$$\text{Usig}: \sum_{n=0}^{\infty} P_n = 1 \Rightarrow C = \sum_{0}^{\infty} \exp(-E_n/k_B T)$$

- Thus the probability of finding the oscillator in the n'th excited state

$$\boxed{P_n = \frac{\exp(-E_n/k_B T)}{\sum_{0}^{\infty} \exp(-E_n/k_B T)}}$$

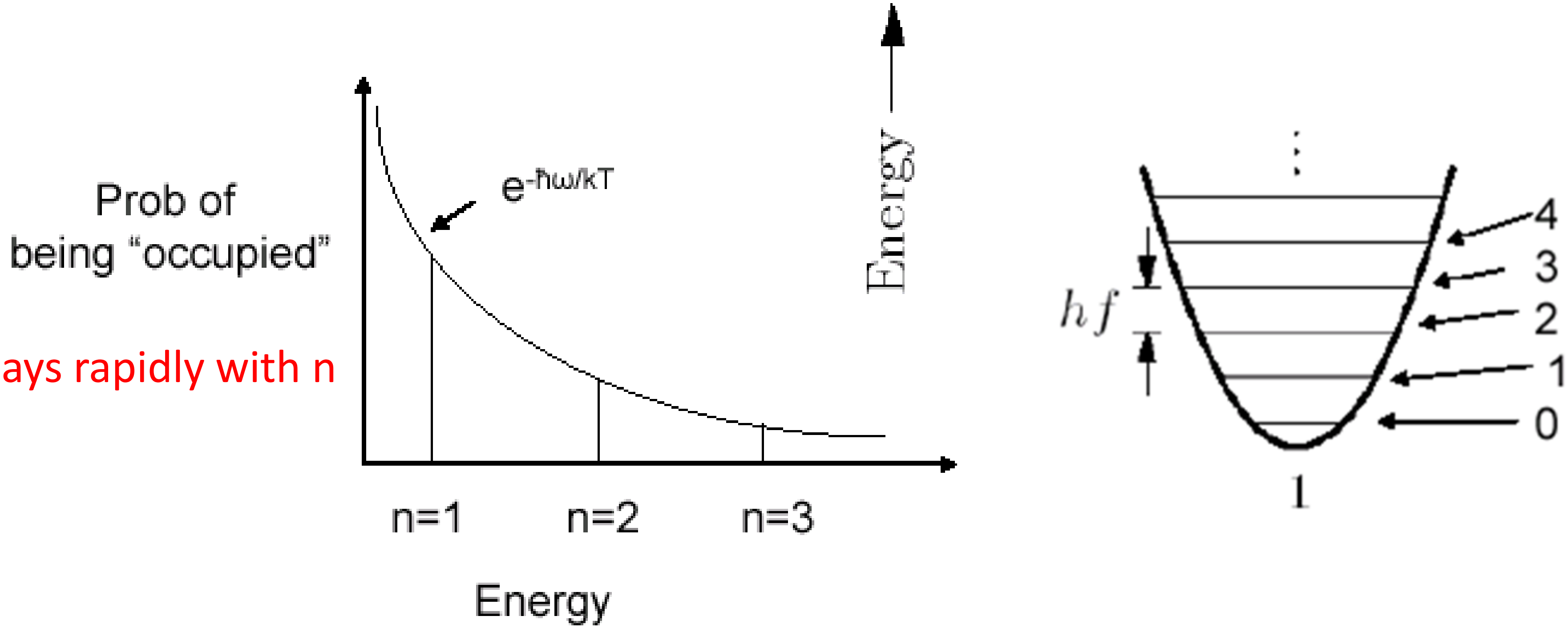
Harmonic oscillator probability of thermally excited states

- The probability of finding the oscillator in the n’th excited with energy

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

$$P_n = \frac{\exp(-n\hbar\omega/k_BT)}{\sum_0^\infty \exp(-n\hbar\omega/k_BT)}$$

- What does this look like?



Note that it decays rapidly with n

Average number of excited modes at temperature T

- Average occupation number at temperature T is thus:

< > denotes thermal average, so T is implicit in the notation

$$\langle n \rangle \equiv \sum_{0}^{\infty} P_n n$$

This is the expectation value of n.

$$\boxed{\langle n \rangle = \frac{\sum_{n=0}^{\infty} n \exp(-n\hbar\omega / k_B T)}{\sum_{n=0}^{\infty} \exp(-n\hbar\omega / k_B T)}}$$

How can we do this sum?

1. We know that:

$$\sum_{0}^{\infty} x^n = \frac{1}{1-x}$$

Geometric series

$$\text{replace } x \to \exp(-n\hbar\omega / k_B T)$$

DENOMINATOR

$$\boxed{\sum_{n=0}^{\infty} \exp(-n\hbar\omega / k_B T) = \frac{1}{1-e^{-\hbar\omega/k_B T}}}$$

Average number of excited modes at temperature T

- We can use this result, and a trick, to calculate the numerator:

$$\sum_0^\infty s x^s = \frac{\partial}{\partial x}\left(\sum_0^\infty x^s\right) = \frac{\partial}{\partial x}\left(\frac{1}{1-x}\right) = \frac{x}{(1-x)^2}$$

Compare to Planck's model for photons

$$\Rightarrow \boxed{\sum_0^\infty n\exp(-n\hbar\omega/k_BT) = \frac{\exp(-\hbar\omega/k_BT)}{(1-\exp(-\hbar\omega/k_BT))^2}}$$

Putting it all together:

$$\boxed{\begin{aligned}\langle n\rangle &= \frac{\text{numerator}}{\text{denominator}}\\ &= \frac{x/(1-x)^2}{1/(1-x)} = \frac{x}{1-x}\end{aligned}}$$

$\Rightarrow$

Planck distribution:

$$\boxed{\langle n\rangle = \frac{1}{\exp(\hbar\omega/k_BT)-1}}$$

Max Planck
1858 -1947

Note: This is different from the Bose Einstein distribution:

$$\boxed{\langle n\rangle = \frac{1}{\exp(\hbar\omega/k_BT-\mu)-1}}$$

μ Chemical potential

Average Kinetic energy of oscillator at temperature T

$$\langle n \rangle = \frac{1}{\exp(\hbar\omega / k_B T) - 1}$$

- This is the average number of excitations in a mode with frequency ω at temperature T.
- We can therefore use this to calculate the total energy of the lattice and from this obtain the specific heat.

$$E(T) = \hbar\omega(\langle n \rangle + 1/2) = \hbar\omega\left(\frac{1}{\exp(\hbar\omega / k_B T) - 1} + 1/2\right)$$

High T limit: :

$$E(T) = \langle n \rangle \hbar\omega = \xrightarrow[T=\infty]{} k_B T$$

Same as classical result!!

Low T limit: :

$$E(T) = \langle n \rangle \hbar\omega = \xrightarrow[T=0]{} \hbar\omega \exp(-\hbar\omega / k_B T)$$

No excitations at T=0

But very different from classical result

Einstein's result for the specific heat

$$\boxed{E(T) = \hbar\omega(\langle n\rangle + 1/2) = \hbar\omega\left(\frac{1}{\exp(\hbar\omega/k_BT)-1} + 1/2\right)}$$

- Heat capacity of HO

$$C_V = \left.\frac{dE}{dT}\right|_V = k_B\frac{x^2\exp(x)}{(\exp(x)-1)^2} \qquad \boxed{x \equiv \frac{\hbar\omega}{k_BT}}$$

Einstein model

- The heat capacity of a system consisting of 3N HO of frequency ω

$$\boxed{C_V = \sum_1^{3N} k_B\frac{x^2\exp(x)}{(\exp(x)-1)^2} = 3Nk_B\frac{x^2\exp(x)}{(\exp(x)-1)^2}}$$

Einstein's model predictions

$$\boxed{C_V = 3Nk_B \frac{x^2 \exp(x)}{(\exp(x)-1)^2}}$$

$$\boxed{x \equiv \frac{\hbar\omega}{k_B T}}$$

- High T limit:

$$\boxed{\begin{gathered} x \xrightarrow[T\to\infty]{} 0; \quad \exp(x) \xrightarrow[T\to\infty]{} 1+x \\ C_V \xrightarrow[T\to\infty]{} 3Nk_B \frac{x^2(1+x)}{(x)^2} \xrightarrow[T\to\infty]{} 3Nk_B \end{gathered}}$$

Classical (Dulong Petit) result!!

- Low T limit:

$$\boxed{\begin{gathered} x \xrightarrow[T\to 0]{} \infty; \quad \exp(x)-1 \xrightarrow[T\to 0]{} \exp(x) \\ C_V \xrightarrow[T\to 0]{} 3Nk_B x^2 \exp(-x) \propto e^{-\frac{\hbar\omega}{k_B T}} \end{gathered}}$$

Heat capacity in Einstein model compared to experiment

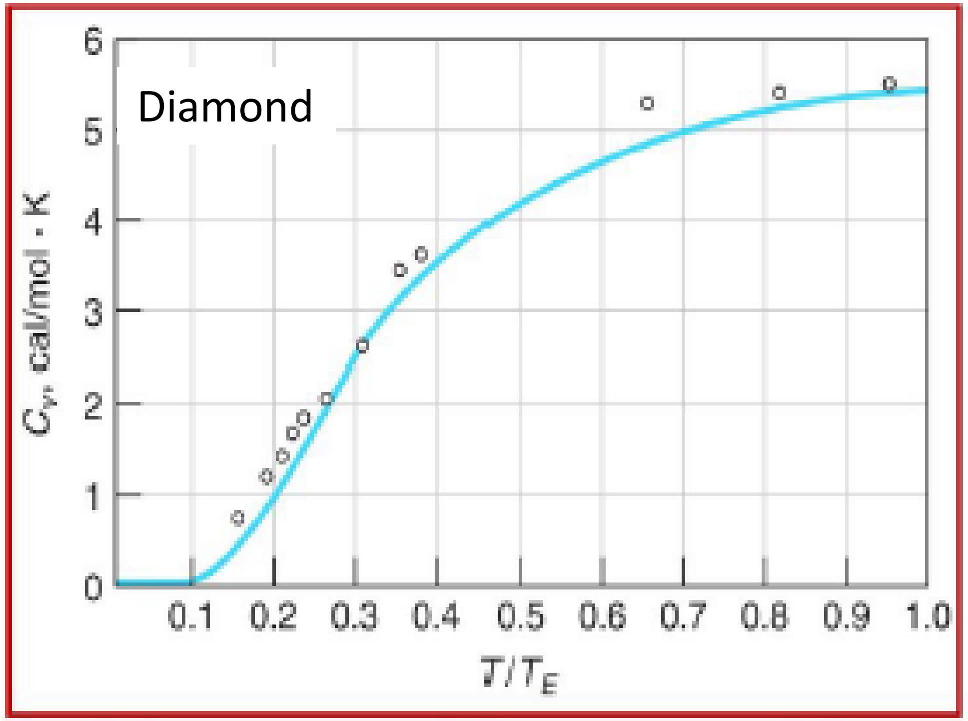
$$C_V = 3Nk_B \frac{(\beta\hbar\omega)^2 e^{\beta\hbar\omega}}{(e^{\beta\hbar\omega}-1)^2}$$

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

$$C_V = 3Nk_B \frac{(T_E/T)^2 e^{T_E/T}}{(e^{T_E/T}-1)^2}$$

$$T_E \equiv \frac{\hbar\omega}{k_B}$$

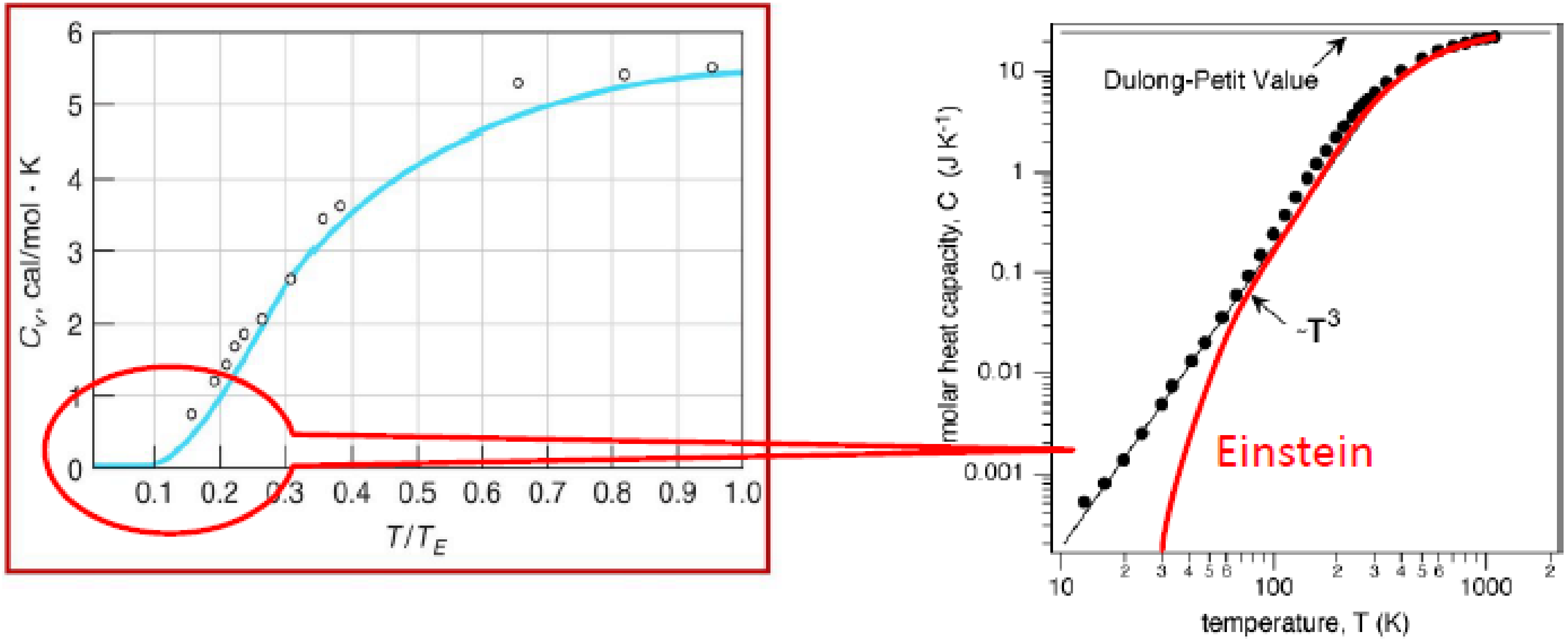
Single parameter fit !



Experiment vs. Einstein's theory. $T_E = 1320K$ – the only fitting parameter.

A. Einstein, *Annalen der Physik* 22, 180 (1907)

Limitations of Einstein.s model



A. Einstein, *Annalen der Physik* 22, 180 (1907)

- Not a bad approximation to experimental data but not perfect.
- At low T heat capacity is much too low

(Experiment: $C \propto T^3$ rather than $C \propto e^{-\frac{\hbar\omega}{k_B T}}$)

- This is not that surprising- ω is not constant for most vibration modes!

But the model works reasonably well for optical modes where frequency is almost constant.

- To do this right we need to take into account multiple oscillator frequencies– Debye model .

Summary

Early models for the specific heat of solids.

Scorecard so far :

- Boltzmann model – based on energy equipartition for classical particles.
  - Works well at high T but fails at low T.
- Einstein's model: - assumes N independent quantum oscillators (bosons) with Planck statistics
  - Works well at high T
  - Underestimates C at low T

Next time we will see how Debye 'fixed' the low T problem in Einstein's model by assuming harmonic oscillators with frequencies given by a linear dispersion of sound waves.

Limitations of Einstein model

Einstein's model ignores the fact that the ions are coupled together –coupled oscillators.

- For coupled oscillators, the calculation of the partition function may look rather difficult.
- But a system of N coupled 3D oscillators is equivalent to a system of 3N independent 1D oscillators.
- The price to be paid is that the independent oscillators are not of the same frequency; the normal modes of vibration of a solid have a wide range of frequencies.
- These modes are not related to the motion of single atoms, but to the collective motion of all atoms in the crystal – vibrational modes or sound waves.

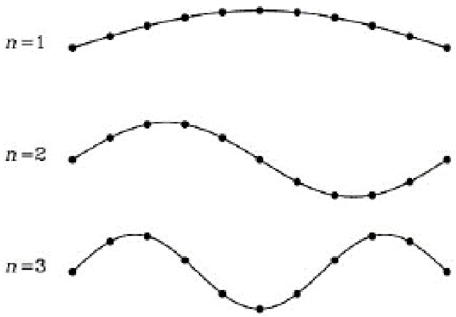
Need to consider a broad spectrum of $\boldsymbol{\omega}$ and not a single characteristic frequency as in the Einstein's model:

$$\boxed{E(T) = \sum_i \langle n_i \rangle \hbar \omega_i}$$

Debye's theory of Heat capacity

Debye's model (1912)

- Treats the solid as a continuum, i.e., the atomic structure is ignored.
- A continuum has vibrational modes of arbitrary low frequencies, and at sufficiently low T only these low-ω modes are excited.
- The low-ω modes are simply standing sound waves, they should be quantized the same way as Planck had quantized light waves in 1900.



The continuum model works well at low T (the characteristic energy of excitations is ~T), where the wavelength is much greater than the inter-atomic distance a:

$$\boxed{E = \hbar\omega = \hbar \mathrm{v} k = \mathrm{v}\frac{h}{\lambda} \approx k_B T}$$

$$\lambda = \frac{h\mathrm{v}}{k_B T} = [T = 1K] \sim \frac{6.6\cdot 10^{-34} \times 2\cdot 10^{3}}{1.4\cdot 10^{-23} \times 1} \sim 10^{-7} m = 0.1 \mu m >> a$$

Assumptions: $\boxed{\omega = vk}$

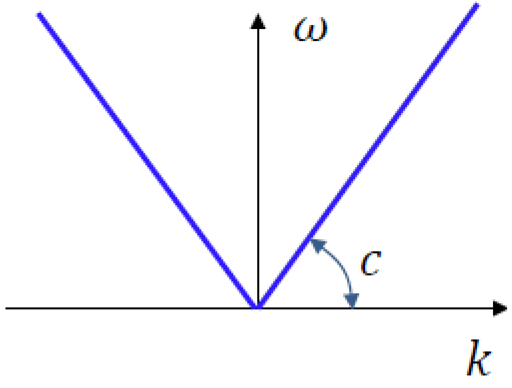
- all sound waves propagate with the same speed c (not the speed of light)
- 3 different modes – one longitudinal two transverse

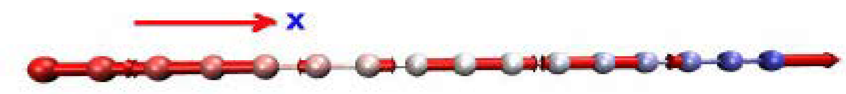
➢ - at low T the discreteness can be ignored!!

Continuum approximation

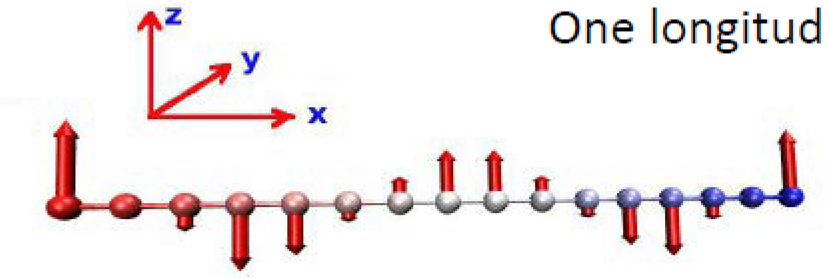
Isotropic medium: $u_n = u_{n0} e^{i(\vec{k}\cdot\vec{r} - \omega t)}$

Dispersion relation is linear $\omega = ck$





One longitudinal mode: $\vec{u}_n \,||\, \vec{k}$



Two transverse modes: $\vec{u}_n \perp \vec{k}$

We neglect the difference in the speed of propagation of longitudinal and transverse modes. In reality the phase velocity of traverse vibrations is always smaller than that for longitudinal ones - smaller restoring force (in many metals the longitudinal waves travel approx. twice as fast as the transverse ones).

In anisotropic lattices, elastic waves are combinations of longitudinal and transverse oscillations (except for a few directions of k, such as [100] in simple cubic lattice)

Einstein – quantum (low T) model

Energy of Einstein solid:

$$E = \sum_{i=1}^{3N} \hbar\omega\left(n_i + \frac{1}{2}\right)$$

n_i - the number of energy quanta in the i^{th} oscillator

Calculate $<n_i>$ the mean occupation number in the n’th level.

From statistical mechanics :
The partition function for an oscillator of frequency ω in it’s the n’th energy level

$$Z = \sum_{n=0}^{\infty} \exp\left(-\frac{E_n}{k_B T}\right)$$

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

Recall:

$$\boxed{\langle E\rangle = -\frac{\partial \ln Z}{\partial \beta}}$$

$$\boxed{\langle E\rangle = \left(\langle n\rangle + \frac{1}{2}\hbar\omega\right)}$$

Bose Einstein statistics

$$\boxed{\langle n\rangle = \frac{1}{\exp(\hbar\omega / k_B T) - 1}}$$

Debye's Calculation Following Planck

Debye assumed that the oscillation modes were waves with frequencies ω(k) = v|k| with v the sound velocity.
For each k there should be 3 oscillation modes, one for each direction of motion.
He wrote an expression analogous to Einstein's

$$\langle E\rangle \;=\; 3\sum_{\mathbf{k}} \hbar\omega(\mathbf{k}) \left(n_B(\beta\hbar\omega(\mathbf{k})) + \frac{1}{2}\right)$$

Each excitation mode is a boson of frequency ω(k) and it is occupied on average $n_B(\beta\hbar\omega(k))$ times.

For a large enough sample the sum can be converted to an integral .
We simplify the problem by using "Born-Von-Karman" boundary conditions.
In one dimension: instead of having a sample of length L with actual ends, we imagine that the two ends are connected together making the sample into a circle.

- The periodic boundary condition means that, any wave in this sample e^{ikr} is required to have the same value for a position r as it has for r + L (we have gone all the way around the circle). This then restricts the possible values of k to:

$$\boxed{k = \frac{2\pi}{L}n} \xrightarrow{\text{1D}} \boxed{\sum_k \to \frac{L}{2\pi}\int_{-\infty}^{\infty} dk} \xrightarrow{\text{3D}} \boxed{\sum_{\mathbf{k}} \to \frac{L^3}{(2\pi)^3}\int d\mathbf{k}}$$

Each k point occupies a segment of length L/2π

Each k point occupies a volume $(L/2\pi)^3$

Debye's Calculation Following Planck

Taking the continuum limit:

$$\begin{aligned}\langle E\rangle &= 3\sum_{\mathbf{k}}\hbar\omega(\mathbf{k})\left(n_B(\beta\hbar\omega(\mathbf{k}))+\frac{1}{2}\right)\\ &= 3\frac{L^3}{(2\pi)^3}\int d\mathbf{k}\,\hbar\omega(\mathbf{k})\left(n_B(\beta\hbar\omega(\mathbf{k}))+\frac{1}{2}\right)\end{aligned}$$

Assuming spherical symmetry, we integrate out the angular dependence $\int d\mathbf{k} \rightarrow 4\pi\int_0^\infty k^2 dk$

And using $k=\omega/v$

$$\langle E\rangle = 3\frac{4\pi L^3}{(2\pi)^3}\int_0^\infty \omega^2 d\omega(1/v^3)(\hbar\omega)\left(n_B(\beta\hbar\omega)+\frac{1}{2}\right)$$

Rewrite ion terms of density of states *g(ω)*: .

$$\langle E\rangle = \int_0^\infty d\omega\, g(\omega)(\hbar\omega)\left(n_B(\beta\hbar\omega)+\frac{1}{2}\right)$$

the number of modes with frequencies between ω and ω + dω is given by g(ω)dω.

Density of States: .

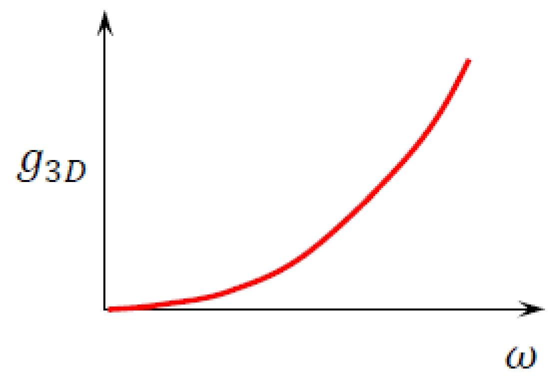
$$g(\omega) = N\left[\frac{12\pi\omega^2}{(2\pi)^3 n v^3}\right] = N\frac{9\omega^2}{\omega_d^3}$$

- n is the density of atoms, and $nL^3=N$
- *ω_D is the Debye frequency*

$$\omega_d^3 = 6\pi^2 n v^3$$

Debye's Calculation Following Planck

$$\langle E \rangle = \int_0^\infty d\omega\, g(\omega)(\hbar\omega)\left(n_B(\beta\hbar\omega) + \frac{1}{2}\right) \qquad g(\omega) = N\left[\frac{12\pi\omega^2}{(2\pi)^3 n v^3}\right] = N\frac{9\omega^2}{\omega_d^3}$$

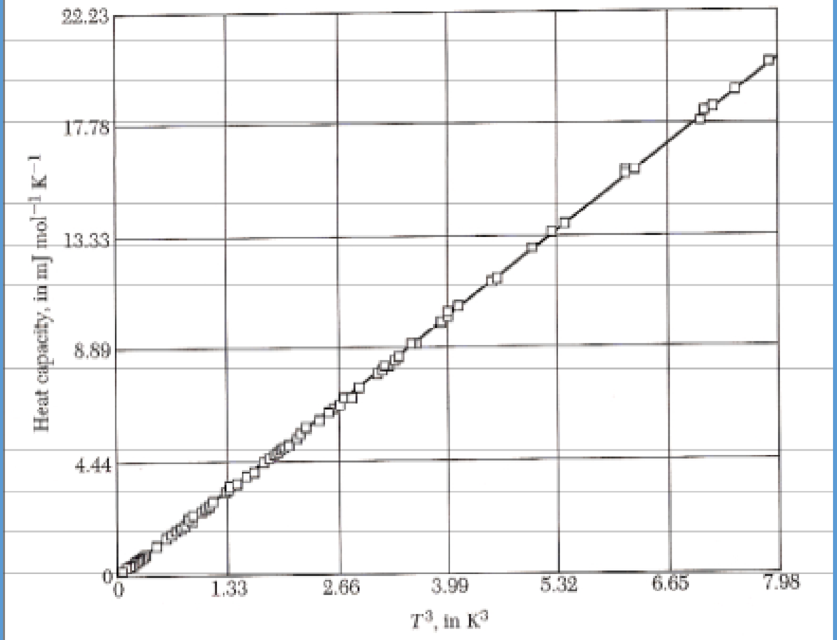


$$\boxed{x \equiv \beta\hbar\omega} \Rightarrow \langle E \rangle = \frac{9N\hbar}{\omega_d^3(\beta\hbar)^4}\int_0^\infty dx\, \frac{x^3}{e^x - 1} \quad + \quad T \text{ independent constant}$$

$$\Rightarrow \boxed{\langle E \rangle = 9N\frac{(k_B T)^4}{(\hbar\omega_d)^3}\frac{\pi^4}{15} \quad + \quad T \text{ independent constan}}$$

$$\boxed{C = \frac{\partial\langle E \rangle}{\partial T} = N k_B \frac{(k_B T)^3}{(\hbar\omega_d)^3}\frac{12\pi^4}{5} \sim T^3}$$

Gives the correct T^3 dependence at low T!!

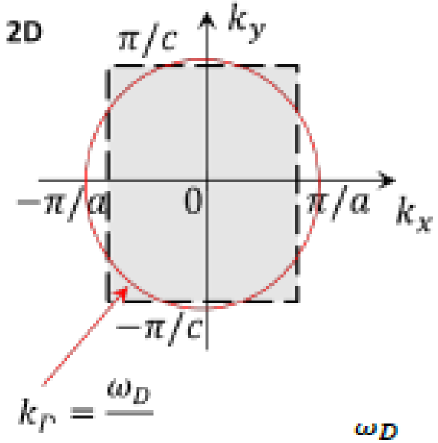


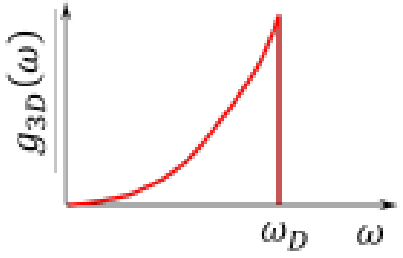
Low T heat capacity of solid Argon plotted against T^3 Finegold and Philips (1968)

Debye's correction for high T

Because of finite distance between atoms in a crystal, it does not make sense to allow arbitrary large k (i.e. arbitrary small λ) – should be a high-$\boldsymbol{k}$ ($\boldsymbol{\omega}$) cut-off.

Debye introduced an ad hoc cut-off: at high T the average energy <E> should be 3Nk_BT (the total number of modes times the energy per mode).





Total number of modes (per unit volume)
$n = N/L^3$ is the density of atoms

$$3n = \int_0^{\omega_D} g(\omega)\,d\omega$$

- cutof condition

$$\langle E\rangle = \int_0^{\omega_D} \langle n(\omega)\rangle \hbar\omega\, g(\omega)\,d\omega$$

High-T limit: $\frac{1}{e^{\beta\hbar\omega}-1} \approx (\beta\hbar\omega)^{-1}$

$$\langle E\rangle = k_BT\int_0^{\omega_D} \frac{3}{2\pi^2}\frac{\omega^2}{c^3}\,d\omega = \frac{1}{2\pi^2}\frac{k_BT}{c^3}(\omega_D)^3 = 3nk_BT$$

All 3N modes are excited, the energy of each mode ($\propto$ its amplitude squared) $\approx k_BT$.

$$\omega_D = (6\pi^2 n)^{1/3} c$$

- the ***Debye frequency***, $\boldsymbol{\omega_D}$

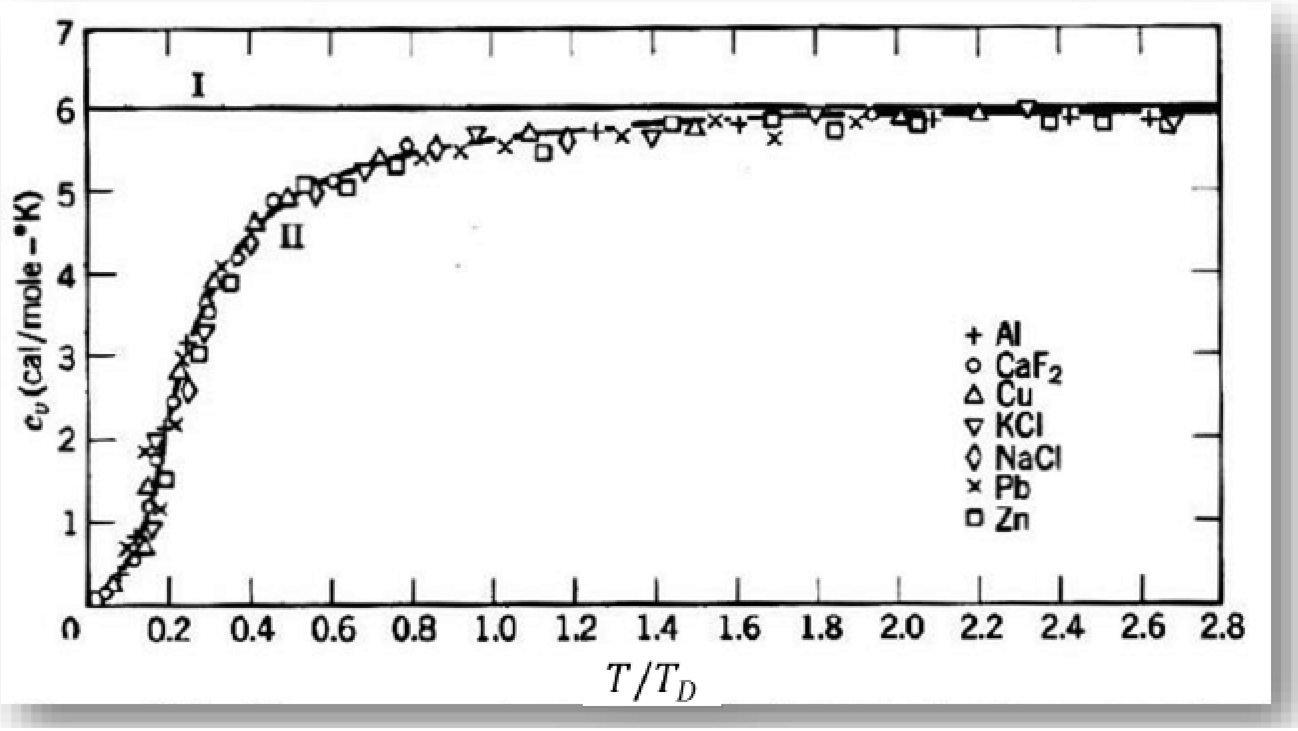
The cut-off value of $k = (6\pi^2 n)^{1/3}$ is on the order of $\frac{\pi}{a} \sim n^{1/3}$, as it should be.

Debye's specific heat compared experiment

Low T ($T \ll T_D$) $$C = \frac{2}{5}\frac{\pi^2 k_B{}^4}{(\hbar c)^3}T^3 = \frac{12\pi^4}{5}R\left(\frac{T}{T_D}\right)^3$$

High T ($T \gtrsim T_D$) $$C = 3R$$

T_D is usually determined by fitting the exp. data on specific heat.



$$\omega_{cutoff} \sim c\frac{\pi}{a}$$

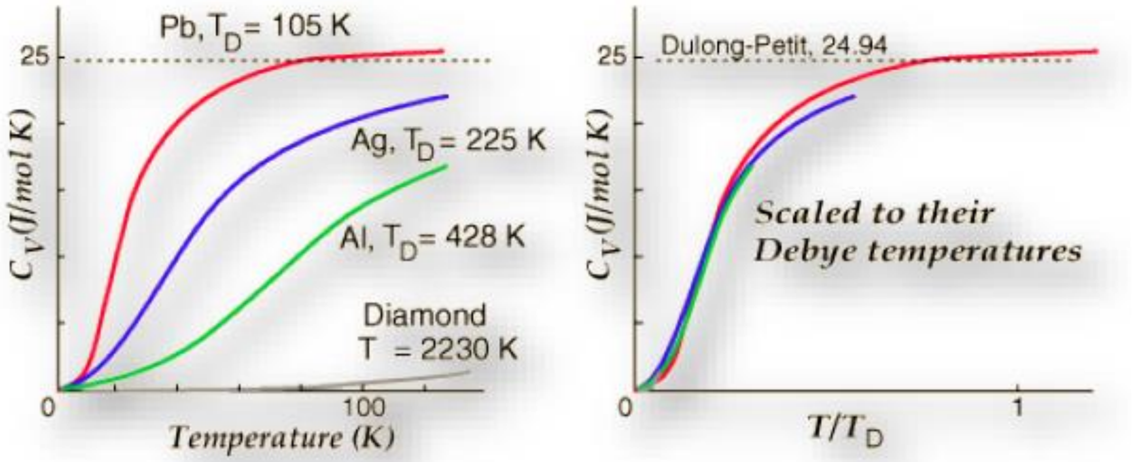
$c \sim 3\ km/s$, $a \sim 0.2\ nm$, $\omega_{cutoff} \sim 5 \cdot 10^{13}\ rad^{-1}$

Compare with the max. sound $\omega \sim 2\pi \cdot 10^4\ rad^{-1}$

The Debye Temperature

$$T_D = \frac{\hbar\omega_D}{k_B} = \frac{\hbar}{k_B}(6\pi^2 n)^{1/3}\mathrm{v}$$

The greater the sound speed and the density of ions, the higher the Debye temperature. If the temperature is normalized by T_D, the data for different materials collapse onto a universal dependence.

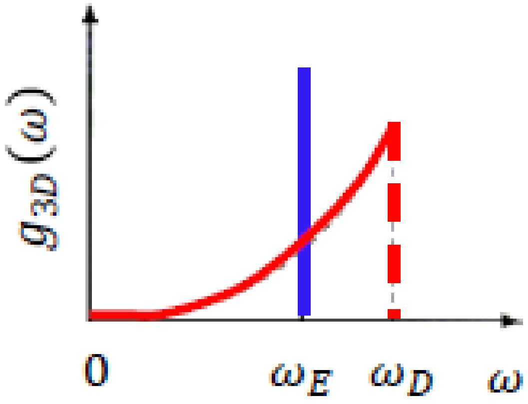


T_D varies from ~$105K$ for lead (soft, low c) to ~$2200K$ for diamond (hard, high c) .

Aluminium	428 K
Beryllium	1440 K
Cadmium	209 K
Caesium	38 K
Carbon	2230 K
Chromium	630 K
Copper	343.5 K
Gold	170 K
Iron	470 K
Lead	105 K

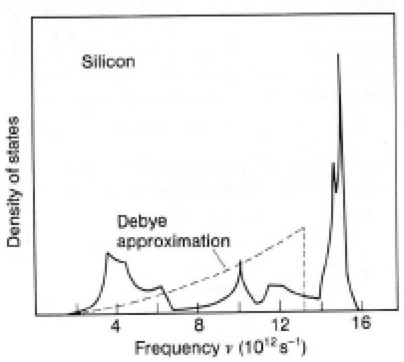
T_D plays similar role for phonons as T_F plays for electrons: it separates the high-T (classical) and the low-T (quantum) regime. In the case of electrons in metals, T_F~$10^4 K$ so only quantum regime is encountered. For phonons T_D~$10^2 - 10^3 K$, and both classical and quantum behavior can be observed.

Limitations of the Debye Theory



- The dependence $g_{3D}(\omega) \propto \omega^2$ was obtained by ignoring the discreteness of matter. In reality, $g_{3D}(\omega) \propto \omega^2$ holds only for low ω ($\lambda \gg a$). At ω~ω_D we will need to modify the dispersion relation and the corresponding density of states.
- The speed of sound is assumed to be the same for all polarizations of acoustic waves, which is not true.

The real phonon spectra are very complicated, and T_D is treated as an experimental fitting parameter.
Our goal will be to (qualitatively) understand the spectra.



Summary

- Boltzmann: classical approach (no energy quantization), works well at $k_B T \gg \hbar\omega_D$;
- Einstein: quantum ($k_B T \gtrless \hbar\omega_D$), independent oscillators, oversimplified DoS (just one ω_E) and, as a result, underestimation of E and C at low T;
- Debye: quantum, coupled oscillators = broad range of ω, DoS is more realistic but still not quite right because discreteness is not treated consistently.

Density of States: important concept that we will extensively in the course.

Einstein – quantum (low T) model

Energy of Einstein solid:

$$E = \sum_{i=1}^{3N} \hbar\omega \left(n_i + \frac{1}{2} \right)$$

n_i - the number of energy quanta in the i^{th} oscillator

Calculate $<n_i>$ the mean occupation number in the n'th level.

From statistical mechanics :
The partition function for an oscillator of frequency ω in it's the n'th energy level

$$\begin{aligned} Z &= \sum_{n=0}^{\infty} \exp\left(-\frac{E_n}{k_B T}\right) \\ &= \sum_{n=0}^{\infty} \exp\left(-\frac{(n+1/2)\hbar\omega}{k_B T}\right) \\ &= \frac{1}{2\sinh\left(\frac{\hbar\omega}{2k_B T}\right)} \\ &= \frac{1}{2\sinh\left(\frac{\beta\hbar\omega}{2}\right)} \end{aligned}$$

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

Recall:

$$\boxed{\langle E \rangle = -\frac{\partial \ln Z}{\partial \beta} = \left(\langle n \rangle + \frac{1}{2} \hbar\omega \right)}$$

Bose Einstein statistics

$$\boxed{\langle n \rangle = \frac{1}{\exp(\hbar\omega / k_B T) - 1}}$$

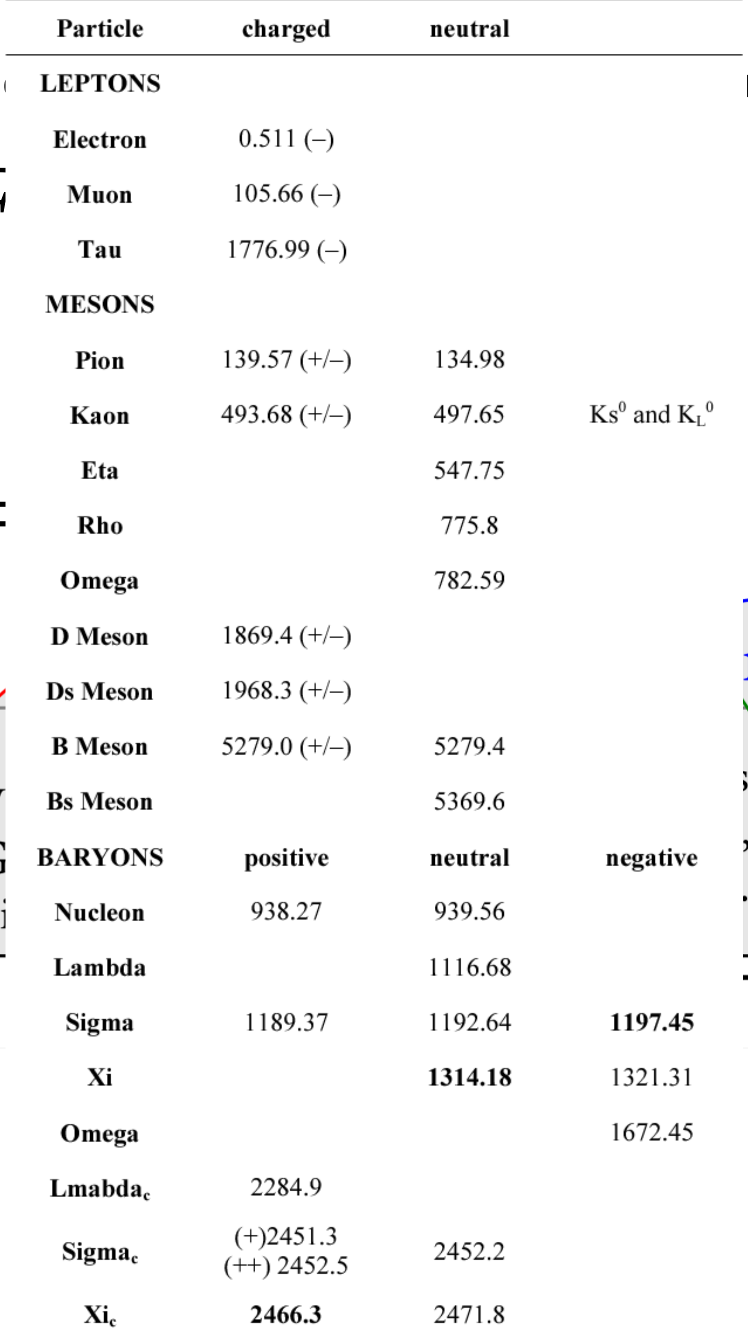
Fermi Dirac statistics

$$\boxed{\langle n \rangle = \frac{1}{\exp(\hbar\omega / k_B T) + 1}}$$

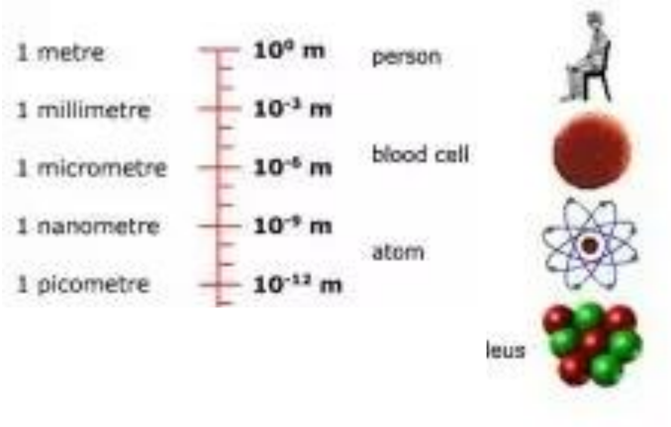
Parti nal forces

F

E :

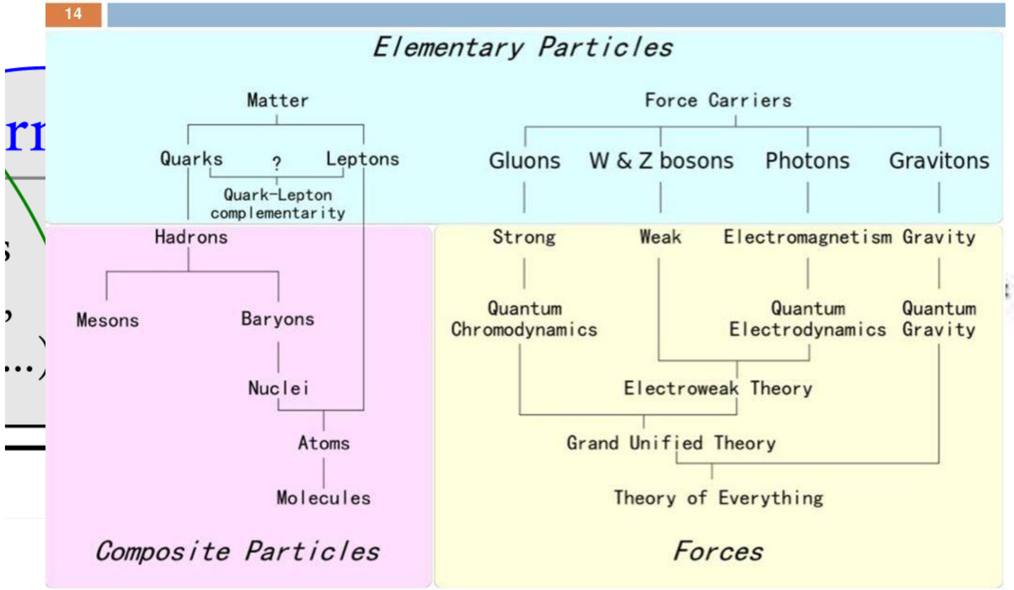


Particle	charged	neutral	
LEPTONS			
Electron	0.511 (–)		
Muon	105.66 (–)		
Tau	1776.99 (–)		
MESONS			
Pion	139.57 (+/–)	134.98	
Kaon	493.68 (+/–)	497.65	Ks^0 and $K_L{}^0$
Eta		547.75	
Rho		775.8	
Omega		782.59	
D Meson	1869.4 (+/–)		
Ds Meson	1968.3 (+/–)		
B Meson	5279.0 (+/–)	5279.4	
Bs Meson		5369.6	
BARYONS	**positive**	**neutral**	**negative**
Nucleon	938.27	939.56	
Lambda		1116.68	
Sigma	1189.37	1192.64	**1197.45**
Xi		**1314.18**	1321.31
Omega			1672.45
$Lmabda_c$	2284.9		
$Sigma_c$	(+)2451.3 (++) 2452.5	2452.2	
Xi_c	**2466.3**	2471.8	

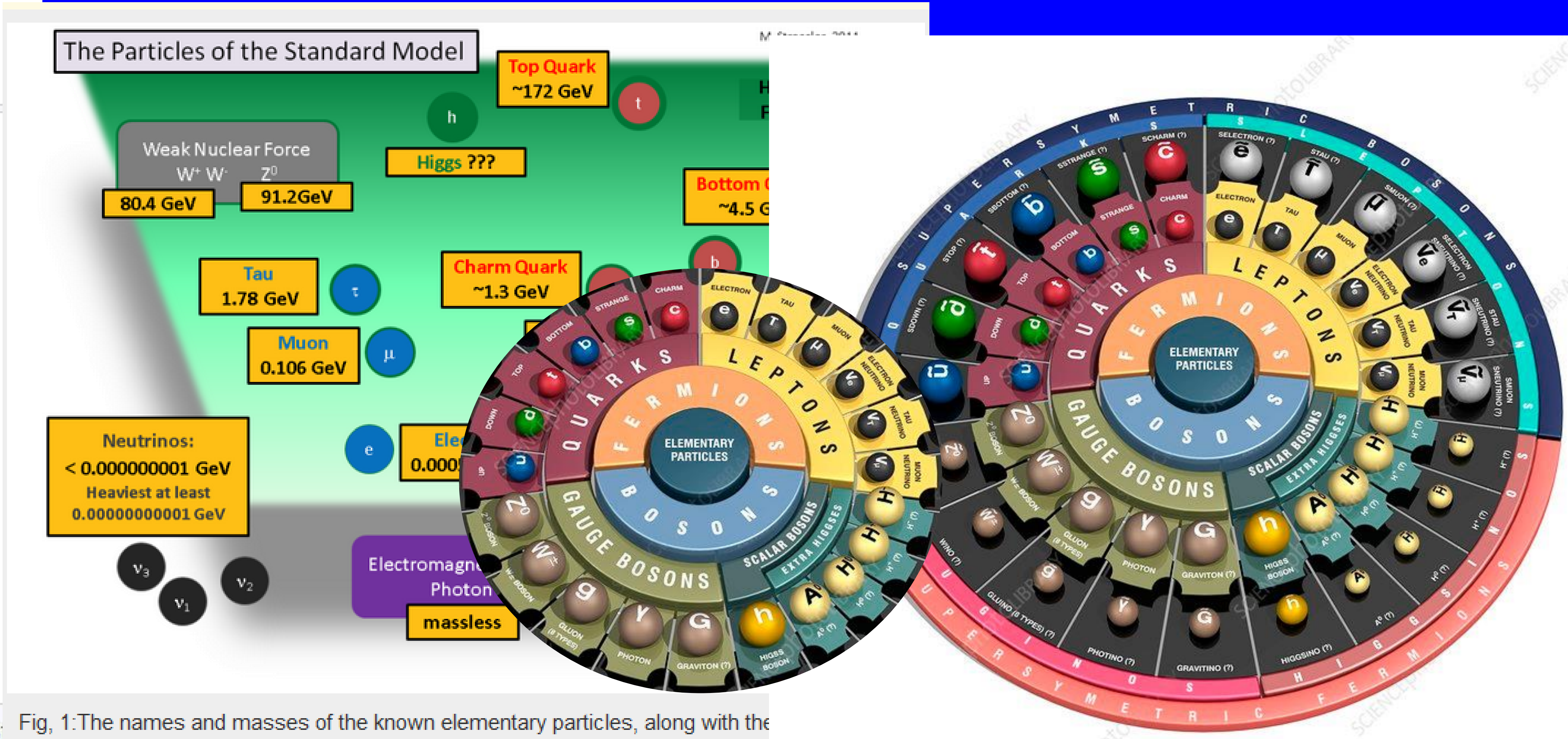


scale

Big Theory Chart



Condensed matter vacuum



S

Fig, 1:The names and masses of the known elementary particles, along with the
The universe's non-zero Higgs field is evoked by the green sea. Particle masse
mass-energies E = m c-squared) are shown, in units of a GeV, which is a few pe
the mass-energy of the lightest atom (hydrogen). Neutrino masses haven't yet been nailed down.
To avoid clutter, the gravitational force (and its carrier the presumed graviton) is not shown.

P. W. Anderson's principles

The description of the properties of materials rests on two principles:

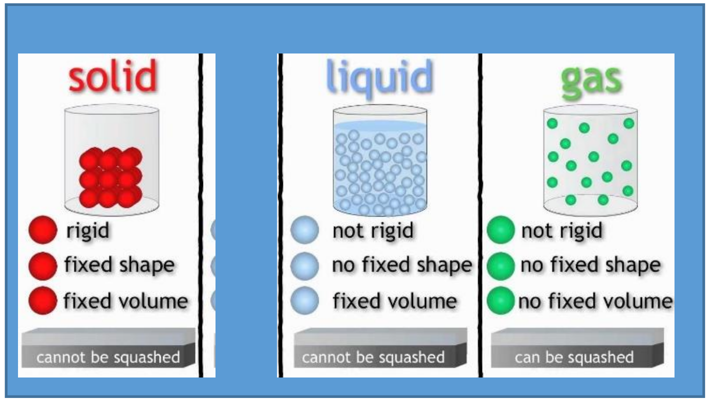
- Adiabatic continuity. Complicated systems may be replaced by simpler systems that have the same essential properties in the sense that the two systems may be adiabatically deformed into each other without changing qualitative properties.

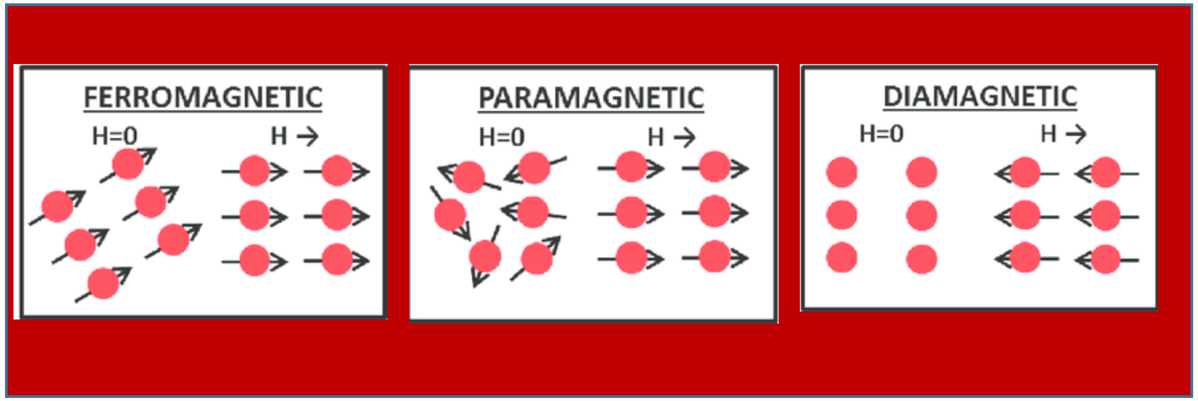
Example: Landau's Fermi liquid theory. The low-energy properties of strongly interacting electrons are the same as those of non-interacting fermions with renormalized parameters.

- Spontaneously broken symmetry. Phase transitions into states with qualitatively different properties can often be characterized by broken symmetries.

Example: Crystal versus Liquid – broken translation and rotation symmetries; Ferromagnet versus paramegnet broken rotational symmetry and time-reversal

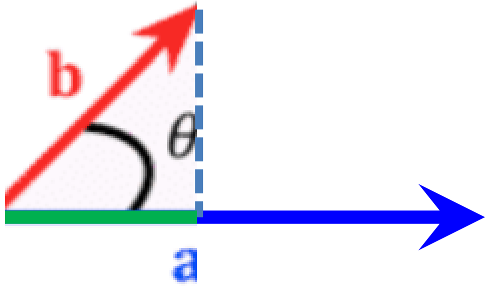
- Topological order – recently added to the list – Lifshitz transitions change in number of Fermi surfaces





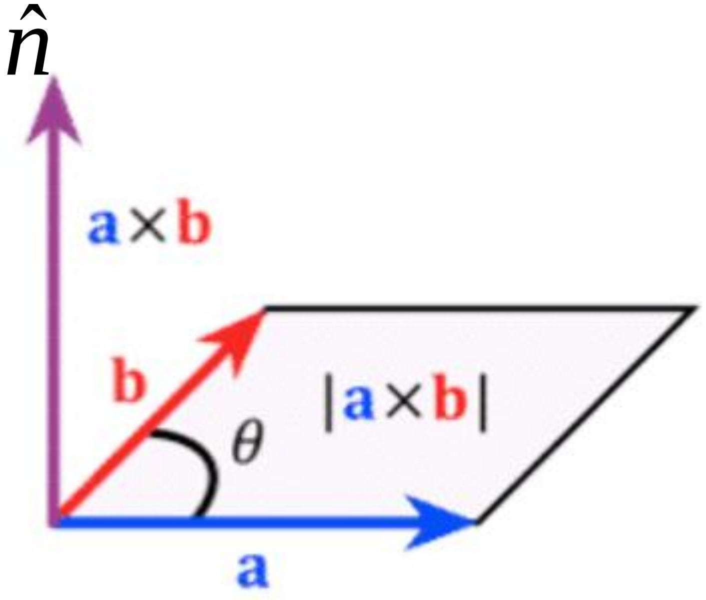
Dot (Scalar) product

$$\vec{a} \cdot \vec{b} = \left|\vec{a}\right| \cdot \left|\vec{b}\right| \cos\theta$$



Cross (vector) product

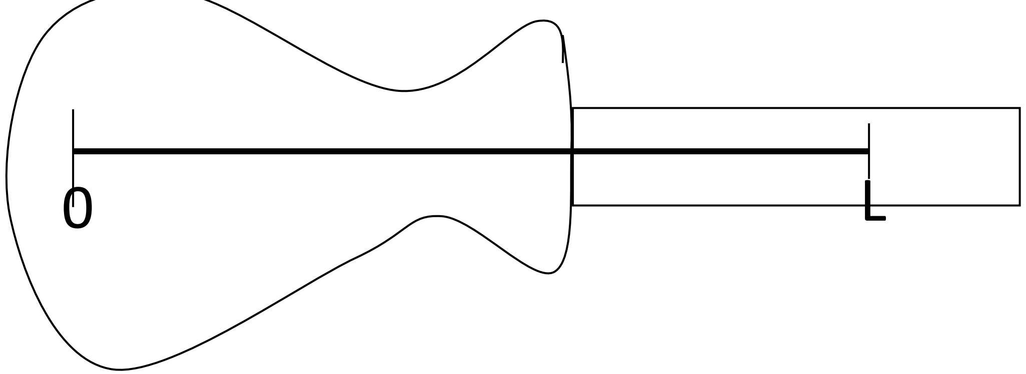
$$\vec{a}\times\vec{b} = \hat{n}\left|\vec{a}\right|\cdot\left|\vec{b}\right|\sin\theta$$



$$c = \begin{vmatrix} i & j & k \\ a_1 & a_2 & a_3 \\ b_1 & b_2 & b_3 \end{vmatrix}$$

$$\begin{aligned} c = {} & [(a_2 \times b_3) - (a_3 \times b_2)]\, i \; + \\ & [(a_3 \times b_1) - (a_1 \times b_3)]\, j \; + \\ & [(a_1 \times b_2) - (a_2 \times b_1)]\, k \end{aligned}$$

$$\boxed{\frac{\partial^2 y}{\partial x^2} = \frac{1}{v^2}\frac{\partial^2 y}{\partial t^2}}$$



Functional form of solution?

y(x,t) = Asin(kx)cos(ωt) + Bcos(kx)sin(ωt)

Boundary conditions?

I. y(x,t) = 0 at x=0 and x=L

At x=0: y(x,t) = Bsin(ωt) = 0 → only works if B=0

y(x,t) = Asin(kx)cos(ωt)

Evaluate y(x,t)=0 at x=L. What are possible values for k?

a. k can have any positive or negative value

b. π/(2L), π/L, 3π/(2L), 2π/L …

c. π/L

d. π/L, 2π/L, 3π/L, 4π/L …

e. 2L, 2L/2, 2L/3, 2L/4, ….

Answer is d: k=nπ/L

Boundary conditions put constraints on k …

causes *quantization of k and λ!!!*

Dispersion

- The group velocity is $u_{\mathrm{gr}} = \dfrac{d\omega}{dk}$
- For a de Broglie wave: $E = hf = \hbar(2\pi f) = \hbar\omega$

  $p = \hbar k$

- The group velocity of a de Broglie wave packet is thus:

$$u_{gr} = \frac{d\omega}{dk} = \frac{dE}{dp}$$

Using: $E = \sqrt{(pc)^2 + (mc^2)^2}$

$$\Longrightarrow \boxed{u_{\mathrm{gr}} = \frac{dE}{dp} = \frac{pc^2}{E}}$$

Group velocity and phase velocity

- The group velocity is $u_{\mathrm{gr}} = \dfrac{d\omega}{dk}$

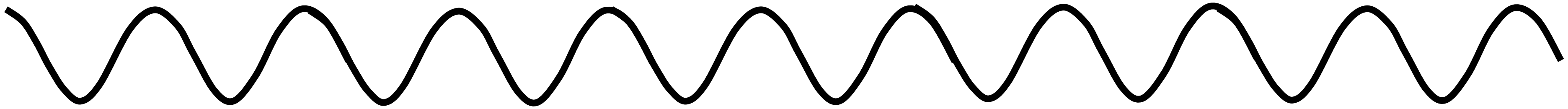
- The relationship between the phase velocity and the group velocity is

$$u_{\mathrm{gr}} = \frac{d\omega}{dk} = \frac{d}{dk}\left(v_{\mathrm{ph}} k\right) = v_{\mathrm{ph}} + k\frac{dv_{\mathrm{ph}}}{dk}$$

- Hence the group velocity may be greater or less than the phase velocity. A medium is called **nondispersive** when the phase velocity is the same for all frequencies and equal to the group velocity.

Plane Waves vs. Wave Packets

$$\Psi(x,t) = A\exp\left[i\left(kx-\omega t\right)\right]$$



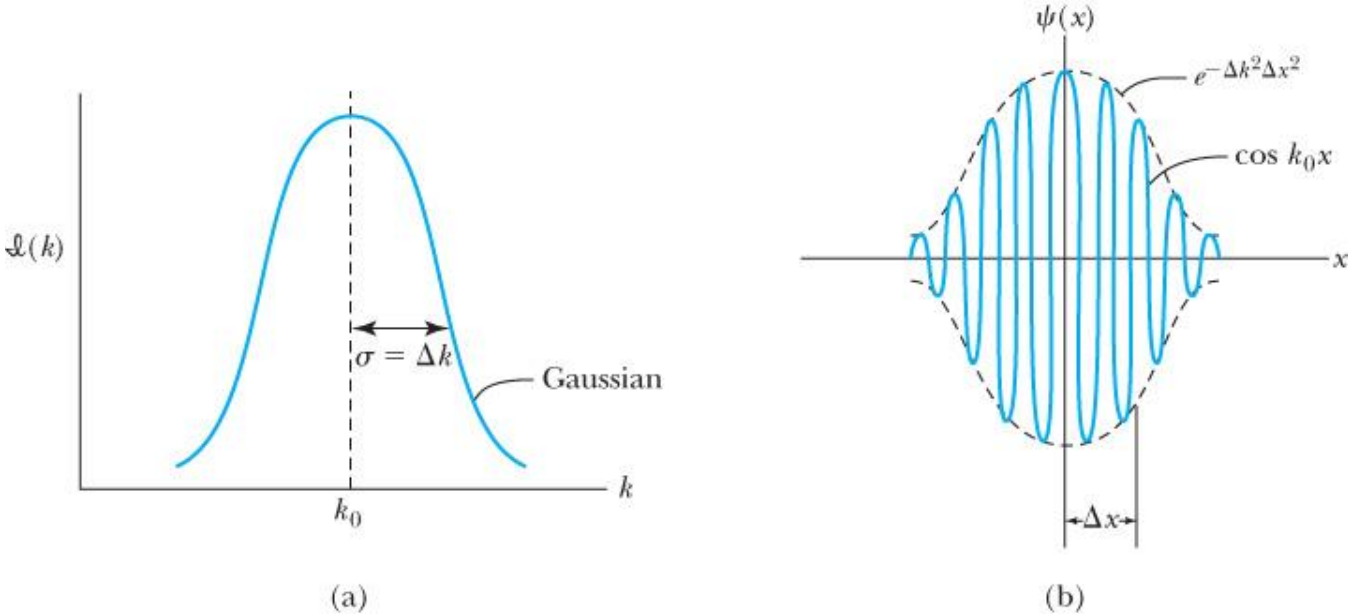
$$\Psi(x,t) = \sum_n A_n \exp\left[i\left(k_n x-\omega_n t\right)\right]$$

Which one looks more like a particle?

Gaussian Function

- A Gaussian wave packet describes the envelope of a pulse wave.

$$\Psi(x,0)=\Psi(x)=Ae^{-\Delta k^2x^2}\cos(k_0x)$$



- The localization of the wave packet over a small region to describe a particle requires a large range of wave numbers. Conversely, a small range of wave numbers cannot produce a wave packet localized within a small distance.

$$\boxed{\Delta k\ \Delta x=\frac{1}{2}\quad \Delta\omega\ \Delta t=\frac{1}{2}}$$

Normalization and Probability

- The probability $P(x)\,dx$ of a particle being between x and $x + dx$:

$$P(x)\,dx = \Psi^*(x,t)\,\Psi(x,t)\,dx$$

here Ψ^* denotes the complex conjugate of Ψ

- The probability of the particle being between x_1 and x_2 is given by

$$P = \int_{x_1}^{x_2} \Psi^* \Psi \; dx$$

- The wave function must also be normalized so that the probability of the particle being somewhere on the x axis is 1.

$$\int_{-\infty}^{\infty} \Psi^*(x,t)\,\Psi(x,t)\; dx = 1$$