INTERNATIONAL INSTITUTE OF INFORMATION TECHNOLOGY

HYDERABAD

Science-1: prep notes

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General pointers

1. State of system: 3-dimensional Cartesian coordinate system.
   - scalar quantities (mass, temperature)
   - vector quantities (position vector, velocity and momentum, angular momentum and torque)
2. Vector calculus:
   - vector equalities, addition
   - vector dot product, cross products
   - gradient of a scalar function
   - line integrals: circulation and curl of vector fields
   - surface integrals: flux and divergence of vector fields

Laws of Newton

1. Ist Law: Inertia. Inertial frames. Uniform rectilinear motion of an object in absence of forces
2. IInd Law: Definition of momentum. Rate of change of momentum equals the net external force on the object
3. IIIrd Law: For central forces, the reaction is equal and opposite to action

Great generality of these laws of motion to all kinds of phenomena. Spurred by advances in mathematics.

Work, kinetic energy.

Work done on an object by application of external force $\vec{F}(t)$ is given by:

$$W = \int_{t_1}^{t_2} \vec{F}(t) \cdot d\vec{r}(t)$$

- Using Newton IInd Law, we get $W = \int_1^2 \frac{d\vec{p}}{dt} \cdot \vec{v}(t)dt = \frac{1}{2}mv_2^2 - \frac{1}{2}mv_1^2 = K_2 - K_1$

Defining $K = \frac{1}{2}mv^2$ as kinetic energy, we see force acting on system changes the kinetic energy of the system.

Conservative forces, potential energy

- If the force is conservative, i.e. $\vec{F}(\vec{r}) = -\nabla U(\vec{r})$, then $W = \int_1^2 (-\nabla U) \cdot d\vec{r} = -(U_2 - U_1)$.
- Thus conservative forces have an associated potential energy function U
- For conservative forces, the above shows that work W is path-independent, depending only on end-point potential energies
- $W = K_2 - K_1 = -(U_2 - U_1)$
- Thus, $K_1 + U_1 = K_2 + U_2$. Law of conservation of mechanical energy

Law of conservation of linear momentum

For a vector $\vec{s}$, if $\vec{F} \cdot \vec{s} = 0$, then

- $\vec{F} \cdot \vec{s} = \frac{d\vec{p}}{dt} \cdot \vec{s} = \frac{d}{dt}\left(\vec{p} \cdot \vec{s}\right)$
- $\vec{F} \cdot \vec{s} = 0$ implies $\left(\vec{p} \cdot \vec{s}\right)$ is a constant
- Thus momentum in the direction of $\vec{s}$ is conserved

Torque & Angular momentum and its conservation

- Angular momentum about origin: $\vec{L} \equiv \vec{r} \times \vec{p}$
- Torque $\vec{N} \equiv \frac{d}{dt}\vec{L} = \frac{d\vec{r}}{dt} \times \vec{p} + \vec{r} \times \frac{d\vec{p}}{dt}$
$$\vec{N} = \vec{v} \times m\vec{v} + \vec{r} \times \vec{F} = 0 + \vec{r} \times \vec{F}$$
$$\vec{N} = \frac{d}{dt}\vec{L} = \vec{r} \times \vec{F}$$
- $\vec{N} \cdot \vec{s} = 0 \implies \frac{d}{dt}\left(\vec{L}.\vec{s}\right) = 0;$
Conservation of Angular momentum along the direction of zero torque.

For conservative forces, show conservation of energy

- $E = T(\vec{v}(t)) + U(\vec{r}(t), t) \implies \frac{d}{dt}E = \frac{d}{dt}T + \frac{d}{dt}U$
- $\frac{d}{dt}T = m\vec{v} \cdot \frac{d}{dt}\vec{v} = m\vec{v} \cdot \vec{a} = \vec{v} \cdot \vec{F}$
- $\frac{d}{dt}U(\vec{r}, t) = \sum_\alpha \frac{\partial U}{\partial x_\alpha}\frac{dx_\alpha}{dt} + \frac{\partial U}{\partial t} = \vec{v} \cdot \nabla U + \frac{\partial U}{\partial t}$
- $\frac{d}{dt}E = \frac{d}{dt}(T + U) = \vec{v} \cdot (\vec{F} + \nabla U) + \frac{\partial U}{\partial t}$

$\frac{d}{dt}E = \frac{\partial U}{\partial t} \implies E =$constant when $U \equiv U(\vec{r})$

Galilean Relativity

All inertial frames have same form of mechanical law.

Two inertial frames, K and K' having relative velocity v. Then, a particle having $\vec{u}$ in K-frame, $\vec{u}'$ in K'-frame. Then

$$\vec{u}' = \vec{u} - \vec{v}$$

Thus, clearly $\frac{d\vec{p}'}{dt} = \frac{d\vec{p}}{dt}$. This gives

$$\vec{F}' = \vec{F}$$

Hence, all mechanical laws remain in same form in both inertial frames.

Problem solving strategy

- Identify forces, draw free body diagram
- "balance forces" to satisfy constraints
- set up dynamical equations (Use IInd/IIIrd Laws and/or use conservation laws)
- solve math of dynamical equations, with appropriate boundary conditions

Examples: next slide

Single particle, constrained motion

- Need to introduce ‘balancing’ forces. Examples:
  - block moving on a horizontal plane. “normal force”
  - block moving down inclined plane.

For Simple Harmonic Oscillator, find EoM

For Simple Harmonic Oscillator, find EoM

- Hooke's law: $F(x) = -kx$, EoM as $m\ddot{x} = -kx$
- Rewrite as: $\ddot{x}(t) + \omega_0^2 x(t) = 0$, with $\omega_0 = \sqrt{\frac{k}{m}}$
- Differential equation: second order. Linear in x
- One standard practice: convert to two first order differential equation. With $p = m\dot{x}$
  two equations $\frac{d}{dt}p(t) = -kx$ and $\frac{d}{dt}x(t) = p(t)/m$
- $\frac{d}{dt}(x, p) = (p/m, -kx)$, with $(x(0), p(0)) = (x_0, p_0)$
- Conservation of energy, $E = \frac{1}{2m}p^2 + \frac{1}{2}mx^2$
- Note: solution is $x(t) = A_+ e^{i\omega_o t} + A_- e^{-i\omega_o t}$
- Phase diagram: $x(t)$ vs $p(t)$

Show that SHO is applicable for other systems near ‘minima’

Limitations of Newtonian Mechanics

- Handling of constraints (will return to this later)
- Galilean Invariance (Newtonian Relativity) violated by EM: Special Theory of Relativity

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Reasons & postulates of Special Theory of Relativity

- Electromagnetic phenomena seemingly in violation
  - EM wave equation is not Galilean invariant
  - same phenomena seen differently in inertial frames
    - Moving coil, magnet at rest: magnetic field exerts forces ($qv \times B$) on charges in coil, generating current
    - moving magnet, coil at rest: time varying magnetic flux creates electric field on charges (motive emf, Faraday's Law)
- Speed of light is same in all inertial frames (expts)

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Postulates of Special Theory of Relativity (Einstein 1905)

- Same physical laws in all inertial frames
- Speed of light is same value in all inertial frames

Events simultaneous in all frames? NO!

Concept: Relativity of simultaneity.

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Observer located at the middle of a train, receives flash from front and back of train; flashes set off at same time.

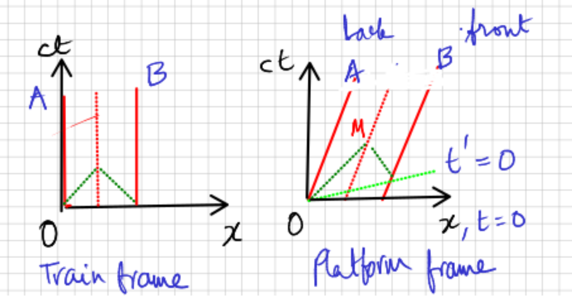

Figure: Space-time diagrams in (left) train-fixed frame and (right) platform-fixed frame, with *c* being same value in both.
Red lines are for front, back and mid-points of train.
Green lines are for light and have same slope in both plots.

How do space-time coordinates transform?

Frame K' with relative velocity v w.r.t. frame K

$$\begin{aligned} x' &= \gamma\,(x - vt) \\ y' &= y \\ z' &= z \\ t' &= \gamma\,(t - \frac{xv}{c^2}) \end{aligned} \quad \Longleftrightarrow \quad \begin{aligned} x &= \gamma\,(x' + vt') \\ y &= y' \\ z &= z' \\ t &= \gamma\,(t' + \frac{x'v}{c^2}) \end{aligned}$$

$$\gamma = \frac{1}{\sqrt{1 - \frac{v^2}{c^2}}}$$

$K-$frame the event $e = (x, t)$ has transformed $K'-$frame coordinates $e' = (x', t')$

Space-time invariant has same value in both frames:
$(\Delta s)^2 = (\Delta x)^2 + (\Delta y)^2 + (\Delta z)^2 - (c\Delta t)^2$

Notes on Lorentz transform

K'-frame is moving with velocity v w.r.t. K-frame

- Given an event $e = (x, y, z, t)$, use forward transform to get $e' = (x', y', z', t')$
- Strategy is to use difference in events as experimental measurable
- Note: interchaning prime with unprimed variables and changing v to $-v$ gives Inverse Lorentz Transform. This is an important symmetry!

What is time difference between ticks of a clock as measured from a moving frame?

Take events, $e_0 = (0, 0)$ and $e_1 = (0, \tau_0)$, $e_2 = (0, 2\tau_0), \cdots$
(i.e. ticking of the clock stationary in K-frame)

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In K'-frame, using Lorentz transform, we get $e'_n = (-\gamma v n\tau_0, \gamma n t_0)$.

Hence time difference between two consecutive ticks of the stationary clock will be measured in K'-frame as $\gamma(n-(n-1))t_0 = \gamma t_0$.

This effect is known as Time dilation

What is the length of a rod as measured from moving frame?

Back end of rod: $e_1 = (0, t)$ and
front-end of rod $e_2 = (L_0, t)$ for any t
To measure rod length in K'−frame, we need to find $e'_{1,2}$
with $t'_1 = t'_2$

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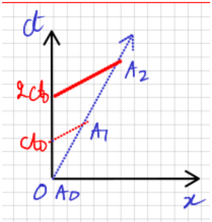
$\Delta x' = \gamma(\Delta x - v\Delta t)$
The forward transform involves knowing unprimed quantities , but we do not know which t to use to get x'), we will use inverse Lorentz transform: $x = \gamma(x' + vt')$, giving us $x_{1,2} = \gamma(x'_{1,2} + vt'_{1,2})$ and thus
$\Delta x = x_2 - x_1 = \gamma(\Delta x' + v \cdot 0)$
This gives us

$$\Delta x = \gamma \Delta x' \implies L_0 = \gamma L' \implies L' = L_0\sqrt{1 - \frac{v^2}{c^2}}$$

This is known as Length Contraction

What is the frequency measured by a moving observer?



$$A_0 = (0,0) \implies A'_0 = (0,0)$$

$$A_1 : ct = x + ct_0 \;\&\; x = vt \implies ct_1 = \frac{ct_0}{c-v}$$

$$A_2 : ct = x + 2ct_0 \;\&\; x = vt \implies ct_2 = \frac{2ct_0}{c-v}$$

$$A_1 = \left(\frac{vct_0}{c-v}, \frac{ct_0}{c-v}\right) \implies A'_1 = \left(0, \gamma\left[\frac{ct_0}{c-v} - \frac{v}{c^2}\frac{vct_0}{c-v}\right]\right)$$

$$\nu' = \frac{1}{\Delta t'} = \nu\sqrt{\frac{1-\beta}{1+\beta}}$$

Frequency shift is velocity dependent; velocity of stars

What about moving rod and a moving clock?

Symmetry: both moving and stationary observer will say exactly same thing about other!

- stationary clock is measured to have “longer time difference between consequtive ticks” by moving observer
- a stationary observer will measure a moving clock to have ”longer time difference between consecutive ticks”
- a stationary rod is measured to be shorter than its rest length by moving observer
- a moving rod is measured to be shorter than its rest length by stationary observer

Derive relative velocity formulae

Particle with $x(t) = ut$, what is its velocity in K' frame?

$$x' = \gamma(x - vt) \implies \frac{dx'}{dt} = \gamma(\frac{dx}{dt} - v)$$

$$t' = \gamma\left(t - x\frac{v}{c^2}\right) \implies \frac{dt'}{dt} = \gamma(1 - \frac{dx}{dt}\frac{v}{c^2})$$

$$\frac{dx'}{dt'} = \frac{u_x - v}{1 - \frac{u_x v}{c^2}}$$

$$\frac{dy'}{dt'} = \frac{u_y}{\gamma\left(1 - \frac{u_x v}{c^2}\right)}$$

$$\frac{dz'}{dt'} = \frac{u_z}{\gamma\left(1 - \frac{u_x v}{c^2}\right)}$$

What is the relativistic momentum?

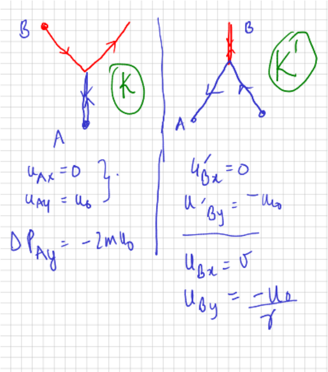


Figure: In $K-$frame (K'-frame), particle A (B) is has u_0 velocity.

Momentum change of A is $-2mu_0$, but NOT for B!
Having $\vec{p} = \gamma(u)\, m\vec{u}$, solves this issue.

From momentum, find energy of particle.

Show $K = (\gamma_u - 1)mc^2$, and hence suggest $E_0 = mc^2$.
Also $E^2 = (pc)^2 + (mc^2)^2$

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$$W = \int_1^2 F \cdot dr = \int_1^2 \frac{d\vec{p}}{dt} \cdot \vec{u}dt = \int_1^2 \frac{d(\gamma m\vec{u})}{dt} \cdot \vec{u}dt$$

After a bit of math, $W = \int_1^2 \frac{d}{dt}(\gamma mc^2)dt = (\gamma(u) - 1)mc^2$,
to get from rest to velocity $\vec{u}$.
Since $W = K_2 - K_1$, we get $K = (\gamma(u) - 1)mc^2$
Hence, total energy $E = \gamma mc^2$, rest mass energy
$E_0 = mc^2$, gives $K = E - E_0$

Since $E = \gamma mc^2$, and $p^2 = \gamma^2 m^2 u^2$, we get
$E^2 - p^2c^2 = \gamma^2 m^2 c^4 (1 - u^2/c^2) = m^2 c^4$
Energy formula: $E^2 = (pc)^2 + (mc^2)^2$ for free particle

Space-time invariant

- Events: $e_1 = (x_1, y_1, z_1, t_1)$ and $e_2 = (x_2, y_2, z_2, t_2)$
- Define $(\Delta s)^2 = (\Delta x)^2 + (\Delta y)^2 + (\Delta z)^2 - c^2(\Delta t)^2$
- Lorentz Tranform: $x' = \gamma(x - \beta ct),\ ct' = \gamma(ct - x\beta)$, $y' = y$, $z' = z$ with $\beta = v/c$
- Define $(\Delta s')^2 = (\Delta x')^2 + (\Delta y')^2 + (\Delta z')^2 - c^2(\Delta t')^2$
- $(\Delta s')^2 =$ $\gamma^2 \left[(\Delta x - \beta c\Delta t)^2 - (c\Delta t - \beta \Delta x)^2\right] + (\Delta y)^2 + (\Delta z)^2$ $=\gamma^2(1 - \beta^2)\left[(\Delta x)^2 + c^2(\Delta t)^2\right] + (\Delta y)^2 + (\Delta z)^2$ $= (\Delta s)^2$
- Space-time 4-vector $\vec{s} = (x, y, z, ict)$
- If $(\Delta s)^2 < 0$, an inertial frame exists where both events happen at same position but at different times. Time-like interval. Allows for casual relationships between two events.
- If $(\Delta s)^2 > 0$, space-like interval. Both can happen at same time, but at different spatial locations.

Show electric and magnetic effects are equivalent by STR.

Consider a infinite line of charges with density λ on x-axis, and a charge q at a distance d from this "wire" of charges. All charges at rest. The charge q will experience a force $\vec{F} = q\vec{E}$ directly away from the wire ('repelling' force).

Consider now a frame K' where all the charges are moving to right ($+x-$axis) with velocity v. Now the charge q will experience two forces
(a) 'repelling' electric force
(b) 'attractive' magnetic force

Due to length contraction in K'-frame, density of charges is larger ($\lambda' > \lambda$) and hence the repelling electric force is larger. But the 'new' magnetic force exactly cancels the part that is in excess to case of stationary charges!

Equivalence of electric and magnetic effects (continued)

- Additional reference: https://tinyurl.com/4x2629nv, where force on two parallel line of charges are analysed from two inertial frames
- Maxwell laws of electromagnetism showed that magnetic fields result from time-varying electric fields (due to currents, Biot-Savart Law) and electric fields result from time-varying magnetic fields (Faraday's Law). Maxwell laws demonstrate the connection between electricity and magnetism.
- Special theory of relativity goes one step further: electric forces and magnetic forces are the same phenomena viewed from different inertial frames.

Review: One particle Newtonian Mechanics

- Identify forces, draw free body diagram
- “balance forces” to satisfy constraints
- set up dynamical equations (Use IInd/IIIrd Laws and/or use conservation laws)
- solve math of dynamical equations, with appropriate boundary conditions

Examples: get Equations of Motion

1. Freely falling body, $\vec{F} = m(0, 0, -g) = m\frac{d^2}{dt^2}(x, y, z)$
2. Charged particle in magnetic field: $\vec{F} = q\vec{v} \times \vec{B}$
3. Block sliding down an incline (no friction)
4. Simple pendulum

Note: In Ex: 4 (5) constraint force is (is not) constant

From EoM to path properties

- Newton's laws: forces change state of system
  $\frac{d}{dt}(x, v) = (v, F/m)$ for each time point t,
- Ex: Harmonic Oscillator (1-dim): $F(x) = -kx = m\ddot{x}$
  Trajectory $x(t) = A\cos(wt),\ p(t) = -Amw\sin(wt)$
  Alternate description $(x/A)^2 + (p/B)^2 = 1$
  Describes whole path, not just at single time
- Ways to get path description:
  - Conservation laws $E = T + U$ along path
  - Straight line path for free particle
  - Also, for free particle minimum average kinetic energy path $T_{avg} = \frac{1}{t_2 - t_1} \int_{t_1}^{t_2} dt\ T(t)$.
- Fermat minimum time principle for path of light:
  Snell's Law of refraction at interface between medium

Hand-wavy derivation of a path principle

- $F = \dot{p} \implies [F(t) - \dot{p}(t)] \cdot \eta(t) = 0$
- $J \equiv \int_1^2 [F - \dot{p}] \cdot \eta(t)\, dt$.
  For true path $(x^*(t), v^*(t))$, $J = 0$
- $J[\eta] = \int_1^2 [-\frac{\partial U}{\partial x} - m\dot{v}] \cdot \eta\, dt$
- Use $\frac{d}{dt}(v \cdot \eta) = \dot{v} \cdot \eta + v \cdot \dot{\eta}$ to get
  $J = \int_1^2 [-\nabla U \cdot \eta - m\frac{d}{dt}(v \cdot \eta) + mv \cdot \dot{\eta}]dt$
- Set $\eta(t_{1,2}) = 0$. Giving $J = \int_1^2 [-\nabla U \cdot \eta + mv \cdot \dot{\eta}]dt$
- Set $\eta(t) = x(t) - x^*(t)$, i.e. small variation of path from true path. $\delta x(t) = \eta(t), \delta v = \dot{\eta}(t)$
- $L(x, v) = -U(x) + mv^2/2 \implies J = \int_1^2 \delta L(x, v)dt$
- Action $S \equiv \int_1^2 L(x, v)dt$, thus $J = \delta S = 0$ for true path
- Principle of stationary action: $\delta S = 0$

Issues with derivation

- Issue-1: When constraints present, $F = -\nabla U + F_C$.
  But F_C is not included in above derivation
  Note that $F_c(t) \cdot dx^*(t) = 0$ on true path
- Issue-2: Non-simple constraints Ex: Pendulum
- Mathematically rigorous derivation of
  "Euler-Lagrange equations" MT-C7.6
  - $F_k = m\frac{d^2}{dt^2}x_k = m_k\frac{d^2}{dt^2}x_k$
  - $x_k \equiv x_k(\{q\}, t) \implies$

    $$\dot{x}_k = \sum_m \frac{\partial x_k}{\partial q_m}\dot{q}_m + \frac{\partial x_k}{\partial t} \quad \& \quad \frac{\partial \dot{x}_k}{\partial \dot{q}_n} = \frac{\partial x_k}{\partial q_n}$$
  - After a bit of algebra, using $L = T - U$

    $\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_k}\right) = \frac{\partial L}{\partial q_k}, \quad \forall k$
- Action $S = \int_{t_1}^{t_2} dt\, L(\{q_k\}, \{\dot{q}_k\}, t)$. Then

$$\delta S = 0 \iff \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_k}\right) = \frac{\partial L}{\partial q_k}, \quad \forall k$$

Calculus of variations: Find stationary soln.

- $J = \int_{x_A}^{x_B} dx \; f\left(y(x), \frac{dy}{dx}(x); x\right)$,
  find $y(x)$ s.t. J is extremum, with fixed $y(x_{A,B}) = y_{A,B}$
- Path space parametrization: $y(\alpha, x) = y(0, x) + \alpha\eta(x)$
- $J(\alpha) = \int_{x_1}^{x_2} f\left(y(\alpha, x), y'(\alpha, x); x\right) dx \implies$
  for true path $y(0, x)$, we have $\frac{\partial J}{\partial \alpha}|_{(\alpha=0)} = 0$
- With $y = y_0 + \alpha\eta$, we have $\frac{\partial y}{\partial \alpha} = \eta$, $\frac{\partial y'}{\partial \alpha} = \frac{d\eta}{dx}$
- $\frac{\partial J}{\partial \alpha} = \frac{\partial}{\partial \alpha} \int_{x_1}^{x_2} dx \; f(y, y'; x)$, with $y(\alpha), y'(\alpha)$
-

$$\frac{\partial J}{\partial \alpha} = \int_{x_1}^{x_2} dx \; \left(\frac{\partial f}{\partial y} \frac{\partial y}{\partial \alpha} + \frac{\partial f}{\partial y'} \frac{\partial y'}{\partial \alpha} \right) = \int_{x_1}^{x_2} \left(\frac{\partial f}{\partial \alpha} \eta + \frac{\partial f}{\partial y'} \frac{d\eta}{dx} \right)$$

Calculus of variations (cntd.)

- $\frac{d}{dx}\left(\frac{\partial f}{\partial y'}\eta\right) = \eta\frac{d}{dx}\frac{\partial f}{\partial y'} + \frac{\partial f}{\partial y'}\frac{d\eta}{dx}$
- Thus for $\eta(t_{1,2}) = 0$, we get

$$\frac{\partial J}{\partial \alpha} = \int_{x_1}^{x_2} dx \left(\frac{\partial f}{\partial y} - \frac{d}{dx}\frac{\partial f}{\partial y'}\right)\eta(x)$$

- Setting $\frac{\partial J}{\partial \alpha} = 0$, for every η then gives:

$$\frac{\partial f}{\partial y} = \frac{d}{dx}\frac{\partial f}{\partial y'}$$

This is the famous Euler-Lagrange equation, with $f \equiv f\,(y(x), y'(x); x)$

Euler equation of 'second' kind

$f \equiv f(y(x), y'(x))$, hence $\frac{\partial f}{dx} = 0$, then $f - y'\frac{\partial f}{\partial y'}$ =constant

$$df = \frac{\partial f}{\partial y} dy + \frac{\partial f}{\partial y'} dy' + \frac{\partial f}{dx} dx \implies \frac{df}{dx} = y' \frac{\partial f}{dy} + y'' \frac{\partial f}{\partial y'} + \frac{\partial f}{\partial x}$$

Use E-L equation $\frac{d}{dx}\frac{\partial f}{\partial y'} = \frac{\partial f}{\partial y}$ to get

$$\frac{df}{dx} = \frac{d}{dx}\left(y' \frac{\partial f}{\partial y'}\right) + \frac{\partial f}{\partial x}$$

Brachistochrone problem MT-C6-Ex:6.2

What is the shortest time curve for the particle travel while starting from rest at point A to reach point B with $z_A > z_B$?

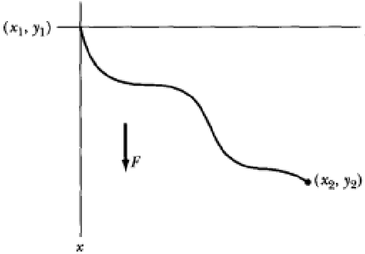


FIGURE 6-3 Example 6.2. The *brachistochrone* problem is to find the path of a particle moving from (x_1, y_1) to (x_2, y_2) that occurs in the least possible time. The force field acting on the particle is F, which is down and constant.

$$mv^2/2 = mgx \implies v = \sqrt{2gx},\ ds = vdt = \sqrt{dx^2 + dy^2}$$

$$T = \int_1^2 \frac{\sqrt{dx^2+dy^2}}{\sqrt{2gx}} = \int_{x_1}^{x_2} dx \frac{\sqrt{1+y'^2}}{\sqrt{2gx}}$$

Path Principle: General Pointers

- Generalize to N-particle systems.
  $L = KE - PE = \sum_{k=1}^{N} \frac{1}{2} m_k v_k^2 - U(\{r_k\}_{k=1}^{N})$
- $S = \int_1^2 dt\ L(\{r_k\}, \{v_k\}), \delta S = 0$ over paths.
  $\{r_k\} \mapsto q_j$ (transformation of coordinates) still has
  $\delta S = 0$ with $S = \int_1^2 dt\ L'(\{q_j\}, \{\dot{q}_j\})$
  This is the power of stationary action
- Now,

$$\frac{\partial J}{\partial \alpha} = \int_{t_1}^{t_2} dt\ \left(\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}_k} \right) - \frac{\partial L}{\partial q_k} \right) \cdot \eta_k(t)$$

  we can derive equation of motion in q_j as

$$L(\{q_k\}, \{\dot{q}_k\}) \text{ has } \frac{d}{dt} \frac{\partial L}{\partial \dot{q}_k} = \frac{\partial L}{\partial q_k}, \forall k$$

- NOTE: [MT] has direct derivation from $F = ma$

Generalised coordinates

- Simple pendulum MT-E7.2
- Wall of death MT-E7.4
- block sliding down raising incline MT-P7-11

Simple Pendulum MT-E7.2

For the simple pendulum, derive E-L EoM

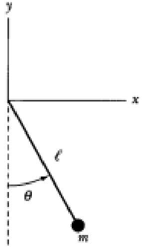


FIGURE 7-1 Example 7.2. A simple pendulum of length ℓ and bob of mass m.

- single generalised coordinates θ
- $L = \frac{1}{2}m(l\dot{\theta})^2 - (-mgl\cos\theta) = \frac{1}{2}ml^2\dot{\theta}^2 + mgl\cos\theta$
- $\frac{\partial L}{\partial \dot{\theta}} = ml^2\dot{\theta}$ and $\frac{\partial L}{\partial \theta} = -mgl\sin\theta$
- E-L: $ml^2\ddot{\theta} = -mgl\sin\theta$
- For small osciallatons, we get $\ddot{\theta} = -w^2\theta$, a simple harmonic oscillator

Wall of death MT-E7.4

See: https://www.youtube.com/shorts/HKS31wOunY8
(MT-C9-Example 7.4) Particle travelling on a cone of half-angle α subject to gravitational force. Find EoM.

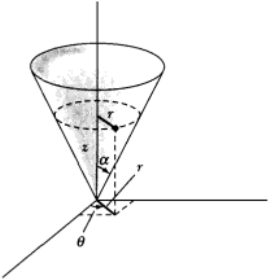


FIGURE 7-2 Example 7.4. A smooth cone of half-angle α. We choose r, θ, and z as the generalized coordinates.

$z = r \cot\alpha$, hence $(x, y, z) = (r\cos\theta, r\sin\theta, r\cot\alpha)$
Clearly, only two generalized coord. required! r and θ

Wall of death (continued)

- $v^2 = \dot{x}^2 + \dot{y}^2 + \dot{z}^2 = \dot{r}^2 + r^2\dot{\theta}^2 + \dot{r}^2 \cot^2\alpha = \dot{r}^2 \csc^2\alpha + r^2\dot{\theta}^2$
- $U = mgz = mgr\cot\alpha$
- $L = \frac{1}{2}m(\dot{r}^2 \csc^2\alpha + r^2\dot{\theta}^2 - mgr\cot\alpha)$
- $\frac{\partial L}{\partial\theta} = 0$ and $\frac{\partial L}{\partial\dot{\theta}} = mr^2\dot{\theta} =$constant [Angular momentum about z-axis is conserved]
- $\frac{\partial L}{\partial r} = mr\dot{\theta}^2 - mg\cot\alpha$ and $\frac{\partial L}{\partial\dot{r}} = m\dot{r}\csc^2\alpha$
- E-L for r is thus, $m\ddot{r}\csc^2\alpha = mr\dot{\theta}^2 - mg\cot\alpha$ which is $\ddot{r} - r\dot{\theta}^2\sin^2\alpha + \frac{1}{2}\sin(2\alpha) = 0$

Block sliding down raising incline MT-P7.12

A block is located on an incline whose angle is increasing linearly with time. Find EoM

- Angle of incline $\theta = \alpha t$
- Distance of block from point of rotation along incline q
- $L = \left(\frac{1}{2}m\dot{q}^2 + \frac{1}{2}m(q\dot{\theta})^2\right) - mgq\sin\theta$
  $L = \frac{1}{2}m\dot{q}^2 + \frac{1}{2}mq^2\alpha^2 - mgq\sin(\alpha t) = L(q, \dot{q}, t)$
- $\frac{\partial L}{\partial \dot{q}} = m\dot{q} \implies \frac{d}{dt}\frac{\partial L}{\partial \dot{q}} = m\ddot{q}$
- $\frac{\partial L}{\partial q} = mq\alpha^2 - mg\sin(\alpha t)$

Thus the equation of motion is:

$$\ddot{q} = \alpha^2 q - g\sin(\alpha t)$$

ML: training as variational problem

Given data set $\{x_k, y_k\}$ find function f s.t. $y = f(x)$
Standard methodology is to minimize $J = \int dx\, [y - f_\theta(x)]^2$

Alain & Bengio, Journal of Machine Learning Research 15 (2014) 3743

Appendix C. Calculus of Variations

Theorem 2 *Let p be a probability density function that is continuously differentiable once and with support $\mathbb{R}^d$ (i.e., $\forall x \in \mathbb{R}^d$ we have $p(x) \neq 0$). Let $\mathcal{L}_{\sigma^2}$ be the loss function defined by*

$$\mathcal{L}_{\sigma^2}(r) = \int_{\mathbb{R}^d} p(x) \left[\|r(x) - x\|_2^2 + \sigma^2 \left\| \frac{\partial r(x)}{\partial x} \right\|_F^2 \right] dx$$

for $r : \mathbb{R}^d \to \mathbb{R}^d$ assumed to be differentiable twice, and $0 \leq \sigma^2 \in \mathbb{R}$ used as factor to the penalty term.

Let $r^*_{\sigma^2}(x)$ denote the optimal function that minimizes $\mathcal{L}_{\sigma^2}$. Then we have that

$$r^*_{\sigma^2}(x) = x + \sigma^2 \frac{\partial \log p(x)}{\partial x} + o(\sigma^2) \quad as \quad \sigma^2 \to 0.$$

Moreover, we also have the following expression for the derivative

$$\frac{\partial r^*_{\sigma^2}(x)}{\partial x} = I + \sigma^2 \frac{\partial^2 \log p(x)}{\partial x^2} + o(\sigma^2) \quad as \quad \sigma^2 \to 0.$$

Both these asymptotic expansions are to be understood in a context where we consider $\{r^*_{\sigma^2}(x)\}_{\sigma^2 \geq 0}$ to be a family of optimal functions minimizing $\mathcal{L}_{\sigma^2}$ for their corresponding value of σ^2. The asymptotic expansions are applicable point-wise in x, that is, with any fixed x we look at the behavior as $\sigma^2 \to 0$.

(part 1 of the proof)

We make use of the Euler-Lagrange equation from the Calculus of Variations. We would refer the reader to either (Dacorogna, 2004) or Wikipedia for more on the topic. Let

$$f(x_1, \ldots, x_n, r, r_{x_1}, \ldots, r_{x_n}) = p(x) \left[\|r(x) - x\|_2^2 + \sigma^2 \left\| \frac{\partial r(x)}{\partial x} \right\|_F^2 \right]$$

E-L with undetermined multipliers

Constraints $f_k(\{x\}, t) = 0$
Example of disk rolling down the incline in next slide.

$$\frac{\partial L}{\partial q_j} - \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_j}\right) + \sum_k \lambda_k(t)\frac{\partial f_k}{\partial q_j} = 0$$

$$g(y, \theta) = y - R\theta = 0 \qquad (6.73)$$

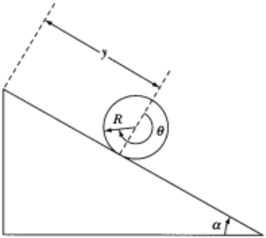


FIGURE 6-7 Example 6.5. A disk rolls down an inclined plane without slipping.

Figure: Disk rolling without slipping

Example: Disk rolling down incline MT-E7.9

- Generalized coordinates y and θ
- Constraint $g(y, \theta) = y - R\theta = 0$; $\quad \frac{\partial g}{\partial y} = 1, \ \frac{\partial g}{\partial \theta} = -R$
- $L = \left(\frac{1}{2}M\dot{y}^2 + \frac{1}{2}I\dot{\theta}^2\right) - Mg(-y \sin\alpha) = L(y, \dot{y}, \dot{\theta})$
- $$\frac{\partial L}{\partial y} - \frac{d}{dt}\frac{\partial L}{\partial \dot{y}} + \lambda\frac{\partial f}{\partial y} = 0$$
  $$\frac{\partial L}{\partial \theta} - \frac{d}{dt}\frac{\partial L}{\partial \dot{\theta}} + \lambda\frac{\partial f}{\partial \theta} = 0$$
- $Mg\sin\alpha - M\ddot{y} + \lambda 1 = 0$ and
  $0 - I\ddot{\theta} - \lambda R = 0$
  $y - R\theta = 0$
- Eliminate λ: $\lambda = -I\ddot{\theta}/R = -I\ddot{y}/R^2$, which gives
  $Mg\sin\alpha - M\ddot{y} - I\ddot{y}/R^2 = 0$
  $$\ddot{y} = \left(\frac{M}{M + I/R^2}\right) g \sin\alpha$$

Comparison: Newtonian and Lagrangian formulations

	Newtonian	Lagrangian
Equation of Motion	$m_k \frac{d^2}{dt^2} x_k = F_k$	$\frac{d}{dt} \frac{\partial L}{\partial \dot{q}_k} = \frac{\partial L}{\partial q_k}$
Order of diff. equation	Second order	Second order
Coordinates	Cartesian only	generalised coordinates
Interactions via	using forces	using energies
Constraints	'balancing' forces	naturally or by equation of constraints

Time symmetry leads to Conservation of Energy

Time symmetry: A path is 'translated' time, and has no change in value of Lagrangian,i.e. when $\frac{\partial L}{\partial t} = 0$

$$\frac{dL}{dt} = \nabla_q L \cdot dq + \nabla_{\dot{q}} L \cdot d\dot{q} + \frac{\partial L}{\partial t}$$

which gives

$$\frac{d}{dt}\left(L - \dot{q} \cdot \nabla_{\dot{q}} L\right) = \frac{\partial L}{\partial t} = 0$$

This shows that $H = \sum_k q_k p_k - L =$ constant when $\frac{\partial L}{\partial t} = 0$
Show that $H = E$ when $L = mv^2/2 + U(x)$ proving energy is conserved

Translation symmetry leads to Conservation of Momentum

Translation symmetry: A path 'translated' in space, has no change in value of Lagrangian i.e. $\delta L = 0$ for $\delta \vec{r}$ in path

$$\delta L = \nabla_x L \cdot \delta x + \nabla_{\dot{x}} L \cdot \delta \dot{x} = 0$$

Now noting that translation means that$\delta \dot{x} = 0$, we get

$$\delta L = \nabla_x L \cdot \delta x = 0 \implies \frac{\partial L}{\partial x_i} = 0$$

which from EL equations, give $\frac{d}{dt}\frac{\partial L}{\partial v_i} = 0 \implies mv_i =$ constant!

Rotational symmetry

Rotational Symmetry: A path "rotated" in space, has no change in value of Lagrangian $\delta\vec{r} = \delta\vec{\theta} \times \vec{r}$ and hence $\delta\vec{v} = \delta\vec{\theta} \times \vec{v}$

HOMEWORK Show $\delta L = 0 \implies \vec{r} \times \vec{p} =$ constant

See MT-7.9

Hamiltonian Dynamics

- $p_k = \frac{\partial L}{\partial \dot{q}_k}$, whose solution gives $\dot{q}_k = \dot{q}_k(q_k, p_k, t)$
- $H = \sum_k p_k \dot{q}_k - L(q_k, \dot{q}_k, t)$ can be seen as Legrende transform of L to replace variable $\dot{q}_k$
- $H \equiv H(\{q_k\}, \{\dot{q}_k\}, t)$ i.e. natural variables: q_k and p_k
- dH with $H(q_k, p_k, t)$ and $H = \sum_k p_k \dot{q}_k - L(q_k, \dot{q}_k, t)$
- Hamilton equation of motion

$$\dot{q}_k = \frac{\partial H}{\partial p_k}, \quad \dot{p}_k = -\frac{\partial H}{\partial q_k}, \quad \forall k$$

- p_k and q_k are treated equivalently.
- for each k, two first-order differential equations

Two body problem: m_1, m_2 & gravity [MT:C8]

- $L = \frac{1}{2} m_1 v_1^2 + \frac{1}{2} m_2 v_2^2 - U(|r_1 - r_2|)$
  Two particle system: 6 coordinates (and 6 velocities)
- Choose appropriate generalised coordinates
  - Center of Mass: $\vec{R} = \frac{m_1}{M}\vec{r}_1 + \frac{m_2}{M}\vec{r}_2$
  - Diff vector: $\vec{r} = \vec{r}_1 - \vec{r}_2$
- With $\vec{R}$ and $\vec{r}$, we find: $L = \frac{1}{2} M \dot{\vec{R}}^2 + \frac{1}{2}\mu\dot{\vec{r}}^2 - U(r)$
- Set $\dot{\vec{R}} = 0$ (Why?). And $\vec{r}$ as 2d vector (Why?):
  $L = \frac{1}{2}\mu(\dot{r}^2 + r^2\dot{\theta}^2) - U(r) = L(r, \dot{r}, \theta, \dot{\theta})$
  generalised coordinates r and θ: 1 particle in 2D
- $\frac{\partial L}{\partial \theta} = 0 \implies \frac{\partial L}{\partial \dot{\theta}} = \ell$, a constant. Thus
  $\mu r^2 \dot{\theta} \implies \ell = r \cdot r\dot{\theta} = \ell$, Kepler's second law
- $\frac{\partial L}{\partial \dot{r}} = \mu\dot{r}$ and $\frac{\partial L}{\partial r} = \mu r\dot{\theta}^2 - U'(r)$. Thus,
  $\mu\ddot{r} = \mu r\dot{\theta}^2 - U'(r) \implies \mu\ddot{r} = \ell^2/(\mu r^3) - U'(r)$
  (a) Circular orbit (b) non-circulur orbit

Two body problem: continued

- $\mu r^2\dot{\theta} = \ell$ a constant; AND $\mu\ddot{r} = \ell^2/(\mu r^3) - U'(r)$
- $H = K + U = \frac{1}{2}\mu(\dot{r}^2 + r^2\dot{\theta}^2) + U(r) = \frac{1}{2}\mu\dot{r}^2 + \frac{\ell^2}{\mu r^2} - \frac{Gm_1m_2}{r}$
- $U_{eff} = \frac{\ell^2}{\mu r^2} - \frac{Gm_1m_2}{r}$

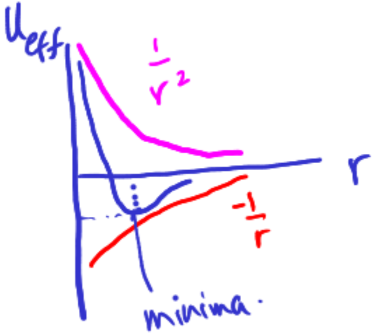


Figure: U_{eff} has a minima

Two body problem: continued

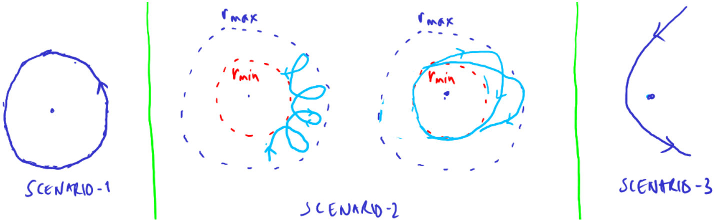


Figure: Scenarios for total energy H

- Scenario-1: $\dot{r} = 0 \implies H = U^*_{eff}$. This has r =constant, $\dot{\theta} = \frac{\ell}{\mu r^2}$ =constant. This means the trajectory is a circle with constant angular velocity
- Scenario-2: $H \in (U^*_{eff}, 0]$, the particle will be oscillate between two values of r. Closed orbits for $n = -1, 2$
- Scenario-3: $H > 0$. Particle is NOT confined, Particle Swings by!

Two-body problem continuedMT:C8-S7

- Closed orbits for PE$\sim r^n$, only n=-1 (gravitational) and n=2 (SHO) in general case
- Gravitational case:
  $H = \frac{1}{2}\mu(\dot{r}^2 + r^2\dot{\theta}^2) - \frac{k}{r} = E \implies \dot{r} = \sqrt{\frac{2}{\mu}(E + \frac{k}{r}) - \frac{l^2}{\mu^2 r^2}}$
- Using $d\theta = \frac{\dot{\theta}}{\dot{r}}\, dr$ and $\dot{\theta} = \ell/(\mu r^2)$ we get

$$\theta(r) = \int \frac{\ell/r^2}{\sqrt{2\mu(E - \frac{k}{r} - \frac{l^2}{2\mu r^2})}} dr$$

  suggeting $u = 1/r$, which upon integration gives :

$$\frac{\alpha}{r} = 1 + \epsilon\cos\theta,\ \text{with } \alpha = \frac{l^2}{\mu k}, \epsilon = \sqrt{1 + \frac{2El^2}{\mu k^2}}$$

Solutions: (a) $E < 0$ an ellipse (or special case: circle), (b) parabola $E = 0$ and (c) hyperbola for $E > 0$

Two body problem: implications on solar system

- Kepler 'derived' this three laws using incorrect forces (several errors magically cancel to give a law that matches Tycho Brache's and his observations)
- Newton proved that his Law of Universal Gravitation will result in Kepler's law for *any* two body system and hence solar systems
- This problem can be considered as one of the origin problems of several fields of calculus and analysis
- Lagrange and Poincare made significant contributions to analysis of trajectories
- Perturbations to two body trajectories of planets have been explained by presence of nearby 'large' planets.

Solar system

- Ancients knew and recognised planets: mercury, venus, earth mars, jupiter and saturn. These are visible to eye and move reasonaly fast.
- Uranus (which is visible to naked eye) is so slow that it was thought to be a faint star till Hershel's careful measurements showed it to orbit sun.
- Unaccounted perturbations to Uranus orbit was postulated to be due to a yet undiscovered planet, which was quickly discovered at the approximate location given by mathematical calculations.
- Pluto was postulated based on perturbations to Neptune's orbit starting from 1840's. Discovery in 1930. Advancements in telescopes (1990's) showed that several bodies of similar size of Pluto forming the Kupier belt. In 2006, Pluto is 'downgraded' to a planetoid.

Three body problem: no closed solutions

A good overview:
`https://en.wikipedia.org/wiki/Three-body_problem`
No general solutions possible. However, special situations have known solutions with closed orbits.

Multi-particle systems: Center of Mass

Consider a system of N particles, with masses $\{m_k\}$, position vectors $\{\vec{r}_k\}$, velocities $\{\vec{v}_k\}$ etc..

- Total mass of system $M = \sum_{k=1}^{N} m_k$
- Center of Mass (CoM) is defined as:
  $\vec{R} = \frac{1}{M}\sum_{k=1}^{N} m_k \vec{r}_k$
- Momentum of particle k is $\vec{p}_k = m_k \vec{v}_k$
- Total linear momentum of system, $\vec{P} \equiv \sum_k \vec{p}_k$
- Total angular momentum of system, $\vec{L} \equiv \sum_k \vec{r}_k \times \vec{p}_k$
- Net Torque about origin of system, $\vec{N} \equiv \sum_k \vec{r}_k \times \vec{F}_k$
  Check that $\vec{N} \equiv \frac{d}{dt}\vec{L}$ gives above expression for $\vec{N}$

Collection of particles

Forces:

- $F_k = F_k^e + F_k^i$ (external and internal forces, resp.)
- $F_k^i = \sum_j F_{k \leftarrow j}$ (internal interactions)
- For central forces $F_{k \leftarrow j} = -F_{j \leftarrow k}$
  - $\sum_k F_k^i = \sum_{\langle j,k \rangle} F_{k \leftarrow j} = 0$!
  - $\sum_k r_k \times F_k^i = \sum_{\langle j,k \rangle} r_k \times F_{k \leftarrow j} = 0$!

Effects of these forces:

- Net force: $F = \sum_k F_k = \sum_k F_k^e$
- Effective mass M at Center of Mass position $\vec{R}$
- Overall motion: $M \frac{d^2}{dt^2} \vec{R} = \vec{F}$
- Angular momentum: $\vec{L} = \vec{L}_{CoM} + \vec{L}^i_{CoM}$
- Internal forces are central $\implies$ the total internal torque is zero!

Show $\vec{P}$ conserved, when no external forces

Show $\vec{P}$ conserved, when no external forces

- $\frac{d}{dt}\vec{P} = \frac{d}{dt}\left[\sum_k m_k \vec{v}_k\right] = \sum_k m_k \frac{d^2}{dt^2}\vec{r}$
- $\vec{R} = \frac{1}{M}\sum_k m_k \vec{r}_k \implies \frac{d^2}{dt^2}\vec{R} = \frac{1}{M}\frac{d^2}{dt^2}\sum_k m_k \vec{r}_k = \frac{1}{M}\frac{d^2}{dt^2}\vec{P}$
- $\frac{d}{dt}\vec{P} = \frac{d}{dt}\left[\sum_k \vec{p}_k\right] = \sum_k \vec{F}_k$ = net force on system
- If no external forces then
  - $\vec{F}_k = \sum_{j \neq k} \vec{F}_{k \leftarrow j}$, inter-particle interactions only
  - $\sum_k \vec{F}_k = \sum_k \sum_{j \neq k} \vec{F}_{k \leftarrow j} = \sum_{\langle j,k \rangle} \left(\vec{F}_{k \leftarrow j} + \vec{F}_{j \leftarrow k}\right) = 0!$
  - Hence $\frac{d}{dt}\vec{P} = 0$, $\vec{P}$ is a conserved quantity
- When external forces exist, following math similar to above argument, it can be shown that:
  - Define net external force $\vec{F}_{ext} = \sum_k \vec{F}_{k,ext}$
  - $\frac{d}{dt}\vec{P} = \vec{F}_{ext}$
  - And hence $M\frac{d^2}{dt^2}\vec{R} = \vec{F}_{ext}$

Show $\vec{L}$ conserved when no external forces

Show $\vec{L}$ conserved when no external forces

- $r_k = R + r'_k \implies v_k = V + v'_k$
- $L = \sum_k r_k \times p_k = \sum_k m_k(R + r'_k) \times (V + v'_k)$
  which gives $L = MR \times V + \sum_k r'_k \times p'_k$
  Angular momentum= L of CoM + L_{system} about CoM
- $\frac{d}{dt}L = \frac{d}{dt}\sum_k \vec{r}_k \times \vec{p}_k = \sum_k \left[\frac{d}{dt}\vec{r}_k \times \vec{p}_k + \vec{r}_k \times \frac{d}{dt}\vec{p}_k\right]$
- $\frac{d}{dt}\vec{L} = \sum_k [0 + r_k \times F_k] \implies N = \sum_k r_k \times F_k$
- for every particle k, force $F_k = F_{k,ext} + \sum_{j\neq k} F_{k\leftarrow j}$
- $\frac{d}{dt}L = \sum_k r_k \times F^e_k = \sum_k N^e_k$
  Rate of change of L = sum external torque
  If no enxternal torque, angular momentum of system is conserved

Show energy is conserved

Show energy is conserved

- $W = \int_{t_1}^{t_2} \sum_k F_k(t) \cdot dr_k(t) = \sum_k \int_{t_1}^{t_2} m_k \frac{dv_k}{dt} \cdot v_k dt = T_2 - T_1$
  where $T \equiv \sum_k \frac{1}{2} m_k v_k^2$
- Center of Mass: $r_k = R + r'_k,\ v_k = V + v'_k$
- $v_k^2 = V^2 + 2v'_k \cdot V + {v'_k}^2$
- $T = \sum_k \frac{1}{2} m_k v_k^2 = \frac{1}{2} M V^2 + 0 + \sum_k \frac{1}{2} m_k {v'_k}^2$
  KE of system = CoM KE + System KE in CoM frame
- $F_k = F_k^e + \sum_{j \neq k} F_{k \leftarrow j}$
- $W = \sum_k \int_1^2 (F_k^e + F_k^i) \cdot dr_k$
- If $U_{j,k}^i = U(r_k, r_j)$ then $F_{j \leftarrow k} - = -Fk \leftarrow k$
- unfinished

Summary: Multi-particle systems MT:C9.1-9.5

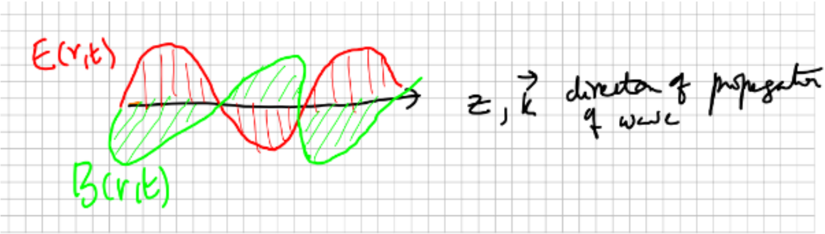
- Center of Mass of collection of particles
- Total momentum of system: $\vec{P} \equiv \sum_k p_k = \vec{P}_{CoM}$
- Net force on system $\vec{F} = M\frac{d}{dt}\vec{P}$
  If there are no external forces, linear momentum of system is conserved and equals the CoM momentum
- Total angular momentum of system about origin:
  $\vec{L} \equiv \sum_k L_k = \sum_k r_k \times p_k = R_{CoM} \times P_{CoM} + \sum_k r'_k \times p'_k$
  = CoM L about origin + sum of particle L'_k about CoM
- Net torque on system $N = \frac{d}{dt}L$ For central forces, net interal torque must vanish
- KE of system equals sum of CoM KE and sum of KE of each partcle in CoM frame
- For a conservative system, the total energy is constant in absence of external forces.

Light

1. Huygens proposed waver theory of light (1690AD)
2. Newton's treatise (Opticks 1705AD): proposed corpuscular theory of light
3. Refraction, diffraction, internal reflection etc were of considerable importance
4. Spectacles were 'normal' technology of the time
5. Young (1801AD): Double slit experiment support for wave theory of light. Also find wavelength of light source.
6. Fresnel's mathematical Huygens-Fresnel Theory (1818AD) conclusively sets up light as wave
7. Maxwell Equations (1860's AD): In vacuum, give wave equations for $\vec{E}$ and $\vec{B}$

Light in vacuum

1. $\frac{d^2}{dt^2}\vec{E} = \frac{1}{\mu_0\epsilon_0}\nabla^2\vec{E}$ and same for $\vec{B}$
2. PLANE WAVE SOLUTIONS
3. $\vec{E} = \vec{E}_0 e^{i(kz-wt)}$, propagating along z-axis
4. $\vec{B} = \frac{k}{w}(\hat{z} \times \vec{E}_0)$, that is $\vec{B}_0 = \vec{E}_0$
5. Transverse waves, $c^2 = \frac{1}{\mu_0\epsilon_0}$ and $\nu\lambda = c$
6. Superposition of plane waves is also solution: Polarization.



Light: color depends on wavelength

1. Wavelength from using Diffraction gratings (like Youngs Double slit)
2. Visible range (Human): Red 800 nm, Blue 400 nm
3. Sunlight, after refraction from prism, is found to contain non-visible infra-red radiation and some ultra-violet radiation
4. When metals are heated to high temperature, they emit light and cool off (even beyond convective cooling, if present)
5. Spectrum at a temperature is independent of metal used
6. Kirchhoff: formulated Black body problem: What is the spectrum of black-body? Major technological importance, scientific enquiry

Black body radiation

1. Stefan-Boltzamann Radioactive power law: $P = \sigma T^4$
2. Wein Displacement Law: $\lambda_{max} T =$constant
3. Wein Distribution law (1896AD): $I(\nu) \propto \nu^3 e^{-b\nu/T}$,
4. Rayleigh-Jeans law(1899AD): $I(\nu) \propto \nu^2 T$

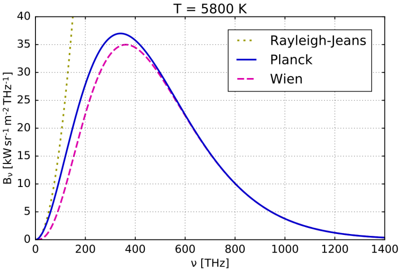


Figure: Wein's formula is good fit for large ν and Ralyeigh's for small ν

Planck's Black body radiation formula

1. Planck (1894-1900AD): Attempted to get an expression / model that could fit all frequencies: fresh data from his experimental colleagues for small ν
2. Planck's model required statistical mechanics, and that energy levels of a particular frequency be discrete for good expt fit:

$$I(\nu) = \frac{2h\nu^3}{c^2}\frac{1}{e^{\frac{h\nu}{kT}} - 1}$$

3. Planck: a better model will remove quantization of energy
4. First instance of quantization of energy $E(\nu) = nh\nu$

Photoelectric Effect (Hertz 1887AD)

- In vacuum, charged metal objects discharge their charge when (UV) light falls on it
- Counter-intuitive results unexplained by contemporary physics
- Einstein (1905AD): proposes a model that uses Planck energy quantization. Light packet (photon) falling on metal knocks-off an electron with remainder energy into kinetic energy of electron
  $h\nu = KE_{max} + W$

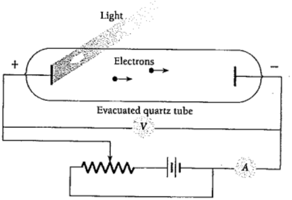


Figure 2.9 Experimental observation of the photoelectric effect.

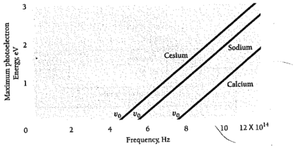
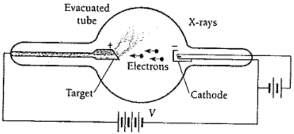
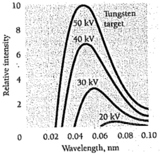


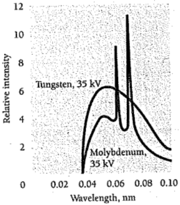
Figure 2.12 Maximum photoelectron kinetic energy KE_{max} versus frequency of incident light for three metal surfaces.

X-ray production: inverse photoelectric effect

1 High KE electrons impinge on metal, light is emitted

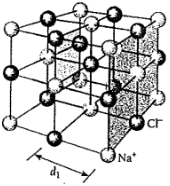






1 X-Ray's are light of very small wavelength (0.1nm)

2 X-Ray Diffraction probes chemical structure



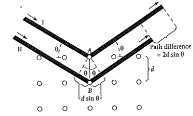
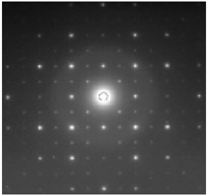


Figure 2.20 X-ray scattering from a cubic crystal.



Compton Expt: Photon as particle: confirmation

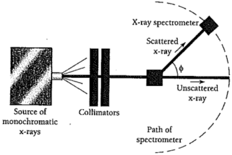


Figure 2.23 Experimental demonstration of the Compton effect.

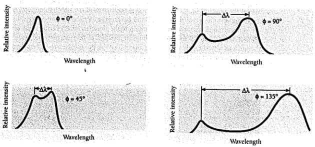
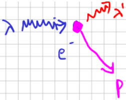
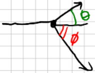


Figure 2.24 Experimental confirmation of Compton scattering. The greater the scattering angle, the greater the wavelength change, in accord with Eq. (2.21).





① Energy conservation: $\frac{hc}{\lambda} + m_e c^2 = \frac{hc}{\lambda'} + \sqrt{p^2c^2 + m_e^2c^4}$

② x-momentum conservation: $\frac{h}{\lambda} = \frac{h}{\lambda'}\cos\theta + p\cos\phi$

③ y-Momentum Conservation: $\frac{h}{\lambda'}\sin\theta = p\sin\phi$

③ In expt, light falls on graphite and scattered light is collected. ie λ, λ', and θ are known.

ⓐ $p^2\cos^2\theta + p^2\sin^2\theta = \left(\frac{h}{\lambda} - \frac{h}{\lambda'}\cos\theta\right)^2 + \left(\frac{h}{\lambda'}\sin\theta\right)^2 = \boxed{\left(\frac{h}{\lambda}\right)^2 + \left(\frac{h}{\lambda'}\right)^2 - \frac{2h^2}{\lambda\lambda'}\cos\theta = p^2}$

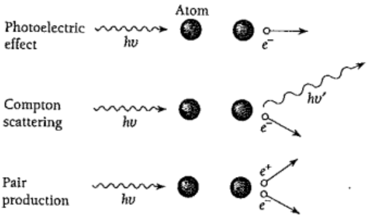
ⓑ $\boxed{p^2c^2 + m_e^2c^4 = \left(\frac{hc}{\lambda} - \frac{hc}{\lambda'} + m_e c^2\right)^2}$

ⓒ Combing ⓐ and ⓑ to eliminate p. gives $\boxed{\lambda' - \lambda = \frac{h}{mc}(1-\cos\theta)}$

Inspired elastic scattering
RAMAN suggested inelastic scattering of photon
← NOBEL 1930.

Summary: Light

1. Light as wave: Young's Double slit,, X-Ray Diffraction
2. Light as particle: Photoelectric, Compton Effects
3. LIGHT WAVE-PARTICLE DUALITY:
   Light is both a wave and a particle
4. wavelength , frequency ν, speed $c = \lambda\nu$
5. Mass $m = 0$, $E = pc$. Planck's $E = h\nu \implies p = \frac{h}{\lambda}$



de Broglie hypothesis: matter waves (1924AD)

1. Inspired by wave-particle duality of light, de Broglie proposed wave-particle duality of particles. Specifically, that a wave of wavelength $\lambda = \frac{h}{p}$ is associated with matter having momentum p
2. Einstein strongly supported this idea, and experiments conclusively showed that particles (electrons) show diffraction pattern when scattered off crystals (just like X-Rays). Also, show interference patterns in double slit experiment.
3. Extending this idea, Schrodinger found the "wave equation" for such a wave, that is now called "Schrodinger Equation" (1926AD). This equation is for ALL quantum mechanics currently in use, it is QM equivalent to Newtons "F=ma"

Davisson-Gremer Experiment: Particle Diffraction

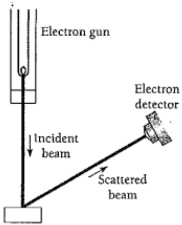


Figure 3.6 The Davisson-Germer experiment.

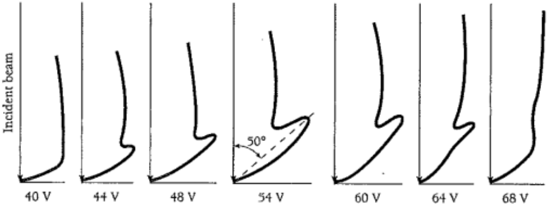


Figure 3.7 Results of the Davisson-Germer experiment, showing how the number of scattered electrons varied with the angle between the incoming beam and the crystal surface. The Bragg planes of atoms in the crystal were not parallel to the crystal surface, so the angles of incidence and scattering relative to one family of these planes were both 65° (see Fig. 3.8).

Figure: Davisson-Gremer expt. Diffraction peaks of electrons from the Nickel crystal surface

For Nickel crystal $d = 0.091\ nm$, $\theta = 65^{\mathrm{deg}}$.
Using $n\lambda = 2d\sin\theta$ gives $\lambda = 0.165\ nm$.
54 eV electrons have $\lambda = \frac{h}{p} = \frac{h}{\sqrt{2m\ KE}} = 0.166\ nm$

Matter waves, $\lambda = \frac{h}{p}$

1. For $1\mu g$ mass moving at $1\mu m/s$,
$\lambda \sim 10^{-34}/(10^{-9} * 10^{-6}) = 10^{-20} m$!
(electron, $m_e = 9.1 \times 10^{-31} kg$, proton=$1.6 \times 10^{-27} kg$).
2. Regime of small: in energy/ momentum / mass
3. NOTE: MACROSCOPIC SYSTEMS also
4. Localization of wave: particle behavior: group wave
5. 1D wave: $A \cos(2\pi x/\lambda + 2\pi\nu t) = A\cos(kx + wt)$
Amplitude A, $k = 2\pi/\lambda$, $w = 2\pi\nu$

Matter waves: group wave

Superposition is also a solution:

$$A\cos(wt - kx) + A\cos((w + \Delta w)t - (k + \Delta k)x)$$
$$\sim 2A\cos(wt - kx)\cos\left(\frac{\Delta w}{2}t - \frac{\Delta k}{2}x\right)$$

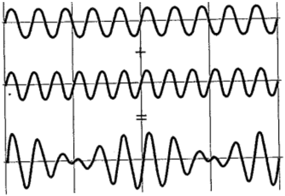


Figure 3.4 Beats are produced by the superposition of two waves with different frequencies.

Figure: Individual waves of velocity $v_p = \frac{w}{k}$. Resulting gruop wave $v_g = \frac{\Delta w}{\Delta k}$

Matter waves: group wave (2)

Many individual waves, more localization in group wave

$$w = 2\pi\nu = 2\pi\frac{E}{h} = \frac{2\pi\gamma mc^2}{h}. \text{ And } \; k = \frac{2\pi}{\lambda} = \frac{2\pi}{h}p = \frac{2\pi\gamma mv}{h}$$

with $\gamma = 1/\sqrt{1 - v^2/c^2}$

Phase velocity $v_p = \frac{w}{k} = \frac{c^2}{v}$

Group velocity $v_g = \frac{dw}{dk} = \frac{dw/dv}{dk/dv} = v$

Uncertainity Principle

Waves have a fundamental property: $\Delta x \Delta k > \frac{1}{2}$
Using de Broglie: $k = \frac{2\pi}{\lambda} = \frac{2\pi p}{h}$ which gives

$$\Delta x \cdot \Delta p \geq \frac{1}{2}\hbar$$

This is the famous Heisenberg Uncertainty principle (1927AD) "It is impossible to determine *precisely both* the position and momentum of a particle simultaneously"

Such uncertainty exists for every pair of complementary variables: E and t

Example: Particle in the box problem:

Old Quantum Theory

- Plank (1900AD) hypothesized: energy of oscillator is quantized $E = nh\nu$
- Bohr (1913AD) hypothesized: angular momentum of electron quantized $mvr = nh/2\pi, \; n = 1, 2, 3, \cdots$ for electron in Hydrogen atom; this is the famous Bohr model
- Somerfield (and his group) attempted to explain multi-electron atoms by postulating additional quantization conditions; this is extension of Bohr's model for Hydrogen

Quantization conditions were proposed ad hoc (pulled out of a hat like a magician), and was quite unsatisfactory

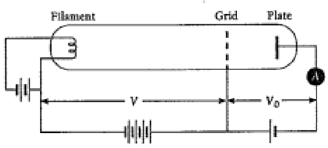
Bohr Model of Hydrogen atom (1913AD)

Electron orbiting the fixed nucleus:

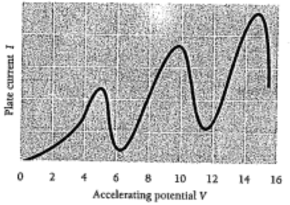
1. Postulate: $mvr = n\hbar$: Angular momentum is quantized
2. Orbit of electron around hydrogen: $2\pi r = n\lambda$ with de Broglie wave $\lambda = \frac{h}{mv}$, which gives $mvr = n\hbar$
3. $E = \frac{1}{2}mv^2 - K\frac{e^2}{r}$ and balancing electrostatic force with centrifugal force gives: $\frac{mv^2}{r} = K\frac{e^2}{r^2} \implies mv^2 = Ke^2/r$. Thus $E = -\frac{1}{2}K\frac{e^2}{r}$
4. $mvr = n\hbar$ and $mv^2 = Ke^2/r$, gives: $v = \frac{Ke^2}{n\hbar}$, $r = \frac{(n\hbar)^2}{mKe^2}$, thus $E = -R\frac{1}{n^2}$, with $R = \frac{K^2me^4}{2\hbar^2}$
5. $E_n - E_m = -R\left(\frac{1}{n^2} - \frac{1}{m^2}\right)$. Gives good fit to Lyman, Balmer, Paschen and Pfund series for Hydrogen atom

Frank-Hertz experiment(1913AD)

Electrons, in a vacuum tube, sent through vapor (of mercury).



1 Apparatus for the Franck-Hertz experiment.



Results of the Franck-Hertz experiment, showing critical potentials i

Light of 253.6nm is emitted; this corresponds exactly to KE of 4.9eV electron. Confirmation of the basic ideas behind Bohr model for hydrogen atom

Quantum Theory: math formulation

1. Insists that there a "wave function" $\Psi(x,t)$ that is state of the system; it can be complex function
2. It satisfies Schrodinger equation (evolution of Ψ)

$$i\hbar\frac{d}{dt}\Psi(x,t) = \hat{H}\Psi(x,t)$$

3. Born Postulate: $|\Psi^(x,t)|^2 dx$ is probability of finding system at x at time t
4. Every experimental observable has an operator, and expectation value can be calculated by

$$\langle A\rangle = \int dx \Psi^*(x,t)\hat{A}\,\Psi(x,t)$$

5. Measurement and collapse of wave function

Motivate proof of Schrodinger Equation

Consider a matter wave for a 'free' particle

1. Waves satisfy wave equation: $\nabla^2\psi(x) + k^2\psi(x) = 0$ where $k = 2\pi/\lambda$
2. de Broglie: $\lambda = \frac{h}{p}$, gives us: $\nabla^2\psi(x) + (\frac{p}{\hbar})^2\psi(x) = 0$
3. Suggestion: $\psi(x) = \exp\left(ipx/\hbar\right)$
4. For free particle $E = \frac{p^2}{2m}$ which using (2) can be written as:

$$E = -\frac{1}{\psi}\frac{\hbar^2}{2m}\nabla^2\psi(x) \implies -\frac{\hbar^2}{2m}\nabla^2\psi(x) = E\psi(x)$$

and for a particle in a potential as: $E = \frac{p^2}{2m} + V(x)$ giving us Time Independent Schrodinger Equation:

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V(x)\right)\psi(x) = E\psi(x)$$

Another motivating derivation

1. Wave can be represented as $\Psi(x,t) = \exp i(kx - wt)$
2. de Broglie: $k = \frac{2\pi}{\lambda} = \frac{p}{\hbar}$
3. Planck-Einstein: $E = h\nu \implies w = \frac{\nu}{2\pi} = \frac{E}{\hbar}$
4. $\Psi(x,t) = \exp \frac{i}{\hbar}(px - Et)$, matter wave of particle with momentum p and energy E
5. $\frac{\partial \Psi}{\partial t} = -\frac{i}{\hbar} E\ \psi$, and $\frac{\partial^2 \Psi}{\partial x^2} = -\frac{1}{\hbar^2} p^2 \Psi$
6. Now using $E = \frac{p^2}{2m}$, we get $i\hbar \frac{\partial \Psi}{\partial t} = (-\frac{\hbar^2}{2m}\frac{\partial^2 \Psi}{\partial x^2})$
7. Extending for particle in a potential $V(x)$, with $E = \frac{p^2}{2m} + V(x)$:

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

Features of Schrodinger equation

1. Linearity and Superposition: $a_1\Psi_1(x,t) + a_2\Psi_2(x,t)$ also satisfies Schrodinger equation, if $i\hbar\frac{\partial}{\partial t}\Psi_i(x,t) = \hat{H}\Psi_i(x,t)$ for $i = 1, 2$
2. Normalization: $a_1\Psi_1 + a_2\Psi_2$ is normalized if $|a_1|^2 + |a_2|^2 = 1$
3. Stationary Solutions: $\Psi(x,t) = \psi(x)\chi(t)$ satisfy $\hat{H}\psi(x) = E\psi(x)$ and $\chi(t) = \chi(0)\exp\left(-iEt/\hbar\right)$
4. Operators: $\hat{x} = x$ and $\hat{p}_x = -i\hbar\frac{\partial}{\partial x}$ (next slide), $\hat{K} = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)$ and finally $\hat{E} = \hat{H} = \hat{K} + V(x)$
5. Expectation values

$$\langle\hat{A}\rangle = \int \psi^* \hat{A}\psi$$

6. Correspondence principle: CM limit for QM problems

Momentum operator

$$\langle p_x \rangle = m\frac{\partial}{\partial t}\langle x \rangle = m\frac{\partial}{\partial t}\int\, dx\; \Psi^*(x,t)\; x\; \Psi(x,t)$$

1. SE gives $i\hbar\Psi_t = -C\Psi_{xx} + V\Psi$ and $-i\hbar\Psi_t^* = -C\Psi_{xx}^* + V\Psi^*$
2. $\langle v_x \rangle = \int\, dx\; x(\Psi^*\Psi_t + \Psi_t^*\Psi) = -C\frac{1}{i\hbar}\int\, dx\; x(\Psi^*\Psi_{xx} - \Psi\Psi_{xx}^*)$ $=-\frac{C}{i\hbar}\int\, dx\; x\partial_x(\Psi^*\Psi_x - \Psi\Psi_x^*)$
3. Using uv-rule for integration, we get $\langle v_x \rangle = +\frac{C}{i\hbar}\int\, dx\; (\Psi^*\Psi_x - \Psi\Psi_x^*)$ $=2\frac{C}{i\hbar}\int\, dx\; \Psi^*\frac{\partial}{\partial x}\Psi$

Hence $\hat{v}_x = \hat{p}_x/m = \frac{2C}{i\hbar}\frac{\partial}{\partial x}$, with $C = \hbar^2/(2m)$, we get $\hat{p}_x = \frac{h}{i}\frac{\partial}{\partial x}$

All operators can be expressed in position and momentum operators! $\hat{K}(\hat{r},\hat{p})$

Particle in 1-D box

1. Particle confined to $x \in [0, L]$. So potential $V(x) = 0 \forall x \in [0, L]$ and $V(x) = \infty \forall x \notin [0, L]$
2. Region-1 $R_1 : x \in (-\infty, 0)$, $R_2 : x \in [0, L]$ and $R_3 : x \in [L, \infty)$
3. SE is $-CD_{xx}\psi(x) + V(x)\psi(x) = E\psi(x)$, $C = \hbar^2/2m$
4. For R_1 and R_3, we have LHS of SE having $V(x) = \infty$ while RHS is finite. Only possible solution: $\psi(x) = 0$!
5. For R_2, we get $-CD_{xx}\psi = E\psi \implies D_{xx}\psi = -k^2\psi$ where $k = \sqrt{2mE/\hbar^2}$ is a real number. This has solutions $\psi(x) = A\cos(kx) + B\sin(kx)$.
6. Boundary conditions-1: boundary $R_1 : R_2$ gives $0 = A.1 + B.0 \implies A = 0$
7. Boundary conditions-2: boundary $R_2 : R_3$ gives $B\sin(kL) = 0 \implies kL = \pi n$ where n=1,2,3,4...
8. Solution: $\psi(x) = 0 \forall x \notin [0, L]$ and $\psi(x) = B\sin(\frac{\pi n x}{L}) \forall x \in [0, L]$ with

Particle in 1-D box (2)

Above condition for k gives $E_n = n^2 E_1$, with $E_1 = h^2/(8mL^2)$ and the wave function $\psi_n(x) = B\sin(n\pi x/L)$. Requiring $\int_{-\infty}^{\infty} |\psi(x)|^2 \, dx = 1$ gives $B = \sqrt{2/L}$

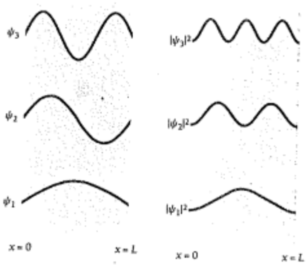


Figure: Particle in 1-D box. Left $\psi(x)$ and Right $\psi^2(x)$. Notice the number of nodes in the wave function.

Particle in 3-D box

Box is defined to have $x \in [0, L_x],\ y \in [0, L_y],\ z \in [0, L_z]$.
Potential $V(x, y, z) = 0$ inside the box and $V = \infty$ outside.

$$-C(D_{xx}+D_{yy}+D_{zz})\psi(x, y, z)+V(x, y, z)\psi(x, y, z) = E\psi(x, y, z)$$

Outside the box, $V = \infty$, so $\psi = 0$! Now for inside the box, we use the ansatz of Separation of variables:
$\psi(x, y, z) = \psi_1(x)\psi_2(y)\psi_3(z)$ gives us

$$-C(\psi_2\psi_3\ D_{xx}\psi_1 + \psi_1\psi_3\ D_{yy}\psi_2 + \psi_1\psi_2 D_{zz}\psi_3) = E\psi_1\psi_2\psi_3$$

$$\frac{D_{xx}\psi_1}{\psi_1} + \frac{D_{yy}\psi_2}{\psi_2} + \frac{D_{zz}\psi_3}{\psi_3} = -\frac{E}{C}$$

And thus PiB in x, y and z variables. So

$$\psi(x, y, z) = \sqrt{\frac{2^3}{L_x L_y L_z}} \sin\frac{n_1\pi x}{L_x}\ \sin\frac{n_2\pi y}{L_y}\ \sin\frac{n_3\pi z}{L_y}$$

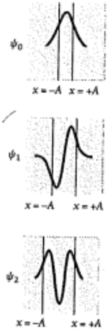
with Energy $E = \left(\frac{n_1^2}{L_x^2} + \frac{n_2^2}{L_y^2} + \frac{n_3^2}{L_z^2}\right)\frac{h^2}{8m}$

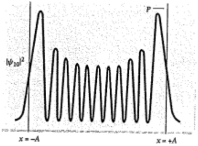
Harmonic Oscillator

1. SE: $-C\psi_{xx} + \frac{1}{2}kx^2\psi(x) = E\psi(x)$,
2. Choose $x = by$ to get $-C\psi_{yy}/b^2 + \frac{1}{2}kb^2y^2\psi = E\psi$,
3. Rearrange: $\psi_{yy} - \frac{kb^4}{C}y^2\psi + \frac{Eb^2}{C}\psi = 0$. Now choosing b so that $kb^4/C = 1$ and $\alpha = Eb^2/C = \alpha$, we get $\psi_{yy} + (\alpha - y^2)\psi = 0$
4. When $y \to \pm\infty$, we get $\psi_{yy} - y^2\psi = 0$, which in turn suggests $\psi \sim \exp dy^2$, with $4d^2 = 1$. We choose $\psi \sim \exp(-y^2/2)$
5. Ansatz: $\psi(y) = f(y)\exp(-y^2/2)$. This gives us $\psi_y = \exp(-y^2/2)(f_y - yf)$ and $\psi_{yy} = \exp(-y^2/2)(-y(f_y - yf) + (f_{yy} - yf_y - f))$
6. Thus SE $\psi_{yy} - y^2\psi + \alpha\psi = 0$ becomes: $\exp(-y^2/2)\,(f_{yy} - 2yf_y + (\alpha - 1)f) = 0$. Set $f(y) = \sum_n a_ny^n$, to get $a_{n+2} = \frac{2n+1-\alpha}{(n+1)(n+2)}a_n$

Harmonic (2)

1. Thus $\psi = \exp(-y^2/2) f(y)$ converges when $2n + 1 - \alpha = 0$ for integer n. For $\alpha = 2n + 1$, $\psi_n(y) = \exp(-y^2/2) f_n(y)$, f_n is polynomial of order n
2. $n = 0,\ \alpha = 1$, we get $a_2 = 0$ and hence $f_0 = 1$
3. $n = 1,\ \alpha = 3$, we get $f_1 = 2y$
4. $n = 2, \alpha = 4$, we get $f_2 = 4y^2 - 2$

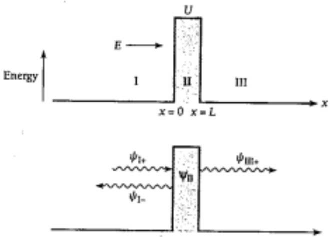




Harmonic Oscillator (2)

Tunneling

1. In SHO, non-zero probability beyond classical turning points (with KE¡0!)
2. Starting in Region-1 with energy $E < U$, classically the particle cannot penetrate Region-2.



3. Conditions at boundaries: $x = 0$ and $x = L$:
   1. ψ must be continuous
   2. Derivative $d\psi/dx$ must be continuous

The tunnel effect

1. Region-1: $D_{xx}\psi_I + C_1 E\psi_1 = 0$, with $C_1 = 2m/\hbar^2$
   1. $\psi_I = A\exp(ik_1 x) + B\exp(-ik_1 x)$, $k_1 = \sqrt{2mE/\hbar^2}$
2. Region-2: $D_{xx}\psi_{II} + C_1(E - U)\psi_{II} = 0$
   1. $\psi_{II} = C\exp(k_2 x) + D\exp(-k_2 x)$, $k_2 = \sqrt{2m(U - E)/\hbar^2}$
3. Region-3: $D_{xx}\psi_{III} + CE\psi_{III} = 0$
   1. $\psi_{III} = F\exp(ik_1 x)$ (only the +ve direction wave)
4. Boundary conditions:
   1. $\psi_I(x = 0) = \psi_{II}(x = 0) \implies A + B = C + D$
   2. $D_x\psi_I(x = 0) = D_x\psi_{II}(x = 0) \implies ik_1(A - B) = k_2(C - D)$
   3. $\psi_{II}(x = L) = \psi_{III}(x = L) \implies C\exp(k_2 L) + D\exp(-k_2 L) = F\exp(ik_1 L)$
   4. $D_x\psi_{II}(x = L) = D_x\psi_{III}(x = L) \implies k_2(C\exp(k_2 L) - D\exp(-k_2 L) = k_1(F\exp(ik_1 L)$

Tunnel effect (3)

$$\left(\frac{A}{F}\right) = \left[\frac{1}{2} + \frac{i}{4}\left(\frac{k_2}{k_1} - \frac{k_1}{k_2}\right)\right]e^{(ik_1+k_2)L} + \left[\frac{1}{2} - \frac{i}{4}\left(\frac{k_2}{k_1} - \frac{k_1}{k_2}\right)\right]e^{(ik_1-k_2)L} \quad (5.95)$$

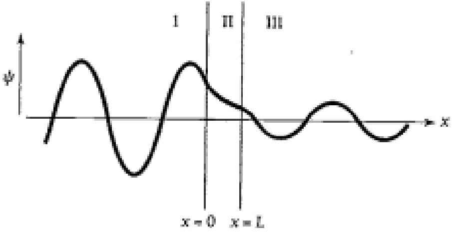


Figure 5.14 At each wall of the barrier, the wave functions inside and outside it must match up perfectly, which means that they must have the same values and slopes there.

Transmission coefficient $T \sim e^{-2k_2 L}$
Scanning Electron Microscope (SEM) uses principle of tunneling: surface topography and composition

Hydrogen Atom

$$\textbf{SE:} \; -\frac{\hbar^2}{2m}(\psi_{xx}+\psi_{yy}+\psi_{zz})+V(x,y,z)\psi = E\psi$$

$$\frac{1}{r^2}\frac{\partial}{\partial r}(r^2\frac{\partial\psi}{\partial r})+\frac{1}{r^2\sin\theta}\left(\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right)+\frac{\partial^2\psi}{\partial\phi^2}\right)+\frac{2m}{\hbar^2}(E-V)\,\psi=0$$

Ansatz: Separation of variables: $\psi(r,\theta,\phi) = R(r)\Theta(\theta)\Phi(\phi)$

$$\frac{\sin^2\theta}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)+\frac{\sin\theta}{\Theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right)+$$

$$\frac{1}{\Phi}\frac{d^2\Phi}{d\phi^2}+\frac{2mr^2\sin^2\theta}{\hbar^2}\left(\frac{e^2}{4\pi\epsilon_0 r}+E\right)=0$$

Note Φ appears in only one term!

$$\frac{1}{\Phi}\frac{d^2\Phi}{d\phi^2}=-m_l^2 \implies \Phi(\phi)=A\,e^{im_l\phi}$$

Note: $\Phi(\phi)=\Phi(\phi+2\pi n)$ requires integer squared $-m_l^2$!

Hydrogen atom (2)

Note that the third term depends on $\Phi(\phi)$ alone, so equating it to $-m_l^2$, we get are small rearrangement:

$$\frac{1}{R}\frac{d}{dR}(r^2\frac{dR}{dr})+\frac{2mr^2}{\hbar^2}(K\frac{e^2}{r}+E) = \frac{m_l^2}{\sin^2\theta}-\frac{1}{\Theta\sin\theta}\frac{d}{d\theta}(\sin\theta\frac{d\Theta}{d\theta})$$

which gives, after equating both sides to $l(l+1)$:

$$\frac{m_l^2}{\sin^2\theta} - \frac{1}{\Theta\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right) = l(l+1)$$

$$\frac{1}{R}\frac{d}{dR}(r^2\frac{dR}{dr}) + \frac{2mr^2}{\hbar^2}(K\frac{e^2}{r} + E) = l(l+1)$$

Hydrogen atom (3)

1. $\Phi(\phi) = Ae^{im_l\phi}$, where $m_l = 0, \pm 1, \pm 2, \cdots$
2. $\Theta(\theta)$ depends on both m_l^2 and l , it can be shown that $m_l = 0, \pm 1, \pm 2, \cdots, \pm l$
3. $R(r)$ depends on both l and a new quantum number n, such that $l = 0, 1, 2, \cdots (n-1)$
4. So $\psi(r, \theta, \phi) = R_{n,l}(r)\Theta_{l,m_l}(\theta)\Phi_{m_l}(\phi)$
5. n : Principal quantum number (shell): Energy
6. l: Orbital quantum number (subshell): Angular momentum magnitude
7. m: Magnetic quantum number: direction of angular momentum

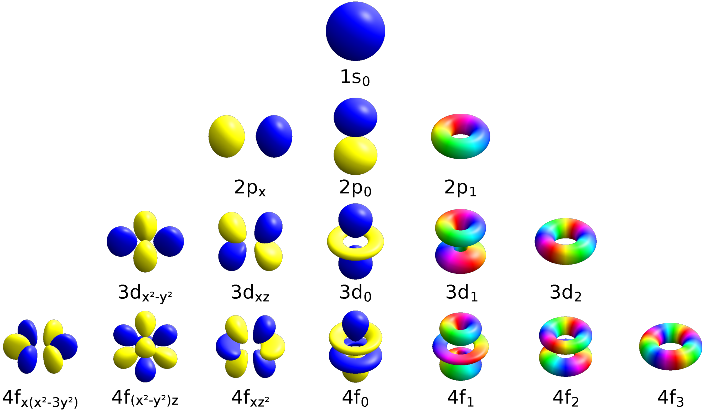
Hydrogen (4)

Table 6.1 Normalized Wave Functions of the Hydrogen Atom for $n = 1$, 2, and 3*

n	l	m_l	$\Phi(\phi)$	$\Theta(\theta)$	$R(r)$	$\psi(r, \theta, \phi)$
1	0	0	$\frac{1}{\sqrt{2\pi}}$	$\frac{1}{\sqrt{2}}$	$\frac{2}{a_0^{3/2}} e^{-r/a_0}$	$\frac{1}{\sqrt{\pi}\, a_0^{3/2}} e^{-r/a_0}$
2	0	0	$\frac{1}{\sqrt{2\pi}}$	$\frac{1}{\sqrt{2}}$	$\frac{1}{2\sqrt{2}\, a_0^{3/2}} \left(2 - \frac{r}{a_0}\right) e^{-r/2a_0}$	$\frac{1}{4\sqrt{2\pi}\, a_0^{3/2}} \left(2 - \frac{r}{a_0}\right) e^{-r/2a_0}$
2	1	0	$\frac{1}{\sqrt{2\pi}}$	$\frac{\sqrt{6}}{2} \cos\theta$	$\frac{1}{2\sqrt{6}\, a_0^{3/2}} \frac{r}{a_0} e^{-r/2a_0}$	$\frac{1}{4\sqrt{2\pi}\, a_0^{3/2}} \frac{r}{a_0} e^{-r/2a_0} \cos\theta$
2	1	± 1	$\frac{1}{\sqrt{2\pi}} e^{\pm i\phi}$	$\frac{\sqrt{3}}{2} \sin\theta$	$\frac{1}{2\sqrt{6}\, a_0^{3/2}} \frac{r}{a_0} e^{-r/2a_0}$	$\frac{1}{8\sqrt{\pi}\, a_0^{3/2}} \frac{r}{a_0} e^{-r/2a_0} \sin\theta\, e^{\pm i\phi}$
3	0	0	$\frac{1}{\sqrt{2\pi}}$	$\frac{1}{\sqrt{2}}$	$\frac{2}{81\sqrt{3}\, a_0^{3/2}} \left(27 - 18\frac{r}{a_0} + 2\frac{r^2}{a_0^2}\right) e^{-r/3a_0}$	$\frac{1}{81\sqrt{3\pi}\, a_0^{3/2}} \left(27 - 18\frac{r}{a_0} + 2\frac{r^2}{a_0^2}\right) e^{-r/3a_0}$
3	1	0	$\frac{1}{\sqrt{2\pi}}$	$\frac{\sqrt{6}}{2} \cos\theta$	$\frac{4}{81\sqrt{6}\, a_0^{3/2}} \left(6 - \frac{r}{a_0}\right) \frac{r}{a_0} e^{-r/3a_0}$	$\frac{\sqrt{2}}{81\sqrt{\pi}\, a_0^{3/2}} \left(6 - \frac{r}{a_0}\right) \frac{r}{a_0} e^{-r/3a_0} \cos\theta$
3	1	± 1	$\frac{1}{\sqrt{2\pi}} e^{\pm i\phi}$	$\frac{\sqrt{3}}{2} \sin\theta$	$\frac{4}{81\sqrt{6}\, a_0^{3/2}} \left(6 - \frac{r}{a_0}\right) \frac{r}{a_0} e^{-r/3a_0}$	$\frac{1}{81\sqrt{\pi}\, a_0^{3/2}} \left(6 - \frac{r}{a_0}\right) \frac{r}{a_0} e^{-r/3a_0} \sin\theta\, e^{\pm i\phi}$
3	2	0	$\frac{1}{\sqrt{2\pi}}$	$\frac{\sqrt{10}}{4} (3\cos^2\theta - 1)$	$\frac{4}{81\sqrt{30}\, a_0^{3/2}} \frac{r^2}{a_0^2} e^{-r/3a_0}$	$\frac{1}{81\sqrt{6\pi}\, a_0^{3/2}} \frac{r^2}{a_0^2} e^{-r/3a_0} (3\cos^2\theta - 1)$
3	2	± 1	$\frac{1}{\sqrt{2\pi}} e^{\pm i\phi}$	$\frac{\sqrt{15}}{2} \sin\theta\cos\theta$	$\frac{4}{81\sqrt{30}\, a_0^{3/2}} \frac{r^2}{a_0^2} e^{-r/3a_0}$	$\frac{1}{81\sqrt{\pi}\, a_0^{3/2}} \frac{r^2}{a_0^2} e^{-r/3a_0} \sin\theta\cos\theta\, e^{\pm i\phi}$
3	2	± 2	$\frac{1}{\sqrt{2\pi}} e^{\pm 2i\phi}$	$\frac{\sqrt{15}}{4} \sin^2\theta$	$\frac{4}{81\sqrt{30}\, a_0^{3/2}} \frac{r^2}{a_0^2} e^{-r/3a_0}$	$\frac{1}{162\sqrt{\pi}\, a_0^{3/2}} \frac{r^2}{a_0^2} e^{-r/3a_0} \sin^2\theta\, e^{\pm 2i\phi}$

*The quantity $a_0 = 4\pi\epsilon_0\hbar^2/me^2 = 5.292 \times 10^{-11}$ m is equal to the radius of the innermost Bohr orbit.

Hydrogen atom (5)



Hydrogen atom (6): Transitions

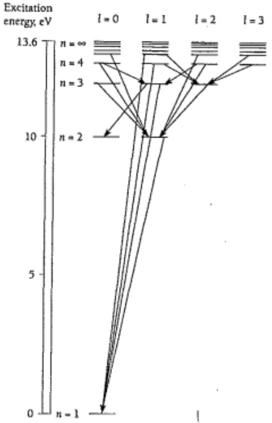
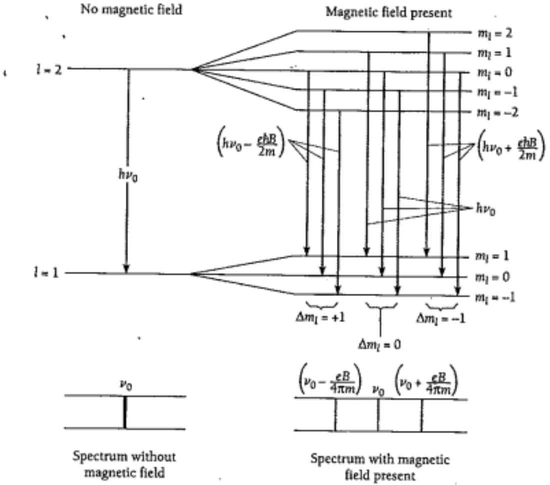


Figure 6.13 Energy-level diagram for hydrogen showing transitions allowed by the selection rule $\Delta l = \pm 1$. In this diagram the vertical axis represents excitation energy above the ground state.

Figure: Energy level diagram for hydrogen atom, showing allowed transitions $\Delta l = \pm 1$, given by $\int dx \, \psi_f^* \, (ex) \psi_i \neq 0$

Zeeman effect: magnetic dipole of atom interacts with external magnetic field

$$\tau = \mu B \sin\theta, \;\; U_m = m_l \frac{e\hbar}{2m} B$$



Multi-electron atoms: from Hydrogen atom solution

1. SE for multi-electron atoms: Only numerical methods.
2. Wave function can have even/odd symmetry:
   $\psi(x_1 = a, x_2 = b) = \pm\, \psi(x_1 = b, x_2 = a)$
3. Electron spin is also quantized: quantun number m_s
4. Exclusion Principle: No two electrons can have same set of quantum numbers (n, l, m_l, m_s)

Table 7.1 Quantum Numbers of an Atomic Electron

Name	Symbol	Possible Values	Quantity Determined
Principal	n	$1, 2, 3, \ldots$	Electron energy
Orbital	l	$0, 1, 2, \ldots, n-1$	Orbital angular-momentum magnitude
Magnetic	m_l	$-l, \ldots, 0, \ldots, +l$	Orbital angular-momentum direction
Spin magnetic	m_s	$-\frac{1}{2}, +\frac{1}{2}$	Electron spin direction

Periodic Table

Table 7.2

The Periodic Table of the Elements

The number above the symbol of each element is its atomic number, and the number below its name is its average atomic mass. The elements whose atomic masses are given in parentheses do not occur in nature but have been created in nuclear reactions. The atomic mass in such a case is the mass number of the most long-lived radioisotope of the element.

Elements with atomic numbers 110, 111, 112, 114, and 116 have also been created but not yet named.

Period	Group 1	2											3	4	5	6	7	8
1	1 H Hydrogen 1.008																	2 He Helium 4.003
2	3 Li Lithium 6.941	4 Be Beryllium 9.012											5 B Boron 10.81	6 C Carbon 12.01	7 N Nitrogen 14.01	8 O Oxygen 16.00	9 F Fluorine 19.00	10 Ne Neon 20.18
3	11 Na Sodium 22.99	12 Mg Magnesium 24.31				Transition metals							13 Al Aluminium 26.98	14 Si Silicon 28.09	15 P Phosphorus 30.97	16 S Sulfur 32.07	17 Cl Chlorine 35.45	18 Ar Argon 39.95
4	19 K Potassium 39.10	20 Ca Calcium 40.08	21 Sc Scandium 44.96	22 Ti Titanium 47.88	23 V Vanadium 50.94	24 Cr Chromium 52.00	25 Mn Manganese 54.94	26 Fe Iron 55.8	27 Co Cobalt 58.93	28 Ni Nickel 58.69	29 Cu Copper 63.55	30 Zn Zinc 65.39	31 Ga Gallium 69.72	32 Ge Germanium 72.59	33 As Arsenic 74.92	34 Se Selenium 78.96	35 Br Bromine 79.90	36 Kr Krypton 83.80
5	37 Rb Rubidium 85.47	38 Sr Strontium 87.62	39 Y Yttrium 88.91	40 Zr Zirconium 91.22	41 Nb Niobium 92.91	42 Mo Molybdenum 95.94	43 Tc Technetium (98)	44 Ru Ruthenium 101.1	45 Rh Rhodium 102.9	46 Pd Palladium 106.4	47 Ag Silver 107.9	48 Cd Cadmium 112.4	49 In Indium 114.8	50 Sn Tin 118.7	51 Sb Antimony 121.8	52 Te Tellurium 127.6	53 I Iodine 126.9	54 Xe Xenon 131.3
6	55 Cs Cesium 132.9	56 Ba Barium 137.3		72 Hf Hafnium 178.5	73 Ta Tantalum 180.9	74 W Tungsten 183.9	75 Re Rhenium 186.2	76 Os Osmium 190.2	77 Ir Iridium 192.2	78 Pt Platinum 195.1	79 Au Gold 197.0	80 Hg Mercury 200.6	81 Tl Thallium 204.4	82 Pb Lead 207.2	83 Bi Bismuth 209.0	84 Po Polonium (209)	85 At Astatine (210)	86 Rn Radon (222)
7	87 Fr Francium (223)	88 Ra Radium 226.0		104 Rf Rutherfordium (261)	105 Db Dubnium (262)	106 Sg Seaborgium (263)	107 Ns Nielsbohrium (262)	108 Hs Hassium (264)	109 Mt Meitnerium (266)								Halogens	Inert gases
	Alkali metals																	

Lanthanides (rare earths)

57 La Lanthanum 138.9	58 Ce Cerium 140.1	59 Pr Praseodymium 140.9	60 Nd Neodymium 144.2	61 Pm Promethium (145)	62 Sm Samarium 150.4	63 Eu Europium 152.0	64 Gd Gadolinium 157.3	65 Tb Terbium 158.9	66 Dy Dysprosium 162.5	67 Ho Holmium 164.9	68 Er Erbium 167.3	69 Tm Thulium 168.9	70 Yb Ytterbium 173.0	71 Lu Lutetium 175.

Spin-orbit coupling

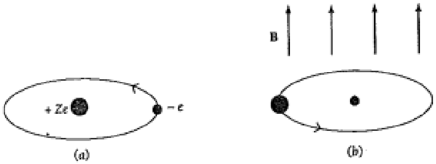
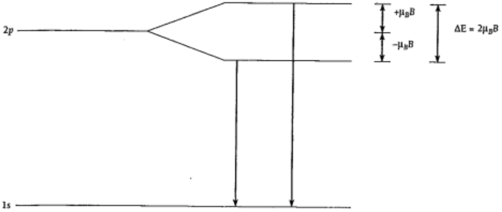


Figure 7.13 (a) An electron circles an atomic nucleus, as viewed from the frame of reference of the nucleus. (b) From the electron's frame of reference, the nucleus is circling it. The magnetic field the electron experiences as a result is directed upward from the plane of the orbit. The interaction between the electron's spin magnetic moment and this magnetic field leads to the phenomenon of spin-orbit coupling.



igure 7.14 Spin-orbit coupling splits the $2p$ state in the hydrogen atom into two substates ΔE apart. The result is a doublet two closely spaced lines) instead of a single spectral line for the $2p \rightarrow 1s$ transition.

Energy level ordering

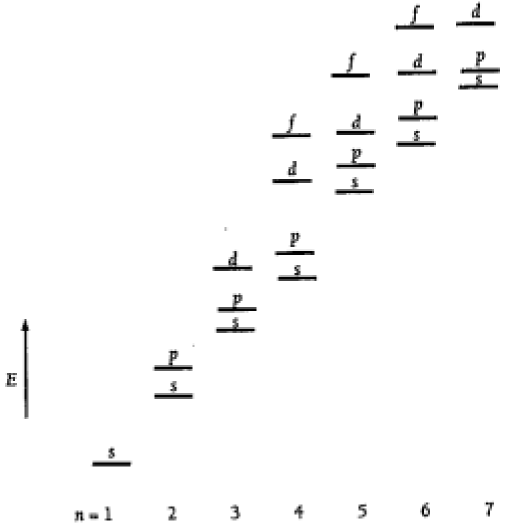
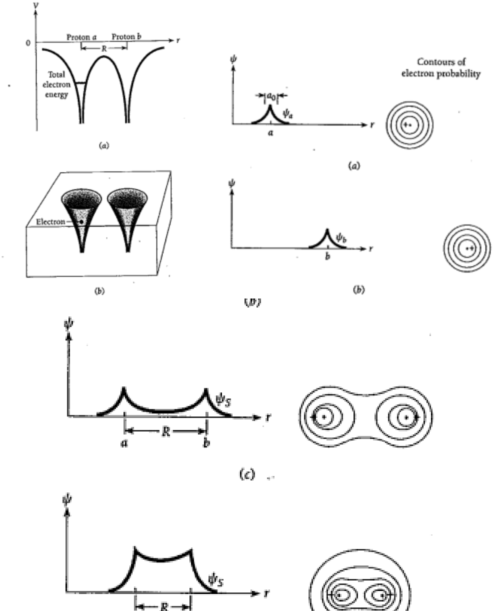


Figure 7.12 The sequence of quantum states in an atom. Not to scale.

Molecular Covalent Bond



Statistical Mechanics

- Atoms / molecules approximated as interacting particles (Lennard-Jones, electrostatic, bonds (as springs) etc)
- Classical mechanics reasonably model dynamics
- ISSUE: $N \sim 10^{23}$ atoms. Too large for tracking numerically
- Statistics is the way to go
- Statistical Mechanics: child of Boltzmann, based on strong belief on reality of atoms
- Statistical Mechanics gives a probabilistic description of system, moving away from deterministic Classical Mechanics. This was major sticking point/contention of its acceptability among Boltzmann's contemporary scientists (thermodynamics, mechanics)

Simple Harmonic oscillator

- $m\ddot{x} = -kx \implies x = A\cos(wt), w = \sqrt{k/m}$
- $x = A\cos(wt) \implies p = m\dot{x} = -Amw\sin(wt)$
- $E = \frac{1}{2}kx^2 + \frac{1}{2m}p^2 = \frac{1}{2}kA^2$
- phase plot (x vs p): point on 'circle' with angle wt. Phase-point $\mathbf{x} = (x, p)$ visits all points equally
- Make a probabilistic statement: "Equal probability for system to be in any of the *possible* phase points"

A mathematically rigorous proof for Hamiltonian systems: Louivlle theorem for phase space density (in an ensemble) $\frac{d}{dt}\rho(q_k, p_k, t) = 0$

Postulates of statistical mechanics

- State of system $\mathbf{x} = \left(\{\vec{r}_k\}_{k=1}^{N}, \{\vec{p}_k\}\right)_{k=1}^{N}$, $\mathbf{x} \in \mathcal{R}^{6N}$. Phase-space point
- POSTULATE: "Equal a priori probability of states with equal energy"
- EQUIVALENTLY: "probability of state $\mathbf{x}$ is proportional to $e^{-E(x)/kT}$". This is commonly known as Boltzmann Law.
- Ensemble: a collection of states consistent with thermodynamic constraint
  - Micro-canonical: particles, volume and energy
  - Canonical: particles, volume and temperature
  - Constant pressure, temperature and particles
  - Grand canonical: chemical potential, volume and temperature
- POSTULATE: (Ergodicity) Time average equals Ensemble average

Canonical ensemble: general setup

- phase point $\mathbf{x} \in \mathcal{R}^{3N} \times \mathcal{R}^{3N}$ (generalized coordinate, generalized momentum space)
- $p(\mathbf{x}) \propto e^{-E(\mathbf{x})/kT} = \frac{1}{Z} e^{-E(\mathbf{x})/kT}$
- Partition function $Z = \int d\mathbf{x}\; e^{-E(\mathbf{x})/kT} = \frac{1}{Z} e^{-\beta E}$, $\beta = 1/kT$
- $\langle E \rangle = \int d\mathbf{x}\; p(\mathbf{x}) E(\mathbf{x}) = -\frac{\partial}{\partial \beta} \ln Z$
- Reminder Gibbs-Helmholtz relation in Thermodynamics:

$$U = \left(\frac{\partial (A/T)}{\partial (1/T)} \right)_{V,N}$$

We identify $A/kT = -\ln Z + \phi(V, N)$, setting $\phi = 0$

- $A = -kT \ln Z$, all thermodynamics from this relation!

Degeneracy of energy level, Entropy

- $A = -kT \ln Z = -kT \int d\mathbf{x} \exp -\frac{E(\mathbf{x})}{kT}$
- $Z = \int_{E_0}^{\infty} dE \; W(E) \exp(-E/kT)$
- Integrand is gaussian with peak $\bar{E}$
  $Z = e^{-\bar{E}/kT} W(\bar{E}) \Delta E$ where ΔE is spread
- $S = (U - A)/T = (\bar{E} + kT \ln Z)/T = k \ln \left[W(\bar{E}) \Delta E \right]$
- Entropy S is thus a measure of number of states assailable to system given by $S(T) = k \ln W(\bar{E}) \Delta E$ where $\bar{E}$ and spread ΔE both are T dependent
- Microcanonical (const E,V,N): has
  $S(E, V, N) = k \ln W(E)$
- uncertainty principle $\Delta x \Delta p_x \geq h$. So gives volume of each state is given by $\Delta x \Delta p_x = h$

System of non-interacting particles

Ideal system i.e. identical non-interacting (independent) particles at temperature T

- Total energy $E = \sum E_k$ where E_k is KE of particle k
- Probability density $p(\mathbf{x}) = \Pi_{k=1}^{N} p_1(\mathbf{x}_k)$,
- $p_1(\mathbf{x}_k) = \frac{1}{Z_1} e^{-E_1(\mathbf{x}_k)/kT}$ with $Z_1 = \int d\mathbf{x}_k \; e^{-E_1(\mathbf{x}_k)/kT}$
- Barometric Law: $E_1 = mgh \implies \rho(h) \propto exp(\frac{mgh}{kT})$
- Maxwell-Boltzmann distribution:
  $E_1 = \frac{1}{2} m\vec{v} \cdot \vec{v} \implies p_1(\vec{v}) \propto exp(-\frac{mv^2}{2kT})$

System of non-interacting particles (cntd.

Equi-partition theorem:

- $Z_1 = \int d\mathbf{x_1} e^{-p_1^2/2mkT}$
- $d\mathbf{x} = d\vec{r} d\vec{p} = \int dx \int dy \int dz \int dp_x \int dp_y \int dp_z$
- $Z_1 = \left[\int d\vec{r} 1\right] \left[\int d\vec{p}\ e^{-p^2/2mkT}\right] =$
  $V \left[\int_{-\infty}^{+\infty} dp_x e^{-p_x^2/2mkT}\right]^3 = V \left(\sqrt{2\pi mkT}\right)^3$
  $Z_1 \propto T^{3/2}$
- $\langle E_1 \rangle = -\frac{\partial ln Z_1}{\partial \beta} = \frac{3}{2} kT$
- for N Particle system
  - $\langle E \rangle = \frac{3}{2} Nk\ T = \frac{3}{2} RT$
  - $Z_N = (Z_1)^N \implies p = -\left(\frac{\partial A}{\partial V}\right)_{T,N} = kT\frac{N}{V}$
- Every quadratic term in energy contributes $\frac{1}{2}kT$

Grand-canonical ensemble statistics: Ideal systems i.e. non-interacting particles

- Constant chemical potential μ, volume V and Temperature T.
  Varying number of particles N
- each state can have occupancy of:
  - $n_s = 0, 1 \implies$ Fermi-Dirac statistics
  - $n_s = 0, 1, 2, \cdots, N \implies$ Bose-Einstein statistics
- Occupation probability: $prob(n_s) = \frac{1}{\exp\left(\frac{E_s - \mu}{kT}\right) \pm 1}$, with
  - $+$ sign for Fermi-Dirac statistics
  - $-$ sign for Bose-Einstein statistics
  - When 1 is removed in denominator, we get Boltzmann statistics

$\pm$ sign in occupation statistics

1. Maxwell-Boltzmann works well for system of identical particles that can be distinguished
2. $\psi_1 = \psi_a(1)\psi_b(2)$ and $\psi_2 = \psi_a(2)\psi_b(1)$ violates non-distinguishably
3. $\psi_B = \frac{1}{\sqrt{2}}(\psi_a(1)\psi_b(2) + \psi_a(2)\psi_b(1))$ has even symmetry $\psi_B(1,2) = \psi_B(2,1)$
    1. Apparent increment of probability!
4. $\psi_F = \frac{1}{\sqrt{2}}(\psi_a(1)\psi_b(2) - \psi_a(2)\psi_b(1))$ has odd symmetry $\psi_F(1,2) = -\psi_F(2,1)$
    1. Apparent decrement of probability! (infact zero probability at same positions)

Black-body radiation: Boson photon gas

$$\textbf{Ralyeigh-Jeans: } u(\nu)d\nu = \frac{8\pi\nu^2 kT}{c^2} d\nu$$

- Standing wave: $j_x^2 + j_y^2 + j_z^2 = \left(\frac{2L}{\lambda}\right)^2$, set $j = \sqrt{j_x^2 + j_y^2 + j_z^2}$
- Number of standing waves: $g(j)dj = 2 \cdot \frac{1}{8} \cdot 4\pi j^2 dj$
- $j = \frac{2L}{\lambda} = \frac{2L\nu}{c}$
- Density of standing waves: $G = \frac{1}{V} g \implies G(\nu)d\nu = \frac{8\pi\nu^2}{c^3} d\nu$
- If energy per wave is kT, the energy density is thus: $u(\nu)d\nu = \frac{8\pi\nu^2}{c^3} kT\, d\nu$

Note that this has a major issue! $U_{total} = \int u(\nu)\, d\nu = \infty$

Planck Radiation Formula

Planck assumed that walls of black body are made of oscillators; to calculate average energy of an oscillator of frequence ν (called $\bar{E}(\nu)$) that could keep energy finite Planck after several attempts was 'cornered' to assume that energy of oscillator is not continuous but is given by $nh\nu$. This gives:

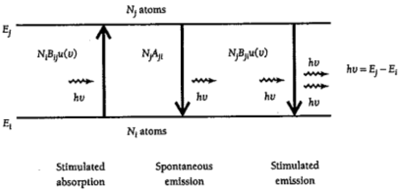
$$\bar{E} = \sum_n nh\nu \frac{e^{-nh\nu/kT}}{Z} = \frac{h\nu}{e^{h\nu/kT} - 1}$$

This average energy per oscillator gives energy of the cavity as:

$$u(\nu)d\nu = \frac{8\pi h}{c^3} \frac{\nu^3}{e^{h\nu/kT} - 1} d\nu$$

matching experimental data over the whole range of ν

LASER



$$N_{i\to j} = N_{j\to i} \text{ EQUILIBRIUM}$$

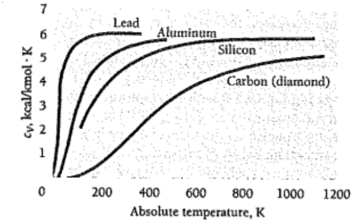
$$N_{i\to j} = N_i B_{ij} u(\nu) \text{ and } N_{j\to i} = N_j \left(A_{ij} + B_{ij} u(\nu)\right)$$

$$u(\nu) = \frac{A_{ji}/B_{ji}}{\frac{N_i}{N_j}\cdot\frac{B_{ij}}{B_{ji}} - 1}$$

- Stimulated emission: same probability as absorption (i.e $B_{ji} = B_{ij}$)
- Ratio of spontaneous and stimulated emission is ν^3, from $A_{ji} = B_{ji} \cdot \frac{8\pi h\nu^3}{c^3}$

Specific heat of solids

- CM model of solid: Particles oscillate about their mean position, i.e.each atom is a 3-d oscillator. Thus each has energy $3 \cdot 2 \cdot \frac{1}{2}kT$
- For $E = 3NkT$, the system has $C_v = 3Nk$, a constant



- Einstein (1907AD) suggested: $\bar{E} = \frac{h\nu}{e^{h\nu/kT}-1}$ and hence for $T \to 0$, we get $C_v = \propto \left(\frac{h\nu}{kT}\right)^2 e^{-h\nu/kT}$

Electrons in metal

1. Electrons are fermions, thus $n_{FD}(\epsilon) = \frac{1}{e^{(\epsilon-\epsilon_F)/kT}+1}$
2. $g(j)dj = \pi j^2 dj$, with $j = \frac{2L}{\lambda} = \frac{2Lp}{h} = \frac{2L\sqrt{2m}}{h}\sqrt{\epsilon}$
3. This gives us

$$g(\epsilon)d\epsilon \propto \sqrt{\epsilon}\, d\epsilon \implies n(\epsilon) \propto \frac{\sqrt{\epsilon}}{e^{(\epsilon-\epsilon_F)/kT}+1} d\epsilon$$

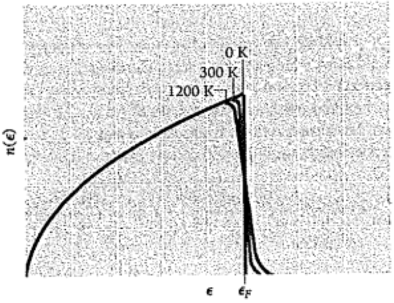


Figure 9.11 Distribution of electron energies in a metal at various temperatures.