1. The action principle

- For small $\delta s \in \mathbb{R}$, $f(s+\delta s)=f(s)+\frac{df(s)}{ds}\delta s+R(s,\delta s)$ With $\delta f:=f(s+\delta s)-f(s)$, $\delta f=\frac{df(s)}{ds}\delta s+R(s,\delta s)$, with

$$\lim_{\delta s \to 0} \frac{R(s,\delta s)}{\delta s} = 0$$

So δf vanishes to first order in δs , so $R(s,\delta s)$ can be written as $O\!\left((\delta s)^2\right)$. At the extrema of $f,\frac{df(s)}{ds}=0$ so $\delta f=O\!\left((\delta s)^2\right)$

- **Functional**: map from functions to \mathbb{R}
- y(t) stationary for functional S if

$$\frac{dS[y(t) + \varepsilon z(t)]}{d\varepsilon} \Big|_{\varepsilon=0} = 0$$

for every smooth z(t) with z(a)=z(b)=0. We use the notation $\delta y(t)=\varepsilon z(t)$. y(t) is called a path.

• Action principle (variational principle): paths described by particles are stationary paths of S:

$$\delta S \coloneqq S[x + \delta x] - S[x] = O((\delta x)^2)$$

for arbitrary smooth small deformations $\delta x(t)$ around true path x(t).

• Fundamental lemma of the calculus of variations: Let f(x) be continuous in [a, b]and

$$\int_a^b f(x)g(x)\,\mathrm{d}x = 0$$

for every smooth g(x) in [a, b] with g(a) = g(b) = 0. Then f(x) = 0 in [a, b].

Notation:

$$\frac{\partial L}{\partial x} = \frac{\partial L(r,s)}{\partial r} \mid_{(r,s) = (x(t),\dot{x}(t))}, \quad \frac{\partial L}{\partial \dot{x}} = \frac{\partial L(r,s)}{\partial s} \mid_{(r,s) = (x(t),\dot{x}(t))}$$

• For a path q and a Lagrangian $L(q,\dot{q})$, the action for the path is

$$S = \int_{t_0}^{t_1} L\big(\underline{q}(t),\underline{\dot{q}}(t)\big)) \,\mathrm{d}t$$

• The action above satisfies

$$0 = \delta S = \int_{t_0}^{t_1} \left(\sum_{i=1}^{N} \frac{\partial L}{\partial q_i} \delta q_i + \sum_{i=1}^{N} \frac{\partial L}{\partial \dot{q}_i} \delta \dot{q}_i \right) \mathrm{d}t$$

• Euler-Lagrange equation:

$$\frac{\partial L}{\partial x} - \frac{d}{dt} \left(\frac{\partial L}{\partial \dot{x}} \right) = 0$$

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• The arguments in a Lagrangian, x and \dot{x} , are independent:

$$\frac{\partial x}{\partial \dot{x}} = \frac{\partial \dot{x}}{\partial x} = 0$$

- Configuration space, \mathcal{C} : set of all possible instantaneous confingrations of a physical system. (Includes positions but not velocities).
- For configuration space \mathcal{C} of system \mathcal{S} , S has $\dim(\mathcal{C})$ degrees of freedom.
- Generalised coordinates: A set of coordinates in configuration space.
- Notation: *q* shows results holds for arbitrary choices of generalised coordinates.
- Euler-Lagrange equation for configuration space \mathcal{C} :

$$\frac{\partial L}{\partial q_i} - \frac{d}{dt} \Bigg(\frac{\partial L}{\partial \dot{q}_i} \Bigg) = 0 \quad \forall i \in \{1,...,\dim(\mathcal{C})\}$$

• For system with kinetic energy $T(\underline{q},\underline{\dot{q}})$ and potential energy $V(\underline{q})$, the Lagrangian for the system is

$$L\big(q,\dot{q}\big) = T\big(q,\dot{q}\big) - V\big(q\big)$$

• Ignorable coordinate q_i : Lagrangian does not depend on q_i :

$$\frac{\partial L(q_1,...q_N,\dot{q}_1,...\dot{q}_N)}{\partial q_i} = 0$$

• Generalised momentum of coordinate q_i :

$$\boldsymbol{p}_i\coloneqq\frac{\partial L}{\partial \dot{q}_i}$$

• Generalised momentum of ignorable coordinate is conserved.

2. Symmetries, Noether's theorem and conservation laws

• Transformation depending on ε : family of smooth maps $\varphi(\varepsilon): \mathcal{C} \to \mathcal{C}$ with $\varphi(0)$ the identity map. Can be written as

$$\boldsymbol{q_i} \rightarrow \boldsymbol{q_i}' = \boldsymbol{\phi_i} \big(\boldsymbol{q_1},...,\boldsymbol{q_N}, \boldsymbol{\varepsilon} \big)$$

where the ϕ_i are a set of $N=\dim(\mathcal{C})$ functions representing the transformation in the given coordinate system. Change in velocities is

$$\dot{q}_i \rightarrow \frac{d}{dt} \phi_i$$

• Generator of φ :

$$\frac{d\varphi(\varepsilon)}{d\varepsilon}\mid_{\varepsilon=0}=\varphi'(0)$$

• In any coordinate system,

$$\boldsymbol{q}_i \rightarrow \boldsymbol{\phi}_i \big(\underline{\boldsymbol{q}}, \boldsymbol{\varepsilon}\big) = \boldsymbol{q}_i + \varepsilon \boldsymbol{a}_i \big(\underline{\boldsymbol{q}}\big) + O(\varepsilon^2)$$

where

$$a_i = rac{\partial \phi_i \left(\underline{q}, arepsilon
ight)}{\partial arepsilon} \mid_{arepsilon = 0}$$

So the generator of the transformation is a_i .

· For velocities,

$$\dot{\boldsymbol{q}}_i \rightarrow \dot{\boldsymbol{q}}_i + \varepsilon \dot{\boldsymbol{a}}_i \big(\boldsymbol{q}_1,...,\boldsymbol{q}_N,\dot{\boldsymbol{q}}_1,...,\dot{\boldsymbol{q}}_N\big) + O(\varepsilon^2)$$

generated by \dot{a}_i .

• Equations of motion don't change when total derivative of function of coordinates and time is added to Lagrangian:

$$L \rightarrow L + \frac{dF \left(q_1,...,q_N,t\right)}{dt}$$

doesn't change equations of motion.

• Transformation $\varphi(\varepsilon)$ is **symmetry** if for some F(q,t),

$$L \rightarrow L' = L \big(\phi \big(q_1, \varepsilon \big), ..., \phi \big(q_N, \varepsilon \big) \big) = L + \varepsilon \frac{dF \big(q_1, ..., q_N, t \big)}{dt} + O(\varepsilon^2)$$

F(q,t) defined up to a constant.

- For ignorable coordinate q_i , transformation $q_i \to q_i + c_i$ is symmetry since q_i doesn't appear in Lagrangian and \dot{q}_i stays invariant. So F=0 here and $a_k=\delta_{ik}$.
- Noether's theorem: Let a symmetric transformation be generated by $a_i \big(q_1, ..., q_N \big)$, so

$$L \rightarrow L + \varepsilon \frac{dF \left(q_1, ..., q_N, t\right)}{dt} + O (\varepsilon^2)$$

Then

$$Q \coloneqq \left(\sum_{i=1}^N a_i \frac{\partial L}{\partial \dot{q}_i}\right) - F$$

is conserved (so $\frac{dQ}{dt} = 0$).

- Q is called **Noether charge**.
- Given Lagrangian $L(q,\dot{q},t)$, energy is

$$E \coloneqq \left(\sum_{i=1}^N \dot{q}_i \frac{\partial L}{\partial \dot{q}_i}\right) - L$$

- Along path q(t) satisfying equations of motion,

$$\frac{dE}{dt} = -\frac{\partial L}{\partial t}$$

• So energy conserved iff Lagrangian doesn't depend explicitly on time.

3. Normal modes

• Canonical kinetic term: of the form $T = \frac{1}{2} \sum_{i=1}^{n} \dot{q}_{i}^{2}$.

• Normal mode: solution to $\ddot{\underline{q}}+A\underline{q}=0$, associated with eigenvalue $\lambda^{(i)}>0$ of A, of form

$$\underline{q}(t) = \underline{v}^{(i)} \bigg(\alpha^{(i)} \cos \! \left(\sqrt{\lambda^{(i)}} t \right) + \beta^{(i)} \sin \! \left(\sqrt{\lambda^{(i)}} t \right) \bigg)$$

• **Zero mode**: solution to $\ddot{q} + Aq = 0$, associated with eigenvalue $\lambda^{(i)} = 0$ of A, of form

$$q(t) = \underline{v}^{(i)} \left(\alpha^{(i)}t + \beta^{(i)}\right)$$

• Instability: solution to $\ddot{q}+Aq=0$, associated with eigenvalue $\lambda^{(i)}<0$ of A, of form

$$\underline{q}(t) = \underline{v}^{(i)} \bigg(\alpha^{(i)} \cosh \bigg(\sqrt{-\lambda^{(i)}} t \bigg) + \beta^{(i)} \sinh \bigg(\sqrt{-\lambda^{(i)}} t \bigg) \bigg)$$

• When no instabilities, general solution is superposition (sum) of normal modes and zero modes.

4. Fields and the wave equation

· Generalised Euler-Lagrange equations for fields:

$$\frac{\partial \mathcal{L}}{\partial u} - \frac{\partial}{\partial x} \left(\frac{\partial \mathcal{L}}{\partial u_x} \right) - \frac{\partial}{\partial t} \left(\frac{\partial \mathcal{L}}{\partial u_t} \right) = 0$$

and for n fields $u^{(i)}$:

$$\frac{\partial \mathcal{L}}{\partial u^{(i)}} - \frac{\partial}{\partial x} \left(\frac{\partial \mathcal{L}}{\partial u_x^{(i)}} \right) - \frac{\partial}{\partial t} \left(\frac{\partial \mathcal{L}}{\partial u_t^{(i)}} \right) = 0 \quad \forall i$$

• If fields don't depend on (t, x) but on d coordinates x_i ,

$$rac{\partial \mathcal{L}}{\partial u^{(i)}} - \sum_{k=1}^d rac{\partial}{\partial x_k} \Biggl(rac{\partial \mathcal{L}}{\partial u_k^{(i)}}\Biggr)$$

where $u_k^{(i)}=\frac{\partial u^{(i)}}{\partial x_k}$ • Massless scalar field Lagrangian:

$$\mathcal{L} = \frac{1}{2}\rho u_t^2 - \frac{1}{2}\tau u_x^2$$

 ρ is **density**, τ is **tension**. The field u is the **massless scalar**.

• Equation of motion for massless scalar field is

$$\rho u_{tt} - \tau u_{xx} = 0$$

which rearranges to wave equation:

$$u_{tt} = c^2 u_{xx}$$

where $c^2 = \tau / \rho$.

• D'Alembert's solution to wave equation:

$$u(x,t) = f(x - ct) + g(x + ct)$$

f(x-ct) corresponds to a wave moving to the right with speed c, g(x+ct) corresponds to a wave moving to the left with speed c.

• If $u(x,0) = \varphi(x)$ and $u_t(x,0) = \psi(x)$ then

$$u(x,t) = \frac{1}{2}(\varphi(x-ct) + \varphi(x+ct)) + \frac{1}{2c} \int_{x-ct}^{x+ct} \psi(s) \, \mathrm{d}s$$

• In field theory, symmetry is transformation

$$u \to u' = u + \varepsilon a(u)$$

such that $\delta \mathcal{L} = O(\varepsilon^2)$. a(u) generates the transformation.

- Note: often, x_0 chosen to be t.
- Let $u_i = \frac{\partial u}{\partial x_i}$, generalised momentum vector is

$$\underline{\Pi} \coloneqq \left(\frac{\partial \mathcal{L}}{\partial u_0}, ..., \frac{\partial \mathcal{L}}{\partial u_d}\right)$$

• Noether current associated to transformation generated by a is

$$J=a\Pi$$

• If \underline{J} associated to symmetry,

$$\underline{\nabla} \cdot \underline{J} = \sum_{i=0}^{d} \frac{\partial J_i}{\partial x_i} = 0$$

• (Noether) charge density:

$$Q := J_0$$

• For d = 1, charge contained in interval (a, b):

$$Q_{(a,b)} = \int_a^b \mathcal{Q} \, \mathrm{d}x$$

• For d = 1,

$$\frac{dQ_{(a,b)}}{dt} = J_1(a) - J_1(b)$$

• Noether charge is total charge over all space. For d=1:

$$Q\coloneqq Q_{(-\infty,\infty)}=\int_{-\infty}^\infty J_0\,\mathrm{d}x$$

• If d=1 and $\lim_{x \to \pm \infty} J_1 = 0$,

$$\frac{dQ}{dt} = 0$$

• Energy-momentum tensor:

$$T_{ij} \coloneqq \frac{\partial \mathcal{L}}{\partial u_i} \frac{\partial u}{\partial x_i} - \delta_{ij} \mathcal{L}$$

• Energy density:

$$\mathcal{E} := T_{00}$$

• Conservation law for energy-momentum tensor:

$$\sum_{j=0}^{d} \frac{\partial T_{ij}}{\partial x_j} = 0$$

- Energy flux: T_{tx} .
- Dirichlet boundary condition for wave equation: $u_t(0,t)=0$ (so u(0,t)=0 as u has shift symmetry) which gives

$$u(x,t) = f(x - ct) - f(-x - ct)$$

Here, waves reflected off boundary and turned upside down.

• Neumann (free) boundary condition: $u_x(0,t) = 0$ which gives

$$u(x,t) = f(x - ct) + f(-x - ct)$$

So waves reflected off boundary and not turned upside down.

- Junction conditions:
 - *u* continuous at 0:

$$\lim_{\varepsilon \to 0^+} u(\varepsilon,t) = \lim_{\varepsilon \to 0^-} u(\varepsilon,t)$$

• Energy conservation across junction:

$$\frac{d}{dt} \Bigl(\lim_{\varepsilon \to 0} T(-\varepsilon, \varepsilon) \Bigr) = \lim_{\varepsilon \to 0} \left(T_{tx} \right)_{x = -\varepsilon} - \lim_{\varepsilon \to 0} \left(T_{tx} \right)_{x = \varepsilon}$$

• Ansatz for wave function with spring at junction at x = 0:

$$u(x,t) = \begin{cases} \operatorname{Re}((e^{ipx} + Re^{-ipx})e^{-ipct}) & \text{if } x \leq 0 \\ \operatorname{Re}(Te^{ip(x-ct)}) & \text{if } x > 0 \end{cases}$$

5. The Hamiltonian formalism

- **State** of classical system at given instant in time is complete set of data that fully fixes future evolution of system.
- **Phase (state) space** of system is space of all possible states system can be in at instant in time.
- Hamiltonian formalism parameterises phase space as generalised coordinates $\underline{q}(t)$ and associated generalised momenta p(t).
- When going from Lagrangian to Hamiltonian formalism, define generalised momentum as

$$\boldsymbol{p}_i \coloneqq \frac{\partial L\big(\underline{q},\underline{\dot{q}},t\big)}{\partial \dot{q}_i}$$

• Poisson bracket of f(q, p, t) and g(q, p, t):

$$\{f,g\} \coloneqq \sum_{i=1}^n \left(\frac{\partial f}{\partial q_i} \frac{\partial g}{\partial p_i} - \frac{\partial f}{\partial p_i} \frac{\partial g}{\partial q_i} \right)$$

where n is dimension of configuration space (half dimension of phase space). Position and momentum treated as independent when taking partial derivatives.

- · Properties of Poisson bracket:
 - Antisymmetric: $\{f, g\} = -\{g, f\}$.
 - Linear: $\{af + bg, h\} = a\{f, h\} + b\{g, h\}.$
 - Leibniz identity: $\{fg, h\} = f\{g, h\} + g\{f, h\}$.
 - Jacobi identity: $\{\{f,g\},h\}+\{\{h,f\},g\}+\{\{g,h\},f\}=0$.
- Let $\mathcal P$ be phase space, $\mathcal F$ be set of functions from $\mathcal P$ to $\mathbb R$.
- Hamiltonian flow defined by $f:\mathcal{P}\to\mathbb{R}$ is infinitesimal transformation on \mathcal{F} given by

$$\Phi_f^{(e)}: \mathcal{F} \to \mathcal{F}, \quad \Phi_f^{(e)}(g) \coloneqq g + \varepsilon \{g,f\} + O(\varepsilon^2)$$

- $\Phi_f^{(e)}$ is **generator** of map from $\mathcal P$ to $\mathcal P$:

$$\Phi_f^{(e)} \Big(\boldsymbol{q}_i \Big) = \boldsymbol{q}_i + \varepsilon \frac{\partial f}{\partial \boldsymbol{p}_i} + O(\varepsilon^2)$$

$$\Phi_f^{(e)}\!\left(\boldsymbol{p}_i\right) = \boldsymbol{p}_i - \varepsilon \frac{\partial f}{\partial q_i} + O\!\left(\varepsilon^2\right)$$

• Noether charge $Q = \left(\sum_{i=1}^n a_i p_i\right) - F$ generates symmetry transformation via Hamiltonian flow:

$$\Phi_Q^{(e)}\!\left(q_i\right) = q_i + \varepsilon\!\left\{q_i,Q\right\} + O(\varepsilon^2) = q_i + \varepsilon a_i + O(\varepsilon^2)$$

• Hamiltonian gives energy:

$$H = \left(\sum_{i=1}^n p_i \dot{q}_i\right) - L$$

• Hamilton's equations of motion:

$$\dot{\boldsymbol{q}}_{i}=\left\{\boldsymbol{q}_{i},\boldsymbol{H}\right\}=\frac{\partial\boldsymbol{H}}{\partial\boldsymbol{p}_{i}},\quad \dot{\boldsymbol{p}}_{i}=\left\{\boldsymbol{p}_{i},\boldsymbol{H}\right\}=-\frac{\partial\boldsymbol{H}}{\partial\boldsymbol{q}_{i}}$$

• Time evolution of f(q, p) generated by H:

$$\frac{df}{dt} = \{f, H\}$$

If *f* depends explicitly on time,

$$\frac{df}{dt} = \frac{\partial f}{\partial t} + \{f, H\}$$

• Relation between Hamiltonian and Lagrangian:

$$\frac{\partial H\big(\underline{q},\underline{p},t\big)}{\partial t}\mid_{q,p} = -\frac{\partial L\big(\underline{q},\underline{\dot{q}},t\big)}{\partial t}\mid_{q,\dot{q}}$$

• If function Q doesn't depend explicitly on time, $\{H,Q\}=0$ so Hamiltonian left invariant by transformation generated by Q:

$$\Phi_Q(H) = H + \varepsilon \{Q,H\} + O\bigl(\varepsilon^2\bigr) = H + O\bigl(\varepsilon^2\bigr)$$

6. Wave function and probabilities

- Wave function: continuous, complex function of position x and time t: $\psi(x,t)$.
- Probability density to find particle at time t and position x: $P(x,t) = |\psi(x,t)|^2$, with

$$\int_{-\infty}^{\infty} P(x,t) \, \mathrm{d}x = 1$$

If this integral exists, ψ is **square-normalisable**. If integral equal to 1, ψ is **normalised**. Probability of finding particle in interval (a, b) is

$$\int_a^b P(x,t) \, \mathrm{d}x$$

• **Expectation value** of f(x):

$$\langle f(x) \rangle = \int_{-\infty}^{\infty} f(x) P(x, t) \, \mathrm{d}x$$

- Uncertainty in position: $\Delta x = \sqrt{\langle x^2 \rangle \langle x \rangle^2}$
- Infinite potential well in 0 < x < L:

$$V(x) = \begin{cases} 0 & \text{if } 0 < x < L \\ \infty & \text{otherwise} \end{cases}$$

Wave function vanishes in regions $x \leq 0$ and $x \geq L$. Eigenfunctions for this potential are

$$\varphi_n(x) = \sqrt{\frac{2}{L}} \sin\!\left(\frac{n\pi x}{L}\right)$$

- Wave function collapse: if position is measured to be x_0 , wave function becomes very localised around at x_0 , and measurement immediately afterwards will also yield x_0 .
- $\langle x \rangle$ is not average of repeated measurements of same particle, but average of measurements of many particles with same wave function.

7. Momentum and Planck's constant

· Position operator:

$$\hat{x} = x$$

• Momentum operator:

$$\hat{p}=-i\hbar\frac{\partial}{\partial x}$$

where \hbar is **reduced Planck constant**.

Commutator:

$$[\hat{x},\hat{p}] := \hat{x}\hat{p} - \hat{p}\hat{x} = i\hbar$$

• Expectation value of momentum for wave function ψ :

$$\langle \psi \rangle = \int_{-\infty}^{\infty} \overline{\psi(x,t)} \hat{p} \psi(x,t) \, \mathrm{d}x = -i\hbar \int_{-\infty}^{\infty} \overline{\psi(x,t)} \frac{\partial}{\partial x} \psi(x,t) \, \mathrm{d}x$$

• Expection value of function of momentum:

$$\langle f(p) \rangle = \int_{-\infty}^{\infty} \overline{\psi(x,t)} f(\hat{p}) \psi(x,t) \, \mathrm{d}x$$

• Momentum uncertainty:

$$\Delta p = \sqrt{\langle p^2
angle - \langle p
angle^2}$$

• Heisenberg's uncertainty principle: for any normalised wave function,

$$\Delta x \Delta p \ge \frac{\hbar}{2}$$

8. Schrodinger's equation

• Hamiltonian operator:

$$\widehat{H} = \frac{\widehat{p}^2}{2m} + V(x) = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x)$$

Corresponds to measurements of energy.

• Schrodinger's equation:

$$i\hbar\frac{\partial\psi(x,t)}{\partial t} = \widehat{H}\psi(x,t)$$

9. The Hilbert space

- Hermitian inner product on vector space V: map $\langle \cdot, \cdot \rangle : V \times V \to \mathbb{C}$ satisfying:
 - $\langle v, w \rangle = \overline{\langle w, v \rangle}$.
 - $\langle v, a_1 w_1 + a_2 w_2 \rangle = a_1 \langle v, w_1 \rangle + a_2 \langle v, w_2 \rangle$.
 - $\langle a_1v_1+a_2v_2,w\rangle=\overline{a_1}\langle v_1,w\rangle+\overline{a_2}\langle v_2,w\rangle$
 - $\langle v, v \rangle \ge 0$ for all v and $\langle v, v \rangle = 0 \Longleftrightarrow v = 0$.
- Set of continuous square-integrable wave functions forms complex vector space. So $a_1\psi_1+a_2\psi_2$ is also square-integrable.
- Hermitian inner product of two wave functions:

$$\langle \psi_1, \psi_2 \rangle = \int_{-\infty}^{\infty} \overline{\psi_1(x)} \psi_2(x) \, \mathrm{d}x$$

• If $\left\{ \varphi_n(x) \right\}$ is orthonormal basis so $\langle \varphi_m, \varphi_n \rangle = \delta_{mn}$, then any vector can be expressed

$$\psi(x) = \sum_{n} c_n \varphi_n(x)$$

where $c_m = \langle \varphi_m, \psi \rangle$. Hermitian product is then

$$\langle \psi_1, \psi_2 \rangle = \sum_i \overline{\psi_1(x)} \psi_2(x) = \sum_n \overline{c}_{1,n} c_{2,n}$$

So squared norm of ψ is $|\psi|^2 = \langle \psi, \psi \rangle = \sum_n |c_n|^2$.

10. Hermitian operators

• For vector space V, **linear operator** is map $A:V\to V$ with

$$A(a_1v_1 + a_2v_2) = a_1(Av_1) + a_2(Av_2)$$

- · Any linear combination or composition of linear operators is linear operator.
- Matrix elements of linear operator for orthonormal basis $\{e_j\}$: $A_{ij} = \langle e_i, Ae_j \rangle$.
- Adjoint A^{\dagger} : $\langle v_1, Av_2 \rangle = \langle A^{\dagger}v_1, v_2 \rangle$. Adjoint has matrix elements which are conjugate of transpose of original matrix.
- Properties of adjoint:
 - $\bullet \ \ (\overline{a_1}A_1 + a_2A_2)^\dagger = \overline{a_1}A_1^\dagger + \overline{a_2}A_2^\dagger.$
 - $(A_1 A_2)^{\dagger} = A_2^{\dagger} A_1^{\dagger}$.
- Hermitian operator: linear operator that is equal to adjoint. Matrix is Hermitian: $A_{ij} = \overline{A_{ji}}$.
- Position and momentum operators Hermitian, w.r.t. orthonomal basis of wave functions $\left\{\varphi_n(x)\right\}.$

11. The spectrum of a Hermitian operator

- Wave function ψ_a is **eigenfunction** of Hermitian differential operator A with **eigenvalue** a if $A\psi_a(x) = a\psi_a(x)$.
- Expectation value of Hermitian operator:

$$\langle A \rangle = \langle \psi, A\psi \rangle = \int_{-\infty}^{\infty} \overline{\psi(x)} A\psi(x) dx$$

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- If ψ_a is eigenfunction, $\langle A \rangle = a$ and $\langle A^n \rangle = a^n.$ So uncertainty $\Delta A = 0.$
- Let A Hermitian operator.
 - Eigenvalues are real and
 - + $\boldsymbol{\psi}_1, \boldsymbol{\psi}_2$ eigenfunctions of A with distinct eigenvalues are orthogonal.
- If A has discrete spectrum, can choose orthonormal basis of eigenfunctions $\left\{ \varphi_n(x) \right\}$ with eigenvalues a_n . Then any wave function can be written as $\psi(x) = \sum_n c_n \varphi_n(x)$ where $c_n = \langle \varphi_n, \psi \rangle$. Can interpret $|c_n|^2$ as probability of measurement of A yielding a_n .
- Dirac delta function:

$$\delta(a) = \begin{cases} 0 & \text{if } a \neq 0 \\ \infty & \text{if } a = 0 \end{cases}$$

with $\int_{-\infty}^{\infty} \delta(a) da = 1$ and

$$\int^\infty \delta(a-a')f(a')\,\mathrm{d}a'=f(a)$$

• Limit definition of Dirac delta function: limit as $\varepsilon \to 0^+$ of

$$\delta_{arepsilon}(a) = rac{1}{arepsilon\sqrt{\pi}}e^{-a^2/arepsilon^2}$$

• Delta funtion is Fourier transform of 1:

$$\delta(a) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{iaa'} \, \mathrm{d}a'$$

• If A has continuous spectrum (eigenvalues $a \in \mathbb{R}$) then can choose basis of eigenfunctions $\varphi_a(x)$ with $\langle \varphi_a, \varphi_{a'} \rangle = \delta(a-a')$. Can uniquely expand wave function

$$\psi(x) = \int_{-\infty}^{\infty} c(a) \varphi_a(x) \, \mathrm{d}a$$

where $c(a) = \langle \varphi_a, \psi \rangle$. Norm of wave function is

$$\langle \psi, \psi
angle = \int_{-\infty}^{\infty} \left| c(a) \right|^2 \mathrm{d}a$$

For normalised wave function,

$$\int_{-\infty}^{\infty} |c(a)|^2 = 1$$

so treat $|c(a)|^2$ as probability distribution for measurements of A.

12. Postulates of quantum mechanics

- · Postulates of quantum mechanics:
 - Particle described by normalised wave function $\psi(x)$.
 - Measurable quantities represented by Hermitian operators A(x, p), constructed from polynomial/real analytic functions of position and momentum operators:

$$\begin{split} \hat{x} &= x, \\ \hat{p} &= -i\hbar \frac{\partial}{\partial x} \end{split}$$

- Possible outcomes of measurement of A are given by its eigenvalues a. If spectrum discrete, $\left\{a_j\right\}$, then choose eigenfunction basis $\varphi_j(x)$ with $\langle \varphi_i, \varphi_j \rangle = \delta_{ij}$. Then probability of finding measurement as eigenvalue a_j is $\left|\langle \varphi_j, \psi \rangle\right|^2$. If spectrum continuous, $a \in \mathbb{R}$, choose eigenfunctions $\varphi_a(x)$ with $\langle \varphi_a, \varphi_{a'} \rangle = \delta(a-a')$, then probability of finding measurement as eigenvalue a is $\left|\langle \varphi_a, \psi \rangle\right|^2$.
- If measurement of A yields eigenvalue a_j (or a), wave function immediately afterwards is $\varphi_j(x)$ (or $\varphi_a(x)$). **Note**: in continuous case, wave function immediately afterwards not square-normalisable.
- If no measurements made, ψ evolves in time according to Schrödinger equation:

$$i\hbar \frac{\partial \psi(x,t)}{\partial t} = \widehat{H}\psi(x,t)$$

• For discrete spectrum, expectation value of A is

$$\langle A \rangle = \sum_{j} a_{j} P_{j}$$

for eigenvalues a_{j} , $P_{j}=\left|c_{j}\right|^{2}$ is probability of measurement being a_{j} .

• For continuous spectrum, expectation value of A is

$$\langle A \rangle = \int_{-\infty}^{\infty} a P(a) \, \mathrm{d}a$$

where $P(a) = |c(a)|^2$ is probability distribution.

13. Commutators and uncertainty principle

• Commutator of operators A, B:

$$[A, B] = AB - BA$$

- Properties of commutator:
 - **Anti-symmetry**: [A, B] = -[B, A].
 - Linearity: $[a_1A_1 + a_2A_2, B] = a_1[A_1, B] + a_2[A_2, B]$.
 - [A, BC] = B[A, C] + [A, B]C.
 - Jacobi identity: [A, [B, C]] + [B, [C, A]] + [C, [A, B]] = 0.
- If [A, B] = 0, possible to find orthonormal basis of wave functions which are eigenfunctions of A and B.
- A, B compatible if [A, B] = 0.
- Generalised uncertainty principle: for any square-normalisable wave function,

$$\Delta A \Delta B \geq \frac{1}{2} |\langle [A,B] \rangle|$$

• Anti-commutator: $\{A, B\} = AB + BA$.

14. Energy revisited

- Eigenfunctions of Hamiltonian are **bound states** if classical solution is bounded in space.
- Let $V(x) \geq V_0$ for all $x \in \mathbb{R}$. Then if wave function normalised, $\langle H \rangle > V_0$.
- If $\psi(x)$ is normalised eigenfunction of H with eigenvalue E, then $E > V_0$.
- **Zero-point energy**: smallest eigenvalue $E > V_0$.
- Spectrum of Hamiltonian is non-degenerate.

15. Stationary states

- Solution to Schrodinger's equation is $\psi(x,t) = \varphi(x)e^{-iEt/\hbar}$ where $\varphi(x)$ is eigenfunction of Hamiltonian with eigenvalue E. This solution is **stationary wave function**.
- Full solution to Schrodinger's equation:

$$\psi(x,t) = \sum_j c_j \varphi_j(x) e^{-iE_j t/\hbar}$$

where $\{\varphi_j(x)\}$ is orthonormal basis of Hamiltonian eigenfunctions with eigenvalues E_j , c_j are coefficients of initial wave function expansion:

$$\psi(x,0) = \sum_j c_j \varphi_j(x)$$

Probability of energy measurement being E_j is $P_j = \left| \langle \varphi_j, \psi \rangle \right|^2 = \left| c_j \right|^2$.

• Time-independent Schrodinger equation:

$$\widehat{H}\varphi(x) = E\varphi(x)$$

where $\varphi(x)$ is Hamiltonian eigenfunction with eigenvalue (energy) E.

16. Case study: the free particle

• If V(x) = 0, eigenfunction of \hat{p} is eigenfunction of \hat{H} .

17. Two particle systems

• For two particles in one dimension, wave function is $\psi(x_1,x_2)$, probability density is $P(x_1,x_2)=|\psi(x_1,x_2)|^2$: probability of finding particle one in (a,b) and particle two in (c,d) is

$$\int_a^b \int_c^d P(x_1, x_2) \, \mathrm{d}x_1 \, \mathrm{d}x_2$$

• Probability of finding particle one in (a, b) is

$$P(x_1) = \int_a^b P(x_1, x_2) \, \mathrm{d}x_2$$

(similarly for particle two).

- If both positions measured as $\tilde{x}_1, \tilde{x}_2,$ wave function collapses to product of position eigenfunctions:

$$\psi_{\rm before}(x_1,x_2) \rightarrow \psi_{\rm after}(x_1,x_2) \propto \delta(x_1-\tilde{x}_1)\delta(x_2-\tilde{x}_2)$$

• If only particle one measured,

$$\psi_{\text{before}}(x_1, x_2) \rightarrow \delta(x_1 - \tilde{x}_1) \psi_{\text{before}}(\tilde{x}_1, x_2)$$

• Hamiltonian for two particles with zero potential:

$$\widehat{H}=-rac{\hbar^2}{2m}rac{\partial}{\partial x_1^2}-rac{\hbar^2}{2m}rac{\partial}{\partial x_2^2}$$

Eigenfunctions are product are single-particle eigenfunctions:

$$\varphi(x_1,x_2) = \frac{2}{L} \sin \left(\frac{n\pi x_1}{L}\right) \sin \left(\frac{m\pi x_2}{L}\right)$$

Eigenvalues are sum of eigenvalues of single-particle Hamiltonians.

• Wave function separable if can be written as product of function of x_1 and function of x_2 .

• **Entangled states**: when measurement of one particle affects subsequent measurement of other particle. Occurs for non-separable wave functions.

18. Simple harmonic oscillator

• Simple harmonic oscillator potential:

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

where ω is angular frequency.

- If V has minimum at $x=x_0$ and $|x-x_0|$ small, $m\omega^2\approx \frac{1}{2}V^{\prime\prime}(x_0)$ by Taylor expanion of V(x) around x_0 .
- Energy spectrum of Hamiltonian for simple harmonic oscillator is $E_n=\hbar\omega (n+\frac{1}{2})$

19. The continuity equation

· Probability current density:

$$J\coloneqq rac{\hbar}{2mi}ig(\overline{\psi}\partial_x\psi-\psi\partial_x\overline{\psi}ig)$$

• Continuity equation:

$$\partial_t P + \partial_x J = 0$$

where $P(x,t) = |\psi(x,t)|^2$.

• Probability current vanishes for square-normalisable wave functions.

20. Scattering problems

• When particle has to cross potential, for $t\to -\infty$, $\psi(x,t)\to \psi_I(x,t)$ is incoming wavepacket, then it scatters from the potential, as $t\to \infty$, tends to sum of reflected and transmitted wavepackets:

$$\psi(x,t) \to \psi_{\scriptscriptstyle R}(x,t) + \psi_{\scriptscriptstyle T}(x,t)$$

As $t \to \infty$, reflected and transmitted wavepackets don't interfere.

• Probability of reflection is

$$R = \lim_{t o \infty} \int_{-\infty}^{\infty} \left| \psi_R(x,t) \right|^2 \mathrm{d}x$$

Probability of transmission is

$$T = \lim_{t \to \infty} \int_{-\infty}^{\infty} \left| \psi_T(x,t) \right|^2 \mathrm{d}x$$

R+T=1 if ψ normalised.

21. Tunnelling

- Finite step potential: for $V_0>0$

$$V(x) = \begin{cases} 0 & \text{if } x < 0 \\ V_0 & \text{if } x \ge 0 \end{cases}$$

- Scattering occurs when particle has energy $E > V_0$.
- Tunnelling occurs when particle has energy $0 < E < V_0$.
- For scattering, Hamiltonian eigenfunctions are

$$\varphi(x) = \begin{cases} e^{ikx} + re^{-ikx} & \text{if } x < 0 \\ te^{ik'x} & \text{if } x \ge 0 \end{cases}$$

where
$$k=\sqrt{2mE/\hbar^2},\,k'=\sqrt{2m(E-V_0)/\hbar^2}$$

- Determine r and t by using that ψ and $\partial_x \psi$ continuous at x = 0.
- Finite barrier potential:

$$V(x) = \begin{cases} 0 & \text{if } x < 0 \\ V_0 & \text{if } 0 \le x \le L \\ 0 & \text{if } x > L \end{cases}$$

• For tunnelling, Hamiltonian eigenfunctions are

$$\varphi(x) = \begin{cases} e^{ikx} + re^{-ikx} & \text{if } x < 0 \\ te^{-\kappa x} & \text{if } x \ge 0 \end{cases}$$

where $\kappa = \sqrt{2m(V_0 - E) / \hbar^2}$. Coefficients r and t found by replacing $k' \to i\kappa$.

22. Momentum-space wave function

• Momentum-space wave function:

$$ilde{\psi}(p) = rac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \psi(x) e^{-ipx/\hbar} \, \mathrm{d}x$$

satisfies

$$\psi(x) = rac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} ilde{\psi}(p) e^{ipx/\hbar} \, \mathrm{d}p$$

• For momentum-space wave function, position and momentum act as operators

$$\hat{x} = i\hbar \frac{\partial}{\partial p}$$

$$\hat{p} = p$$

• Momentum probability density: $\tilde{P}(p) = \left| \tilde{\psi}(p) \right|^2$. Probability of momentum measurement being a is

$$\int_a^b \tilde{P}(p) \, \mathrm{d}p$$

• Momentum expectation value of f(p):

$$\langle f(p) \rangle = \int_{-\infty}^{\infty} f(p) \tilde{P}(p) \, \mathrm{d}p$$

• Position expectation value of f(x):

$$\langle f(x) \rangle = \int_{-\infty}^{\infty} \overline{\tilde{\psi}(p)} f\bigg(i\hbar \frac{\partial}{\partial p}\bigg) \tilde{\psi}(p) \, \mathrm{d}p$$

- + $\psi(x)$ normalised iff $\tilde{\psi}(p)$ normalised.
- Translating $\psi(x)$ by x_0 multiplies $\tilde{\psi}(p)$ by $e^{-ipx_0/\hbar}$. Translating $\tilde{\psi}(p)$ by p_0 multiplies $\psi(x)$ by $e^{ip_0x/\hbar}$.