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 $\delta f \coloneqq f(s+\delta s) - f(s)$, $\delta f = \frac{df(s)}{ds}\delta s + R(s,\delta s)$, 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 $O\Big((\delta s)^2\Big)$
- At the extrema of f, $\frac{df(s)}{ds} = 0$ so $\delta f = O\Big((\delta s)^2\Big)$
- **Functional**: map from functions to $\mathbb{R}$
- $y(t)$ **stationary** for functional S if

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

  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 (an action functional):

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

  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**:

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

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

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

- 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**:

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

- 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 confiugratinons 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: $\underline{q}$ shows results holds for arbitrary choices of generalised coordinates.
- **Euler-Lagrange equation for configuration space $\mathcal{C}$**:

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

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

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

- **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:

$$p_i := \frac{\partial L}{\partial \dot{q}_i}$$

- 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

$$q_i \to q_i{}' = \phi_i(q_1, ..., q_N, \varepsilon)$$

  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

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

- **Generator of φ**:

$$\frac{d\varphi(\varepsilon)}{d\varepsilon}\,|_{\varepsilon=0} = \varphi'(0)$$

- In any coordinate system,

$$q_i \to \phi_i(\underline{q}, \varepsilon) = q_i + \varepsilon a_i(\underline{q}) + O(\varepsilon^2)$$

  where

$$a_i = \frac{\partial \phi_i(\underline{q}, \varepsilon)}{\partial \varepsilon} \mid_{\varepsilon=0}$$

So the generator of the transformation is a_i.

- For velocities,

$$\dot{q}_i \to \dot{q}_i + \varepsilon \dot{a}_i(q_1, ..., q_N, \dot{q}_1, ..., \dot{q}_N) + O(\varepsilon^2)$$

generated by $\dot{a}_i$.

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

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

doesn't change equations of motion.

- Transformation $\varphi(\varepsilon)$ is **symmetry** if for some $F(\underline{q}, t)$,

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

$F(\underline{q}, t)$ 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 $a_i(q_1, ..., q_N)$, so

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

Then

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

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

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

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

- Along path $\underline{q}(t)$ 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

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

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

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

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

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

- 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,

$$\frac{\partial\mathcal{L}}{\partial u^{(i)}} - \sum_{k=1}^{d}\frac{\partial}{\partial x_k}\left(\frac{\partial\mathcal{L}}{\partial u_k^{(i)}}\right)$$

  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

$$\underline{J} = a\underline{\Pi}$$

- 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**:

$$\mathcal{Q} \coloneqq J_0$$

- 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**:

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

- **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:

$$\frac{d}{dt}\Big(\lim_{\varepsilon \to 0^+} E(-\varepsilon, \varepsilon)\Big) = \lim_{\varepsilon \to 0^+} (T_{tx})_{x=-\varepsilon} - \lim_{\varepsilon \to 0^+} (T_{tx})_{x=\varepsilon}$$

- **Ansatz for wave function with spring at junction at $x = 0$**:

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

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 $\underline{p}(t)$.
- When going from Lagrangian to Hamiltonian formalism, define **generalised momentum** as

$$p_i := \frac{\partial L(\underline{q}, \underline{\dot{q}}, t)}{\partial \dot{q}_i}$$

- **Poisson bracket** of $f(\underline{q}, \underline{p}, t)$ and $g(\underline{q}, \underline{p}, t)$:

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

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 $\mathcal{P}$:

$$\Phi_f^{(e)}(q_i) = q_i + \varepsilon\frac{\partial f}{\partial p_i} + O(\varepsilon^2)$$

$$\Phi_f^{(e)}(p_i) = p_i - \varepsilon\frac{\partial f}{\partial q_i} + O(\varepsilon^2)$$

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

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

- **Hamiltonian** gives **energy**:

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

- **Hamilton's equations of motion**:

$$\dot{q}_i = \{q_i, H\} = \frac{\partial H}{\partial p_i}, \quad \dot{p}_i = \{p_i, H\} = -\frac{\partial H}{\partial q_i}$$

- Time evolution of $f(\underline{q},\underline{p})$ 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**:

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

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

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

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**:

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

- **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**:

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

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

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

8. Schrodinger's equation

- **Hamiltonian operator**:

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

  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:
  - $\langle v, w \rangle = \overline{\langle w, v \rangle}$.
  - $\langle v, a_1 w_1 + a_2 w_2 \rangle = a_1 \langle v, w_1 \rangle + a_2 \langle v, w_2 \rangle$.
  - $\langle a_1 v_1 + a_2 v_2, w \rangle = \overline{a_1} \langle v_1, w \rangle + \overline{a_2} \langle v_2, w \rangle$
  - $\langle v, v \rangle \geq 0$ for all v and $\langle v, v \rangle = 0 \iff v = 0$.
- 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 $\{\varphi_n(x)\}$ 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

$$A(a_1 v_1 + a_2 v_2) = a_1(Av_1) + a_2(Av_2)$$

- 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:
  - $(a_1 A_1 + a_2 A_2)^\dagger = \overline{a_1} A_1^\dagger + \overline{a_2} A_2^\dagger$.
  - $(A_1 A_2)^\dagger = A_2^\dagger A_1^\dagger$.
- **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 $\{\varphi_n(x)\}$.

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:

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

.

- 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
  - ψ_1, ψ_2 eigenfunctions of A with distinct eigenvalues are orthogonal.
- If A has discrete spectrum, can choose orthonormal basis of eigenfunctions $\{\varphi_n(x)\}$ 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 $\int_{-\infty}^{\infty} \delta(a)\,\mathrm{d}a = 1$ and

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

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

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

- **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

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

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:

$$\hat{x} = x,$$

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

  - Possible outcomes of measurement of A are given by its eigenvalues a. If spectrum discrete, $\{a_j\}$, 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

$|\langle\varphi_j, \psi\rangle|^2$. 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 $|\langle\varphi_a, \psi\rangle|^2$.

- 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 Schrodinger 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, $P_j = |c_j|^2$ is probability of measurement being a_j.

- For continuous spectrum, expectation value of A is

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

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 $\widehat{H}$.

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:

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

- If only particle one measured,

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

- Hamiltonian for two particles with zero potential:

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

  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, $m\omega^2 \approx \frac{1}{2}V''(x_0)$ by Taylor expanion of $V(x)$ around x_0.
- Energy spectrum of Hamiltonian for simple harmonic oscillator is $E_n = \hbar\omega\left(n + \frac{1}{2}\right)$

19. The continuity equation

- **Probability current density**:

$$J := \frac{\hbar}{2mi}\left(\overline{\psi}\partial_x\psi - \psi\partial_x\overline{\psi}\right)$$

- **Continuity equation**:

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

  where $P(x,t) = |\psi(x,t)|^2$.
- Probability current vanishes as $x \to \pm\infty$ 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:

$$\psi(x,t) \to \psi_R(x,t) + \psi_T(x,t)$$

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

- Probability of reflection is

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

  Probability of transmission is

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

  $R + T = 1$ if ψ normalised.

21. Tunnelling

- **Finite step potential**: for $V_0 > 0$

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

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

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

  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**:

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

- For tunnelling, Hamiltonian eigenfunctions are

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

  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**:

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

  satisfies

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

- 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 $a < p < b$ 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 $f(x)$:

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

- $\psi(x)$ 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 $e^{ip_0x/\hbar}$.