

# 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

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

So  $\delta f$  vanishes to first order in  $\delta s$ , so  $R(s, \delta s)$  can be written as  $O((\delta s)^2)$

- At the extrema of  $f$ ,  $\frac{df(s)}{ds} = 0$  so  $\delta f = O((\delta s)^2)$
- **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  $S$ :

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

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

$$\int_a^b f(x)g(x) dx = 0$$

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

- **Notation:**

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

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

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

- The action above satisfies

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

- **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 configurations of a physical system. (Includes positions but not velocities).
- For configuration space  $\mathcal{C}$  of system  $\mathcal{S}$ ,  $\mathcal{S}$  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  $\mathcal{C}$ :**

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

- 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  $q_i$ :

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

- **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  $\varepsilon$ :** family of smooth maps  $\varphi(\varepsilon) : \mathcal{C} \rightarrow \mathcal{C}$  with  $\varphi(0)$  the identity map. Can be written as

$$q_i \rightarrow q_i' = \phi_i(q_1, \dots, q_N, \varepsilon)$$

where the  $\phi_i$  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  $\varphi$ :**

$$\left. \frac{d\varphi(\varepsilon)}{d\varepsilon} \right|_{\varepsilon=0} = \varphi'(0)$$

- In any coordinate system,

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

where

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

So the generator of the transformation is  $a_i$ .

- For velocities,

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

generated by  $\dot{a}_i$ .

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

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

doesn't change equations of motion.

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

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

$F(\underline{q}, t)$  defined up to a constant.

- For ignorable coordinate  $q_i$ , transformation  $q_i \rightarrow q_i + c_i$  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  $a_i(q_1, \dots, q_N)$ , so

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

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:**

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

$\rho$  is **density**,  $\tau$  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

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

- In field theory, **symmetry** is transformation

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

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

$$\underline{\Pi} := \left( \frac{\partial \mathcal{L}}{\partial u_0}, \dots, \frac{\partial \mathcal{L}}{\partial u_d} \right)$$

- **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:**

$$\mathcal{Q} := J_0$$

- For  $d = 1$ , **charge contained in interval**  $(a, b)$ :

$$Q_{(a,b)} = \int_a^b \mathcal{Q} \, dx$$

- For  $d = 1$ ,

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

- **Noether charge** is total charge over all space. For  $d = 1$ :

$$Q := Q_{(-\infty, \infty)} = \int_{-\infty}^{\infty} J_0 \, dx$$

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

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

- **Energy-momentum tensor:**

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

- **Energy density:**

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

- **Conservation law for energy-momentum tensor:**

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

- **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:

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

- Energy conservation across junction:

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

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

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

## 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  $g(\underline{q}, \underline{p}, t)$ :

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

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  $f : \mathcal{P} \rightarrow \mathbb{R}$  is infinitesimal transformation on  $\mathcal{F}$  given by

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

- $\Phi_f^{(e)}$  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  $H$ :

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

In  $f$  depends explicitly on time,

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

- **Relation between Hamiltonian and Lagrangian:**

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

- 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

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

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

$$\int_a^b P(x, t) dx$$

- **Expectation value of  $f(x)$ :**

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

- **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  $\psi$ :**



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

- **Expection value of function of momentum:**

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

- **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:**

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

Corresponds to measurements of energy.

- **Schrodinger's equation:**

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

## 9. The Hilbert space

- **Hermitian inner product on vector space  $V$ :** map  $\langle \cdot, \cdot \rangle : V \times V \rightarrow \mathbb{C}$  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:**

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

- 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

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

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

## 10. Hermitian operators

- For vector space  $V$ , **linear operator** is map  $A : V \rightarrow V$  with

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

- Any linear combination or composition of linear operators is linear operator.
- Matrix elements of linear operator** for orthonormal basis  $\{e_j\}$ :  $A_{ij} = \langle e_i, A e_j \rangle$ .
- Adjoint**  $A^\dagger$ :  $\langle v_1, A v_2 \rangle = \langle A^\dagger v_1, v_2 \rangle$ . 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. orthonormal basis of wave functions  $\{\varphi_n(x)\}$ .

## 11. The spectrum of a Hermitian operator

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

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

- .
- If  $\psi_a$  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
  - $\psi_1, \psi_2$  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  $\int_{-\infty}^{\infty} \delta(a) da = 1$  and

$$\int_{-\infty}^{\infty} \delta(a - a') f(a') da' = f(a)$$

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

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

- **Delta function is Fourier transform of 1:**

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

- 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

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

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

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

For normalised wave function,

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

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,  $\psi$  evolves in time according to Schrodinger equation:

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

- 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

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

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**:  $[a_1 A_1 + a_2 A_2, B] = a_1 [A_1, B] + a_2 [A_2, B]$ .
  - $[A, BC] = B[A, C] + [A, B]C$ .
  - **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  $P_j = |\langle \varphi_j, \psi \rangle|^2 = |c_j|^2$ .

## 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

$$\int_a^b \int_c^d P(x_1, x_2) dx_1 dx_2$$

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

$$P(x_1) = \int_a^b P(x_1, x_2) dx_2$$

(similarly for particle two).

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

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

- If only particle one measured,

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

- Hamiltonian for two particles with zero potential:

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

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  $\omega$  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 expansion 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:**

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

- **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  $t \rightarrow -\infty$ ,  $\psi(x, t) \rightarrow \psi_I(x, t)$  is incoming wavepacket, then it scatters from the potential, as  $t \rightarrow \infty$ , tends to sum of reflected and transmitted wavepackets:

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

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

- Probability of reflection is

$$R = \lim_{t \rightarrow \infty} \int_{-\infty}^{\infty} |\psi_R(x, t)|^2 dx$$

Probability of transmission is

$$T = \lim_{t \rightarrow \infty} \int_{-\infty}^{\infty} |\psi_T(x, t)|^2 dx$$

$R + T = 1$  if  $\psi$  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  $\psi$  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  $k' \rightarrow i\kappa$ .

## 22. Momentum-space wave function

- **Momentum-space wave function:**

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

satisfies

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

- 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:**  $\tilde{P}(p) = |\tilde{\psi}(p)|^2$ . Probability of momentum measurement being  $a < p < b$  is

$$\int_a^b \tilde{P}(p) dp$$

- Momentum expectation value of  $f(p)$ :

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

- Position expectation value of  $f(x)$ :

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

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