

## 1 The Nature of Light

The photoelectric effect. Einstein proposed that

$$eV_0 = E_k = h\nu - W.$$

where  $V_0$  is the stopping potential,  $E_k$  is the energy of the electron.  $W$  is the work function

The Compton effect is given by

$$\lambda' - \lambda = \frac{1}{mc} (1 - \cos\theta)$$

The wave and particle properties of a quanta:

(1) Quantized (particle-like): Quanta are discrete and can be counted.

(2) Superposition (wave-like): Quanta obeys linear equations of motion.

(3) Energy and angular frequency (connection of wave and particle). The Planck formula says

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

(4) Momentum and wave number (connection of wave and particle): The de-Broglie formula tells

$$p = \frac{\hbar}{\lambda} = \hbar k.$$

## 2 The Quantum Wave Functions

A quantum state  $|\Psi\rangle$  is described by a wave function  $\Psi(x, t)$ .

Born's rule: The wave function is a probability amplitude,  $|\Psi(x, t)|^2$  is the probability density. The probability to find the particle between  $x$  and  $x + dx$  is  $|\Psi(x, t)|^2 dx$ .

Normalization:

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

Plane waves: for constant  $V$ , we have

$$\Psi_p(x, t) = \frac{1}{\sqrt{2\pi\hbar}} e^{i(px - Et)/\hbar}$$

where  $p = \hbar k$  and  $E = \hbar\omega$ .

Completeness:

$$\Psi(x, t) = \sum_n C_n f_n(x)$$

Operators:  $\hat{x} = x$ ,  $\hat{p} = -\frac{\hbar}{i} \frac{\partial}{\partial x}$ . The expectation value.

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

$$\langle \hat{p} \rangle = \int_{-\infty}^{\infty} \Psi^*(x, t) \hat{p} \Psi(x, t) dx$$

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

## 3 Observables and Measurements

An observable is represented by an operator  $\hat{O}$  in quantum mechanics. The observables are required to be Hermitian operators:  $\hat{O}^\dagger \equiv (\hat{O}^*)^T = \hat{O}$ . We have

$$\hat{O}\Psi_\lambda(x) = \lambda\Psi_\lambda(x),$$

where  $\lambda$  is the eigenvalue,  $\Psi_\lambda(x)$  is the eigenstate.

For example, for the plane waves,

$$\hat{p}\Psi_p(x) = p\Psi_p(x).$$

For position eigenstate, we have

$$x\Psi_q(x) = q\Psi_q(x).$$

the solution is  $\Psi_q(x) = \delta(x - q)$ .

For superpositions when measuring  $\hat{O}$ , we decompose the general state in eigenstate. For observables taking discrete results:

$$\psi(x) = \sum_i C_i \psi_{\lambda_i}(x).$$

The probability for the measurement outcome being  $\lambda_i$  is  $|C_i|^2$ . After the measurement, the wave function collapses to  $\psi_{\lambda_i}$ .

For observables taking continuous results.

$$\psi(x) = \int C(\lambda) \psi_{\lambda} d\lambda$$

The probability density for the measurement outcome being  $\lambda$  is  $|C(\lambda)|^2$ . After the measurement, the wave function collapses to  $\psi_{\lambda}$ .

For example, for the plane wave,

$$\psi(x, t) = \int_{-\infty}^{\infty} C(p) \psi_p(x, t) dp.$$

For position measurement,

$$\psi(x) = \int_{-\infty}^{\infty} \psi(q) \delta(x-q) dq.$$

#### 4 The Uncertainty Principle

Uncertainty of the state's position  $\sigma_x \equiv \sqrt{\langle (x - \langle x \rangle)^2 \rangle} = \sqrt{\langle x^2 \rangle - \langle x \rangle^2}$ .

Uncertainty of the state's momentum  $\sigma_p \equiv \sqrt{\langle (\hat{p} - \langle \hat{p} \rangle)^2 \rangle} = \sqrt{\langle \hat{p}^2 \rangle - \langle \hat{p} \rangle^2}$ .

Heisenberg's uncertainty principle:

$$\sigma_x \sigma_p \geq \frac{\hbar}{2}$$

For example, for plane waves:  $\psi_p = \frac{1}{\sqrt{2\pi\hbar}} e^{ipx/\hbar}$ ,  $\sigma_p=0$  and  $\sigma_x=\infty$ .

For a Gaussian wave packet

$$\psi(x) = \frac{1}{\sqrt{6\sigma\sqrt{2\pi}}} e^{-\frac{x^2}{4\sigma^2}}$$

Note that  $\langle \hat{p} \rangle = 0$ ,  $\langle \hat{p} \rangle^2 = \hbar^2/(4\sigma^2)$ . Thus  $\sigma_x \sigma_p = \hbar/2$ .

#### 5 The Schrödinger Equation

The Schrödinger equation is given by

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

$\hat{H} \equiv -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V$  is the Hamiltonian, thus the Schrödinger equation can also be written as

$$i\hbar \frac{\partial \Psi}{\partial t} = \hat{H} \Psi.$$

The spreading wave packet: Suppose we have  $V=0$ . The wave function

$$\Psi(x, t) = \frac{6}{\sqrt{2\pi(6^2 + \beta^2 t^2)}} e^{ikx - i\omega t} e^{-\frac{(x - v_g t)^2}{4(6^2 + \beta^2 t^2)}}$$

where  $v_g \equiv \hbar k/m$ ,  $\beta \equiv \hbar k^2/2m$ ,  $\omega \equiv \hbar k^2/2m$  and  $6$  is a free parameter indicating the spatial spread of  $\Psi$  at  $t=0$ . This is known as the Gaussian wave packet, as

$$|\Psi(x, t)|^2 = \frac{6}{\sqrt{2\pi(6^2 + \beta^2 t^2)}} e^{-\frac{6^2(x - v_g t)^2}{2(6^2 + \beta^2 t^2)}}$$

The spatial spread of the wave function is

$$\sigma_x(t) = \sqrt{6^2 + \frac{\beta^2 t^2}{6^2}}.$$

Time-independent Schrödinger equation

$$\hat{H}\Psi = E\Psi.$$

And  $\Psi(x, t) = e^{-iEt/\hbar} \psi(x)$ .

The standard boundary condition for  $\psi$ : 1.  $\psi$  is always continuous 2.  $d\psi/dx$  is continuous except at points where the potential is infinite.

A step in potential: Now consider

$$V(x) = \begin{cases} V_1, & \text{if } x < x_0 \\ V_2, & \text{if } x > x_0 \end{cases}$$

I. Scattering state:  $E > V_1$  and  $E > V_2$ . The Schrödinger equation writes

$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} = (E - V)\psi \Rightarrow \frac{d^2\psi}{dx^2} = -k^2\psi$$

The solution for the ODE is

$$\psi(x) = Ae^{ikx} + Be^{-ikx}, \text{ where } k = \frac{\sqrt{2m(E-V)}}{\hbar}.$$

So for this situation we have

$$\psi(x) = \begin{cases} Ae^{ik_1 x} + Be^{-ik_1 x}, & k_1 = \frac{\sqrt{2m(E-V_1)}}{\hbar}, \text{ if } x < x_0 \\ Ce^{ik_2 x} + De^{-ik_2 x}, & k_2 = \frac{\sqrt{2m(E-V_2)}}{\hbar}, \text{ if } x > x_0 \end{cases}$$

We assume that the wave comes from  $x < x_0$ , then  $D=0$ . Applying the boundary condition, we have

$$Ae^{ik_1 x_0} + Be^{-ik_1 x_0} = Ce^{ik_2 x_0}$$

$$Ak_1 e^{ik_1 x_0} - Bk_1 e^{-ik_1 x_0} = Ck_2 e^{ik_2 x_0}.$$

Then

$$Ae^{ik_1 x_0} = \frac{k_1 + k_2}{2k_1} Ce^{ik_2 x_0}, \quad Be^{-ik_1 x_0} = \frac{k_1 - k_2}{2k_1} Ce^{ik_2 x_0}.$$

Thus

$$C = \frac{2k_1}{k_1 + k_2} e^{i(k_1 - k_2)x_0} A, \quad B = \frac{k_1 - k_2}{2k_1} e^{i(k_1 + k_2)x_0} C = \frac{k_1 - k_2}{k_1 + k_2} e^{2ik_1 x_0} A.$$

II. Bound state:  $V_1 < E < V_2$ .

For  $x < x_0$ , we still have  $\psi(x) = Ae^{ik_1 x} + Be^{-ik_1 x}$ ,  $k_1 = \sqrt{2m(E-V_1)}/\hbar$

For  $x > x_0$ , the Schrödinger equation reads

$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} = (E - V_2)\psi \Rightarrow \frac{d^2\psi}{dx^2} = k^2\psi$$

Then the solution is

$$\psi(x) = Ce^{kx} + De^{-kx}, \text{ where } k = \frac{\sqrt{-2m(E-V_2)}}{\hbar}$$

$C$  has to be 0 or else  $\psi \rightarrow \infty$  as  $x \rightarrow \infty$ . Thus

$$\psi(x) = De^{-kx}, \quad x > x_0.$$

Infinite potential well Consider

$$V(x) = \begin{cases} \infty, & \text{if } x < x_1 \text{ or } x > x_2 \\ V, & \text{if } x_1 < x < x_2. \end{cases}$$

The Schrödinger equation reads

$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} = (E - V)\psi$$

Thus the solution is

$$\psi(x) = Acoskx + Bsinkx, \text{ where } k = \frac{\sqrt{2m(E-V)}}{\hbar}.$$

Since  $\psi(x_1) = \psi(x_2) = 0$ , then

$$\begin{aligned} \psi(x_1) = Acoskx_1 + Bsinkx_1 &= 0, \quad \psi(x_2) = Acoskx_2 + Bsinkx_2 = 0, \\ \Rightarrow \frac{coskx_1}{sinkx_1} &= \frac{coskx_2}{sinkx_2} \Rightarrow sinkx_2 coskx_1 - sinkx_1 coskx_2 = sin[k(x_2 - x_1)] = 0. \end{aligned}$$

Thus we have

$$k(x_2 - x_1) = n\pi, \quad n = 1, 2, 3, \dots$$

Also,

$$B = -\frac{Acoskx_1}{sinkx_1}$$

Thus

$$\psi(x) = Acoskx - \frac{Acoskx_1 \cdot sinkx}{sinkx_1} = -A \sin[k_1(x - x_1)]$$

Normalization gives that

$$\int_{x_1}^{x_2} |A|^2 \sin^2(kx - kx_0) dx = |A|^2 \cdot \left[ \frac{x}{2} - \frac{\sin(2k(x-x_0))}{4k} \right]_{x_1}^{x_2}$$
$$= |A|^2 \frac{x_2 - x_1}{2} = 1$$

Thus,

$$A = \pm \sqrt{\frac{2}{x_2 - x_1}}.$$

Then,

$$\Psi_n(x) = \pm \sqrt{\frac{2}{x_2 - x_1}} \sin\left(\frac{n\pi}{x_2 - x_1}(x - x_0)\right).$$

And the energy is given by

$$E_n = \frac{\hbar^2 n^2 \pi^2}{2m(x_2 - x_1)} + V$$

## 6 Identical Particle

The existence of identical particles is a fundamental principle in quantum mechanics. The two-particle wave function  $\Psi(x_1, x_2, t)$  means that the probability to find one particle at  $(x_1, x_1 + dx)$  and the other particle at  $(x_2, x_2 + dx)$  is  $|\Psi(x_1, x_2, t)|^2 dx_1 dx_2$ .

Two kinds of multi-particle wave functions:

I. Symmetric wave function with  $\Psi(x_1, x_2, t) = \Psi(x_2, x_1, t)$ . Such particles are called bosons, representing the force, like photons, gravitons.

II. Anti-symmetric wave functions with  $\Psi(x_1, x_2, t) = -\Psi(x_2, x_1, t)$ . Such particles are called fermions, representing the building blocks of matter, like electrons, quarks.

### 2 The Hydrogen Atom

Balmer found a formula for the Hydrogen spectrum for visible light frequencies

$$\frac{1}{\lambda} = R_H \left( \frac{1}{4} - \frac{1}{n^2} \right), n=3,4,5\dots$$

Rydberg proposed a general formula for Hydrogen

$$\frac{1}{\lambda} = R_H \left( \frac{1}{m^2} - \frac{1}{n^2} \right), n=m+1, m+2, \dots$$

Bohr's model: Classically, the force acting on the electron is

$$F = m \frac{v^2}{r} = \frac{1}{4\pi\epsilon_0} \frac{e^2}{r^2} \Rightarrow mv^2 = \frac{1}{4\pi\epsilon_0} \frac{e^2}{r}$$

The energy of the electron is

$$E_e = \frac{1}{2}mv^2 + V(r) = -\frac{1}{2}mv^2.$$

The frequency of the electron is

$$\nu_e = \frac{v}{2\pi r}$$

Emitting photons, the electron move from the orbital to  $\infty$ , its energy becomes 0. Thus

$$0 - E_e = nh\nu$$

Bohr suggests that  $\nu = \frac{\nu_e}{2} = \frac{v}{4\pi r}$ , then  
 $mvr = \frac{nh}{2\pi}$ .

Since  $r = \frac{e^2}{4\pi\epsilon_0 m v^2}$ , we have

$$\nu = \frac{e^2}{2n\epsilon_0 h} \Rightarrow E_e(n) = -\frac{me^4}{8\epsilon_0^2 h^2 n^2}.$$

Hence

$$\boxed{\nu = c R_H \left( \frac{1}{n_1^2} - \frac{1}{n_2^2} \right), R_H = -\frac{me^4}{8\epsilon_0^2 h^2 c}}$$

Solving the Schrödinger equation for the Hydrogen atom:  $n$  is the principle quantum number,  $\ell$  is the azimuthal quantum number,  $m$  is the magnetic quantum number. They satisfies

$$\boxed{n = 1, 2, \dots, \ell = 0, 1, \dots, n-1, m = 0, \pm 1, \pm 2, \dots, \pm \ell}$$

The energy is

$$\boxed{E = \frac{E_1}{n}, E_1 = -\frac{me^4}{32\pi^2 \epsilon_0^2 \hbar^2}}$$

For each set of  $n, \ell, m$ , there're two electron states (spin up and spin down). In general, for a given  $n$ , there are  $2n^2$  state. The states with the same  $n$  is said to be in the same shell; the states with the same  $n$  and  $\ell$  is said to be in the same orbital.

The s orbital has greater probability density at both small  $r$  and larger than p. d.

For energy conservation, the frequency of the photon emitted or absorbed is

$$\boxed{\nu = \frac{E_{n'} - E_n}{h}}$$

where the two states must satisfy  $\Delta \ell = \pm 1, \Delta m_\ell = 0, \pm 1$ .

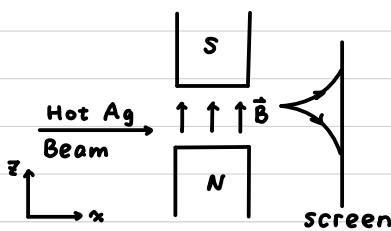
### 3 The Periodic Table

Pauli's exclusion principle: If one orbital is filled, the other electrons in the atom must be put in other orbitals.

Screening effect: In a hydrogen atom, for the same  $n$ ,  $E_s = E_p = E_d = E_f$ . In a multiple electron atom, for the same  $n$ ,  $E_s < E_p < E_d < E_f$ . since higher angular momentum means farther away from the nuclei and thus more screening.

## 1 Spin

### 1.1 The Stern-Gerlach Experiment



The magnetic potential energy  $U = -\vec{\mu} \cdot \vec{B}$ ,

where  $\vec{\mu}$  is the magnetic moment,  $\vec{B}$  is the magnetic field.

The Stern-Gerlach experiment: measuring the magnetic moment of atoms.

Outcome: 1. One beam splits into two beams with equal strength

2. This indicates that a Ag atom has a magnetic moment  $\vec{\mu}$ .

Interpretation: 1.  $|\vec{\mu}|$  is quantized.

2. Before measurement,  $\vec{\mu}$  should point to random directions

The external magnetic field measures the z-component  $\mu_z$  of atoms. The states collapse to one of the two eigenstates with eigenvalues  $\pm |\vec{\mu}|$ .

Call  $| \uparrow \rangle$  with eigenvalue  $|\vec{\mu}|$ , and  $| \downarrow \rangle$  with eigenvalue  $-|\vec{\mu}|$ .

An electron has magnetic moment.

### 1.2 The Quantum Mechanics of Spin

A basis:  $| \uparrow \rangle, | \downarrow \rangle$ . And  $| \rightarrow, \leftarrow, \otimes, \odot \rangle = \frac{1}{\sqrt{2}}(| \uparrow \rangle + e^{i\phi}| \downarrow \rangle)$ .

Write  $| \rightarrow \rangle = \frac{1}{\sqrt{2}}(| \uparrow \rangle + | \downarrow \rangle)$ ,  $| \leftarrow \rangle = \frac{1}{\sqrt{2}}(| \uparrow \rangle - | \downarrow \rangle)$

$| \otimes \rangle = \frac{1}{\sqrt{2}}(| \uparrow \rangle + i| \downarrow \rangle)$ ,  $| \odot \rangle = \frac{1}{\sqrt{2}}(| \uparrow \rangle - i| \downarrow \rangle)$ .

A spinstate is a building block of information – a quantum bit (qubit).

A general state can be written as

$$| \psi \rangle = \cos \frac{\theta}{2} | \uparrow \rangle + e^{i\phi} \sin \frac{\theta}{2} | \downarrow \rangle,$$

where  $0 \leq \theta \leq \pi$ ,  $0 \leq \phi \leq 2\pi$ . Two real parameters are used to describe the state.

Spin states in state vectors

$$\begin{aligned} | \uparrow \rangle &= \begin{pmatrix} 1 \\ 0 \end{pmatrix}, & | \downarrow \rangle &= \begin{pmatrix} 0 \\ 1 \end{pmatrix} \\ | \rightarrow \rangle &= \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}, & | \leftarrow \rangle &= \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix} \\ | \otimes \rangle &= \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ i \end{pmatrix}, & | \odot \rangle &= \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -i \end{pmatrix}. \end{aligned}$$

Inner product of spin states: Suppose  $| \psi \rangle = \begin{pmatrix} a \\ b \end{pmatrix}$ ,  $| \chi \rangle = \begin{pmatrix} c \\ d \end{pmatrix}$ , define

$$\langle \psi | = \begin{pmatrix} a \\ b \end{pmatrix}^T = (a^*, b^*),$$

then  $\langle \psi | \chi \rangle = (a^* b^*) \begin{pmatrix} c \\ d \end{pmatrix} = a^* c + b^* d$ .

Normalization and orthogonality of spin states

$$\langle \uparrow | \uparrow \rangle = \langle \downarrow | \downarrow \rangle = \langle \rightarrow | \rightarrow \rangle = \langle \leftarrow | \leftarrow \rangle = \langle \otimes | \otimes \rangle = \langle \odot | \odot \rangle = 1,$$

and

$$\langle \uparrow | \downarrow \rangle = \langle \downarrow | \uparrow \rangle = \langle \otimes | \odot \rangle = \langle \odot | \otimes \rangle = 0.$$

Pauli matrices are operator for spin measurements in z, x, y directions:

$$\sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad \sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

Using Pauli matrices to build operators for measurement in a general direction  $\hat{n}$

$$\sigma(\hat{n}) = \sum_i \hat{n}_i \sigma_i = \hat{n} \cdot \hat{\sigma}$$

The probability to find the spin up state  $| \uparrow \rangle$  is

$$P_{\uparrow} = \langle \psi | \frac{1 + \sigma_3}{2} | \psi \rangle$$

The probability to find a spin  $| \psi \rangle$  along the  $\hat{n}$  direction after a measurement is

$$P_{\hat{n}} = \langle \psi | \frac{1 + \sigma(\hat{n})}{2} | \psi \rangle$$

Pauli matrices acting on spin states:

$$\sigma_3 | \uparrow \rangle = | \uparrow \rangle, \quad \sigma_3 | \downarrow \rangle = -| \downarrow \rangle.$$

$$\sigma_1 | \uparrow \rangle = | \downarrow \rangle, \quad \sigma_1 | \downarrow \rangle = | \uparrow \rangle.$$

$$\sigma_2 | \uparrow \rangle = i | \downarrow \rangle, \quad \sigma_2 | \downarrow \rangle = -i | \uparrow \rangle.$$

Note that "1" represents the identity matrix.

## 2 Multiple Spins and Their Entanglement

### 2.1 Multiple Spins, Entanglements and Quantum Computing

States with two spins:  $| \uparrow\uparrow \rangle, | \uparrow\downarrow \rangle, | \downarrow\uparrow \rangle, | \downarrow\downarrow \rangle$ .

A general state is  $|\Psi\rangle = \alpha_1| \uparrow\uparrow \rangle + \alpha_2| \uparrow\downarrow \rangle + \alpha_3| \downarrow\uparrow \rangle + \alpha_4| \downarrow\downarrow \rangle$ .

The state contains two qubits of information. There are four complex numbers. deducting normalization and overall phase, we have  $4 \times 2 - 2 = 6$  real parameters to describe the state.

Generally, for  $n$  qubits of information, a general state is described by  $2^{n+1}-2$  real parameters. The qubits contain much more information in entanglements. Independent measurements can be represented by two sets of Pauli matrices, one acting on particle 1,  $\sigma_i$ , and the other acting on particle 2,  $T_i$ . The probability to find particle 1 in direction  $\hat{n}$  and particle 2 in direction  $\hat{m}$  in a state is

$$P = \langle \Psi | \frac{1+\sigma(\hat{n})}{2} \frac{1+T(\hat{m})}{2} | \Psi \rangle$$

### 2.2 The Einstein-Podolsky-Rosen (EPR) Paradox



Prepare a state (singlet state)  $|S\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$  and take the two particles far apart each other.

Suppose A, B measure the spin of the particles along the  $z$ -direction immediately after receiving the particles.

$$P_{\uparrow\uparrow} = \langle S | \frac{1+\sigma_z}{2} \frac{1+\tau_z}{2} | S \rangle = 0, P_{\uparrow\downarrow} = \langle S | \frac{1-\sigma_z}{2} \frac{1-\tau_z}{2} | S \rangle = 0.$$

$$P_{\downarrow\uparrow} = \langle S | \frac{1+\sigma_z}{2} \frac{1-\tau_z}{2} | S \rangle = \frac{1}{2}, P_{\downarrow\downarrow} = \langle S | \frac{1-\sigma_z}{2} \frac{1+\tau_z}{2} | S \rangle = \frac{1}{2}.$$

A, B find that they have equal chance to find the state spin up or spin down. If they meet, they will find their results is correlated - if one  $\uparrow$ , the other must  $\downarrow$ . The correlation doesn't depend on the measurement direction. As long as they're measuring the same direction, then one  $\uparrow$ , the other  $\downarrow$ . Before A, B meet, they consider their results random. Thus A cannot encode any classical information in what she choose to measure and let B know immediately.

### 2.3 The Bell's Inequality and its Violation

A local variable theory: 1. Hidden variables 2. Local

One consequence of the classical logic is

$$N(A \cdot \neg B) + N(B \cdot \neg C) \geq N(A \cdot \neg C)$$

$N$  denotes the number of states satisfying the condition.

A: Measuring particle 1 along the  $z$ -axis and get positive spin

B: Measuring particle 1 along  $45^\circ$  in  $x-z$  plane and get positive spin

C: Measuring particle 1 along the  $x$ -axis and get positive spin

$\neg A$ : Measuring particle 2 along the  $z$ -axis and get positive spin

$\neg B$ : Measuring particle 2 along  $45^\circ$  in  $x-z$  plane and get positive spin

$\neg C$ : Measuring particle 2 along the  $x$ -axis and get positive spin

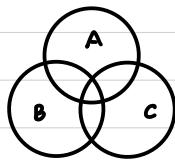
The above is known as the Bell's Inequality.

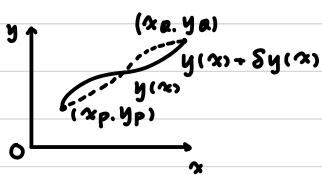
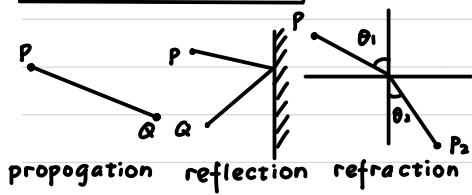
$$P(A \cdot \neg B) = \frac{1}{4}(1 - \frac{1}{\sqrt{2}}) \approx 0.073$$

$$P(B \cdot \neg C) = \frac{1}{4}(1 - \frac{1}{\sqrt{2}}) \approx 0.073$$

$$P(A \cdot \neg C) = \frac{1}{4} = 0.25$$

The classical logic is violated. Thus the quantum information stored in the entanglement cannot be mimicked by local hidden variables





### Taylor expansion

$$f(a) = f(0) + f'(0)a + \frac{f''(0)}{2!}a^2 + \dots$$

$$\sqrt{1+(y'+(\delta y)')^2} = \frac{k}{\sqrt{1+k^2}} \cdot \frac{dk}{da} = \frac{k}{\sqrt{1+k^2}}$$

Integration by parts

$$d(uv) = u dv + v du$$

$$= u dv = d(uv) - v du.$$

### 1 Fermat's Principle of Light

**Light propagation problem:** Given two fixed points  $P$  and  $Q$ , how does light propagate between those points. Fermat proposed that: Light travels between two given points along the path of extremal time.

A path can be a function, say  $y = y(x)$ .  $T$  is the light propagation time  $T$ .  $T$  is a functional of  $y$ , denoted as  $T[y]$ .

To find the extremal path, vary the path by  $y(x) \rightarrow y(x) + \delta y(x)$ , where  $\delta y$  is an arbitrary infinitesimal function,  $\delta y(x_p) = 0$ ,  $\delta y(x_Q) = 0$  (boundary conditions).

The functional variation

$$\delta T \equiv T[y + \delta y] - T[y]$$

A path with extremal time must have  $\delta T = 0$  for all the possible variations  $\delta y(x)$ .

**Light propagation in the vacuum.** The propagation time

$$T = \int_{t_p}^{t_Q} dt = \frac{1}{c} \int_{x=x_p}^{x=x_Q} \sqrt{dx^2 + dy^2} = \frac{1}{c} \int_{t_p}^{t_Q} \sqrt{1 + \left(\frac{dy}{dx}\right)^2} dx.$$

Vary  $y(x) \rightarrow y(x) + \delta y(x)$ . By Taylor expansion

$$\sqrt{1 + \left(\frac{d[y(x) + \delta y(x)]}{dx}\right)^2} = \sqrt{1 + (y' + (\delta y)')^2} = \sqrt{1 + (y')^2 + \frac{y'}{\sqrt{1+(y')^2}} \frac{d\delta y}{dx} + O((\delta y)^2)}.$$

Thus we have

$$\begin{aligned} \delta T[y] &= T[y + \delta y] - T[y] = \frac{1}{c} \int_{x_p}^{x_Q} \frac{y'}{\sqrt{1+(y')^2}} \frac{d\delta y}{dx} dx \\ &= \frac{1}{c} \int_{x_p}^{x_Q} \left\{ \frac{d}{dx} \left( \frac{y'}{\sqrt{1+(y')^2}} \delta y \right) - \delta y \frac{d}{dx} \left( \frac{y'}{\sqrt{1+(y')^2}} \right) \right\} dx \\ &\underline{\delta y[x_p] = 0, \delta y[x_Q] = 0} - \frac{1}{c} \int_{x_p}^{x_Q} \delta y \frac{d}{dx} \left( \frac{y'}{\sqrt{1+(y')^2}} \right) dx \end{aligned}$$

$\delta T = 0$  requires that

$$\frac{d}{dx} \left( \frac{y'}{\sqrt{1+(y')^2}} \right) = 0 \rightarrow y' = \text{const}$$

Hence light travels with straight line.

### 2 Principle of Extremal Action

**The action principle:** A theory is defined by an action  $S$ . The equation of motion of the theory corresponds to the extremal action  $\delta S = 0$ .

**Action principle in Newtonian mechanics:** Given a potential  $V(q)$ .

$q(t)$  is the position. Define an action

$$S[q] = \int_{t_1}^{t_2} dt \left[ \frac{1}{2} m \dot{q}^2 - V(q) \right]$$

Vary  $q(t) \rightarrow q(t) + \delta q(t)$ .  $\delta q(t_1) = \delta q(t_2) = 0$ .

$$\delta S = \int_{t_1}^{t_2} dt \left[ m \dot{q} \delta \dot{q} - \frac{dV}{dq} \delta q \right] = \int_{t_1}^{t_2} dt \left[ \frac{d}{dt} (m \dot{q} \delta \dot{q}) - m \ddot{q} \delta q - \frac{dV}{dq} \delta q \right]$$

The first term vanishes because of the boundary conditions. The last two terms hold for all  $\delta q(t)$ , and thus

$$m \ddot{q} + \frac{dV}{dq} = 0$$

This is just the Newton's second law.

In general, consider a Lagrangian  $L = L(q_i, \dot{q}_i, t)$ , where  $i = 1, 2, \dots, N$ .  $q_i$  denotes the position of the  $i$ -th particle and the action is defined as

$$S = \int L(q_i, \dot{q}_i, t) dt$$

The variation

$$\begin{aligned} \delta S &= \sum_i \left\{ \left( \frac{\partial L}{\partial q_i} \delta \dot{q}_i + \frac{\partial L}{\partial \dot{q}_i} \delta q_i \right) dt \right\} \\ &= \sum_i \left\{ \left[ \frac{d}{dt} \left( \frac{\partial L}{\partial \dot{q}_i} \delta q_i \right) - \frac{d}{dt} \left( \frac{\partial L}{\partial q_i} \right) \delta \dot{q}_i - \frac{\partial L}{\partial q_i} \delta q_i \right] dt \right\} \end{aligned}$$

Then we obtain the Euler-Lagrangian equation

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

$$f(x_0 + \Delta x) - f(x_0) = f'(x_0) \Delta x + O((\Delta x)^2)$$

### 3 Symmetry and Conservation Laws

A symmetry of a theory is a transformation under which the theory does not change. Consider an infinitesimal transformation

$$q_i \rightarrow \tilde{q}_i = q_i + \epsilon \delta q_i$$

If the action doesn't change

$$\delta S = \int L(\tilde{q}_i, \dot{\tilde{q}}_i, t) dt - \int L(q_i, \dot{q}_i, t) dt = 0$$

Example: time translation, to test if the prediction of a theory is time independent. The time translation:

$$q_i(t) \rightarrow \tilde{q}_i(t) = q_i(t + \epsilon \delta t) = q_i(t) + \epsilon \dot{q}_i(t) \delta t, \delta q_i = \dot{q}_i(t) \delta t$$

If the Lagrangian doesn't depend on  $t$ ,  $L(q_i, \dot{q}_i, t) = L(q_i, \dot{q}_i)$ , the theory is time translation invariant. Considering a constant  $\epsilon$ .

$$\delta q_i = \dot{q}_i \delta t, \delta \dot{q}_i = \ddot{q}_i \delta t$$

$$\delta L = L(q_i + \epsilon \dot{q}_i \delta t, \dot{q}_i + \epsilon \ddot{q}_i \delta t) - L(q_i, \dot{q}_i) = \left[ \frac{\partial L}{\partial q_i} q_i + \frac{\partial L}{\partial \dot{q}_i} \dot{q}_i \right] \epsilon \delta t = \epsilon \frac{d(L \delta t)}{dt}$$

This is indeed a symmetry.

A symmetry leaves the action invariant and changes the Lagrangian by at most a total derivative:  $\delta L = -\epsilon dL/dt$  for some  $L$ . The conserved quantity is

$$Q = q + \sum_i \frac{\partial L}{\partial \dot{q}_i} \delta q_i$$

When the equation of motion is used,  $\dot{Q} = 0$  (conservation law)

Under time translation,  $q = -L \delta t$ . The conserved quantity is the Hamiltonian

$$H \equiv \frac{Q}{\delta t} = \sum_i \frac{\partial L}{\partial \dot{q}_i} q_i - L$$

$$L = \sum_i \frac{1}{2} \dot{q}_i^2 - V(q_1, \dots, q_n)$$

Then the conserved quantity is

$$H = \sum_i \frac{1}{2} \dot{q}_i^2 + V$$

### 4 The Hidden Quantum Reality

The particle "tries" all possible paths and "takes" the extremal one.

In quantum mechanics, the probability for the particle to propagate from A to B is

$$P = |A|^2$$

where  $A$  is the probability amplitude.

$$A \propto \sum_{\text{all paths}} e^{iS/\hbar}$$

In classical mechanics  $S \gg \hbar$ . Near  $\delta S = 0$  different paths do not cancel.

### The first law of thermodynamics

$$dE = TdS - pdV$$

For an isolated system consisting of  $n$  subsystems, for each subsystem  $i$  define

$$\Delta S_i = \frac{\Delta Q_i}{T}$$

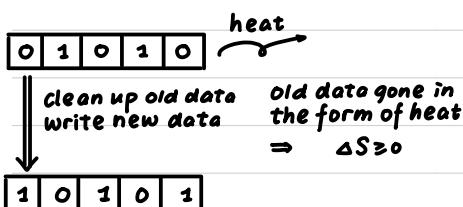
where  $\Delta Q_i$  is the heat flowing into the subsystem if the process is reversible.

The entropy of the system satisfies the second law of thermodynamics

$$\Delta S = \sum_{i=1}^n \Delta S_i \geq 0 \quad ("= " \text{when reversible})$$

$S$  is a quantity describing the state of the system.

past now future  
 ↓ have some process into memory ↓ have no memory



The gate keeper only allows molecules with  $v > v_0$  to enter the right part and molecules with  $v < v_0$  to enter the left part.

### 1 The Statistical Entropy

Two subsystems A, B in an isolated system. A, B can exchange heat but each has fixed volume and fixed particle number. The total energy  $E = E_A + E_B$  is fixed. A, B are in thermal equilibrium individually. When  $T_A = T_B$ , the whole system is in equilibrium. Then

$$\frac{dS_A}{dE_A} = \frac{dS_B}{dE_B}$$

Assume that each microscopic state has equal chance to appear. The partition of A, B should correspond a maximal number of microscopic states, to maximize its probability to appear. Denote the number of possible microscopic states of A and B as  $\Omega_A(E_A)$ ,  $\Omega_B(E_B)$ . The total number of states is

$$\Omega = \Omega_A(E_A) \times \Omega_B(E_B).$$

Let  $\Omega$  to be extremal,

$$0 = \frac{d\Omega}{dE_A} = \Omega_B \frac{d\Omega_A}{dE_A} \rightarrow \Omega_A \frac{d\Omega_B}{dE_B} \frac{dE_B}{dE_A} = \Omega_B \frac{d\Omega_A}{dE_A} - \Omega_A \frac{d\Omega_B}{dE_B}.$$

This gives that

$$\frac{d\ln \Omega_A}{dE_A} = \frac{d\ln \Omega_B}{dE_B}.$$

Thus we can conclude that

$$S = k_B \ln \Omega.$$

where  $k_B \approx 1.38 \times 10^{-23} \text{ J/K}$  is the Boltzmann constant.

### 2 The Arrow of Time

At the level of a fundamental particle, there's no difference between past and future, because of symmetry ( $t \leftrightarrow -t$ , left  $\leftrightarrow$  right, particle  $\leftrightarrow$  anti-particle).

A psychological arrow of time: we remember things in the past, not the future. Getting the brain prepared to remember needs increase of entropy. Thus the psychological time arrow agrees with the thermodynamic arrow, defined by  $\Delta S \geq 0$ . A few effects which are not time reversal invariant: collapse of wave function, radiation of charge, black holes absorbs matter, weak interaction, cosmological expansion.

### 3 Entropy and Information

Two possibilities for the demon:

(1) It has a large memory to record all the molecular data. The cost of making the gas from disordered to ordered is to make the demon's brain from ordered to disordered.

(2) The demon has 1 bit of memory. He has to erase the state of a previous molecule and remember a new one. Landauer proposed that to erase one bit of information, the minimal entropy generated is  $k_B \ln 2$ .

In both (1), (2), 2nd law isn't broken.

The information content is given by

$$h(p) = \log_2 \frac{1}{p}$$

where  $p$  is the probability for an event to happen. The unit of information is bit.

The information entropy is defined as the weighted average information content for all possible outcomes. The Shannon entropy is defined as

$$H(X) = \sum_{i \in X} p_i \log_2 \frac{1}{p_i}$$

In physics, the information entropy is the Gibbs entropy:

$$S = (k_B \ln 2) \times H$$

where  $p_i$  in  $H$  is the physical microscopic states.