

Non-relativistic quantum mechanics

Wave mechanics;

- free particles can be described by wave packets which can be decomposed into a Fourier integral of plane waves

$$\psi(\vec{x}, t) \propto \exp[i(\vec{k} \cdot \vec{x} - \omega t)]$$

From wave-particle duality (de Broglie): $\lambda = h/p$
or $\vec{k} = \vec{p}/\hbar$

Angular frequency of a plane wave (Einstein): $E = \hbar \omega$
 $\hbar = 1$ (natural units) $\Rightarrow \vec{k} = \vec{p}$, $\omega = E$

①
plane wave $\psi(\vec{x}, t) = N \exp[i(\vec{p} \cdot \vec{x} - E \cdot t)] = N \exp[i p^\mu x_\mu]$

Classical physics: $E, p \rightarrow$ dynamical variables (time-dependent real numbers)

QM: dynamical variables of a QM state obtained from the wavefunction

Classical

QM

time-dependent variables $\rightarrow$ t -independent operators
acting on t -dependent wavefunction

In QM the wavefunction is postulated to contain all the info. about the system

- a physical observable A corresponds to the action of a QM operator $\hat{A}$ on the wavefunction

$$\begin{array}{ccc} & \hat{A}\psi = a\psi & \\ \text{operator} \nearrow & & \nwarrow \text{eigenvalues (must be real)} \end{array}$$

a -real $\Rightarrow \hat{A}$ is Hermitian:

$$\int \psi_1^* \hat{A} \psi_2 d\tau = \int [\hat{A} \psi_1]^* \psi_2 d\tau$$

The plane wave from ① with E and $\vec{p} \Rightarrow \hat{E}$ and $\hat{\vec{p}}$ operators?

$$\hat{\vec{p}} = -i\nabla \quad \text{and} \quad \hat{E} = i\frac{\partial}{\partial t}$$

$$\hat{\vec{p}}\psi = -i\nabla\psi = \vec{p}\psi \quad ; \quad \hat{E}\psi = i\frac{\partial}{\partial t}\psi = E\psi$$

Classical mechanics

$$E = H = T + V = \frac{\vec{p}^2}{2m} + V \rightarrow \text{hamiltonian}$$

QM: time-dependent Schrödinger equation

$$i\frac{\partial \psi(\vec{x}, t)}{\partial t} = \hat{H}\psi(\vec{x}, t) \quad ; \quad \hat{H}_{NR} = -\frac{\nabla^2}{2m} + \hat{V}$$

non-relativistic

For a 1D system: (only x)

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi(\vec{x}, t)}{\partial x^2} + \hat{V}\psi(\vec{x}, t)$$

Probability density and probability current

Physical interpretation of the wavefunction $\psi(\vec{x}, t)$:

- $\psi^* \psi d^3\vec{x}$ - probability of finding the particle represented by ψ in the volume element $d^3\vec{x}$

$\Rightarrow \rho(\vec{x}, t) = \psi^*(\vec{x}, t) \psi(\vec{x}, t)$ - const if no decay is allowed

Conservation of probability $\rightarrow$ continuity equation

Two ingredients of the continuity equation:

- probability density $\rho(\vec{x}, t)$

- probability current (flux) density $\vec{j}(\vec{x}, t)$

$\Rightarrow$ flux of prob. across an elemental surface $d\vec{S}$: $\vec{j} \cdot d\vec{S}$

The rate of change of probability is related to the net flux leaving the surface by:

$$\frac{\partial}{\partial t} \int_V \rho dV = - \int_S \vec{j} \cdot d\vec{S}$$

Using the divergence theorem:

$$\frac{\partial}{\partial t} \int_V \rho dV = - \int_V \vec{\nabla} \cdot \vec{j} dV \Rightarrow \boxed{\vec{\nabla} \cdot \vec{j} + \frac{\partial \rho}{\partial t} = 0} \quad \text{continuity equation}$$

Divergence theorem (Gauss - Ostrogradsky)

Surface integral of a vector field over a closed surface (flux through the surface) is equal to the volume integral of the divergence over the region inside the surface

$$\int_V (\vec{\nabla} \cdot \vec{F}) dV = \oint_S (\vec{F} \cdot \hat{n}) dS$$

In non-rel. QM we can get $\rho(\vec{x}, t)$ by using Schrödinger eq.

$$\textcircled{1} \quad i\partial_t \psi = -\frac{1}{2m} \nabla^2 \psi \quad \textcircled{2} \quad -i\partial_t \psi^* = -\frac{1}{2m} \nabla^2 \psi^*$$

$$\psi^* \times \textcircled{1} - \psi \times \textcircled{2}$$

$$-\frac{1}{2m} (\psi^* \nabla^2 \psi - \psi \nabla^2 \psi^*) = i(\psi^* \partial_t \psi + \psi \partial_t \psi^*)$$

$$-\frac{\nabla \cdot (\psi^* \nabla \psi - \psi \nabla \psi^*)}{2m} = i\partial_t (\psi^* \psi) = i\partial_t \rho$$

$$\downarrow \quad \vec{j}(\vec{x}, t) = \frac{1}{2mi} (\psi^* \nabla \psi - \psi \nabla \psi^*)$$

$$\text{The plane wave } \psi(\vec{x}, t) = N e^{i(\vec{p} \cdot \vec{x} - Et)}$$

$$\rho(\vec{x}, t) = |N|^2 \rightarrow \text{constant probability density}$$

$$\vec{j}(\vec{x}, t) = \frac{\vec{p}}{m} \cdot |N|^2 = |N|^2 \vec{v} \rightarrow \text{non-relativistic velocity}$$

Time dependence and conserved quantities

$$\hat{H}\psi_i(\vec{x}, t) = E_i \psi_i(\vec{x}, t)$$

Time evolution $i\partial_t \psi_i(\vec{x}, t) = E_i \psi_i(\vec{x}, t)$

We can split the wavefunction: $\psi_i(\vec{x}, t) = \phi_i(\vec{x}) \cdot e^{-iE_i t}$

For a QM state $|\psi\rangle \rightarrow$ can have more D.o.F. (e.g. spin)
the expectation value of an operator $\hat{A}$ is

$$\langle \hat{A} \rangle = \langle \psi | \hat{A} | \psi \rangle = \int \psi^\dagger \hat{A} \psi d^3\vec{x}$$

Time evolution:

$$\frac{d\langle \hat{A} \rangle}{dt} = \int \left[\frac{\partial \psi^\dagger}{\partial t} \hat{A} \psi + \psi^\dagger \hat{A} \frac{\partial \psi}{\partial t} \right] d^3\vec{x}$$

Assumed no time dependence of the operator $\hat{A}$

$$\begin{aligned} \Rightarrow \frac{d\langle \hat{A} \rangle}{dt} &= 0 = \int \left[\left(\frac{\hat{H}}{i} \psi \right)^\dagger \hat{A} \psi + \psi^\dagger \hat{A} \left(\frac{\hat{H}}{i} \psi \right) \right] d^3\vec{x} = \\ &= i \int \left[\psi^\dagger \hat{H}^\dagger \hat{A} \psi + \psi^\dagger \hat{A} \hat{H} \psi \right] d^3\vec{x} = i \int \psi^\dagger (\hat{H} \hat{A} - \hat{A} \hat{H}) \psi d^3\vec{x} \end{aligned}$$

$$\Rightarrow [\hat{H}, \hat{A}] = 0 \Rightarrow \boxed{\frac{d\langle \hat{A} \rangle}{dt} = i \langle [\hat{H}, \hat{A}] \rangle}$$

If an observable commutes with $\hat{H}$ then it doesn't change in time $\Rightarrow$ conserved quantity!

For an eigenvalue of $\hat{H}$ the expectation value of any operator is constant

Eigenvalues known as stationary states!

A state $|\psi\rangle$ can be expressed using the complete set of states formed from the eigenvalues of $\hat{H}$

$$|\psi\rangle = \sum_i c_i |\psi_i\rangle \rightarrow \text{time evolution given by } e^{-iE_i t}$$

$$|\psi(\vec{x}, t)\rangle = \sum_i c_i |\phi_i(\vec{x})\rangle e^{-iE_i t}$$

If two observables commute, they can be known simultaneously

$$[\hat{A}, \hat{B}] = 0$$

If $[\hat{A}, \hat{B}] \neq 0$ it is not possible to define a simultaneous eigenstate of the two operators and the limit to which $\hat{A}$ and $\hat{B}$ can be known is:

$$\Delta A \Delta B \geq \frac{1}{2} |\langle [\hat{A}, \hat{B}] \rangle| \rightarrow \text{uncertainty principle}$$

$$(\Delta A)^2 = \langle \hat{A}^2 \rangle - \langle \hat{A} \rangle^2$$

$$[\hat{x}, \hat{p}_x] = i(\hbar) \Rightarrow \Delta x \Delta p_x \geq \frac{\hbar}{2}$$

The Klein - Gordon equation

- We need a relativistic formulation of QM so that we can compute decay rates and cross sections of elementary particles

- The Schrödinger equation depends differently on time and space (1st derivative in time, 2nd in space) and is therefore not Lorentz-invariant

* can't provide a good description of relativistic particles!
 * consequence of the non-relativistic relationship between energy and momentum: $E = \frac{p^2}{2m}$

- First attempt is by just writing Einstein energy-momentum relationship:

$$E^2 = \vec{p}^2 + m^2$$

in the form of operators: $\hat{E}^2 \Psi(\vec{x}, t) = \hat{\vec{p}}^2 \Psi(\vec{x}, t) + m^2 \Psi(\vec{x}, t)$

$$\hat{\vec{p}} = -i\vec{\nabla} ; \hat{E} = i\partial_t \Rightarrow \partial_t^2 \Psi = \vec{\nabla}^2 \Psi - m^2 \Psi \quad (1)$$

$$\Rightarrow \boxed{(\partial_\mu \partial^\mu + m^2) \Psi = 0} \quad \partial_\mu \partial^\mu = \partial_t^2 - \partial_x^2 - \partial_y^2 - \partial_z^2$$

(Klein - Gordon equation)

KG equation: plane wave solution

$$\psi(\vec{x}, t) = N e^{-i(\vec{p} \cdot \vec{x} - Et)}$$

which when substituted gives $E^2 \psi = p^2 \psi + m^2 \psi$

Energy of the particle described by a plane wave: $E = \pm \sqrt{p^2 + m^2}$

In classical mechanics: $E < 0$ states can be discarded (unphysical)

In QM: all solutions must form a complete set of states

$\Rightarrow E < 0$ solutions can't be discarded and not clear how to interpret them

Probability density and flux (continuity equation)

$$\psi^* \times \textcircled{1} - \psi \times \textcircled{1}^*$$

$$\psi^* \partial_t^2 \psi - \psi \partial_t^2 \psi^* = \psi^* (\nabla^2 \psi - m^2 \psi) - \psi (\nabla^2 \psi^* - m^2 \psi^*)$$

$$\Rightarrow \partial_t (\psi^* \partial_t \psi - \psi \partial_t \psi^*) = \nabla \cdot (\psi^* \vec{\nabla} \psi - \psi \vec{\nabla} \psi^*)$$

$$g = i(\psi^* \partial_t \psi - \psi \partial_t \psi^*) \quad \vec{j} = -i(\psi^* \vec{\nabla} \psi - \psi \vec{\nabla} \psi^*)$$

i is added to make sure $g, \vec{j}$ are real

For plane wave: $g = 2|N|^2 E$ and $\vec{j} = 2|N|^2 \vec{p} \Rightarrow$

Can be written as: $j^M = 2|N|^2 p^M$

$E < 0$ solutions $\Rightarrow$ negative probability density!

$\Rightarrow$ KG equation does not provide good description of single particle states for a relativistic system

The Dirac equation (1928)

- search for alternative formulation of relativistic QM

- very successful:

* solved the problem with $E < 0$ solutions

* natural description of spin and magnetic moment of spin $1/2$ fermions

Dirac looked for an equation first order in ∂_t and ∂_x

$$\hat{E}\Psi = (\vec{\alpha} \cdot \vec{\hat{p}} + \beta m)\Psi$$

$$i\partial_t \Psi = (-i\alpha_x \partial_x - i\alpha_y \partial_y - i\alpha_z \partial_z + \beta m)\Psi \quad (2)$$

The equation must be valid for relativistic particles $\Rightarrow$ must satisfy KG equation as well

Squaring (2) we get

$$-\partial_t^2 \Psi = (i\alpha_x \partial_x + i\alpha_y \partial_y + i\alpha_z \partial_z - \beta m)(i\alpha_x \partial_x + i\alpha_y \partial_y + i\alpha_z \partial_z - \beta m)\Psi$$

$$\Rightarrow \partial_t^2 \Psi = \alpha_x^2 \partial_x^2 \Psi + \alpha_y^2 \partial_y^2 \Psi + \alpha_z^2 \partial_z^2 \Psi - \beta^2 m^2 \Psi + (\alpha_x \alpha_y + \alpha_y \alpha_x) \partial_x \partial_y \Psi \\ + (\alpha_y \alpha_z + \alpha_z \alpha_y) \partial_y \partial_z \Psi + (\alpha_z \alpha_x + \alpha_x \alpha_z) \partial_z \partial_x \Psi + i(\alpha_x \beta + \beta \alpha_x) m \partial_x \Psi \\ + i(\alpha_y \beta + \beta \alpha_y) m \partial_y \Psi + i(\alpha_z \beta + \beta \alpha_z) m \partial_z \Psi \quad (3)$$

For (3) to reduce to (1) we need the following conditions:

$$1. \alpha_x^2 = \alpha_y^2 = \alpha_z^2 = \beta^2 = I \rightarrow \text{unit matrix}$$

$$2. \alpha_i \beta + \beta \alpha_i = 0$$

$$3. \alpha_i \alpha_j + \alpha_j \alpha_i = 0 \quad (i \neq j)$$

fully defines the algebra of the Dirac equation

2. and 3. can't be satisfied if α_i and β are numbers but must be matrices

Can be shown that they have eigenvalues ± 1 and a trace of 0 $\Rightarrow$ even dimensions. Then using that $\hat{H}$ is hermitian it follows that α_i, β must be 4×4 matrices

(for demonstration check page 83-84 in Chapter 4 of the Thomson book)

Dirac Hamiltonian: $\hat{H}_D = (\vec{\alpha} \cdot \vec{p} + \beta m)$ $\rightarrow 4 \times 4$ matrix of operators
for massless particles
no need for the β term

H_D acts on a 4-component Dirac spinor $\psi = \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{pmatrix}$

The wavefunction has 4-degrees of freedom
- consequence of requiring the QM wavefunction to satisfy the Dirac eq. and to be consistent with KG eq.

If all particles are massless $\vec{\alpha}$ could be represented by the Pauli matrices $\Rightarrow$ 2-component spinors (Weyl spinors)

- We choose the Dirac-Pauli representation of $\vec{\alpha}$ and β
- The physical prediction of the Dirac eq. does not depend on the representation
- The physics is defined by the algebra

Probability density and current flux

$$(-i\hbar_x \partial_x - i\hbar_y \partial_y - i\hbar_z \partial_z + \beta m)\Psi = (i\partial_t)\Psi \quad DE$$

$$i\partial_x \Psi^\dagger \hbar_x^\dagger + i\partial_y \Psi^\dagger \hbar_y^\dagger + i\partial_z \Psi^\dagger \hbar_z^\dagger + m\Psi^\dagger \beta^\dagger = -i\partial_t \Psi^\dagger \quad DE^\dagger$$

$$\Psi^\dagger DE - DE^\dagger \Psi$$

$$-i\Psi^\dagger \vec{\alpha} \cdot \vec{\nabla} \Psi + m\Psi^\dagger \beta \Psi - i\vec{\nabla} \Psi^\dagger \cdot \vec{\alpha} \Psi - m\Psi^\dagger \beta^\dagger \Psi = i\Psi^\dagger \partial_t \Psi + i\partial_t \Psi^\dagger \Psi$$

$$\text{We use: } \Psi^\dagger \vec{\alpha} \cdot \vec{\nabla} \Psi + \vec{\nabla} \Psi^\dagger \cdot \vec{\alpha} \Psi = \vec{\nabla}(\Psi^\dagger \vec{\alpha} \Psi) \text{ and}$$

$$\Psi^\dagger \partial_t \Psi + \partial_t \Psi^\dagger \Psi = \partial_t(\Psi^\dagger \Psi)$$

$$\Rightarrow \vec{\nabla}(\Psi^\dagger \vec{\alpha} \Psi) + \partial_t(\Psi^\dagger \Psi) = 0 \quad (\text{continuity equation})$$

$$\rho = \Psi^\dagger \Psi = \sum_{i=1}^4 |\psi_i|^2 \quad \vec{j} = \Psi^\dagger \vec{\alpha} \Psi$$

All solutions have a positive energy density!

Covariant form of DE

$$\Rightarrow \beta \times DE$$

$$i\beta\hbar_x\partial_x\psi + i\beta\hbar_y\partial_y\psi + i\beta\hbar_z\partial_z\psi + i\beta\partial_t\psi - \beta^2 m\psi = 0$$

$$\mu^0 = \beta \quad \mu^1 = \beta\hbar_x \quad \mu^2 = \beta\hbar_y \quad \mu^3 = \beta\hbar_z$$

$$\Rightarrow \boxed{(i\mu^\mu\partial_\mu - m)\psi = 0 \quad (\beta^2 = I) \quad \mu = 0, 1, 2, 3}$$

μ^μ matrices are not 4-vectors but constant matrices!

μ -matrices properties:

$$\{\mu^\mu, \mu^\nu\} = \mu^\mu\mu^\nu + \mu^\nu\mu^\mu = 2g^{\mu\nu}$$

$$(\mu^0)^2 = I, \quad (\mu^i)^2 = -I \quad (i=1, 2, 3) \Rightarrow \mu^\mu\mu^\nu = -\mu^\nu\mu^\mu \quad (\text{for } \mu \neq \nu)$$

$$(\mu^0)^\dagger = \mu^0, \quad (\mu^i)^\dagger = -\mu^i$$

$$\mu^0 = \beta = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix} \quad \mu^i = \beta\hbar_i = \begin{pmatrix} 0 & \sigma_i \\ -\sigma_i & 0 \end{pmatrix}$$

Solutions to the DE

- identify explicit forms of the wavefunction that can be used in the matrix element computation

First look at general plane wave solutions for a free particle

$$\Psi(\vec{x}, t) = u(E, \vec{p}) e^{i(\vec{p} \cdot \vec{x} - Et)}$$

$\uparrow$
4-component Dirac spinor

$$\Psi(\vec{x}, t) \text{ satisfies DE: } (i\gamma^\mu \partial_\mu - m)\Psi = 0$$

The derivatives act only on the argument of the exponent

$$\partial_0 \Psi = -iE \Psi \quad \partial_i \Psi = i p_i \Psi \quad (i=1, 2, 3)$$

$$\Rightarrow (\gamma^\mu p_\mu - m)u = 0 \quad (5)$$

$$\text{Particle at rest: } p=0 \Rightarrow \Psi = u(E, 0) e^{-iEt} \quad (6)$$

$$\Rightarrow \text{Substituting (6) in (5): } E \gamma^0 u = m u$$

$$E \begin{pmatrix} 1 & & & \\ & 1 & & \\ & & -1 & \\ 0 & & & -1 \end{pmatrix} \begin{pmatrix} \phi_1 \\ \phi_2 \\ \phi_3 \\ \phi_4 \end{pmatrix} = m \begin{pmatrix} \phi_1 \\ \phi_2 \\ \phi_3 \\ \phi_4 \end{pmatrix} \Rightarrow$$

4 orthogonal solutions

$$u_1(E, 0) = N \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

$$u_2(E, 0) = N \begin{pmatrix} 0 \\ 1 \\ 0 \\ 1 \end{pmatrix}$$

$E = m, E > 0$

$$u_3(E, 0) = N \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}$$

$$u_4(E, 0) = N \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$$

$E = -m, E < 0$

N - normalisation

$u_1 - u_4$ are also eigenstates of the $\hat{S}_z$ operator!

u_1, u_2 : spin-up and -down^{states} for positive energy solutions

u_3, u_4 : spin-up and -down states for negative energy solutions