

Recall the motivation for the Schrödinger Eqn.

1923: Louis de Broglie — suggests material particles can act like waves.

$$\Psi(\vec{x}, t) = A \exp\left[i(\vec{k} \cdot \vec{x} - \omega t)\right] \text{ for free particle}$$

\vec{k} ← wavevector ω ← angular frequency

$$\left. \begin{array}{l} \vec{p} = \hbar \vec{k} \\ E = \hbar \omega \end{array} \right\} \text{Einstein-de Broglie relations.}$$

(1925-1926: Heisenberg, Born, Jordan, Pauli
— Matrix Quantum Mechanics)

1926: Schrödinger eqn.

$$E = \frac{\vec{p}^2}{2m} \text{ together w/ Einstein-de Broglie relations}$$

Consistent w/ plane wave solutions if.

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \Psi$$

To include interactions, postulate the general relationship $\left. \begin{array}{l} E \rightarrow i\hbar \frac{\partial}{\partial t} \\ \vec{p} \rightarrow -i\hbar \nabla \end{array} \right\}$ consistent w/ discussion above.

$$E = \frac{\vec{p}^2}{2m} + V(\vec{x}) \rightarrow \boxed{i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \Psi + V(\vec{x}) \Psi}$$

- Nonrelativistic Schrödinger Eqn.

1926: Following the logic of the non-relativistic Schrödinger Eqn, Schrödinger, Klein, Gordon wrote down the Relativistic Schrödinger Eqn = Klein-Gordon Eqn

$$E^2 = \vec{p}^2 c^2 + m^2 c^4 \rightarrow \boxed{-\hbar^2 \frac{\partial^2 \psi}{\partial t^2} = -\hbar^2 c^2 \nabla^2 \psi + m^2 c^4 \psi}$$

Plane-Wave Solutions: $\psi(\vec{x}, t) = A \exp[i(\vec{k} \cdot \vec{x} - \omega t)] + B \exp[-i(\vec{k} \cdot \vec{x} - \omega t)]$

where $\boxed{\hbar^2 \omega^2 = \hbar^2 \vec{k}^2 c^2 + m^2 c^4}$

- Dispersion Relation
- relates frequency and wavevector.

Q: Can the relativistic wavefunction ψ have a probabilistic interpretation as in non-relativistic QM?

A: No.

Non-relativistic: $i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \psi + V(\vec{x}) \psi$ (1)

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

Multiply (1) by ψ^* , (2) by ψ , and subtract:

$$i\hbar \left(\psi^* \frac{\partial \psi}{\partial t} + \psi \frac{\partial \psi^*}{\partial t} \right) = -\frac{\hbar^2}{2m} (\psi^* \nabla^2 \psi - \psi \nabla^2 \psi^*)$$

$$i\hbar \frac{\partial}{\partial t} |\psi|^2 = -\frac{\hbar^2}{2m} \nabla \cdot (\psi^* \nabla \psi - \psi \nabla \psi^*)$$

$$\frac{\partial}{\partial t} |\psi|^2 + \frac{\hbar}{m} \nabla \cdot \text{Im}(\psi^* \nabla \psi) = 0$$

- Resembles current conservation $\frac{\partial \rho}{\partial t} + \nabla \cdot \vec{J} = 0$

$\rho = |\psi|^2 = \text{probability density}$

$\vec{J} = \frac{\hbar}{m} \text{Im}(\psi^* \nabla \psi) = \text{probability current}$

Integrate current conservation eqn over \vec{x} :

$$\int_V d^3x \frac{\partial \rho}{\partial t} = - \int_V d^3x \nabla \cdot \vec{J}$$

$$= - \int_{\partial V} d^2x \hat{n} \cdot \vec{J} = 0 \text{ as } V \rightarrow \mathbb{R}^3 \text{ (all space)}$$

$$\frac{d}{dt} \int d^3x \rho(\vec{x}, t) = \boxed{\frac{d}{dt} \int d^3x |\psi|^2 = 0}$$

① Hence, the total probability is conserved.

If $\int d^3x |\psi(\vec{x}, t)|^2 = 1$ at some time t , then the same is true at all times.

② Also note that $|\psi|^2 \geq 0$.

Conditions ① and ② are the reason $|\psi|^2$ may be interpreted as a probability density.

Repeat for the relativistic wavefunction:

$$-\hbar^2 \frac{\partial^2 \psi}{\partial t^2} = -\hbar^2 c^2 \nabla^2 \psi + m^2 c^4 \psi \quad (1')$$

$$-\hbar^2 \frac{\partial^2 \psi^*}{\partial t^2} = -\hbar^2 c^2 \nabla^2 \psi^* + m^2 c^4 \psi^* \quad (2')$$

Multiply (1') by $i\psi^*$, (2') by $i\psi$, and subtract.

$$\rightarrow \boxed{i \frac{\partial}{\partial t} (\psi^* \frac{\partial \psi}{\partial t} - \psi \frac{\partial \psi^*}{\partial t}) = i c^2 \nabla \cdot (\psi^* \nabla \psi - \psi \nabla \psi^*)}$$

This is of the form $\frac{\partial \rho}{\partial t} + \nabla \cdot \vec{J} = 0$, with

$$\rho = \frac{i\hbar}{2mc^2} (\psi^* \frac{\partial \psi}{\partial t} - \psi \frac{\partial \psi^*}{\partial t}) = \frac{-\hbar}{mc^2} \text{Im} (\psi^* \frac{\partial \psi}{\partial t})$$

$$\vec{J} = \frac{-i\hbar}{2m} (\psi^* \nabla \psi - \psi \nabla \psi^*) = \frac{\hbar}{m} \text{Im} (\psi^* \nabla \psi)$$

$$(1) \frac{d}{dt} \int d^3x \rho = \frac{d}{dt} \int d^3x \operatorname{Im} \left(\psi^* \frac{\partial \psi}{\partial t} \right) = 0$$

The quantity $\int d^3x \operatorname{Im} \left(\psi^* \frac{\partial \psi}{\partial t} \right)$ is conserved,

but the density $\rho = \operatorname{Im} \left(\psi^* \frac{\partial \psi}{\partial t} \right)$ is not positive semidefinite.

→ The analogy of condition (2) for the nonrelativistic probability density is not satisfied.

Hence, ρ is not a probability density in this case.

Other difficulties w/ the Klein-Gordon eqn:

- Including electromagnetic coupling, predictions for fine structure of hydrogen spectrum disagree w/ detailed measurements by Paschen.

- There are negative-energy solutions $E = \pm \sqrt{\vec{p}^2 c^2 + m^2 c^4}$
→ There is no ground state. What would prevent a state from decaying to successively lower energy states?

The Dirac Equation (1928)

Dirac reasoned that the essential difference between the relativistic and non-relativistic Schrödinger eqns is that the former is 2nd order in time derivatives, while the latter is 1st order.

Q: Can an eqn of the form $i\hbar \frac{\partial \Psi}{\partial t} = H \Psi$ be consistent with Lorentz invariance?

A: Yes, if there are enough Ψ 's and H is a matrix of differential operators.

Lorentz invariance relates spatial and time coordinates, so conjecture that H is linear in spatial derivatives.

$$i\hbar \frac{\partial \Psi}{\partial t} = -i\hbar c \left(\alpha^1 \frac{\partial \Psi}{\partial x^1} + \alpha^2 \frac{\partial \Psi}{\partial x^2} + \alpha^3 \frac{\partial \Psi}{\partial x^3} \right) + \beta mc^2 \Psi$$

- Dirac Equation

If α^i were just c-numbers (complex numbers) then the Dirac eqn would not transform consistently under rotations of the coordinates.

What if α^i, β are $N \times N$ matrices, and Ψ has N components?

$$i\hbar \frac{\partial \psi_j}{\partial t} = -i\hbar c \sum_{k=1}^N \left(\alpha^1 \frac{\partial}{\partial x^1} + \alpha^2 \frac{\partial}{\partial x^2} + \alpha^3 \frac{\partial}{\partial x^3} \right) \psi_k + \sum_{k=1}^N \beta_{jk} mc^2 \psi_k$$
$$\equiv \sum_{k=1}^N H_{jk} \psi_k$$

Iterating the Dirac eqn,

$$\begin{aligned}
 -\hbar^2 \frac{\partial^2 \psi}{\partial t^2} &= -\hbar^2 c^2 \sum_{k,l=1}^3 \frac{\alpha^k \alpha^l + \alpha^l \alpha^k}{2} \frac{\partial^2 \psi}{\partial x^k \partial x^l} \\
 &+ \frac{\hbar mc^3}{i} \sum_{k=1}^3 (\alpha^k \beta + \beta \alpha^k) \frac{\partial \psi}{\partial x^k} \\
 &+ \beta^2 m^2 c^4 \psi
 \end{aligned}$$

To recover $E^2 = \vec{p}^2 c^2 + m^2 c^4$ for plane wave solutions, we arrange that each component of ψ satisfy the Klein-Gordon eqn,

$$-\hbar^2 \frac{\partial^2 \psi}{\partial t^2} = -\hbar^2 c^2 \nabla^2 \psi + m^2 c^4 \psi$$

In that case, (1) $\boxed{\alpha^k \alpha^l + \alpha^l \alpha^k = 2\delta^{kl} \mathbb{1}_{N \times N}}$

Kronecker delta = $\begin{cases} 1 & \text{if } k=l \\ 0 & \text{if } k \neq l \end{cases}$

(2) $\boxed{\alpha^k \beta + \beta \alpha^k = 0}$

(3) $\boxed{\beta^2 = \mathbb{1}_{N \times N}}$

• It follows from (1) and (3) that $(\alpha^k)^2 = \beta^2 = \mathbb{1}_{N \times N}$

→ $\boxed{\text{eigenvalues of } \alpha^k, \beta \text{ are } \pm 1}$

• $0 = (\alpha^k \beta + \beta \alpha^k) \beta = \alpha^k + \beta \alpha^k \beta$

$\text{Tr } \alpha^k = -\text{Tr } \beta \alpha^k \beta = -\text{Tr } \beta^2 \alpha^k = -\text{Tr } \alpha^k$

→ $\boxed{\text{Tr } \alpha^k = 0}$ cyclicity of trace $\beta^2 = \mathbb{1}_{N \times N}$

• Similarly, $0 = \alpha^k (\alpha^k \beta + \beta \alpha^k) = \beta + \alpha^k \beta \alpha^k$

→ $\boxed{\text{Tr } \beta = 0}$

- $\text{Tr } \alpha^k = \sum (\text{eigenvalues of } \alpha^k) = 0$
 \rightarrow # +, - eigenvalues equal. Similarly for β
 \Rightarrow α^k, β must be even-dimensional matrices.

- H Hermitian \rightarrow α^k, β Hermitian matrices

In summary, we need 4 mutually anticommuting, even-dimensional Hermitian matrices.

2x2 Hermitian matrices: spanned by 3 mutually anticommuting Pauli matrices σ^k and the unit matrix $\mathbb{1}$.
 \rightarrow 2x2 is out.

(However, note that if the mass $m=0$, then there is no matrix β in the Dirac eqn, and we would only need 3 matrices \rightarrow the Pauli σ -matrices would work.)

What about 4x4 matrices?

Dirac basis: $\alpha^k = \begin{pmatrix} 0 & \sigma^k \\ \sigma^k & 0 \end{pmatrix}$ $\beta = \begin{pmatrix} \mathbb{1} & 0 \\ 0 & -\mathbb{1} \end{pmatrix}$

Each entry is a 2x2 matrix

$$\sigma^1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \sigma^2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \sigma^3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

What about the probability density?

$$i\hbar \frac{\partial \psi}{\partial t} = -i\hbar c \sum_{k=1}^3 \alpha^k \frac{\partial \psi}{\partial x^k} + \beta mc^2 \psi \quad (1'')$$

$$-i\hbar \frac{\partial \psi^\dagger}{\partial t} = i\hbar c \sum_{k=1}^3 \frac{\partial \psi^\dagger}{\partial x^k} \alpha^k + mc^2 \psi^\dagger \beta \quad (2'')$$

Left-multiply (1'') by ψ^\dagger , right-multiply (2'') by ψ ,
subtract:

$$i\hbar \left(\psi^\dagger \frac{\partial \psi}{\partial t} + \frac{\partial \psi^\dagger}{\partial t} \psi \right) = -i\hbar c \sum_{k=1}^3 \left(\psi^\dagger \alpha^k \frac{\partial \psi}{\partial x^k} + \frac{\partial \psi^\dagger}{\partial x^k} \alpha^k \psi \right)$$

$$\boxed{\frac{\partial}{\partial t} (\psi^\dagger \psi) + c \sum_{k=1}^3 \frac{\partial}{\partial x^k} (\psi^\dagger \alpha^k \psi) = 0}$$

This is of the form $\frac{\partial \rho}{\partial t} + \nabla \cdot \vec{J} = 0$, with

$$\rho = \psi^\dagger \psi$$

$$J^k = c \psi^\dagger \alpha^k \psi, \quad k=1,2,3$$

Note that $\rho \geq 0$ and is conserved, so it is a candidate for a probability density.