Quantum mechanics

Time evolution of the state of the system is described by Schrödinger equation:

$$i\hbar \frac{\partial}{\partial t} |\psi, t\rangle = H |\psi, t\rangle$$

where $H$ is the hamiltonian operator representing the total energy. For a free, spinless, nonrelativistic particle we have:

$$H = \frac{1}{2m} P^2$$

in the position basis, $P = -i\hbar \partial / \partial x$ and S.E. is:

$$i\hbar \frac{\partial}{\partial t} \psi(x, t) = -\frac{\hbar^2}{2m} \nabla^2 \psi(x, t)$$

where $\psi(x, t) = \langle x | \psi, t \rangle$ is the position-space wave function.

Relativistic generalization?

Obvious guess is to use relativistic energy-momentum relation:

$$H = +\sqrt{P^2 c^2 + m^2 c^4}, \quad H = mc^2 + \frac{1}{2m} P^2 + \ldots$$

Schrödinger equation becomes:

$$i\hbar \frac{\partial}{\partial t} \psi(x, t) = +\sqrt{-\hbar^2 c^2 \nabla^2 + m^2 c^4} \psi(x, t)$$

Not symmetric in time and space derivatives 😞

Attempts at relativistic QM

A proper description of particle physics should incorporate both quantum mechanics and special relativity.

However historically combining quantum mechanics and relativity was highly non-trivial.

Today we review some of these attempts.

The result of this effort is relativistic quantum field theory - consistent description of particle physics.
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Schrödinger equation becomes:

\[ i\hbar \frac{\partial}{\partial t} \psi(x, t) = +\sqrt{-\hbar^2 c^2 \nabla^2 + m^2 c^4} \psi(x, t) \]

Applying \( i\hbar \frac{\partial}{\partial t} \) on both sides and using S.E. we get

\[ -\hbar^2 \frac{\partial^2}{\partial t^2} \psi(x, t) = \left(-\hbar^2 c^2 \nabla^2 + m^2 c^4\right) \psi(x, t) \]

Klein-Gordon equation looks symmetric 😊

Special relativity

(Physics is the same in all inertial frames)

Space-time coordinate system: \( x^\mu = (ct, \mathbf{x}) \)

Define: \( x_\mu = (-ct, \mathbf{x}) \)

or \( x_\mu = g_{\mu\nu} x^\nu \) where \( g_{\mu\nu} = \begin{pmatrix} -1 & 1 \\ 1 & 1 \end{pmatrix} \)

is the Minkowski metric tensor. Its inverse is:

\( g^{\mu\nu} = \begin{pmatrix} -1 & -1 \\ -1 & 1 \end{pmatrix} \)

\( g^{\mu\nu} g_{\nu\rho} = \delta^{\mu\rho} \)

that allows us to write: \( x^\mu = g^{\mu\nu} x_\nu \)

Interval between two points in space-time can be written as:

\[ ds^2 = (x - x')^2 - c^2(t - t')^2 = g_{\mu\nu}(x - x')^\mu(x - x')^\nu = (x - x')^\mu(x - x')_\mu \]

General rules for indices:

- Repeated indices, one superscript and one subscript are summed; these indices are said to be contracted.
- Any uncontracted indices (not summed) must match in both name and height on left and right side of any valid equation.

Two coordinate systems (representing inertial frames) are related by

\[ \bar{x}^\mu = \Lambda^\mu_\nu x^\nu + a^\mu \]

Lorentz transformation matrix

Interval between two different space-time points is the same in all inertial frames:

\[ (\bar{x} - \bar{x}')^2 = g_{\mu\nu}(\bar{x} - \bar{x}')^\mu(\bar{x} - \bar{x}')^\nu = g_{\rho\sigma}(\bar{x} - \bar{x}')^\rho(\bar{x} - \bar{x}')^\sigma = (x - x')^2, \]

which requires:

\[ g_{\mu\nu} \Lambda^\mu_\rho \Lambda^\nu_\sigma = g_{\rho\sigma} \]
Notation for space-time derivatives:

\[ \partial_\mu = \frac{\partial}{\partial x^\mu} = \left( \frac{1}{c} \frac{\partial}{\partial t}, \nabla \right) \]
\[ \partial^\mu = \frac{\partial}{\partial x_\mu} = \left( -\frac{1}{c} \frac{\partial}{\partial t}, \nabla \right) \]

matching-index-height rule works: \( \partial^\mu x^\nu = g^{\mu\nu} \)

For two coordinate systems related by \( \bar{x}^\mu = \Lambda^\mu_\nu x^\nu + a^\mu \)

derivatives transform as: \( \bar{\partial}^\mu = \Lambda^\mu_\nu \partial^\nu \)

which follows from

\[ \bar{\partial}^\mu \bar{x}^\nu = (\Lambda^\rho_\mu \partial^\mu)(\Lambda^\sigma_\nu \partial^\nu + a^\nu) = \Lambda^\rho_\mu \Lambda^\sigma_\nu (\partial^\mu x^\nu) = \Lambda^\rho_\mu \Lambda^\sigma_\nu g^{\mu\nu} = g^{\rho\sigma} \]

Is K-G equation consistent with relativity?

Physics is the same in all inertial frames: the value of the wave function at a particular space-time point measured in two inertial frames is the same:

\[ \psi(x) = \bar{\psi}(\bar{x}) \]

This should be true for any point in the space-time and thus a consistent equation of motion should have the same form in any inertial frame.

Is that the case for Klein-Gordon equation?

Klein-Gordon equation: in 4-vector notation:

\[ -\hbar^2 c^2 \partial_0^2 \psi(x) = \left( -\hbar^2 c^2 \nabla^2 + m^2 c^4 \right) \psi(x) \]

\[ \Box = \partial^2 \equiv \partial^\mu \partial_\mu = -\partial_0^2 + \nabla^2 \]

in 4-vector notation:

\[ (-\partial^2 + m^2 c^2/\hbar^2) \psi(x) = 0 \]

Is it equivalent to:

\[ (-\bar{\partial}^2 + m^2 c^2/\hbar^2) \bar{\psi}(\bar{x}) = 0 \]

Since

\[ \bar{\partial}^2 = g_{\mu\nu} \bar{\partial}^\mu \bar{\partial}^\nu = g_{\mu\nu} \Lambda^\mu_\rho \Lambda^\nu_\sigma \partial^\rho \partial^\sigma = \partial^2 \]

\[ \bar{\partial}^\mu = \Lambda^\mu_\nu \partial^\nu \]

K-G eq. is manifestly consistent with relativity!

Is K-G consistent with quantum mechanics?

Schrödinger equation (first order in time derivative) leaves the norm of a state time independent. Probability is conserved:

\[ \langle \psi, t | \psi, t \rangle = \int d^3x \langle \psi, t | x \rangle \langle x | \psi, t \rangle = \int d^3x \psi^*(x) \psi(x) = \int d^3x \rho(x) \]

\[ \frac{\partial}{\partial t} \langle \psi, t | \psi, t \rangle = \int d^3x \frac{\partial \rho}{\partial t} = - \int d^3x \nabla \cdot j = - \int_S j \cdot dS = 0 \]

Gauss's law

\[ j(x) = 0 \text{ at infinity} \]

\[ \frac{\partial \rho}{\partial t} = \psi \frac{\partial \psi}{\partial t} + \psi^* \frac{\partial \psi^*}{\partial t} \]

\[ = \frac{i\hbar}{2m} \psi^* \nabla^2 \psi - \frac{i\hbar}{2m} \psi \nabla^2 \psi^* \]

\[ = \frac{i\hbar}{2m} \nabla \cdot (\psi^* \nabla \psi - \psi \nabla \psi^*) \equiv - \nabla \cdot j \]
Is K-G consistent with quantum mechanics?

Schrödinger equation (first order in time derivative) leaves the norm of a state time independent. Probability is conserved:

\[
\langle \psi, t | \psi, t \rangle = \int d^3 x \langle \psi, t | x \rangle \langle x | \psi, t \rangle = \int d^3 x \psi^*(x) \psi(x) = \int d^3 x \rho(x)
\]

\[
\frac{\partial}{\partial t} \langle \psi, t | \psi, t \rangle = \int d^3 x \frac{\partial \rho}{\partial t} = - \int d^3 x \nabla \cdot j = - \int_S j \cdot dS = 0
\]

Klein-Gordon equation is second order in time derivative and the norm of a state is NOT in general time independent. Probability is not conserved.

Klein-Gordon equation is consistent with relativity but not with quantum mechanics.

\[
(H^2)_{ab} = c^2 P_j P_k (\alpha^j \alpha^k)_{ab} + mc^2 P_j (\alpha^j \beta + \beta \alpha^j)_{ab} + (mc^2)^2 (\beta^2)_{ab}
\]

\[
(\alpha^j \beta + \beta \alpha^j)_{ab} \text{ can be written as anticommutator } \{\alpha^j, \beta\}_{ab}
\]

and also \( \alpha^j \alpha^k \) can be written as \( \frac{1}{2} \{\alpha^j, \alpha^k\} \).

Eigenvalues of \( \hat{H}^2 \) should satisfy the correct relativistic energy-momentum relation:

\[
(H^2)_{ab} = (P^2 c^2 + m^2 c^4) \delta_{ab}
\]

and so we choose matrices that satisfy following conditions:

\[
\{\alpha^j, \alpha^k\}_{ab} = 2 \delta^{jk} \delta_{ab}, \quad \{\alpha^j, \beta\}_{ab} = 0, \quad (\beta^2)_{ab} = \delta_{ab}
\]

it can be proved (later) that the Dirac equation is fully consistent with relativity.

we have a relativistic quantum mechanical theory!

**Discussion of Dirac equation**

- to account for the spin of electron, the matrices should be 2x2 but the minimum size satisfying above conditions is 4x4 - two extra spin states

- \( H \) is traceless, and so 4 eigenvalues are: \( E(p), E(p), -E(p), -E(p) \)

\[
E(p) = (+p^2 c^2 + m^2 c^4)^{1/2}
\]

- negative energy states no ground state also a problem for K.-G. equation

Dirac’s interpretation: due to Pauli exclusion principle each quantum state can be occupied by one electron and we simply live in a universe with all negative energy states already occupied.

Negative energy electrons can be excited into a positive energy state (by a photon) leaving behind a hole in the sea of negative energy electrons. The hole has a positive charge and positive energy antiparticle (the same mass, opposite charge) called positron (1927)
Quantum mechanics as a quantum field theory

Consider Schrödinger equation for n particles with mass m, moving in an external potential U(x), with interparticle potential V(x₁ - x₂)

\[ i\hbar \frac{\partial}{\partial t} \psi = \left[ \sum_{j=1}^{n} \left( -\frac{\hbar^2}{2m} \nabla_j^2 + U(x_j) \right) + \sum_{j=1}^{n} \sum_{k=1}^{n} V(x_j - x_k) \right] \psi \]

\( \psi = \psi(x_1, \ldots, x_n; t) \) is the position-space wave function.

It is equivalent to:

\[ H = \int d^3x \ a^\dagger(x) \left( -\frac{\hbar^2}{2m} \nabla^2 + U(x) \right) a(x) + \frac{1}{2} \int d^3x \ d^3y \ V(x - y)a^\dagger(x)a^\dagger(y)a(y)a(x) \]

\[ |\psi, t\rangle = \int d^3x_1 \ldots d^3x_n \ \psi(x_1, \ldots, x_n; t)a^\dagger(x_1) \ldots a^\dagger(x_n)|0\rangle \]

If and only if \( \psi = \psi(x_1, \ldots, x_n; t) \) satisfies S.E. for wave function!

\( a(x) \) is a quantum field and \( a^\dagger(x) \) its hermitian conjugate;

they satisfy commutation relations:

\[ [a(x), a(x')] = 0 , \]
\[ [a^\dagger(x), a^\dagger(x')] = 0 , \]
\[ [a(x), a^\dagger(x')] = \delta^3(x - x') \]

\( |0\rangle \) is the vacuum state

\[ a(x)|0\rangle = 0 \]

\( a^\dagger(x_1)|0\rangle \) state with one particle at \( x_1 \)

\( a^\dagger(x_1)a^\dagger(x_2)|0\rangle \) state with one particles at \( x_1 \) and another at \( x_2 \)

Total number of particles is counted by the operator:

\[ N = \int d^3x \ a^\dagger(x)a(x) \] commutes with H!