Path integrals

Free particle example

\[
\langle x | e^{-\frac{i}{\hbar} H t} | x' \rangle = \\
\lim_{N \to \infty} \int dx_1 \ldots dx_N \left(\frac{m}{2\pi i \hbar} \right)^N e^{i \frac{m}{\hbar} \frac{1}{2} \sum_{n=1}^{N} \frac{m}{2} \left(\frac{x_{n+1} - x_n}{\Delta t}\right)^2 \Delta t} \delta(x' - x_N)
\]

define

\[
K(x_i, x_i; \Delta t) = \left(\frac{m}{2\pi i \hbar} \right)^{\frac{1}{2}} e^{i \frac{m}{\hbar} \frac{1}{2} \left(\frac{(x_i - x_i')}{\Delta t}\right)^2 \Delta t}
\]

with this notation the expression above becomes

\[
= \lim_{N \to \infty} \int K(x_N, x_{N-1}; \Delta t) K(x_{N-1}, x_{N-2}; \Delta t) \ldots \int K(x_2, x_1; \Delta t) \, dx_2 \ldots dx_N
\]

consider

\[
\int K(x, x'; \Delta t) \, dx' \, K(x', x''; \Delta t_2) = \\
\frac{1}{(2\pi \hbar)^2 \sqrt{\Delta t_1 \Delta t_2}} \int \, dx'' \, e^{-\frac{1}{i \hbar} \frac{m}{2} \left(\frac{\dot{x}^2}{\Delta t_1} + \frac{\dot{x'}^2}{\Delta t_2}\right)}
\]

\[
\frac{x^2}{\Delta t_1} + \left(\frac{1}{\Delta t_1} + \frac{1}{\Delta t_2}\right) \dot{x} \dot{x'} + 2 \dot{x} \left(\frac{\dot{x}}{\Delta t_1} + \frac{\dot{x}'}{\Delta t_2}\right) + \frac{\dot{x'}^2}{\Delta t_2}
\]
when we do the integral

\[ I = \int e^{\frac{i}{2\hbar} \left( x^2 \left( \frac{1}{\Delta t} + \frac{1}{\Delta t_i} \right) - 2x' \left( \frac{x}{\Delta t_i} - \frac{x''}{\Delta t_i} \right) \right)} \]

note \( \frac{1}{\Delta t} + \frac{1}{\Delta t_i} = \frac{\Delta t_i + \Delta t}{\Delta t \Delta t_i} \); completing the square in the integral gives

\[ I = \int e^{\frac{i}{2\hbar} \frac{\Delta t_i + \Delta t}{\Delta t \Delta t_i} \left( x' - \frac{\Delta t_i \Delta t}{\Delta t \Delta t_i} \left( \frac{x}{\Delta t} - \frac{x''}{\Delta t} \right)^2 - \frac{i}{2\hbar} \left( \frac{\Delta t_i + \Delta t}{\Delta t \Delta t_i} \right)^2 \left( \frac{x}{\Delta t} + \frac{x''}{\Delta t} \right)^2 \right)} \]

doing the gaussian integral gives

\[ I = \sqrt{\frac{2\pi \hbar \Delta t \Delta t_i}{-i m (\Delta t_i, \Delta t)}} e^{-\frac{i}{\hbar} \frac{1}{2} \frac{\Delta t_i \Delta t}{\Delta t \Delta t_i} \left( \frac{x'}{\Delta t} \right)^2 + \frac{x'}{\Delta t} + 2x'x'' \frac{1}{\Delta t \Delta t_i} } \]

\[ = \sqrt{\frac{2\pi \hbar \Delta t \Delta t_i}{-i m (\Delta t_i, \Delta t)}} e^{-\frac{i}{\hbar} \frac{1}{2} \frac{\Delta t_i \Delta t}{\Delta t \Delta t_i} \left( \frac{x'}{\Delta t} \right)^2 + 2x'x'' + x''^2 \frac{\Delta t_i}{\Delta t} } \]

putting everything together we get

\[ \int K(x, x', \Delta t_i) dx' K(x', x'', \Delta t_i) = \]

\[ = \frac{m}{2\pi \hbar} \sqrt{\frac{1}{\Delta t \Delta t_i}} e^{-\frac{i}{\hbar} \frac{1}{2} \frac{\Delta t_i \Delta t}{\Delta t \Delta t_i} \left( \frac{x'}{\Delta t} \right)^2 - \frac{x'}{\Delta t} + 2x'x'' \frac{1}{\Delta t \Delta t_i} } \]

\[ \times \sqrt{\frac{m}{2\pi \hbar} \frac{1}{(\Delta t_i + \Delta t) \hbar}} e^{i m \frac{1}{2\hbar} \left( \frac{\Delta t_i + \Delta t - \Delta t_i}{\Delta t \Delta t_i} \right) - 2x'x'' + x''^2 \frac{\Delta t_i + \Delta t - \Delta t_i}{\Delta t_i} } \]
\[
\begin{align*}
&= \sqrt{\frac{m}{2\pi i\hbar (\Delta t_1 + \Delta t_2)}} \ e^{\frac{i}{\hbar} \frac{m}{2} \left( \frac{x - x''}{\Delta t_1 + \Delta t_2} \right)^2 (\Delta t_1 + \Delta t_2)} \\
&= K(\mathbf{x}, \mathbf{x}'' \Delta t_1 + \Delta t_2)
\end{align*}
\]

It follows that
\[
\int K(\mathbf{x}_{n+1}, \mathbf{x}_n \Delta t) \ dx_n = \frac{\ dx_3 \ K(x_3, x_1 \Delta t) \ dx_3 \ K(x_1, x_1 \Delta t)}{K(x_3, x_1, 2\Delta t)} \frac{\ dx_2 \ K(x_2, x_1, \Delta t) \ dx_2 \ K(x_1, x_1, \Delta t)}{K(x_1, x_1, 3\Delta t)}
\]

\[
K(x_{n+1}, x_{N \Delta t}) = K(x_{n+1}, x_t)
\]

which is exactly
\[
-\frac{i \ p^2}{2m} \ t
\]

\[
\int <\mathbf{x}_{n+1} | p > \ dx \ e^{-ip \mathbf{x}_t} <p | \mathbf{x}_t>
\]

Comment - note
\[
\int K(\mathbf{x}, \mathbf{x}' \Delta t) \ dx' = \sqrt{\frac{m}{2\pi i\hbar t}} \ e^{\frac{i}{\hbar} \frac{m}{2} \left( \frac{\mathbf{x} - \mathbf{x}'}{t} \right)^2} \ dx'
\]

\[
= \sqrt{\frac{m}{2\pi i\hbar t}}, \ \sqrt{-i\hbar} = 1
\]
This means

\[ \int K(x_{n+1}, x_1, t) \, dx_1 = 1 = \]

\[ \int K(x_{n+1}, x_n, \Delta t) \, dx_n \int K(x_n, x_{n-1}, \Delta t) \, dx_{n-1} \]

\[ - \int K(x_2, x_1, \Delta t) \, dx_1 \]

If there is a potential term, then it becomes

\[ \int K(x_{n+1}, x_n, \Delta t) - \int K(x_2, x_1, \Delta t) \, dx_1 \]

\[ - \frac{1}{\hbar} \int \psi^* \nabla \psi \, \Delta t \]

Interpretation of Nathansohn Jusens:

\[ K(x_{n+1}, x_n, \Delta t) \, dx_n \quad dx_2 \quad K(x_2, x_1, \Delta t) \, dx_1 \]

is complex probability of a path being within \( dx_1 \) of \( x_1 \) at time \( t_1 \), \( dx_2 \) of \( x_2 \) at time \( t_1 \), \( \ldots \), \( dx_n \) of \( x_n \) at time \( t_n \).
\[ e^{-\frac{i}{\hbar} \int V(x) \, dt} \sim e^{-\frac{i}{\hbar} \int V(x(t)) \, dt} \]

It is a functional that assigns a weight to each set \( x, \Delta x \quad x, \Delta x \).

In this case, the path integral is reinterpreted as the expectation of a potential functional of paths between \( x_i \) and \( x_{i+1} \) with respect to a complex probability distribution on a space of paths.

This interpretation makes mathematical sense, unlike the interpretation as an integral.
Dirac Equation

\[ \text{i} \hbar \frac{\partial \Psi}{\partial t} = H \Psi = \left( -\frac{\hbar^2}{2m} \nabla^2 + V \right) \Psi \]

\[ \text{i} \hbar \frac{\partial \Psi}{\partial t} = \text{energy} \]

\[ -\text{i} \hbar \nabla = \text{momentum} \]

In special relativity the energy and momentum are related by

\[ E = \sqrt{p^2 c^2 + m^2 c^4} \]

This suggests the following generalization of the Schrödinger equation

\[ \text{i} \hbar \frac{\partial \Psi}{\partial x} = \left( \sqrt{-\hbar^2 c^2 \nabla^2 + m^2 c^4} + V \right) \Psi \]

This equation is called the relativistic Schrödinger equation.

There are a number of reasons why it was rejected.
- * physics - did not give the correct electron magnetic moment

- * non-symmetric treatment of space and time derivatives

It has some good qualities:

+ * energy is positive

+ * generalizes to many particle systems

+ * follows from symmetry considerations

+ * probability conserved in time

In order to get a more symmetric treatment of space and time derivatives:

\[ h_\text{\textsuperscript{2}} \frac{\partial^2 \psi}{\partial t^2} + \hbar^2 \nabla^2 + m^2 c^4 \psi = 0 \]

This equation is called the Klein-Gordon - Schroedinger equation.
This equation has several problems.

Since the equation is symmetric under $E \rightarrow -E$, it has negative energy solutions.

This means that small corrections could lead to catastrophic decays.

A second problem with the Klein Gordon equation is that probabilities are not conserved in time.

Normally:

$$\frac{\partial^2}{\partial t^2} \int \psi^* \psi \ dx^3 =$$

$$\int \left( \frac{\partial \psi^*}{\partial t} \psi + \psi^* \frac{\partial \psi}{\partial t} \right) =$$

$$\int \frac{i}{\hbar} (\mathcal{H} \psi^* : \psi - \frac{i}{\hbar} \psi^* \mathcal{H} \psi)$$

Since $\mathcal{H}$ is Hermitian,

$$= -i \hbar \int \psi^* (\mathcal{H} - \mathcal{H}) \psi = 0$$

This cancellation does not happen with equations that have 2 time derivatives.
The third problem was that it did not correctly predict the magnetic moment of the electron.

Dirac's proposal:

1. Equation should be first order in time derivatives in order to have conserved probabilities.

2. Equation should be linear in space derivatives so space and time are treated symmetrically.

3. Hamiltonian should be Hermitian to have real eigenvalues:

\[ i \hbar \frac{\partial}{\partial t} \psi = -i \hbar c \vec{A} \cdot \vec{D} \psi + \beta mc^2 \]

This will still have to lead to

\[ E^2 = p^2 c^2 + m^2 c^4 \]
\[(\imath \hbar \frac{\partial}{\partial t})(\imath \hbar \frac{\partial}{\partial t}) = \]
\[\left(-\imath \hbar \vec{\alpha} \cdot \vec{\nabla} \psi + \beta mc^2 \psi \right) \]
\[\left(-\imath \hbar \vec{\alpha} \cdot \vec{\nabla} \left(\imath \hbar \frac{\partial \psi}{\partial t}\right) + \beta mc^2 \left(\imath \hbar \frac{\partial \psi}{\partial t}\right) \right) = \]
\[\left(-\imath \hbar \vec{\alpha} \cdot \vec{\nabla} \psi \right) \left(-\imath \hbar \vec{\alpha} \cdot \vec{\nabla} + \beta mc^2 \right) \psi \]
\[+ \beta mc^2 \left(-\imath \hbar \vec{\alpha} \cdot \vec{\nabla} + \beta mc^2 \right) \psi = \]
\[- \hbar^2 c^2 (\vec{\alpha} \cdot \vec{\nabla}) (\vec{\alpha} \cdot \vec{\nabla}) - \imath \hbar mc^2 \vec{\alpha} \cdot \vec{\nabla} \beta \]
\[- \imath \hbar mc^2 \beta \vec{\alpha} \cdot \vec{\nabla} + \beta^2 m^2 c^4 \psi \]

This can be written as:

\[- \frac{\hbar^2 c^2}{2} (\delta_{ij} \alpha_i \alpha_j + \alpha_i \alpha_j) \nabla_i \nabla_j \psi \]
\[- \imath \hbar mc^2 \left( (\beta \vec{\alpha} + \alpha \beta \vec{\alpha}) \cdot \vec{\nabla} \right) \psi \]
\[+ \beta^2 m^2 c^4 \psi \]

This should become:

\[- \hbar^2 c^2 \nabla^2 \psi + m^2 c^4 \psi.\]
This requires

\[ \alpha_i \alpha_j + \alpha_j \alpha_i = 2 \delta_{ij} \]

\[ \beta \bar{\alpha} + \bar{\alpha} \beta = 0 \]

\[ \beta^2 = 1 \]

These equations cannot be satisfied with numbers. Dirac considered these as matrices

1. The matrices must be Hermitian to have real eigenvalues and conserved probabilities \( e^{-iHt} \) must be unitary.

2. \( \alpha_i^2 = \beta^2 = 1 \) the eigenvalues of these 4 matrices must be \( \pm 1 \)

3. Since the anticommutate, \( AB = -BA \)

\[ \text{Tr}(AB) = \text{Tr}(BA) = -\text{Tr}(BA) \]

\[ \text{Tr}(A) = \text{Tr}(AB^2) = \text{Tr}(BAB) = -\text{Tr}(AB^2) = -\text{Tr}A \]

This requires \( \text{Tr}(A) = 0 \) and must have the same number of \( +1 \) and \( -1 \) eigenvalues \( \Rightarrow \dim A \) is even.
The simplest case would be \( N = 2 \), in that case there are only 3 independent traceless anticommuting independent matrices - the Pauli matrices.

\( N = 4 \) is this simplest possibility. Direct choice

\[
\bar{\alpha} = \begin{pmatrix} 0 & \bar{\sigma} \\ \bar{\sigma} & 0 \end{pmatrix} \quad \beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}
\]

With these choices, \( \Psi(x) \) becomes a 4 component object

\[
i \hbar \frac{\partial \psi_i}{\partial t} = \sum_j \left( -i \hbar (\alpha_x)_{ij} \frac{\partial}{\partial x} - i \hbar (\alpha_y)_{ij} \frac{\partial}{\partial y} - i \hbar (\alpha_z)_{ij} \frac{\partial}{\partial z} \right) \beta_m c^1 \psi_i
\]
Dirac's original form of the equation is
\[
\text{i} \hbar \frac{\partial \psi}{\partial t} = \left( -\text{i} \hbar c \vec{\alpha} \cdot \vec{\nabla} + \beta mc^2 \right) \psi
\]
This can be expressed in the equivalent form by multiplying by \( \beta \)
\[
\text{i} \hbar \beta \frac{\partial \psi}{\partial t} = \left( -\text{i} \hbar c \vec{\beta} \cdot \vec{\nabla} + mc^2 \right) \psi
\]
\[
\left( \text{i} \hbar \beta \frac{\partial}{\partial t} + \text{i} \hbar c \vec{\beta} \cdot \vec{\nabla} - mc^2 \right) \psi = 0
\]
Let \( P_\mu \equiv \left( \text{i} \hbar \frac{1}{c} \frac{\partial}{\partial t}, \text{i} \hbar \vec{\nabla} \right) \)
\( \gamma^\mu \equiv (\beta, \vec{\beta} \vec{\alpha}) \)
Then the equation takes on the form
\[
\left( c \frac{\partial}{\partial t} \gamma^\mu P_\mu - mc^2 \right) \psi = 0
\]
while the matrices \( \gamma^\mu = \beta \vec{\alpha} \) are no longer all Hermitian
\[
\beta^2 = 1
\]
\[
\beta \alpha_i \beta \alpha_j = -\beta \cdot \alpha_i \alpha_j \beta = \beta \alpha_i \alpha_j \beta = -\beta \alpha_i \alpha_j
\]
\( \vec{\beta} \alpha_i \beta \alpha_i = -\beta^2 \alpha_i \alpha_i = -1 \)
It follows that
\[
\Theta^\mu_\nu = \left\{ \begin{array}{c} 2 & \mu = \nu = 0 \\ -2 & \mu = \nu \neq 0 \\ 0 & \mu \neq \nu \end{array} \right.
\]
plane wave solutions

\[ \psi(t) = \psi(x) e^{\frac{-i}{\hbar} E t + i \frac{\mathbf{p} \cdot \mathbf{x}}{\hbar}} \]

\[ (\gamma^\mu p_\mu - m c^2) \psi(x) e^{\frac{-i}{\hbar} E t + i \frac{\mathbf{p} \cdot \mathbf{x}}{\hbar}} \]

\[ (\gamma^\nu i \hbar c (\gamma^\mu p_\mu - m c^2) \psi(x) e^{\frac{-i}{\hbar} E t + i \frac{\mathbf{p} \cdot \mathbf{x}}{\hbar}} ) = \]

\[ (\gamma^\nu E - c \mathbf{\bar{\gamma} \cdot \mathbf{p}} - m c^2) \psi = 0 \]

to find the solution not

\[ (\gamma^\nu E - c \mathbf{\bar{\gamma} \cdot \mathbf{p}} - m c^2) (\gamma^\nu E - c \mathbf{\bar{\gamma} \cdot \mathbf{p}} + m c^2) = \]

\[ E^2 - \mathbf{p}^2 c^2 - m^2 c^4 = 0 \]

so if \( E = \pm \sqrt{\mathbf{p}^2 c^2 + m^2 c^4} \) then

\[ (\gamma^\nu E - c \mathbf{\bar{\gamma} \cdot \mathbf{p}} + m c^2) \gamma(x) = \psi(x) \]

\[ \psi(t) = \psi(x) e^{\frac{-i}{\hbar} (\sqrt{\mathbf{p}^2 c^2 + m^2 c^4} E t + i \frac{\mathbf{p} \cdot \mathbf{x}}{\hbar})} \]

is a plane wave solution. To get explicit solutions note

\[ \gamma^0 = \beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \]

\[ \mathbf{\bar{\gamma}} = \beta \mathbf{\bar{\gamma}} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & \bar{\gamma} \\ \bar{\gamma} & 0 \end{pmatrix} = \begin{pmatrix} 0 & \bar{\gamma} \\ \bar{\gamma} & 0 \end{pmatrix} \]
\[ Y^0 E - c^2 \beta \bar{p} + mc^2 = \]

\[
\begin{pmatrix}
 E-mc^2 & 0 & -c \beta & -c(p_x-ip_y) \\
 0 & E-mc^2 & -c(p_x+ip_y) & c \beta \\
 -c \beta & c(p_x+ip_y) & -E-mc^2 & 0 \\
 c(p_x+ip_y) & -c \beta & 0 & -E-mc^2
\end{pmatrix}
\]

each column of this matrix corresponds to a plane wave solution.

Remarks

1. There are 4 solutions.
2. 2 have positive energy, 2 have negative energy.
3. The 2 solutions to each energy are associated with spin components — solutions of the Dirac equation are spin 1/2 particles.

* The Dirac equation does not resolve the problem of negative energy states.

* Because they are fermions — Dirac proposed that all of the negative energy states are filled.
From it becomes possible to excite a negative energy electron - it leaves a hole with an effective positive charge.

Dirac used this to predict the existence of antielectrons.

Antielectrons were found.

The negative energy states are still a problem. If we have bound states of a negative energy proton and negative energy electron as negative energy bosons - they are not protected by the exclusion principle.

Resolution

The Dirac equation is correctly interpreted as a classical field equation like Maxwell's equations.

Quantizing both the EM and Dirac fields results in a theory called quantum electrodynamics, which is one of the most precisely tested theories of physics.