Notes on covariant quantization

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1 Introduction

In standard quantum mechanics, quantum states provide probability distributions for the outcomes of any possible measurement on a system at time t. Alongside with the rule for time evolution, they provide a complete description of a system.

We propose to consider instead generalized quantum states defined in spacetime which provide the probability distributions for the outcomes of any possible measurement at any given spacetime point. The standard space-like quantum states can be retrieved foliating the four dimensional quantum states at fixed times.

The covariant approach could be useful for example in the quantization of gravity where the geometry of spacetime (and consequently the distinction between time and space) is not fixed a priori.

2 Classical mechanics

Let's start by considering a point particle in classical mechanics. In standard Lagrangian mechanics, the state of the particle is described by its coordinates $(t, q^i(t))$[1], the system is governed by the Lagrangian

$$\mathcal{L} = \mathcal{L}(q^i, t) = \mathcal{L}(q^i, \partial_t q^i, t)\,, \tag{1}$$

and the equations of motion can be derived by the Lagrange equations

$$\frac{\partial \mathcal{L}}{\partial q^i} = \partial_t \frac{\partial \mathcal{L}}{\partial(\partial_t q^i)}\,. \tag{2}$$

We can consider instead coordinates in spacetime parametrized by the proper time τ: $(\tau, q^\mu(\tau))$[2], the Lagrangian of the system then becomes

$$\mathcal{L} = \mathcal{L}(q^\mu, t) = \mathcal{L}(q^\mu, \partial_\tau q^\mu, \tau)\,, \tag{3}$$

and the Lagrange equations

$$\frac{\partial \mathcal{L}}{\partial q^\mu} = \partial_\tau \frac{\partial \mathcal{L}}{\partial(\partial_\tau q^\mu)}\,. \tag{4}$$

[1] i runs over the spatial dimensions.

[2] μ runs over the spacetime dimensions: $\mu = 0 \to$ time dimension, $\mu > 0 \to$ spatial dimensions.

In standard Hamiltonian formulation the conjugate momenta π_i and Hamiltonian $\mathcal{H}$ are defined as

$$\pi_i \equiv \frac{\partial \mathcal{L}}{\partial(\partial_t q^i)}\,, \qquad \mathcal{H} = \pi_i \partial_t q^i - \mathcal{L}(q^i, t)\,, \tag{5}$$

and the equation of motions are given by the Hamilton equations

$$\frac{dq^i}{dt} = \frac{\partial \mathcal{H}}{\partial \pi_i}\,, \qquad \frac{d\pi_i}{dt} = -\frac{\partial \mathcal{H}}{\partial q^i}\,. \tag{6}$$

In covariant formulation, by introducing the four-velocity $u^\mu = \partial_\tau q^\mu$, the conjugate momenta and Hamiltonian are defined as

$$\pi_\mu \equiv \frac{\partial \mathcal{L}}{\partial u^\mu}\,, \qquad \mathcal{H} = \pi_\mu u^\mu - \mathcal{L}(q^\mu, \tau)\,, \tag{7}$$

and the Hamilton equations become

$$\frac{dq^\mu}{d\tau} = \frac{\partial \mathcal{H}}{\partial \pi_\mu}\,, \qquad \frac{d\pi_\mu}{d\tau} = -\frac{\partial \mathcal{H}}{\partial q^\mu}\,. \tag{8}$$

3 Quantum mechanics (covariant formulation)

We want to consider a quantum formulation based on generalize quantum states defined in spacetime. The axioms of quantum mechanics can then be rewritten as

1. The state of an isolated system is represented at proper time τ by a state vector $|\psi(\tau)\rangle$ of an Hilbert space $\mathscr{H}$.
2. An observable A is described by an Hermitian operator $\hat{A}$ whose eigenvectors form a basis of $\mathscr{H}$: $\hat{A}\,|\psi\rangle = a_n\,|a_n\rangle$.
3. The result fo a measurement of A must be an eigenvalue of $\hat{A}$.
4. The probability of observing the eigenvalue a_n (at proper time τ) is $P(a_n, \tau) = |\langle a_n|\psi(\tau)\rangle|^2$.
5. After the measurement the state $|\psi\rangle$ collapse in the eigenvector $|a_n\rangle$
6. The proper time evolution of the state $|\psi(\tau)\rangle$ is governed by the Schrödinger equation

   $$i\hbar \frac{d}{d\tau}\,|\psi(\tau)\rangle = \hat{H}(\tau)\,|\psi(\tau)\rangle\ . \tag{9}$$

   Covariant canonical quantization prescribes that coordinates x^μ and momenta p_μ are replaced by operators $\hat{x}^\mu$, $\hat{p}_\mu$ which obey the commutation relations

   $$[\hat{x}^\mu, \hat{p}_\nu] = i\hbar\delta^\mu_\nu\,, \qquad [\hat{x}^\mu, \hat{x}_\nu] = 0\,, \qquad [\hat{p}^\mu, \hat{p}_\nu] = 0\,. \tag{10}$$

   These imply

   $$\hat{x}^\mu \equiv x^m u\,, \qquad \hat{p}_\mu \equiv -i\hbar\partial_\mu\,. \tag{11}$$

   To make an analogy between covariant classical and quantum mechanics, we could say that

- In classical mechanics, $x^\mu(\tau)$ represents the world-line of the particle, it gives its time and space coordinates for any proper time τ.
- In quantum mechanics, $\psi(x^\mu, \tau)$ represents the world-state of the particle, it gives the probability of finding the particle at time t and position x^i for any proper time τ.

4 Examples

We apply the above formalism to a few simple examples

4.1 Classical particle in electromagnetic field

The covariant Lagrangian for a particle in electromagnetic field is

$$\mathcal{L} = \frac{1}{2} m u_\mu(\tau) u^\mu(\tau) + q u_\mu(\tau) A_\mu(\tau) , \tag{12}$$

where q is the particle charge and A_μ the electromagnetic four-potential. From Eq. (7), the conjugate momentum and Hamiltonian turn out to be

$$pi_\mu = m u_\mu + q A_\mu , \qquad \mathcal{H} = \frac{1}{2m} \left(\pi_\mu - q A_\mu\right)^2 , \tag{13}$$

and by solving the Hamilton equations (8), one obtains the Lorentz force

$$\partial_\tau \pi_\mu = q u^\nu \partial_\mu A_\nu \Rightarrow m \partial_\tau u_\mu = q u^\nu (\partial_\mu A_\nu - \partial_\nu A_\mu) . \tag{14}$$

4.2 Quantum covariant hydrogen atom

Let's apply the covariant quantization to the study of the hydrogen atom. The Hamiltonian of a charged particle in electrostatic central potential is

$$\mathcal{H} = \frac{1}{2m} \left(p_\mu - q A_\mu\right)^2 , \tag{15}$$

where the central potential is given by

$$A_\mu = A_0 = \frac{e}{4\pi\epsilon_0 r} . \tag{16}$$

The momentum p_μ under canonical quantization becomes

$$p_\mu = m u_\mu + q A_\mu \rightarrow \hat{P}_\mu = -i\hbar\partial_\mu - q A_\mu = -i\hbar D_\mu , \tag{17}$$

which is invariant under gauge transformation. The covariant Hamiltonian operator is

$$\hat{\mathcal{H}} = \frac{1}{2m} \left(\hbar^2 \partial_0^2 - \hbar^2 \partial_i^2 - i\hbar \frac{qe}{4\pi\epsilon_0 r} \partial_0 - \frac{q^2 e^2}{(4\pi\epsilon_0 r)^2 r^2} \right) , \tag{18}$$

to be compared with the Hamiltonian in standard quantum mechanics

$$\hat{\mathcal{H}} = \left(-\frac{\hbar^2}{2m} \partial_i^2 - \frac{qe}{4\pi\epsilon_0 r} \right) . \tag{19}$$

The eigenstate equation for the Hamiltonian is

$$\hat{\mathcal{H}}\psi = E\psi \,. \tag{20}$$

Since we are dealing with a central spherical potential, it is simpler to work in spherical coordinates. By separation of variable, the wave function ψ becomes

$$\psi(t, r, \theta, \phi) = T(t)R(r)Y(\theta, \phi) \,. \tag{21}$$

Expressing the derivatives in spherical coordinates, Eq. (20) becomes

$$\begin{aligned}
&(\hbar^2\partial_0^2 - i\hbar\frac{\alpha qe}{r}\partial_0)T = \lambda T \,, \\
&\frac{1}{r^2}\partial_r(r^2\partial_r)R = \left[\gamma - \frac{1}{\hbar^2}\left(2mE + \lambda + \alpha^2\frac{q^2e^2}{r^2}\right)\right]R \,, \\
&\frac{1}{r^2\sin\theta}\partial_\theta(\sin\theta\partial_\theta + \frac{1}{r^2\sin^2\theta}\partial_\phi^2)Y = -\gamma Y \,,
\end{aligned} \tag{22}$$

where $\alpha = (4\pi\epsilon_o)^{-1}$. As in the standard formulation, the solution of the angular equation are the spherical harmonics

$$Y = Y_l^m(\theta, \phi) \,, \qquad \gamma = \frac{l(l+1)}{r^2} \,. \tag{23}$$

By using the Fourier transform of T in the temporal equation, we obtain the solution

$$T(t) = Ae^{-i\omega t} \,, \qquad \lambda = -\omega\hbar\left(\omega\hbar - \alpha\frac{qe}{r}\right) \,. \tag{24}$$

Substituting the value for γ and λ the radial equation becomes

$$\frac{1}{r^2}\partial_r(r^2\partial_r)R = \left[\frac{l(l+1)}{r^2} - \frac{1}{\hbar^2}\left(2mE - \omega\hbar\left(\omega\hbar - \alpha\frac{qe}{r}\right) + \alpha^2\frac{q^2e^2}{r^2}\right)\right]R \,, \tag{25}$$

to be compared with the standard radial equation

$$\frac{1}{r^2}\partial_r(r^2\partial_r)R^S = \left[\frac{l(l+1)}{r^2} - \frac{2m}{\hbar^2}\left(E + \alpha\frac{qe}{r}\right)\right]R^S \,. \tag{26}$$

The general conformal and standard solutions can be written as

$$\begin{aligned}
\psi(x^\mu, \tau) &= e^{-\frac{i}{\hbar}E\tau}T(t)R(r)Y(\theta, \phi) \\
\psi^S(x^i, t) &= e^{-\frac{i}{\hbar}Et}R^S(r)Y(\theta, \phi) \,.
\end{aligned} \tag{27}$$

For non-relativistic regimes we expect the covariant solution to coincide with the standard solution

$$v \ll c \;\rightarrow\; \frac{dt}{d\tau} = \gamma \approx 1 \;\rightarrow\; t = \tau \;\rightarrow\; \psi(x^\mu, \tau) = \psi^S(x^i, t) \,. \tag{28}$$

By setting $\omega = -\frac{2m}{\hbar}$, the conformal solution at order α becomes

$$\psi(x^\mu, \tau) = e^{-\frac{i}{\hbar}(E-2m)t}R^S(r)Y(\theta, \phi) \qquad O(\alpha) \,. \tag{29}$$

To solve the radial equation consider the substitution $u = rR(r)$, this gives

$$\partial_r^2 u = \left(\delta^2 + \frac{\beta}{r} + \frac{\gamma}{r^2}\right) u \,, \tag{30}$$

where

$$\delta^2 = \omega^2 - \frac{2mE}{\hbar^2} \,, \quad \beta = \frac{\omega\alpha q e}{\hbar c} \,, \quad \gamma = (l(l+1) - \eta) \,, \quad \eta = \left(\frac{\alpha q e}{\hbar c}\right)^2 \,. \tag{31}$$

As in the standard case approach, by studying the asymptotic solutions at $r \to \inf$, $r \to 0$ one arrive at the expression

$$u(r) \simeq C e^{-\delta r} r^{l+1-\frac{\eta}{2l+1}} G(r) \,, \qquad G(r) = \sum_n A_n r^n \,, \tag{32}$$

and by substituting this expression in the radial equation, a recurrence relation for the A_n is found

$$A_n = \frac{\delta(2n - 1 + \sqrt{1+4\gamma}) + \beta}{n(n + \sqrt{1+4\gamma})} A_{n-1} \,. \tag{33}$$

To avoid divergences at $r \to \inf$, the series must be truncated. This happens if some $A_n = 0$, which implies

$$E_{nl} = \frac{\omega^2}{2m}\left(\hbar^2 - \left(\frac{\alpha q e}{2c(n + l - \frac{\eta}{2l+1})}\right)^2\right) \,. \tag{34}$$

The first energy level is $n = 1$, $l = 0$ ($n = 0$ diverges at $r = 0$) for an atom of atomic number Z is

$$E_{10} = \frac{\omega^2}{2m}\left(\hbar^2 - \left(\frac{\alpha q Z e}{2c(1-\eta)}\right)^2\right) \,, \tag{35}$$

and the corresponding radial solution

$$R_{10}(r) = C_{10} e^{-\delta r} r^{\frac{1}{2}(-2+\sqrt{5-4\eta})} \,. \tag{36}$$

This solution diverges at $r = 0$ if $\eta > 1$ i.e. $Z > 137$ as expected from the theory of relativistic Coulomb potential.