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PARTICLES AND FIELDS
Frédéric Schuller, Michael Neumann-Spallart\textsuperscript{1}, Renaud Savalle\textsuperscript{2}

It is the aim of this lecture to recall how, in relativistic quantum physics, negative energy states are avoided by adopting the field viewpoint. For this purpose we chose as the simplest possible case that of an uncharged particle obeying the Klein-Gordon equation. The essential arguments developed here then apply equally to the case of more general systems.

Negative energy states, causality

In quantum mechanics we associate a particle with a wave function $\Psi(x,t)$ depending on time and space coordinates $t$ and $x$ respectively. The wave functions are solutions of a differential equation known as the Schrödinger equation. In a heuristic way this equation can be derived by replacing the energy and momentum of the particle by operators, according to the relations

$$E = -i\hbar \frac{\partial}{\partial t} \text{ and } p = -i\hbar \nabla$$

For a particle we then have in the non relativistic case $E - \frac{p^2}{2m} = 0$ yielding

\begin{equation}
\left( \frac{\partial}{\partial t} - \frac{i\hbar}{2m} \nabla^2 \right) \Psi = 0
\end{equation}

(1)

In the relativistic case we start from the relation

$$E^2 = m^2c^4 + p^2c^2$$

and obtain, after inserting the relevant differential operators

\begin{equation}
\left( -\frac{1}{c^2} \frac{\partial^2}{\partial t^2} + \nabla^2 \right) \Psi - \frac{m^2c^2}{\hbar^2} \Psi = 0
\end{equation}

(2)

This relativistic version of the Schrödinger equation is called the Klein-Gordon equation. It is important to note that in contrast to the non relativistic eq.(1) the Klein-Gordon equation contains the second time derivative meaning that it allows for negative energy solutions. Using from now on natural units $\hbar = 1$, $c = 1$, we write explicitly

\begin{equation}
\left( -\frac{\partial^2}{\partial t^2} + \nabla^2 \right) \Psi - m^2\Psi = 0
\end{equation}

(3)

Setting

$$\Psi(x,t) = \psi(x)e^{-iEt}$$

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Eq. (3) reduces to
\( (E^2 - p^2)\psi - m^2 \psi = 0 \)
where we have used \( \nabla^2 = -p^2 \).

For plane wave solutions with \( p^2 = \text{const} \), we then have the energy relations

(5a) \( E^2 = (p^2 + m^2) \)

(5b) \( E = \pm \sqrt{p^2 + m^2} \)

Hence there are negative energy solutions. The question arises whether these solutions cannot be discarded as non-physical. But in that case we would not have a complete set of basis functions since these solutions are part of it. In actual calculations this could yield erroneous results. Furthermore, in a less obvious way, omitting these solutions leads to a violation of the principle of causality as we shall demonstrate now.

Consider the amplitude \( A(t) = \langle x | e^{-itH} | x_0 \rangle \) for the evolution of a free particle from an initial to a final position during the time interval \( t \). Discarding negative energy states this amplitude would be

(6) \( A(t) = \langle x | e^{-it\sqrt{p^2 + m^2}} | x_0 \rangle = \int d^3p \langle x|p\rangle e^{-it\sqrt{p^2 + m^2}} \langle p|x_0 \rangle \)

Inserting the wave functions

(7) \( \langle x|p\rangle = \frac{1}{(2\pi)^{3/2}} e^{ip\cdot x} ; \langle p|x_0 \rangle = \frac{1}{(2\pi)^{3/2}} e^{-ip\cdot x} \)

We have

(8) \( A(t) = \frac{1}{(2\pi)^3} \int d^3pe^{ip\cdot(x-x_0)} e^{-it\sqrt{p^2 + m^2}} \)

Using polar coordinates as follows:
\( p \cdot (x - x_0) = p|x - x_0|cos\theta \); \( d^3p = 2\pi p^2 sin\theta d\theta \)

We arrive after integration over \( \theta \) at the expression

(9) \( A(t) = \frac{1}{2\pi|x-x_0|} \int pdp sin(p|x - x_0|)e^{-it\sqrt{p^2 + m^2}} \)

For simplicity we set \( X = |x - x_0| \). With a convergence factor \( e^{-\Lambda\sqrt{p^2 + m^2}} \), \( \Lambda > 0 \), inserted the value of this integral is known [1]. Setting \( b = it + \Lambda \) its value is proportional to the Bessel function
\( K_2[m(X^2 + b^2)^{1/2}] \) up to a rational function of \( X \) and \( t \). For large values of its argument the Bessel function reduces essentially to the exponential \( e^{-m(X^2+b^2)^{1/2}} \) [2], leading for \( \Lambda = 0 \) to the result

\[ \text{result} \]
Given this factor in the expression of $A(t)$ we have a non zero amplitude outside the light cone, thus violating the principle according to which space like separated events cannot be causally connected. Consequently violation of the causality principle occurs if only positive energy functions are taken into account.

There are however other shortcomings contained in the relativistic particle theory. One could argue that any positive energy state must be unstable since after some time the particle would fall into a lower energy state, in the same way as an atomic electron in an excited state falls into the ground state after some short life time. In the case of fermions this can be prevented by assuming, following Dirac, that all negative energy states are occupied already. This situation is due to the fact that, according to the Pauli principle, each state can only receive one electron. The completely filled negative states constitute the Dirac sea.

Moreover, this picture has led Dirac to the prediction of the positron, i.e. a positively charged electron, appearing as a hole in the Dirac sea when by some process an electron is removed from it.

It is however possible to give a less artificial description of relativistic quantum particles by adopting the field viewpoint which shall be presented now.

Lagrangian field method

We consider a field function $\phi$ depending on the time-space vector $x = (t, \mathbf{x})$ with components $x^\alpha, \alpha = 0, 1, 2, 3$. Distinguishing between contravariant and covariant components, $x'^\alpha, x_\beta$ respectively, we further have $x^\alpha = g^{\alpha\beta} x_\beta$ and a similar relation with $g^{\alpha\beta} = g_{\alpha\beta} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$. As usual, Greek indices belong to the Minkowski four-space, Latin ones to ordinary space.

In analogy with classical mechanics, we introduce a Lagrange function, having here the character of a density, given by the expression $\mathcal{L}(\phi, \phi_\alpha)$, where we have set $\phi_\alpha = \partial_\alpha \phi = \frac{\partial \phi}{\partial x^\alpha}$. Note also the complementary relation $\phi^\alpha = \partial^\alpha \phi = \frac{\partial \phi}{\partial x^\alpha}$. We now define an action integral $S$ over a region $\Omega$ bordered by a closed surface $\Sigma(\Omega)$, as follows:

$$ (11) S(\Omega) = \int_\Omega d^4x \mathcal{L}(\phi, \phi_\alpha) $$

Varying this integral in the usual way according to the relation
(12) $\delta S(\Omega) = \int_\Omega d^4x \left\{ \frac{\partial L}{\partial \phi} \delta \phi + \frac{\partial L}{\partial \phi_{\alpha \beta}} \delta \phi_{\alpha \beta} \right\}$

And using the identities
\[ \partial_\alpha \left( \frac{\partial L}{\partial \phi_{\alpha \beta}} \delta \phi \right) = \partial_\alpha \left( \frac{\partial L}{\partial \phi_{\alpha \beta}} \right) \delta \phi + \frac{\partial L}{\partial \phi_{\alpha \beta}} \partial_\alpha \delta \phi \]
\[ ; \quad \partial_\alpha \delta \phi = \delta \phi_{\alpha \beta} \]

we arrive at
(13) $\delta S(\Omega) = \int_\Omega d^4x \left\{ \left( \frac{\partial L}{\partial \phi} - \partial_\alpha \left( \frac{\partial L}{\partial \phi_{\alpha \beta}} \right) \right) \delta \phi + \partial_\alpha \left( \frac{\partial L}{\partial \phi_{\alpha \beta}} \delta \phi \right) \right\}$

The last term in the parenthesis can be seen as the four-divergence of a four-vector proportional to $\delta \phi$. Therefore, with Gauss’s theorem it can be transformed into a surface integral over the border $\Sigma(\Omega)$. Since the Lagrange method postulates $\delta \phi = 0$ at the surface, this term disappears. On the other hand, if the action integral $S$ has to be an extremum, $\delta S$ must vanish for any value of $\delta \phi$. This leads to the familiar Euler-Lagrange equations
(14) \[ \frac{\partial L}{\partial \phi} - \partial_\alpha \frac{\partial L}{\partial \phi_{\alpha \beta}} = 0 \]

or more explicitly
(15) \[ \frac{\partial L}{\partial \phi} - \frac{\partial}{\partial x^\alpha} \left( \frac{\partial L}{\partial (\phi_{\alpha \beta})} \right) = 0 \]

These equations apply to classical fields, e.g. one component of the electromagnetic vector potential, as well as to wave functions in particle quantum mechanics.

As an example let us therefore consider the Klein-Gordon wave function.

Setting
(16) \[ L = \frac{1}{2} \{ (\phi_{\alpha \beta} \phi_{\alpha}^\beta) - m^2 \phi^2 \} \]

We write $\phi_{\alpha \beta} \phi_{\alpha}^\beta = g^{\alpha \beta} \phi_{\beta}^2$ and hence
\[ \partial_\alpha \frac{\partial L}{\partial \phi_{\alpha \beta}} = \frac{1}{2} \partial_\alpha g^{\alpha \beta} \phi_{\beta}^2 = \frac{1}{2} \{ \partial_\alpha \phi_{\alpha \beta} - \partial_\alpha \phi_{\alpha}^2 \} = \left( \frac{\partial^2}{\partial t^2} - \nabla^2 \right) \phi \]
yielding with $\frac{\partial L}{\partial \phi} = -m^2 \phi$ the Klein-Gordon equation
(17) \[ \left( \frac{\partial^2}{\partial t^2} - \nabla^2 + m^2 \right) \phi = 0 \]

The Hamiltonian

In order to establish a link with classical mechanics, we first conceive the space coordinates $x_i$ as a countable set, each element occupying an infinitesimal space segment $\delta x_i$.

Considering the classical expression of the Hamiltonian
(18) \[ H = \sum_i p_i \dot{q}_i - L \]

with the canonical variable $p_i$ obeying the relation
We have the correspondence
\[ \dot{q}_i \rightarrow \dot{\phi}_i; \quad p_i = \frac{\partial L}{\partial \dot{\phi}_i}, \quad \delta x_i = \pi_i \delta \phi_i \]
defining the canonical variable
\[ \pi_i = \frac{\partial L}{\partial \dot{\phi}_i} \]
With these definitions we obtain for the classical relation (18) the following equivalent expression:
\[ H = \sum_i \left( \pi_i \dot{\phi}_i - L_i \right) \delta x_i \]
Switching now to the limit of continuous space coordinates, this result takes the form
\[ H = \int d^3x \left\{ \pi(x) \dot{\phi}(x) - L(\phi, \phi_{,\alpha}) \right\} = \int d^3x \mathcal{H}(x) \]
where \( \mathcal{H} \) represents the Hamiltonian density
\[ \mathcal{H}(x) = \pi(x) \dot{\phi}(x) - L \]
with \( \pi(x) \) the canonical momentum given by
\[ \pi(x) = \frac{\partial L}{\partial \dot{\phi}} \]
Let us consider as an example the Klein-Gordon case.
According to eq.(16) the Lagrange density can be written as
\[ \mathcal{L} = \frac{1}{2} \left( \dot{\phi}^2 - (\nabla \phi)^2 - m^2 \phi^2 \right) \]
We then have \( \pi(x) = \dot{\phi} \) and hence
\[ \mathcal{H}(x) = \dot{\phi}^2 - \frac{1}{2} \dot{\phi}^2 + \frac{1}{2} (\nabla \phi)^2 + \frac{1}{2} m^2 \phi^2 - \frac{1}{2} \left( \dot{\phi}^2 + (\nabla \phi)^2 + m^2 \phi^2 \right) \]
Second quantization
Simply speaking, a given wave function is quantized if it is replaced by an operator. This is familiar in quantum electro-dynamics where e.g. one component of the vector potential is replaced by photon creation and annihilation operators. A similar procedure can be applied to quantum mechanical wave functions and in this latter case one then talks of second quantization, since the wave functions are obtained already by a first quantization procedure. Note however that the term second quantization is not universally accepted.
Here we consider again as an example the Klein-Gordon case, which constitutes the simplest one, as it concerns spinless particles like \( K \) or \( \pi \) mesons.
Let us first switch from \( x \) space to \( p \) space by introducing the following transformations:
(27a) \[ \phi(x, t) = \int \frac{d^3p}{(2\pi)^3} e^{ip \cdot x} \phi(p, t) \]

(27b) \[ \nabla \phi(x, t) = \int \frac{d^3p}{(2\pi)^3} e^{ip \cdot x} ip \phi(p, t) \]

(27c) \[ \dot{\phi}(x, t) = \pi(x, t) = \int \frac{d^3p}{(2\pi)^3} e^{ip \cdot x} \pi(p, t) \]

The Hamiltonian density then takes the form

(28) \[ \mathcal{H}(x) = \int \frac{d^3p}{(2\pi)^3} \int \frac{d^3p'}{(2\pi)^3} e^{i(p + p' \cdot x)} \frac{1}{2} \{ \pi(p)\pi(p') + (-pp' + m^2)\phi(p)\phi(p') \} \]

Since we want to quantize the system by replacing wave functions by operators in the Schrödinger picture, we disregard t in this expression.

Integrating over the space coordinates, we thus arrive at the following expression for the Hamiltonian in terms of functions in p space:

(29) \[ H = \int d^3x \mathcal{H}(x) = \int \frac{d^3p}{(2\pi)^3} \left\{ \pi(p)\pi(-p) + \omega_p^2 \phi(p)\phi(-p) \right\} \]

With

(30) \[ \omega_p^2 = p^2 + m^2 \]

To obtain eq.(29) we have made use of the relation

\[ \int d^3xe^{i(p + p' \cdot x)} = \delta^3(p + p') \]

The parenthesis inside the integral of eq.(29) reminds one of the Hamiltonian \( \frac{1}{2} (p^2 + \omega^2q^2) \) of a harmonic oscillator.

In the latter case quantization is achieved by introducing creation and destruction operators \( a^\dagger, a \), according to the relation

\[ q = \frac{1}{\sqrt{2\omega}}(a + a^\dagger) ; \quad p = -i \sqrt{\frac{\omega}{2}} (a - a^\dagger) \]

with the commutator \([a, a^\dagger] = 1\)

We therefore try in eq.(29) the substitutions

(31a) \[ \pi(p) = -i \sqrt{\frac{\omega_p}{2}} (a_p - a_p^\dagger) \]

(31b) \[ \phi(p) = \frac{1}{\sqrt{2\omega_p}} (a_p + a_p^\dagger) \]

The parenthesis inside the integral in eq.(29) is then found to be given by the expression

\[ \{ \} = \omega_p (a_p a_p^\dagger + a_p^\dagger a_p - p) \]
Since complete summation over $p$ takes place, we can disregard the minus signs of the indices and write
\[
\{ \} = \omega_p (a_p a_p^+ + a_p^+ a_p) = 2\omega_p \left( a_p^+ a_p + \frac{1}{2} [a_p, a_p^+] \right)
\]
We thus obtain for the Hamiltonian the following result
\[ (32) \quad H = \int \frac{d^3p}{(2\pi)^3} \omega_p \left( a_p^+ a_p + \frac{1}{2} [a_p, a_p^+] \right) \]
According to general rules of quantum physics, the commutation relation for canonical variables takes in the present case the following form:
\[ (33) \quad [\phi(x), \pi(x')] = i\delta^3(x - x') .\]
Inserting into the commutator the transformation relations given by eq.'s (27a,c) we write
\[ (34) \quad [\phi(x), \pi(x')] = \int \frac{d^3p}{(2\pi)^3} \int \frac{d^3p'}{(2\pi)^3} e^{ip\cdot x} e^{ip'\cdot x'} [\phi(p), \pi(p')] \]
Substituting for $\phi(p), \pi(p')$ the expressions given by eq.'s (31a,b) we obtain after a lengthy but straightforward calculation
\[ (35) \quad [\phi(p), \pi(p')] = \frac{i}{2} \left( [a_p', a_{-p}^+] + [a_p, a_{-p'}^+] \right) \]
Adopting the trial rule
\[ (36) \quad [a_p, a_p^+] = (2\pi)^3 \delta^3(p - p') \]
Eq.(35) reduces to
\[ (37) \quad [\phi(p), \pi(p')] = i(2\pi)^3 \delta^3(p + p') \]
Substituting this result into eq.(34) we recover the commutation relation of eq.(33). This confirms the validity of the trial rule of eq.(36).
In the field equations developed above the number of particles concerned is not specified.
Let us now be more specific by introducing single particle states $|p> \}$ assumed to constitute an orthonormal set in a given inertial frame. Acting with the Hamiltonian of eq.(32) on one of these states, e.g. $|p_1> \}$, and using eq.(36) for the commutator, we obtain the formal expression
\[ (38) \quad H|p_1> = \omega_{p_1} |p_1> + \left( \int \frac{d^3p}{(2\pi)^3} \frac{1}{2} a_p^+ \right) \delta^3(0) |p_1> \]
The second term on the r.h.s.of this equation contains the infinite quantity $\delta^3(0)$ and moreover it involves an infinite sum over energies $\omega_p/2$. Mostly this term can be considered as some sort of ground state energy $E_0$ which cannot be detected experimentally and thus
be ignored. Note however that a similar term occurring in QED plays an important part in several physical processes as will be shown below.

In order to establish the time dependence of the operators $\phi$ and $\pi$ one has to replace them by Heisenberg operators according to the relation

$$\phi(x, t) = e^{iHt} \phi e^{-iHt} \text{ and similarly for } \pi(x, t).$$

Starting from the expressions (31a,b) we evaluate the corresponding Heisenberg operators of $a_p$ and $a_p^\dagger$ as follows:

Acting on an eigenstate $|p> \text{ of } H$, according to eq.(38), the infinite zero-point energy term cancels in the operator product since it is a c number. We are thus left with the expression

$$e^{iHt} a_p e^{-iHt} |p> = e^{-i\omega_p t} a_p |p>$$

using $e^{iHt} a_p |p> = |0> = a_p |p>$. Similarly we have

$$e^{iHt} a_p^\dagger e^{-iHt} |0> = e^{i\omega_p t} a_p^\dagger |0>$$

Hence the requested operator equations are

(39a) $a_p (t) = e^{-i\omega_p t} a_p$

(39b) $a_p^\dagger (t) = e^{i\omega_p t} a_p^\dagger$

With eq.(31b) the quantized form of eq.(27a) becomes

(40) $\phi(x, t) = \int \frac{d^3p}{(2\pi)^3} \frac{1}{\sqrt{2\omega_p}} \left( a_p e^{-i\omega_p t} e^{ip \cdot x} + a_p^\dagger e^{i\omega_p t} e^{-i\omega_p t} \right)$

Where eq.’s (39a,b) have been used.

Introducing the Lorentz invariant scalar product

$$px = p_0 x_0 - p \cdot x \text{ in four space, with } p_0 = \omega_p \text{ and } x_0 = t,$$

We obtain for the quantized field the expression

(41) $\phi(x, t) = \int \frac{d^3p}{(2\pi)^3} \frac{1}{\sqrt{2\omega_p}} \left( a_p e^{-ip \cdot x} + a_p^\dagger e^{ip \cdot x} \right)$.

Causality again.

As mentioned earlier, two points $x, y$ with space like separation $(x - y)^2 < 0$ are not causally connected. This means that in this case, which corresponds to the region outside the light cone, the commutator $[\phi(x), \phi(y)]$ must vanish.

Starting from eq.(41) the commutator is given by the expression
where the operator commutation rule of eq.(36) has been used. In order to obtain zero for this quantity, the inversion transformation \( x - y \rightarrow -(x - y) \) has to be applied to the second integral. However, this is only legitimate if this transformation leaves the value of the integral invariant. This we shall discuss now. First set \( x - y = \Delta = (\Delta_0, \Delta) \), with \( \Delta_0 = \Delta t \), \( \Delta = \Delta x \). Then we have
\[
\Delta \cdot (x - y) = p_0 \Delta_0 - p \cdot \Delta \quad ; \quad p_0 = \omega_p
\]
Now define a space like surface \([3]\)
\[
\Delta_0^2 - \Delta^2 = -K^2 \quad ; \quad K > 0
\]
Without loss of generality we can restrict ourselves to the plane \((\Delta_0, \Delta_1)\) where the surface of eq.(44) appears as the curve
\[
\Delta_0^2 - \Delta_1^2 = -K^2 \quad \text{see figure}
\]
Now take a particular point \((\Delta_0, \Delta_1)\) on this curve and rotate the coordinate frame in both terms of eq.(42) from \((\Delta_0, \Delta_1)\) to \((\Delta'_0, \Delta'_1)\)
One then has the relations
\[
\Delta_1 = \Delta'_1 \cos \varphi \quad ; \quad \cos \varphi = \frac{\Delta_1}{\sqrt{\Delta_0^2 + \Delta_1^2}}
\]
Hence the transformed quantities are
\[
\Delta'_0, \Delta'_1 = \frac{1}{\cos \varphi} \Delta_0, \Delta'_2 = \Delta'_3 = \Delta_3
\]
yielding the following result in terms of rotated quantities:
\[
e^{-ip \cdot (x - y)} - e^{ip \cdot (x - y)} \rightarrow e^{-ip' \cdot \Delta'} - e^{ip' \cdot \Delta'}
\]
Now the cumbersome factor \( e^{ip_0 \Delta_0} \) has disappeared and the transformation \( \Delta' \rightarrow -\Delta' \) leaves the value of the second integral unchanged, since in this integral one can change the sign of the integration variable without affecting its value. The fact that for any point on a given curve the corresponding coordinate rotation can be made, and that this is true for any curve, proves the statement that the commutator vanishes at any point outside the light cone.
Inside the light cone, i.e. for time like separations, the commutator does not vanish so that in this region points can be causally connected. It is however interesting to note that the
corresponding commutator is invariant with respect to proper Lorentz transformations as shown e.g. in ref.[3].

![Diagram](image)

**Fig. 1**

Note finally, that in many calculations the infinite energy of the vacuum state is eliminated by performing normal ordering of operators. It consists in reshuffling operator products in such a way that destruction operators always stand on the right of creation operators.

Generalizations [4]

Particles obeying the Klein-Gordon equation do not bear any electric charges. In order to treat charged particles, complex wave functions have to be introduced into the theory. Even more profound modifications are necessary in the case of electrons according to the Dirac theory. Here, due to the presence of spin, wave functions are represented by spinors consisting of four functions as components of a vector. An even more striking difference occurs if second quantization is performed. In this case, the fermion character of the particle is taken into account in postulating for the field operators anti-commutation rules instead of the commutation rules pertaining to bosons.
However, the general idea of avoiding negative energy states by means of second quantization, already applied to the Klein-Gordon case, remains essentially the same in this and other situations.

Bibliography


