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Off-Shell Relativistic Quantum Mechanics and Formulation of Dirac's Equation Using Characteristic Matrices

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It is argued that the Klein–Gordon equation is an equation for characteristic functions, i.e., Fourier-transformed Wigner functions, not for wave functions. This statement is derived starting from the off-shell formulation of relativistic quantum mechanics by expressing the condition that the mass of the particle is exactly known. A particular class of solutions of the Klein–Gordon equation is formed by the integrable superpositions of pure momentum states. A direct sum of four copies of the associated Gelfand–Naimark–Segal representation is considered. Then one can derive from the Klein–Gordon equation an equation for spinor wave functions. Solutions of the latter equation are in one-to-one correspondence to the solutions of the Fourier-transformed Dirac equation. Finally, the equation is reformulated as an equation for characteristic matrices.

1. INTRODUCTION

Aparicio *et al.* (1995) review various proper time formulations of relativistic quantum mechanics (RQM). In most approaches the proper time is a scalar parameter. Often wave equations with second-order space-time derivatives are considered. The present paper adopts the equation introduced independently by Johnson (1969, 1971) and Moses (1969). The equation contains a first-order derivative with respect to proper time. Time and space coordinates are treated on the same footing by introducing a four-vector of position operators $\mathbf{Q}_\mu$ and associated momentum operators $\mathbf{P}_\mu$, $\mu = 0, 1, 2, 3$. In particular, one has $\mathbf{Q}_0 = c\mathbf{t}$ and $\mathbf{P}_0 = \mathbf{E}/c$ with $\mathbf{t}$ the time operator and $\mathbf{E}$ the

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energy operator. The generator of the proper time evolution of a free particle is proportional to the mass operator $\mathbf{m}$, which is given by

$$\mathbf{m} = \frac{1}{c}\sqrt{\sum_{\mu=0}^{3} g_{\mu\mu}\mathbf{P}_\mu^2} \tag{1.1}$$

The present paper combines Johnson's formalism with the C^*-algebraic approach. The C^*-algebra of canonical commutation relations (CCR) is generated by the bounded operators

$$\mathbf{W}(p, q) = \exp[i\hbar^{-1} \sum_{\mu} g_{\mu,\mu}(p_\mu \mathbf{Q}_\mu + q_\mu \mathbf{P}_\mu)] \tag{1.2}$$

indexed by parameters p and q in four-space $\mathbb{R}^4$. This algebra is often called the Weyl algebra. It has already been used to describe a quantized relativistic particle (Carey *et al.*, 1977). Following Moyal (1947), the function f given by

$$f(p, q) = \langle \mathbf{W}(p, q) \rangle \tag{1.3}$$

is called the characteristic function of the state of the particle. Here $\langle\cdot\rangle$ denotes the quantum mechanical expectation value. The Fourier transform of f is the Wigner function, if it exists.

An important advantage of the formalism, besides mathematical rigor, is the ease with which singular physical states can be described. These singular states appear in the present context when particles with exact mass are described. Indeed, the momentum states considered in Section 7 are described by characteristic functions of the form $f(p, q) = \delta_{p,0}\phi(q)$. Clearly, such singular states cannot be described by Wigner functions.

There seems to be a consensus in the literature that the Klein–Gordon equation is not an equation for wave functions, but rather an equation for classical fields. The statement here is that it is a quantum mechanical equation, more precisely, an equation for characteristic functions of the form given above. The advantage of this interpretation is that with a characteristic function is associated a state which has a quantum probabilistic interpretation in the C^*-algebraic sense. In particular, the state is positive and normalized. The particle has exact mass m and a classical probability distribution of momenta. As expected from the canonical commutation relations, in combination with the exact knowledge of the mass, the particle is delocalized in space-time.

From the Klein–Gordon equation one can derive the Dirac equation in a straightforward manner, as was first shown by van der Waerden (see, e.g., Sakurai, 1967). This derivation can be made in terms of characteristic functions. It is, however, more convincing if the Hilbert space representation of solutions of the Klein–Gordon equation is constructed first. Next the transition from Klein–Gordon to Dirac is made by indroducing Dirac spinors, i.e., 4-tuples of wave functions. At this point it will be shown that there is a one-to-one correspondence between the Dirac-like equation of the present paper and the known solutions of the Fourier-transformed Dirac equation. The final result of the paper is an equation for 4-by-4 matrices of functions, which will be called characteristic matrices hereafter.

Several interesting questions raised by the present approach will be answered in a forthcoming publication. Although all equations of the present paper are covariant by construction, it is interesting to do the symmetry analysis in an explicit manner because it is known from conventional on-shell RQM that this reveals the nature of the quantum particles described by the theory.

The next step is the transition from the description of free particles to that of particles in an electromagnetic field. Finally, the transition from a one-particle to a many-particle theory looks promising for more than one reason. The present formalism has already a quantum-probabilistic interpretation in the one-particle case, which is not the case for the conventional on-shell theory. Also the formalism of Weyl algebras and characteristic functions allows us to introduce a many-particle description in a natural way via the concept of quasi-free states, (Manuceau *et al.*, 1968).

Sections 2–4 introduce the necessary notations. Section 5 discusses the Weyl transform, the relation between characteristic functions and Wigner functions, and the proper time equation of motion for characteristic functions in case of a free particle. These topics are not needed for the remainder of the paper. Their discussion is added for convenience of the reader. In Section 6 equations are derived which express the conditions under which a characteristic function describes a particle with exactly known mass m. This leads in Section 7 to the Klein–Gordon equation for characteristic functions, after introduction of the concept of momentum states. In Section 8 a Hilbert space representation of the Weyl algebra corresponding to solutions of the Klein–Gordon equation is constructed. This is used in Section 9 to make the transition toward a Dirac equation. In the final section the Dirac equation is reformulated as an equation for characteristic matrices.

2. OFF-SHELL RQM

In the Hilbert space approach to RQM it is obvious to start with the Hilbert space $\mathscr{H} = \mathscr{L}^2(\mathbb{R}^4, \mathbb{C})$ of square-integrable complex functions over four-space $\mathbb{R}^4$. The zeroth component of the position q_0 is proportional to the time t: $q_0 = ct$ (c is the speed of light). In this Hilbert space the time and position operators are multiplication operators: $\mathbf{Q}_\mu\psi(q) = q_\mu\psi(q)$, $\mu = 0, 1, 2, 3$. Obviously, the time operator $\mathbf{T}$ satisfies $\mathbf{Q}_0 = c\mathbf{T}$. A wave function ψ is a normalized element of the Hilbert space. It is uniquely determined by the state of the particle, up to a complex phase factor. An immediate consequence is that a particle has both time and position uncertainty, while in the standard approach the time is a parameter chosen by the observer. The momentum operators are given by

$$\mathbf{P}_\mu = g_{\mu,\mu} i\hbar \frac{\partial}{\partial q_\mu} \tag{2.1}$$

(the metric tensor g has nonzero elements $g_{0,0} = 1$ and $g_{1,1} = g_{2,2} = g_{3,3} = -1$). The energy operator $\mathbf{E}$ is given by $\mathbf{E} = c\mathbf{P}_0$.

For each Lorentz transformation Λ and each shift $a \in \mathbb{R}^4$ a unitary operator $\mathbf{U}_{\Lambda,a}$ of $\mathcal{H}$ is determined by

$$\mathbf{U}_{\Lambda,a}\psi(q) = \psi(\Lambda q + a) \tag{2.2}$$

for all $\psi \in \mathcal{H}$, $q \in \mathbb{R}^4$ (note that the Jacobian of Λ equals 1). The map $(\Lambda, a) \to \mathbf{U}_{\Lambda,a}$ is a unitary representation of the Poincaré group.

The mass operator $\mathbf{m}$ is given by (1.1). It is invariant under the action of the Poincaré group. Mathematically, $\mathbf{m}$ is a function of the commuting self-adjoint operators $\mathbf{P}_\mu$, $\mu = 0, 1, 2, 3$. Hence its existence follows from the spectral theorem. Note that $\mathbf{m}$ can be written as $\mathbf{m} = \mathbf{m}_1 + i\mathbf{m}_2$ with $\mathbf{m}_1$ and $\mathbf{m}_2$ commuting positive operators. In fact, one can split the Hilbert space into two orthogonal components $\mathcal{H}_1$ and $\mathcal{H}_2$ with the property that $\sum_{\mu=0}^{3} g_{\mu\mu}\mathbf{P}_\mu^2$ is positive on $\mathcal{H}_1$ and negative on $\mathcal{H}_2$. Then $\mathbf{m}$ equals $\mathbf{m}_1$ on $\mathcal{H}_1$ and $i\mathbf{m}_2$ on $\mathcal{H}_2$. On physical grounds one could require that the mass operator is positive, in which case wave functions representing a physical particle should belong to $\mathcal{H}_1$. This restriction does not introduce any problems since $\mathcal{H}_1$ is Poincaré-invariant. For representations of the CCR the full Hilbert space is needed (see the next section).

3. THE ALGEBRA OF THE CCR

The notion of the algebra of canonical commutation relations goes back to Weyl and von Neumann (see Emch, 1984, Section 8.3). The formalism of Weyl algebras was developed by Segal. The C^*-algebraic formulation is due to Manuceau (1968; see also Carey *et al.*, 1977). An introductory text is found in Petz (1990).

The C^*-algebra is generated by operators

$$\{\mathbf{W}(p, q): p, q \in \mathbb{R}^n\} \tag{3.1}$$

[in (Moyal 1947) the notation $\mathbf{M}(\tau, \theta)$ is used instead of $\mathbf{W}(p, q)$]. These operators satisfy the relations

$$\begin{aligned} \mathbf{W}(0, 0) &= \mathbb{I} \\ \mathbf{W}(p, q)\mathbf{W}(p', q') &= \mathbf{W}(p + p', q + q') \exp[i\sigma(p, q; p', q')/2\hbar] \end{aligned} \tag{3.2}$$

where σ is a nondegenerate simplectic form [i.e., σ is bilinear and antisymmetric, $\sigma(x, y) = 0$ for all y implies $x = 0$].

In the present case of relativistic quantum mechanics of a single particle it is obvious to take $n = 4$ and

$$\sigma(p, q; p', q') = \sum_{\mu} g_{\mu,\mu}(p_\mu q'_\mu - q_\mu p'_\mu) \tag{3.3}$$

For a given number of degrees of freedom n, there is only one irreducible representation of the algebra of the CCR for which all maps

$$\lambda \in \mathbb{R} \to \mathbf{W}(\lambda p, \lambda q) \tag{3.4}$$

are continuous. In the present case, this representation is (formally) given up to unitary equivalence by expression (1.2). A definition which is more convenient than (1.2) is

$$\mathbf{W}(p, q) = e^{-ipgq/2\hbar} e^{ipg\mathbf{Q}/\hbar} e^{iqg\mathbf{P}/\hbar} \tag{3.5}$$

Useful relations are

$$[\mathbf{W}(p, q), \mathbf{P}_\mu] = p_\mu \mathbf{W}(p, q), \qquad [\mathbf{W}(p, q), \mathbf{Q}_\mu] = -q_\mu \mathbf{W}(p, q) \tag{3.6a}$$

and

$$\mathbf{W}(p, q)\mathbf{W}(p', q') = e^{i\sigma(p,q;p',q')/2\hbar}\mathbf{W}(p + p', q + q') \tag{3.6b}$$

4. CHARACTERISTIC FUNCTIONS

In the present context, the interest in the algebra of the CCR arises from the fact that it also has representations for which the maps (3.4) are not necessarily continuous. In particular, one is interested in representations used in on-shell RQM. These will be obtained by considering physical states of the system which do not correspond with a normalized wave function ψ in $\mathcal{L}^2(\mathbb{R}^4, \mathbb{C})$. Now, starting from a wave function ψ, the characteristic function of the state of the particle is defined as a complex-valued function f given by

$$f(p, q) = \langle \mathbf{W}(p, q) \rangle = \langle \psi | \mathbf{W}(p, q) | \psi \rangle \tag{4.1}$$

(two notations are used for the inner product of the Hilbert space; they are related by $\langle \phi | A | \psi \rangle = (A\psi, \phi)$). If the representation of the algebra of the CCR is continuous, then also the function f is continuous in p and q. By dropping the condition that f should be continuous one can enlarge the set of physical states. It turns out that the largest interesting set of states corresponds to the set of all f satisfying the following conditions:

- Normalization:

$$f(0, 0) = 1 \tag{4.2a}$$

- Positivity condition:

$$\sum_{j,k=1}^{n} \overline{\lambda_j}\lambda_k e^{-i\sigma(p_j,q_j;p_k,q_k)/2\hbar} f(p_j - p_k, q_j - q_k) \geq 0 \tag{4.2b}$$

for all possible choices of $\lambda_1, \ldots, \lambda_n \in \mathbb{C}$, $p_1, q_1, \ldots, p_n, q_n \in \mathbb{R}^4$.

Note that the function f must be defined everywhere, but need not to be continuous. Under the conditions (4.2) there exists a mathematical state on the C^*-algebra of the CCR. Such a state is the generalization of a probability measure, and as such it has a (quantum) probabilistic interpretation. However, the quantum expectation $\langle A \rangle$ of an observable A is not always defined. The expectation values of polynomials in the position and momentum operators are obtained by taking partial derivatives of f. For example, if the function $q_\mu \to f(0, q)$ is n times differentiable with respect to q_μ at $q = 0$ then

$$\langle P_\mu^n \rangle = \left(- i\hbar g_{\mu,\mu} \frac{\partial}{\partial q_\mu} \right)^n f(0, q) \bigg|_{q=0} \tag{4.3}$$

Similarly, if the function $p_\mu \to f(p, q)$ is n times differentiable with respect to p_μ at $p = 0$, then the nth moment of the position is given by

$$\langle Q_\mu^n \rangle = \left(-i\hbar g_{\mu,\mu} \frac{\partial}{\partial p_\mu} \right)^n f(p, 0) \bigg|_{p=0} \tag{4.4}$$

Since the function f does not need to be differentiable the average position and momentum of the particle are not always defined. Weyl (1928) tried to solve this problem using distributions. This formalism is avoided in the present paper, but is briefly discussed in the next section.

Before going on, note that the $\mathbf{W}$ operators transform under an element (Λ, a) of the Poincaré group as

$$\mathbf{U}_{\Lambda,a}^* \mathbf{W}(p, q) \mathbf{U}_{\Lambda,a} = e^{i\hbar^{-1}pga} \mathbf{W}(\Lambda p, \Lambda q) \tag{4.5}$$

The characteristic function $f(p, q)$ transforms into

$$f(p, q) \to (\mathbf{W}(p, q)\mathbf{U}_{\Lambda,a}\psi, \mathbf{U}_{\Lambda,a}\psi) = e^{i\hbar^{-1}pga} f(\Lambda p, \Lambda q) \tag{4.6}$$

5. PROPER TIME EVOLUTION

The Weyl transform of an observable A is a complex function $a \equiv a(p, q)$, which can be defined through (Weyl, 1931; Moyal 1947; de Groot, 1974)

$$A = \hbar^{-4} \int dp \int dq\ \tilde{a}(p, q)\mathbf{W}(p, q) \tag{5.1}$$

where $\tilde{a} \equiv \tilde{a}(p, q)$ is the Fourier transform of a,

$$\tilde{a}(p, q) = \hbar^{-4} \int dp' \int dq'\ e^{i\hbar^{-1}pgq'} e^{-i\hbar^{-1}p'gq} a(p', q') \tag{5.2}$$

The expectation value of an observable A is then formally given by

$$\begin{aligned} \langle A \rangle &= \hbar^{-4} \int dp \int dq\ \tilde{a}(p, q) f(p, q) \\ &= \hbar^{-4} \int dp' \int dq'\ a(p', q')\rho(p', q') \end{aligned} \tag{5.3}$$

where

$$\rho(p', q') = \hbar^{-4} \int dp \int dq\ e^{i\hbar^{-1}pgq'} e^{-i\hbar^{-1}p'gq} f(p, q) \tag{5.4}$$

ρ is called the Wigner function. It is the Fourier transform of the characteristic function f.

Using the Weyl transform, it is easy to obtain the proper time evolution of the characteristic function f of a free particle. The generator of the proper time evolution is $\mathbf{m}c^2$ [Moses (1969) proposed to use $\mathbf{m}_1$ instead of $\mathbf{m}$ because the latter is not self-adjoint; Johnson (1969) restricts physical states to wave functions in $\mathcal{H}_1$]. A short calculation gives

$$e^{i\hbar^{-1}\mathbf{m}c^2\tau} = \int_{\mathbb{R}^4} dq\ \beta_\tau(q)\mathbf{W}(0, q) \tag{5.5}$$

with

$$\beta_\tau(q) = (2\pi)^{-4} \int_{\mathbb{R}^4} dk\ e^{-ikgq}\ e^{ic\tau\kappa(k)} \tag{5.6}$$

and $\kappa(q) = (\sum_{\mu=0}^{3} g_{\mu,\mu} q_\mu^2)^{1/2}$. Hence we obtain

$$\begin{aligned} f_\tau(p, q) &= (\mathbf{W}(p, q)\psi_\tau, \psi_\tau) \\ &= (\mathbf{W}(p, q)e^{i\hbar^{-1}\mathbf{m}c^2\tau}\psi, e^{i\hbar^{-1}\mathbf{m}c^2\tau}\psi) \\ &= \int_{\mathbb{R}^4} dq' \int_{\mathbb{R}^4} dq''\ \beta_\tau(q')\ \overline{\beta_\tau(q'')}(\mathbf{W}(p, q)\mathbf{W}(0, q')\psi, \mathbf{W}(0, q'')\psi) \end{aligned}$$

$$= \int_{\mathbb{R}^4} dq' \int_{\mathbb{R}^4} dq'' \, \beta_\tau(q') \, \overline{\beta_\tau(q'')} \, e^{ipg(q'+q'')/2\hbar} f(p, q + q' - q'')$$

$$= \int_{\mathbb{R}^4} dq' \, e^{ipgq'/2\hbar} \xi_\tau(p, q') f(p, q + q') \tag{5.7}$$

with

$$\xi_\tau(p, q) = (2\pi)^{-4} \int_{\mathbb{R}^4} dk \, e^{-ikgq} \, e^{ic\tau\kappa(k)} \, e^{\overline{-ic\tau\kappa(k - p/\hbar)}} \tag{5.8}$$

It is a solution of the equation of motion

$$i\hbar \frac{d}{d\tau} f_\tau(p, q) = \int_{\mathbb{R}^4} dq' \, e^{-ipgq'/2\hbar} \, \zeta(p, q') f_\tau(p, q - q') \tag{5.9}$$

with

$$\zeta(p, q) = -\hbar c (2\pi)^{-4} \int_{\mathbb{R}^4} dk \, e^{ikgq} \, (\kappa(k) - \overline{\kappa(k - p/\hbar)}) \tag{5.10}$$

Note that

$$f_\tau(0, 0) = \int_{\mathbb{R}^4} dq \, \xi_\tau(0, q) f(0, q) \tag{5.11}$$

which, in general, is not equal to 1. Hence the function f_τ is not properly normalized. This is a consequence of the fact that the mass operator $\mathbf{m}$ is not self-adjoint. Only when the characteristic function f corresponds to a wave function in $\mathcal{H}_1$ (or a superposition of such wave functions) does one expect normalization to be conserved. Conversely, if the generator of proper time evolution is $\mathbf{m}_1 c^2$, then the definition of κ should be replaced by

$$\begin{aligned} \kappa(l) &= \left(\sum_{\mu=0}^{3} g_{\mu,\mu} l_\mu^2 \right)^{1/2} \qquad && \text{if} \quad \sum_{\mu=0}^{3} g_{\mu,\mu} l_\mu^2 \geq 0 \\ &= 0 && \text{otherwise} \end{aligned} \tag{5.12}$$

In that case (5.8) yields $\xi_\tau(0, q) = \delta(q)$, so that (5.11) implies that $f_\tau(0, 0) = f(0, 0)$.

6. MASS STATES IN RQM

Let us now derive the conditions under which the function f describes a particle with exact mass m. No such solution can be found in the off-shell Hilbert space formulation because the mass operator $\mathbf{m}$ has a purely continuous spectrum. It does not have any eigenstate in $\mathscr{L}^2(\mathbb{R}^4, \mathbb{C})$.

A short calculation using (3.5) gives

$$\frac{\partial}{\partial q_\mu}(e^{ipgq/2\hbar}\mathbf{W}(p, q)) = e^{ipgq/2\hbar}\mathbf{W}(p, q)\frac{i}{\hbar}(g\mathbf{P})_\mu \tag{6.1}$$

and hence

$$\begin{aligned}\frac{\partial^2}{\partial q_\mu^2}(e^{ipgq/2\hbar}\mathbf{W}(p, q)) &= \frac{\partial}{\partial q_\mu}(e^{ipgq/2\hbar}\mathbf{W}(p, q))\frac{i}{\hbar}(g\mathbf{P})_\mu \\ &= e^{ipgq/2\hbar}\mathbf{W}(p, q)\frac{-1}{\hbar^2}\mathbf{P}_\mu^2\end{aligned} \tag{6.2}$$

The d'Alembertian is denoted by

$$\Box_q \equiv \sum_{\mu=0}^{3} g_{\mu,\nu}\frac{\partial^2}{\partial q_\mu^2} \tag{6.3}$$

Using (6.2), (6.3), and the definition of the mass operator $\mathbf{m}$ in (1.1), one obtains for suitable wave functions ψ

$$\Box_q(e^{ipgq/2\hbar}\langle\psi|\mathbf{W}(p, q)|\psi\rangle) = -\frac{c^2}{\hbar^2}e^{ipgq/2\hbar}\langle\psi|\mathbf{W}(p, q)\mathbf{m}^2|\psi\rangle \tag{6.4}$$

Take now a sequence of wave functions ψ which approximate an exact eigenstate of $\mathbf{m}$ with eigenvalue m. The expectation values $\langle\psi|\mathbf{W}(p, q)|\psi\rangle$ then accumulate to a function f which satisfies the equation

$$\Box_q(e^{ipgq/2\hbar}f(p, q)) = -\frac{c^2}{\hbar^2}m^2 e^{ipgq/2\hbar}f(p, q) \tag{6.5}$$

The latter equation can be written out as

$$\begin{aligned}&-\hbar^2\Box_q f(p, q) - \hbar^2\sum_{\mu=0}^{3} g_{\mu,\mu}\left(i\hbar^{-1}p_\mu g_{\mu,\mu}\frac{\partial}{\partial q_\mu} - \frac{1}{4\hbar^2}p_\mu^2\right)f(p, q) \\ &= m^2c^2 f(p, q)\end{aligned} \tag{6.6a}$$

Also the complex conjugate equation should hold. After changing the signs of p and q it becomes

$$\begin{aligned}&-\hbar^2\Box_q f(p, q) - \hbar^2\sum_{\mu=0}^{3} g_{\mu,\mu}\left(-i\hbar^{-1}p_\mu g_{\mu,\mu}\frac{\partial}{\partial q_\mu} - \frac{1}{4\hbar^2}p_\mu^2\right)f(p, q) \\ &= m^2c^2 f(p, q)\end{aligned} \tag{6.6b}$$

By adding and subtracting both equations one obtains

$$\sum_{\mu=0}^{3} p_\mu \frac{\partial f}{\partial q_\mu} = 0 \tag{6.7a}$$

and

$$-\hbar^2 \Box_q f(p, q) = (m^2c^2 + \frac{1}{4} |p|^2) f(p, q) \tag{6.7b}$$

Let us postulate that a relativistic particle is in a state with exact mass m if it is described by a characteristic function f which satisfies conditions (6.7). Condition (6.7b) generalizes the Klein–Gordon equation, which is discussed in the next section.

7. MOMENTUM STATES IN RQM

Momentum states in nonrelativistic quantum mechanics represent particles with exact momentum (Fannes *et al.*, 1974). Their characteristic function is of the form $f(p, q) = \delta_{p,0}\phi(q)$, where $\delta_{p,0}$ is the Kronecker symbol, which equals one if $p = 0$ and zero otherwise. The positivity and normalization requirements (4.2) become:

Normalization:

$$\phi(0) = 1 \tag{7.1a}$$

Positivity condition:

$$\sum_{j,k=1}^{n} \overline{\lambda_j}\lambda_\kappa \phi(q_j - q_\kappa) \geq 0 \tag{7.1b}$$

for all choices of $\lambda_1, \ldots, \lambda_n \in \mathbb{C}$ and $q_1, \ldots, q_n \in \mathbb{R}^4$.

The condition (6.7a) is satisfied automatically. Hence, a state of this type describes a particle with exact mass m if (6.7b) is satisfied. The latter equation simplifies to:

Exact mass condition:

$$-\hbar^2 \Box_q \phi(q) = m^2c^2\phi(q) \tag{7.1c}$$

Equation (7.1c) is known as the Klein–Gordon equation.

Any $k \in \mathbb{R}^4$ which satisfies $|\hbar k|^2 = m^2c^2$ determines a solution ϕ of equations (7.1) by

$$\phi(q) = \exp(ikgq) \tag{7.2}$$

From (4.3) it follows that $\langle P_\mu^n \rangle = (\hbar k)^n$, $n \geq 0$. Hence the solution describes a particle with mass m and exact 4-momentum $\hbar k$. On the other hand, the position of this particle is not defined. The solutions of the form $f(p, q) = \delta_{p,0}\phi(q)$ with ϕ given by (7.2) are pure momentum states.

A more general class of solutions of conditions (7.1) is formed by the integrable superpositions of pure momentum states:

$$\begin{aligned}\phi(q) = \int_{\mathbb{R}^3} dk \exp\left(-i\sum_{\mu=1}^{3} q_\mu k_\mu\right) \\ \times\{[\exp(iq_0\sqrt{|k|^2+m^2c^2/\hbar^2})]\tilde{\phi}_0(k) \\ + [\exp(-iq_0\sqrt{|k|^2+m^2c^2/\hbar^2})]\tilde{\phi}_1(k)\}\end{aligned} \tag{7.3}$$

with $\tilde{\phi}_0$, $\tilde{\phi}_1$ any normalized pair of nonnegative integrable functions

$$\tilde{\phi}_\kappa(k) \geq 0, \quad \kappa = 0,1, \qquad \int_{\mathbb{R}^3} dk\, (\tilde{\phi}_0(k) + \tilde{\phi}_1(k)) = 1 \tag{7.4}$$

for which

$$\int_{\mathbb{R}^3} dk\, k_\mu^2 \tilde{\phi}_\kappa(k) < \infty, \qquad \mu = 0, \ldots, 4, \quad \kappa = 0,1 \tag{7.5}$$

The latter condition is required to ensure that ϕ is twice differentiable so that the l.h.s. of (7.1c) is well defined. If (7.1c) is interpreted in the distributional sense, then (7.5) is not needed.

The average energy and momentum of this particle satisfy

$$\begin{aligned}\langle E^n\rangle &= c\int_{\mathbb{R}^3} dk\, (\hbar^2|k|^2 + m^2c^2)^{n/2}[\tilde{\phi}_0(k) + (-1)^n\, \tilde{\phi}_1(k)] \\ \langle P_\alpha^n\rangle &= \int_{\mathbb{R}^3} dk\, (\hbar k_\alpha)^n[\tilde{\phi}_0(k) + \tilde{\phi}_1(k)], \qquad \alpha = 1, 2, 3\end{aligned} \tag{7.6}$$

provided that the integrals converge. Hence (7.3) describes a superposition of momentum states. Both positive and negative energy states can contribute.

8. HILBERT SPACE REPRESENTATION OF MOMENTUM STATES

The Gelfand–Naimark–Segal representation (Dixmier, 1964) corresponding to the state (7.3) is constructed as follows. Let $\mathcal{H}$ be the Hilbert space of wave functions

$$\begin{pmatrix}\psi_{0,p}\\ \psi_{1,p}\end{pmatrix}(k) \tag{8.1}$$

for which

$$\sum_{p\in\mathbb{R}^4}\int_{\mathbb{R}^3} dk\,\left(\left|\psi_{0,p}(k)\right|^2 + \left|\psi_{1,p}(k)\right|^2\right) < \infty \tag{8.2}$$

Define multiplication operators $\mathbf{P}_\mu$, $\mu = 0,\ldots, 3$, by

$$\mathbf{P}_0\begin{pmatrix}\psi_{0,p}(k)\\ \psi_{1,p}(k)\end{pmatrix} = \left(\sqrt{\hbar^2|k|^2 + m^2c^2} + p_0\right)\begin{pmatrix}\psi_{0,p}(k)\\ -\psi_{1,p}(k)\end{pmatrix} \tag{8.3}$$

$$\mathbf{P}_\alpha\begin{pmatrix}\psi_{0,p}(k)\\ \psi_{1,p}(k)\end{pmatrix} = (\hbar k_\alpha + p_\alpha)\begin{pmatrix}\psi_{0,p}(k)\\ \psi_{1,p}(k)\end{pmatrix}, \qquad \alpha = 1, 2, 3$$

Define unitary operators $\mathbf{U}_p$, $p \in \mathbb{R}^4$, by

$$\mathbf{U}_p\begin{pmatrix}\psi_{0,p'}\\ \psi_{1,p'}\end{pmatrix}(k) = \begin{pmatrix}\psi_{0,p'+p}\\ \psi_{1,p'+p}\end{pmatrix}(k) \tag{8.4}$$

Now let

$$\mathbf{W}(p, q) = \mathbf{U}_p e^{iqg\,(\mathbf{P}-p/2)/\hbar} \tag{8.5}$$

The operators $\mathbf{W}(p, q)$ generate a representation of the algebra of CCR. Let the wave function ψ be given by

$$\psi_{\kappa,p}(k) = \delta_{p,0}(\tilde{\phi}_\kappa(k))^{1/2}, \qquad \kappa = 0, 1 \tag{8.6}$$

Then one calculates

$$\begin{aligned}\langle\psi|\mathbf{W}(p, q)|\psi\rangle &= \sum_{p'\in\mathbb{R}^4}\int_{\mathbb{R}^3} dk\left\langle\begin{matrix}\psi_{0,p'+p}(k)\\ \psi_{1,p'+p}(k)\end{matrix}\right|e^{iqg(\mathbf{P}-p/2)/\hbar}\left|\begin{matrix}\psi_{0,p'}(k)\\ \psi_{1,p'}(k)\end{matrix}\right\rangle\\ &= \delta_{p,0}\int_{\mathbb{R}^3} dk\left\langle\begin{matrix}(\tilde{\phi}_0(k))^{1/2}\\ (\tilde{\phi}_1(k))^{1/2}\end{matrix}\right|e^{iqg\mathbf{P}/\hbar}\left|\begin{matrix}(\tilde{\phi}_0(k))^{1/2}\\ (\tilde{\phi}_1(k))^{1/2}\end{matrix}\right\rangle\\ &= \delta_{p,0}\phi(q)\end{aligned} \tag{8.7}$$

with ϕ given by (7.3). This shows that in this representation the state of the particle is represented by a wave function ψ.

Finally note that the Klein–Gordon equation (7.1c) can be written as

$$\begin{aligned}&\sum_{\mu=0}^{3} g_{\mu,\mu}\langle\psi\left|e^{iqg\mathbf{P}/\hbar}\mathbf{P}_\mu^2\right|\psi\rangle\\ &\quad = m^2c^2\langle\psi\right|e^{iqg\mathbf{P}/\hbar}\left|\psi\rangle \qquad \text{for all}\quad q \in \mathbb{R}^4\end{aligned} \tag{8.8}$$

The equation is rather trivial since any wave function ψ in this representation satisfies by construction

$$\sum_{\mu=0}^{3} g_{\mu,\mu} (P_\mu - p_\mu)^2 \psi_{\kappa,p} = m^2c^2\psi_{\kappa,p}, \qquad \kappa = 0, 1, \quad p \in \mathbb{R}^4 \tag{8.9}$$

Hence, wave functions of the form (8.6) satisfy

$$\sum_{\mu=0}^{3} g_{\mu,\mu}\mathbf{P}_\mu^2\psi = m^2c^2\psi \tag{8.10}$$

The latter equation implies (8.8).

9. DIRAC'S EQUATION

Construct a new representation of the CCR which is the direct sum of four identical copies of the previous representation. The wave function ψ in (8.7) is now replaced by a Dirac spinor

$$\psi = \begin{pmatrix} \psi_0 \\ \psi_1 \\ \psi_2 \\ \psi_3 \end{pmatrix} \qquad \text{with } \sum_{\mu=0}^{3} \|\psi_\mu\|^2 = 1 \tag{9.1}$$

Each ψ_μ is itself of the form (8.1).

The Pauli matrices are defined by

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{9.2}$$

The identity matrix is denoted σ_0, so that any 2-by-2 matrix can be written as a linear combination $\sum_{\mu=0}^{3}\lambda_\mu\sigma_\mu$. Note that the product of two Pauli matrices is again a Pauli matrix (or the identity matrix σ_0) up to a scalar factor.

Introduce matrices γ_μ, $\mu = 0, 1, 2, 3$, by

$$\gamma_0 = \begin{pmatrix} 0 & \mathbb{I}_2 \\ \mathbb{I}_2 & 0 \end{pmatrix}, \qquad \gamma_\alpha = \begin{pmatrix} 0 & -\sigma_\alpha \\ \sigma_\alpha & 0 \end{pmatrix}, \quad \alpha = 1, 2, 3 \tag{9.3}$$

[this is the so-called Weyl representation of the γ-matrices; see, e.g., Scharf (1989, Section 1.2)]. They satisfy the anticommutation relations

$$\gamma_\mu\gamma_\nu + \gamma_\nu\gamma_\mu = 2g_{\mu,\nu} \tag{9.4}$$

Replace now equation (8.10) with the more restrictive equation

$$\sum_{\mu=0}^{3} \gamma_\mu g_{\mu,\mu} \mathbf{P}_\mu \psi = mc\psi \tag{9.5}$$

That (9.5) implies (8.10) for each of the components of ψ can be seen as follows. If ψ is a solution of (9.5), then one has

$$\left(\sum_{\mu=0}^{3} \gamma_\mu g_{\mu,\mu} \mathbf{P}_\mu \right)^2 \psi = m^2\, c^2 \psi \tag{9.6}$$

Using (9.4), we can write the l.h.s. of (9.6) as $\Sigma\, g_{\mu,\mu} \mathbf{P}_\mu^2 \psi$. Hence (9.6) reduces to (8.10).

Equation (9.5) is the Dirac equation, except that it differs from it because the momentum operators $\mathbf{P}_\mu$ appearing in (9.5) are not the differential operators $i\hbar g_{\mu,\mu} \partial/\partial q_\mu$, $\mu = 0, \ldots, 3$. The motivation for introducing (9.5) is that there exists a representation of the Lorentz group which leaves the equation invariant. The solutions of (9.5) can be mapped onto the well-known solutions of the Dirac equation. Indeed, the general solution of (9.5) of the form $\psi_p = \delta_{p,0} \psi_0$ ($p \in \mathbb{R}^4$) is a superposition of four wave functions, two with positive and two with negative energy:

$$\begin{aligned} \psi_0(k) = {} & \begin{pmatrix} \psi_0(k) \\ 0 \end{pmatrix} \otimes \begin{pmatrix} mc \\ 0 \\ \hbar k_0 + \hbar k_3 \\ \hbar k_1 + i\hbar k_2 \end{pmatrix} + \begin{pmatrix} \psi_1(k) \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 0 \\ mc \\ \hbar k_1 - i\hbar k_2 \\ \hbar k_0 - \hbar k_3 \end{pmatrix} \\ & + \begin{pmatrix} 0 \\ \psi_2(k) \end{pmatrix} \otimes \begin{pmatrix} \hbar k_0 + \hbar k_3 \\ \hbar k_1 + i\hbar k_2 \\ -mc \\ 0 \end{pmatrix} + \begin{pmatrix} 0 \\ \psi_3(k) \end{pmatrix} \otimes \begin{pmatrix} \hbar k_1 - i\hbar k_2 \\ \hbar k_0 - \hbar k_3 \\ 0 \\ -mc \end{pmatrix} \end{aligned} \tag{9.7}$$

In the conventional approach the general solution of the Dirac equation is the Fourier transform of (9.7) [see, e.g., Scharf (1989), expression (1.4.35)].

10. CHARACTERISTIC MATRICES

From equation (9.5) one can derive an equation for characteristic functions as follows. Using (8.5), we can write it as

$$\sum_{\mu=0}^{3} \gamma_\mu \frac{\hbar}{i} \frac{\partial}{\partial q_\mu} \mathbf{W}\ (0,\, q)\psi = mc\mathbf{W}(0,\, q)\psi \tag{10.1}$$

Now introduce 4 by 4 matrices $\Phi(p, q)$ by

$$\Phi_{\nu',\nu}(p, q) = \langle\psi_{\nu'}\left|\mathbf{W}(p, q)\right|\psi_{\nu}\rangle \tag{10.2}$$

Φ is called a characteristic matrix hereafter. Equation (10.1) implies the following matrix equation:

$$\sum_{\mu=0}^{3} \frac{\hbar}{i} \frac{\partial}{\partial q_{\mu}} \gamma_{\mu}\Phi(0, q) = mc\Phi\,(0, q) \tag{10.3}$$

This equation is the analog of Dirac's equation for characteristic matrices. By iterating the equation, one verifies that each of the 16 elements of the matrix Φ satisfies the Klein–Gordon equation (7.1c).

A further generalization of (10.3) is

$$\sum_{\mu=0}^{3} \left(i\hbar \frac{\partial}{\partial q_{\mu}} + \frac{i}{2} g_{\mu,\mu} p_{\mu} \right) \gamma_{\mu}\Phi(p, q) + mc\Phi(p, q) = 0 \tag{10.4a}$$

By iterating this equation one verifies that each of the 16 elements of the characteristic matrix Φ satisfies equation (6.7b), provided that also the equation

$$\sum_{\mu=0}^{3} p_{\mu} \frac{\partial}{\partial q_{\mu}} \Phi\,(p, q) = 0 \tag{10.4b}$$

is satisfied. Finally, note that Φ should satisfy the normalization condition

$$\mathrm{Tr}\ \Phi(0.0) = 1 \tag{10.4c}$$

and the positivity condition

$$\sum_{j,k} e^{-i\sigma(p_j,q_j;p_k,q_k)/2\hbar}\ \mathrm{Tr}\ \lambda_j^{*}\Phi(p_j - p_k, q_j - q_k)\lambda_k \geq 0 \tag{10.4d}$$

for all possible choices of complex 4-by-4 matrices $\lambda_1, \ldots, \lambda_n$, and of p_1, $q_1, \ldots, p_n, q_n \in \mathbb{R}^4$.

Equations (10.4) describe a spin-1/2 particle with exact mass m. The characteristic function of the particle is given by

$$f(p, q) = \delta_{p,0}\ \mathrm{Tr}\ \Phi(q) \tag{10.5}$$

It describes the position and momentum of the particle, while the characteristic matrix includes also information about the internal state of the particle. In fact, Φ determines a mathematical state on the tensor product of the Weyl algebra with the Clifford algebra C_4. The relevant observables are

$$\mathbf{W}(p, q) \otimes \sigma_{\nu} \otimes \sigma_{\nu'} \tag{10.6}$$

where the $\sigma_\nu \otimes \sigma_{\nu''}$ act on the four-component wave functions as

$$\sigma_\nu \otimes \sigma_0 = \begin{pmatrix} \sigma_\nu & 0 \\ 0 & \sigma_\nu \end{pmatrix}, \qquad \sigma_\nu \otimes \sigma_1 = \begin{pmatrix} 0 & \sigma_\nu \\ \sigma_\nu & 0 \end{pmatrix} \tag{10.7}$$
$$\sigma_\nu \otimes \sigma_2 = \begin{pmatrix} 0 & -i\sigma_\nu \\ i\sigma_\nu & 0 \end{pmatrix}, \qquad \sigma_\nu \otimes \sigma_3 = \begin{pmatrix} \sigma_\nu & 0 \\ 0 & -\sigma_\nu \end{pmatrix}$$

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