A FORMAL DEFINITION OF CARRIERS

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Abstract. We give a formal definition of the carrier density which represents an elementary type of physical object.

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1. Introduction

In [1, 2] we have presented a derivation of a Density Functional Theory (DFT) from first principles. It was shown to be an independent and fundamental formulation for the description of an extended system in space. Our approach was also shown to contain the standard features of DFT. The methodology deduces the theory from the consideration of a distribution of action over space–time within a general framework we have called START. For this purpose we introduced the concept of carrier density. In the present paper we give a formal definition of the carrier density which represents an elementary type of physical object. The procedure will allow a systematic study of the role of auxiliary amplitude functions in the theory.

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In a series of papers [3, 4] we have developed a comprehensive theory of matter which has followed this scheme

$$\begin{array}{ccc}
 & SPACE + TIME + ACTION & \\
 & + & \\
 & FUNDAMENTAL\ PRINCIPLES & \\
 & and & \\
 & POSTULATES & \\
 & \Downarrow & \\
 & START\ GEOMETRY & \\
 & \Downarrow & \\
 & Density\ Functional\ Theory & \\
\swarrow & \downarrow & \searrow \\
General\ Relativity & Quantum\ Mechanics & Standard\ Model
\end{array}$$

In this program the principles refer to the existence of a unified geometry for space, time and action. A fundamental principle is also the requirement of the state of the system to be that of the least action. The postulates, to the geometrical union of the manifold of those variables through the systematic use of the concept of carriers and to the requirement that exchanges of action should occur in Planck's quanta.

1.1. Mass, Charges, Action, Space and Time

In our formalism **"action"**, as a fundamental variable, is distributed among a set of **carrier (of action) fields**. An action density $\breve{\alpha}(\mathbf{x}, t)$ is the fundamental concept defining all three: space (parametrized by the vector $\mathbf{x}$), time (parametrized by the scalar t) and action density (parametrized by the scalar valued analytical function $\breve{\alpha}(\mathbf{x}, t)$) as **primitive** concepts from which all other physical quantities will be derived or at least related directly or indirectly. The different forms of distributing the action among these carriers define the carriers themselves. Here as in our study of General Relativity and related theories (see [3, 4]) action (action density) is given the status of an independent variable (function).

1.2. Definition of Carrier Fields

Within our fundamental formulation we will have to define properties of the fields we call "carriers".

A carrier-domain $\mathcal{B}$ is a connected open set whose elements can be put into bijective correspondence with the points of a region (domain in some instances) $\mathbf{B}$ of an Euclidean point space $\mathbb{E}$ (In continuum mechanics the elements of $\mathcal{B}$ are assumed to exist by themselves, in our presentation this term is merely part of the description of a carrier-domain.). $\mathbf{B}$ is referred to as a configuration of $\mathcal{B}$; the point in $\mathbf{B}$ to which a given element of $\mathcal{B}$ corresponds is said to be "*occupied*" by that *element.* If $\mathcal{X}$ denotes a representative *element* of $\mathcal{B}$ and $\mathbf{x}$ the position relative to an origin $\mathbf{0}$ of the point $\mathbf{x}$ occupied by $\mathcal{X}$ in $\mathbf{B}$, the preceding statement implies the existence of a function $\theta : \mathcal{B} \rightarrow \mathbf{B}_0$ ($\mathbf{B}_0$, stands for the totality of the positions relative to $\mathbf{0}$ of the points of $\mathbf{B}$) and its inverse $\Theta : \mathbf{B}_0 \longrightarrow \mathcal{B}$ such that

$$\mathbf{x} = \theta(\mathcal{X}), \qquad \mathcal{X} = \Theta(\mathbf{x}). \tag{1.1}$$

In a motion of a carrier-domain the configuration changes with time. Let t be a real variable, denoting time, and $I \in \mathbb{R}$ an interval (not necessarily bounded). If with each value of t in I, there is associated a unique configuration $\mathbf{B}_t$, of a carrier-domain $\mathcal{B}$, the family of configurations $\{\mathbf{B}_t : t \in I\}$ is called a motion of $\mathcal{B}$. This definition entails the existence of functions $\phi : \mathcal{B} \otimes I \rightarrow (\mathbf{B}_t)_0$ and $\Phi : \{(\mathbf{x}, t) : t \in I, \mathbf{x} \in (\mathbf{B}_t)_0\} \longrightarrow \mathcal{B}$ such that

$$\mathbf{x} = \phi(\mathcal{X}, t), \quad \mathcal{X} = \Phi(\mathbf{x}, t). \tag{1.2}$$

In a motion of $\mathcal{B}$ a typical element $\mathcal{X}$ occupies a succession of points which together form a curve in $\mathbf{E}$. This curve is called the path of $\mathcal{X}$ and is given parametrically by equation (1.2). The rate of change $\mathbf{v}$ of $\mathbf{x}$ in relation to t is called the velocity of the element $\mathcal{X}$. As in continuum mechanics (our definitions run parallel to those of an extended body in continuum mechanics, see for example Spencer 1980 [16]) the velocity and the acceleration of $\mathcal{X}$ can be defined as the rates of change with time of position and velocity respectively as $\mathcal{X}$ traverses its path, here and there "Kinematics" is this study of motion *per se*, regardless of the description in terms of physical forces causing it. The primitive concepts concerned are *position, time* and *carrier*, the latter abstracting into mathematical terms intuitive ideas about aggregations of matter capable of motion and deformation. The set of constitutive properties of the carriers, described below, will give useful, formal, existence to this concept.

Equations (1.2) depict a motion of a carrier-domain as a sequence of correspondences between elements of $\mathcal{B}$ and points. The points are identified by their positions relative to a selected origin $\mathbf{0}$ and the definitions provide a similar means of recognizing elements of $\mathcal{B}$. At each $\mathcal{X}$ a scalar quantity is given, called carrier density $\varrho(\mathcal{X})$, such that if $\mathbf{x} = \phi(\mathcal{X}, t)$ then $\varrho(\mathcal{X}) \to \rho(\mathbf{x},t)$ defines a scalar field called local carrier density.

As mentioned a carrier will have physical significance through its set of properties. The value of the density of a carrier field can be defined through a set of fundamental scalar constants (main examples: mass and charges) such that the integral of the product of these constants and the density gives the experimentally attributed value of a property for that carrier. The density might become an indirect observable through the repeated measurement of those properties, but it is not an observable in itself. We will use an example. A carrier field identified with an electron will have a density $\rho(\mathbf{x}, t)$ and if the property is Q we will obtain the definition $Q = \int_{\underline{\mathrm{V}}} q(\mathbf{x}, t) d\mathbf{x} = \int_{\underline{\mathrm{V}}} Q\rho(\mathbf{x}, t) d\mathbf{x}$ for all t in the system's volume $\underline{\mathrm{V}}$, which defines that Q is a constant property (in space and time) for that field (otherwise the variable quantity $q(\mathbf{x}, t)$ can be called "the density of Q ") The set of properties $\{Q\}$ characterizes a carrier field and in turn establishes the conditions for a density field to correspond to an acceptable carrier. This is for example the case of electromagnetism, and its daughter theory: elementary particles theory, where the set {mass, electric charge, weak charge, strong charge, spin} defines the 'elementary particle' one is dealing with.

1.3. INTERACTION TENSOR

In $\mathcal{B}$ the carrier has as only properties its existence, whereas in $\mathbf{B}$ the carrier c has a distribution characterized by the density $\rho_c(\mathbf{x}, t)$. There is no restriction in defining a reference space $\mathbf{B}_R$ where the carrier exists in the points $\mathbf{x}$ with constant density $\rho^{(0)}$ occupying a volume V_0 such that $\rho^{(0)} V_0 = 1$, these two quantities are unobservable as far as any "observation" requires an "interaction", only then the distribution acquires a meaningful space dependence as a function, by definition, of an *external interaction* $\mathbf{V}(\mathbf{x}, t)$, which will be defined below. Here it is important to state that as a result of this interaction, and of the attributed properties of the carrier, the density evolves into a current: $\rho^{(0)} \Longrightarrow \overrightarrow{j_c^V}(\mathbf{x}, t)$. The first considerations are that $\rho^{(0)}$ is defined in a given proper frame of reference $\mathbf{E}^{(0)}$ with vectors $\{e_0^{(0)}, e_1^{(0)}, e_2^{(0)}, e_3^{(0)}\}$ and then a reference carrier's density current is defined in those points as $j^{(0)} = \rho^{(0)} e_0^{(0)}$, second that in the **observers** frame of reference $\mathbf{E}$ with vectors $\{e_0, e_1, e_2, e_3\}$, as a result of the modification of the distribution caused by the interaction, the carrier's density current is given by

$$\overrightarrow{j_c^V}(\mathbf{x}, t) = \mathbf{R}_c^V(\mathbf{x}, t) \mathbf{S}_c^V(\mathbf{x}, t; \mathbf{x}') \mathbf{R}_c^{(0)} \rho^{(0)} (\mathbf{x}') \, e_0^{(0)},$$

with time-like component $\rho_c^V(\mathbf{x}, t) = \overrightarrow{j_c^V}(\mathbf{x}, t) \cdot e_0$.

That is in density functional theory the density itself is characterized by the properties of the carrier and the self-organization of the carrier which adapts to the external interactions. Let us analyze this.

Let $\mathbf{x}$ be the position of an arbitrary point $\mathcal{X}$ relative to an origin $\mathbf{o}$ and let $\mathbf{S}(\mathbf{x}, t; \mathbf{x}')$ and $\mathbf{R}(\mathbf{x}, t)$ be respectively a positive definite symmetric tensor and a proper orthogonal tensor fields on $\mathbf{E}$. First we give geometrical interpretations of the actions of $\mathbf{S}$ and $\mathbf{R}$ on $\mathbf{x}$.

- $\mathbf{S}$ admits an spectral representation ($\mathbf{I} = \sum(\mathbf{p}_r \otimes \mathbf{p}_r)$)

  $$\mathbf{S}(\mathbf{x}, t; \mathbf{x}') = \mathbf{S}(\mathbf{x}, t; \mathbf{x}') \sum(\mathbf{p}_r \otimes \mathbf{p}_r) = \sum \lambda_r(\mathbf{x}, t; \mathbf{x}')(\mathbf{p}_r \otimes \mathbf{p}_r)$$

  with λ_r and p_r the eigenvalues and eigenvectors of $\mathbf{S}$. The λ_r being positive and the associated proper vectors forming an orthonormal basis $\mathbf{p} = \{\mathbf{p}_r\}$ of $\mathbf{E}$. Hence

  $$\begin{aligned}\mathbf{S}\mathbf{x}' &= \sum \lambda_r(\mathbf{x}, t; \mathbf{x}')(\mathbf{p}_r \otimes \mathbf{p}_r)\mathbf{x}' \\ &= \sum \lambda_r(\mathbf{x}, t; \mathbf{x}')(\mathbf{p}_r \cdot \mathbf{x}')\mathbf{p}_r = \sum \lambda_r(\mathbf{x}, t; \mathbf{x}')x_r\mathbf{p}_r\end{aligned}$$

  where x_r are the coordinates of $\mathbf{x}'$ in the Cartesian system $(\mathbf{o}, \mathbf{p})$. In geometrical terms, therefore, the action of S on $\mathbf{x}'$ is to map $\mathbf{x}'$ into the point $\mathbf{x}(\mathbf{x}', t)$ having position $\mathbf{S}\mathbf{x}'$ relative to $\mathbf{o}$ and coordinates $\lambda_r(\mathbf{x}, t; \mathbf{x}')x_r$ in the system $(\mathbf{o}, \mathbf{p})$. The distance of every point of E from the coordinate plane $x_1 = 0$ is changed by the positive factor $\lambda_1(\mathbf{x}, t; \mathbf{x}')$, (being increased if $\lambda_1 > 1$ and reduced if $0 < \lambda_1 < 1$), and distances from the planes $x_2 = 0$ and $x_3 = 0$ through $\mathbf{o}$ are likewise multiplied by $\lambda_2(\mathbf{x}, t; \mathbf{x}')$ and $\lambda_3(\mathbf{x}, t; \mathbf{x}')$ respectively. The tensor $\mathbf{S}(\mathbf{x}, t; \mathbf{x}')$ accordingly gives rise to a transformation of E consisting of proportional extensions, or stretches, of amounts $\lambda_r(\mathbf{x}, t; \mathbf{x}')$, in the mutually orthogonal directions defined by the unit proper vectors p_r. These directions are known as the principal axes of $\mathbf{S}$.

- The antisymmetric tensor $\mathbf{R}(\mathbf{x}, t)$ can be expressed in the form

  $$\mathbf{R}(\mathbf{x}, t) = \mathbf{p} \otimes \mathbf{p} + (\mathbf{q} \otimes \mathbf{q} + \mathbf{r} \otimes \mathbf{r}) \cos\theta(\mathbf{x}, t) - (\mathbf{q} \otimes \mathbf{r} - \mathbf{r} \otimes \mathbf{q}) \sin\theta(\mathbf{x}, t)$$

  where $-\pi < \theta(\mathbf{x}, t) < \pi$ and $\{\mathbf{p}, \mathbf{q}, \mathbf{r}\}$ is an orthonormal basis of $\mathbf{E}$. Hence

  $$\begin{aligned}\mathbf{R}\mathbf{x} = \mathbf{y} &= \{\mathbf{p} \otimes \mathbf{p} + (\mathbf{q} \otimes \mathbf{q} + \mathbf{r} \otimes \mathbf{r}) \cos\theta - (\mathbf{q} \otimes \mathbf{r} - \mathbf{r} \otimes \mathbf{q}) \sin\theta\}\mathbf{x} \\ &= p\mathbf{p} + (q\cos\theta(\mathbf{x}, t) + r\sin\theta(\mathbf{x}, t))\mathbf{q} + (r\cos\theta(\mathbf{x}, t) - q\sin\theta(\mathbf{x}, t))\mathbf{r}\end{aligned}$$

with $p = x \cdot p$, $q = x \cdot q$ and $r = x \cdot r$. In the rectangular Cartesian coordinate system with origin $\mathbf{o}$ and base vectors $\mathbf{p}, \mathbf{q}, \mathbf{r}$ and the points $\mathbf{y}$ with position $\mathbf{Rx}$ relative to $\mathbf{o}$ have coordinates $(p, \Re\, z, \Im\, z)$ and $(p, \Re\, ze^{i\theta}, \Im\, ze^{i\theta})$ respectively, where $z = q + ir$, and $\mathbf{x}$ is carried into $\mathbf{y}$ by rotating the radius vector $\overrightarrow{\mathbf{ox}}$ through an angle $\theta(\mathbf{x}, t)$ about the axis $\overrightarrow{\mathbf{oc}}$. The action of $\mathbf{R}(\mathbf{x}, t)$ on $\mathbf{x}$ may therefore be interpreted as a **rotation** in E of amount $\theta(\mathbf{x}, t)$ about the axis through $\mathbf{o}$ in the direction defined by $\mathbf{p}$.

Now we give a *physical interpretation* to the transformations $\mathbf{S}(\mathbf{x}, t)$ and $\mathbf{R}(\mathbf{x}, t)$.

- The positive definite symmetric tensor $\mathbf{S}^V(\mathbf{x}, t; \mathbf{x}')$ describe the spatial distributions of the carriers density which should minimize the action of the system according to our physical principle that the state of the system should be that corresponding to a stationary action. Otherwise the reference distribution being arbitrary we can replace the deformation it defines by a scale factor $S^V(\mathbf{x}, t)$ which describes the final carrier density distribution.
- The orthogonal tensor $\mathbf{R}^V(\mathbf{x}, t)$ describes the additional local rotation of the distribution arising from the effect of the external interaction.
- It could be convenient to write the actual density distribution in the form

  $$\rho^V(\mathbf{x}, t) = \mathbf{R}^V(\mathbf{x}, t) S^V(\mathbf{x}, t) \mathbf{R}^{(0)} \rho^{(0)},$$

  where the $\mathbf{R}^{(0)}$ describes the reference state of rotation of the carrier distribution. This reference rotation (a constant for an elementary carrier as defined in the next section) will be called *spin of the carrier* in accordance with the usual nomenclature. When the density $\rho(\mathbf{x}, t)$ is described below this additional orthogonal tensor $\mathbf{R}^{(0)}$ will acquire its full physical significance. As a result of the definitions above we could in fact write

  $$S^V(\mathbf{x}, t) = S^V(\mathbf{V}(\mathbf{x}, t)),\ \mathbf{R}^V(\mathbf{x}, t) = \mathbf{R}^V(\mathbf{V}(\mathbf{x}, t)),$$

  for the interaction tensors.
- The carriers density current can be written, if a representation is given of $\mathbf{S}(\mathbf{x}, t)$ and $\mathbf{R}(\mathbf{x}, t)$, as

  $$\begin{aligned} \overrightarrow{j^V}(\mathbf{x}, t) &= S^V(\mathbf{x}, t) \mathbf{R}^V(\mathbf{x}, t) \mathbf{R}^{(0)} \rho^{(0)} e_0^{(0)} \\ &= \widehat{\Psi}^V(\mathbf{x}, t) \rho^{(0)} e_0^{(0)} = \Psi^V(\mathbf{x}, t) \rho^{(0)} e_0^{(0)} \left(\Psi^V(\mathbf{x}, t)\right)^\dagger, \end{aligned}$$

the last form which will acquire full meaning below with the carrier current amplitude function operators $\Psi^V(\mathbf{x},t)$ and $\left(\Psi^V(\mathbf{x},t)\right)^\dagger$ being multivector or matrix representations of the extensions and Lorentz (Poincaré) transformations defined by Ψ^V.

Density Functional Theory is then a theory which describes the self-organization of a carrier distribution upon the influence of an external interaction, represented by the potential $V(\mathbf{x},t)$, as seen by a given observer represented by a geometric frame of reference.

The carrier current amplitude function

Here we want to show explicitly the multi-vector content of the carrier current amplitude function. We have considered that associated with each matter field, there is a distribution current field $e_\mu j^\mu(\ x)$, such that, denoting by $x= e_\mu x^\mu$ points in the observers frame of reference,

$$e_\mu j^\mu(\mathbf{x}) = \rho^{(0)} e_0^{(0)}, \tag{1.3}$$

assuming that there exists a (local) frame $e_\mu^{(0)}$ where the carrier distribution is at rest. The frame $e_\mu^{(0)}$ is related to the observers frame e_μ through the local Lorentz transformation with representation

$$e_\mu^{(0)} = R(\mathbf{x}) e_\mu R^{-1}(\mathbf{x}), \quad R^{-1} = R^\dagger, \tag{1.4}$$

then (1.3) becomes

$$e_\mu j^\mu(\mathbf{x}) = \rho^{(0)} R(\mathbf{x}) e_0 R^{-1}(\mathbf{x}), \tag{1.5}$$

we multiply (1.5) by $R(\mathbf{x})$ on the right,

$$e_\mu j^\mu(\mathbf{x}) R(\mathbf{x}) = \rho^{(0)} R(\mathbf{x}) e_0, \tag{1.6}$$

and use the multi-vector double projector $P_{+\uparrow}$, with the properties (best choice for a massive carrier)

$$P_{+\uparrow} = e_0 P_{+\uparrow} = P_{+\uparrow} e_0 \quad \text{and} \quad \mathrm{P}_{+\uparrow} = \mathrm{P}_{+\uparrow} \mathrm{i} \mathrm{e}_1 \mathrm{e}_2, \tag{1.7}$$

to obtain

$$e_\mu j^\mu R(\mathbf{x}) P_{+\uparrow} = \rho^{(0)} R(\mathbf{x}) P_{+\uparrow} i e_0 e_1 e_2. \tag{1.8}$$

Here, the ie_1e_2 factor is to be kept for further reference to $P_{+\uparrow}$ having been chosen as the appropriate projector, other choices could have been made. The up arrow refers to e_{12} as the direction of spin up and the plus sign to the choice of 'positive' carrier mass m_0 when energy-momentum is considered.

Now assume that there is a function

$$\Psi(\mathbf{x}) = A(\mathbf{x})R(\mathbf{x})P_{+\uparrow} \ \in \widehat{C}_{1,3}, \tag{1.9}$$

where $\widehat{C}_{1,3}$ is the space–time multivector algebra (basis vectors $\{e_\mu; \mu, \nu = 0, 1, 2, 3\}$, with $e_0^2 = -e_1^2 = -e_{2_3}^2 = -e_3^2 = 1$ and the definition property $e_\mu e_\nu = -e_\nu e_\mu$, we also use the notation $e_{0j} = e_0 e_j = \mathbf{e_j}$ $(i, j, k = 1, 2, 3)$ and $e_5 = e_0 e_1 e_2 e_3 = e_{0123}$) and such that (1.8) can be written

$$e_\mu j^\mu \Psi(\mathbf{x}) = \rho^{(0)} \Psi(\mathbf{x}) i e_0 e_1 e_2. \tag{1.10}$$

In the reference 'rest' frame of the field $R(\mathbf{x}) = 1$. We could also set the reference carrier density to $\rho^{(0)} = \rho^{(0)}(\mathbf{x}) = 1/A^2(\mathbf{x})$, replacing also $j^\mu \Longrightarrow j^\mu/A^2(\mathbf{x})$, resulting in $\rho = j^0 = \Psi(\mathbf{x}) e_0 (\Psi(\mathbf{x}))^\dagger$. Notice that $m_0 c j^\mu = p^\mu$, the energy-momentum components, and, with this $m_0 c$ factor included, (1.8) becomes an equation for the p^μ. Also the needed eigenvalue choice $\Psi(\mathbf{x}) i e_0 e_1 e_2 = \Psi(\mathbf{x})$ defines the sign of the mass and the intrinsic angular momentum of the carrier.

The function $\Psi(\mathbf{x}) = \Psi^V(\mathbf{x})$ in (1.9) explicitly contains then four main contributions: the existence of the carriers' field in $A(\mathbf{x}) = A^V(\mathbf{x})$; the observer's description of the relative motion of the field in $R(\mathbf{x})$ a (local) Lorentz transformation, the reference to a preferred sign of m_0 and, writing $R(\mathbf{x}) = R^V(\mathbf{x}) R^{(0)}$ intrinsic angular momentum (spin through $R^{(0)}$ and $P_{+\uparrow}$). The density $\rho(\mathbf{x}) = j^0(\mathbf{x})$ must be **an acceptable density** in the presence of the external potential $V(\mathbf{x})$, this is defined below. This derivation from first principles [1, 2] is also an explanation of the reason for considering a geometric (multi-vector) analysis.

1.4. COMPOSITE, DECOMPOSABLE, AVERAGE AND AVERAGE DESCRIPTION OF CARRIERS

There are several forms of analyzing the density. Each one allows a physical interpretation. For example:

- A *composite* carrier is defined as one for which the density

$$\rho_C(\mathbf{x}, t) = \sum_c A^c \rho_c(\mathbf{x}, t), \tag{1.11}$$

with the definition of each of the $\rho_c(\mathbf{x},t)$ being meaningful as a description of a carrier itself. In particular we can choose $\int_V \rho_c(\mathbf{x},t)d\mathbf{x} = \mathbf{1}$ and $A^c{=}N_c$.

- Similarly a *non-decomposable* carrier is defined as one for which (1.11) applies but for which the meaning of each of the $\rho_c(\mathbf{x},t)$ can not be defined without reference to the global $\rho_C(\mathbf{x},t)$.
- A (*non-decomposable) elementary* carrier is one for which a single $\rho_c(\mathbf{x},t)$ is all it is needed; in this case we emphasize the discrete nature of an elementary carrier, but we do not assume a point–like or any internal structure for them.
- An *average* carrier is defined as one for which its density can be described as ($W = \sum_{c=1,n} A^c$)

$$\rho_A(\mathbf{x},t) = \frac{1}{W}\sum_{c=1,n} A^c \rho_c(\mathbf{x},t), \tag{1.12}$$

with the definition of the $\rho_c(\mathbf{x},t)$ being meaningful as a description of a carrier itself. Similarly an *average description of a carrier* can be defined either as a space average over carrier descriptions as in (1.12) or as a time average of a description, or sum of descriptions ($\overline{W} = \sum_{c=1,n} \frac{1}{\tau}\int_{t=t_0}^{t=t_0+\tau} A^c(t)dt$, the choice $\overline{W} = 1$ presents less handling problems)

$$\overline{\rho(\mathbf{x})} = \frac{1}{\overline{W}}\sum_{c=1,n}\frac{1}{\tau}\int_{t=t_0}^{t=t_0+\tau} A^c(t)\rho_c(\mathbf{x},t)dt. \tag{1.13}$$

The introduction of restrictions (definitions) on the $A^c(t)\rho_c(\mathbf{x},t)$ terms defines the desired properties of the carriers. For example (with an Euler-Lagrange multiplier) a term of the form:

$$A^c(t)\rho_c(\mathbf{x},t) = \left(B_{ij}\,(t)\right)^c \left(\psi^i(\mathbf{x},t)\right)^\dagger \psi^j(\mathbf{x},t)$$

can be used (see below) to introduce symmetry properties and interaction possibilities.

1.5. SPACE, TIME AND ACTION

We already stated that in our theory space and time are fundamental, primordial, concepts. The geometrical unification of these concepts into a space–time coordinate manifold $\mathbf{X} = (\mathbf{x}, ct)$ and the introduction of a metric defining an interval ds^2 requires the introduction of a universal constant: the speed of light c. As we will also use action as a fundamental concept we need another universal constant $\kappa = d_0/h$. We construct κ from a fundamental distance d_0 and a fundamental unit of action we will choose to be Planck's action constant h.

The concept of **charges** appears in the theory first of all from the necessity to define the objects which exchange action among them in order to give a formal meaning to the principle that action will be exchanged in integer units of the Planck constant, second to relate the carriers among themselves defining the interaction through the bilinear form containing the products of pairs of charges, one type of charge for each one of the desired interactions. In this context for an electron-like carrier both mass and electric charge belong to the generic name of 'charges'. This full program can obviously not be achieved if the formulation is not suitable to contain the deduction of the theory of elementary particles itself, giving a geometric meaning to this theory. This will be mentioned in the paper but the reader is referred to our previous publications on this matter. To agree with standard formulations energy $E = \partial\breve{\alpha}/\partial t$ and momentum $p_i = \partial\breve{\alpha}/\partial x^i$ are the fundamental rates of change of the primitive concept of action. Otherwise we are presenting ideas which unify existing theories in the sense that we transform the theories from an inductive to a deductive class, also we suggest a well defined procedure to create future structures of theoretical physics.

Hermann Minkowski in his 1908 Address to the 80th Assembly of German Natural Scientists and Physicians, at Cologne, presented his mathematical formulation of Special Relativity in a talk he called *Space and Time*, introducing a fundamental axiom:

> .-*The substance of any world-point may always, with the appropriate determination of space and time, be looked upon as at rest.*

In our present formulation the quantity which was called "substance" by Minkowski is identified with the concept of "action density $\breve{\alpha}$" with a well defined physical and mathematical formulation, that is we include "substance" in the list of formal terms of physics. It is also appropriate to say that the concept of **matter**, hitherto formally undefined, acquires proper formal definition in the context of the different structural theories we have derived from START before and here, in a form which corresponds to a geometrization of Minkowski's fundamental axiom. Action density will be described as a sum of contributions over carriers, $\breve{\alpha} = \sum_{\mathrm{c}} \breve{\alpha}_c$ and then the contributions to energy-momentum, that is the rates of change of action over space-time directions, will also be sums over carriers c and over collections of carriers $\{\mathrm{c}_i\}$ when the choice was made to consider them as interacting carriers. Both the density function $\breve{\alpha}(\mathbf{X})$ and the splitting among carrier fields will be considered analytically well behaved functions.

Energy–Momentum–Stress

The derivatives of action with respect to time and to space (3-dimensions) generate a space–time vector which is termed "energy–momentum vector" $p_\mu^{(0)}$. These derivatives are nevertheless to be defined with respect to a given observer with local basis vectors $e_\mu^{(0)}$, for any other observer with local basis vectors e_μ the components of the energy momentum vector will be given by a new set of values p_μ, related to the first ones by Lorentz transformations. The best procedure is to define a vector valued function of a vector named the energy–momentum–stress tensor field $T(\mathbf{x},t)$ which will, upon application on the e_μ give the corresponding components of the energy–momentum vector

$$p_\mu(\mathbf{x},t) = T(\mathbf{x},t)\,[e_\mu]\,.$$

There are contributions to the action $\breve{\alpha}$ which have no space or time derivatives, this correspond to intrinsic contributions which give rise, for example, to the spin angular momentum.

1.6. Carriers as Action Carriers in START

We need to partition the different distributions of action over space–time by considering a set of contributions by a collection of scalar fields of "carriers" in such a form that the total action density in space–time is the sum of the action attributed to the carriers which, in that given point of space–time, have a non null field. For a given observer the carrier field c is defined to have an energy density $\frac{1}{N_\mathrm{c}}\mathcal{E}_\mathrm{c}\rho_\mathrm{c}$ with $\mathcal{E}_\mathrm{c}$ a constant in space and N_c the integer number of carrier units of type c. The density $\rho_\mathrm{c}(\mathbf{x},t)$ is required to obey $\int_{\underline{\mathtt{V}}} \rho_\mathrm{c}(\mathbf{x},t)d\mathbf{x} = N_\mathrm{c}$ in the system's volume $\underline{\mathtt{V}}$.

In order to make direct contact with standard formulations of physics we assume that the variables and fields associated to the concepts of space, time and action have the same mathematical relations as they have in those formulations. A fundamental, immediate, result is that energy and momentum as the rate of change of action with respect to time or to space are natural, primary, geometric concepts. Also the second derivatives of the action distribution are natural candidates to be the field strengths when expressed per unit carrier charges. This is particularly important in the gauge theory approach, where the rate of change of the action distribution, described through an auxiliary amplitude function, has contributions difficult to describe, as is often the case, as averages of the energy-momentum of some hypothetical point carriers. We also make a sharp distinction between action density and Lagrangian density. A Lagrangian density contains a description of the action distribution and a set of constrains for the formulation of a theory, a Lagrangian density is already a part of a particular theory.

Action is in our approach one of the properties of a distribution describing, in relation to an observer, the contents of the physical world in space–time. The concept of Physical Phenomena refers to the existence and change of this distribution. Physics corresponds to the description of the action distribution and its changes in relation to a given observer.

For a given observer the energy of a system $\mathcal{E} = \sum_{\mathrm{c}} N_{\mathrm{c}} \mathcal{E}_{\mathrm{c}}$ is at a given time a description dependent weighted by N_{c} sum of constants $\mathcal{E}_{\mathrm{c}}$, assumed to be distributed among the different carriers $\{\mathrm{c}\}$ and can furthermore, for theoretical needs, be described as a sum of contributions per carrier. A more general formulation, not developed here, would consider that the N_{c} could be variable real numbers $N_{\mathrm{c}} = N_{\mathrm{c}}(t)$. The simplest, almost universal, type of distribution of the energy per carrier $\mathcal{E}_{\mathrm{c}}$ of type c is into the isolated carrier at rest constitution energy $\mathcal{E}_0$, the position dependent kinetic energy $\mathcal{E}_k(\mathbf{X})$, and the position dependent sum of potential energies $\mathcal{E}_v(\mathbf{X})$ then

$$\mathcal{E}_{\mathrm{c}}(t) = \mathcal{E}_0^{\mathrm{c}} + \mathcal{E}_k^{\mathrm{c}}(\mathbf{X}) + \mathcal{E}_v^{\mathrm{c}}(\mathbf{X}) + \mathcal{E}_\Delta^{\mathrm{c}}(\mathbf{X}). \tag{1.14}$$

It is precisely this distribution (1.14) which defines the carrier for a given observer. $\mathcal{E}_0^{\mathrm{c}}$ defines the basic carrier, $\mathcal{E}_k^{\mathrm{c}}(\mathbf{X})$ the state of motion relative to the observer, and $\mathcal{E}_v^{\mathrm{c}}(\mathbf{X})$ the relation between that carrier and the rest of the system as defined by the observer. *The* $\mathcal{E}_\Delta^{\mathrm{c}}(\mathbf{X})$ *term is required to make* $\mathcal{E}_{\mathrm{c}}$ *a position independent constant, this is needed to have a meaningful definition of the carriers of type* c.

For a given carrier charge q_{c} (of type Q) an interaction field intensity $\mathbf{E}^i_{Q,\mathrm{c}}(\mathbf{X})$ contributing to the energy per carrier, can be defined from the second derivatives of the action, defined as arising from that interaction for that carrier. This second derivatives in turn may have further derivatives, with respect to space or time coordinates. The invariant definition, given that the integrated action A of a system is invariant under a space–time Lorentz transformation, would be $A = \sum_{\mathrm{c}} N_{\mathrm{c}} A_{\mathrm{c}}$, this is because $\mathcal{E}_{\mathrm{c}} = \partial A_{\mathrm{c}} / \partial t$ is not invariant but observer dependent and this imposes structural mathematical restrictions on the energy densities $\mathcal{E}_{\mathrm{c}}$ and, consequently, on $\mathcal{E}_0^{\mathrm{c}}$, $\mathcal{E}_k^{\mathrm{c}}$ and $\mathcal{E}_v^{\mathrm{c}}$. This not only because energy is a component of an invariant four–vector but also because the partition of energy among carriers has to be observer dependent.

Because the rate of change of momenta is related to the classical concept of force, these geometric features are the geometrical representation of potentials and their derivatives, the second derivatives of the action are then correctly termed strength fields or force fields.

Notice that within the concept of interaction the rates of change of action are to be expressed per unit charge and represent those contributions arising from sums over carriers other than the one under consideration. The action is to be considered as distributed among interacting carriers, and the concept of charges of the carriers is required for this purpose.

The local energy density $\mathcal{E}_c(\mathbf{x},t)$ would then be

$$\mathcal{E}_c(\mathbf{x},t) = \rho_{\mathrm{c}}(\mathbf{x},t)\mathcal{E}_{\mathrm{c}}\,(t) = \rho_{\mathrm{c}}(\mathbf{x},t)\left\{\mathcal{E}_0^{\mathrm{c}} + \mathcal{E}_k^{\mathrm{c}}(\mathbf{X}) + \mathcal{E}_v^{\mathrm{c}}(\mathbf{X}) + \mathcal{E}_\Delta^{\mathrm{c}}(\mathbf{X})\right\},$$

where usually the term $\mathcal{E}_v^{\mathrm{c}}(\mathbf{X}) = \mathcal{E}_v^{\mathrm{c}}\left\{\rho_{\mathrm{c}}(\mathbf{x},t),(\mathbf{X})\right\}$ is itself considered a functional of the density. This is fundamental in the variational definition of interaction potentials $V(x) \equiv \partial\mathcal{E}_v^{\mathrm{c}}(\mathbf{X})/\partial\rho_{\mathrm{c}}(\mathbf{x},t)$.

1.7. DYNAMICAL PROPERTIES OF THE DENSITY

Using the parametrization of the amplitude function

$$\Psi(\mathbf{x},t) = A(\mathbf{x},t)\exp[iS(\mathbf{x},t)/\hbar],$$

and the condition of a current density

$$\frac{\partial\rho}{\partial t} + \nabla\cdot\mathbf{j} = 0,$$

we can introduce the definition of $\mathbf{v}$, a velocity-like vector, such that $\mathbf{j} = \rho\mathbf{v}$ which allows writing a dynamical equation

$$\begin{aligned} m\rho\frac{d\mathbf{v}}{dt} &= -\rho\nabla(V + V_\rho), \\ \frac{d\mathbf{v}}{dt} &= \frac{\partial\mathbf{v}}{\partial t} + (\mathbf{v}\cdot\nabla)\mathbf{v}, \\ \frac{\partial\rho}{\partial t} &= -\nabla\cdot(\rho\mathbf{v}), \end{aligned}$$

again $\rho = |A|^2$, also $\mathbf{v} = \nabla S/m$ where we use the definition $V_\rho = -\hbar^2\nabla^2 A/2mA$, and

$$m\frac{\partial}{\partial t}(\rho \upsilon_\mu) = \sum_{v} \nabla_v \left\{ m\rho\upsilon_\mu \upsilon_v + \widetilde{T}^{(\rho)}_{\mu v} \right\} - \rho\nabla_\mu V,$$

defining energy-momentum-stress tensor

$$\widetilde{T}^{(\rho)}_{\mu v} = -\frac{\hbar^2}{4m}\nabla^2\rho\delta_{\mu v} + \frac{\hbar^2}{4m}\frac{\nabla_\mu\rho\nabla_v\rho}{\rho}.$$

or, from the amplitude function

$$\mathbf{u} = -i\frac{\hbar}{m}\frac{\nabla\Psi}{\Psi} = \mathbf{v} + i\mathbf{v}_i, \text{where } \mathbf{v}_i = -\frac{\hbar}{2m}\nabla\ln\rho \text{ and } \frac{d\langle\mathbf{v}\rangle}{dt} = \frac{-\langle\nabla V\rangle\,.}{m}$$

and the equation for the current

$$m\frac{d}{dt}\int \mathbf{j}(\mathbf{x})d\mathbf{x} = -\int \rho(\mathbf{x})\nabla V(\mathbf{x})d\mathbf{x}.$$

With the, by construction, condition $\langle \mathbf{x}\times\nabla V_\rho\rangle = 0$. In the non relativistic limit and in the presence of an external electromagnetic field $(\varphi, \mathbf{A})$ (see [1, 2]) and the field intensities $\mathbf{E} = -\nabla\varphi - \frac{1}{c}\frac{\partial\mathbf{A}}{\partial t}$, $\mathbf{B} = \nabla\times\mathbf{A}$

$$\frac{1}{2m}\left(-i\hbar\nabla + \frac{e}{c}\mathbf{A}\right)^2\Psi + V\Psi - e\varphi\Psi = i\hbar\frac{\partial\Psi}{\partial t},$$

$$m\rho\frac{d\mathbf{v}}{dt} + \rho\left(e\mathbf{E} + \frac{e}{c}\mathbf{v}\times\mathbf{B}\right) = -\rho\nabla(V + V_\rho),$$

to obtain a fundamental formal definition of the velocity in terms of the local action per carrier and the external vector field

$$\mathbf{v} = \frac{1}{m}\left(\nabla S + \frac{e}{c}\mathbf{A}\right).$$

Here the sum in the parenthesis is fixed but the individual terms are defined up to a gauge transformation.

2. Action Density

In this section we shall present our fundamental concepts as an Action **Density** Functional Theory and discuss the origin and consequences of the formulation of an Action **Amplitude** Function Theory.

For the study of the distribution of action we consider that:

a) In the space–time–action picture, where the basic mathematical properties of space-time are assumed to correspond to the physical space-time, the action density $\breve{\alpha}(\mathbf{x}, t)$ is inhomogeneously distributed, corresponding to the different material objects to which this action corresponds, in a possible relative motion in the spatial directions with speeds $0 \leq v \leq c$. The sets of distributions which move with relative velocities $0 \leq v < c$ with respect to a given observer are called matter-like. (**Note**: *for some particular descriptions an auxiliary time–average distribution of action* $\langle\breve{\alpha}\rangle_{av}$ *can be used, with restrictions, to account for practical or discretional lack of the knowledge of the time dependence of* $\breve{\alpha}$).

b) The matter-like energy distributions are to be considered as sources of (infinite extension, in principle) decaying deformations of action distribution of several types: first, a part A_0 uniformly decaying with distance, which observers will interpret as gravitation; second, of a collection $(A, B, C, ...)$ of vortical fields, superimposed on the A_0 part, which can be felt selectively by responses of the given internal vortices of other matter-like distributions. This second property is not given *a priori* but it is a consequence of the intrinsic nature which the desired description attributes to the objects, as developed below.

c) We introduce now a third fundamental concept: energy–momentum carriers. At a macroscopic level the energy carrier is defined by a density distribution and by the integral properties of the distribution. We shall keep this concept without considering that the distribution could be reduced to a point singularity in space (line in space–time). We shall, anyhow, use the (not very fortunate) name **carrier density** for this quantity, the main reason being that its integral will be taken to be, as mentioned above, an integer. An extra reason is the definition of identical carriers as a density in a space volume V_s such that at time $t = t'$

$$\int_{V_s} \rho_b d\mathbf{x} = n_b, \quad h \int_{\mathbf{V}_s} \partial_t a_b d\mathbf{x} = \int_{V_s} \rho_b \varepsilon_b d\mathbf{x} = n_b \varepsilon_b = E_b, \tag{2.15}$$

and $E_{t'} = \left[\sum_b E_b\right]_{t'}$ for a collection $\{b\}$ of (by practical construction) independent types of carriers. In agreement with our freedom of description we could also allow the n_b not to be integers, provided $E_{t'}$ is not changed.

2.1. CLASSIFICATION OF ACTION (ENERGY) CARRIERS

The definition of energy carrier in (2.15) is useful in general. In the development of different theories the action can be partitioned among carriers (carriers of action which we will call carriers type $\mathfrak{a}$ below). Subsequently the energy–momentum will be partitioned into the carrier fields. When interactions are considered there is the possibility of an arbitrary momentum distribution per carrier. In this case there is the additional possibility for the energy–momentum attributed to a specific carrier fields to present relative or intrinsic rotational distributions, even if non-solenoidal fields can not be directly derived from a scalar action, given that $curl(div(\breve{\alpha}(\mathbf{x}))) = 0$.

Then a second type of carriers will be those for which the energy–momentum itself is partitioned into the carrier fields. The energy distributed as in the last terms of (2.15), but allowing the momentum field to posses a rotational distribution $curl(\mathbf{p}(\mathbf{x})) \neq 0$, and by necessity $div(curl(\mathbf{p}(\mathbf{x}))) = 0$. This second type of carriers, whose definition allows a larger type of interactions, will be called carriers type $\mathfrak{b}$.

A third type $\mathfrak{c}$ of carriers has been present in the systematic development of the theory, for sets of carriers which are collectively of type $\mathfrak{b}$, even if for each carrier a further splitting of the field intensities is made which violates basic symmetries [1, 3].

The carriers of type $\mathfrak{a}$ are those considered in standard (Newtonian) mechanics and in the ordinary formulation of General Relativity where only the total energy-momentum content is considered. The carriers of type $\mathfrak{b}$ are those considered here and in standard electrodynamics where the splitting of the energy-momentum content is considered. The carriers of type $\mathfrak{c}$ are those considered in the standard model of elementary particles where symmetry breaking interactions are admissible.

2.2. The Density

The conditions to be obeyed by the analytical function carrier density $\rho_{\mathrm{c}}(\mathbf{x}, t)$ are:

D1.- $\rho_{\mathrm{c}}(\mathbf{x}, t)$ is a real quantity $\rho_{\mathrm{c}}(\mathbf{x}, t) \subset \mathbb{R}$.

D2.- The density $0 \leq \rho_{\mathrm{c}}(\mathbf{x}, t) < \infty$ in order to represent a finite amount of action.

D3.- The derivatives of the density $-\infty < \partial_\mu \rho_{\mathrm{c}}(\mathbf{x}, t) < +\infty$ in order to represent a finite amount of energy–momentum.

Theorem 1 *If* $\Psi(\mathbf{x}, t)$ *is an analytical quadratic integrable complex or multivector function, conditions D1, D2 and D3 are fulfilled identically if* $\rho_{\mathrm{c}}(\mathbf{x}, t) =$

$|\Psi_c(\mathbf{x},t)|^2$. *Here* $|f|^2$ *means the real quadratic form of any more general function* f*, even if* f *itself is not necessarily a real function and we define: if* $|f|^2 = f^+ f$ *then* $\partial_\mu |f|^2 = (\partial_\mu f^+)f + f^+(\partial_\mu f)$.

Condition D1 is fulfilled by the definition $\rho_c(\mathbf{x},t) = |\Psi_c(\mathbf{x},t)|^2$, D2 by the requirement of quadratic integrability, D3 by the definition $\partial_\mu |f|^2 = (\partial_\mu f^+)f + f^+(\partial_\mu f)$ and the analytical properties of $\Psi(\mathbf{x},t)$. It is seen that the conditions D1, D2, D3 and $\int_V \rho_c(\mathbf{x},t)d\mathbf{x} = N_c$ correspond to the $\Psi(\mathbf{x},t)$ being quadratic integrable Hilbert functions. In any Lagrangian type formulation this last definition of ρ can be used as a condition introduced via a Lagrange multiplier.

Gauge freedom

Carrier density and density of action should be gauge invariant physical quantities, thus we need to develop a procedure which can allow gauge freedom, that is, a procedure which allows for arbitrary, but correct and useful, descriptions.

Because the definition of carrier density depends on the attributed energy per carrier we can not separate the definition of the gauge, in a form compatible to the basic concept that the energy–momentum components are obtained by using the operator $i\hbar\partial_\mu$, from the definition of the carriers themselves.

The definition required by D1, D2 and D3 above $\rho_c = |\Psi_c|^2$, allows gauge independence. A set of Lagrange conditions and multipliers can be used to define the carriers and their desired properties. This procedure can be carried at any level of description, hence the universality of mathematical descriptions presented here, which in fact give a self existing status to density functional theory. There should be no confusion from the fact that $\rho_c = |\Psi_c|^2$, here proposed for density functional theory, is formally equivalent to the use of Wave Equations in Quantum Mechanics. This equivalence will be shown below to have far reaching consequences.

3. Considerations About Density Functional Theory

Density functional theory [5], in a form useful for the study of the electronic structure of atoms, molecules and condensed matter, can be systematically derived and formulated. Nevertheless in all cases hitherto, as a quantum theory, it is developed in the context of quantum mechanics and its wave functions, after considering the properties of the density operators, with particular emphasis on three aspects as follows: (a) definitions and existence theorems, (b) rules for constructing density functionals, and (c) methodology.

DFT is frequently considered then not as a fundamental theory but as an approximation scheme within Quantum Mechanics because the density functionals and some aspects of the methodology (mainly for the study of condensed matter) require the use of formal and numerical approximations. Otherwise it is a successful approach to study and describe small, medium size and large systems.

The now traditional presentation of density-functional theory states first, following Hohenberg and Kohn [6], that there is a unique functional to compute the total energy for a system with N electrons interacting with an external potential $\upsilon(x)$ (in their ground state),

$$E\left[\upsilon,\gamma\right]=E_{\upsilon}\left[\gamma\right]=F\left[\gamma\right]+\int\upsilon(\mathbf{x})\gamma(\mathbf{x},\mathbf{x})d\mathbf{x}, \tag{3.16}$$

where γ is the reduced first-order density operator, and $F\left[\gamma\right]$ is defined:

$$F\left[\gamma\right]=T\left[\gamma\right]+V_{e-e}\left[\gamma\right]. \tag{3.17}$$

$T\left[\gamma\right]$ is the kinetic-energy functional and $V_{e-e}\left[\gamma\right]$ is the total electron-electron interaction energy. Both functionals are well defined but unknown.

On the other hand, the second Hohenberg-Kohn theorem states that for whatever other approximated electron density $\gamma'\left(\mathbf{x}\right)$ the energy functional obeys the following inequality for the exact ground-state density

$$E_{\upsilon}\left[\gamma'\right]\geq E_{\upsilon}\left[\gamma\right]. \tag{3.18}$$

A variational procedure can then be proposed to find both γ and E

$$\delta\left[E_{\upsilon}\left[\gamma\right]-\mu\left(\int\gamma\left(\mathbf{x}\right)d\mathbf{x}-N\right)\right]=0, \tag{3.19}$$

where μ is a Lagrange multiplier associated with the restriction of having N particles in the system. It has been argued that this constraint is enough for the development and use of the theory, but recent evidence indicates that other constraints are needed [7, 8, 9, 10], this is in accordance with our present approach.

The one density γ can be written within the one-particle approximation, considering that for each 'particle' of the system there is at least one auxiliary function ψ_i, such that [11]

$$\gamma\left(\mathbf{x},\mathbf{x}'\right)=\sum_i n_i\left|\psi_i\left(\mathbf{x}\right)\right\rangle\left\langle\psi_i\left(\mathbf{x}'\right)\right|.$$

It is fundamental that in this approximation the total number of electrons can also be expressed as a density functional

$$N = N\left[\gamma\right] = \int \gamma\left(\mathbf{x},\mathbf{x}\right) d\mathbf{x}, \tag{3.20}$$

using the diagonal part of γ.

In the present paper the $\psi_i\left(\mathbf{x}\right)$ are precisely auxiliary functions, as defined above, with no other purpose but to define N quasi-particle states in the system.

A. Appendix

A.1. Schrödinger Amplitude Functions in START

The freedom of description of the energy-momentum partitioning is a fundamental issue in the construction of physical theories. Since at least the XIXth century an action function was introduced which was useful for this purpose, in the XXth century the de Broglie phase factor $\exp(i\triangle a/\hbar)$ [14] allowed the freedom of energy-momentum description and the use of the gauge fields. Later the concept of non-commuting gauge fields was successfully introduced to describe a larger set of energy-momentum partitioning among carriers (fundamental interactions). We follow now the Schrödinger procedure.

1. Let the Schrödinger (1926) definition $S(\mathbf{x},t)$ of action in terms of an auxiliary function $\Psi(\mathbf{x},t)$ be

$$S(\mathbf{x},t) = K\ln\Psi(\mathbf{x},t) = -K\ln\Psi^{\dagger}(\mathbf{x},t),$$

that is: action is considered a sum of terms. The action $S(\mathbf{x},t)$ is requested to correspond to the stationary states of the system to be described, this if ensured through a variational optimization procedure.

2. Let the carrier density ρ be the real quantity

$$\rho(\mathbf{x},t) = \Psi^{\dagger}(\mathbf{x},t)\Psi(\mathbf{x},t),$$

where $\rho(\mathbf{x},t)$, Ψ and $\Psi^{\dagger}$ are: unique-valued, continuous and twice-differentiable, with the condition $\rho(\mathbf{x},t)|_{\text{space boundary}} = 0$.

3. Let the canonically conjugated variables be: $(\mathbf{x},t)$ and $\Box S = iK\Box\ln\Psi = -iK\Box\ln\Psi^{\dagger}$, with, again, $\Box = e^{\mu}\partial_{\mu}$ the space-time gradient operator.

4. The local energy description be ($\mathcal{E}_0$ is not a density)

$$K^2\frac{(\Box\Psi^\dagger)\cdot(\Box\Psi)}{\Psi^\dagger\Psi}c^2=\mathcal{E}^2-(Pc)^2=(\mathcal{E}_0)^2=\left(m_0c^2\right)^2,$$

with the Lagrangian (density of energy and constrain) function

$$J=K^2(\Box\Psi^\dagger)\cdot(\Box\Psi)c^2-\left(m_0c^2\right)^2\Psi^\dagger\Psi,$$

and variationally search for the extremum energy $\mathcal{E}$ (minimum of action for a stationary state system) $\delta J=0$ to obtain from the standard variational approach

$$K^2\left[\Psi^\dagger\left(\Box^2\Psi\right)+\left(\Box^2\Psi^\dagger\right)\Psi\right]=m_0c^2\Psi^\dagger\Psi,$$

and the equation for the auxiliary function Ψ

$$K^2\Box^2\Psi=\left(m_0c^2\right)^2\Psi.$$

(In the case where an interaction is assumed to exist $(E-V)^2-(Pc-eA)^2=\left(m_0c^2\right)^2$).
From the Schrödinger variational search for the minimum of action for a stationary state system $\delta J=0$ we obtain the Schrödinger-Klein-Gordon Equation (SKG), (consider first V=A=0) it is

$$\left[K^2\left(\frac{\partial^2}{\partial t^2}-\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)c^2\right)-\left(m_0c^2\right)^2\right]\Psi=0. \qquad \text{(A.21)}$$

We must emphasize that in the relativistic (and in the non relativistic) case we obtain, through the Schrödinger optimization procedure, the Ψ (or $\Psi^\dagger$) function which minimizes the action of the system. The geometric factorization of the operator in the SKG equation transforms it into the Dirac equation. In the next section we follow an alternative procedure which illustrates directly the meaning of the components of the Schrödinger Amplitude Function.

A.2. LINEAR FORM OF THE SCHRÖDINGER-KLEIN-GORDON EQUATION

We want to express the Schrödinger-Klein-Gordon equation (SKG, A.21) in the linear form

$$\hat{H}_{linear}\psi=m_0c^2\psi. \qquad \text{(A.22)}$$

Consider the simple case of the free carrier, that is, of the equation (here $k^2 = (m_0 c/\hbar)^2$, $i^2 = -1$)

$$\frac{1}{c^2}\frac{\partial^2}{\partial t^2}\psi - \nabla^2\psi + k^2\psi = 0, \tag{A.23}$$

and write (following a procedure analog to that of Charlier, Bérard, Charlier and Fristot [13] to obtain a Schrödinger-like equation from the SKG)

$$\psi = \sum_{a=1}^{m} \phi_a, \tag{A.24}$$

$$\frac{\partial\psi}{\partial x_\mu} = \sum_{a=1}^{m} c_\mu^a \phi_a,$$

$m = 8$ in order to have a faithful representation of both definitions and the coefficients are given by the matrix

$$c_\mu^a = ik \begin{pmatrix} +1 & +1 & +1 & +1 & -1 & -1 & -1 & -1 \\ +1 & -1 & +1 & -1 & -1 & +1 & -1 & +1 \\ +1 & +1 & -1 & -1 & +1 & +1 & -1 & -1 \\ +1 & -1 & -1 & +1 & +1 & -1 & -1 & +1 \end{pmatrix},$$

with these definitions we write the 4 equations

$$\frac{\partial}{\partial x_\mu}\sum_{a=1}^{m}\phi_a = -ik\sum_{a=1}^{m} c_\mu^a \phi_a,$$

and use them in equation (A.21,A.23) to obtain:

$$\sum_\mu \frac{\partial}{\partial x_\mu}\sum_{a=1}^{8} c_\mu^a \phi_a = -ik\sum_{a=1}^{m}\phi_a,$$

which is a linear form of the energy-momentum conservation equation (A.21).

If a representation of the same relation is given through the use of a set of real 8×8 or complex 4 × 4 matrices γ^μ, [$2\mathbb{C}(2)$] we obtain the Dirac equation. The Dirac equation is thus a faithful representation of the linearized form of the Schrödinger–Klein–Gordon equation.

Observe that the fact that we can now define a d'Alembertian operator

$$\Box = \gamma^\mu \partial\mu,$$

allows the generation of a Clifford algebra representation of the full geometry of space–time through the definition

$$\gamma\left(e^{\mu}\right)=\gamma^{\mu},$$

of the matrix representation of the geometric algebra of space–time. The γ^{μ} faithfully obey the same relations as the basis vectors e^{μ}. The set of 8×8 real matrices $\gamma^{\mu}=\gamma\left(e^{\mu}\right)\subset[2\mathbb{R}(4)]$ representing the e^{μ} is, for example,

$$\gamma^0=\begin{pmatrix} &&&&1&&& \\ &&&&&1&& \\ &&&&&&1& \\ &&&&&&&1 \\ 1&&&&&&& \\ &1&&&&&& \\ &&1&&&&& \\ &&&1&&&& \end{pmatrix} \quad \gamma^2=\begin{pmatrix} &&&&&&1& \\ &&&&&&&1 \\ &&&&1&&& \\ &&&&&1&& \\ &&\text{-1}&&&&& \\ &&&\text{-1}&&&& \\ \text{-1}&&&&&&& \\ &\text{-1}&&&&&& \end{pmatrix}$$

$$\gamma^1=\begin{pmatrix} &&&&&&&1 \\ &&&&&&\text{-1}& \\ &&&&&\text{-1}&& \\ &&&&1&&& \\ &&&\text{-1}&&&& \\ &&1&&&&& \\ &1&&&&&& \\ \text{-1}&&&&&&& \end{pmatrix} \quad \gamma^3=\begin{pmatrix} &&&&1&&& \\ &&&&&1&& \\ &&&&&&\text{-1}& \\ &&&&&&&\text{-1} \\ \text{-1}&&&&&&& \\ &\text{-1}&&&&&& \\ &&1&&&&& \\ &&&1&&&& \end{pmatrix}$$

The chiral representation Dirac matrices γ^{μ} and wave function Ψ are obtained trough the mapping.

$$\begin{pmatrix}1&0\\0&1\end{pmatrix}=1,\begin{pmatrix}0&1\\-1&0\end{pmatrix}=i.$$

Representations of algebras are not unique, but they are related by similitude transformations.

A.3. The First Order Equation as a Factorization-Projection

The deduced equations which are first order in the space–time derivatives can also be analyzed as a factorization and projection procedure. Consider again the equation for the optimized function to obtain the least action state of the system of independent equivalent carriers (again $k^2=(m_0c/\hbar)^2$, $i^2=-1$)

$$\frac{1}{c^2}\frac{\partial^2}{\partial t^2}\psi - \nabla^2\psi + k^2\psi = 0, \tag{A.25}$$

and propose the factorization of the operator in the Dirac sense ($\Box = \gamma^\mu \partial\mu$)

$$(\Box + ik)(\Box - ik)\psi = (\gamma^\mu\partial\mu + ik)(\gamma^\mu\partial\mu - ik)\psi, \tag{A.26}$$

defining the projected function

$$\Psi = (\gamma^\mu\partial\mu - ik)\psi \tag{A.27}$$

which obeys, by construction, the well known Dirac equation

$$(\gamma^\mu\partial\mu + ik)\Psi = 0 \tag{A.28}$$

showing that the, **optimized to obtain the least action, complete solution of the linear equation,** auxiliary function Ψ is a non–scalar function (which depends on the representation ($\gamma(e_\mu) = \gamma^\mu$) of the geometry) containing information about the action and about the energy–momentum relationship through the $m_0 c$ and the space–time derivatives of the action.

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