The Significance of Density in
the Structure of Quantum Theories

E. Comay*

School of Physics and Astronomy
Raymond and Beverly Sackler Faculty of Exact Sciences
Tel Aviv University
Tel Aviv 69978
Israel

PACS No: 11.10.Ef, 03.70.+k, 03.65.Pm

Abstract:

It is proved that density plays a crucial role in the structure of quantum field theory. The Dirac and the Klein-Gordon equations are examined. The results prove that the Dirac equation is consistent with density related requirements whereas the Klein-Gordon equation fails to do that. Experimental data support these conclusions.
The present work reviews very briefly the first steps taken by the standard method of constructing a quantum field theory. Then, the need for a self-consistent expression for density is discussed. Later, this general analysis is examined for the specific cases of a Dirac field and of Klein-Gordon (KG) fields. The discussion contains new results proving the significant role of density in the structure of quantum field theory. Some concluding remarks follow.

Herein, units where $\hbar = c = 1$ are used. The metric is diagonal and its entries are $(1,-1,-1,-1)$. Greek indices run from 0 to 3. The subscript symbol $\mu$ denotes the partial differentiation with respect to $x^\mu$. An upper dot denotes a differentiation with respect to time. Only one kind of dimension is required for the system of units used here. Thus, dimensions of a variable are denoted by an expression of the form $[L^n]$, where the letter $[L]$, enclosed by square brackets, denotes the unit of length (and should be distinguished from the Lagrangian $L$).

A standard method of constructing a quantum field theory (see e.g. [1], Section 11.3) begins with the equation of motion of the specific field discussed

$$\hat{O}\psi = 0,$$  \hspace{1cm} (1)

where the operator $\hat{O}$ denotes the field’s equation. At this point, a Lagrangian density $L$ is defined. This Lagrangian density yields an expression for the action of the system

$$I = \int L d^4x.$$  \hspace{1cm} (2)

$L$ is defined so that an application of the variational principle to its action reproduces (1).

The Hamiltonian density can be derived from the Lagrangian density $L$. 
Thus,

\[ \mathcal{H} = \dot{\psi} \frac{\partial \mathcal{L}}{\partial \dot{\psi}} - \mathcal{L}. \]  

(3)

A spatial integration of (3)

\[ H = \int \mathcal{H} d^3x \]  

(4)
yields the Hamiltonian for the field equation (1).

An alternative and equivalent procedure can be taken. In this case, the Lagrangian \( L \) is obtained as the spatial integral of the Lagrangian density \( \mathcal{L} \) and the Hamiltonian is derived from this Lagrangian. These alternatives are equivalent and, as shown below, both require a self-consistent expression for density.

These steps provide the basis for other steps taken for accomplishing the structure of the theory. The objective of this work is to analyze the physical meaning of the operations that begin with (1) and end with (4). The structure of (1) can be treated in a mathematical sense as an eigenfunction/eigenvalue problem. The following analysis aims to show how expressions obtained along the way from (1) to (4) acquire physical meaning and physical constraints as well.

The left hand side of (2) is dimensionless. Therefore, since the dimension of \( d^4x \) is \( [L^4] \), one concludes that the dimension of the Lagrangian density \( \mathcal{L} \) is \( [L^{-4}] \). It follows that the form of the operator \( \hat{O} \) of (1) boils down to the Lagrangian density and affects the dimension of the wave function. Thus, one realizes that the construction of the Lagrangian density changes the meaning of the wave function: in (1) it is a complex mathematical function whereas in the Lagrangian density it acquires dimensions. This point is used below in an analysis of two specific cases, the Dirac field and the Klein-Gordon fields.

Now let us turn to the integral (4) where the Hamiltonian \( H \) is obtained
from the Hamiltonian density $\mathcal{H}$. For this end, the form of the Lagrangian density $\mathcal{L}$ should be examined. Since the operator $\hat{O}$ is independent of the wave function, one finds from the Euler-Lagrange equation

$$
\frac{\partial}{\partial x} \frac{\partial \mathcal{L}}{\partial \psi_{,\mu}} - \frac{\partial \mathcal{L}}{\partial \psi} = 0
$$

(5)

that the Lagrangian density is a quadratic (or bilinear) function of the wave function $\psi$. Evidently, the equation of motion (1) retains its form if one multiplies the Lagrangian density $\mathcal{L}$ by a numerical factor. On the other hand, the Hamiltonian (4) represents energy and, for a given system, it should have a specific eigenvalue.

This problem is settled by means of a normalization procedure where the wave function $\psi$ is multiplied by a normalization factor which guarantees that the integral (4) takes the correct value. Thus, there is a need for a physically selfconsistent expression for density.

Now, the integral of density is a Lorentz scalar, because the particle is found in all Lorentz frames. Hence, one may take the requirements for particle density from electrodynamics where an expression for charge density is readily found (see [2], pp. 69-73). Thus, in a quantum theory, density must satisfy the following requirements:

A. The dimension of density is $[L^{-3}]$.

B. Density is the 0-component of a 4-vector $j^\mu$.

C. This 4-vector satisfies the continuity equation

$$
j_{,\mu}^\mu = 0.
$$

(6)

These points are known for a very long time. Here they are used in an analysis of the Dirac and the KG fields. In particular, a new aspect of
these requirements is shown here. Thus, it is proved that requirements A-C are necessary, but not sufficient, conditions for constructing a self-consistent expression for density of a quantum field theory.

Let us begin with an analysis of the Dirac field. Here, the matter part of the Lagrangian density is (see [1], p. 84)

\[ \mathcal{L} = \bar{\psi} \left( \gamma^{\mu} \left( i \partial_{\mu} - e A_{\mu} \right) - m \right) \psi, \]  

(7)

As is well known, a 4-current is defined for the Dirac field

\[ j^{\mu} = \bar{\psi} \gamma^{\mu} \psi. \]  

(8)

This 4-current satisfies requirements A-C. The density of (8)

\[ \rho = \bar{\psi} \gamma^{0} \psi = \psi \dagger \psi \]  

(9)

has been used recently (see [3], Section 2) in an analysis of the Dirac field. The results are:

1. The conserved 4-current depends on \( \psi \) and on the corresponding \( \bar{\psi} \), and is independent of the external field \( A_{\mu} \). Hence, one can use the positive definite density \( \psi \dagger \psi \) and construct an orthonormal basis for the Hilbert space of solutions. This basis is not affected by changes of external quantities.

2. The Dirac Hamiltonian operator is easily extracted from the Hamiltonian density and is free of \( \psi, \bar{\psi} \) and their derivatives. An examination of the fundamental quantum mechanical equation

\[ H \psi = i \frac{\partial \psi}{\partial t}. \]  

(10)

proves that this property is consistent with the linearity of quantum mechanics and with the superposition principle as well.
3. Since the Dirac Lagrangian density is linear in the time-derivative $\partial \psi / \partial t$, the corresponding Hamiltonian density does not contain derivatives of $\psi$ with respect to time. The same is true for the Hamiltonian differential operator which is extracted from the Hamiltonian density. Hence, in the case of a Dirac particle, the fundamental quantum mechanical relation (10) takes the standard form of an explicit first-order partial differential equation. Here a derivative with respect to time is equated to an expression which is free of time derivatives. This property does not hold for Hamiltonians that depend on time derivative operators.

4. If the Dirac Hamiltonian is substituted into (10) then one finds that it agrees completely with the Dirac equation obtained as the Euler-Lagrange equation of the Lagrangian density of the Dirac field. This property means that the Dirac’s Euler-Lagrange equation does not impose additional restrictions on the Hamiltonian’s eigenfunctions and on their corresponding eigenvalues.

5. The term $e A^\mu$ of the Dirac Hamiltonian correctly represents electromagnetic interactions.

These results prove that the construction of the Dirac Hamiltonian proceeds in a straightforward manner and that self-consistent expressions are obtained. It is shown below that results of the KG field are inconsistent with points 1-5 above.

Now let us turn to the KG equation. Here one finds two kinds of fields: one kind of fields uses complex wave functions and the second kind uses real wave functions. The former is used for describing charged KG particles and the latter is used in the Yukawa Lagrangian density. The discussion begins
with the complex fields.

The Lagrangian density of the complex KG fields can be found in Section 3 of [4] (The following expressions are written in units where \( \hbar = c = 1 \))

\[
\mathcal{L} = (\phi^*_0 - ieV\phi^*)(\phi_{,0} + ieV\phi) - \sum_{k=1}^{3} (\phi^*_k + ieA_k\phi^*)(\phi_{,k} - ieA_k\phi) - m^2\phi^*\phi. \tag{11}
\]

Here, as usual, the symbol \( \phi \) denotes the KG wave function. \( V \) and \( A_k \) denote the scalar and the vector potentials, respectively. Using, methods which have become standard, the Authors of [4] obtain the Hamiltonian density

\[
\mathcal{H} = (\phi^*_0 - ieV\phi^*)(\phi_{,0} + ieV\phi) + \sum_{k=1}^{3} (\phi^*_k + ieA_k\phi^*)(\phi_{,k} - ieA_k\phi) + m^2\phi^*\phi. \tag{12}
\]

A 4-current is obtained for this theory and it is shown that it satisfies requirements A-C obtained earlier in this work. Thus, the density of this 4-current is (see eq. (42) therein)

\[
\rho = i(\phi^*\phi_{,0} - \phi^{*}_{,0}\phi) - 2eV\phi^*\phi. \tag{13}
\]

and the corresponding 3-current is (see eq. (43) therein)

\[
\mathbf{j} = i((\nabla\phi^*)\phi - \phi^*\nabla\phi) - 2e\mathbf{A}\phi^*\phi. \tag{14}
\]

An examination of the Hamiltonian density (12) reveals an alarming aspect. Thus, (12) contains time derivatives of the wave function. It follows that if a Hamiltonian can be constructed then the Hamiltonian density is expressed in terms of the Hamiltonian whereas in (4) the Hamiltonian is expressed in terms of the Hamiltonian density. Certainly, this is an undesirable situation. However, it is proved below such a Hamiltonian does not exist.

The problem of extracting a covariant differential operator for the Hamiltonian of the complex KG field is discussed in Section 3 of [3], where it is proved that this task cannot be accomplished. The proof examines the highest time derivatives of \( \phi^* \), \( \phi \) in the Hamiltonian density (12) and in the
density (13). For (12) one finds a symmetric expression $\phi^*_{0}\phi_{0}$ whereas the density (13) contains the antisymmetric term $\phi^*\phi_{0} - \phi^*_{0}\phi$. Using self-evident arguments, one infers from these properties that there is no covariant differential operator for the complex KG equation. This conclusion is consistent with the contents of the available literature.

Let us turn now to the problem of constructing a Hamiltonian matrix of the KG equation. Here one should define a self-consistent inner product $(\phi^*_i, \phi_j)$ for the Hilbert space and construct an appropriate orthonormal basis. This basis is used in a calculation of the Hamiltonian matrix elements. Hence, the density expression (13) must be used. It is proved below that such an inner product cannot be constructed for the complex KG field.

Consider 2 states of a positively charged particle written in spherical polar coordinates

$$\phi_0(t, r, \theta, \varphi) = e^{i\omega_0 t} f_0(r) Y_{00}(\theta, \varphi),$$
$$\phi_1(t, r, \theta, \varphi) = e^{i\omega_1 t} f_1(r) Y_{10}(\theta, \varphi).$$

where $Y_{lm}$ are the ordinary spherical harmonics (see [5], pp. 510, 511). The radial functions $f_i(r)$ belong to the lowest energy of the corresponding angular momentum. Hence, they do not change sign and $f_i(r) \geq 0$. Using the expression for density (13), one examines the inner product of these functions in the case where the external potential $V$ vanishes. In this case, one finds that the density is

$$\rho = i(\phi^*_0\phi_{1,0} - \phi^*_0\phi_{1})$$

Substituting (15) and (16) into the density (17) and performing the integration, one finds

$$\int (\omega_0 + \omega_1) \phi_0(t, r, \theta, \varphi)\phi_1(t, r, \theta, \varphi)r^2 sin(\theta) dr d\theta d\phi = 0,$$
where the null result is obtained from the orthogonality of the spherical harmonics $Y_{00}(\theta, \varphi)$ and $Y_{10}(\theta, \varphi)$.

Now, let us examine these states in the case where an external positively charged particle moves towards the origin along the z-axis and $z > 0$. Hence, in this case, the external potential $V$ varies in space-time and so does the density (13). Substituting the new expression for the density into the integral (18), one finds after a straightforward calculation that the orthogonality of $\phi_0$ and $\phi_1$ is destroyed. Indeed, the contribution of the last term of (13) to the inner product is

$$U = \int -2e^{\phi_0(t, r, \theta, \varphi)} V \phi_1(t, r, \theta, \varphi) r^2 \sin(\theta) dr d\theta d\varphi$$

(19)

Let us examine the integrand at two volume elements defined at points $P_1(r, \theta, \varphi)$ and $P_2(r, \pi - \theta, \varphi)$, where $\theta < \pi/2$. The product $\phi_0 \phi_1$ changes sign at $P_1, P_2$. On the other hand, $V(r, \theta, \varphi) > V(r, \pi - \theta, \varphi)$. Hence, $U \neq 0$ and the inner product is destroyed.

This result proves that it is impossible to construct a self-consistent inner product for the Hilbert space of complex KG functions. It follows that a Hamiltonian matrix cannot be constructed for this field.

This discussion completes the proof that the complex KG field has no self-consistent expression for density and that its Hamiltonian cannot be constructed. Another result is that requirements A-C are only necessary conditions for a physically self-consistent expression for density of a quantum field. Indeed, the 4-vector whose entries are (13) and (14) satisfies requirements A-C (see Section 3 of [4]) but it is physically unacceptable.

Let us turn to the case of the real KG field. Using the results of the complex KG equation, one concludes that, in this case, there is no expression for density. Indeed, substituting $\phi^* = \phi$ in (13), and remembering that a real
KG field cannot carry charge, one finds that the density of a real KG field vanishes identically [6].

The foregoing discussion can be used for a derivation of another discrepancy of the KG equation. Here the dimension of the field function is examined. Thus, in the Lagrangian density of the Dirac field (7), the dimension of the operator is \([L^{-1}]\). Hence, since the dimension of the Lagrangian density is \([L^{-4}]\), one finds that the dimension of the Dirac field function is \([L^{-3/2}]\). On the other hand, the dimension of the operator in the KG Lagrangian density is \([L^{-2}]\). Hence, the dimension of the KG field function is \([L^{-1}]\). Therefore, it is concluded that the nonrelativistic limit of the KG equation disagrees with the Schroedinger equation, because here \(\psi^*\psi\) represent density (see [7], p. 54) and \(\psi\) has the dimension \([L^{-3/2}]\).

An examination of contemporary textbooks on quantum field theory indicates that, at least in the case of the KG equation, the validity of a density expression is generally taken for granted when the Hamiltonian is derived from the Hamiltonian density (see e.g. [1], p. 26; [8], pp. 21, 22; [9], pp. 16-19 etc.). This work proves that density plays a significant role in the structure of quantum theories and that it deserves an appropriate discussion in textbooks.

The issues of the Dirac and the KG equations has a long history of debates. In particular, Dirac maintained his opinion stating that the KG equation has no physical merits (see [8], pp. 7, 8 and [10]). Other people have adopted a different opinion and most (if not all) of contemporary textbooks discuss the KG field as a physically meaningful field. For the most of the time elapsed, this controversy was based on pure theoretical arguments. This situation has changed during the last decades because new experimental data have been accumulated. Thus, the KG field function \(\phi\) depends on a single
set of space-time coordinates. Hence, like the Dirac field $\psi$, it describes a
structureless pointlike particle. Now, experimental data tell us that unlike
Dirac particles (electrons, muons, quarks etc.), the existence of pointlike KG
particles has not been established. In particular, it is now recognized that $\pi$
mesons, which are regarded as the primary example of a KG particle, contain
a pair of quark and antiquark and are not pointlike particles.

This state of affairs help people take the right course and seek for theo-
retical arguments that explain why Nature is so unkind to the KG theory.
References:

* Email: elic@tauphy.tau.ac.il
  Internet site: http://www-nuclear.tau.ac.il/~elic

[1] J. D. Bjorken and S.D. Drell, *Relativistic Quantum Fields* (McGraw-Hill, New York, 1965).

[2] L. D. Landau and E. M. Lifshitz, *The Classical Theory of Fields* (Pergamon, Oxford, 1975).

[3] E. Comay, Apeiron 12, no. 1, 26 (2005).

[4] W. Pauli and V. Weisskopf, Helv. Phys. Acta, 7, 709 (1934). English translation: A. I. Miller *Early Quantum Electrodynamics* (University Press, Cambridge, 1994). pp. 188-205.

[5] A. de-Shalit and I. Talmi, *Nuclear Shell Theory* (Academic, New York, 1963).

[6] V. B. Berestetskii, E. M. Lifshitz and L. P. Pitaevskii *Quantum Electrodynamica* (Pergamon, Oxford, 1982). (See middle of p. 42.)

[7] L. D. Landau and E. M. Lifshitz, *Quantum Mechanics* (Pergamon, London, 1959).

[8] S. Weinberg, *The Quantum Theory of Fields* (University Press, Cambridge, 1995). Vol. 1.

[9] M. E. Peskin and D. V. Schroeder, *An Introduction to Quantum Field Theory* (Addison-Wesley, Reading, Mass., 1995).

[10] P. A. M. Dirac *Mathematical Foundations of Quantum Theory*, Editor A. R. Marlow (Academic, New York, 1978). (See pp. 3,4).