

The Significance of Density in the Structure of Quantum Theories

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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.

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1. Introduction

The simplest state of a massive particle is probably the state where it is motionless and free of interaction with external fields.

Information about the particle's position abides by the quantum mechanical uncertainty relations. Hence, the particle is located within a certain volume and an expression for its density is required for a quantum mechanical description of its state. Since wave functions of the Hilbert space are used in the Fock space, one concludes that this requirement also holds for quantum field theory.

A related issue is the description of such a state in quantum field theory. Thus, let us review 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^μ . 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 dimension of length (and should be distinguished from the Lagrangian L).

A standard method of constructing a quantum field theory (see e.g. Bjorken et al. 1965, Section 11.3) begins with the equation of motion of the specific field discussed

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

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

$$I = \int \mathcal{L} d^4x. \quad (2)$$

\mathcal{L} is defined so that an application of the variational principle to its action reproduces the equations of motion (1).

The Hamiltonian density can be derived from the Lagrangian density \mathcal{L} . Thus,

$$\mathcal{H} = \dot{\psi} \frac{\partial \mathcal{L}}{\partial \dot{\psi}} - \mathcal{L}. \quad (3)$$

A spatial integration of (3)

$$H = \int \mathcal{H} d^3x \quad (4)$$

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 procedures taken for accomplishing the final form of the theory's structure. 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.

2. The Physical Aspect of the Procedure

In the system of units used here $\hbar = 1$ and the action on 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 outcome and its consequences are 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

$$\frac{\partial}{\partial x^\mu} \frac{\partial \mathcal{L}}{\partial \psi_{,\mu}} - \frac{\partial \mathcal{L}}{\partial \psi} = 0 \quad (5)$$

that the Lagrangian density is a quadratic (or bilinear) function of the wave function ψ . 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 the well known normalization procedure where the wave function ψ 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 frames. Hence, one may take the requirements for particle density from electrodynamics where an expression for charge density is readily found (see Landau et al. 2005). 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^μ .
- C. This 4-vector satisfies the continuity equation

$$j^\mu_{,\mu} = 0. \quad (6)$$

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.

3. The Dirac Field

Let us begin with an analysis of the Dirac field. Here, the matter part of the Lagrangian density is (see Bjorken et al. 1965, p. 84)

$$\mathcal{L} = \bar{\psi}[\gamma^\mu(i\partial_\mu - eA_\mu) - m]\psi, \quad (7)$$

The Hamiltonian density is derived from the Lagrangian density (7) by the well known relation (see Bjorken et al. 1965, p. 87)

$$\begin{aligned}\mathcal{H} &= \sum \psi_{,0} \frac{\partial \mathcal{L}}{\partial \psi_{,0}} - \mathcal{L} \\ &= \psi^\dagger [\boldsymbol{\alpha} \cdot (-i\nabla - e\mathbf{A}) + \beta m + eV] \psi,\end{aligned}\quad (8)$$

where the summation runs on $\psi_{,0}$ and $\bar{\psi}_{,0}$. (Note that $\bar{\psi}_{,0}$ is not found in (7).) As is well known, a 4-current is defined for the Dirac field

$$j^\mu = \bar{\psi} \gamma^\mu \psi. \quad (9)$$

This 4-current satisfies requirements A-C. The density of (9) is

$$\rho = \bar{\psi} \gamma^0 \psi = \psi^\dagger \psi. \quad (10)$$

This expression has been used recently (see Comay 2005, Section 2) in an analysis of the Dirac field. The results are:

1. The conserved 4-current depends on ψ and on the corresponding $\bar{\psi}$, and is independent of the external field A_μ . 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. Since the Dirac Lagrangian density (7) is *linear* in the time-derivative $\partial\psi/\partial t$, the corresponding Hamiltonian density (8) does not contain derivatives of ψ with respect to time. The same is true for the Hamiltonian differential operator which is extracted from the Hamiltonian density. Thus,

one removes the particle's density $\psi^\dagger\psi$ from the Hamiltonian density (8) and obtains the Dirac Hamiltonian in the form of a differential operator

$$H = \boldsymbol{\alpha} \cdot (-i\nabla - e\mathbf{A}) + \beta m + eV \quad (11)$$

3. The Dirac Hamiltonian operator is free of ψ , $\bar{\psi}$ and of their derivatives. Let us substitute it in the fundamental quantum mechanical equation

$$H\psi = i\frac{\partial\psi}{\partial t}. \quad (12)$$

This expression is consistent with the linearity of quantum mechanics and with the superposition principle as well. Hence, in the case of a Dirac particle, the fundamental quantum mechanical relation (12) 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 (11) is substituted into (12) 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 (see Comay 2005, Section 2). 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 eA^μ 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 1-3, 5 above. (The KG fields do not also satisfy point 4 above. However, this aspect is not directly related to density. Hence, it is not discussed below.)

4. The Klein-Gordon Fields

Now let us turn to the KG equation. Here one finds two kinds of fields: one kind 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 is (see Pauli et al. 1934, section 3)

$$\mathcal{L} = (\phi_{,0}^* - ieV\phi^*)(\phi_{,0} + ieV\phi) - \sum_{k=1}^3 (\phi_{,k}^* + ieA_k\phi^*)(\phi_{,k} - ieA_k\phi) - m^2\phi^*\phi \quad (13)$$

(The quoted expressions are rewritten in units where $\hbar = c = 1$.) Here, as usual, the symbol ϕ denotes the KG wave function. V and A_k denote the scalar and the vector potentials, respectively. Using, methods which have become standard, Pauli et al. (1934,

section 3) obtain the following Hamiltonian density

$$\mathcal{H} = (\phi_{,0}^* - ieV\phi^*)(\phi_{,0} + ieV\phi) + \sum_{k=1}^3 (\phi_{,k}^* + ieA_k\phi^*)(\phi_{,k} - ieA_k\phi) + m^2\phi^*\phi \quad (14)$$

A 4-current is obtained for this theory and it is shown by Pauli et al. (1934, section 3) that it satisfies requirements A-C which can be found above, near the end of Section 2. Thus, the density of this 4-current is (see eq. (42) therein)

$$\rho = i(\phi^*\phi_{,0} - \phi_{,0}^*\phi) - 2eV\phi^*\phi. \quad (15)$$

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

$$\mathbf{j} = i((\nabla\phi^*)\phi - \phi^*\nabla\phi) - 2e\mathbf{A}\phi^*\phi. \quad (16)$$

It turns out that (15) may be either positive or negative. Hence, it is usually called "charge density".

An examination of the Hamiltonian density (14) reveals an alarming aspect. Thus, (14) 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 that such a Hamiltonian does not exist.

The problem of extracting a covariant differential operator for the Hamiltonian of the complex KG field is discussed (Comay 2005, Section 3). It is proved there that this task cannot be accomplished. The proof examines the highest time derivatives of ϕ^* , ϕ in the Hamiltonian density (14) and in the density (15).

For (14) one finds the product $\phi_{,0}^*\phi_{,0}$ which is *symmetric* with respect to ϕ, ϕ^* , whereas the density (15) contains the *antisymmetric* term $\phi^*\phi_{,0} - \phi_{,0}^*\phi$. Using self-evident arguments, one infers from these properties that *for the complex KG field, there is no covariant differential operator representing the Hamiltonian*. 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 (ϕ_i^*, ϕ_j) for the Hilbert space and construct an appropriate orthonormal basis. This basis is used in a calculation of the Hamiltonian's matrix elements. Hence, the density expression (15) 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

$$\phi_0(t, r, \theta, \varphi) = e^{-i\omega_0 t} f_0(r) Y_{00}(\theta, \varphi), \quad (17)$$

$$\phi_1(t, r, \theta, \varphi) = e^{-i\omega_1 t} f_1(r) Y_{10}(\theta, \varphi). \quad (18)$$

where Y_{lm} are the ordinary spherical harmonics (see de-Shalit et al. 1963). The radial functions $f_i(r)$ belong to the lowest energy of the corresponding angular momentum. Hence, they do not change sign (Bransden et al. 2000) and $f_i(r) \geq 0$. Using the expression for density (15), one examines the inner product of these functions in the case where the external potential V vanishes. In this case, one finds for the density operator

$$\rho = i(\phi_0^*\phi_{1,0} - \phi_{0,0}^*\phi_1). \quad (19)$$

Substituting (17) and (18) into the density (19) and performing the integration, one finds

$$\int (\omega_0 + \omega_1) \phi_0(t, r, \theta, \varphi) \phi_1(t, r, \theta, \varphi) r^2 \sin(\theta) dr d\theta d\phi = 0, \quad (20)$$

where the null result is obtained from the orthogonality of the spherical harmonics $Y_{00}(\theta, \varphi)$ and $Y_{10}(\theta, \varphi)$. Hence, ϕ_0 and ϕ_1 are orthogonal in the Hilbert space.

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 (15). Substituting the new expression for the density into the integral (20), one finds after a straightforward calculation that the orthogonality of ϕ_0 and ϕ_1 is destroyed. Indeed, the contribution of the last term of (15) to the inner product is

$$U = \int -2e\phi_0(t, r, \theta, \varphi) V \phi_1(t, r, \theta, \varphi) r^2 \sin(\theta) dr d\theta d\phi \quad (21)$$

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 $\theta < \pi/2$. At these points the product $\phi_0\phi_1$ takes the same absolute value but its sign changes (because Y_{10} contains the factor $\cos(\theta)$ and Y_{00} is independent of θ). On the other hand, $V(r, \theta, \varphi) > V(r, \pi - \theta, \varphi)$, because the distance from the approaching charge to P_1 is smaller than that of P_2 . Hence, in (21) the contribution of the $z > 0$ half of the entire space is not compensated by that of the $z < 0$ half and $U > 0$. This result is inconsistent with the null value obtained in (20). This example demonstrates that in

the case of a complex KG charged field, the inner product of the Hilbert space is destroyed.

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

This discussion completes the proof showing 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 (mentioned near the end of Section 2) are only necessary conditions for a physically self-consistent expression for density of a quantum field. Indeed, the 4-vector whose entries are (15) and (16) satisfies requirements A-C (see Pauli et al. 1934, section 3) but it is proved above that this 4-vector 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 (15), and remembering that a real KG field cannot carry charge, one finds that the density of a real KG field vanishes identically (Berestetskii et al. 1982).

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 (Landau et al. 1959) and ψ has the dimension [$L^{-3/2}$].

5. Conclusions

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. Bjorken et al. 1965, p. 26; Weinberg 1995, pp.21, 22; Peskin et al. 1995, 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.

Another aspect of this matter is that, in principle, a massive particle can be in a motionless state and a physical theory should be able to describe its location. (This argument does not hold for photons, which are massless particles.) A quantum mechanical theory of a massive particle accomplishes this requirement by means of a self-consistent expression for density. Since wave functions of the Hilbert space are elements of the Fock space, one concludes that this requirement also holds for quantum field theory.

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 Weinberg 1995, pp. 7, 8 and Dirac 1978). 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 ϕ depends on a single set of space-time coordinates. Hence, like the Dirac field ψ , 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 π 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 helps people take the right course and seek for theoretical arguments that explain why experimental data do not support the existence of KG particles.

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