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On the Crucial Role of the Variational Principle in Quantum Theories

Eliahu Comay

Charactell Ltd., Tel-Aviv, Israel Email: elicomay@post.tau.ac.il

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Abstract

The paper shows that the variational principle serves as an element of the mathematical structure of a quantum theory. The experimentally confirmed properties of the corpuscular-wave duality of a quantum particle are elements of the analysis. A Lagrangian density that yields the equations of motion of a given quantum theory of a massive particle is analyzed. It is proved that if this Lagrangian density is a Lorentz scalar whose dimension is $\begin{bmatrix} L^4 \end{bmatrix}$ then the associated action consistently defines the required phase of the quantum particle. The $\begin{bmatrix} L^4 \end{bmatrix}$ dimension of this Lagrangian density proves that also the quantum function $\psi(x^\mu)$ has dimension. This result provides new criteria for the acceptability of quantum theories. An examination of the first order Dirac equation demonstrates that it satisfies the new criteria whereas the second order Klein-Gordon equation fails to do that.

Keywords

Quantum Theories, Lagrangian Density, Corpuscular-Wave Duality, Dimension of the Quantum Function, The Correspondence Principle

1. Introduction

A physical theory has two primary elements: it has a self-consistent mathematical structure and it describes adequately data which are obtained from experiments that are included in the theory's domain of validity. The present work concentrates on the mathematical structure of quantum theories of electromagnetic interactions. Like any other physical theory, it takes few experimental data as elements that the theory must satisfy. The discussion shows that these requirements lead to a quite unique mathematical structure of the theory. The results provide another example

of Wigner's well known statement about *the unreasonable effectiveness of mathematics in the natural sciences* [1].

Special relativity is a well established theory. In particular, modern accelerators produce particles whose velocity is very close to the speed of light. The design of these machines and the data which are obtained from them are consistent with the laws of special relativity. It means that accelerators provide an astronomical number of experimental tests which are consistent with special relativity. Therefore, it is assumed here that the required quantum theory must take a relativistic covariant form.

This work aims to derive the structure of a quantum theory of an *elementary massive* particle. Historically, the first purpose of quantum theories was to describe experimental data of the electron. As a matter of fact, the electron is the most well-known elementary massive particle and it provides many kinds of experimental data. Hence, the ample electronic data enable to carry out many different tests of the validity of its quantum theory. This issue is very useful because a physical theory becomes unacceptable if it is inconsistent with even one kind of well established experiment that is included within its domain of validity.

Physical principles play an important role in the search for new physical theories because they provide general requirements that should be satisfied by any new theoretical candidate. The title of this work indicates that it discusses the variational principle. The correspondence principle is also used in the following discussion and the meaning of this principle is explained before it is applied.

Units where $\hbar=c=1$ are used. Greek indices run from 0 to 3 and Latin indices run from 1 to 3. The metric is diag. (1, -1, -1, -1). Relativistic expressions are written in the standard notation. Square brackets $[\]$ denote the dimension of the enclosed expression. In a system of units where $\hbar=c=1$ there is just one dimension, and the dimension of length, denoted by $[\ L\]$, is used. In particular, energy and momentum take the dimension $[\ L^{-1}\]$ and the electric charge is a dimensionless pure number. The value of the electron's charge is $e^2 \simeq 1/137$. The second section discusses hierarchical relations between physical theories and the significance of the correspondence principle. The role of the variational principle in the structure of quantum theories is explained in the third section. The experimental information used in the analysis is shown in the fourth section. The fifth section proves the validity of a new reason for the need of the variational principle. The sixth section describes specific results which are derived from the variational principle. The last section contains concluding remarks.

2. Hierarchical Relationships between Physical Theories

An essential feature of an acceptable physical theory is the existence of a domain of validity where the theory describes properly experimental results. For example,

it is well known that Newtonian mechanics yields good predictions in cases where the particles' velocity is much smaller than the speed of light and if quantum effects can be ignored. These restrictions define the domain of validity of Newtonian mechanics.

The founders of quantum mechanics have recognized that the classical limit of quantum mechanics should be consistent with classical physics. And indeed, a proof showing that the classical limit of quantum mechanics agrees with classical physics was published in 1927 (see the Ehrenfest theorem in [2], pp. 25-27, 136-138). This matter can be found in many textbooks. For example: "classical mechanics must therefore be a limiting case of quantum mechanics" (see [3], p. 84). A general discussion of this topic is presented in pp. 1-6 of [4].

Let A,B denote two physical theories and D_A,D_B denote their domain of validity, respectively. If $D_A \subset D_B$ then these domains of validity can be used for a definition of hierarchical relationships between A,B. It means that theory B is good in A cases where theory A is good, but not vice versa. In this case the rank of theory B is higher than that of theory A. For example, the rank of special relativity is higher than that of Newtonian mechanics.

Generally the hierarchical relationship between two theories is obtained in cases where D_A is relevant to a limit of a certain variable. For example, the domain of validity of Newtonian mechanics is relevant to the limit $v_i \rightarrow 0$, where v_i is the velocity of the ith particle. In this case, formulas of special relativity boil down to corresponding formulas of Newtonian mechanics. The domain of validity of Newtonian mechanics holds not only for the case where $v_i = 0$ because the continuity of expressions indicates that if $v_i \ll c$ then errors of Newtonian mechanics are smaller than measurements' errors and this theory is acceptable. The limit process used for the definition of D_A means that the correspondence between theories A, B relies on a solid mathematical basis.

The relationship $D_A \subset D_B$ means that theory B has a more profound meaning than that of theory A. However, the merits of theory A should not be underestimated because an appropriate limit of expressions of theory B must be consistent with the corresponding expressions of theory A. It means that theory A provides theoretical constraints on the acceptability of theory B. These constraints are useful in an examination of the acceptability of new theoretical ideas. They are related to a certain limit of a variable that defines the domains of validity of the two theories. Therefore, these constraints belong to the mathematical structure of the theories.

The hierarchical relationships between the following quantum theories are discussed in this work: non-relativistic quantum mechanics (QM), relativistic quantum mechanics (RQM) and quantum field theory (QFT). Here the hierarchical rank of RQM is higher than that of QM because QM is restricted to cases where the particles' velocity v_i (or in a quantum parlance p_i/m_i) is much smaller than the speed of light. RQM is restricted to cases where the number of particles can be regarded as a constant of the motion whereas QFT

discusses cases where additional particle-antiparticle pairs are included in the system. For example, experiments show that a non-negligible probability of the existence of quark-antiquark pairs is found in the proton (see [5], p. 282). Therefore, QFT should be used for a description of the proton structure. **Figure 1** illustrates the hierarchical relations between these theories. Here the domains of validity of the three theories are represented by the corresponding rectangles which satisfy the following relations $QM \subset RQM \subset QFT$.

The relationships between QFT and QM is recognized in the literature. For example: "First, some good news: quantum field theory is based on the same quantum mechanics that was invented by Schroedinger, Heisenberg, Pauli, Born, and others in 1925-26, and has been used ever since in atomic, molecular, nuclear and condensed matter physics" (see [6], p. 49). In this work, these constraints are called Weinberg correspondence principle.

In the physical literature the relationship between QM and classical physics is sometimes called the Bohr correspondence principle (see [2], p. 4). The philosophical literature discusses general aspects of the correspondence between theories and this topic is called the generalized correspondence principle [7].

3. The Role of the Variational Principle in Quantum Theories

Items of the following list mention briefly examples that point out the relevance of the variational principle, its Lagrangian density \mathcal{L} and the associated action \mathcal{S} to quantum theories. These items are not new and it is shown here that they can be found in textbooks. Furthermore, the variational principle has a mathematical structure and it means that one can prove the correctness of these items.

- The variational principle is used in a demonstration of the consistence of the classical limit of quantum mechanics with classical physics (see e.g. [3], section 32; [8], pp. 19-21).
- The discussions in the previous references also show that in the classical limit, the wave function of a quantum particle takes the following form

$$\psi = Ae^{iS/\hbar}, \tag{1}$$

where *S* is the action of the given Lagrangian. In the units used herein $\hbar = 1$ and it can be removed from (1).

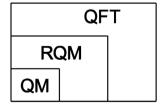


Figure 1. A chain of three rectangles that represent domains of validity of three quantum theories, respectively. The figure shows that a smaller rectangle is included in a larger rectangle (see text).

- An application of the Lagrangian that is used in the variational principle yields a definition of canonical momenta, where each of which is related to a generalized coordinates (see e.g. [9], p. 16). It can be shown that the Poisson brackets of a classical Hamiltonian and a dynamical variable correspond to an appropriate commutation relations of quantum mechanics (see e.g. [3], section 21; [8], pp. 26-28).
- The Noether theorem (see [10]) proves that a conservation law of a physical quantity corresponds to an appropriate invariance of the Lagrangian with respect to a certain transformation. Analogous relations are found for the Lagrangian density of QFT (see [6], pp. 306-314; [11], pp. 17-22).
- Relativistically covariant QFT equations are obtained from a Lagrangian density that is a Lorentz scalar (see [6], p. 300). This property emphasizes the significance of this kind of Lagrangian density.
- The variational principle is also used in other fields of physics. For example, textbooks prove that Newtonian mechanics can be derived from this principle (see [9, 12]).

The main objective of this work is to show that the foregoing items do not cover all aspects of the relevance of the variational principle to quantum theories. Consequences of the new applications of the variational principle are discussed.

4. Experimental Elements Used in the Analysis

The following fundamental experimental data are a combination of two features of a quantum particle. Some experiments show that it has corpuscular properties whereas other experiments show that it has wave properties (see [2], pp. 1-3; [13] p. 59). The combination of these properties is called corpuscular-wave duality. In classical physics this duality is a contradiction. Indeed, in classical physics an elementary particle is point-like (see [14], pp. 46-47) whereas a wave has a spatial distribution. Therefore, a new theory which is consistent with this duality is required.

The following discussion shows how these requirements lead to the structure of quantum theories. In particular, the primary role of the variational principle is derived.

5. Properties of Relativistic Quantum theories

The primary experimental properties of a quantum particle which are described in the previous section are used here for a construction of the main elements of a quantum theory. This task is done stepwisely.

• In order to be consistent with the pointlike property of an elementary quantum particle, the theory describes it by means of a wave function whose form is

$$\psi(x^{\mu}),$$
 (2)

where x^{μ} denotes a *single* set of four space-time coordinates. The following

argument explains why the form of (2) describes an elementary pointlike particle.

Take for example the ground state of the positronium, which is a bound state of an electron and a positron. This object, which has a non-vanishing volume, is described by a function of the form $\psi(t, x_1, x_2)$, where x_1, x_2 denote the three spatial coordinates of the electron and the positron, respectively. This example shows that in order to describe a composite non-pointlike particle one needs more than four space-time degrees of freedom.

As a matter of fact, the form of (2) is used in QFT textbooks in expressions for the Lagrangian density of any elementary quantum particle [6] [11] [15]. This issue means that there is a consensus about this requirement.

• In order to be consistent with the wave properties of a quantum particle, the function $\psi(x^{\mu})$ must have a phase factor. The de Broglie work has proven that the argument of the phase factor of a free quantum particle takes the form $(\mathbf{k} \cdot \mathbf{x} - \omega t)$, where

$$\mathbf{k} = \mathbf{p}/\hbar; \quad \omega = E/\hbar$$
 (3)

and *p*, *E* denote the particle's linear momentum and energy, respectively. Historically, de Broglie published his relations (3) before they were experimentally confirmed (see [2], p. 3; [8], pp. 48-49). This is certainly an example of a successful theoretical work.

- The wave properties of the quantum function (2) show that it must satisfy a wave equation.
- A wave function of a free particle that travels in the x-direction and satisfies the de Broglie relations can be written as a linear combination of the following expressions (see [2], p. 18)

$$\cos(kx - \omega t)$$
, $\sin(kx - \omega t)$, $\exp(\pm i(kx - \omega t))$ (4)

The first and the second expressions of (4) are real functions whereas the last expression is a complex function.

The following argument proves that real functions cannot describe a massive quantum particle. Let us use the real functions of (4) and examine a massive quantum particle which is in a field free region. In a particular inertial frame this particle is at rest and its linear momentum p = 0. Substituting this value and (3) into (4), one finds that in this frame the general form of a real wave function of a massive quantum particle is

$$\psi(t,x) = A\sin(\omega t) + B\cos(\omega t) = C\sin(\omega t - \delta), \tag{5}$$

where A,B,C and δ are appropriate real constant numbers. It follows that for every integer N, there is an instant when $\omega t - \delta = N\pi$ and the wave function of (5) vanishes throughout the entire 3-dimensional space. The following argument proves that this function is unacceptable. In the non-relativistic QM the particle's density is $\psi^*\psi$. It means that if ψ vanished throughout the entire 3-dimensional space then the particle does not exist. The Weinberg

correspondence principle and the limiting process prove that this result also holds for higher quantum theories because these theories must use ψ as a factor for the definition of density.

For these reasons, the phase factor of the quantum function of a motionless particle must be complex and the last expression of (4) shows that this function takes the form

$$\psi = e^{i\Phi} \chi(x, y, z). \tag{6}$$

The foregoing argument holds for a motionless particle. Such a particle is in a state which is the limit of states of particles that move inertially in a field-free region and their velocity tends to zero. Hence, a quantum function of particles that move inertially in a field-free region must be complex, because the limit of real functions is a real function.

Furthermore, a field-free region is the limit of regions where the intensity of the interaction tends to zero. Therefore, using a similar argument, one finds that the general state of a quantum particle is described by a complex function. This issue is also discussed in [16].

• Let us examine the power series of the phase factor of the quantum function (6)

$$e^{i\Phi} = 1 + i\Phi + \cdots \tag{7}$$

Now, a very well known law of physics states that all terms of a physically acceptable expression must have the same dimension, and, in a relativistic theory, they must also satisfy covariance. Since each of the numbers 1,i on the right hand side of (7) is a dimensionless Lorentz scalar, one concludes that also the phase Φ must be a dimensionless Lorentz scalar. The following argument explains how these constraints are satisfied.

ullet Let us use the variational principle and a Lagrangian density ${\cal L}$ that yields the required equations of the given quantum particle. The case of a Dirac particle is used here as an illustration of this issue

$$\mathcal{L}_{D} = \overline{\psi} \left[\gamma^{\mu} i \partial_{\mu} - m \right] \psi - \frac{1}{16\pi} F^{\mu\nu} F_{\mu\nu} - e \overline{\psi} \gamma^{\mu} A_{\mu} \psi. \tag{8}$$

Here $\overline{\psi} = \psi^{\dagger} \gamma^{0}$. The first term of (8) represents a free Dirac particle, the second term represents free electromagnetic fields and the last term represents the interaction between a Dirac charged particle and electromagnetic fields (see [11], p. 84, [15], p. 78).

The action of (8) is obtained from its 4-dimensional integral

$$S = \int \mathcal{L}_D d^4 x. \tag{9}$$

The action S and \hbar have the same dimension (see e.g. [8], p. 20, Equation (6.1)). It follows that in the unit system used herein where $\hbar=1$, the action is a dimensionless Lorentz scalar. Evidently, d^4x is a Lorentz scalar whose dimension is $\left[L^4\right]$ (see [14], p. 21). Hence, the action (9) proves that the Lagrangian density \mathcal{L} of a quantum particle must be a Lorentz scalar whose

dimension is $\left[L^4 \right]$. These constraints are imposed on an acceptable theory of a quantum particle. This kind of action can be used for the particle's phase. This general result is an extension of (1) which applies to the classical limit of the wave function.

The foregoing discussion proves that the action which is obtained from the Lagrangian density of a quantum theory can be used as the required phase of a quantum particle if the Lagrangian density is a Lorentz scalar whose dimension is $[L^4]$. The Weinberg correspondence principle proves that this conclusion holds for QM, RQM and QFT. Item 5 of section 3 indicates that the need for a Lorentz scalar Lagrangian density is already documented in the literature. The required $[L^4]$ dimension of the Lagrangian density is the main subject of the following discussion.

6. Discussion

This section describes some results that demonstrate powerful consequences of the requirement of a Lagrangian density whose dimension is $\lfloor L^4 \rfloor$.

Let us take the Lagrangian density of a Dirac electron (8). Its dimension is $\left[L^4\right]$ and in the unit system used herein c=1 and the dimension of each component of the partial derivatives ∂_{μ} is $\left[L^1\right]$. It follows that the dimension of the product $\bar{\psi}\psi$ is $\left[L^3\right]$. This is the dimension of density and indeed, the theory of a Dirac particle yields a consistent expression for a conserved 4-current

$$j^{\mu} = \overline{\psi}\gamma^{\mu}\psi; \quad j^{\mu}_{\mu} = 0. \tag{10}$$

It is well known that density is the 0-component of the 4-current $j^0 = \psi^{\dagger} \psi$ (see [17], pp. 23, 24).

The following product of the Schroedinger wave function $\psi^*\psi$ denotes density and it is used in a consistent expression for density-current (see [8], p. 54; [13], pp. 117-120). This result shows that the Dirac equation is consistent with the Weinberg correspondence principle of section 2. In particular, a construction of a Hilbert space is a requirement that should be satisfied by a consistent quantum theory (see [6], p. 49). The consistent expression for density of a Dirac particle (10) enables a construction of a Hilbert space for a Dirac electron, where the required inner product of two functions is $\int \psi_i^{\dagger} \psi_j d^3 x$.

In the case of quantum theories, the dimension $\left[L^4\right]$ of the Lagrangian density provides a simple proof of the role of the electromagnetic 4-potential in the interaction term of an electric charge. Indeed, the laws of Maxwellian electrodynamics prove that electromagnetic interaction is proportional to the charge. Therefore, in a quantum theory it should be proportional to the charge density whose dimension is $\left[L^3\right]$. Hence, due to the $\left[L^4\right]$ dimension of the Lagrangian density, the dimension of the electromagnetic factor of the interaction term must be $\left[L^1\right]$. This is the dimension of the electromagnetic potentials. By contrast, this argument proves that the electromagnetic field tensor $F^{\mu\nu}$ is unsuitable for this purpose because it is the 4-curl of the

4-potential and its dimension is $\lceil L^2 \rceil$.

The Dirac equation is a first order differential equation. As a matter of fact, one can find in the literature quantum equations of the second order. The Klein-Gordon (KG) equation is a quite simple example of this kind of equations. The KG function is a Lorentz scalar and its Lagrangian density is (see [18], p. 198 of the English translation)

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

The KG equation is derived from (11) (see Equation (39) therein)

$$\left(\frac{\partial}{\partial t} - ieV\right) \left(\frac{\partial}{\partial t} - ieV\right) \phi = \sum_{k=1}^{3} \left(\frac{\partial}{\partial x^{k}} + ieA_{k}\right) \left(\frac{\partial}{\partial x^{k}} + ieA_{k}\right) \phi + m^{2} \phi \tag{12}$$

and the KG density is (see Equation (42) therein)

$$\rho = i \left(\phi^* \phi_{,0} - \phi_{,0}^* \phi \right) - 2eV \phi^* \phi. \tag{13}$$

The product of two derivatives of the KG Lagrangian density (11) proves that the dimension of the KG function ϕ is $\left[L^{-1}\right]$. Therefore, the following inconsistencies arise.

- The dimension of the product $\phi^*\phi$ of the KG function is $\left[L^2\right]$. On the other hand it is shown earlier in this section that the dimension of the corresponding product of the Schroedinger functions is $\left[L^3\right]$. Hence, the KG function is inconsistent with the Weinberg correspondence principle because the continuity of a limit process does not alter the discrete value of the wave function's dimension.
- The dimension $[L^2]$ of the product $\phi^*\phi$ of the KG function explains why its expression for density (13) contains a derivative with respect to time. Hence, unlike the case of the non-relativistic QM, one *cannot* use density of a KG function and construct a Hilbert space in the Heisenberg picture where the quantum function is time-independent (see [3], p. 112; [11], p. 6). This is another violation of the Weinberg correspondence principle.
- The KG Lagrangian density (11) contains a second order term of the potentials. For example, a factor V^2 of the electric potential is obtained from the first term on the right hand side of (11). By contrast, Maxwell equations are derived from a Lagrangian density that depends *linearly* on the 4-potential (see [14], pp. 78, 79). Hence, the KG Lagrangian density (11) is inconsistent with Maxwellian electrodynamics.

These problematic results support Dirac lifelong objection to the KG equation (see [19], pp. 3,4). It can be shown that analogous problems hold in other kinds of second order quantum equations (see [20], Section 4).

7. Concluding Remarks

This work examines some aspects of the relevance of the variational principle to the mathematical structure of quantum theories. The experimentally confirmed corpuscular-wave duality is the basis of the analysis. This analysis focuses on the role of a consistent expression for the phase factor of a given quantum function. For this end, the paper examines a Lagrangian density which depends on a quantum function whose form is $\psi(x^{\mu})$. It is proved that each term of this Lagrangian density must be a Lorentz scalar whose dimension is $[L^4]$. The results show that such a Lagrangian density yields an action that can be used as the phase of a quantum particle. Moreover, it is shown that the $[L^4]$ dimension of the Lagrangian density defines a specific dimension for the quantum function $\psi(x^{\mu})$. The correspondence principle proves that the dimension of the quantum function provides a new kind of constraint that an acceptable quantum theory must satisfy. It is shown that the Dirac first order quantum theory complies with this constraint. By contrast, problems arise in the case of second order quantum theories, like that of the KG equation.

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