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Chapter

Lagrangian Quantum Mechanics: A Fully Relativistic Theory of Atomic Structure

Richard Oldani

Abstract

A fully relativistic formulation of quantum mechanics is derived by introducing a Lagrangian density of the fields between the excited and ground states and taking the action integral. The change in action, or photon, is a four-dimensional localization of fields that is defined symmetrically with respect to the field boundaries. Due to this photon model, we interpret the three mathematical formulations of atomic structure, matrix mechanics, wave mechanics, and path integrals, as different mathematical methods of describing the superposed physical components of an excited state: nucleus, electron, and photon. Recent experiments with slow and stopped light are shown to support this theoretical interpretation. The derivation of quantum theory with respect to fields requires new interpretations of the uncertainty principle, correspondence principle, complementarity, and force.

Keywords: quantum mechanics, relativity theory, uncertainty principle, correspondence principle, complementarity

1. Introduction

Nonrelativistic quantum mechanics is commonly expressed by using a Hamiltonian function, with the total energy of an atomic system given by the sum of the kinetic and potential energies. If the atom is in an excited state the energy resides at the location of the electron. The electron in an excited state has a potential energy that is converted into a photon as it decays, so emission is a statistical event that occurs at a particular point in time. Because photon creation occurs at a single point in time, the electron must be in two energy states simultaneously. The two states correspond to a single time, so emission is described by non-covariant means even though we know that it is Lorentz invariant. Although nonrelativistic methods are used to describe atomic structure, they are not a necessary requirement of quantum mechanical formalism. As Dirac stated in the first ever paper on quantum electrodynamics, "The theory is nonrelativistic only on account of the time being counted throughout as a c-number [classically], instead of being treated symmetrically with the space coordinates" [1]. The use of a continuous time parameter to describe microscopic phenomena could easily mask the way time functions in atomic structure. The practice should be closely questioned because time is the least understood of the variables in quantum mechanics. Furthermore there are grounds to support a different approach to quantum mechanics using Lagrangian mechanics. It is not

only more fundamental than Hamiltonian mechanics, but if we begin with an action principle by taking the time integral of a Lagrangian, it is in agreement with special relativity theory.

2. Excitation

We begin an attempt to understand the role of continuous time in quantum mechanics by describing emission as a sequence of events that are relativistically correct. Consider a uniform distribution of atomic oscillators immersed in a coherent or partially coherent radiation field with an outer electron that occupies either of two allowable energy states $|1\rangle$ or $|2\rangle$. The radiation field is conceived of as classical, consisting of many oscillating wave train fields superimposed on the oscillators. The system may be described by a Lagrangian density that is a function of oscillator fields φ_r and radiation fields $\partial_\mu \varphi$. If Hamilton's principle is applied macroscopically to an arbitrary classical region of space-time Ω, we obtain the usual expression:

$$S(\Omega) = \int_\Omega L(\varphi_r, \partial_\mu \varphi) d\Omega \tag{1}$$

The behavior of the radiation field may be described by a Lagrangian density microscopically as well. The amplitude of the field at the local level fluctuates randomly, either reinforcing or canceling, thereby causing the electron to oscillate with respect to the nucleus. If the fields are of insufficient intensity to raise the electron from $|1\rangle$ to $|2\rangle$, the uncertainty relations do not apply and the electron oscillates without radiating. However, if they are sufficiently intense, the electron will resonate at the excitation energy emitting a photon with each amplitude of the wave. When this happens radiation is emitted with double the frequency of the incident wave (see **Figure 1**).

Emission by atomic oscillators is referred to as "nonlinear" if excitation is thought to be quantum mechanical or "spontaneous" if it is thought to be governed by the macroscopic Maxwell's equations [2]. The use of microscopic Maxwell's equations in a Lagrangian density allows emission to be described by a distribution of locally superposed fields that includes continuous, statistical, and quantum mechanical properties in a single model.

Due to the generality of the assumptions, examples of frequency doubling should be common in nature occurring at many energy levels. This is in fact the case, and it is most clearly evident when laser light is passed through a crystal [3]. It is also readily observed using incoherent light in scattering experiments as secondary radiation [4]. On the other hand, when an energy quantum is completely absorbed, an electron will be expelled due to the photoelectric effect, and no frequency change is observed. We see in these examples evidence that the Lagrangian provides a versatile model for the description of electromagnetic phenomena.
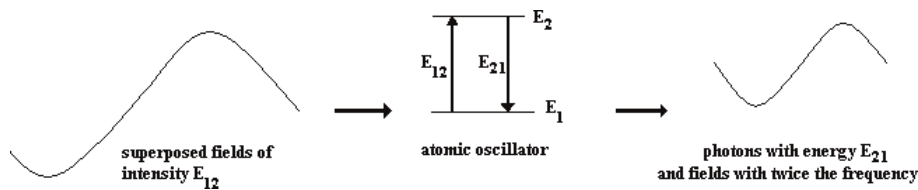

superposed fields of intensity E_{12} atomic oscillator   photons with energy E_{21} and fields with twice the frequency

Figure 1.
Frequency doubling.

3. Decay

The first appearance of a Lagrangian in quantum mechanics is in a paper by Dirac. "We ought to consider the classical Lagrangian not as a function of the coordinates and velocities but rather as a function of the coordinates at time t and the coordinates at time t+dt" [5]. Rather than specify emission as an event that occurs at a particular point in time, Dirac is seeking compatibility with relativity theory by calculating the change in action of the electron over a space-time interval. That idea resulted in an interpretation of electron transitions as a "sum over histories" of all possible paths from one diagonalized steady state to another [6]. Although calculations made with the path integral method are accurate, they include serious theoretical problems resulting from the renormalization methods used to deal with infinities that have so far prevented a complete theory from being formulated. At a later point in the same paper, Dirac provides a possible way out of this difficulty by proposing a complementary description of quantum mechanics in terms of a "vibrating medium." The idea begins from a classical vantage point. "We introduce at each point of space-time a Lagrangian density, which must be a function of the coordinates and their first derivatives with respect to x, y, z, and t, corresponding to the Lagrangian in particle theory being a function of coordinates and velocities. The integral of the Lagrangian density over any (four-dimensional) region of space-time must then be stationary for all small variations of the coordinates inside the region, provided the coordinates on the boundary remain invariant." To obtain the quantum analogue, he divided the classical region into a number of very small subregions; however, the idea was never pursued to completion. We shall investigate that line of reasoning in more detail by describing fields over a four-dimensional region of space-time with respect to invariant field boundaries coincident with the steady states.

The excited states of an atom should be described discretely in time. As Dirac pointed out, discrete time is symmetric with the spatial coordinates allowing the emission and absorption of radiation to be described relativistically. A relativistic formulation is desirable in order to make quantum mechanics compatible with special relativity theory. To formulate a fully relativistic description of emission, we begin with a Lagrangian density $L(\phi_i, \phi_{i,\mu})$ that is a function of the coordinates and their first derivatives. Then the action integral of the Lagrangian density over a particular region of space-time must be stationary for all small variations of the continuous coordinates in the region provided the discrete coordinates on the boundary remain invariant. Let three-dimensional surfaces R_1 and R_2 representing the diagonalized coordinates be erected and then used together with the discrete time period $t_2 - t_1$ as field boundaries to define a region of space-time between $|2\rangle$ and $|1\rangle$. Integrating from $|2\rangle$ to $|1\rangle$ yields a relativistic formulation of emission that is invariant, the same for all observers:

$$S[\varphi_i(t)] = \int\limits_{R_2}^{R_1}\int\limits_{t_2}^{t_1} L(\varphi_i, \varphi_{i,\mu})d^3x\,dt = h \qquad (2)$$

The end points of the electron's path are located on equipotential, space-like surfaces, and the action minimum is not equal to zero as in classical theory, but to Planck's constant h. The action $S[\varphi_i(t)]$ in (2) is functional, a function of the values of coordinates on the *discrete* boundary of the space-time surface R_2 which is in turn a function of the *continuous* space-time variables of the fields within the surface.

Solving for the action, we obtain solutions for localized energy or equivalently, photon creation; due to a transformation of field:

$$E\tau = h \tag{3}$$

Solutions of Equation (3) are determinations of energy and time between exact four-dimensional field boundaries, so they are also exact. In the case of time periods, this has been confirmed to the limits of experimental accuracy by atomic clocks that can operate for many billions of years without significant error [7]. Thus field energy from a laser is absorbed by the lattice of ytterbium atoms and localized within a four-dimensional field boundary. The emission and absorption energies E_{21} and E_{12} have also long been assumed to be exact by astronomers when employed for the measurement of distant star composition. Emission and absorption spectra, together with a red shift, often require billions of years before they are observed, thereby reflecting the precise role of energy and time in natural phenomena.

From (2), a model of atomic structure may be constructed. The three field sources present in excited atomic states, electron, proton, and photon, superpose linearly and are momentarily stabilized in steady states. Although force is an unnatural concept in quantum mechanics, it may be interpreted with respect to the field boundaries that separate point sources by a careful consideration of (2). Thus the force on a bound electron due to the potential is equal to the continuously distributed excitation energy divided by the distance between field boundaries. In order for quantum mechanical forces to agree with relativity theory, we need only require that the action integral be invariant for all potentials both free and bound.

Whereas the quantum mechanical force of bound states is due to well-defined field boundaries, the force due to instantaneous exchanges of momentum, such as occurs in the Compton effect, may be interpreted as a result of the encounter of a single, exact field boundary (x_o, y_o, z_o, t_o) with a material point. Wave properties, on the other hand, occur in free space when field boundaries have no reference point, so they cannot be observed at all. Thus we interpret complementarity as the different ways that fields and its field boundaries interact with matter.

4. Interpretation of mathematical models

4.1 Fully relativistic quantum mechanics

A fully relativistic description of excited atomic states specifies discrete four-dimensional field boundaries and continuous localized fields between the boundaries. Excited atomic states, electron, photon, and nucleus, are interpreted as a linear superposition of three field sources with respect to their electrostatic and electromagnetic field components. Recent experiments, referred to by the authors as "photon capture" and "photon storage," support the accuracy of this theoretical interpretation [8]. In these experiments light coherence is converted to atomic coherence and back again, so the photon in localized form must be present in excited atomic states from the time energy is absorbed until it is emitted. We describe the linear properties of atomic structure by introducing a wavelike field source ε, the localized photon, into our description of excited atomic states. The modified Hamiltonian is now given by

$$H = T + \varepsilon + V \tag{4}$$

and the Lagrangian is similarly given by

$$L = T + \varepsilon - V \tag{5}$$

where T represents the bound electron's energy, ε represents the energy of a "captured" photon, and V represents the potential energy due to the nucleus/proton. Each of the three field sources possesses a unique vector field, that is, a field with definite field geometry that is delimited from the others by field boundaries, where plus and minus signs indicate the linear superposition of delimited fields.

Eqs. (4) and (5) contain the essence of quantum mechanics as a three-body problem in real space as opposed to current descriptions based on a two-body system in abstract space. The use of an abstract space is necessary for nonrelativistic descriptions of atomic structure since the photon is not treated as an independent particle. The equations revert to their classical form when the influence of ε is negligible or equivalently when field boundaries are no longer determinable. To see whether the model accurately describes atomic structure, we shall compare it to the existing mathematical models.

4.2 The path integral formulation

From (5), it is postulated that the contribution of two energies is summed and one is subtracted to give the transition energy. In the path integral formulation, there are in fact two contributions that are summed, one determined by the paths and the other by the phase. In Feynman's words, "The paths contribute equally in magnitude, but the phase of their contribution is the classical action (in units of $\hbar$)" [9]. The computation of the total energy is not complete, however, until contributions to the potential V due to self-energy are subtracted away by renormalizing. Therefore the mathematical structure of the Lagrangian in nonrelativistic quantum mechanics indicates the existence of three contributions and is in agreement with (5). It differs fundamentally from the fully relativistic Lagrangian method described here in its interpretation of space-time. Eq. (2) treats space and time equivalently as real parameters for both the integration limits and the region between them. On the other hand, the path integral formulation uses abstract forms of space and time to describe the region between the steady states since the paths follow all trajectories and for all times.

4.3 Matrix mechanics

In quantum mechanics, observables are determined by pairs of states, while in classical theory they refer to the same state. This is especially evident in matrix mechanics which describes the atom as a twofold infinite, denumerable array of virtual oscillators, where observables are vectors in Hilbert space whose magnitude defines a spectral line intensity, or transition amplitude, and whose direction corresponds to either an absorption or an emission. Although the physical model consists of two ideal particles, the virtual harmonic oscillators, the matrix elements include three field components: the fields of the two ideal particles and a spectral line intensity due to photon superpositions. All three components of the modified Hamiltonian given by Eq. (4) are present but with respect to classical space and time. In nonrelativistic theory, photons are singularities that correspond to pairs of states, whereas conformance with relativity theory requires that the photon be spatially and temporally extended. Fields are localized by exact four-dimensional

field boundaries separated from each other in space-time, while in nonrelativistic quantum mechanics, field boundaries do not exist.

Because Heisenberg's uncertainty relations use a continuous time parameter, they are only valid when events are defined with respect to specific observers, but not in general for all observers. When interpreted according to Eq. (2) by a fully relativistic theory, we conclude that indeterminacy is due to measurements performed with a non-singular, spatially and temporally extended probe, the photon. This may be compared to the case in classical mechanics of measurements that are performed with a coarsely defined standard. In quantum mechanics, the standard of measurement is the photon, and no matter how high its energy, it cannot be used to localize a point particle more precisely than its wavelength. On the other hand, localizations in atomic clocks occur four-dimensionally with respect to *both* field boundaries, so they occur without measurable error.

4.4 Wave mechanics

In the wave mechanical interpretation of quantum mechanics, field boundaries are not specified. Nevertheless fields are a part of wave functions, and field boundaries must be included in a fully relativistic theory of electrodynamics. To satisfy that requirement, we interpret the wave function $\Psi\left(\vec{r},t\right)$ as combining an electron or other particle, and a force $\varepsilon\left(\vec{r},t\right)$, that are separated by field boundaries. A wave function composed in this manner as a composite of two physical components may be used to describe the interaction of particles in both bound and free states. Whereas in classical theory forces are three-dimensional vectors with direction and magnitude, in a fully relativistic theory they are four-dimensional and symmetric in the coordinates. They have orientation in space-time, but not direction, with magnitude determined by the instantaneous separation of field boundaries according to (1). Thus force is the continuous application of a discrete form. All interactions of electrodynamics may be conceived of in this way in terms of fields and their boundaries.

5. Discussion

Although the wave function contains all that can be known about a particle, the preceding fully relativistic interpretation of atomic structure indicates the presence of internal characteristics that are *in principle* unknown to observers. The field model, described by (1) and confirmed experimentally by slow or stopped light phenomena, includes internal processes in its description of the wave function that are temporarily restricted from external expression due to field boundaries. The characteristics cannot be accessed because the fields vanish at the field boundaries. Due to the unobserved processes, quantum theory predicts the occurrence of instantaneous action-at-a-distance events such as the collapse of the wave function and other macroscopic phenomena that exist outside of our consciousness. However, if wave functions are interpreted in a fully relativistic theory, we conclude that these phenomena are only unusual when interpreted in abstract space with respect to continuous time parameters.

The detection events that form the basis of optical theory are due to energy emissions that occur at singular points in time and are referred to as "photons" due to their discrete nature. If energy absorption evolves according to Eq. (2), as the integration of a Lagrangian density over a region of space-time, then excitation is a

continuous process that results from field superposition during the discrete time period τ. Therefore in a fully relativistic theory, interference effects are due to the instantaneous reinforcement and cancelation of superposed photons of the type described in (2), and the statistical nature of quantum mechanics that is observed in experiments such as double-slit interference is due to time averages. A fully relativistic optical theory will account for interference effects as they evolve in real space and time.

6. Conclusion

It has long been asserted that classical physics is inadequate for describing quantum mechanical phenomena. Consequently experimental results are explained by introducing complementarity and the correspondence principle. However, the problem is not that classical theory is deficient, but it is the insistence on using singularities in a nonrelativistic theory. If the photon's fields are singular, wave and particle properties seem to appear out of nowhere, and experimental results have an intrinsically defined uncertainty. But if the photon is instead described as a localization of fields, uncertainty and duality are accounted for by physical characteristics, fields and field boundaries, and complementarity has a classically derived meaning. A similar explanation is possible for the correspondence principle which specifies the point where a two-particle classical system must be replaced by a three-particle quantum mechanical system to explain what is observed. It may seem to be an acceptable practice to describe particles as singularities propagating and interacting continuously in time, but in a fully relativistic theory the photon cannot be singular. Rather it is a four-dimensional localization of fields defined symmetrically in space-time that determines electron behavior in bound states and also in free space by means of four-dimensional forces.

The mathematical framework surrounding quantum mechanics is precisely the type of description that is expected when a particle of zero mass is absorbed by a two-particle system. The particle properties of the photon are overwhelmed by the other two such that it is impossible to distinguish it independently of them. Sometimes the influence of its continuous properties is more evident (wave mechanics); at other times its discrete properties are prominent (matrix mechanics); and in path integral formulations, the exact field boundaries of bound states are manifested. Each of the three formulations of nonrelativistic quantum mechanics provides a unique perspective to atomic structure by emphasizing a different physical aspect of the three field sources. This may be compared to the simpler three-dimensional practice in architecture of providing three visual perspectives to a building. Each one provides a partial view, and when taken together they give an improved understanding of the structure as a whole. The "whole" of quantum mechanics is given of course by Lagrangian quantum mechanics.

Author details

Richard Oldani
Illinois Institute of Technology, Clymer, NY, USA

*Address all correspondence to: oldani@juno.com

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