


Fundamental formulation of light-matter interactions revisited

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The basic physics disciplines of Maxwell's electrodynamics and Newton's mechanics have been thoroughly tested in the laboratory, but they can nevertheless also support nonphysical solutions. The unphysical nature of some dynamical predictions is demonstrated by the violation of symmetry principles. Symmetries are fundamental in physics since they establish conservation principles. The procedures explored here involve gauge transformations that alter basic symmetries, and these alterations are possible because gauge transformations are not necessarily unitary despite the widespread assumption that they are. That gauge transformations can change the fundamental physical meaning of a problem despite the preservation of electric and magnetic fields is a universal proof that potentials are more basic than fields. These conclusions go to the heart of physics. Problems are not evident when fields are perturbatively weak, but the properties demonstrated here can be critical in strong-field physics where the electromagnetic potential becomes the dominant influence in interactions with matter.

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I. INTRODUCTION

The unfamiliar properties of electromagnetism to be described here can be overlooked when the electromagnetic field is no more than a perturbative influence in physical processes. However, when the electromagnetic field is the dominant influence, then these properties become profoundly important. The ever-expanding use of powerful lasers imparts a fundamental significance to these unfamiliar properties.

Current beliefs about electromagnetism that are challenged here come from the following demonstrations: (i) electromagnetic potentials convey more physical information than electric and magnetic fields, (ii) reliance on electric and magnetic fields can introduce basic errors, (iii) gauge transformations alter the properties of a physical system, (iv) gauge transformations are not unitary, (v) concepts such as the adiabaticity property in laser phenomena are false and wasteful, (vi) a proposed nondipole correction is unphysical, and (vii) predictions that follow from the solutions of Maxwell's equations can be unphysical. From these results, it is a corollary that Newton's mechanics can also support unphysical solutions.

An ancillary matter is the objection to the widespread use of an intensity parameter that lacks Lorentz invariance, but is held to be descriptive of otherwise covariantly described phenomena.

It is emphasized that neglect of basic electrodynamic principles in applications to strong-field laser processes has caused important hindrances to the development of the discipline. These hindrances continue, and can lead to needless delays in the development of this large and expanding field of study.

II. GAUGE TRANSFORMATIONS ALTER PHYSICAL PROPERTIES

The fact that gauge transformations can fundamentally alter the physical identity of a system is evident even in the elementary problem of an electron immersed in a uniform constant electric field \mathbf{E}_0 .

A possible set of potentials to describe the field is

$$\phi = -\mathbf{r} \cdot \mathbf{E}_0, \quad \mathbf{A} = \mathbf{0}. \quad (1)$$

The Lagrangian that describes the electron in the field is independent of time. By Noether's theorem [1], this means that energy is conserved. Another possible gauge for the description of the constant field is

$$\phi = 0, \quad \mathbf{A} = -c\mathbf{E}_0 t. \quad (2)$$

The Lagrangian for an electron with the field described by Eq. (2) has time dependence, but is independent of the spatial coordinate \mathbf{r} . In this case, energy is not conserved but momentum is conserved.

The potentials (1) and (2) have different symmetries, and represent different physical situations. These differences are produced by the gauge transformation.

An important case that possesses only one gauge that satisfies all relevant symmetries was examined in Ref. [2]. The electromagnetic field examined is a plane-wave field, such as that of a laser beam. The symmetry that is present in that case is the propagation property, which requires that the field can depend on the spacetime 4-vector x^μ only as a scalar product with the propagation 4-vector k^μ :

$$\varphi \equiv k^\mu x_\mu = \omega t - \mathbf{k} \cdot \mathbf{r}, \quad (3)$$

where ω is the field frequency and \mathbf{k} is the propagation 3-vector. When a scalar potential ϕ such as that from a Coulomb potential is also present, then the sole possible gauge satisfying the necessary symmetry is the radiation gauge (also

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called Coulomb gauge), where the 3-vector component \mathbf{A} is descriptive of the plane-wave field, and the scalar potential ϕ describes the binding potential, so that the total 4-potential is

$$A^\mu : (\phi^{\text{scalar}}, \mathbf{A}^{\text{plane wave}}). \quad (4)$$

III. GAUGE TRANSFORMATIONS ARE NOT NECESSARILY UNITARY

The starting point here is the property known as form invariance, where the Schrödinger equation has the same form when expressed in terms of the gauge-transformed potentials as it does in the original gauge. See, for example, Ref. [3]. Form invariance under a gauge transformation generated by the operator U can be written as

$$\tilde{H} - i\hbar\partial_t = U(H - i\hbar\partial_t)U^{-1}, \quad (5)$$

where \tilde{H} is the transformed Hamiltonian. This gives the gauge-transformed Hamiltonian

$$\tilde{H} = UHU^{-1} - i\hbar U(\partial_t U^{-1}). \quad (6)$$

This means that the gauge transformation cannot be a unitary transformation if U is time-dependent.

For laser-related problems, the time dependence of the field imparts time dependence to any gauge transformation employed. Such transformations are not, in general, unitary.

IV. ELECTROMAGNETIC POTENTIALS ARE MORE FUNDAMENTAL THAN ELECTRIC AND MAGNETIC FIELDS

The primacy of potentials over fields was first established by the Aharonov-Bohm effect [4,5]. This relates to a specific example: the deflection of an electron beam as it moves in the field-free region around a solenoid. It is the potential that causes the deflection, since there is a potential but no field outside the solenoid. That quantum result stood for many years as the sole example of the fundamental role of electromagnetic potentials. A more general case is the demonstration [2] that there exists an unphysical solution of the Maxwell equations for a plane-wave field propagating in the vacuum. This has consequences that are both quantum and classical.

Furthermore, as shown in the following section, when a solution of the Maxwell equations is unphysical, then the properties of the potentials are necessary to distinguish physical from unphysical solutions. This is a universal proof that potentials are more fundamental than fields.

V. SOLUTIONS OF MAXWELL EQUATIONS ARE NOT NECESSARILY PHYSICAL

A single unphysical solution of Maxwell's equations is sufficient to demonstrate that such unphysical solutions can exist. The example selected here is significant since it has been proposed or employed for practical laser-induced processes.

The symmetry condition that applies to all plane-wave fields, such as laser fields, comes from the Einstein principle [6] that the speed of light in vacuum is the same in all inertial frames of reference. This was referred to above as the propagation property. Its mathematical statement is that the spacetime 4-vector x^μ can occur only as the scalar product

φ defined in Eq. (3); that is, the vector potential describing a plane wave must have the form $A^\mu(\varphi)$.

A gauge transformation of the electromagnetic field is generated by the function Λ :

$$A^\mu \rightarrow \tilde{A}^\mu = A^\mu + \partial^\mu \Lambda. \quad (7)$$

The only constraints on Λ are that it be a scalar function and that it satisfies the homogeneous wave equation

$$\partial^\mu \partial_\mu \Lambda = 0. \quad (8)$$

This is sufficient to preserve the electric and magnetic fields. If A^μ satisfies the Lorenz condition $\partial^\mu A_\mu = 0$, the same will be true of \tilde{A}^μ . Now consider the generating function [7]

$$\Lambda = -A^\mu x_\mu, \quad (9)$$

which leads to the gauge-transformed potential

$$\tilde{A}^\mu = -k^\mu (x^\nu A'_\nu), \quad (10)$$

where A'_ν is the total derivative of A_ν with respect to φ : $A'_\nu = (d/d\varphi)A_\nu$. Equation (10) takes a familiar form if the initial gauge for A^μ is the radiation gauge. A pure plane-wave field is described in the radiation gauge by the 4-vector

$$A^\mu(\varphi) : (0, \mathbf{A}(\varphi)). \quad (11)$$

The gauge-transformed 4-vector is then

$$\tilde{A}^\mu = -\hat{k}^\mu \mathbf{r} \cdot \mathbf{E}(\varphi), \quad \hat{k}^\mu \equiv \frac{k^\mu}{\omega/c}, \quad (12)$$

where \hat{k}^μ is the unit propagation 4-vector that lies on the light cone.

The form (12) resembles the dipole-approximation scalar potential $\mathbf{r} \cdot \mathbf{E}(t)$ that is so ubiquitous in length-gauge atomic, molecular, and optical (AMO) physics. This is the reason why it was examined in Ref. [7] in an attempt to provide a rigorous basis for the Keldysh approximation [8] of strong-field atomic physics. It was rejected in Ref. [7] on multiple grounds, the most obvious of which is that it violates the Einstein principle. The violation is evident in Eq. (10) from the appearance of x^ν in isolation from the propagation 4-vector, and the presence of the 3-vector \mathbf{r} in Eq. (12) that requires an origin for a fixed spatial coordinate system that is contrary to the nature of a freely propagating plane-wave field. Nevertheless, the fields are preserved by the gauge transformation (9), and so are the Lorenz condition $\partial^\mu A_\mu = 0$ and the transversality condition $k^\mu A_\mu = 0$ [7].

The 4-potential in Eq. (10) or (12) has the curious feature that it lies on the light cone. A plane-wave field is described by a spacelike 4-potential, not one that is lightlike. Furthermore, a fundamental property of a charged particle in interaction with a plane-wave field is the ponderomotive energy [9–11] U_p , which is proportional to $A^\mu A_\mu$. However, since k^μ is self-orthogonal,

$$k^\mu k_\mu = 0, \quad (13)$$

the \tilde{A}^μ of Eq. (10) or (12) predicts a zero ponderomotive energy for any charged particle.

For all of these reasons, Eqs. (10) and (12) are unphysical. Nevertheless, they are arrived at by a valid gauge transformation from a proper plane-wave 4-potential, meaning that

they predict the same electric and magnetic fields, and hence they satisfy the same Maxwell equations, since the Maxwell equations depend only on the fields, not on the potentials. This is proof that Maxwell's equations can support unphysical solutions.

Equations (10) and (12) were first proposed and discussed in Ref. [7], where the above-mentioned problems were noted, and Eqs. (10) and (12) were rejected as unphysical. However, a Heidelberg group [12] took note of these equations and applied them to practical problems on the grounds that they described correctly the electric and magnetic fields of laser beams. Also, a Norwegian group [13], apparently without knowledge of Ref. [7], proposed these equations as a way of introducing nondipole corrections into the study of laser-induced reactions.

While Eq. (10) or (12) is not acceptable for a properly formulated theory, it is possible that qualitative information can be attainable from it. It was used in Ref. [14] to estimate the onset of magnetic effects, which it established correctly.

VI. SOLUTIONS OF NEWTON'S EQUATIONS ARE NOT NECESSARILY PHYSICAL

Newtonian physics is based on forces, and electromagnetic forces are dependent on electric and magnetic fields, as given by the Lorentz force expression

$$\mathbf{F} = q\left(\mathbf{E} + \frac{\mathbf{v}}{c} \times \mathbf{B}\right). \quad (14)$$

Hence, the reasoning applied to show the possibility of unphysical solutions of the Maxwell equations applies as well to Newton's equations.

Alternative formulations of classical mechanics, such as the Lagrangian, Hamiltonian, Hamilton-Jacobi, etc., are based on potentials, and hence they convey more information than a force-based theory like Newton's mechanics. This explains the common practice in mechanics textbooks to show that potential-based formalisms imply the Newtonian formalism, but the reverse is never shown.

VII. PRACTICAL CONSEQUENCES

When approximations are employed in the study of a physical process, results can be inefficient and possibly erroneous if basic symmetries are not observed. An example from strong-field physics is the phenomenon known as above-threshold ionization (ATI), which refers to the observation [15] that ionization by an intense laser beam can exhibit processes of photon number in addition to, or in place of, the lowest allowed order predicted by perturbation theory. AMO physics has experienced accurate and reliable results from perturbation theory, and the observation of ATI came as a shock to the AMO community. A recent assessment by prominent researchers [16] of this unexpected result can be paraphrased in abbreviated form as "... multiphoton ionization experiments using intense infrared pulses found the then-amazing result that an ionizing electron often absorbed substantially more photons than the minimum needed for ionization. This puzzling behavior led to the term... ATI... The problem was ultimately solved by computer simulations and the semiclassical recollision model." Citations of the relevant

theory place the date for eventual understanding of the 1979 experiment at 1993, a span of 14 years.

The important fact here is that both analytical and numerical studies employed the dipole approximation, which has the effect of replacing the propagating laser field by an oscillatory electric field. This loses the propagation symmetry that is at the heart of the strong-field processes described above.

From the point of view of propagating fields, the significant contribution of many photon orders at high field intensities is obvious, and noted long before the 1979 experiment. For example, in bound-bound transitions, there is the 1970 statement [17] "...as the intensity gets very high ... higher order processes become increasingly important." For photon-multiphoton pair production in 1971 [18], "... an extremely high-order process can... dominate the lowest order...". For interband transitions in band-gap solids in 1977 [19], "...high-order processes can be more probable than lower-order processes when the intensity is sufficiently high." The 1980 ionization paper [20], written before the ATI experiment, describes ATI in detail. Other high-intensity phenomena, such as channel closing and stabilization, are also discussed in the early papers just cited.

A. Nondipole corrections

The difficulty of Eq. (10) or (12) for the introduction of nondipole corrections has been discussed above. A valuable laboratory project would be to determine the limitations on such an approach.

A fully relativistic propagating strong-field theory is certainly applicable for all nondipole, magnetic field, and relativistic studies. The construction of such a theory was elaborated in Ref. [21] for the Klein-Gordon case, and implemented in detail in Ref. [22] for the Dirac case.

B. Local constant field approximation (LCFA)

The LCFA is an example of how field-based criteria can differ from potentials-based criteria. One justification of the LCFA follows from the field-based observation that the two Lorentz invariants of plane-wave fields,

$$\mathbf{E}^2 - \mathbf{B}^2 = 0, \quad \mathbf{E} \cdot \mathbf{B} = 0, \quad (15)$$

can be satisfied by constant crossed fields [23,24].

When viewed from the standpoint of potentials, the potentials that describe constant crossed fields $\mathbf{E}_0, \mathbf{B}_0$ are

$$\phi = -\mathbf{r} \cdot \mathbf{E}_0, \quad \mathbf{A} = -\frac{1}{2} \mathbf{r} \times \mathbf{B}_0, \quad (16)$$

$$|\mathbf{E}_0| = |\mathbf{B}_0|, \quad \mathbf{E}_0 \perp \mathbf{B}_0. \quad (17)$$

These potentials are unrelated to the $A^\mu(\varphi)$ requirement for propagating fields.

C. Low-frequency limit of a plane wave

Plane waves are characterized by the fact that they propagate in vacuum at the speed of light. This feature is independent of frequency. There is a line of reasoning, adopted for many years in the strong-field community, that there exists a zero-frequency limit of plane waves, and this limit is simply a constant electric field. This is inferred from the dipole

approximation, so that there is no magnetic field present, distinguishing it from the LCFA.

There is no such thing as a zero-frequency plane wave. Plane waves propagate at the speed of light, independently of frequency. An example of a plane-wave phenomenon of extremely low frequency is the Schumann resonance [25]. This is a naturally occurring phenomenon in which powerful lightning strikes generate extremely low-frequency radio waves that resonate in the cavity formed by the Earth's surface and the ionosphere. The lowest mode of this cavity is 7.83 Hz, corresponding to a wavelength about equal to the circumference of the Earth. On a laboratory scale, a plane wave with a wavelength equal to the circumference of the Earth would appear to be a constant field. Yet neither a constant crossed field nor a constant electric field can spread its influence over the entire planet.

A pernicious consequence of the concept of a low-frequency limit of a laser field as being a constant electric field was its use as a criterion for judging the worth of analytical approximations. For many years, a zero-frequency limit equivalent to a constant electric field was regarded as a feature of sufficient importance to reject any theory that did not possess that property. See, for example, Ref. [26]. This limit was regarded as an adiabatic limit, and the qualitative stance was adopted that low-frequency fields should exhibit this adiabaticity. In actuality, the $\omega \rightarrow 0$ limit of plane waves is relativistic [27], not adiabatic. It is the relativistic property of propagation at the speed of light that distinguishes the Schumann resonance from a constant field phenomenon.

It is impossible to estimate the cost in valuable research resources of the long-term application of the adiabaticity test as a basic criterion, but it is undoubtedly considerable.

VIII. CENTRAL ROLE OF A^μ

The basic properties of a propagating field can be described entirely by the 4-vector potential. This makes possible a covariant statement of those properties, including the identity of the coupling constant of strong-field physics.

The 4-vector potential enters the description of propagating fields in the three fundamental expressions:

$$\partial^\mu A_\mu = 0, \quad (18)$$

$$k^\mu A_\mu = 0, \quad (19)$$

$$z_f \sim A^\mu A_\mu. \quad (20)$$

The first is the Lorenz condition, second is the transversality condition, and the third enters into the definition of the strong-field coupling constant z_f . The implications of Eq. (20) seem to be little known, but they are perhaps the most direct expressions of the ascendancy of potentials over fields.

The Lorenz condition can be expanded into

$$\partial^\mu A_\mu = \frac{\partial}{\partial t} \phi - \nabla \cdot \mathbf{A} = 0. \quad (21)$$

In the radiation (or Coulomb) gauge, where the scalar potential ϕ applies only to longitudinal potentials, the Lorenz condition for the propagating field reduces to $\nabla \cdot \mathbf{A} = 0$, which is often used as the identifying condition for the radiation gauge.

The expression (19) is the covariant transversality condition. This is readily shown to infer geometrical transversality: $\mathbf{k} \cdot \mathbf{E} = 0$ and $\mathbf{k} \cdot \mathbf{B} = 0$.

The coupling constant of strong-field physics was identified [9,10] long ago. Strong-field physics as a separate discipline was established (see Appendix A in Ref. [28]) as a consequence of the demonstration by Dyson [29] that standard quantum electrodynamics (QED) does not possess a convergent perturbation expansion. This raised the question of the convergence properties of an external-field theory, which represents a strong-field situation in which the number of photons present during an interaction is large. The expansion parameter of standard QED is the fine-structure constant α . A convergence study of the external-field theory revealed the fact that every appearance of α involved the same intensity-dependent factor. That is, the expansion parameter is not α , but rather the product of α with that factor. This product was labeled z in the original studies [9,10], since an expansion parameter must be extended into the complex plane to find the singularities that limit convergence, and z is often used to label a complex number. In more recent work, z was relabeled z_f to indicate that it is the intensity parameter for free electrons as opposed to two new parameters z (nonperturbative intensity parameter) and z_1 (bound-state intensity parameter) that arises when scalar potentials exist through interactions of the electron with binding potentials in addition to the plane-wave field. See Sec. 1.3 in Ref. [30] for further discussion.

In current terminology, the coupling constant is written

$$z_f = 2U_p/mc^2, \quad (22)$$

where U_p is the ponderomotive energy, defined as

$$U_p = \frac{e^2}{2mc^2} \langle |A^\mu A_\mu| \rangle. \quad (23)$$

The angle brackets denote an average over a full cycle of the field, and the absolute value is taken because A^μ is a spacelike 4-vector.

The quantity z_f just identified as the coupling constant for strong laser fields is known as an intensity parameter for strong fields, but its additional role as the coupling constant seems to have escaped general attention.

From Eq. (23), the ponderomotive energy and hence z_f are Lorentz invariants. If z_f is to be a proper coupling constant, it must also be gauge-invariant, and this is not apparent in (23). However, when A^μ describes a propagating field, then U_p has been shown [11,31] to be gauge-invariant.

An objection is raised here to an intensity parameter that has found acceptance in the relativistic strong-field literature. The quantity $A^\mu A_\mu$ is rendered as $|\mathbf{E}^2|/\omega^2$, and then, since the square seems unnecessary, the parameter is commonly written as proportional to E/ω . The intent apparently is to introduce the electric field in the belief that it is more fundamental than the 4-vector potential. In addition to its inappropriate emphasis on the electric field rather than on the 4-vector potential, this convention is objectionable in a theory that is founded on covariant expressions. Lorentz invariance is lost because Lorentz transformation properties of the electric field E are not the same as for the frequency ω . The quantity z_f of Eq. (22) is Lorentz-invariant, gauge-invariant, and covariant.

It is not possible to express $A^\mu A_\mu$ in terms of fields. When a quantity can be stated with fields it is always possible to convert it to potentials because fields are found from potentials by differentiation—a local procedure. To convert a quantity stated entirely with potentials, any attempt to convert the expression to fields will fail because such a procedure requires integration, which is nonlocal.

The z_f parameter also occurs in the intensity-dependent mass-shell condition for the electron in a strong field. The usual mass shell of QED is

$$p^\mu p_\mu = (mc)^2. \quad (24)$$

However, all the early studies of strong-field interactions [9,10,32–35] found the shifted-mass equation

$$p^\mu p_\mu = (mc)^2(1 + z_f). \quad (25)$$

Sarachik and Schappert find [36] that the altered mass shell expression (25) also exists with classical strong fields.

A further implication of z_f becomes clear when it is expressed in terms of the photon density ρ . This expression has the form [11]

$$z_f = \alpha \rho V, \quad (26)$$

with the fine-structure constant α multiplied by the number of photons contained in an effective interaction volume V . This volume is approximately a cylinder of radius given by the electron Compton wavelength and a length λ given by the wavelength of the plane-wave field. The Compton wavelength is the expected interaction length for a free electron, but λ is a macroscopic length in most laboratory applications. This

is a way to understand why $\omega \rightarrow 0$ (or $\lambda \rightarrow \infty$) leads to relativistic behavior and not adiabatic behavior.

The fundamental quantity $A^\mu A_\mu$ is expressed directly in terms of the 4-vector potential A^μ . There is no equivalent expression in terms of the electric field. This simple compelling fact supports the primacy of potentials over fields.

IX. THE PATH AHEAD

As laser intensities increase and as low-frequency capabilities improve, the lessons contain herein are basic. In brief, one must consider the true electromagnetic properties of very strong fields, including especially the requirements that follow from the propagation property. The dipole approximation, long a reliable feature of AMO physics, is not to be trusted, and new criteria must be adopted that are consonant with relativistic behavior. The penalty for a waste of research resources that was mentioned in connection with the explanation of ATI by a transverse-field method 14 years earlier than in terms of the dipole approximation, and the fallacious adiabaticity demand that also delayed progress by many years, is a caution that also applies to the LCFA model. Guidance in research activities allows for some investigation of the limits of applicability of the proposed nondipole correction of Eq. (10) or (12), but always with the knowledge that it lacks support as a reliable method.

Perhaps most important of all is the need to be aware that electromagnetic potentials are the essential determinants of the nature of electromagnetic phenomena, and that a dependence on electric and magnetic fields carries existential risks.

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