Low-frequency failure of the Göppert-Mayer gauge transformation and consequences for the Strong-Field Approximation

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Abstract

The Göppert-Mayer (GM) gauge transformation, of central importance in atomic, molecular, and optical physics since it connects the length gauge and the velocity gauge, becomes unphysical as the field frequency declines towards zero. This is not consequential for theories of transverse fields, but it is the underlying reason for the failure of gauge invariance in the dipole-approximation version of the Strong-Field Approximation (SFA). This failure of the GM gauge transformation explains why the length gauge is preferred in analytical approximation methods for fields that possess a constant electric field as a zero-frequency limit.
The Strong-Field Approximation (SFA) is the basic analytical method for the treatment of the interaction of nonperturbatively strong laser fields with atoms and molecules, but it is known to be gauge-dependent. It is important to note from the outset that results obtained herein apply only to theories that make a priori use of the dipole approximation. Such theories are identifiable by the fact that a zero-frequency limit exists, and that this limit corresponds to a constant electric field. In other words, this work applies only to longitudinal fields. Thus theories that are derived from propagating-wave formalisms are excluded, since such transverse-field theories have extremely low-frequency radio waves as a low frequency limit.

Gauge dependence of the SFA is probably shown most clearly in Ref. [1], where the length gauge (LG) results are plausible, but the velocity gauge (VG) results are not. This long-known lack of gauge invariance has led to statements of alarm, such as “... the SFA is not gauge invariant, which is really bad news for a theory.” [2] (emphasis from the original.) Another expression of concern is: “...how can a noninvariant theory be used for the calculation of observables?” [3].

The approach taken here for examination of the gauge problem is entirely general, with no dependence on the particular properties of any problem or class of problems beyond the statement that the field is treated as a longitudinal field (or the equivalent statement that the field has a zero-frequency limit corresponding to a static electric field). We start with a re-derivation of the known result [4, 5] that the static electric field can be described only within a unique gauge if all physical constraints are to be satisfied. A nominally alternative gauge is discarded on the grounds that it violates the physical condition that a charged particle in a static electric field represents a system for which total energy is conserved. It is then shown that this unphysical gauge arises from a Göppert-Mayer (GM) gauge transformation from the length gauge to the velocity gauge as applied to an oscillatory electric field in the zero frequency limit. This establishes the unphysical nature of the GM gauge transformation when zero frequency is a possibility. This is consequential in that photoelectron spectra that extend to zero frequency are a necessary part of any strong-field, nonperturbative problem. The GM gauge transformation from the LG to the VG is thus shown to be unphysical in the zero-frequency limit, leaving the LG as the only physical alternative. The two constraints of strong fields and the accessibility of a zero-frequency limit are all that is necessary to confirm the LG as the only physical gauge for the SFA in the form appropriate to oscillatory
Consider a static electric field with the amplitude $E_0$. It is known from electrostatics that this field can be specified by the scalar and vector potentials

$$\phi = -r \cdot E_0, \quad A = 0.$$  \hspace{1cm} (1)

A gauge transformation can be accomplished by a scalar generating function $\Lambda$ subject only to the constraint that the generating function satisfy the homogeneous wave equation

$$\partial^\mu \partial_\mu \Lambda = 0.$$  \hspace{1cm} (2)

The 4-vector potential following from a gauge transformation is

$$\tilde{A}^\mu = A^\mu + \partial^\mu \Lambda,$$  \hspace{1cm} (3)

which is equivalent to the transformed scalar and 3-vector potentials

$$\tilde{\phi} = \phi + \frac{1}{c} \partial t \Lambda,$$  \hspace{1cm} (4)

$$\tilde{A} = A - \nabla \Lambda.$$  \hspace{1cm} (5)

It is well-known that the representation of a static electric field by a scalar potential alone, as in Eq. (1) can be gauge-transformed so that the field can be described by a vector potential alone by using the generating function

$$\Lambda = c t r \cdot E_0,$$  \hspace{1cm} (6)

which leads to the new potentials

$$\tilde{\phi} = 0, \quad \tilde{A} = -c t E_0.$$  \hspace{1cm} (7)

The potentials in Eq. (7) are unphysical in the sense that a charged particle subject to those potentials is described by Lagrangian and Hamiltonian functions that possess explicit time dependence; and explicit time dependence of these system functions is a clear indicator that total energy is not conserved. This contrasts with the time independence of the potentials in Eq. (1), signifying energy conservation.

The formal foundations for Noether’s Theorem connecting symmetries with physical conservation laws are expressed in terms of the Lagrangian function. (See, for example, Ref.
The potentials (1) lead to a Lagrangian that has no explicit dependence on time, and thereby demonstrates energy conservation, whereas the potentials (7) signify a Lagrangian that depends explicitly on the time, and is thus unphysical.

The GM gauge transformation is usually expressed in terms of the vector potential that arises after the transformation. That is, the generator of the GM gauge transformation is usually written as

$$\Lambda^{GM} = -\mathbf{r} \cdot \tilde{\mathbf{A}}.$$  

(8)

This is exactly what follows from Eqs. (6) and (7), so the above discussion amounts to concluding that the GM gauge transformation is unphysical when $\omega = 0$.

Problems described by nonperturbative methods such as tunneling methods [7–10], have spectra that are always inclusive of zero frequency. This is straightforward to describe within the LG, but the extension to $\omega \to 0$ defies treatment within the VG.

The failure of the GM gauge transformation has no significance for transverse fields, such as laser fields. Such fields are propagating fields that do not have a zero frequency limit in the same sense as longitudinal fields. Propagating fields have extremely low-frequency radio fields as the limit when $\omega \to 0$ [5, 11]. The limit point of $\omega = 0$ cannot be achieved for a variety of (inter-related) reasons: propagation is not defined when $\omega = 0$; the magnetic field must always have the same magnitude as the electric field (in Gaussian units), so it can never be set to zero when the electric field is nonzero; $\omega \to 0$ implies wavelength $\lambda \to \infty$; the ponderomotive energy $U_p$ for a transverse field is proportional to $1/\omega^2$, so infinite energy must be supplied; there is no gauge freedom at all for propagating fields [4, 5]; and so on.

The overall conclusion is that the LG is the sole physical gauge for oscillatory electric fields when the zero-frequency limit must be considered.

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