PHYSICAL REVIEW A VOLUME 22, NUMBER 2 AUGUST 1980

Gauges for intense-field electrodynamics

Howard R. Reiss
*Department of Physics, University of Arizona, Tucson, Arizona 85721**
and Department of Physics, The American University, Washington, D.C. 20016†
(Received 10 December 1979)

For all gauges of the Göppert-Mayer type, the two-body Schrödinger equation for charged particles in a plane-wave electromagnetic field fails to separate into center-of-mass and relative-coordinate equations when the field is sufficiently intense.

I. INTRODUCTION

It was shown recently[1] that, for both charged and neutral two-body bound-state systems, "crossed" vector potential terms occur in the electric-field gauge which prevent separation of the Schrödinger equation into center-of-mass and relative-coordinate equations when the field intensity is high. This difficulty does not arise in Coulomb gauge (radiation gauge). The so-called electric-field gauge[2] is the simplest generalization to full space and time dependence of the Göppert-Mayer gauge,[3] which is a long-wavelength approximation.[4] It is the main purpose of this paper to show that this conclusion about intense-field difficulties in the electric-field gauge is true of all gauges of Göppert-Mayer type.

The procedure used is first to show that the separation problem that arises in the electric-field (EF) gauge exists as well in a quite different generalization of the Göppert-Mayer (GM) gauge. The other GM-type gauge employed is the Fiutak (F) gauge.[5] EF gauge is the simplest generalization of GM gauge to full space and time-coordinate dependence, whereas F gauge is a generalization of GM gauge which is more useful for dealing with multipole expansions. The common features of EF and F gauges are then used to extend the conclusions to all gauges of GM type.

Section II gives a brief discussion of the potentials and fields in GM, EF, and F gauges and Sec. III contains a treatment of the separability properties of the two-body Schrödinger equation.

II. POTENTIALS AND FIELDS

The general conditions stated in Ref. 1 are adopted here again. That is, the electromagnetic fields are taken to be plane-wave, source-free external fields describable by a four-vector potential A^μ. A gauge transformation of the four-potential is given by

$$A^\mu \to A^\mu + \partial^\mu \chi \,. \tag{1}$$

The Coulomb and EF gauges satisfy the transversality condition

$$k_\mu A^\mu = 0 \,, \tag{2}$$

and the Lorentz condition[6]

$$\partial_\mu A^\mu = 0 \,, \tag{3}$$

so that the gauge-transformation function connecting them satisfies the homogeneous wave equation

$$\partial_\mu \partial^\mu \chi = 0 \,. \tag{4}$$

In Eq. (2), k^μ is the propagation four vector of the field. The relativistic notation is one with a time-favoring real metric. That is, the metric tensor signature is 1, −1, −1, −1. Units with $\hbar = c = 1$ are used.

The starting gauge from which transformations are considered is the Coulomb (or radiation) gauge, in which the potentials are

$$A^0 = 0 \,, \quad \vec{A} = \vec{A}(k\cdot x) = \vec{A}(t, \vec{r}) \,, \tag{5}$$

with

$$k\cdot x \equiv k_\mu x^\mu = \omega t - \vec{k}\cdot\vec{r} \,, \tag{6}$$

and from Eqs. (2) and (3),

$$\vec{k}\cdot\vec{A} = 0 \,, \quad \vec{\nabla}\cdot\vec{A} = 0 \,. \tag{7}$$

Transformations to GM, EF, and F gauges are defined by the generating functions

$$\chi_{GM} = \vec{r}\cdot\vec{A}(t) \,, \tag{8a}$$

$$\chi_{EF} = \vec{r}\cdot\vec{A}(t,\vec{r}) = -x\cdot A(k\cdot x) \,, \tag{8b}$$

$$\chi_F = \int_0^1 du\, \vec{r}\cdot\vec{A}(t, u\vec{r}) \,. \tag{8c}$$

A covariant form is shown only for χ_{EF}, since the others are inherently noncovariant. The difference between Eq. (8a) and (8b) or (8c) is simply that the long-wavelength approximation[4] is used in Eq. (8a). In other words, the size of the bound system is presumed to be so small as compared to a wavelength that, in Eq. (6), one can take

$$|\vec{k}\cdot\vec{r}| \ll 1 \,, \quad k\cdot x \approx \omega t \,. \tag{9}$$

When Eq. (9) is satisfied, Eqs. (8b) and (8c) both reduce to Eq. (8a). Therefore, EF and F gauges

 © 1980 The American Physical Society

can both be regarded as generalizations of the GM gauge.

The potentials which follow from Eqs. (1), (5), and (8) are

$$A^o_{\rm GM}=-\vec{r}\cdot\vec{E}(t)\,,\quad \vec{A}_{\rm GM}=0\,; \tag{10a}$$

$$A^o_{\rm EF}=-\vec{r}\cdot\vec{E}(t,\vec{r})\,,\quad \vec{A}_{\rm EF}=-\vec{k}\omega^{-1}\vec{r}\cdot\vec{E}(t,\vec{r})\,; \tag{10b}$$

$$A^o_{\rm F}=-\int_0^1 du\,\vec{r}\cdot\vec{E}(t,u\vec{r})\,,\quad \vec{A}_{\rm F}=-\int_0^1 duu\,\vec{r}\times\vec{B}(t,u\vec{r})\,. \tag{10c}$$

The salient feature of the GM gauge is its lack of a vector potential. This is clearly a deficiency, since a time-dependent electromagnetic field obviously cannot be completely described by only a single component; but it is a defect of consequence only when multipolar corrections are required, and/or the field is intense.[1] The potentials of EF gauge satsify Eqs. (2) and (3) exactly, but the F gauge potentials do not. The fact that F gauge is neither transverse nor a Lorentz gauge is of no formal consequence, but it is an inconvenient loss of properties useful in analytical manipulations.

The long-wavelength forms of Eqs. (10a)–(10c) are

$$A^o_{\rm GM}=-\vec{r}\cdot\vec{E}(t)\,,\quad \vec{A}_{\rm GM}=0\,; \tag{11a}$$

$$A^o_{\rm EF}\approx-\vec{r}\cdot\vec{E}(t)\,,\quad \vec{A}_{\rm EF}\approx-\vec{k}\omega^{-1}\vec{r}\cdot\vec{E}(t)\,; \tag{11b}$$

$$A^o_{\rm F}\approx-\vec{r}\cdot\vec{E}(t)\,,\quad \vec{A}_{\rm F}\approx-\tfrac{1}{2}\vec{r}\times\vec{B}(t)\,. \tag{11c}$$

The F gauge long-wavelength vector potential can also be written in terms of electric fields as

$$A_{\rm F}\approx-\tfrac{1}{2}\vec{k}\omega^{-1}\vec{r}\cdot\vec{E}(t)+\tfrac{1}{2}\vec{E}(t)\omega^{-1}\vec{k}\cdot\vec{r}\,, \tag{11d}$$

when the plane-wave relation

$$\vec{B}=\omega^{-1}\vec{k}\times\vec{E} \tag{12}$$

is used. The scalar potentials in Eqs. (11a)–(11c) are all equal, but the vector potentials are not. In particular, the presence of a vector potential is vitally important when field intensity is high, which underlines the importance of not introducing the long-wavelength approximation too early. Even though the generating functions, Eqs. (8a)–(8c), are all the same in the long-wavelength case, the resulting vector potentials are not the same. The operations of carrying out the gauge transformation and going to the long-wavelength limit are not commutative.

The electric field is found from

$$\vec{E}=-\vec{\nabla}A^o-\partial_t\vec{A}\,, \tag{13}$$

where from Eqs. (10a)–(10c),

$$-\vec{\nabla}A^o_{\rm GM}=\vec{E}(t)\,,\quad -\partial_t\vec{A}_{\rm GM}=0\,; \tag{14a}$$

$$-\vec{\nabla}A^o_{\rm EF}=\vec{E}(t,\vec{r})-\vec{k}\omega^{-1}\vec{r}\cdot\partial_t\vec{E}(t,\vec{r})\,,\quad -\partial_t\vec{A}_{\rm EF}=\vec{k}\omega^{-1}\vec{r}\cdot\partial_t\vec{E}(t,\vec{r})\,; \tag{14b}$$

$$-\vec{\nabla}A^o_{\rm F}=\int_0^1 du\,\vec{E}(t,u\vec{r})-\int_0^1 duu\,\vec{k}\omega^{-1}\vec{r}\cdot\partial_t\vec{E}(t,u\vec{r})\,,\quad -\partial_t\vec{A}_{\rm F}=\vec{E}(t,\vec{r})-\int_0^1 du\,\vec{E}(t,u\vec{r})+\int_0^1 duu\,\vec{k}\omega^{-1}\vec{r}\cdot\partial_t\vec{E}(t,u\vec{r})\,. \tag{14c}$$

The two terms in Eq. (13) are evaluated separately in Eqs. (14a)–(14c) in order to show the presence of components in the longitudinal ($\vec{k}$) direction arising from the scalar potential used by itself. These longitudinal components are exactly canceled by vector potential contributions.

The magnetic field is found from

$$\vec{\nabla}\times\vec{A}_{\rm GM}=0\,, \tag{15a}$$

$$\vec{\nabla}\times\vec{A}_{\rm EF}=\omega^{-1}\vec{k}\times\vec{E}(t,\vec{r})\,, \tag{15b}$$

$$\vec{\nabla}\times\vec{A}_{\rm F}=\vec{B}(t,\vec{r})\,. \tag{15c}$$

The results of Eqs. (15b) and (15c) are, of course, identical in view of Eq. (12). The great deficiency of the GM gauge shows glaringly in Eq. (15a). With no vector potential, there can be no magnetic field. Yet, for a true plane wave, magnetic and electric fields are of equal magnitude. This is not normally of consequence in the long-wavelength, nonrelativistic situation appropriate to most problems in atomic and molecular physics; but when the field is intense, the magnetic field (and hence the vector potential) is vitally important.[1]

III. SEPARABILITY OF EQUATIONS OF MOTION

The essential conclusion of Sec. VI of Ref. 1 is that the presence of a strongly position-coordinate-dependent vector potential in the two-body Schrödinger equation in EF gauge, makes it impossible to separate the equation into independent center-of-mass and relative-coordinate equations when the field intensity is high. Exactly the same conclusion holds true for F gauge. When the two-body Schrödinger equation for particles of masses m_1, m_2 and charges e_1, e_2 is expressed in F gauge, and then written in terms of the center-of-mass coordinate $\vec{R}$ and relative coordinate $\vec{r}$, the result is

$$\begin{aligned} i\partial_t\psi(\vec{r},\vec{R}) = [& -e_t\vec{E}\cdot\vec{R} - e_r\vec{E}\cdot\vec{r} \\ & + (1/2m_t)(-i\vec{\nabla}_R + \tfrac{1}{2}e_t\vec{R}\times\vec{B} + \tfrac{1}{2}e_r\vec{r}\times\vec{B})^2 \\ & + (1/2m_r)(-i\vec{\nabla}_r + \tfrac{1}{2}e_r\vec{R}\times\vec{B} + \tfrac{1}{2}e_e\vec{r}\times\vec{B})^2 \\ & + V(r)]\psi(\vec{r},\vec{R}) , \end{aligned} \tag{16}$$

in exact analogy to Eq. (63) of Ref. 1. In Eq. (16), the long-wavelength form of F gauge is used, as in Eq. (11c), $\vec{B}$ means $\vec{B}(t)$, and the total mass and charge (m_t, e_t), reduced mass and charge (m_r, e_r), and effective charge (e_e) are defined in Eqs. (54), (55), and (64) of Ref. 1. Equation (16) has the crossed vector potential term $\frac{1}{2}e_r\vec{r}\times\vec{B}$ which appears with the $-i\vec{\nabla}_R$ operator, and the term $\frac{1}{2}e_r\vec{R}\times\vec{B}$ which accompanies the $-i\vec{\nabla}_r$ operator. These crossed vector potential terms are completely negligible at ordinary field intensities, but block the separation of variables in Eq. (16) when field intensity is high. Since the separation-blocking terms are of exactly the same order of magnitude as the corresponding EF gauge terms explored in Ref. 1 (since $|\vec{E}| = |\vec{B}|$), the consequences are the same. The conclusions in Eqs. (67) and (69) of Ref. 1 are that $z_m \ll 1$ for separability, where z_m is an intensity parameter which may be written as[1]

$$z_m = e^2\langle\vec{E}^2\rangle/2m^2\omega^2 = e^2\langle\vec{B}^2\rangle/2m\omega^2 \tag{17}$$

for a plane wave in a nonrelativistic problem. The angular brackets in Eq. (17) refer to a time average over a wave period.

The separability problem in EF and F gauges is generic to all gauges of the GM type. The reason is the multiplicative position vector that appears in the potentials, as shown in Eqs. (10) and (11). This is a consequence of its appearance in the gauge-transformation functions of Eq. (8). The two-body Schrödinger equation separates without difficulty in Coulomb gauge because the only position dependence is in the argument of the vector potential, and not in a multiplicative factor. When Eq. (9) is satisfied, separation in Coulomb gauge is entirely unambiguous and multipole corrections will always be small, regardless of field intensity. However, no matter how large the wavelength as compared to the size of the bound system, a sufficiently high field intensity, as measured by z_m, makes any generalization of the GM gauge unusable.

---

*Present address.

†Permanent address.

[1]H. R. Reiss, Phys. Rev. A 19, 1140 (1979).

[2]This name was chosen because both scalar and vector potentials can be expressed very naturally in terms of the electric-field vector. However, the potentials could also be rewritten in terms of the magnetic field, and it must be kept clearly in mind that the expressions are potentials and not fields.

[3]M. Göppert-Mayer, Ann. Phys. (Leipzig) 9, 273 (1931).

[4]In Ref. 1, the terms "dipole approximation" and "long-wavelength approximation" were used interchangeably, as is often done. They are not identical, and the distinction is important in the intense-field case. As shown by the inadequacy of the GM gauge, a simple electric-dipole approximation is not valid when fields are intense. I wish to thank D. H. Kobe for raising this issue.

[5]J. Fiutak, Can. J. Phys. 41, 12 (1963).

[6]Equations (2) and (3) are equivalent in Coulomb gauge. The correspondence between these conditions remains in EF gauge, but it is much less direct.