N94-10596

NON-GAUGE PHASE TRANSFORMATIONS IN QUANTUM TRANSITION AMPLITUDES

H. R. Reiss
Department of Physics, The American University
Washington, DC 20016-8058, USA

Abstract

The prescription for introducing a gauge transformation into a quantum transition amplitude, nominally well known, contains an ambiguous feature. It is presumed by some authors that an appropriate transformation of the phase of a wave function will generate the associated gauge transformation. It is shown that this is a necessary but not sufficient step. Examples from the literature are cited to show the consequences of the failure of this procedure. One must distinguish between true gauge transformations and unitary transformations within a fixed gauge.

1. Introduction

The necessary procedure to introduce a change of gauge in quantum mechanics is quite standard [1,2]. (We adopt the terminology that the phrase "gauge transformation" implies the so-called "gauge transformation of the second kind" [1].) This quantum-mechanical procedure begins with a change in the potentials employed to represent an electromagnetic field, and then associates with these altered potentials a changed interaction Hamiltonian and a particular phase transformation of the wave function. Some practitioners presume the inverse: that the phase transformation of the wave function will always imply that a gauge transformation has been done. It is the aim of this paper to show that this inverse procedure does not necessarily produce a gauge transformation, and that significant misinterpretations can occur thereby.

When a non-gauge-changing unitary transformation (a "phase transformation") is presumed to actually produce a gauge transformation, it may not have practical ill consequences. In some cases, it simply induces an identity transformation in the

PRECEDING PAGE BLANK NOT FILMED

transition amplitude. The outcome is less benign when the non-gauge phase transformation is interpreted as a gauge transformation, and used to infer further physical conclusions. For example, this has led to the concept that one particular gauge is more fundamental than others. These difficulties are discussed in Sec. 3 after a review of basic information in Sec. 2.

2. Formal Background

The approach taken here is that of semi-classical electrodynamics. Quantization of the field is not necessary for present purposes. Both relativistic and non-relativistic formulations will be used; relativistic because matters are clearer in that context, and non-relativistic because that is where the difficulties have actually occurred. It is presumed throughout that the fields and the gauge-transformation functions are explicitly time dependent.

A gauge transformation of the electromagnetic four-vector potential A^μ by the real, scalar generating function Λ is accomplished by

$$A^\mu \rightarrow A^{G\mu} = A^\mu - \partial^\mu \Lambda \tag{2.1}$$

or the non-relativistic equivalent

$$\phi \rightarrow \phi^G = \phi - \partial\Lambda/\partial(ct) \tag{2.2}$$

$$\vec{A} \rightarrow \vec{A}^G = \vec{A} + \vec{\nabla}\Lambda, \tag{2.3}$$

where $A^\mu=(\phi,\vec{A})$. This is accompanied in quantum mechanics by a change in the phase of the wave function induced by the unitary transformation

$$\Psi \rightarrow \Psi^G = U\Psi, \tag{2.4}$$

with

$$U = exp(ie\Lambda). \tag{2.5}$$

When one wishes to change the gauge in which a transition amplitude is expressed, it is necessary to know how the Hamiltonian is transformed. It follows directly from the Schrödinger equation that this transformed Hamiltonian operator is given by

$$H^G - i\hbar\partial/\partial t = U\,(H - i\hbar\partial/\partial t)\,U^\dagger, \tag{2.6}$$

or, equivalently, by [3,4]

$$H^G = UHU^\dagger - i\hbar\dot{U}U^\dagger = UHU^\dagger + i\hbar U\dot{U}^\dagger, \tag{2.7}$$

where the dot on the U indicates the time derivative. The Dirac analog of this Schrödinger result is instructively simple. From the Dirac equation

$$(i\partial\!\!\!/ - eA\!\!\!/ - m)\Psi = 0, \tag{2.8}$$

one obtains

$$U(i\partial\!\!\!/ - eA\!\!\!/ - m)U^{\dagger}U\Psi = (i\partial\!\!\!/ - eA\!\!\!/^{G} - m)\Psi^{G} = 0, \tag{2.9}$$

where $A\!\!\!/ \equiv \gamma^{\mu}A_{\mu}$, and A_{μ}^{G} is given by Eq.(2.1).

The transition amplitude employed will be the generic form

$$(S-1)_{fi} = -(i/\hbar)\int dt\ (\Phi_f, H_I\Psi_i), \tag{2.10}$$

which is commonplace in scattering theory, but is useful also in bound-state problems. It represents a physical situation in which the transition-inducing electromagnetic field is not present at asymptotic times, i.e., there is no field present at large negative times when the initial state is prepared and at large positive times when final measurement of the transition products is made. The state Φ is one with no electromagnetic field present. Its Hamiltonian will be called H_0. The state Ψ satisfies the Schrödinger equation with full interaction. In other words,

$$(i\hbar\partial_t - H_0)\Phi = 0, \tag{2.11}$$

$$(i\hbar\partial_t - H)\Psi = 0, \tag{2.12}$$

$$H = H_0 + H_I. \tag{2.13}$$

For the usual problem in which an atomic or molecular potential V is present at asymptotic times, as distinct from the electromagnetic field whose application causes transitions, one can state

$$H_0 = (p^2/2m)+V,\ H_I = (1/2m)(e\vec{p}\cdot\vec{A}/c + e\vec{A}\cdot\vec{p}/c + e^2A^2) + e\phi \tag{2.14}$$

in an arbitrary gauge, where no stipulation has been made as to how the field is to be represented by scalar or vector potentials, or a combination of both. To be as straightforward as possible in this formalism, it is required that the field is to be turned on and off adiabatically, so that one can require the vector potential at both positive and negative asymptotic times to be the same (nominally zero). This restriction is known [3-8] to assure that the same physical result will arise from the transition amplitude in Eq.(2.10) in different gauges, but with the use of exactly the same non-interacting wave function Φ_f, regardless of the choice of gauge for H_I and Ψ_i.

Finally, the relativistic transition amplitude analogous to

Eq.(2.10) is stated [9]

$$(S-1)_{fi} = -(i/\hbar) \int d^4x \, \bar{\Phi}_f e\not{A}\Psi_i, \tag{2.15}$$

where $\bar{\Phi}$ is the Dirac adjoint $\bar{\Phi}\equiv\Phi^\dagger\gamma^0$, and a static binding potential is singled out, so that the non-interacting and interacting Dirac equations are, respectively,

$$(i\partial\!\!\!/ - \gamma^0 V - m)\Psi = 0 \tag{2.16}$$

$$(i\partial\!\!\!/ - e\not{A} - \gamma^0 V - m)\Psi = 0. \tag{2.17}$$

3. Statement of the Problem

Whereas there is really no ambiguity in the information reviewed in Sec. 2, the way in which it is employed in the literature is not uniform. A simple unifying concept which serves to characterize the inconsistencies which arise is to note that they all stem from the improper notion that a gauge-change-like unitary transformation applied to the wave function is a guarantee that a gauge change has actually occurred.

Possibly the simplest example of this problem occurred in connection with the demonstration [10,11] that the substitution $\Psi\approx U\Phi$ in Eq.(2.10) (for a particular choice of U) can give a good approximation for certain classes of transitions in which dressing by a low frequency field is present. The result of this approximation is that Eq.(2.10) becomes

$$(S-1)_{fi} = -(i/\hbar) \int dt \, (\Phi_f, H_I U \Phi_i). \tag{3.1}$$

This has, however, been characterized as a gauge transformation [12] solely on the grounds of the presence of the unitary factor U, even though there is no transformation at all of the interaction Hamiltonian H_I.

Another example is a procedure intended to change the gauge in which a transition amplitude is expressed in a fashion which is purported to be "manifestly gauge invariant". The device employed is simply to insert a unit operator into the transition amplitude in the form of $U^\dagger U$. Then the U factors are attached to the wave functions, and a gauge transformation is presumed to be accomplished. (A clear example of this is in Ref.13.) Equation (2.10) would then become

$$\begin{aligned}(S-1)_{fi} &= -(i/\hbar) \int dt \, (\Phi_f, H_I U^\dagger U \Psi_i) \\ &= -(i/\hbar) \int dt \, ((U\Phi_f), (UH_I U^\dagger)(U\Psi_i)).\end{aligned} \tag{3.2}$$

Since the wave functions now bear the unitary transformation factors U as in Eq.(2.4), they are regarded by some authors as being in a new gauge.

There are several defects with the above procedure. One is

the fact that the non-interacting wave function Φ is transformed as well as the interacting wave function Ψ. This fact has been noted by some authors, and concluded to be necessary [13-18]. A corollary of this procedure is that there then exists a preferred gauge, since only in one gauge is it possible to have the non-interacting wave function appear without its unitary transformation factor. The preferred gauge normally selected is the so-called "length gauge", or "EF" gauge, where the dipole-approximation interaction Hamiltonian is $H_I=-e\vec{E}\cdot\vec{r}$. For example, the statement is made that [14] "... the textbook wave functions can, in general, only be applied in the $\vec{E}\cdot\vec{r}$ formalism ...". The presumed necessity to apply a field-dependent gauge transformation factor to represent a non-interacting state in any gauge other than the length gauge has been termed an oxymoron [19].

Another problem with the procedure expressed in Eq.(3.2) is that the interaction Hamiltonian is not properly stated. The true gauge-transformed interaction Hamiltonian follows from Eq.(2.6) or (2.7), taken together with Eq.(2.13). By contrast, the form

$$H_I^P = UH_IU^\dagger \tag{3.3}$$

is simply a unitary (or phase) transformation of the operator H_I. It is not the gauge-transformed interaction Hamiltonian. The actual gauge-transformed interaction Hamiltonian is given by

$$H_I^G = UH_IU^\dagger + (UH_0U^\dagger - H_0) + i\hbar\dot{U}U^\dagger. \tag{3.4}$$

The clearest way to see the true meaning of Eq.(3.2) is to employ the relativistic form given in Eq.(2.15). The lack of second order differential operators in the Dirac equation and the simple form $e\not{A}$ for the interaction term makes the relativistic form especially clear for formal purposes. The procedure analogous to Eq.(3.2) employed in Eq.(2.15) gives

$$\begin{aligned}(S-1)_{fi} &= -(i/\hbar)\int d^4x\ \bar{\Phi}_f e\not{A}U^\dagger U\Psi_i \\ &= -(i/\hbar)\int d^4x\ (\overline{U\Phi}_f)e\not{A}(U\Psi_i),\end{aligned} \tag{3.5}$$

since U always commutes with $e\not{A}$. Equation (3.5) shows plainly that there is no gauge transformation at all. The interaction term remains identically the same as the original, and does not transform to the new gauge as would follow from Eq.(2.1).

The procedure in Eq.(3.5), as in Eq.(3.2), is simply a unitary transformation within a fixed gauge.

4. Resolution of the Problem

The resolution of the ambiguities discussed above is straightforward. One simply states a transition amplitude in an unspecified gauge, containing all four components of the electromagnetic potential function, as given in, for example,

Eq.(2.15). In a particular gauge, designated by the superscript (a), this is

$$(S-1)_{fi} = -(i/\hbar) \int d^4x \, \bar{\Phi}_f e\not{A}^{(a)} \Psi_i^{(a)}. \tag{4.1}$$

In gauge (b), it is

$$(S-1)_{fi} = -(i/\hbar) \int d^4x \, \bar{\Phi}_f e\not{A}^{(b)} \Psi_i^{(b)}. \tag{4.2}$$

The non-interacting state Φ_f is the same in both instances since it is independent of the field. This is the type of transparent gauge invariance that has also been given the name "manifest gauge invariance" [19], although that description is risky, since the same phrase means different things to different researchers. A better name would be "strong gauge invariance", since it so strongly stresses the complete equivalence of all gauges.

There is no clear algebraic transformation that connects Eq.(4.1) with (4.2). Nevertheless, they must be equivalent if all gauges are equally valid. This has been shown by calculation of practical examples [6,7] as well as by the demonstration [3] that the formal difference between the expressions which are the non-relativistic analogs of Eqs.(4.1) and (4.2) has a null result.

The mis-identification of the simple phase transformation in Eq.(3.2) or (3.4) as a gauge transformation follows from an attempt to achieve algebraic identity between transition amplitudes in different gauges. What is achieved instead is simply a unitary transformation within a fixed gauge.

Another motivation for employing Eq.(3.3) as a gauge-transformed interaction Hamiltonian in place of Eq.(3.4) makes use of arguments [14,15] involving dependence on the dipole approximation and on the preferred use of the $\vec{E}\cdot\vec{r}$ interaction. Such arguments are inherently risky. One cannot view as fundamental a formalism which depends critically on an interaction which cannot extend to very strong fields or to the presence of significant magnetic influences.

5. Acknowledgment

Support for this work comes from the National Science Foundation under Grant No. PHYS-9113926.

References

[1] J. M. Jauch and F. Rohrlich, *The Theory of Photons and Electrons* (Addison-Wesley, Cambridge, MA, 1955).

[2] C. Cohen-Tannoudji, J. Dupont-Roc, and G. Gilbert, *Photons and Atoms* (Wiley, New York, 1989).

[3] Y. Aharonov and C. K. Au, Phys. Rev. A **20**, 1553 (1979).

[4] Y. Aharanov and C. K. Au, Phys. Lett. **86A**, 269 (1981).

[5] E. A. Power and S. Zienau, Philos. Trans. Roy. Soc. **251**, 427 (1959).

[6] J. J. Forney, A. Quattropani, and F. Bassani, Nuovo Cimento **37B**, 78 (1977).

[7] F. Bassani, J. J. Forney, and A. Quattropani, Phys. Rev. Lett. **39**, 1070 (1977).

[8] G. Grynberg and E. Giacobino, J. Phys. B **12**, L93 (1979).

[9] J. D. Bjorken and S. D. Drell, *Relativistic Quantum Mechanics* (McGraw-Hill, New York, 1964).

[10] H. R. Reiss, Phys. Rev. A **1**, 803 (1970).

[11] H. R. Reiss, Phys. Rev. A **39**, 2449 (1989).

[12] C. Cohen-Tannoudji, J. Dupont-Roc, C. Fabre, and G. Grynberg, Phys. Rev. A **8**, 2747 (1973).

[13] C. Leone, S. Bivona, R. Burlon, F. Morales, and G. Ferrante, Phys. Rev. A **40**, 1828 (1989).

[14] W. E. Lamb, R. R. Schlicher, and M. O. Scully, Phys. Rev. **36**, 2763 (1987).

[15] K. H. Yang, Ann. Phys. (N.Y.), **101**, 62 (1976).

[16] J. Bergou, J. Phys. B **16**, L647 (1983).

[17] G. P. Arrighini, C. Guidotti, and N. Durante, Nuovo Cimento **9D**, 1219 (1987).

[18] R. Burlon, C. Leone, F. Trombetta, and G. Ferrante, Nuovo Cimento **9D**, 1033 (1987).

[19] J. L. Friar and S. Fallieros, Phys. Rev. C **34**, 2029 (1986).