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Equivalence of path dependence and gauge dependence

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Abstract. The equivalence of path dependence and gauge dependence is established by showing that, for every set of the path dependent expansion coefficients of a wavefunction, there exists one identical set of the conventional, gauge dependent expansion coefficients of a wavefunction in another gauge. This equivalence is further demonstrated through simple examples of a quantum particle interacting with a classical radiation field in the dipole approximation.

1. Introduction

Recently Feuchtwang *et al* (1982, 1984a, b) and Kazes *et al* (1983), in an effort to understand the $A \cdot p$ versus $r \cdot E$ controversy raised by Lamb (1952) and the more fundamental question of gauge transformations and gauge invariance in quantum mechanics, rediscovered the path dependent procedure (PDP) of constructing transition probabilities, first formulated by DeWitt (1962). They proposed the PDP in their 1982 paper, and used it to criticise the gauge invariant formulation (GIF) (Yang 1976a), apparently unaware that the PDP suffers from the ambiguity of path dependence (Lee *et al* 1983) and that the PDP and the closely related path-averaging procedure had been examined in Yang (1976a) in which the GIF was first proposed. Later in Kazes *et al* (1983) and Feuchtwang *et al* (1984a, b) they realised the path dependence of the PDP, but insisted that their transition probabilities were gauge independent and path dependent.

The insistence that a quantity can be simultaneously gauge independent and path dependent seems to imply that the 'path property,' whatever it may be, is a fundamental property in quantum mechanics. This would be of great interest to theoretical physics, especially concerning the fundamental symmetry properties of the Schrödinger equation. Furthermore, the insistence that path dependent quantities can be interpreted as transition probabilities seems also to suggest that, somehow, one path can be experimentally distinguished from another. (Feuchtwang *et al* and Kazes *et al* take the traditional point of view that gauge dependent quantities cannot be experimentally measured and hence cannot be interpreted as transition probabilities.)

The history of the path dependent procedure is quite interesting. DeWitt (1962), in a dispute with Aharonov and Bohm (AB) on their interpretation of the significance of potentials in the AB effect (Aharonov and Bohm 1959, 1961), first constructed what he called the gauge independent wavefunction and potentials, apparently unaware of their path dependence. (This dispute was settled on the observation of Aharonov and Bohm (1962, 1963) that the AB effect could be regarded as a result of either the local interaction of charges with potentials or the nonlocal interaction of charges with fields.)

DeWitt's gauge independent wavefunction and potentials were later shown to be path dependent by Mandelstam (1962) who also used the formalism to quantise electromagnetic fields.

The first work to hint at a relation between gauge dependence and path dependence was by Belinfante (1962), who conjectured that a path was just a 'gauge'. Because of this insight he set out to devise the path averaging procedure, in an attempt to get rid of this path dependence. By averaging the path dependent potentials over the paths he chose, he obtained the potentials in the Coulomb gauge. Three years later, Rohrlich and Strocchi (1965), who were not satisfied with Belinfante's choice of noncovariant paths, applied the procedure to average over covariant paths. They obtained the potentials in the Lorentz gauge.

These two studies show a very important point. It is that the path dependent potentials cannot be gauge independent. This is because all quantities used in the path averaging are functions only of the electromagnetic fields and paths. If the path dependent potentials are truly gauge independent, the results from the path averaging must remain gauge independent and cannot be expressed in terms of potentials in the Coulomb or Lorentz gauge.

Because the path dependent potentials cannot be gauge independent, it then follows from consideration with the Schrödinger equation that the path dependent wavefunction cannot be gauge independent. Furthermore, since the eigenfunctions of the unperturbed Hamiltonian have neither gauge nor path dependence, the expansion coefficients of the path dependent wavefunction in this basis set of functions therefore cannot be gauge independent.

Another point of value also developed from the dispute between DeWitt and AB. Aharonov and Bohm (1962, 1963) commented that DeWitt's formalism did not fundamentally solve the gauge problem in quantum mechanics, but only put it in a different disguise.

The purpose of this paper is to prove the complete equivalence of the gauge dependence and the path dependence. In § 2, we first review the gauge dependence of the conventional expansion coefficients of the wavefunction. (All necessary proofs can be found in the references quoted therein.) Then, we review the $A \cdot p$ versus $r \cdot E$ controversy and point out its underlying reasons. In § 3, we first review the path dependent procedure as currently used by Feuchtwang *et al.* Then we establish the complete equivalence of the path dependence and the gauge dependence by showing that, for every set of the path dependent expansion coefficients of a wavefunction with an arbitrary choice of the path, there exists one identical set of the conventional, gauge dependent expansion coefficients of a wavefunction in a different gauge. The wavefunction, Hamiltonian and potentials in this other gauge will be constructed from the original wavefunction, potentials and choice of path. This equivalence is later demonstrated in three simple examples of a charged particle in eracting with a classical radiation field in the dipole (i.e., long wavelength) approximation. Finally, we present our conclusions in § 4.

2. The conventional interpretation and the $A \cdot p$ versus $r \cdot E$ controversy

In this section, we shall briefly review the conventional approach to the problem of constructing the quantum mechanical probability amplitudes and probabilities, which is what Lamb (1952) called 'the usual interpretation', and how it leads to the $A \cdot p$

versus $\mathbf{r} \cdot \mathbf{E}$ controversy. The underlying reason for this controversy has now been well understood. It is because the conventional expansion coefficients are gauge dependent, or stated differently, the 'unperturbed' Hamiltonian is, in general, not a true physical quantity (Yang 1976a, 1982a, b, Cohen-Tannoudji *et al* 1977, Kobe and Smirl 1978, Park 1979, Lee and Albrecht 1983). Nevertheless, we shall review its basic contents here for our discussion of the path dependent method recently rediscovered by Feuchtwang *et al* and Kazes *et al*.

2.1. The conventional interpretation

Let us assume a nonrelativistic, spinless quantum particle of mass m and charge e subject to an electrostatic field $\mathbf{E}_0(\mathbf{r}) = -\nabla V_0(\mathbf{r})$ (e.g., the Coulombic field due to the nuclear charge) and a laser radiation field $\mathbf{E}(\mathbf{r}, t)$ and $\mathbf{B}(\mathbf{r}, t)$. If we use two sets of potentials (\mathbf{A}^g, Φ^g) and $(\mathbf{A}^{g'}, \Phi^{g'})$ to represent the laser field, then

$$\begin{aligned} \mathbf{E} &= -\nabla\Phi^g - c^{-1} \partial\mathbf{A}^g/\partial t = -\nabla\Phi^{g'} - c^{-1} \partial\mathbf{A}^{g'}/\partial t, \\ \mathbf{B} &= \nabla \times \mathbf{A}^g = \nabla \times \mathbf{A}^{g'}. \end{aligned} \quad (2.1)$$

These two sets of potentials are then related by a gauge transformation:

$$\mathbf{A}^{g'} = \mathbf{A}^g + \nabla\chi^{g'g}(\mathbf{r}, t), \quad \Phi^{g'} = \Phi^g - c^{-1} \partial\chi^{g'g}(\mathbf{r}, t)/\partial t. \quad (2.2)$$

The Schrödinger equations for these two gauges are:

$$i\hbar \partial\Psi^g/\partial t = H^g\Psi^g, \quad H^g = (\mathbf{p} - e\mathbf{A}^g/c)^2/2m + eV_0 + e\Phi^g; \quad (2.3)$$

$$i\hbar \partial\Psi^{g'}/\partial t = H^{g'}\Psi^{g'}, \quad H^{g'} = (\mathbf{p} - e\mathbf{A}^{g'}/c)^2/2m + eV_0 + e\Phi^{g'}. \quad (2.4)$$

It then follows that

$$\Psi^{g'}(\mathbf{r}, t) = U^{g'g}\Psi^g(\mathbf{r}, t), \quad U^{g'g}(t) = \exp[ie\chi^{g'g}(\mathbf{r}, t)/\hbar c]. \quad (2.5)$$

To review the conventional interpretation, we first construct the 'unperturbed' Hamiltonian H_0 by

$$H_0 = \mathbf{p}^2/2m + eV_0, \quad (2.6)$$

and then its eigenvalues $\{\epsilon_j\}$ and the associated orthonormal and complete (assumed) set of eigenfunctions $\{\phi_j^0(\mathbf{r})\}$ by

$$H_0\phi_j^0(\mathbf{r}) = \epsilon_j\phi_j^0(\mathbf{r}), \quad \langle\phi_j^0|\phi_k^0\rangle = \delta_{jk}. \quad (2.7)$$

Note, the superscript '0' in the eigenfunctions is to indicate that these functions have no dependence on the gauges chosen for the Hamiltonians. The conventional interpretation consists of constructing the expansion coefficients $\{c_j^g(t)\}$ for Ψ^g and $\{c_j^{g'}(t)\}$ for $\Psi^{g'}$ by

$$c_j^g(t) = \langle\phi_j^0|\Psi^g(t)\rangle, \quad (2.8)$$

$$c_j^{g'}(t) = \langle\phi_j^0|\Psi^{g'}(t)\rangle, \quad (2.9)$$

and interpreting these expansion coefficients as probability amplitudes for finding the particle in the eigenstates of the 'unperturbed' Hamiltonian H_0 .

There are numerous ways to understand the gauge dependence of these conventional expansion coefficients. Here, we only discuss three, which complement one another.

First, the ‘unperturbed’ Hamiltonian H_0 is in general a nonphysical quantity (Cohen-Tannoudji *et al* 1977) and it is not form invariant under gauge transformations,

$$U^{g'g}H_0(U^{g'g})^\dagger \neq H_0. \tag{2.10}$$

Second, the gauge dependence is shown explicitly through the mathematical expression (Kobe and Smirl 1978, Lee and Albrecht 1983)

$$c_j^{g'}(t) = \sum_k \langle \phi_j^0 | U^{g'g} | \phi_k^0 \rangle c_k^g(t). \tag{2.11}$$

We now discuss the third way, which is perhaps most relevant to our later discussion of the path dependent method. By definition, all electromagnetic potentials are gauge dependent†. Hence, all wavefunctions are gauge dependent and there does not exist a set of ‘gauge independent’ electromagnetic potentials. Because all wavefunctions are gauge dependent, and because the eigenfunctions of the ‘unperturbed’ Hamiltonian have no gauge dependence, it then follows that the conventional expansion coefficients are gauge dependent. As is now clear from our notation, the $\{c_j^g(t)\}$ carry with them faithfully all the gauge dependence of the wavefunction $\Psi^g(\mathbf{r}, t)$. This gauge dependence of the conventional expansion coefficients is what causes the $\mathbf{A} \cdot \mathbf{p}$ versus $\mathbf{r} \cdot \mathbf{E}$ controversy, first raised by Lamb (1952).

2.2. The $\mathbf{A} \cdot \mathbf{p}$ versus $\mathbf{r} \cdot \mathbf{E}$ controversy

In his pioneering work of the measurement of the fine structure spectrum of the hydrogen atom, Lamb (1952) discovered that, when an RF field was used to quench the metastable state, different forms of the interaction Hamiltonian predicted different quenching cross sections. He investigated the two familiar forms of interaction Hamiltonian in the long wavelength and lowest-order approximation in the radiation gauge (R-gauge) and in the electric-field gauge (E-gauge). Under this approximation of the fields ($\mathbf{E}(\mathbf{r}, t) \approx \mathbf{E}(\mathbf{0}, t)$ and $\mathbf{B}(\mathbf{r}, t) \approx \mathbf{0}$), these two sets of potentials are:

$$\mathbf{A}^R(\mathbf{r}, t) = \mathbf{A}^R(\mathbf{0}, t), \quad \Phi^R(\mathbf{r}, t) = 0, \tag{2.12}$$

$$\mathbf{A}^E(\mathbf{r}, t) = 0, \quad \Phi^E(\mathbf{r}, t) = -\mathbf{r} \cdot \mathbf{E}(\mathbf{0}, t), \tag{2.13}$$

with

$$\mathbf{E}(\mathbf{0}, t) = -c^{-1} \partial \mathbf{A}^R(\mathbf{0}, t) / \partial t. \tag{2.14}$$

Lamb then solved for the conventional expansion coefficients $\{c_j^R(t)\}$ and $\{c_j^E(t)\}$ in these two gauges, using the two-state approximation, the rotating-wave approximation and with decay constants added phenomenologically to simulate the spontaneous emissions. By comparing these two sets of solutions with his quenching curves, he concluded that ‘the usual interpretation’ of probability amplitudes was correct only in the E-gauge and that the expansion coefficients $\{c_j^R(t)\}$ in the R-gauge did not generate

† This is because the word ‘gauge’ is used to designate a particular procedure by which a particular set of potentials is constructed from a given field. Thus, the word ‘gauge’ is simply a convenient and necessary mathematical indexation in sorting out a particular set of potentials from the many-to-one correspondence between all potentials for a given field and the field. Hence every set of potentials must carry with it an index or gauge to show how it is constructed and also to distinguish it from all others. For a discussion on this point with similar implications, see Cohen-Tannoudji *et al* (1977). For further information on electromagnetic gauges and their implications in the propagation and other properties of potentials, see Brill and Goodman (1967), Jackson (1975), Yang (1976b, 1981) and Sorg (1981).

the correct (meaning experimental) results. This conclusion of Lamb has stimulated many papers trying to explain or counter-explain his observation. For a list of papers involved in this controversy, see Yang (1982a). For a gauge invariant explanation of Lamb's result, see Yang (1976a), Kobe and Smirl (1978), Park (1979) and Lee and Albrecht (1983). See Cohen-Tannoudji *et al* (1977) and Yang (1982b) for the fundamentals of gauge invariance.

Just from the knowledge in § 2.1, one can understand Lamb's result. It is because the conventional expansion coefficients are gauge dependent. Hence, the interpretation of these coefficients as probability amplitudes cannot be valid in more than one gauge. Lamb's observation only emphasises this point. What is surprising, however, is that there even exists a gauge (the E-gauge) in which the gauge dependent conventional interpretation is physically correct. In order to fully understand this point, one must refer to the relevant literature on gauge invariance quoted earlier.

3. Gauge dependence of the path dependent procedure

In their quest for a procedure of constructing the quantum mechanical transition probabilities that can explain Lamb's results, Feuchtwang *et al* have rediscovered the path dependent procedure. This path dependent method was first formulated by DeWitt (1962) in a slightly different form. The method was later examined carefully by Mandelstam (1962), Belinfante (1962), Rohrlich and Strocchi (1965), Yang (1976a) and, more recently, Lee *et al* (1983). All these authors have found that the method suffers from the ambiguity of path dependence. As a consequence of this path dependence, the transition probabilities cannot be unique even for a single given gauge. (See also Yang (1976a) for a discussion on the path averaging method used by Belinfante and by Rohrlich and Strocchi in their attempt to eliminate this path dependence.)

Belinfante (1962) pointed out in his paper that path dependence was just a 'gauge' dependence (unfortunately without the necessary mathematical proof). In this section, we shall prove exactly Belinfante's insight that path dependence *is* gauge dependence. The proof will be illustrated with explicit examples using the potentials in (2.12) and (2.13).

3.1. Review of the path dependent procedure

Here, we review the path dependent procedure of Feuchtwang *et al* (1982, 1984a, b) and Kazes *et al* (1983). For any arbitrary gauge g with potentials (A^g, Φ^g) , they first construct the phase function $\eta^\Gamma(\mathbf{r}, t)$ by

$$\begin{aligned} \eta^\Gamma(\mathbf{r}, t) &= \int_{(\mathbf{r}_i, t_i)}^{(\mathbf{r}, t)} A_\mu^g[x(\gamma)] dx_\mu(\gamma) \\ &= \int_{(\mathbf{r}_i, t_i)}^{(\mathbf{r}, t)} \{A^g[s(\gamma), \tau(\gamma)] \cdot ds(\gamma) - c\Phi^g[s(\gamma), \tau(\gamma)] d\tau(\gamma)\}, \end{aligned} \quad (3.1)$$

where γ is a parameter designating a particular path starting from (\mathbf{r}_i, t_i) and ending at (\mathbf{r}, t) , along which the line integral of (3.1) is to be evaluated, and Γ is a collection of relevant parameters:

$$\Gamma = \{g, \gamma, (\mathbf{r}_i, t_i)\}. \quad (3.2)$$

The phase in (3.1) is then used to construct a phase-shifted set of basis functions from the eigenfunctions of the unperturbed Hamiltonian by

$$\phi_j^\Gamma(\mathbf{r}, t) = U^\Gamma \phi_j^0(\mathbf{r}), \quad U^\Gamma = \exp(i e \eta^\Gamma / c \hbar). \tag{3.3}$$

This set of complete basis functions is then used to expand the wavefunction $\Psi^g(\mathbf{r}, t)$, resulting in the expansion coefficients $\{b_j^{g\Gamma}(t)\}$:

$$b_j^{g\Gamma}(t) = \langle \phi_j^\Gamma(t) | \Psi^g(t) \rangle, \quad \Psi^g(\mathbf{r}, t) = \sum_j b_j^{g\Gamma}(t) \phi_j^\Gamma(\mathbf{r}, t). \tag{3.4}$$

Feuchtwang *et al* then interpret these expansion coefficients as probability amplitudes for finding the particle in the states defined by (3.3).

Their claim is that the expansion coefficients $\{b_j^{g\Gamma}(t)\}$ are gauge independent but path dependent. This path dependence (not realised in a previous paper (Feuchtwang *et al* 1982)) can be seen easily since the closed line integral,

$$I = \oint A_\mu^g[x(\gamma)] dx_\mu(\gamma),$$

does not vanish for an arbitrary field and for an arbitrary closed loop. In §§ 3.2-6, we shall translate this path dependence into something we know better, the gauge dependence.

3.2. Connection to the conventional procedure

We now show the equivalence of the path dependence and the gauge dependence. First, we rearrange (3.4) in a slightly different form:

$$b_j^{g\Gamma}(t) = \langle U^\Gamma \phi_j^0 | \Psi^g(t) \rangle = \langle \phi_j^0 | (U^\Gamma)^\dagger \Psi^g(t) \rangle. \tag{3.5}$$

Thus, it is obvious that the path dependent coefficients $\{b_j^{g\Gamma}(t)\}$ are identical to the conventional gauge dependent expansion coefficients $\{c_j^{g\Gamma}(t)\}$ defined by

$$c_j^{g\Gamma}(t) \equiv \langle \phi_j^0 | \Psi^{g\Gamma}(t) \rangle, \quad \Psi^{g\Gamma}(\mathbf{r}, t) \equiv (U^\Gamma)^\dagger \Psi^g(\mathbf{r}, t). \tag{3.6}$$

Hence, by construction,

$$c_j^{g\Gamma}(t) = b_j^{g\Gamma}(t), \quad \text{for all } j \text{ and } t. \tag{3.7}$$

This $\Psi^{g\Gamma}(\mathbf{r}, t)$ is a true wavefunction since it satisfies the Schrödinger equation in the gauge $g\Gamma$ (note: we now use $g\Gamma$ as a single gauge index):

$$i \hbar \partial \Psi^{g\Gamma} / \partial t = H^{g\Gamma} \Psi^{g\Gamma}, \quad H^{g\Gamma} = (\mathbf{p} - e \mathbf{A}^{g\Gamma} / c)^2 / 2m + e V_0 + e \Phi^{g\Gamma}, \tag{3.8}$$

where the potentials $\mathbf{A}^{g\Gamma}$ and $\Phi^{g\Gamma}$ in the gauge $g\Gamma$ are

$$\mathbf{A}^{g\Gamma} = \mathbf{A}^g - \nabla \eta^\Gamma, \quad \Phi^{g\Gamma} = \Phi^g + c^{-1} \partial \eta^\Gamma / \partial t. \tag{3.9}$$

The essence of our above finding is as follows. If we start from the arbitrary gauge g , the conventional procedure will generate the conventional expansion coefficients $\{c_j^g(t)\}$. But the path dependent procedure will generate the conventional expansion coefficients $\{c_j^{g\Gamma}(t)\}$ in the gauge $g\Gamma$. Thus, the path dependent procedure does

absolutely nothing different from the conventional procedure except shifting the dependence on one gauge to the dependence on another different gauge†. There is one more defect in the path dependent procedure that is not present in the conventional procedure. It is that the conventional procedure uniquely defines the expansion coefficients for any given gauge, whereas the path dependent procedure cannot uniquely define a single set of expansion coefficients for a given gauge because of the freedom in the choice of path along which the phase function η^Γ is to be evaluated. In the following, we shall use the potentials in (2.12) and (2.13) to illustrate our point just concluded. Note, there is no magnetic field implied in these two sets of potentials. Therefore, the following examples also prove that the path dependent procedure is invalid for cases with $\mathbf{B} = 0$. (When $\mathbf{B} \neq 0$, it is quite obvious that the phase function in (3.1) is path dependent.)

3.3. Example in R-gauge

We now work in the R-gauge with the potentials listed in (2.12). First, we choose the starting point (\mathbf{r}_i, t_i) to be $(\mathbf{0}, 0)$. Next, the path is chosen to consist of two straightline segments from $(\mathbf{0}, 0)$ to (\mathbf{r}, t) as indicated symbolically by

$$\gamma' = (\mathbf{0}, 0) \rightarrow (\mathbf{0}, t) \rightarrow (\mathbf{r}, t) \tag{3.10}$$

where the time-like leg, $(\mathbf{0}, 0) \rightarrow (\mathbf{0}, t)$, has no effect here since $\Phi^R = 0$. Thus

$$\Gamma' = \{\mathbf{R}, \gamma', (\mathbf{0}, 0)\}. \tag{3.11}$$

Substituting (3.11) into (3.1), we get

$$\eta^{\Gamma'}(\mathbf{r}, t) = \int_0^1 d\xi \mathbf{r} \cdot \mathbf{A}^R(\xi \mathbf{r}, t) = \mathbf{r} \cdot \mathbf{A}^R(\mathbf{0}, t). \tag{3.12}$$

Consequently, from (3.9) and (3.12),

$$\mathbf{A}^{R\Gamma'}(\mathbf{r}, t) = \mathbf{0}, \quad \Phi^{R\Gamma'}(\mathbf{r}, t) = -\mathbf{r} \cdot \mathbf{E}(\mathbf{0}, t). \tag{3.13}$$

Thus, we see that the path dependent procedure with the choice of (3.10) and (3.11) in the R-gauge produces the conventional expansion coefficients in the E-gauge.

3.4. Example in E-gauge

We now work in the E-gauge with the potentials specified in (2.13). Again we choose (\mathbf{r}_i, t_i) to be the four-origin $(\mathbf{0}, 0)$. This time, however, the path is chosen to be of two straightline segments as indicated below:

$$\gamma'' = (\mathbf{0}, 0) \rightarrow (\mathbf{r}, 0) \rightarrow (\mathbf{r}, t). \tag{3.14}$$

Note, since $\mathbf{A}^E = 0$ the space-like leg $(\mathbf{0}, 0) \rightarrow (\mathbf{r}, 0)$ has no effect in the E-gauge. Finally, we have

$$\Gamma'' = \{\mathbf{E}, \gamma'', (\mathbf{0}, 0)\}. \tag{3.15}$$

† There is a simpler way to understand the gauge dependence of the $\{b_i^{s\Gamma}\}$. If they are gauge independent as claimed, then $\Psi^{s\Gamma}$ must be a gauge independent wavefunction (because the $\{\phi_i^0\}$ have no gauge dependence) and $H^{s\Gamma}$ a gauge independent Hamiltonian. It then follows that $\mathbf{A}^{s\Gamma}$ and $\Phi^{s\Gamma}$ must be gauge independent potentials, a conclusion contradicting the basic definition that all electromagnetic potentials are gauge dependent (see § 2.1). Note, gauge independent potentials exist if and only if the correspondence between potentials and fields is one-to-one.

Again, from (3.1) and (3.15),

$$\eta^{\Gamma''}(\mathbf{r}, t) = c \int_0^t d\tau \mathbf{r} \cdot \mathbf{E}(\mathbf{0}, \tau) = -\mathbf{r} \cdot \mathbf{A}^R(\mathbf{0}, t), \tag{3.16}$$

where, as indicated above, we have assumed that $\mathbf{A}^R(\mathbf{0}, t')$ vanishes for all $t' \leq 0$. From (3.9) and (3.16), we get

$$\mathbf{A}^{E\Gamma''}(\mathbf{r}, t) = \mathbf{A}^R(\mathbf{0}, t), \quad \Phi^{E\Gamma''}(\mathbf{r}, t) = 0. \tag{3.17}, (3.18)$$

Thus, we see that the path dependent procedure in the E-gauge with the choice of (3.14) and (3.15) generates the conventional expansion coefficients in the R-gauge.

3.5. Implication of (\mathbf{r}_i, t_i) in gauge transformations

We now explore the implications of the starting point of the path integral in the relation between path dependence and gauge transformations. First, we choose the following parameters:

$$(\mathbf{r}_i, t_i) = (\alpha \mathbf{r}, t), \quad \text{real } \alpha, \tag{3.19}$$

$$\gamma''' = (\alpha \mathbf{r}, t) \rightarrow (\mathbf{r}, t), \tag{3.20}$$

$$\Gamma''' = \{\mathbf{R}, \gamma''', (\alpha \mathbf{r}, t)\}. \tag{3.21}$$

Note, the above notation reads as follows: ‘The path dependent method is to be applied in the R-gauge, with the path being a straight line connecting the starting point $(\alpha \mathbf{r}, t)$ to the final point (\mathbf{r}, t) .’

With this choice, we then have

$$\eta^{\Gamma'''}(\mathbf{r}, t) = \int_{\alpha}^1 d\xi \mathbf{r} \cdot \mathbf{A}^R(\xi \mathbf{r}, t) = (1 - \alpha) \mathbf{r} \cdot \mathbf{A}^R(\mathbf{0}, t). \tag{3.22}$$

Hence, the path dependent coefficients are exactly the conventional coefficients in the gauge $g\Gamma'''$ with potentials

$$\mathbf{A}^{R\Gamma'''}(\mathbf{r}, t) = \alpha \mathbf{A}^R(\mathbf{0}, t), \quad \Phi^{R\Gamma'''}(\mathbf{r}, t) = -(1 - \alpha) \mathbf{r} \cdot \mathbf{E}(\mathbf{0}, t). \tag{3.23}$$

Finally we note that if we choose the path in (3.20) with $\alpha = 0$ and apply it to the path dependent procedure in any arbitrary gauge with the *exact* potentials, the path dependent expansion coefficients will be identical to the conventional expansion coefficients in the multipolar gauge (Power and Zienau 1959, Fiutak 1963). Thus, the multipolar gauge formulation, together with the definition of the conventional expansion coefficients, can be regarded as a special case of the path dependent procedure. At this moment, one should also recall that the potentials in the multipolar gauge are gauge dependent, despite the fact that they can be explicitly expressed only in terms of fields.

3.6. No field case

We now show that in the case where both \mathbf{E} and \mathbf{B} vanish, the path dependent procedure is also ambiguous. Since $\mathbf{E} = \mathbf{B} = 0$, there exists a scalar function $\Lambda(\mathbf{r}, t)$ such that $\mathbf{A}^\Lambda = \nabla \Lambda$ and $\Phi^\Lambda = -c^{-1} \partial \Lambda / \partial t$. If we now choose $\Gamma = \{\Lambda, \gamma''', (\alpha \mathbf{r}, t)\}$ where

α and γ^m are those in (3.19) and (3.20), then

$$\eta^\Gamma(\mathbf{r}, t) = \int_{\alpha r}^r ds \cdot \nabla \Lambda(s, t) = \Lambda(\mathbf{r}, t) - \Lambda(\alpha \mathbf{r}, t). \tag{3.24}$$

Thus, the path dependent coefficients are the conventional expansion coefficients in the gauge Λ^Γ with potentials

$$A^{\Lambda^\Gamma}(\mathbf{r}, t) = \nabla \Lambda(\alpha \mathbf{r}, t), \quad \Phi^{\Lambda^\Gamma}(\mathbf{r}, t) = -c^{-1} \partial \Lambda(\alpha \mathbf{r}, t) / \partial t, \tag{3.25}$$

which shows that the path dependent method does not produce the physically correct probabilities except when $\alpha = 0$.

4. Conclusions

We have shown that the path dependent procedure generates the conventional gauge dependent expansion coefficients. This procedure does absolutely nothing different from the conventional procedure except shifting the dependence on one gauge to that on another. To do just that, the path dependent method goes through all the complicated mathematics, all of which can be accomplished by the conventional procedure with just a simple gauge transformation.

The main reason why the path dependent procedure behaves in this way is in its use of the basis functions $\{\phi_j^\Gamma(\mathbf{r}, t)\}$ defined in (3.3). This basis set differs from the set of eigenfunctions $\{\phi_j^0(\mathbf{r})\}$ of the unperturbed Hamiltonian in (2.7) only by a gauge transformation. It then follows from the discussions given by Yang (1976a, § II C, 1982a, §§ 3-5) that the expansion coefficients defined using $\{\phi_j^\Gamma(\mathbf{r}, t)\}$ and the wavefunction will inherit all the mathematical and physical problems of the coefficients defined using $\{\phi_j^0\}$ and the wavefunction.

The deeper problem of the path dependent procedure lies in its lack of clarity in what operator is being measured when the $\{b_j^{g^\Gamma}(t)\}$ are interpreted as probability amplitudes. According to the basic postulates of quantum mechanics (e.g. Messiah 1966), the interpretation of the $\{b_j^{g^\Gamma}\}$ as probability amplitudes requires that the operator being measured is H_0^Γ , where

$$H_0^\Gamma = U^\Gamma H_0 (U^\Gamma)^\dagger = (\mathbf{p} - e \nabla \eta^\Gamma / c)^2 / 2m + e V_0, \tag{4.1}$$

$$H_0^\Gamma \phi_j^\Gamma(\mathbf{r}, t) = \epsilon_j \phi_j^\Gamma(\mathbf{r}, t). \tag{4.2}$$

Moreover, this interpretation also specifies that the values resulting from individual measurements are the eigenvalues $\{\epsilon_j\}$ and the average (mean) value of all measurements is

$$\overline{\epsilon^{g^\Gamma}} = \sum_j \epsilon_j |b_j^{g^\Gamma}(t)|^2 = \langle \Psi^g(t) | H_0^\Gamma | \Psi^g(t) \rangle. \tag{4.3}$$

Thus, the $\{|b_j^{g^\Gamma}(t)|^2\}$ are gauge independent if and only if $d(\overline{\epsilon^{g^\Gamma}}) / dt$ is gauge independent, where

$$d(\overline{\epsilon^{g^\Gamma}}) / dt = \langle \Psi^g | (dH_0^\Gamma / dt)_{H^g} | \Psi^g \rangle \equiv \langle \Psi^g | (\partial H_0^\Gamma / \partial t + [H_0^\Gamma, H^g] / i\hbar) | \Psi^g \rangle. \tag{4.4}$$

As can be expected from our discussions in this paper, one can easily show that, in general, not only is $(dH_0^\Gamma / dt)_{H^g}$ gauge dependent, but also it does not have any

discernible physical behaviour. That is, the operator H_0^Γ is a purely mathematical object, and it does not represent any physically measurable quantities under general conditions.

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Note added in proof. Both sides now agree that equation (23) of Feuchtwang *et al* (1984a) is inconsistent with the gauge invariant formulation (GIF). Hence, their criticism that the energy operator and the GIF probabilities are not uniquely defined is incorrect. They will announce their corrections in the near future.

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