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Gauge transformations, Foldy–Wouthuysen transformations and conservation of energy

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Abstract. The conventional interpretation of the quantum mechanical probability amplitudes and probabilities is examined in detail with respect to gauge transformations and the Foldy–Wouthuysen transformations. It is shown that the conventional interpretation is *gauge dependent* and, when applied to the relativistic (Dirac) and the non-relativistic quantum mechanics, can *not* be consistent with itself through the Foldy–Wouthuysen transformations. It is also shown that these two difficulties are *not* present in a gauge invariant formulation that explicitly incorporates Poynting's theorem and the conservation law of energy into the definition of probability amplitudes.

1. Introduction

The question whether the conventional interpretation of the quantum mechanical probability amplitudes and probabilities is gauge invariant seems to be an open-ended one (e.g. Göppert-Mayer 1931, Leubner and Zoller 1980), accompanied by conflicting claims.

On the one hand, the investigations of Lamb (1952), Power and Zienau (1959) and Kobe (1978) lead one to believe that it is gauge dependent. On the other hand, the *perturbative* results of Fried (1973), Babiker *et al* (1974), Bassani *et al* (1977), Healy (1977a, b, 1978), Power and Thirunamachandran (1977, 1978), Healy and Woolley (1978), Power (1978), Grynberg and Giacobino (1979) and Haller and Sohn (1979) seem to indicate that the conventional interpretation is gauge invariant§.

Our point of view is that these proofs are not conclusive. It is because these two conclusions are derived from *approximate* solutions to the time-dependent Schrödinger equations. Moreover, the approximations involved are different: some include the effects of line widths, some do not, and some do but also with the authors' other 'physical intuitions.' We thus believe that these approximate solutions reflect more of the *approximations* used than of the *exact definition* of the probability amplitudes.

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§ There are too many papers in the literature proving the gauge invariance of the conventional interpretation by using the results from the usual *time-dependent perturbation theory* (or its equivalent). We list here only some recent papers as references. Note, a recent paper by Aharonov and Au (1979) is *not* classified as a *conventional* work here because they do *not* define the probability amplitudes by the eigenfunctions of the '*unperturbed*' Hamiltonian.

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The purpose of this paper is restricted to examining the gauge properties only of the *exact* conventional probability amplitudes and probabilities. This is because we want to separate the question of principle from any approximation. Recently, Kobe and Wen (1980) have illustrated numerically and analytically the gauge dependence of the exact ground-state probability of a one-dimensional simple-harmonic charged oscillator interacting with an external time-varying field in the dipole approximation. Our proofs in this paper will be valid for an arbitrary system.

This paper is divided into seven sections. In § 2, we review the existing textbook materials concerning the gauge invariance of the Schrödinger equation. In § 3, we will use the gauge *invariance* of the Schrödinger equation as the *only* criterion to prove that the exact conventional probability amplitudes and probabilities are gauge dependent. In § 4, we examine another version of the conventional interpretation—the so-called consistent procedure. Here, we will learn that this procedure does not eliminate *all* the gauge dependence in the probability amplitudes and probabilities. It does, however, eliminate all the dependence on the *gauge transformations* between the initial gauge (from which such a procedure starts) and all subsequent gauges. The only gauge dependence of the probability amplitudes and probabilities defined by this procedure in *all* gauges is the initial-gauge dependence.

In § 5 we consider the Foldy–Wouthuysen transformations (Foldy and Wouthuysen 1950) to illustrate that the conventional interpretation, when applied to both the relativistic (Dirac) and the non-relativistic quantum mechanics, cannot be consistent with itself through the Foldy–Wouthuysen transformations.

In § 6 we first review the classical Poynting's theorem and conservation of energy, then we apply them to quantum mechanics to attain the gauge invariant formulation (Yang 1976a, Kobe and Smirl 1978, Leubner and Zoller 1980). Here we will show that this formulation gives probability amplitudes that are gauge invariant and are consistent with the Foldy–Wouthuysen transformations. Finally, in § 7 we discuss some basic reasons for the difficulties encountered by the conventional interpretation and the implication of the gauge invariance of the Schrödinger equation.

2. Gauge invariance of the Schrödinger equation

In this section, we shall review the existing materials on the gauge invariance of the Schrödinger equation and quantum mechanics. All the materials to be presented here contain no new information and can be found in textbooks by, e.g., Bohm (1951), Dicke and Wittke (1960), Merzbacher (1961), Landau and Lifshitz (1965), Gottfried (1966), Sargent *et al* (1977) and Cohen-Tannoudji *et al* (1977).

Let us consider a non-relativistic, spinless particle with mass m and charge e in the presence of a conservative, electrostatic field $\boldsymbol{E}_0(\boldsymbol{r}) = -\nabla V_0(\boldsymbol{r})$ and an electromagnetic radiation field $\boldsymbol{E}(\boldsymbol{r}, t)$ and $\boldsymbol{B}(\boldsymbol{r}, t)$. If we use the potentials $(\boldsymbol{A}, \Phi)$ to represent the time-varying fields, then

$$\boldsymbol{E} = -\nabla\Phi - (1/c)\partial\boldsymbol{A}/\partial t, \qquad \boldsymbol{B} = \nabla \times \boldsymbol{A}. \tag{2.1}$$

The Schrödinger equation in this set of potentials is

$$i\hbar\dot{\Psi}(\boldsymbol{r}, t) = H\Psi(\boldsymbol{r}, t), \tag{2.2}$$

where the Hamiltonian is

$$H = (\boldsymbol{p} - e\boldsymbol{A}/c)^2/2m + eV_0 + e\Phi. \tag{2.3}$$

If we use another set of potentials $(\boldsymbol{A}', \Phi')$ to represent $\boldsymbol{E}$ and $\boldsymbol{B}$, then $(\boldsymbol{A}', \Phi')$ and $(\boldsymbol{A}, \Phi)$ are related to an arbitrary gauge function $\chi(\boldsymbol{r}, t)$ by†

$$\boldsymbol{A}' = \boldsymbol{A} + \nabla\chi \qquad \text{and} \qquad \Phi' = \Phi - (1/c)\partial\chi/\partial t. \tag{2.4}$$

If we use H' and Ψ' to denote the Hamiltonian and wavefunction in $(\boldsymbol{A}', \Phi')$, then

$$\begin{aligned} H' &= (\boldsymbol{p} - e\boldsymbol{A}'/c)^2/2m + eV_0 + e\Phi' \\ &= RHR^\dagger + i\hbar(\partial R/\partial t)R^\dagger, \end{aligned} \tag{2.5}$$

$$\Psi'(\boldsymbol{r}, t) = R\Psi(\boldsymbol{r}, t), \tag{2.6}$$

where

$$R(t) = \exp[ie\chi(\boldsymbol{r}, t)/c\hbar]. \tag{2.7}$$

From (2.6), it is clear that if we restrict ourselves only to *Hermitian* gauge functions, then

$$|\Psi'(\boldsymbol{r}, t)|^2 = |\Psi(\boldsymbol{r}, t)|^2 \qquad \text{for all } \boldsymbol{r} \text{ and } t. \tag{2.8}$$

This relation establishes that both wavefunctions Ψ and Ψ' generate the same probability for finding the particle at position $\boldsymbol{r}$ at time t. That is, they describe *exactly* the same physical behaviour of the charged particle. Hence the Schrödinger equation is gauge invariant because of relation (2.6).

The prevailing misconception is that (2.8) also implies the gauge invariance of the conventional probability of finding the particle in some state (e.g. Fried 1973 paragraphs 1 and 2). It is the purpose of this paper to show the contrary. Our reason is that here two *different* quantities are involved: One is the probability *in some state*, which is a function of *time only*, whereas the probability in (2.8) is that *at position* $\boldsymbol{r}$ at time t. Because of this characteristic difference, what is true for one does not necessarily imply that it is also true for the other. In fact, we shall show in the next two sections that the well known result in (2.6) implies that the conventional probability amplitudes and probabilities are gauge dependent.

3. Gauge dependence of the conventional interpretation

In this section, we shall show that, by using only (2.6), the 'conventional' probability amplitudes and probabilities are gauge dependent. In order to avoid any confusion as to the language used here, we will define what we mean by 'conventional'. For this matter, we strictly distinguish between the 'conventional interpretation' and a *consistent procedure* which will be discussed in the next section. In the literature, these two *different* interpretations are often not distinguished and confusion inevitably results.

In order to define the 'conventional' interpretation, we first construct the 'unperturbed' Hamiltonian by

$$H_0 = \boldsymbol{p}^2/2m + eV_0 \tag{3.1}$$

for our physical situation. From now on, we use $\{\varepsilon_j\}$ for the eigenvalues and $\{\phi_j(\boldsymbol{r})\}$ for the orthonormal and complete (assumed) set of eigenfunctions of H_0. We now define

† Let us stress here that an understanding of gauge transformations in quantum mechanics requires a knowledge of the physical meanings of gauges and gauge transformations in the classical electromagnetic theory (Brill and Goodman 1967, Jackson 1975 pp 220–223, Yang 1976b, 1981a).

the *conventional* expansion coefficients $\{c_j(t)\}$ of wavefunction $\Psi(\boldsymbol{r}, t)$ and $\{c'_j(t)\}$ of $\Psi'(\boldsymbol{r}, t)$ by

$$c_j(t) = \langle \phi_j | \Psi(t) \rangle \qquad \text{and} \qquad c'_j(t) = \langle \phi_j | \Psi'(t) \rangle. \tag{3.2}$$

In other words, the word 'conventional' as used in this paper means using the eigenfunctions of H_0 to define the expansion coefficients *regardless* of the gauges in the Hamiltonians.

Let us now prove that the conventional expansion coefficients are gauge dependent: If $\nabla\chi(\boldsymbol{r}, t) \neq 0$ over a finite region, however small, in which $|\Psi(\boldsymbol{r}, t)|^2 \neq 0$, there does *not* exist a real function $f(t)$, *of time only*, such that the relation

$$c'_j(t) = c_j(t) \exp[\mathrm{i}f(t)] \qquad \text{for all } j \text{ and } t \tag{3.3}$$

is true.

Proof. First assume that (3.3) is true. Then using the completeness of $\{\phi_j\}$, we have

$$\Psi' = \sum_j c'_j \phi_j = \exp[\mathrm{i}f(t)] \left\{ \sum_j c_j \phi_j \right\} = \exp[\mathrm{i}f(t)] \Psi. \tag{3.4}$$

From (2.2) and (3.4), we get

$$\mathrm{i}\hbar\dot{\Psi}' = \exp(\mathrm{i}f)(H - \hbar\dot{f})\Psi = (H - \hbar\dot{f})\Psi'. \tag{3.5}$$

This result implies that H' can be equal to $H - \hbar f$ where f is a function *of time only*, which contradicts our assumption that $\nabla\chi(\boldsymbol{r}, t) \neq 0$. Thus our proof is completed.

Next, let us prove that the conventional *probabilities* are also gauge dependent. For this purpose, let us prove the following first:
If

$$|c'_j(t)|^2 = |c_j(t)|^2 \qquad \text{for all } j \text{ and } t, \tag{3.6}$$

then *for any arbitrary integer n* the relation

$$\langle \Psi(t) | \{ (R^{\dagger} H_0 R)^n - (H_0)^n \} | \Psi(t) \rangle = 0 \qquad \text{for all } t \tag{3.7}$$

must also be true, where R is defined in equation (2.7).

Proof. Since $\{\phi_j\}$ are the complete and orthonormal set of eigenfunctions of H_0 in (3.1), it then follows from (3.6) that

$$\begin{aligned} \langle \Psi' | (H_0)^n | \Psi' \rangle &= \sum_j |c'_j|^2 (\varepsilon_j)^n = \sum_j |c_j|^2 (\varepsilon_j)^n \\ &= \langle \Psi | (H_0)^n | \Psi \rangle. \end{aligned} \tag{3.8}$$

If we substitute the result (2.6) into the left-hand side, we see that (3.7) is true.

The physical implication of (3.7) is that the operators Q_n, defined by

$$Q_n = (R^{\dagger} H_0 R)^n - (H_0)^n, \tag{3.9}$$

are *constants of motion* under the Hamiltonian H. To see if this can be true, let us set $n = 1$; we find

$$Q_1 = (e/2mc)(\boldsymbol{p} \cdot \nabla\chi + \nabla\chi \cdot \boldsymbol{p}) + (e^2/2mc^2)(\nabla\chi)^2, \tag{3.10}$$

and

$$(\mathrm{d}Q_1/\mathrm{d}t)_H \equiv \partial Q_1/\partial t + (1/\mathrm{i}\hbar)[Q_1, H]$$
$$= (e/2mc)(\boldsymbol{p}\cdot\boldsymbol{\nabla}\dot{\chi} + \boldsymbol{\nabla}\dot{\chi}\cdot\boldsymbol{p}) + (e^2/mc^2)(\boldsymbol{\nabla}\chi)\cdot(\boldsymbol{\nabla}\dot{\chi}) - (e^2/mc)(\boldsymbol{\nabla}\chi)\cdot\boldsymbol{\nabla}(V_0+\Phi)$$
$$+ (e/4m^2c)\sum_{j,k=1}^{3}\{[p_j(\nabla_j\nabla_k\chi) + (\nabla_j\nabla_k\chi)p_j + (2e/c)(\nabla_j\chi)(\nabla_j A_k)]$$
$$\times(p_k - eA_k/c) + \mathrm{HC}\}$$
$$+ (e^2/2m^2c^2)\sum_{j,k=1}^{3}\{(\nabla_j\chi)(\nabla_j\nabla_k\chi)(p_k - eA_k/c) + \mathrm{HC}\}. \tag{3.11}$$

In the above equation, $\dot{\chi}$ is $\partial\chi/\partial t$ and HC denotes the Hermitian conjugate. As we can see, $(\mathrm{d}Q_1/\mathrm{d}t)_H$ does not in general vanish if $\boldsymbol{\nabla}\chi \neq 0$. The only exception occurs when $\boldsymbol{\nabla}(V_0+\Phi) = \boldsymbol{\nabla}\dot{\chi} = \boldsymbol{\nabla}\boldsymbol{A} = \boldsymbol{\nabla}\boldsymbol{\nabla}\chi = 0$. For this case, one can use the resulting simplified conditions to derive a relation between c_j and c_j'. (They are simply different Fourier components of the wavefunction Ψ if $V_0 = 0$.)

The above result means that (3.6) cannot be true. This, of course, means that the conventional probabilities are gauge dependent. Hence our proof is completed.

Finally, let us note two important things here. First, all our statements through equation (3.9) also apply to a Dirac particle. The only change that need be done is to use the Dirac unperturbed Hamiltonian and Hamiltonian in (3.10) and (3.11). Second, all our proofs are valid for *arbitrary* potentials of *arbitrary* fields of *arbitrary* frequencies. Hence whether the system is on or off resonance has no bearing on our results here.

4. Consistent procedures with initial-gauge dependence

In the discussions of whether there really is a gauge problem in the conventional interpretation of quantum mechanics, one often runs into arguments stressing the internal consistency in the definition of probability amplitudes (e.g. Mandel 1979)†. It is our purpose in this section to investigate such a procedure and point out that it still leaves a gauge ambiguity unresolved.

In order to see clearly the shortcomings of this procedure, let us first define the (conventional) consistent procedure *with* $(\boldsymbol{A}, \Phi)$ *as the initial gauge* by

$$\tilde{c}_j(t) = \langle\phi_j|\Psi(t)\rangle \qquad \text{and} \qquad \tilde{c}_j'(t) = \langle\tilde{\phi}_j(t)|\Psi'(t)\rangle \tag{4.1}$$

where, using the operator R in (2.7),

$$\tilde{\phi}_j(\boldsymbol{r}, t) = R(t)\phi_j(\boldsymbol{r}). \tag{4.2}$$

In the above expressions, Ψ is the wavefunction in $(\boldsymbol{A}, \Phi)$ and Ψ' in $(\boldsymbol{A}', \Phi')$; and $\{\phi_j(\boldsymbol{r})\}$ are the eigenfunctions of the 'unperturbed' Hamiltonian in (3.1). Let us note that (4.1) is *different* from (3.2) in the construction of the expansion coefficients of the wavefunction Ψ'. From (2.6) and (4.2), it is obvious that

$$\tilde{c}_j(t) = \tilde{c}_j'(t) \qquad \text{for all } j \text{ and all } t. \tag{4.3}$$

† See Healy (1980) and Power and Thirunamachandran (1980) for a counter-argument of Mandel's discussion of the electric dipole approximation.

The only question is whether (4.3) implies that the procedure (4.1) has eliminated *all* the gauge dependence in the expansion coefficients. To see that it does *not*, let us consider another consistent procedure *with* $(\boldsymbol{A}', \Phi')$ *as the initial gauge*. Thus, the expansion coefficients $\{\hat{c}_j\}$ for Ψ and $\{\hat{c}'_j\}$ for Ψ' from this procedure are

$$\hat{c}'_j(t) = \langle \phi_j | \Psi'(t) \rangle \qquad \text{and} \qquad \hat{c}_j(t) = \langle \hat{\phi}_j(t) | \Psi(t) \rangle, \tag{4.4}$$

where, using R in (2.7),

$$\hat{\phi}_j(\boldsymbol{r}, t) = R^{+} \phi_j(\boldsymbol{r}). \tag{4.5}$$

From (2.6) and (4.5), it follows that

$$\hat{c}_j(t) = \hat{c}'_j(t) \qquad \text{for all } j \text{ and all } t. \tag{4.6}$$

Let us now prove that the two consistent procedures in (4.1) and (4.4) still retain some kind of gauge dependence by proving that $\{\tilde{c}_j(t)\}$ and $\{\hat{c}_j(t)\}$ do *not* generate the same probabilities. By equations (3.2) and (4.1), $\tilde{c}_j(t)$ is exactly $c_j(t)$. By (3.2), (4.4) and (4.6), $\hat{c}_j(t)$ is exactly $c'_j(t)$. Since we have shown that $\{c_j(t)\}$ and $\{c'_j(t)\}$ do not generate the same probabilities in § 3, it follows that the consistent procedure in (4.1) or (4.4) does *not* eliminate *all* the gauge dependence in the expansion coefficients.

The reason why (4.1) does not eliminate all gauge dependence is the following. Equation (4.3) indicates that this procedure has eliminated all dependence on the *gauge transformations* between the initial gauge and *all subsequent* gauges. However, the wavefunction $\Psi(\boldsymbol{r}, t)$ depends upon the gauge of $(\boldsymbol{A}, \Phi)$ (e.g. Yang 1976a § II C, Cohen-Tannoudji *et al* 1977) whereas the eigenfunctions $\{\phi_j(\boldsymbol{r})\}$ of the 'unperturbed' Hamiltonian are gauge *independent* (i.e., do not depend on the potentials in the Hamiltonian). It then follows that the coefficients $\{\tilde{c}_j(t)\}$, and hence $\{\tilde{c}'_j(t)\}$, must have dependence on the initial gauge $(\boldsymbol{A}, \Phi)$. As a matter of fact, this author has investigated this point in detail and discussed how this initial-gauge dependence can be eliminated (Yang 1976a §§ II C and D).

5. The Foldy–Wouthuysen transformation

The basic characteristic of the 'conventional' interpretation in (3.2) and the consistent procedure in (4.1) is the use of the eigenfunctions of the 'unperturbed' Hamiltonian (at least once) in the definition of expansion coefficients. The reason why these expansion coefficients are gauge dependent and hence have ambiguous meanings, can be understood from another viewpoint. As has been clearly explained by Cohen-Tannoudji *et al* (1973, 1977), Kobe and Smirl (1978), Grynberg and Giacobino (1979) and Leubner and Zoller (1980), the meanings of the 'unperturbed' Hamiltonian *vary* with the potentials in the Hamiltonians. Furthermore, it is *not in general a true physical quantity* since $\boldsymbol{p}^2/2m$ is not one in general (Cohen-Tannoudji *et al* 1977) (to be discussed in detail in § 7).

Having understood these points, we now wish in this section to add another dimension to the discussion of the interpretation based on one basic principle of quantum mechanics.

The interpretation of quantum mechanics must, in principle, be invariant under all unitary transformations. This is where we bring the Foldy–Wouthuysen (FW) transformation (Foldy and Wothuysen 1950) into play with gauge transformations to illustrate that this principle will be violated if we insist on interpreting the conventional expansion

coefficients as probability amplitudes. (The FW transformations will be useful in the discussions of the gauge invariant formulation in the next section.)

To begin with, let us consider a Dirac particle with rest mass m and charge e in the presence of the fields in § 2. If we use H_0^{D} for the Dirac 'unperturbed' Hamiltonian, and Ψ^{D} and H^{D} for the wavefunction and the Hamiltonian in the gauge of $(\boldsymbol{A}, \Phi)$, then

$$H_0^{\mathrm{D}} = c\boldsymbol{\alpha}\cdot\boldsymbol{p} + \beta mc^2 + eV_0, \tag{5.1}$$

$$H^{\mathrm{D}} = c\boldsymbol{\alpha}\cdot(\boldsymbol{p} - e\boldsymbol{A}/c) + \beta mc^2 + eV_0 + e\Phi. \tag{5.2}$$

Let us use $\{\varepsilon_j^{\mathrm{D}}\}$ and $\{\phi_j^{\mathrm{D}}(\boldsymbol{r})\}$ for the eigenvalues and the orthonormal and complete (assumed) set of eigenfunctions of H_0^{D}. According to (4.1), the consistent expansion coefficients $\{\tilde{c}_j^{\mathrm{D}}\}$ with $(\boldsymbol{A}, \Phi)$ as the initial gauge are

$$\tilde{c}_j^{\mathrm{D}}(t) = \langle\phi_j^{\mathrm{D}}\,|\,\Psi^{\mathrm{D}}(t)\rangle. \tag{5.3}$$

Here, we have used the consistent procedure to eliminate all subsequent gauge dependence.

We now perform an FW transformation U to the Dirac equation and so on to get

$$\mathrm{i}\hbar\dot{\Psi}^U(\boldsymbol{r}, t) = H^U\Psi^U(\boldsymbol{r}, t), \qquad \Psi^U = U\Psi^{\mathrm{D}}, \tag{5.4}$$

and

$$\tilde{c}_j^U(t) = \langle\phi_j^U\,|\,\Psi^U\rangle, \qquad \phi_j^U = U\phi_j^{\mathrm{D}}, \tag{5.5}$$

where if we show only the lowest order terms, the operator U and the Hamiltonian are (Foldy and Wouthuysen 1950):

$$U = \exp(S), \qquad S = (1/2mc)\beta\boldsymbol{\alpha}\cdot(\boldsymbol{p} - e\boldsymbol{A}/c), \tag{5.6}$$

and

$$\begin{aligned} H^U &= UH^{\mathrm{D}}U^\dagger + \mathrm{i}\hbar(\partial U/\partial t)U^\dagger \\ &= \beta mc^2 + \beta(1/2m)[\boldsymbol{\alpha}\cdot(\boldsymbol{p} - e\boldsymbol{A}/c)]^2 + eV_0 + e\Phi + \ldots. \end{aligned} \tag{5.7}$$

Since the Hamiltonian H^U decouples the positive and negative energy components to the order shown above, we can take the positive energy component of (5.4) only to this order. After eliminating the constant term mc^2, we get the Schrödinger equation with the non-relativistic Hamiltonian in (2.3) if we neglect the spin. If we use the consistent procedure with $(\boldsymbol{A}, \Phi)$ as the initial gauge, then the expansion coefficients $\{\tilde{c}_j(t)\}$ are given in (4.1).

The main question now is: Are the non-relativistic coefficients $\{\tilde{c}_j(t)\}$ consistent with the relativistic (Dirac) coefficients $\{\tilde{c}_j^{\mathrm{D}}(t)\}$ in (5.3)?

The answer to this question lies in how the non-relativistic 'unperturbed' Hamiltonian H_0 is obtained from the Dirac 'unperturbed' Hamiltonian H_0^{D}. Let us consider another FW transformation U_0 defined by Foldy and Wouthuysen (1950):

$$U_0 = \exp(S_0), \qquad S_0 = (1/2mc)\beta\boldsymbol{\alpha}\cdot\boldsymbol{p}. \tag{5.8}$$

As is clear from (5.7), the operation of U_0 on H_0^{D} will give the non-relativistic 'unperturbed' Hamiltonian since

$$\begin{aligned} U_0H_0^{\mathrm{D}}(U_0)^\dagger &= \beta mc^2 + \beta(\boldsymbol{\alpha}\cdot\boldsymbol{p})^2/2m + eV_0 + \ldots \\ &= \beta mc^2 + \beta\boldsymbol{p}^2/2m + eV_0 + \ldots. \end{aligned} \tag{5.9}$$

Thus, the eigenfunctions $\{\phi_j(\boldsymbol{r})\}$ of H_0 in (3.1) are mathematically consistent with $\{U_0\phi_j^{\mathrm{D}}(\boldsymbol{r})\}$. This implies that the non-relativistic coefficient $\tilde{c}_j(t)$, for each j, is consistent with the relativistic coefficient $C_j(t)$ defined by

$$C_j(t) \equiv \langle U_0\phi_j^{\mathrm{D}} \mid U\Psi^{\mathrm{D}}\rangle, \tag{5.10}$$

since the non-relativistic wavefunction is consistent with $U\Psi^{\mathrm{D}}$.

Since $U_0 \neq U$ unless $\boldsymbol{A} = 0$, it is obvious that $\{\tilde{c}_j(t)\}$ are in general *not* consistent with $\{\tilde{c}_j^{\mathrm{D}}(t)\}$. This can be seen by, using the unitarity of U first to get $\tilde{c}_j^{\mathrm{D}} = \tilde{c}_j^{U}$,

$$\tilde{c}_j^{\mathrm{D}} - C_j = \langle\phi_j^{\mathrm{D}}|(1 - U_0^{\dagger}U)|\Psi^{\mathrm{D}}\rangle. \tag{5.11}$$

The *only* situation when (5.11) vanishes identically, which implies that $\{\tilde{c}_j\}$ are consistent with $\{\tilde{c}_j^{\mathrm{D}}\}$, is when $U_0 = U$ or $\boldsymbol{A} = 0$. This situation allows *no* magnetic interaction. In theory, it allows *all* electric multipole interactions (e.g. Fiutak 1963). However, it would be physically inconsistent to take into account the electric quadrupole interaction without the magnetic dipole interaction, etc (e.g. Yang 1976a § III A). Thus, only the electric *dipole* interaction is allowed. In other words, only when the Dirac and the non-relativistic Hamiltonians are in the electric dipole form can the procedure in (4.1) yield consistent relativistic (Dirac) and non-relativistic expansion coefficients.

6. The gauge invariant formulation

Before delving into the gauge invariant formulation, let us first review the difficulties encountered by the conventional interpretation defined in (3.2) and the consistent procedure defined in (4.1). We have found that these two different interpretations have: (i) the consistency problem due to different choices of gauge in the conventional interpretation or due to different choices of the initial gauge in the consistent procedure, and (ii) the consistency problem between the relativistic (Dirac) and the non-relativistic expansion coefficients through the FW transformations. Our purpose in this section is to show that the gauge invariant formulation proposed previously (Yang 1976a, Kobe and Smirl 1978, Leubner and Zoller 1980) has the ability to resolve these difficulties†.

The conceptual basis of the gauge invariant formulation is the microscopic Poynting's theorem and *the conservation law of energy* as derived from Maxwell's equations (e.g. Jackson 1975 pp 236–41 especially equations (6.110) and (6.111)). This is because we are dealing with the electromagnetic interaction of the 'basic' constituents of matter. Since the concept of applying Poynting's theorem to quantum mechanics is relatively recent (Yang 1976a), let us first review the theorem within the framework of the classical electromagnetic theory.

6.1. The classical Poynting's theorem

To avoid confusion, let us first state that all symbols in this *sub*section represent *classical* quantities.

Assume that we have two *physically measurable* charge–current distributions $(\rho^s, \boldsymbol{J}^s)$ and $(\rho', \boldsymbol{J}')$. The fields they produce through Maxwell's equations are $(\boldsymbol{E}^s, \boldsymbol{B}^s)$

† Leubner and Zoller (1980) have recently applied the gauge invariant method to resolve some gauge problems in current literature.

and $(\boldsymbol{E}', \boldsymbol{B}')$. For convenience of argument we assume that, during the time interval of concern, ρ^s and $\boldsymbol{J}^s$ vanish *outside* a finite volume τ that has a closed surface σ, and ρ' and $\boldsymbol{J}'$ vanish *inside* τ. This volume τ is assumed to be stationary in our particular reference frame.

If we define E_{field} and $\boldsymbol{S}_{\text{field}}$ by (e.g. Jackson 1975 pp 236–41)

$$E_{\text{field}} = (1/8\pi) \int_\tau \mathrm{d}^3x[(\boldsymbol{E}^s + \boldsymbol{E}')^2 + (\boldsymbol{B}^s + \boldsymbol{B}')^2], \tag{6.1}$$

$$\boldsymbol{S}_{\text{field}} = (c/4\pi)(\boldsymbol{E}^s + \boldsymbol{E}') \times (\boldsymbol{B}^s + \boldsymbol{B}'), \tag{6.2}$$

then Poynting's theorem in the integral form reads

$$\mathrm{d}E_{\text{field}}/\mathrm{d}t + \int_\tau \mathrm{d}^3x \boldsymbol{J}^s \cdot (\boldsymbol{E}^s + \boldsymbol{E}') = -\int_\sigma \mathrm{d}\boldsymbol{\sigma} \cdot \boldsymbol{S}_{\text{field}}. \tag{6.3}$$

where $\mathrm{d}\boldsymbol{\sigma}$ is the unit surface of σ pointing outward.

The conventional interpretation of (6.3) is *conservation of energy*. This interpretation, however, requires that the energy E_{matter} of the matter inside τ be determined by (e.g. Jackson 1975 equation (6.110))

$$\mathrm{d}E_{\text{matter}}/\mathrm{d}t = \int_\tau \mathrm{d}^3x \boldsymbol{J}^s \cdot (\boldsymbol{E}^s + \boldsymbol{E}'). \tag{6.4}$$

Any other definition of E_{matter}, if it is inconsistent with (6.4), violates this conservation law of energy. (Similar arguments can be used for the conservation laws of the linear and the angular momenta.)

Let us now apply the field situation described in § 2 to equations (6.1)–(6.4) to construct two conservation laws of energy. The fields considered consist of a static field $\boldsymbol{E}_0(\boldsymbol{r})$ and a time varying electromagnetic radiation field $\boldsymbol{E}(\boldsymbol{r}, t)$ and $\boldsymbol{B}(\boldsymbol{r}, t)$. Let us use E^T_{field} and $\boldsymbol{S}^T_{\text{field}}$ for the field energy and Poynting's vector when $\boldsymbol{E}' = \boldsymbol{E}_0 + \boldsymbol{E}$ and $\boldsymbol{B}' = \boldsymbol{B}$, and use E^R_{field} and $\boldsymbol{S}^R_{\text{field}}$ when $\boldsymbol{E}' = \boldsymbol{E}$ and $\boldsymbol{B}' = \boldsymbol{B}$. The energy of the matter corresponding to $\boldsymbol{E}' = \boldsymbol{E}_0 + \boldsymbol{E}$ will be denoted by K and that corresponding to $\boldsymbol{E}' = \boldsymbol{E}$ will be denoted by E_T. Thus,

$$\mathrm{d}K/\mathrm{d}t = \int_\tau \mathrm{d}^3x \boldsymbol{J}^s \cdot (\boldsymbol{E}^s + \boldsymbol{E}_0 + \boldsymbol{E}), \tag{6.5}$$

$$\mathrm{d}E_T/\mathrm{d}t = \int_\tau \mathrm{d}^3x \boldsymbol{J}^s \cdot (\boldsymbol{E}^s + \boldsymbol{E}). \tag{6.6}$$

Physically, K conserves with the total field energy and the total field energy flux; it is traditionally labelled *the kinetic* or *mechanical* energy of the matter. The energy E_T conserves with the field energy and the energy flux due to $(\boldsymbol{E}^s + \boldsymbol{E})$ and $(\boldsymbol{B}^s + \boldsymbol{B})$. Since $\boldsymbol{E}$ and $\boldsymbol{B}$ are the time varying fields, it is E_T that is responsible for the conservation with the radiation field energy and the radiation energy flux (Yang 1976a). According to traditional Newtonian mechanics, we shall label E_T *the total energy* of the matter inside τ. This completes our review of the classical conservation law of energy.

6.2. The gauge invariant formulation

The first step in the gauge invariant formulation of quantum mechanics is to solve, *for a given Hamiltonian*, for operators that satisfy equations having a term-by-term

correspondence (Bohr 1928) with those equations determined from the classical con-servation laws (of linear momentum, angular momentum and energy). For example, equations (6.5) and (6.6). Then, these operators are interpreted according to the physical meanings associated with these classical conservation laws. Finally, we use the eigenfunctions of H_B corresponding to E_T in (6.6) to define the expansion coefficients and interpret them as probability amplitudes (Yang 1976a). Let us show how this procedure works. From now on, we neglect the self-interaction.

Let us consider the Dirac Hamiltonian in (5.2) in the gauge of $(\boldsymbol{A}, \Phi)$. If we use K^{D} and H_B^{D} to represent K and E_T in (6.5) and (6.6), then, because $\mathrm{d}K^{\mathrm{D}}/\mathrm{d}t = \partial K^{\mathrm{D}}/\partial t + [K^{\mathrm{D}}, H^{\mathrm{D}}]/\mathrm{i}\hbar$ and so on, these operators are determined by

$$\partial K^{\mathrm{D}}/\partial t + [K^{\mathrm{D}}, H^{\mathrm{D}}]/\mathrm{i}\hbar = \boldsymbol{J}^{\mathrm{D}} \cdot (\boldsymbol{E}_0 + \boldsymbol{E}), \tag{6.7}$$

$$\partial H_B^{\mathrm{D}}/\partial t + [H_B^{\mathrm{D}}, H^{\mathrm{D}}]/\mathrm{i}\hbar = \boldsymbol{J}^{\mathrm{D}} \cdot \boldsymbol{E} \tag{6.8}$$

where $\boldsymbol{J}^{\mathrm{D}}$ is the current operator associated with H^{D} in (5.2) and hence is $ec\boldsymbol{\alpha}$. The solutions are (Yang 1976a, p 71)

$$K^{\mathrm{D}} = c\boldsymbol{\alpha} \cdot (\boldsymbol{p} - e\boldsymbol{A}/c) + \beta mc^2, \tag{6.9}$$

$$H_B^{\mathrm{D}} = K^{\mathrm{D}} + eV_0. \tag{6.10}$$

Thus, H_B^{D} still retains the physical form of the kinetic energy plus the potential energy.

If we use $\{E_j^{\mathrm{D}}(t)\}$ and $\{\Psi_j^{\mathrm{D}}(\boldsymbol{r}, t)\}$ for the eigenvalues and the orthonormal and complete (assumed) set of eigenfunctions of $H_B^{\mathrm{D}}(t)$, then the gauge invariant procedure defines the expansion coefficients of the wavefunction $\Psi^{\mathrm{D}}(\boldsymbol{r}, t)$ by

$$a_j^{\mathrm{D}}(t) = \langle \Psi_j^{\mathrm{D}}(t) | \Psi^{\mathrm{D}}(t) \rangle. \tag{6.11}$$

As we have illustrated in (3.2), (4.1) and (4.4), a complete interpretive procedure requires specification of the expansion coefficients in a different gauge. Thus, we now consider the Dirac Hamiltonian H'^{D} in the gauge of $(\boldsymbol{A}', \Phi')$.

$$H'^{\mathrm{D}} = c\boldsymbol{\alpha} \cdot (\boldsymbol{p} - e\boldsymbol{A}'/c) + \beta mc^2 + eV_0 + e\Phi', \tag{6.12}$$

which has the current operator $\boldsymbol{J}'^{\mathrm{D}} = ec\boldsymbol{\alpha}$. The total energy operator $H_B'^{\mathrm{D}}$ now is

$$H_B'^{\mathrm{D}} = c\boldsymbol{\alpha} \cdot (\boldsymbol{p} - e\boldsymbol{A}'/c) + \beta mc^2 + eV_0 \tag{6.13}$$

since it can be trivially shown that

$$\partial H_B'^{\mathrm{D}}/\partial t + (1/\mathrm{i}\hbar)[H_B'^{\mathrm{D}}, H'^{\mathrm{D}}] = ec\boldsymbol{\alpha} \cdot \boldsymbol{E}. \tag{6.14}$$

If $\{E_j'^{\mathrm{D}}(t)\}$ and $\{\Psi_j'^{\mathrm{D}}(\boldsymbol{r}, t)\}$ are the eigenvalues and the orthonormal set of eigenfunctions of $H_B'^{\mathrm{D}}(t)$, then our expansion coefficients of wavefunction $\Psi'^{\mathrm{D}}(\boldsymbol{r}, t)$ are

$$a_j'^{\mathrm{D}}(t) = \langle \Psi_j'^{\mathrm{D}}(t) | \Psi'^{\mathrm{D}}(t) \rangle. \tag{6.15}$$

Let us now show that the expansion coefficients and the eigen energies are gauge invariant. For this we first note that $H_B'^{\mathrm{D}} = RH_B^{\mathrm{D}}R^{+}$ where R is given in (2.7). Thus, $E_j'^{\mathrm{D}}(t) = E_j^{\mathrm{D}}(t)$ and $\Psi_j'^{\mathrm{D}}(\boldsymbol{r}, t) = R\Psi_j^{\mathrm{D}}(\boldsymbol{r}, t)$. Since $\Psi'^{\mathrm{D}}(\boldsymbol{r}, t)$ and $\Psi^{\mathrm{D}}(\boldsymbol{r}, t)$ are still related by (2.6), it is obvious from (6.11) and (6.15) that $a_j'^{\mathrm{D}}(t) = a_j^{\mathrm{D}}(t)$ for all j and t.

To see that the gauge invariant procedure is also consistent with the FW transformations, let us consider the non-relativistic Hamiltonian of a *spinning* particle in the gauge $(\boldsymbol{A}, \Phi)$:

$$H = (\boldsymbol{p} - e\boldsymbol{A}/c)^2/2m - g(e\hbar/2mc)\boldsymbol{s} \cdot \boldsymbol{B} + eV_0 + e\Phi, \tag{6.16}$$

where s is the spin. (For comparison, we restrict the spin to magnitude $\frac{1}{2}$.) The total energy operator H_B for this Hamiltonian has been obtained before (Yang 1977); it is†

$$H_B = (\boldsymbol{p} - e\boldsymbol{A}/c)^2/2m - g(e\hbar/2mc)\boldsymbol{s}\cdot\boldsymbol{B} + eV_0. \tag{6.17}$$

If we use $\{E_j(t)\}$ and $\{\Psi_j(\boldsymbol{r}, t)\}$ for the eigenvalues and the orthonormal and complete (assumed) set of eigenfunctions of H_B, the expansion coefficients $\{a_j(t)\}$ in the gauge invariant procedure are

$$a_j(t) = \langle \Psi_j(t) | \Psi(t) \rangle. \tag{6.18}$$

That these amplitudes are consistent with those defined in (6.11) can be seen as follows. If we perform an FW transformation on H_B^{D} in (6.10) by U in (5.6), then

$$\begin{aligned} H_B^U = UH_B^{\mathrm{D}}U^\dagger &= \beta mc^2 + \beta(1/2m)[\boldsymbol{\alpha}\cdot(\boldsymbol{p} - e\boldsymbol{A}/c)]^2 + eV_0 + \ldots \\ &= \beta mc^2 + \beta(\boldsymbol{p} - e\boldsymbol{A}/c)^2/2m - \beta(e\hbar/2mc)\boldsymbol{\Sigma}\cdot\boldsymbol{B} + eV_0 + \ldots, \end{aligned} \tag{6.19}$$

where $\boldsymbol{\Sigma}$ is the Dirac 4×4 spin matrix (usually expressed as $\begin{pmatrix}\sigma & 0\\ 0 & \sigma\end{pmatrix}$ in terms of the 2×2 Pauli spin matrix). If we choose $g = 2$ as is the case for the electron without the anomalous moment interaction correction, we see that H_B in (6.17) is consistent with H_B^U. Hence the $\{a_j(t)\}$ are consistent with the $\{a_j^{\mathrm{D}}(t)\}$.

So far we have not included the spin–orbit interaction and the correction to the kinetic energy due to a term proportional to the fourth power of the particle's momentum. How to obtain the gauge invariant formulation for a non-relativistic particle with these relativistic correction terms has been a subject of recent research work. Some initial results can be found in the works by Kobe and Yang (1980), Yang and Hirschfelder (1980) and Yang *et al* (1981).

7. Discussions

At first, it may look like a paradox that the Schrödinger equation, hence quantum mechanics, is gauge invariant whereas the conventional probability amplitudes and probabilities (defined by either (3.2) or (4.1)) are gauge dependent. However, the *true* meaning of the gauge invariance of the Schrödinger equation is the gauge invariance of the absolute value squared of the wavefunctions *at each position at each time, not* the gauge invariance of the wavefunctions themselves. Since the conventional interpretation uses the eigenfunctions of the 'unperturbed' Hamiltonian (at least once) and the wavefunctions to define the probability amplitudes, there is *no* direct relation between the gauge properties of these amplitudes and the gauge invariance of the Schrödinger equation. In fact, the meanings of the conventional amplitudes and probabilities are *completely* determined by the means of the 'unperturbed' Hamiltonian since the wavefunctions are determined by the Schrödinger equation.

It is only very recently that we begin to realise that the meanings of the 'unperturbed' Hamiltonian vary with the potentials in the Hamiltonian (Cohen-Tannoudji *et al* 1973, 1977, Yang 1976a, Kobe and Smirl 1978, Grynberg and Giacobino 1979,

† This example bears out another basic difficulty in the interpretation of quantum mechanics: that the requirement of gauge invariance *alone* is *not* sufficient to determine *uniquely* the *correct* basis functions to be used to define the probability amplitudes (Yang 1976a §§ II C and D). For example, the choice of $H_B = (\boldsymbol{p} - e\boldsymbol{A}/c)^2/2m + eV_0$ for the Hamiltonian in (6.16) also gives *gauge invariant* expansion coefficients. However, this choice does *not* result in physically measurable probabilities since: (i) it violates the conservation of energy, and (ii) it is not consistent with the FW transformations (to be shown in a moment).

Leubner and Zoller 1980). Out of this understanding, a systematic discussion of operators in general, especially the classification of those operators whose meanings do *not* change with the gauges in the Hamiltonian, has just started to emerge (Yang 1976a, Cohen-Tannoudji *et al* 1977, Kobe and Smirl 1978). As has been discussed in detail by Cohen-Tannoudji *et al* (1977), gauge invariant probability amplitudes can result *only if* they are defined by the eigenfunctions of an operator whose meaning is gauge invariant.

That the conventional intrerpretation generates gauge dependent probabilities can be easily understood in this way by looking into the meaning of the 'unperturbed' Hamiltonian. For simplicity let us use a non-relativistic spinless particle as an example to illustrate the essence of the arguments. Let us work with the Hamiltonian in (2.3).

First, we note that the position operator $\boldsymbol{r}$ has a gauge invariant meaning. Thus, the velocity operator $\boldsymbol{v}$ defined to be the total time-derivative† of $\boldsymbol{r}$,

$$\boldsymbol{v} \equiv (\mathrm{d}\boldsymbol{r}/\mathrm{d}t)_H = [\boldsymbol{r}, H]/\mathrm{i}\hbar = (\boldsymbol{p} - e\boldsymbol{A}/c)/m, \tag{7.1}$$

has a gauge invariant meaning (e.g. Cohen-Tannoudji *et al* 1977). Furthermore, the meaning of $eV_0(\boldsymbol{r})$ is also gauge invariant since

$$[\mathrm{d}(eV_0)/\mathrm{d}t]_H = -\tfrac{1}{2}(e\boldsymbol{v}\cdot\boldsymbol{E}_0 + \boldsymbol{E}_0\cdot e\boldsymbol{v}) \tag{7.2}$$

and both $\boldsymbol{v}$ and $\boldsymbol{E}_0$ have gauge invariant meanings. When expressed in terms of the velocity operator $\boldsymbol{v}$, the 'unperturbed' Hamiltonian in (3.1) becomes

$$H_0 = \{\tfrac{1}{2}m\boldsymbol{v}^2 + eV_0\} + (e/2c)(\boldsymbol{v}\cdot\boldsymbol{A} + \boldsymbol{A}\cdot\boldsymbol{v}) + (e\boldsymbol{A})^2/2mc^2. \tag{7.3}$$

The first term, $\frac{1}{2}m\boldsymbol{v}^2 + eV_0$, is gauge invariant and corresponds to the *Newtonian* total energy. The other two terms in (7.3) depend on the potentials in the Hamiltonian. Hence, the meaning of the 'unperturbed' Hamiltonian varies with the potentials in the Hamiltonian. From this, it is no surprise that the probability amplitudes and probabilities defined by the conventional interpretation are gauge dependent‡.

If the time-varying fields are approximated by the *dipole* approximation, i.e., $\boldsymbol{E}(\boldsymbol{r}, t) \approx \boldsymbol{E}(\boldsymbol{0}, t)$ and $\boldsymbol{B}(\boldsymbol{r}, t) \approx 0$, and if we choose the gauge to be such that $\boldsymbol{A}(\boldsymbol{r}, t) = 0$ and $\Phi(\boldsymbol{r}, t) = -e\boldsymbol{r}\cdot\boldsymbol{E}(\boldsymbol{0}, t)$, then according to (7.3), the 'unperturbed' Hamiltonian corresponds to the Newtonian total energy. Thus, the conventional probabilities *in this gauge* are the physically measurable probabilities *during* the interaction. This simple understanding has been applied (Yang 1976a) to explain Lamb's observation (1952) that only the interaction $-e\boldsymbol{r}\cdot\boldsymbol{E}$ gives results in agreement with his experimental data. It has recently been applied by Leubner and Zoller (1980) to resolve some gauge-related difficulties in the current literature.

The gauge invariant formulation is designed to correct this situation by using the eigenfunctions of the total energy operator to define the probability amplitudes. Here, the total energy operator is determined by Poynting's theorem describing the conservation of the particle's energy with the field energy and field energy flux due to the time-varying field. The *probabilities* thus defined have two physically important characteristics. First, they are gauge invariant since Poynting's theorem and the conservation law of energy, and hence the total energy operator, are gauge invariant. Second and more important, they are consistent with this conservation law of energy and hence they are physically measurable.

† The following symbol $(\mathrm{d}/\mathrm{d}t)_H$ is defined in the first line of equation (3.11).

‡ One can also prove that the conventional interpretation is gauge dependent (Yang 1976c) by using the propagation properties of potentials in different gauges (Yang 1976b).

So far we have discussed only the theoretical aspects of the conventional and the gauge invariant formulations. As far as the *exact* probability amplitudes are concerned, they are very different. This brings up another important question: How would the *practical* results from these two formulations compare with each other? (Here one should bear in mind that *all practical* results depend on the approximations used in solving the differential equations for the probability amplitudes. Thus, the statement that is true for one approximation *may not* be appropriate for another.) A recent investigation (Yang 1981b) indicates that, within the framework of *the time-dependent perturbation theory without the effects of the line widths*, the net transition rates predicted by these two formulations are identical†.

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† It should be noted that the *conventional* time-dependent perturbation theory is formulated according to the procedure in (3.2) rather than (4.1) (e.g. Cohen-Tannoudji *et al* 1973, Bassani *et al* 1977, Power and Thirunamachandran 1978, Grynberg and Giacobino 1979).

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