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Representation of the Spin in the Dirac Equation for the Electron

TOYOKI KOGA

3061 *Ewing Avenue, Altadena, California* 91001, U.S.A.

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Abstract

The conventional interpretation of the spin matrices contained in the Dirac equation for the electron is considered to be mostly unintelligible in the operational sense. It is shown that it appears that the interpretation is often illogical. The necessity of a more comprehensible interpretation of the concerned equation is implied.

1. *Introduction*

Pauli's non-relativistic spin matrices were first introduced as analogous to operators representing orbital angular momenta. Constituting the interaction between the electron and an external magnetic field, the matrices were shown to yield the anomalous Zeeman effect and the spin-orbit coupling effect. In the course of derivation of the Dirac equation for the electron, two requirements, the first that the equation must be linear in the operator $\partial/\partial t$ and the second that the equation is covariant under the Lorentz transformation, lead to the introduction of spin matrices almost uniquely. Our confidence in the Dirac equation seems to begin at this point, and the interpretation of the equation has been constructed as to be in accordance with Pauli's spin theory (Dirac, 1967). Accordingly, a considerable amount of information of the spin of the electron has been produced deductively, and one tends to accept it as physically feasible. It is rather surprising, however, to note that there is no direct experimental confirmation of it.† Only being placed in the Dirac equation (or similar wave equations), spin matrices yield effects such as the

† In the theory of metals and in chemistry, spins of electrons play significant roles. But those treatments of spins are more or less semi-classical, and are not precisely based on the concerned spin theory.

anomalous Zeeman effect and the spin-orbit coupling effect, which can be compared with relevant experimental results. Are these few and particular cases sufficient for confirming the feasibility of the entire spin theory? Are we obliged to refrain from searching any other interpretation of the Dirac equation, if it tends to conflict with the interpretation made according to the conventional spin theory? The present study has been motivated by those questions.

As we shall see in Section 2, it is difficult to derive Heisenberg's equations of motion from the Dirac equation for the electron. (Furthermore, there is no direct experimental confirmation of the outcome of Heisenberg's equations of motion governing spin matrices.) Hence it is emphasized that interpretation of spin matrices in the Dirac equation is to be made solely in terms of solutions of the Dirac equation itself. In Section 3, the motion of a free electron is investigated. In Section 4, we re-examine the well-known demonstration that the spin magnetic moment contributes a part of the energy when an electron is placed in an electromagnetic field. In Section 5, we re-examine the conventional statement that two different representations of the same spin observable are equivalent when placed in the Dirac equation.

As noted earlier by Lamb (1969), it is true that almost all expositions of quantum mechanics make use of the notion that some kinds of measurements are possible. That is to accept a conclusion of the mathematical formalism as physically real if it is possible to restate the conclusion in terms of phenomena to be manipulated in the physical world. This approach tends to lead us to make an unbound extension and animation of a fictitious image of reality, particularly when those conclusions are not completely logically obtained.

2. *The Dirac Equation and Heisenberg's Equations of Motion*

We write for the Dirac equation for the electron (Dirac, 1967)

$$\{\beta(i\hbar\, \partial/\partial t - eA_t) + \beta \boldsymbol{\alpha}.(i\hbar c\, \partial/\partial \mathbf{r} + e\mathbf{A}) - mc^2\}\Psi = 0 \qquad (2.1)$$

where $\mathbf{r} = (x, y, z)$, $(\mathbf{A}, iA_t)$ is a 4-vector potential and e the electronic charge ($e < 0$); the α's and β satisfy the following relations:

$$\alpha_x^2 = \alpha_y^2 = \alpha_z^2 = \beta^2 = 1$$

$$\alpha_x\alpha_y + \alpha_y\alpha_x = 0, \qquad \alpha_x\beta + \beta\alpha_x = 0, \text{ etc.} \qquad (2.2)$$

We may represent $\beta, \boldsymbol{\alpha}$, and Ψ as follows:

$$\beta = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}, \qquad \boldsymbol{\alpha} = \rho\boldsymbol{\sigma}, \qquad \Psi = \begin{pmatrix} \Psi_1 \\ \Psi_2 \\ \Psi_3 \\ \Psi_4 \end{pmatrix}$$

where

$$\rho = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix} \qquad \sigma_x = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

$$\sigma_y = \begin{pmatrix} 0 & -i & 0 & 0 \\ i & 0 & 0 & 0 \\ 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \end{pmatrix} \qquad \sigma_z = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \qquad (2.3)$$

The σ's are spin matrices.

According to (2.3), equation (2.1) consists of four simultaneous partial differential equations. If we interchange a pair of σ's in equation (2.1),† we obtain a different set of partial differential equations. By solving the two sets of equations under the same boundary condition, we may obtain two different sets of particular solutions in general. It is conventionally believed, however, that the interchange of the pair of σ's does not cause any difference in the physical implication of equation (2.1). This implies rather clearly that significant solutions and interpretations of the Dirac equation made in quantum mechanics are expected to be so particular and limited that the evident mathematical difference between the aforementioned two sets of equations is physically insignificant.

The above observation suggests further that the knowledge of the electron provided by the conventional interpretation of the Dirac equation might not be precise, if the Dirac equation itself be assumed to be precise for representing the behavior of the electron. In quantum mechanics, however, it is customary to avoid this criticism by showing that those matrices, apparently time-independent in the Dirac equation, vary in time according to Heisenberg's equations of motion which are believed to be derivable from the Dirac equation. As contrary to the belief, it will be shown in the following that Heisenberg's equations of motion are not derivable from the Dirac equation.

In order to find the connection between the Heisenberg picture and the Schrödinger picture, as is well known (Dirac, 1967), it is necessary to define unitary operator T by

$$T = \exp\left[-i \int H(t)\, dt/\hbar\right] \qquad (2.4)$$

† It is necessary to adjust signs so that $\boldsymbol{\sigma} \times \boldsymbol{\sigma} = 2i\boldsymbol{\sigma}$ holds in the vector form.

where $H(t)$ is the Hamiltonian defined in the Schrödinger picture, or in the Dirac equation in this case. An operator v in the Dirac equation yields v_t in the Heisenberg picture according to

$$v_t = T^{-1} v T \tag{2.5}$$

Particularly

$$H_t = T^{-1} H(t) T = H(t) \tag{2.6}$$

Then, considering (2.4) and (2.5), we obtain Heisenberg's equation of motion for v_t:

$$i\hbar\, dv_t/dt = v_t H(t) - H(t) v_t \tag{2.7}$$

In the above derivation of equation (2.7), we notice that operator T can be defined only if the state under consideration can be given as a linear superposition of eigenstates of $H(t)$. (Otherwise, we cannot define $\exp(-iHt/\hbar)$ where H is an operator.) This condition is realized if the energy eigenfunctions concerned constitute a complete and orthonormal set. As is shown in the Appendix, however, the completeness and the orthonormality are not compatible with respect to the energy eigenfunctions satisfying the Dirac equation. Hence the Dirac equation should be interpreted in its own context, without Heisenberg's equations of motion being employed.

The result of the above investigation implies that, if the anisotropy of the electron structure is embodied in the Dirac equation, it should be represented by the anisotropy of the spin matrices. Indeed, the σ's are often regarded as constituting a 3-vector (Dirac, 1967). From this point of view, we may regard $(\beta\boldsymbol{\alpha}, i\beta)$ as a 4-vector and Ψ as a set of scalars, so that the Dirac equation is covariant under the rotational transformation (including the Lorentz transformation) of the coordinate axes.

3. *The Motion of a Free Electron*

We assume

$$(\mathbf{A}, iA_t) = 0 \tag{3.1}$$

in equation (2.1), and consider for the solution of the equation

$$\Psi_\xi = a_\xi \exp\left[-i(Wct - \mathbf{p}\,.\mathbf{r})/\hbar + i\theta_\xi\right] \qquad (\xi = 1, 2, 3, 4) \tag{3.2}$$

where W and $\mathbf{p}$ are respectively numbers for energy and momentum.

For the first case, we assume

$$\left.\begin{array}{ll} p_x \neq 0, & p_y = p_z = 0 \\ \theta_\xi = 0 & \end{array}\right\} \tag{3.3}$$

By substituting (3.1), (3.2) and (3.3) in (2.1), we obtain

$$Wa_1 - p_x a_4 - mca_1 = 0 \tag{3.4}$$

$$Wa_2 - p_x a_3 - mca_2 = 0 \tag{3.5}$$

$$Wa_3 - p_x a_2 + mca_3 = 0 \tag{3.6}$$

$$Wa_4 - p_x a_1 + mca_4 = 0 \tag{3.7}$$

By solving these, we obtain

$$W = \pm(m^2c^2 + p_x^2)^{1/2} \tag{3.8}$$

$$\frac{a_1}{a_4} = \frac{a_2}{a_3} = \frac{p_x}{W - mc} = \frac{W + mc}{p_x} \tag{3.9}$$

The direction in which the component of $\boldsymbol{\sigma}$ has the present state for its eigenstate is found by considering

$$(l\sigma_x + m\sigma_y + n\sigma_z)\Psi = \pm\Psi \tag{3.10}$$

where l, m, n are the direction cosines of the concerned direction. On substituting (3.2) in (3.10) under condition (3.9), we obtain

$$l = \pm 1, \qquad m = n = 0 \tag{3.11}$$

and

$$\Psi_1 = \pm\Psi_2, \qquad \Psi_3 = \pm\Psi_4 \tag{3.12}$$

Under conditions (3.11) and (3.12), Ψ represents the eigenstate of energy and that of σ_x at the same time.

Secondly, if we assume, instead of (3.3),

$$\left.\begin{array}{l} p_y \neq 0, \quad p_x = p_z = 0, \\ \theta_4 - \theta_1 = \theta_2 - \theta_3 = \pi/2 \end{array}\right\} \tag{3.13}$$

we find that Ψ represents the eigenstate of energy and that of σ_y. Similarly, on assuming

$$\left.\begin{array}{l} p_z \neq 0, \qquad p_x = p_y = 0 \\ \theta_\xi = 0 \end{array}\right\} \tag{3.14}$$

we find that Ψ represents the eigenstate of energy and that of σ_z.

Those solutions shown above are well known. Nevertheless, we have repeated them in order to conclude that the spin of a free electron has eigenvalues $\pm\hbar/2$ only in the direction of its motion. It is also noted that this is the unique case in which the Hamiltonian and a component of spin have eigenvalues at the same time, as is seen in the following relation: In general, when $(\mathbf{A}, A_t) = 0$, we have

$$\sigma_x H - H\sigma_x = 2ic\rho(\sigma_z p_y - \sigma_y p_z) \tag{3.15}$$

and σ_x commutes with H, if

$$p_y\Psi = p_z\Psi = 0 \tag{3.16}$$

(In (3.15) and in (3.16), p_y and p_z are operators.)

The above conclusion derived from the Dirac equation is conventionally accepted as of the electron. If one asks the physical significance of the conclusion, however, the answer is not simple. For example, we consider the following: An eigenstate of σ_z can be regarded as a superposition of the two eigenstates of σ_x (or of σ_y). Therefore, if there is a way of observing σ_x with respect to a state which is known to be an eigenstate of σ_z, the state immediately after the measurement will be an eigenstate of σ_x, according to the theory of measurement. According to results of our investigation of the Dirac equation, an eigenstate of σ_z is an eigenstate of momentum with the eigenvalue in the z-direction, and the eigenstate of σ_x is an eigenstate of momentum with the eigenvalue in the x-direction. Therefore, the measurement of the spin made in the above must have changed the momentum also, i.e., the motion of the electron, being initially in the z-direction, changes to be in the x-direction. When the measurement is made only with respect to the spin angular momentum, how can the change of the momentum occur without violating the momentum conservation law? On the other hand, the measurement of the momentum made with respect to the eigenfunction of a component of $\boldsymbol{\sigma}$, e.g. σ_z, must result in a definite value which is in the z-direction, and there is no change of the state after the measurement.

4. *An Approach of Solving the Dirac Equation*

On regarding the Dirac equation as a set of partial differential equations, an approach of solving the Dirac equation may be to reduce the equation to a set of four equations of which each contains only one of the four functions $\Psi_1, \Psi_2, \Psi_3, \Psi_4$. The reduction can be done only by increasing the order of those differential equations. Then, we should note that a solution of the resultant equations does not always satisfy the original Dirac equation. In the following, we shall carry out the reduction in such a way that the covariance under the Lorentz transformation is preserved in the result. In the process of reduction, there will be an opportunity to refer to the well-known demonstration of the existence of the spin magnetic moment.

By writing p_t for $i\hbar\, \partial/\partial t$ and p_x for $-i\hbar c\, \partial/\partial x$, etc., we have for equation (2.1)

$$\{\beta(p_t - eA_t) - \beta\boldsymbol{\alpha}.(\mathbf{p} - e\mathbf{A}) - mc^2\}\Psi = 0 \tag{4.1}$$

According to the investigation made in Section 2, we regard

$$(\beta\boldsymbol{\alpha}, i\beta) \tag{4.2}$$

as a four-vector and Ψ as a scalar. Then, equation (4.1) is covariant under the Lorentz transformation. We consider operator

$$D_1 = \beta(p_t - eA_t) - \beta\boldsymbol{\alpha}.(\mathbf{p} - e\mathbf{A}) + mc^2 \tag{4.3}$$

which is also covariant under the Lorentz transformation. On operating (4.3) on (4.1) from the left-hand side, we obtain

$$\{(p_t - eA_t)^2 - (p - eA)^2 - m^2c^4 + e\hbar c\,\boldsymbol{\sigma}.\mathbf{H} - ie\hbar c\boldsymbol{\alpha}.\,\mathbf{E}\}\Psi = 0 \tag{4.4}$$

where $\mathbf{H}$ = curl $\mathbf{A}$ and $\mathbf{E} = -\partial \mathbf{A}/\partial(ct) - \text{grad}\, A_t$. In view of the process of derivation, equation (4.4) is covariant under the Lorentz transformation.

Noting that

$$(\boldsymbol{\sigma}.\mathbf{H} - i\,\boldsymbol{\alpha}.\mathbf{E})^2 = H^2 - E^2 - 2i\rho\mathbf{E}.\mathbf{H}, \text{etc.}$$

we may reduce equation (4.4) further, by repeating similar treatments, to equations in which matrices $\boldsymbol{\alpha}$, $\boldsymbol{\sigma}$, ρ remain only by being multiplied by higher-order derivatives of A_t, $\mathbf{A}$. It is difficult to eliminate those matrices completely from the resultant equation. Only by ignoring derivatives of A_t and $\mathbf{A}$ of some higher orders, may we do so. On assuming that $\mathbf{E}$ and $\mathbf{H}$ are independent of t and $\mathbf{r}$, and $\mathbf{E} \perp \mathbf{H}$, we operate

$$D_2 = (p_t - eA_t)^2 - (\mathbf{p} - e\mathbf{A})^2 - m^2c^4 - (e\hbar c\,\boldsymbol{\sigma}.\mathbf{H} - ie\hbar c\,\boldsymbol{\alpha}.\mathbf{E})$$

from the left-hand side of (4.4), and obtain

$$\{[(p_t - eA_t)^2 - (\mathbf{p} - e\mathbf{A})^2 - m^2c^4]^2 - e^2\hbar^2c^2(H^2 - E^2)\}\Psi = 0 \quad (4.5)$$

We note the following: (a) Each component of Ψ satisfies the same partial differential equation. (b) If we write for the Dirac equation (2.1)

$$D_0\Psi = 0$$

then we may write for equation (4.5)

$$D_2D_1D_0\Psi = 0 \quad (4.5')$$

Noting that D_2 and D_1D_0 commute mutually, and D_1 and D_0 commute mutually, we may write for (4.5′)

$$D_0D_1D_2\Psi = 0 \quad (4.5'')$$

If solution Ψ of the last equation is known to be $\Psi^{(2)}$, then

$$\Psi^{(0)} = D_1D_2\Psi^{(2)} \quad (4.6)$$

is a solution of the original Dirac equation (2.1). The four components of $\Psi^{(2)}$ are mutually identical. But the four components of $\Psi^{(0)}$ are not so. Also noted is that if $\Psi^{(2)}$ is isotropic, $\Psi^{(0)}$ is not necessarily so.

If Ψ in (4.4) is assumed to be an energy eigenstate, we may substitute W for p_t. With respect to this resultant equation, it is often suggested that $e\hbar c\,\boldsymbol{\sigma}.\mathbf{H}$ implies the existence of the spin magnetic moment. But this interpretation seems to be premature: In this equation, not only $\boldsymbol{\sigma}$ but also $\boldsymbol{\alpha}$ and $\mathbf{p}$ are operators. Furthermore $\mathbf{A}$ and A_t are functions of time and spatial coordinates in general. There is no way to evaluate the eigenvalue of an operator contained in the equation as isolated from the other operators contained in the same equation. For the same reason, it is also premature to conclude that there is no contribution of energy from $ie\hbar c\,\boldsymbol{\alpha}.\mathbf{E}$. Indeed, equation (4.4) cannot be covariant under the Lorentz transformation if the equation does not carry this term of E. Rather the existence of this term of E suggests that the usual interpretation of $e\hbar c\,\boldsymbol{\sigma}.\mathbf{H}$ is overly spontaneous.

If Ψ is an eigenfunction of $(p_t - eA_t)$, then we may have

$$(p_t - eA_t)^2\Psi = [(\mathbf{p} - e\mathbf{A})^2 + m^2c^4 - e\hbar c\,\boldsymbol{\sigma}.\mathbf{H}]\,\Psi$$

But the difficulty of interpreting $e\hbar c\,\boldsymbol{\sigma}.\mathbf{H}$ as isolated from the other operator remains as before.

5. *Equivalency Between Two Representations of the Spin*

In interpretation of the Dirac equation, one often states that the choice of representation of matrices $(\boldsymbol{\alpha}, \beta)$ does not affect the validity of the equation, as long as they satisfy conditions (2.2). First we write for the Dirac equation

$$\{(p_t - eA_t) - \alpha_x(p_x - eA_x) - \alpha_y(p_y - eA_y) - \alpha_z(p_z - eA_z) - \beta mc^2\}\Psi^{(1)} = 0 \quad (5.1)$$

We may replace $(\alpha_x, \alpha_y, \alpha_z)$, for instance, with $(\alpha_x, \alpha_z, -\alpha_y)$ obtaining

$$\{(p_t - eA_t) - \alpha_x(p_x - eA_x) - \alpha_z(p_y - eA_y) + \alpha_y(p_z - eA_z) - \beta mc^2\}\Psi^{(2)} = 0 \quad (5.2)$$

Equation (5.2) is believed to be equivalent to equation (5.1).

Suppose that by solving (5.1) under a certain boundary condition we obtain W for an eigenvalue of p_t. If equation (5.2) under the same boundary condition has the same energy eigenvalue W and the same eigenfunction

$$\Psi^{(2)} = \Psi^{(1)} \quad (5.3)$$

then we have from (5.1) and (5.2)

$$[(\alpha_y - \alpha_z)(p_y - eA_y) + (\alpha_z + \alpha_y)(p_z - eA_z)]\Psi^{(1)} = 0 \quad (5.4)$$

In general, one would not expect such a symmetry as (5.4) in $\Psi^{(1)}$. The quantum-mechanical equivalence does not necessarily require condition (5.3). Instead, it is required that

$$\begin{aligned} \Psi^{(1)*}\Psi^{(1)} &= \Psi^{(2)*}\Psi^{(2)} \\ \Psi^{(1)*}\boldsymbol{\alpha}\Psi^{(1)} &= \Psi^{(2)*}\boldsymbol{\alpha}\Psi^{(2)} \end{aligned} \quad (5.5)$$

Suppose that W is an eigenvalue of p_t with respect to (5.1). By substituting the same value W for p_t in (5.2), we obtain a set of four partial differential equations. Further we suppose that we are able to solve the equations obtaining $\Psi^{(2)}$. Those two sets of solutions, $\Psi^{(1)}$ and $\Psi^{(2)}$, are now required to satisfy (5.5). We notice that those solutions are functionals of $(\mathbf{A}, A_t)$ which may be given arbitrarily. In order to assure the equivalence between (5.1) and (5.2), one has to prove that condition (5.5) is always satisfied if $(\mathbf{A}, A_t)$ are chosen arbitrarily. This proof has never been given and is most unlikely to be possible. In the case of a free electron discussed in Section 3, the proof is easily given. As the field becomes stronger and more complex, the two equations may not be equivalent. Under what condition of the field, do they cease to be equivalent? We do not know.

In the theory of the anomalous Zeeman effect, and also of the spin-orbit coupling, it is customary to take the component of the spin operator in the direction of the concerned magnetic field as diagonal. See Rose (1961), Section 30. In view of the remarkable success of the theory, we may say at least that the above relation between the spin matrices and the magnetic field is feasible in this case. Then it may be of interest to investigate the anomalous Zeeman as based on the Dirac equation in which the component of the spin operator in the z-direction is diagonal and the magnetic field is in the y-direction. (Even when this Dirac equation happens to produce the same result as before, there is no assurance that these two Dirac equations are equivalent in cases of more complex external fields, of course.)

What we need to prove is the equivalence rather than the inequivalence. In view of (5.4), we may say at least that the proof can be positive only under some restrictive conditions. And, against the ordinary belief, one has to recognize that the Dirac equation in a representation of the spin operator is not equivalent to the Dirac equation in another representation of the same spin observable.

6. *Conclusion*

1. Heisenberg's equations of motion are not derivable from the Dirac equation for the electron. Hence, the Dirac equation must be interpreted in terms of its own solutions.

2. A set of spin matrices separated alone from the other operators may be evaluated according to the conventional spin theory. But the result is often operationally untenable.

3. If the anisotropy of the electron structure is embodied in the Dirac equation, the anisotropy must be represented by the anisotropy of the spin matrices. From this point of view, $(\beta\boldsymbol{\alpha}, i\beta)$ must constitute a 4-vector. Then Ψ is a 4-component scalar.

4. In general the Dirac equation given in a representation of the spin observable is not equivalent to the Dirac equation given in another representation of the same observable, even though the equivalency for the purpose of evaluating energy eigenvalues may exist as depending on the characteristics of the external field exerted on the concerned electron. The known success of the Dirac equation in yielding the anomalous Zeeman effect and the spin-orbit coupling effect does not seem to provide a proof of the overall feasibility of the conventional interpretation of the equation.

Appendix

Incompatibility Between the Completeness and the Orthonormality of a set of Multi-Component Wavefunctions (Spinors)

In this appendix, we shall demonstrate that the orthonormality condition considered for a set of energy eigenfunctions satisfying the Dirac equation for the electron is not compatible with the conventional completeness relation of the same set. The difficulty arises from the fact that each state satisfying the

Dirac equation consists of more than one function. For the sake of simplicity, therefore, we suppose that each state consists of two functions, instead of four, in this Appendix.

A set of two-component functions

$$\Psi^{(i)}(X) = (\Psi_1^{(i)}(X), \Psi_2^{(i)}(X)) \qquad i = 1, 2, \ldots, n \tag{A.1}$$

is supposed to satisfy the orthonormality condition

$$\sum_{\sigma=1}^{2} \int \Psi_\sigma^{(i)*}(X)\Psi_\sigma^{(j)}(X)\,dX = \delta_{ij} \tag{A.2}$$

Taking an arbitrary two-component function

$$F(X) = (F_1(X), F_2(X)) \tag{A.3}$$

we anticipate that it is possible for F to be given by

$$F_\sigma(X) = \sum_i a^{(i)}\Psi_\sigma^{(i)} \qquad (\sigma = 1, 2) \tag{A.4}$$

where $a^{(i)}$ is determined by

$$a^{(i)} = \sum_{\sigma=1}^{2} \int F_\sigma(X)\Psi_\sigma^{(i)*}(X)\,dX \tag{A.5}$$

In order to see the validity of (A.4), we first derive from (A.4)

$$\int F_\sigma(X)\Psi_\sigma^{(i)*}(X)\,dX = \sum_j \int a^{(j)}\Psi_\sigma^{(j)}(X)\Psi_\sigma^{(i)*}(X)\,dX$$

(A.5) being substituted in the right hand side,

$$= \sum_j \sum_\rho \int F_\rho(X')\Psi_\rho^{(j)*}(X')\,dX' \int \Psi_\sigma^{(j)}(X)\Psi_\sigma^{(i)*}(X)\,dX \tag{A.6}$$

The validity of (A.6) is assured, if there is a relation

$$\sum_j \Psi_\rho^{(j)*}(X')\Psi_\sigma^{(j)}(X) = \delta_{\rho\sigma}\delta(X - X') \tag{A.7}$$

If F is a particular function chosen specifically, relation (A.6) might be valid, without relying on (A.7). If the choice of F is arbitrary, relation (A.7) is not only sufficient but also necessary; the relation is conventionally called the completeness relation (e.g., Rose, 1961, page 93).

In the following, we shall demonstrate that relation (A.7) is not compatible with the orthonormality condition (A.2). From (A.7), we have

$$\sum_j \Psi_1^{(j)*}(X')\Psi_1^{(j)}(X) = \delta(X - X') \tag{A.8}$$

On operating $\int F_1(X')\,dX'$ on both sides of (A.8), we have

$$\int F_1(X') \sum_i \Psi_1^{(i)*}(X')\Psi_1^{(i)}(X)\,dX' = \int F_1(X')\delta(X - X')\,dX'$$

or

$$\sum_i b_1^{(i)}\Psi_1^{(i)}(X) = F_1(X) \tag{A.9}$$

where

$$b_1^{(i)} = \int F_1(X)\Psi_1^{(i)*}(X)\,dX \tag{A.10}$$

Relations (A.9) and (A.10) imply that the $\Psi_1^{(i)}$'s constitute a complete set of orthonormal *one-component* functions. (Here again, we should note that $F(X)$ is not a particular function chosen specifically.) Similarly we have

$$\sum_i b_2^{(i)}\Psi_2^{(i)}(X) = F_2(X) \tag{A.9$'$}$$

with

$$b_2^{(i)} = \int F_2(X)\Psi_2^{(i)*}(X)\,dX \tag{A.10$'$}$$

By comparing (A.9) and (A.9′) with (A.4), we see that

$$b_1^{(i)} = b_2^{(i)} = a^{(i)} \tag{A.11}$$

must be satisfied. But definition (A.5) requires that

$$b_1^{(i)} + b_2^{(i)} = a^{(i)} \tag{A.12}$$

Relation (A.11) is not compatible with relation (A.12).

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