CHINESE JOURNAL OF PHYSICS VOL. 33, NO. 2 APRIL 1994

Implications of Parity and Time-Reversal Symmetries in Atoms

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(Received November 29,1993)

We have investigated the implications of parity and time-reversal symmetries in atoms. The atomic wave function is expressed as a linear combination of configuration wave functions. If parity symmetry is violated, an atomic state no longer has a definite parity such that both electronic orbitals and configuration weight coefficients contain parity-nonconserving components. Time-reversal symmetry guarantees that the radial wave functions of the large and small components of the Dirac orbital differ in phase by $\pm\pi/2$, and the parity-conserving and parity-nonconserving components of the Dirac orbital differ in phase by $\pm\pi/2$ as well. In addition, time-reversal symmetry implies that the relative phases between parity-conserving configuration weight coefficients are 0 or π, while the relative phases between parity-conserving and parity-nonconserving configuration weight coefficients are $\pm\pi/2$. The absence of permanent electric dipole moments of atoms with definite angular momentum is demonstrated. In addition, the Kramers theorem is elucidated explicitly in the relativistic context. In the multipole expansion of the photon field, the relative phases between the expansion coefficients for the transverse electric multipole potentials and for the magnetic or longitudinal electric multipole potentials are $\pm\pi/2$. Finally, we show that the relative phases between competing transition amplitudes are 0 or π, which leads to constructive or destructive interferences between competing atomic transitions.

PACS. 11.30.Er – Charge conjugation, parity, time reversal, and other discrete symmetries.
PACS. 31.10.+z – General theory of electronic structure, electronic transitions, and chemical binding.
PACS. 32.80.-t – Photon interactions with atoms.

I. INTRODUCTION

Parity and time-reversal symmetries imply that physical laws are invariant under the parity and time-reversal transformations. Traditionally, the dynamics of atoms are described by the coupled Dirac and Maxwell equations, which are parity and time-reversal invariant. The implications of parity symmetry in atoms were first investigated by Wigner [1], who demonstrated that the Laporte selection rule [2] for atomic transitions was a consequence of parity symmetry. Lee and Yang [3] showed that parity and time-reversal symmetries prohibit the existence of permanent electric dipole moments of atoms with definite angular momentum. In 1967 Weinberg, Salam, and Glashow [4,5] proposed the unified theory of weak and electromagnetic interactions, according to which, there is a parity-nonconserving (PNC) potential between electrons and nucleons. The discovery of CP violation [6] in 1964 also predicted time-reversal-violating (TRV) interactions within atoms [7-11]. During the past, decades, many experiments have been performed to test parity and time-reversal symmetries in atoms [12-16]. At the same time, several theoretical approaches have been proposed to calculate PNC and TRV effects in atoms [17-21].

In this paper, we investigate some aspects of the implications of parity and time-reversal symmetries in atoms. In Sec. II, we explore the implications of parity and time-reversal symmetries in the atomic wave functions. The atomic wave function is expressed as a linear combination of configuration wave functions. If parity symmetry is violated, both electronic orbitals and configuration weight coefficients contain PNC components. Time-reversal symmetry guarantees that the radial wave functions of the large and small components of the Dirac orbital differ in phase by $\pm\pi/2$, and the parity-conserving (PC) and PNC components of the Dirac orbital differ in phase by $\pm\pi/2$ as well. In addition, time-reversal symmetry implies that the relative phases between PC configuration weight coefficients are 0 or π, while the relative phases between PC and PNC configuration weight coefficients are $\pm\pi/2$. The Lee-Yang theorem [3] arises naturally as a consequence of the preceding assertions. In addition, the Kramers theorem [22] is elucidated in the relativistic context.

In Sec. III, we explore the implications of parity and time-reversal symmetries in the photon field. In the multipole expansion of the photon field, the relative phases between the expansion coefficients for the transverse electric multipole potentials and for the magnetic or longitudinal electric multipole potentials are $\pm\pi/2$, provided time-reversal symmetry holds.

In Sec. IV, we explore the implications of parity and time-reversal symmetries in atomic transitions. Parity symmetry leads to the parity selection rule for atomic transitions. If parity symmetry is violated, however, transitions between two atomic states contain both PC and PNC components. The interference of these competing transition amplitudes depends on their relative phases. We show that the relative phases between competing transition amplitudes are 0 or π, which leads to constructive or destructive interferences between competing atomic transitions. Conclusions are made in Sec. V. In the Appendix, we present the parity and time-reversal operators for the coupled electron-positron and photon fields.

II. IMPLICATIONS OF PARITY AND TIME-REVERSAL SYMMETRIES IN THE ATOMIC WAVE FUNCTIONS

II-l. The atomic wave function

The atomic wave function Ψ may be expressed as a linear combination of configuration wave functions. If the atomic Hamiltonian does not conserve parity, the wave function contains configurations of both parities:

$$\Psi = \sum_{\alpha} C_{\alpha}\Psi_{\alpha} + \sum_{\bar{\alpha}} C_{\bar{\alpha}}\Psi_{\bar{\alpha}}\,, \tag{2.1}$$

where α and $\bar{\alpha}$ are the configuration indices for the PC and PNC configurations, respectively. The configuration wave functions are built up from Dirac orbitals. We can construct the Dirac orbital as a simultaneous eigenfunction of H_D, K, $\vec{J}^2$,j_z, and $\vec{s}^2$ with eigenvalues ε, $-\kappa$, $j(j+1)$, m, and $1/2(1/2+1)$, respectively, where H_D is the one-electron Dirac Hamiltonian for a central field, and K is defined as

$$K = \gamma^0\left(\vec{\Sigma}\cdot\vec{j} - \frac{1}{2}\right). \tag{2.2}$$

Here γ^0 and $\vec{\Sigma}$ are the Dirac matrices

$$\gamma^0 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \tag{2.3}$$

$$\vec{\Sigma} = \begin{pmatrix} \vec{\sigma} & 0 \\ 0 & \vec{\sigma} \end{pmatrix}, \tag{2.4}$$

where $\vec{\sigma}$ are the Pauli matrices, and the unit entries in γ^0 represent 2×2 unit matrices. Relativistic units are employed in this paper. The total angular-momentum operator $\vec{j}$ is given by

$$\vec{j} = \vec{l} + \vec{s}, \tag{2.5}$$

where the orbital and spin angular-momentum operators are defined as

$$\vec{l} = \vec{r}\times\vec{p}, \tag{2.6}$$

$$\vec{s} = \frac{1}{2}\vec{\Sigma} . \tag{2.7}$$

For a definite κ, the total angular-momentum quantum number j and the orbital angular-momentum quantum number l of the large component, which determines the parity of the Dirac orbital, are given as

$$j = |\kappa| - \frac{1}{2}, \tag{2.8}$$

$$l = \begin{cases} \kappa , & \kappa > 0 , \\ -\kappa - 1 , & \kappa < 0 . \end{cases} \tag{2.9}$$

Dirac orbitals with definite $\varepsilon\kappa m$ take the explicit form

$$u_{\varepsilon\kappa m} = \begin{pmatrix} G_{\varepsilon\kappa}\Omega_{\kappa m} \\ F_{\varepsilon\kappa}\Omega_{-\kappa m} \end{pmatrix} , \tag{2.10}$$

Here $G_{\varepsilon\kappa}$ and $F_{\varepsilon\kappa}$ *are* the radial wave functions of the large and small components. The angular functions $\Omega_{\kappa m}$ in Eq. (2.10) are normalized spherical spinors defined as

$$\Omega_{\kappa m} \equiv \Omega_{jlm} = \sum_{M\mu}\left\langle lM\frac{1}{2}\mu|jm\right\rangle Y_{lM}(\hat{r})\chi_{\mu} , \tag{2.11}$$

where Y_{lM} is the spherical harmonics, and χ_{μ} is the spin eigenfunction with s $=1/2$ and $s_z = \mu$, given, for example, by the two-component Pauli spinor.

II-Z. The parity and time-reversal symmetries

It can be shown that the parity operator for the electron-positron field is given as (see the Appendix)

$$P_e = \gamma^0 P , \tag{2.12}$$

where P is the inversion operator for the spatial coordinates. For an N-electron atom, the parity operator is given as

$$P_a = \prod_{j=1}^{N} \gamma_j^0 P_j , \tag{2.13}$$

where j is the index for the j-th electron. It follows from Eqs. (2.10) and (2.12) that the parity of the Dirac orbital is $(-)^l$. It is interesting to note that because of γ^0 parity symmetry requires the large and small components of the Dirac orbital to be of opposite parities in the spatial coordinates. If parity symmetry is violated, a Dirac orbital contains a PNC component:

$$v_{\varepsilon\kappa m} = u_{\varepsilon\kappa m} + u_{\varepsilon\kappa m}^{PNC} , \tag{2.14}$$

where

$$u_{\varepsilon\kappa m}^{PNC} = \begin{pmatrix} P_{\varepsilon\kappa}\Omega_{-\kappa m} \\ Q_{\varepsilon\kappa}\Omega_{\kappa m} \end{pmatrix} . \tag{2.15}$$

Of course the designation of an orbital v_α by the quantum numbers $\varepsilon_\alpha, \kappa_\alpha$, and m_α is somewhat artificial since it contains components of opposite values of κ. In the following paragraphs we adopt the convention that an orbital v_α is referred to by the quantum numbers $\alpha \equiv (\varepsilon_\alpha, \kappa_\alpha, m_\alpha)$ of its PC component.

The time-reversal operator for the electron-positron field is given as (see the Appendix)

$$T_e = i\gamma^1\gamma^3 CT , \tag{2.16}$$

where C is the complex conjugate operator, and T stands for the inversion operator for the temporal coordinate. For an N-electron atom, the time-reversal operator is given as

$$T_a = i^N \prod_{j=1}^{N} \gamma_j^1 \gamma_j^3 C_j T_j . \tag{2.17}$$

It follows from Eq. (2.16) that the time-reversed state of the Dirac orbital $v_{\varepsilon\kappa m}$ (2.14) is given as

$$\begin{aligned} T_e v_{\varepsilon\kappa m} &= i\gamma^1\gamma^3 \left[\begin{pmatrix} G_{\varepsilon\kappa}^*\Omega_{\kappa m}^* \\ F_{\varepsilon\kappa}^*\Omega_{-\kappa m}^* \end{pmatrix} + \begin{pmatrix} P_{\varepsilon\kappa}^*\Omega_{-\kappa m}^* \\ Q_{\varepsilon\kappa}^*\Omega_{\kappa m}^* \end{pmatrix} \right] \\ &= (-)^{j+l+m+1/2} \left[\begin{pmatrix} G_{\varepsilon\kappa}^*\Omega_{\kappa -m} \\ -F_{\varepsilon\kappa}^*\Omega_{-\kappa -m} \end{pmatrix} - \begin{pmatrix} P_{\varepsilon\kappa}^*\Omega_{-\kappa -m} \\ -Q_{\varepsilon\kappa}^*\Omega_{\kappa -m} \end{pmatrix} \right] , \end{aligned} \tag{2.18}$$

where we have made use of the identities

$$Y_{lM}^* = (-)^M Y_{l-M} , \tag{2.19}$$

$$\langle j_1 m_1 j_2 m_2 | j_3 m_3 \rangle = (-)^{j_1+j_2-j_3} \langle j_1 - m_1 j_2 - m_2 | j_3 - m_3 \rangle . \tag{2.20}$$

11-3. **Phase relations**

Symmetry considerations reveal a phase relation between the Dirac orbital and its time-reversed partner. If the interactions are invariant under time-reversal, the Mamiltonian commutes with the time-reversal operator, i.e.,

$$[H_D, T_e] = 0 . \tag{2.21}$$

It is also straightforward to show that

$$[K, T_e] = 0\,, \tag{2.22}$$

$$[\gamma^0, T_e] = 0\,, \tag{2.23}$$

$$\{\vec{j}, T_e\} = 0\,, \tag{2.24}$$

$$\{\vec{\Sigma}, T_e\} = 0\,. \tag{2.25}$$

It follows from Eqs. (2.21) and (2.22) that the time-reversal transformation will leave the quantum numbers ε and κ unaltered. Furthermore, it follows from Eq. (2.24) that

$$\begin{aligned} j_z T_e v_{\varepsilon\kappa m} &= -T_e j_z v_{\varepsilon\kappa m} \\ &= -m T_e v_{\varepsilon\kappa m}\,, \end{aligned} \tag{2.26}$$

which indicates that the time-reversed Dirac orbital $T_e v_{\varepsilon\kappa m}$ must be proportional to $v_{\varepsilon\kappa-m}$ within an arbitrary phase, i.e.,

$$T_e v_{\varepsilon\kappa m} = e^{i\theta(\varepsilon\kappa m)} v_{\varepsilon\kappa-m}\,, \tag{2.27}$$

because the Dirac orbital is completely specified by the quantum numbers ε, κ, and m.

The phase factor $e^{i\theta(\varepsilon\kappa m)}$ in Eq. (2.27) can be further simplified. The raising and lowering operators are defined as

$$j_+ = j_x + i j_y\,, \tag{2.28}$$

$$j_- = j_x - i j_y\,, \tag{2.29}$$

with the properties

$$j_+|\varepsilon\kappa m\rangle = \sqrt{\left(|\kappa| - m - \frac{1}{2}\right)\left(|\kappa| + m + \frac{1}{2}\right)}\,|\varepsilon\kappa(m+1)\rangle\,, \tag{2.30}$$

$$j_-|\varepsilon\kappa m\rangle = \sqrt{\left(|\kappa| + m - \frac{1}{2}\right)\left(|\kappa| - m + \frac{1}{2}\right)}\,|\varepsilon\kappa(m-1)\rangle\,. \tag{2.31}$$

It follows from Eq. (2.24) that

$$\begin{aligned} T_e j_+ &= T_e(j_x + i j_y) \\ &= -(j_x - i j_y) T_e \\ &= -j_- T_e\,. \end{aligned} \tag{2.32}$$

Operating on Eq. (2.30) from the left by T_e yields

$$
\begin{aligned}
T_e j_+ |\varepsilon\kappa m\rangle &= \sqrt{\left(|\kappa| - m - \tfrac{1}{2}\right)\left(|\kappa| + m + \tfrac{1}{2}\right)}\, T_e |\varepsilon\kappa(m+1)\rangle \\
&= \sqrt{\left(|\kappa| - m - \tfrac{1}{2}\right)\left(|\kappa| + m + \tfrac{1}{2}\right)}\, e^{i\theta[\varepsilon\kappa(m+1)]} |\varepsilon\kappa - (m+1)\rangle .
\end{aligned}
\tag{2.33}
$$

Alternatively, from Eqs. (2.27), (2.31), and (2.32) it follows that

$$
\begin{aligned}
T_e j_+ |\varepsilon\kappa m\rangle &= -j_- T_e |\varepsilon\kappa m\rangle \\
&= -e^{i\theta(\varepsilon\kappa m)} \sqrt{\left(|\kappa| - m - \tfrac{1}{2}\right)\left(|\kappa| + m + \tfrac{1}{2}\right)}\, |\varepsilon\kappa - (m+1)\rangle .
\end{aligned}
\tag{2.34}
$$

Comparison of Eqs. (2.33) and (2.34) reveals

$$
e^{i\theta(\varepsilon\kappa m)} = (-)^m e^{i\theta(\varepsilon\kappa)} , \tag{2.35}
$$

such that Eq. (2.27) reduces to

$$
T_e v_{\varepsilon\kappa m} = (-)^m e^{i\theta(\varepsilon\kappa)} v_{\varepsilon\kappa - m} . \tag{2.36}
$$

From Eqs. (2.18) and (2.36) we conclude that the radial wave functions of the large and small components of the Dirac orbital differ in phase by $\pm\pi/2$. Although this is a well-known fact and goes without saying in relativistic quantum mechanics [23], it arises naturally as a consequence of time-reversal symmetry. In addition, PC and PNC components of the Dirac orbital differ in phase by $\pm\pi/2$. We may therefore choose the phase for the Dirac orbital such that $G_{\varepsilon\kappa}$ and $Q_{\varepsilon\kappa}$ are real, while $F_{\varepsilon\kappa}$ and $P_{\varepsilon\kappa}$ are purely imaginary.

An atomic state of definite energy and total angular momentum is described by the multiconfiguration wave function (2.1). From Eqs. (2.17), (2.18), and (2.20), it follows that the time-reversed state is given as

$$
\begin{aligned}
T_a \Psi(EJM) &= T_a \left[\sum_\alpha C_\alpha \Psi_\alpha(JM) + \sum_{\bar\alpha} C_{\bar\alpha} \Psi_{\bar\alpha}(JM) \right] \\
&= (-)^{J+M+N_v/2} \pi_a \left[\sum_\alpha C_\alpha^* \Psi_\alpha(J-M) - \sum_{\bar\alpha} C_{\bar\alpha}^* \Psi_{\bar\alpha}(J-M) \right] ,
\end{aligned}
\tag{2.37}
$$

where N_v is the number of valence electrons, and π_a stands for the parity of the atomic state in the absence of PNC interactions. In arriving at Eq. (2.37), we have made use of the fact that the coefficients of fractional parentage are real and independent of the magnetic quantum number. The identity (2.20) and the reality of the Clebsch-Gordan coefficients have been exploited as well. Furthermore, in analogy with the inferences leading to Eq. (2.36), it is straightforward to show that

$$
T_a \Psi(EJM) = (-)^M e^{i\theta(EJ)} \Psi(EJ - M) \tag{2.38}
$$

for atomic states with no degeneracy other than that implied by rotational invariance. Comparison of Eqs. (2.37) and (2.38) reveals that the relative phases between PC configuration weight coefficients are 0 or π, while the relative phases between PC and PNC configuration weight coefficients are $\pm\pi/2$. We may therefore choose the phase for the configuration weight coefficient such that the PC and PNC components are real and purely imaginary, respectively.

The preceding assertions concerning the relative phases of the configuration weight coefficients may be established from an alternative point of view. According to the variational principle, the expectation value of the atomic Hamiltonian should be stationary with respect to variations in the configuration weight coefficients; this leads to a system of secular equations:

$$HC = EC. \tag{2.39}$$

Here H stands for the matrix $\{H_{pq}\}$ with elements

$$H_{pq} = \langle \Psi_p(JM)|H|\Psi_q(JM)\rangle, \tag{2.40}$$

and $C = \{C_r\}$ is its eigenvector, whose components in the configuration basis are the configuration weight coefficients. The phases of the matrix elements H_{pq} are relevant to time-reversal symmetry.

It is convenient to introduce an anti-unitary operator Θ_e as:

$$\Theta_e = T_e R_y(\pi), \tag{2.41}$$

where $R_y(\pi)$ stands for the rotation operator associated with a rotation through an angle π about the y-axis. For an N-electron system, we can define

$$\Theta_a = \prod_{j=1}^{N} \Theta_{ej}. \tag{2.42}$$

By making use of the identity (2.20) and

$$Y_{lM}(\pi-\theta, \pi-\phi) = (-)^{l+M} Y_{l-M}(\theta, \phi), \tag{2.43}$$

$$R_y(\pi)\chi_\mu = (-)^{\mu+1/2}\chi_{-\mu}, \tag{2.44}$$

it follows that

$$R_y(\pi)v_{\varepsilon\kappa m} = (-)^{j+m} v_{\varepsilon\kappa-m}. \tag{2.45}$$

Consequently, Eqs. (2.18) and (2.45) yield

$$\Theta_e v_{\varepsilon\kappa m} = (-)^{l+1/2} v_{\varepsilon\kappa m}. \tag{2.46}$$

For an N-electron system, we have therefore

$$\Theta_a \Psi_p(JM) = (-)^{N_v/2} \pi_p \Psi_p(JM) \,, \tag{2.47}$$

If the interactions are invariant under rotations and time-reversal, the atomic Hamiltonian H commutes with 0,. Accordingly, it follows from Eq. (2.47) that

$$\begin{aligned} H_{pq} &= \langle \Psi_p(JM) | H | \Psi_q(JM) \rangle \\ &= \langle \Psi_p(JM) | \Theta_a^\dagger H \Theta_a | \Psi_q(JM) \rangle \\ &= \pi_p \pi_q \langle \Psi_p(JM) | H | \Psi_q(JM) \rangle^* \\ &= \pi_p \pi_q H_{pq}^* \,. \end{aligned} \tag{2.48}$$

Inspection of Eq. (2.48) shows that $H_{\alpha\beta}$ and $H_{\bar{\alpha}\bar{\beta}}$ are real, while $H_{\alpha\bar{\beta}}$ and $H_{\bar{\alpha}\beta}$ are purely imaginary.

It is convenient to define a matrix $S = \{S_{pq}\}$ with

$$S_{pq} = \begin{cases} 1, & p = q = \alpha \,, \\ i, & p = q = \bar{\alpha} \,, \\ 0, & p \neq q \,. \end{cases} \tag{2.49}$$

The similarity transformation

$$H' = SHS^{-1} \tag{2.50}$$

will convert H to a real symmetric matrix. In the meantime, the eigenvectors transform according to

$$C' = SC \,. \tag{2.51}$$

It can be shown that the components of the eigenvectors of a real symmetric matrix differ in phase by 0 or π; this leads to the preceding assertions concerning the relative phases of the configuration weight coefficients.

11-4. The Lee-Yang theorem

As an application of the preceding assertions concerning the properties of the atomic wave functions, an alternative demonstration is given for the Lee-Yang theorem [3]. The permanent electric dipole moment. of an atom is given by

$$\langle \Psi | \vec{r} | \Psi \rangle \,, \tag{2.52}$$

where

$$\vec{r} = \sum_{i=1}^{N} \vec{r}_i \,, \tag{2.53}$$

and Ψ is the atomic wave function in the absence of the electric field.

For an atomic state with magnetic quantum number M, the only nonvanishing component of the electric dipole moment is along the symmetry axis,

$$\langle\Psi|\vec{z}|\Psi\rangle, \tag{2.54}$$

where the spatial coordinate operator $\vec{r}$ has

$$\begin{aligned}\vec{r} &= x\hat{i} = y\hat{j} + z\hat{k} \\ &= \vec{x}+\vec{y}+\vec{z}.\end{aligned}$$

A justification of the above assertion goes as follows. A rotation through an angle π about the z-axis will convert the atomic state Ψ to 9'. Here

$$\begin{aligned}\Psi' &= R_z(\pi)\Psi \\ &= e^{-iM\pi}\Psi,\end{aligned} \tag{2.56}$$

where $R_z(\pi)$ stands for the rotation operator. Accordingly,

$$\begin{aligned}\langle\Psi|\vec{x}|\Psi\rangle &= \langle\Psi|R_z^\dagger(\pi)R_z(\pi)\vec{x}R_z^\dagger(\pi)R_z(\pi)R_z(\pi)\Psi\rangle \\ &= -\langle\Psi|\vec{x}|\Psi\rangle \\ &= 0,\end{aligned} \tag{2.57}$$

where we have made use of the unitarity of the rotation operator and

$$\{R_z(\pi),\vec{x}\} = 0. \tag{2.58}$$

Similarly, the y-component of the electric dipole moment vanishes as well. Consequently, axial symmetry permits of merely the electric dipole moment along the z-axis.

Moreover, an atomic state has a definite parity, provided parity symmetry holds. Accordingly, insertion of $P_a^\dagger P_a = 1$ into Eq. (2.54) yields

$$\begin{aligned}\langle\Psi|\vec{z}|\Psi\rangle &= \langle\Psi|P_a^\dagger P_a\vec{z}P_a^\dagger P_a|\Psi\rangle \\ &= -\langle\Psi|\vec{z}|\Psi\rangle \\ &= 0,\end{aligned} \tag{2.59}$$

where we have made use of the identity

$$\{P_a,\vec{z}\} = 0. \tag{2.60}$$

We therefore conclude that parity symmetry alone prohibits the existence of atomic permanent electric dipole moments for states with axial symmetry.

If the parity symmetry is violated, however, an atomic state no longer has a definite parity. Even so, the atomic permanent electric dipole moment is strictly forbidden, to the extent that time-reversal symmetry holds. A justification of the preceding assertion goes as follows. It follows from Eqs. (2.1) and (2.47) that

$$\begin{aligned}\Theta_a\Psi &= \sum_\alpha C^*_\alpha \Theta_\alpha \psi_\alpha + \sum_{\bar\alpha} C^*_{\bar\alpha}\Theta_\alpha\psi_{\bar\alpha} \\ &= (-)^{N_v/2}\pi_a\left(\sum_\alpha C^*_\alpha\psi_\alpha - \sum_{\bar\alpha} C^*_{\bar\alpha}\psi_{\bar\alpha}\right) \\ &= (-)^{N_v/2}\pi_a\Psi\,,\end{aligned} \tag{2.61}$$

where π_a is the parity of the atomic state in the absence of PNC interactions. In arriving at Eq. (2.61), we have chosen the phase of the configuration weight coefficient such that the PC and PNC components are real and purely imaginary, respectively. Accordingly, insertion of $\Theta_a^\dagger\Theta_a = 1$ into Eq. (2.54) yields

$$\begin{aligned}\langle\Psi|\vec z|\Psi\rangle &= \langle\Psi|\Theta_a^\dagger\Theta_a\vec z\Theta_a^\dagger\Theta_a|\Psi\rangle \\ &= -\langle\Psi|\vec z|\Psi\rangle^* \\ &= -\langle\Psi|\vec z|\Psi\rangle \\ &= 0\,,\end{aligned} \tag{2.62}$$

where we have made use of the identity

$$\{\Theta_a, \vec z\} = 0\,, \tag{2.63}$$

Consequently, we arrive at the important result that time-reversal symmetry alone prohibits the existence of permanent electric dipole moments of atoms with definite angular momentum. Accordingly, a simultaneous breakdown of parity and time-reversal symmetries will manifest itself as permanent electric dipole moments of atoms with definite angular momentum, which will give rise to the linear Stark effect in atoms [13-15].

11-5. **The Kramers degeneracy**

Another consequence of time-reversal symmetry is the Kramers degeneracy [22]. Although this is a well-known fact, for completeness we elucidate the Kramers theorem in the present relativistic formalism. It is evident that the energy eigenstate Ψ and its time-reversed state $T_a\Psi$ are of the same energy eigenvalue, provided time-reversal symmetry holds. If Ψ and $T_a\Psi$ stood for the same state, they would differ at most by a phase factor, namely,

$$T_a\Psi = e^{i\theta}\Psi\,. \tag{2.64}$$

A repeated application of T_a would yield

$$T_a^2\Psi = \Psi\,. \tag{2.65}$$

Nevertheless, this relation never holds for atoms with odd number of electrons, since it follows from Eq. (2.17) that

$$T_a^2 = (-)^N . \tag{2.66}$$

Consequently,

$$T_a^2 \Psi = -\Psi , \tag{2.67}$$

for atoms with odd number of electrons. It is crucial to note that the result is independent of the phase convention of the time-reversal operator. As a result, there is an inherent two-fold degeneracy for atoms with odd number of electrons, provided that there are no magnetic fields present to remove time-reversal symmetry. As a matter of fact, any system with odd number of electrons shares this attribute.

III. IMPLICATIONS OF PARITY AND TIME-REVERSAL SYMMETRIES IN THE PHOTON FIELD

III-1. The photon field

The photon field is described by the four-potential

$$A^\mu = (\phi, \vec{A}) . \tag{3.1}$$

Its components satisfy the Maxwell equation

$$\nabla^2 A^\mu - \frac{\partial^2 A^\mu}{\partial t^2} = 0 , \tag{3.2}$$

with the subsidiary condition

$$\nabla \cdot \vec{A} + \frac{\partial \phi}{\partial t} = 0 . \tag{3.3}$$

Consider the photon field with the harmonic time-dependence exp(-iwt) such that

$$\nabla^2 A^\mu + \omega^2 A^\mu = 0 , \tag{3.4}$$

with the subsidiary condition

$$\nabla \cdot \vec{A} - ik\phi = 0 , \tag{3.5}$$

where $k = \omega$ in the relativistic units. The solutions of Eq. (3.4) can be expressed in terms of multipole potentials:

$$\vec{A} = \sum_{jm\lambda} C_{jm}^{(\lambda)} \vec{A}_{jm}^{(\lambda)} , \tag{3.6}$$

$$\phi = \sum_{jm} C_{jm}^{(-1)} \phi_{jm} , \tag{3.7}$$

where $C_{jm}^{(\lambda)}$ are expansion coefficients depending on the specific form of $\vec{A}$. The scalar potential ϕ_{jm} is

$$\phi_{jm} = i^j \sqrt{\frac{2}{\pi}}\, j_j(kr) Y_{jm}(\theta, \phi)\,, \tag{3.8}$$

and the two transverse and one longitudinal multipole potentials are

$$\vec{A}_{jm}^{(1)} = -\frac{i}{k}\left[\frac{1}{j(j+1)}\right]^{1/2} \nabla \times \vec{L}\phi_{jm}\,, \tag{3.9}$$

$$\vec{A}_{jm}^{(0)} = \left[\frac{1}{j(j+1)}\right]^{1/2} \vec{L}\phi_{jm}\,, \tag{3.10}$$

$$\vec{A}_{jm}^{(-1)} = -\frac{i}{k} \nabla \phi_{jm}\,, \tag{3.11}$$

where $j_l(kr)$ is the spherical Bessel function, and $\vec{L} = -i\vec{r} \times \nabla$.

These potentials are normalized such that

$$\int d^3r \phi_{j'm'}^{*} \cdot \phi_{jm} = \frac{1}{k^2}\delta(k'-k)\delta_{j'j}\delta_{m'm}\,, \tag{3.12}$$

$$\int d^3r \vec{A}_{j'm'}^{(\lambda')*} \cdot \vec{A}_{jm}^{(\lambda)} = \frac{1}{k^2}\delta(k'-k)\delta_{\lambda'\lambda}\delta_{j'j}\delta_{m'm}\,, \tag{3.13}$$

with $\lambda = 0$ or ± 1. Further manipulation leads to the expressions [24]:

$$\begin{aligned} \vec{A}_{jm}^{(1)} &= i^j \left(\frac{2}{\pi}\right)^{1/2} \left[\left(\frac{j+1}{2j+1}\right)^{1/2} j_{j-1}(kr)\vec{Y}_{j(j-1)m}(\hat{r}) \right. \\ &\quad \left. -\left(\frac{j}{2j+1}\right)^{1/2} j_{j+1}(kr)\vec{Y}_{j(j+1)m}(\hat{r})\right]\,, \end{aligned} \tag{3.14}$$

$$\vec{A}_{jm}^{(0)} = i^j \left(\frac{2}{\pi}\right)^{1/2} j_j(kr)\vec{Y}_{jjm}(\hat{r})\,, \tag{3.15}$$

$$\begin{aligned} \vec{A}_{jm}^{(-1)} &= i^{j-1} \left(\frac{2}{\pi}\right)^{1/2} \left[\left(\frac{j}{2j+1}\right)^{1/2} j_{j-1}(kr)\vec{Y}_{j(j-1)m}(\hat{r}) \right. \\ &\quad \left. +\left(\frac{j+1}{2j+1}\right)^{1/2} j_{j+1}(kr)\vec{Y}_{j(j+1)m}(\hat{r})\right]\,, \end{aligned} \tag{3.16}$$

where $\vec{Y}_{jlm}$ are the vector spherical harmonics defined as

$$\vec{Y}_{jlm} = \sum_{q=0,\pm 1} Y_{l(m-q)}\hat{e}_q \langle l(m-q)1q|jm\rangle\,. \tag{3.17}$$

Here $\hat{e}_q$ are spherical unit vectors defined in terms of Cartesian unit vectors by

$$\begin{aligned} \hat{e}_{+1} &= -(1/\sqrt{2}\,)(\hat{e}_x + i\hat{e}_y), \\ \hat{e}_0 &= \hat{e}_z \;, \\ \hat{e}_{-1} &= (1/\sqrt{2}\,)(\hat{e}_x - i\hat{e}_y)\,. \end{aligned} \tag{3.18}$$

111-2. The parity and time-reversal symmetries

It can be shown that the parity operator for the photon field is given as (see the Appendix)

$$P_\gamma = (g^{\mu\nu})P = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} P\,, \tag{3.19}$$

and

$$P\phi_{jm} = (-)^j \phi_{jm}, \tag{3.20}$$

$$P\vec{A}^{(\lambda)}_{jm} = (-)^{j+\lambda}\vec{A}^{(\lambda)}_{jm}\,. \tag{3.21}$$

Consequently, the photon states of definite angular momentum fall into two types of opposite parities:

$$A^\mu_{jm} = A^\mu_{jm}(M) + A^\mu_{jm}(E)\,, \tag{3.22}$$

where the magnetic and electric multipole four-potentials are

$$A^\mu_{jm}(M) = (0, C^{(0)}_{jm}\vec{A}^{(0)}_{jm})\,, \tag{3.23}$$

$$A^\mu_{jm}(E) = (C^{(-1)}_{ijm}\phi_{jm}, C^{(1)}_{ijm}\vec{A}^{(1)}_{ijm} + C^{(-1)}_{jm}\vec{A}^{(-1)}_{jmn})\,, \tag{3.24}$$

which have parities $(-)^{j+1}$ and $(-)^j$, respectively. Note that the magnetic multipole four-potential in (3.23) includes only the transverse multipole potential, while the electric multipole four-potential in (3.24) includes the scalar, transverse, and longitudinal multipole potentials.

The time-reversal operator for the photon field is given as (see the Appendix)

$$T_\gamma = (g^{\mu\nu})CT = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} CT. \tag{3.25}$$

It is convenient to introduce the antiunitary operator Θ_γ as follows:

$$\Theta_\gamma = T_\gamma R_y(\pi)\,. \tag{3.26}$$

BY making use of the identities

$$\phi^*_{jm} = (-)^{j+m}\phi_{j-m}\,, \tag{3.27}$$

$$\vec{A}^{(\lambda)*}_{jm} = (-)^{j+m+1+(|\lambda|+\lambda)/2}\vec{A}^{(\lambda)}_{j-m}\,, \tag{3.28}$$

$$R_y(\pi)\phi_{jm} = (-)^{j+m}\phi_{j-m}\,, \tag{3.29}$$

$$R_y(\pi)\vec{A}^{(\lambda)}_{jm} = (-)^{j+m}\vec{A}^{(\lambda)}_{j-m}\,, \tag{3.30}$$

it follows that

$$\Theta_\gamma A^\mu = \sum_{jm}\left(C^{(-1)*}_{jm}\phi_{jm}, \sum_\lambda (-)^{(|\lambda|+\lambda)/2}C^{(\lambda)*}_{jm}\vec{A}^{(\lambda)}_{jm}\right)\,. \tag{3.31}$$

III-3. Phase relations

Symmetry considerations reveal a phase relation between the expansion coefficients for multipole potentials. Consider a photon state $A^\mu_{\vec{k}q}$ which is the eigenfunction of the momentum operator $\vec{p}$ and helicity operator $\vec{j}\ \vec{p}/|\vec{j}\cdot\vec{p}|$. It is straightforward to show that

$$[\Theta_\gamma, \vec{p}] = 0\,, \tag{3.32}$$

$$[\Theta_\gamma, \vec{j}\cdot\vec{p}/|\vec{j}\cdot\vec{p}|] = 0\,, \tag{3.33}$$

where we have chosen the quantization axis in the $\vec{k}$ direction. We have therefore

$$\Theta_\gamma A^\mu_{\vec{k}q} = e^{i\theta}A^\mu_{\vec{k}q}\,, \tag{3.34}$$

because a photon state is completely specified by $\vec{k}$ and q. Comparison of Eqs. (3.31) and (3.34) shows that

$$C^{(\lambda)*}_{jm} = e^{i\theta}(-)^{(|\lambda|+\lambda)/2}C^{(\lambda)}_{jm}\,. \tag{3.35}$$

Consequently, the relative phases between the expansion coefficients $C^{(1)}_{jm}$ for the transverse electric multipole potentials and $C^{(0)}_{jm}$ for the magnetic multipole potential or $C^{(-1)}_{jm}$ for the longitudinal electric multipole potentials are $\pm\pi/2$. Again this is a well-known fact in classical electrodynamics; however, it arises naturally as a consequence of time-reversal symmetry.

IV. IMPLICATIONS OF PARITY AND TIME-REVERSAL SYMMETRIES IN ATOMIC TRANSITIONS

The transition matrix elements of atoms in the presence of the photon field $A^{\mu}_{\vec{k}q}$ take the form

$$T_{fi} = \left\langle \Psi_f \left| \sum_{k=1}^{N} \gamma_k^0 \gamma_{\mu k} A^{\mu}_{\vec{k}q}(\vec{r}_k) \right| \Psi_i \right\rangle , \tag{4.1}$$

where Ψ_i and Ψ_f are the initial and final states of the atoms, respectively. After substituting Eqs. (3.6),(3.7), and (3.22)-(3.24) into Eq. (4.1), we can express the transition matrix elements as

$$T_{fi} = \sum [T_{fi}(Ej) + T_{fi}(Mj)] , \tag{4.2}$$

where

$$\begin{aligned} T_{fi}(Ej) &= \left\langle \Psi_f \left| \sum_{k=1}^{N} \gamma_k^0 \gamma_{\mu k} A^{\mu}_{jm}(E) \right| \Psi_i \right\rangle \\ &= \left\langle \Psi_f \left| \sum_{k=1}^{N} \left[C_{jm}^{(-1)} \phi_{jm}(\vec{r}_k) - \vec{\alpha}_k \cdot \left(C_{jm}^{(1)} \vec{A}_{jm}^{(1)}(\vec{r}_k) + C_{jm}^{(-1)} \vec{A}_{jm}^{(-1)}(\vec{r}_k) \right) \right] \right| \Psi_i \right\rangle \end{aligned} \tag{4.3}$$

and

$$\begin{aligned} T_{fi}(Mj) &= \left\langle \Psi_f \left| \sum_{k=1}^{N} \gamma_k^0 \gamma_{\mu k} A^{\mu}_{jm}(M) \right| \Psi_i \right\rangle \\ &= -\left\langle \Psi_f \left| C_{jm}^{(0)} \sum_{k=1}^{N} \vec{\alpha}_k \cdot \vec{A}_{jm}^{(0)}(\vec{r}_k) \right| \Psi_i \right\rangle \end{aligned} \tag{4.4}$$

are the electric and magnetic 2^j-pole transition matrix elements, respectively. Here

$$\vec{\alpha} = \gamma^0 \vec{\gamma} . \tag{4.5}$$

Parity symmetry requires

$$\pi_f \pi_i \pi_\gamma = 1 , \tag{4.6}$$

where π_γ refers to the parity of the photon field. This leads to the well-known parity selection rules for the multipole transitions:

$$\pi_f \pi_i (-)^{j+\lambda+1} = 1 , \tag{4.7}$$

where $\lambda = 0$ or 1 correspond to the magnetic or electric 2^j-pole transitions, respectively. Transitions between two atomic states may contain competing components. Parity symmetry permits of mixed transition which contains both magnetic 2^{j-1}-pole and electric 2^j-pole components. If parity symmetry is violated, an atomic state no longer has a definite parity. Therefore, transitions between two atomic states contain both PC and PNC components. PNC interactions in atoms may be studied by investigating the interference between magnetic dipole and PNC electric dipole transitions, which gives rise to the optical rotation effect in heavy atoms [16]. An alternative proposal is to investigate the electric dipole-electric quadrupole interference in muonic atoms, which leads to angular asymmetries of the emmitted photons [25].

The interference between competing transition amplitudes depends on their relative phases. The phase relations of the competing transition amplitudes have been explored by Lloyd [26] and Bouchiat and Bouchiat [27]. An alternative demonstration is given here in the relativistic context. Insertion of $\Theta_a^\dagger \Theta_a = 1$ into Eqs. (4.3) and (4.4) yields

$$\begin{aligned} T_{fi}(Ej) &= \left\langle \Psi_f \left| \Theta_a^\dagger \Theta_a \sum_{k=1}^{N} \gamma_k^0 \gamma_{\mu k} A_{jm}^{\mu}(E) \Theta_a^\dagger \Theta_a \right| \Psi_i \right\rangle \\ &= e^{i\theta} \pi_i \pi_f T_{fi}^*(Ej) , \end{aligned} \tag{4.8}$$

$$\begin{aligned} T_{fi}(Mj) &= \left\langle \Psi_f \left| \Theta_a^\dagger \Theta_a \sum_{k=1}^{N} \gamma_k^0 \gamma_{\mu k} A_{jm}^{\mu}(M) \Theta_a^\dagger \Theta_a \right| \Psi_i \right\rangle \\ &= e^{i\theta} \pi_i \pi_f T_{fi}^*(Mj) , \end{aligned} \tag{4.9}$$

where we have made use of Eq. (3.35) and the identities

$$\{\gamma^\mu, \gamma^\nu\} = 2g^{\mu\nu} , \tag{4.10}$$

$$\Theta_a \phi_{jm} \Theta_a^\dagger = \phi_{jm} , \tag{4.11}$$

$$\Theta_a \vec{A}_{jm}^{(\lambda)} \Theta_a^\dagger = (-)^{(|\lambda|+\lambda)/2+1} \vec{A}_{jm}^{(\lambda)} . \tag{4.12}$$

Comparison between Eqs. (4.8) and (4.9) shows that the relative phases between competing transition amplitudes are 0 or π, which leads to constructive or destructive interferences between competing atomic transitions.

V. CONCLUSIONS

We have investigated some aspects of the implications of parity and time-reversal symmetries in atoms. If parity symmetry is violated, an atomic state no longer has a definite parity such that both electronic orbitals and configuration weight coefficients contain PNC components. Time-reversal symmetry guarantees that the radial wave functions of the large and small components of the Dirac orbital differ in phase by $\pm\pi/2$, and the PC and PNC components of the Dirac orbital differ in phase by $\pm\pi/2$ as well. In addition, time-reversal symmetry implies that the relative phases between PC configuration weight coefficients are 0 or π, while the relative phases between PC and PNC configuration weight coefficients are $\pm\pi/2$. The Lee-Yang theorem arises naturally as a consequence of the preceding assertions. In addition, the Kramers theorem is elucidated in the relativistic context. In the multipole expansion of the photon field, the relative phases between the expansion coefficients for the transverse electric multipole potentials and for the magnetic or longitudinal electric multipole potentials are $\pm\pi/2$. Finally, we show that the relative phases between competing transition amplitudes are 0 or π, which leads to constructive or destructive interferences between competing atomic transitions. Analogous considerations may also be applied to collision, multiphoton, and Auger processes.

ACKNOWLEDGMENTS

One of the authors (Chou) would like to thank Dr. W.-Y. Cheng for invaluable comments and suggestions. This work was supported in part by the National Science Council of the Republic of China under Grant Nos. NSC83-0208-M019-002 and NSC83-0208-M001-007.

APPENDIX: PARITY AND TIME-REVERSAL TRANSFORMATIONS OF THE COUPLED ELECTRON-POSITRON AND PHOTON FIELDS

The equations of motion for the coupled electron-positron and photon fields are the Dirac and Maxwell equations

$$(i\gamma^\mu \partial_\mu - m)u(x) = -e\gamma^\mu A_\mu(x)u(x)\,, \tag{A1}$$

$$\partial_\nu \partial^\nu A^\mu(x) - \partial_\nu \partial^\mu A^\nu(x) = -e\bar{u}(x)\gamma^\mu u(x)\,, \tag{A2}$$

where $u(x)$ and $A^\mu(x)$ are the electron-positron and photon fields, respectively.

The space-time coordinates transform under the parity and time-reversal transformations according to

$$(t,\vec{x}\,) \xrightarrow{P} (t',\vec{x}\,') = (t,-\vec{x}\,)\,, \tag{A3}$$

$$(t,\vec{x}\,) \xrightarrow{T} (t',\vec{x}\,') = (-t,\vec{x}\,)\,. \tag{A4}$$

The most general homogeneous Lorentz transformation between two coordinate systems is a linear transformation

$$x'^{\mu} = a^{\mu}{}_{\nu}\, x^{\nu} \,, \tag{A5}$$

with

$$a^{\mu}{}_{\nu}\, g_{\mu\rho} a^{\rho}{}_{\sigma} = g_{\nu\sigma} \,. \tag{A6}$$

In Eq. (A6) $g_{\mu\nu}$ is the metric tensor with components

$$\begin{aligned} &g_{00} = -g_{11} = -g_{22} = -g_{33} = 1 \,, \\ &g_{\mu\nu} = 0 \qquad \text{for } \mu \neq \nu \,. \end{aligned} \tag{A7}$$

Suppose the interaction is invariant under the Lorentz transformation, there is a transformation law for the field quantities, so that the transformed fields $u'(x')$ and $A'^{\mu}(x')$ satisfy the same equations of motion in the new coordinate system; i. e.,

$$(i\gamma^{\mu}\partial'_{\mu} - m)u'(x') = -e\gamma^{\mu}A'_{\mu}(x')u'(x') \,, \tag{A8}$$

$$\partial'_{\nu}\partial'^{\nu} A'^{\mu}(x') - \partial'_{\nu}\partial'^{\mu} A'^{\nu}(x') = -e\bar{u}'(x')\gamma^{\mu}u'(x') \,, \tag{A9}$$

where

$$u'(x') = \Lambda u(x), \tag{A10}$$

$$A'^{\alpha}(x') = L^{\alpha}{}_{\beta}\, A^{\beta}(x) \,. \tag{A11}$$

Furthermore, relativistic invariance requires the transformations to preserve the absolute values of scalar products between two states. Consequently, the transformation operators must be unitary or antiunitary. We first assume that both transformations (A10) and (A11) are unitary transformations. Substitution of Eqs. (A10) and (A11) into Eqs. (A8) and (A9) yields

$$(ia_{\mu}{}^{\alpha}\, \gamma^{\mu}\partial_{\alpha} - m)\Lambda u(x) = -eL_{\mu}{}^{\beta}\, \gamma^{\mu} A_{\beta}(x)\Lambda u(x) \,, \tag{A12}$$

$$\partial_{\nu}\partial^{\nu} L^{\mu}{}_{\beta}\, A^{\beta}(x) - a_{\nu}{}^{\alpha}\, a^{\mu}{}_{\beta}\, \partial_{\alpha}\partial^{\beta} L^{\nu}{}_{\gamma}\, A^{\gamma}(x) = -eu^{\dagger}(x)\Lambda^{\dagger}\gamma^{0}\gamma^{\mu}\Lambda u(x) \,. \tag{A13}$$

In addition, multiplication of Eqs. (A1) and (A2) from the left by Λ and $L^{\mu}{}_{\beta}$ yields

$$(i\Lambda\gamma^{\alpha}\partial_{\alpha} - m\Lambda)u(x) = -e\Lambda\gamma^{\beta} A_{\beta}(x)u(x) \,, \tag{A14}$$

$$\partial_{\nu}\partial^{\nu} L^{\mu}{}_{\beta}\, A^{\beta}(x) - \partial_{\gamma}\partial^{\beta} L^{\mu}{}_{\beta}\, A^{\gamma}(x) = -eu^{\dagger}(x) L^{\mu}{}_{\beta}\, \gamma^{0}\gamma^{\beta} u(x) \,. \tag{A15}$$

Comparing Eqs. (A14) and (A15) with Eqs. (A12) and (A13) shows that the coupled Dirac and Maxwell equations are invariant under the Lorentz transformations, provided unitary operators A and L can be found which have the properties

$$g_\gamma{}^\alpha\, L^\mu{}_\beta = a_\nu{}^\alpha\, a^\mu{}_\beta\, L^\nu{}_\gamma\,, \tag{A16}$$

$$L^\mu{}_\beta\, \gamma^0\gamma^\beta = \Lambda^\dagger\gamma^0\gamma^\mu\Lambda\,, \tag{A17}$$

$$\begin{aligned}\Lambda\gamma^\beta\Lambda^{-1} &= a_\alpha{}^\beta\gamma^\alpha \\ &= L_\alpha^\beta\,\gamma^\alpha\,.\end{aligned} \tag{A18}$$

These imply

$$L^\alpha{}_\beta = a^\alpha{}_\beta\,, \tag{A19}$$

$$\Lambda^\dagger\gamma^0\Lambda = \gamma^0\,, \tag{A20}$$

$$\Lambda^\dagger\gamma^0\gamma^\alpha\Lambda = a^\alpha{}_\beta\,\gamma^0\gamma^\beta\,. \tag{A21}$$

Whereas if both transformations (A10) and (All) are anti-unitary transformations, the operators A and L can be written in the forms

$$\Lambda = \bar\Lambda C\,, \tag{A22}$$

$$L^\alpha{}_\beta = \bar L^\alpha{}_\beta\, C\,, \tag{A23}$$

where $\bar\Lambda$ and $\bar L$ are unitary operators, and C stands for the complex conjugate operator. Substitution of Eqs. (A22) and (A23) into Eqs. (A8) and (A9) yields

$$(ia_\mu{}^\alpha\,\gamma^\mu\partial_\alpha - m)\bar\Lambda u^*(x) = -e\gamma^\mu\bar L_\mu^\beta\, A_\beta^*(x)\bar\Lambda u^*(x)\,, \tag{A24}$$

$$\partial_\nu\partial^\nu\bar L^\mu{}_\beta\, A^{\beta*}(x) - a_\nu{}^\alpha\, a^\mu{}_\beta\,\partial_\alpha\partial^\beta\bar L^\nu{}_\gamma\, A^{\gamma*}(x) = -eu^{\dagger*}(x)\gamma^{0*}\bar\Lambda^\dagger\gamma^\mu\bar\Lambda u^*(x)\,. \tag{A25}$$

Multiplication of Eqs. (Al) and (A2) from the left by $\bar\Lambda C$ and $\bar L^\mu{}_\beta$ C yields

$$-\bar\Lambda(i\gamma^{\mu*}\partial_\mu + m)u^*(x) = -e\bar\Lambda\gamma^{\mu*}A_\mu^*(x)u^*(x)\,, \tag{A26}$$

$$\partial_\nu\partial^\nu\bar L^\mu{}_\beta\, A^{\beta*}(x) - \partial_\gamma\partial^\beta\bar L^\mu{}_\beta\, A^{\gamma*}(x) = -e\bar L^\mu{}_\beta\, u^{\dagger*}(x)\gamma^{0*}\gamma^{\beta*}u^*(x)\,. \tag{A27}$$

Comparing Eqs. (A26) and (A27) with Eqs. (A24) and (A25) shows that

$$g_\gamma{}^\alpha\,\bar L^\mu{}_\beta = a_\nu{}^\alpha\, a^\mu{}_\beta\,\bar L^\nu{}_\gamma\,, \tag{A28}$$

$$\bar L^\mu{}_\beta\,\gamma^{0*}\gamma^{\beta*} = \bar\Lambda^\dagger\gamma^{0*}\gamma^\mu\bar\Lambda\,, \tag{A29}$$

$$\begin{aligned} \bar{\Lambda}\gamma^{\beta *}\bar{\Lambda}^{-1} &= -a_{\alpha}^{\ \beta}\,7^{\alpha} \\ &= \bar{L}_{\alpha}^{\ \beta}\,\gamma^{\alpha}. \end{aligned} \tag{A30}$$

These imply

$$L^{\alpha}{}_{\beta} = -a^{\alpha}{}_{\beta}\,, \tag{A31}$$

$$\bar{\Lambda}^{\dagger}\gamma^{0}\bar{\Lambda} = \gamma^{0*}\,, \tag{A32}$$

$$\bar{\Lambda}^{\dagger}\gamma^{0}\gamma^{\alpha}\bar{\Lambda} = -a^{\alpha}{}_{\beta}\,\gamma^{0*}\gamma^{\beta *} \tag{A33}$$

It can be shown that $\Lambda^{\dagger}\Lambda$ is positive definite; therefore its trace is greater than zero

$$tr\,\{\Lambda^{\dagger}\Lambda\} > 0. \tag{A34}$$

For unitary transformations the following identities hold:

$$\Lambda^{\dagger}\Lambda = \Lambda^{\dagger}\gamma^{0}\gamma^{0}\Lambda = a^{0}{}_{\beta}\,\gamma^{0}\gamma^{\beta}\,, \tag{A35}$$

$$tr\,\{\Lambda^{\dagger}\Lambda\} = 4a^{0}{}_{0}\,. \tag{A36}$$

Inspection of Eqs. (A34) and (A36) reveals that

$$a^{0}{}_{0} > 0. \tag{A37}$$

Whereas for antiunitary transformations, the analogues of Eq. (A35) and (A36) are

$$\Lambda^{\dagger}\Lambda = \Lambda^{\dagger}\gamma^{0}\gamma^{0}\Lambda = -a^{0}{}_{\beta}\,\gamma^{0*}\gamma^{\beta *}\,, \tag{A38}$$

$$tr\,\{\Lambda^{\dagger}\Lambda\} = -4a^{0}{}_{0}\,. \tag{A39}$$

Inspection of Eqs. (A34) and (A39) reveals that

$$a^{0}{}_{0} < 0. \tag{A40}$$

In conclusion, under the orthchronous Lorentz transformations, the electron-positron and the photon fields transform as

$$u'(x') = \Lambda u(x)\,, \tag{A41}$$

$$A'^{\alpha}(x') = a^{\alpha}{}_{\beta}\,A^{\beta}(x)\,. \tag{A42}$$

The unitary operator _A in Eq. (A41) satisfies the relations (A20) and (A21). One particular orthchronous transformation is the parity transformation (A3). The parity operator for the electron-positron field is given as

$$P_e = e^{i\phi}\gamma^0 P \,, \tag{A43}$$

where P is the inversion operator for the spatial coordinates,

$$Pu(t,\vec{x}\,) = u(t,-\vec{x}\,)\,. \tag{A44}$$

The quantity $e^{i\phi}$ in Eq. (A43) is an arbitrary phase factor. It is customary to set this phase factor equal to 1. The parity operator for the photon field is given by

$$P_\gamma = (g^{\mu\nu})P = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} P\,. \tag{A45}$$

On the other hand, under the antichronous Lorentz transformations, the electron-positron and photon fields transform as

$$u'(x') = \bar{\Lambda} u^*(x)\,, \tag{A46}$$

$$A'^{\alpha}(x') = -a^{\alpha}{}_{\beta}\, A^{\beta *}(x)\,. \tag{A47}$$

The unitary operator $\bar{\Lambda}$ in Eq. (A46) satisfies the relations (A32) and (A33). One particular antichronous transformation is the time-reversal transformation (A4). The time-reversal operator for the electron-positron field is

$$T_e = e^{i\delta}\gamma^1\gamma^3 CT\,, \tag{A48}$$

where T is the inversion operator for the temporal coordinate?

$$Tu(t,\vec{x}\,) = u(-t,\vec{x}\,)\,. \tag{A49}$$

The quantity $e^{i\delta}$ in Eq. (A48) is again an arbitrary phase factor. It is customary to set, this phase factor equal to i. The time-reversal operator for the photon field is given as

$$T_\gamma = (g^{\mu\nu})CT = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} CT. \tag{A50}$$

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