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Photon Wave Functions and the Exact Electromagnetic Matrix Elements for Hydrogenic Atoms

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After reviewing the properties of the photon considered as a quantized particle of zero mass, positive energy, and unit spin, the expansion of the unquantized and quantized electromagnetic fields and vector and scalar potentials in terms of the photon wave functions and creation and destruction operators is reviewed and extended. The most general vector and scalar potentials are obtained through the use of the eigenfunctions of the curl operator. The dichotomy between the photon and wave picture of electromagnetic radiation is discussed and resolved. The results are applied to the calculation of the exact electromagnetic matrix elements and transition probabilities (i.e., with retardation taken into account exactly) for hydrogenic atoms. The exact matrix elements are very simple in form. The notion of multipole radiation of the usual treatments is irrelevant. However, it is shown how multipoles appear as an approximation.

I. INTRODUCTION AND SUMMARY

In previous papers (Refs. 1–4) the author has shown how electromagnetic fields and electromagnetic potentials may be expanded in the wave functions of the photon. In the present paper these expansions are applied to obtain the *exact* matrix elements and transition probabilities for the nonrelativistic, spinless hydrogen atom, taking retardation into account completely. The notion of multipoles of the usual treatments, which arises because one expands the exponential which appears in the matrix elements, plays no role whatever in this approach, since such an expansion is not necessary. Indeed the exact matrix elements will be sufficiently simple to be used directly. The matrix elements were given in a terse summary in Ref. 5. The purpose of the present paper is to provide the derivation.

The application illustrates the power of the use of the expansions of electromagnetic fields and potentials in terms of the photon wave functions. For this reason we shall give a terse review of the subject and then derive the exact matrix elements of the electromagnetic interaction for hydrogenic atoms.

The use of photon wave functions in the expansions of fields and potentials is equivalent to the expansion of these quantities in terms of the irreducible representations of the Poincaré group. The usual treatments of electromagnetic theory in quantum mechanics (or classical physics, for that mater), even when "manifestly covariant" as in Refs. 6—8, ignore the group-theoretical properties of Maxwell's equations, and those who use the traditional methods are obliged to put up with a great deal of unnecessary awkwardness. Thus calculations of the type of the present paper are very difficult using the traditional theory, whereas, by contrast, the use of Poincaré group theory leads very directly to the desired result. A very close analogy to the ignoring of Poincaré group theory for Maxwell's equations would be the ignoring of the theory of the representations of the rotation group in scattering theory, the lack of which would be an extreme handicap indeed!

The present paper is divided into two parts: In Sec. II we review the theory of the expansion of electromagnetic fields and potentials in terms of photon wave functions in both linear and angular-momentum representations. In Sec. III we derive the matrix elements of the electromagnetic interaction $H_I = i(e\hbar/Mc)\vec{A}\cdot\vec{\nabla}$ for hydrogenic atoms.

In previous treatments (see, e.g., Refs. 9–11) they are calculated to an approximation corresponding to an expansion of $e^{i\vec{k}\cdot\vec{x}}$ in powers of $\vec{k}\cdot\vec{x}$ or otherwise. Such approximations are called dipole, quadrupole, etc., approximations. "Allowed" transitions correspond to dipole transitions. We shall now give the *exact* matrix elements. They are seen to be very simple.

Let the vacuum state of the photon field be denoted by $|V\rangle$ and let the one-photon state with energy $E = h\nu$, total angular momentum $j \geq 1$, magnetic quantum number m, and finally helicity $\lambda = \pm 1$, be denoted by $|E, j, m, \lambda\rangle$. The kets satisfy the orthonormality relations

$$\langle V|V\rangle = 1, \quad \langle E, j, m, \lambda|V\rangle = 0, \tag{1}$$
$$\langle E, j, m, \lambda|E', j', m', \lambda'\rangle = E\delta(E - E')\delta_{jj'}\delta_{mm'}\delta_{\lambda\lambda'}.$$

We denote state 1 as that state for which there is no photon and for which the hydrogen atom is in the eigenstate with the principal quantum number n_1, and angular-momentum quantum numbers

j_1, m_1. State 2 is the state for which there is a photon with the quantum numbers E, j, m, λ and for which the atom is in the eigenstate defined by the quantum numbers n_2, j_2, m_2. Though we are considering spinless hydrogenic atoms, the techniques can easily be extended to the case of spin and to the relativistic hydrogen atom. The atomic wave functions for the atomic states will be denoted by $\psi_i(\vec{x}) = R_i(r) Y_{j_i m_i}(\theta, \phi)$, where R_i is the radial wave function which depends on n_i and j_i, and the Y_{jm} are the usual surface harmonics in the notation, for example, of Ref. 12. Then our exact result is the following: Let $\Delta = j_1 - j_2$ and $W = j_1 + j_2$. Furthermore, let $j_j(kr)$ be the spherical Bessel function of j'th order with $k = E/\hbar c$ the wave number of the photon. Then for $j + j_1 + j_2$ even

$$\langle 1|H_I|2\rangle = e^2 a(\alpha/8)^{1/2} i^j (-1)^{m_1} \lambda \left(\frac{(2j+1)(2j_1+1)(2j_2+1)}{\pi j(j+1)}\right)^{1/2} \begin{pmatrix} j & j_1 & j_2 \\ m & -m_1 & m_2 \end{pmatrix} \begin{pmatrix} j & j_1 & j_2 \\ 0 & 0 & 0 \end{pmatrix}$$
$$\times \left[[j(j+1) + \Delta(W+1)] \int_0^\infty j_j(kr) R_1^*(r) \left(\frac{\partial}{\partial r} R_2(r)\right) r\, dr + [-j(j+1) + \Delta(W+1)] \int_0^\infty j_j(kr) \left(\frac{\partial}{\partial r} R_1^*(r)\right) R_2(r) r\, dr \right]. \tag{2a}$$

For $j + j_1 + j_2$ odd we have

$$\langle 1|H_I|2\rangle = e^2 a(\alpha/8)^{1/2} i^{j+1} (-1)^{m_1} k \left(\frac{(2j+1)(2j_1+1)(2j_2+1)}{\pi j(j+1)}\right)^{1/2} [(W-j)(W+j+2)(j+\Delta+1)(j-\Delta+1)]^{1/2}$$
$$\times \begin{pmatrix} j & j_1 & j_2 \\ m & -m_1 & m_2 \end{pmatrix} \begin{pmatrix} j+1 & j_1 & j_2 \\ 0 & 0 & 0 \end{pmatrix} \int_0^\infty j_j(kr) R_1^*(r) R_2(r) r\, dr\,. \tag{2b}$$

In the above, a is the Bohr radius, α is the fine-structure constant, and the usual notation for the Wigner 3-j symbol is used.

The transition probability (that is, transitions per unit time) for the emission of a photon with wave number k, angular momentum given by j and m, and helicity λ is

$$T = (2\pi/\hbar) |(\hbar c k)^{-1}| \langle 1|H_I|2\rangle|^2\,. \tag{3}$$

The factor $(\hbar c k)^{-1}$ appears because of the photon wave function normalization in Eq. (1). Since T is independent of the helicity, the sum over both helicities would give an additional factor of 2.

It is clear that the exact selection rules are obtained by noting that only those photons can be emitted for which $m = m_1 - m_2$ and for which $j = |\Delta|$, $|\Delta|+1, \ldots, W-1, W$. These exact selection rules are, of course, a consequence of the conservation of angular momentum.

The approximate selection rules for "permitted" transitions are obtained by noting that the absolute values of the matrix elements are greatest for $j = 1$. In this case the integrals contain $j_1(kr)$, which gives a larger contribution near the origin ($r = 0$) than the Bessel functions for which $j > 1$. Then, defining "permitted" transitions as those for which $j = 1$, we note that $|\Delta| = 1$, or equivalently, $j_1 = j_2 \pm 1$, which together with $m = m_1 - m_2 = 0, \pm 1$ are the usual selection rules. The electromagnetic field of the emitted photon, whose expression will be derived in the body of the paper from ideas in Ref. 1–4, can also be given. The wave function of the photon is proportional to $\langle 2|H_I|1\rangle = \langle 1|H_I|2\rangle^*$. Let $\vec{k}$ be the propagation vector with the spherical coordinates k, θ, ϕ, i.e.,

$$\vec{k} = k(\sin\theta\cos\phi,\ \sin\theta\sin\phi,\ \cos\phi)\,.$$

For $m = 0$ the θ and ϕ components of the electric field propagating in the $\vec{k}$ direction are

$$E_\phi(\vec{x}, t) = 0, \quad E_\theta(\vec{x}, t) = A\cos(\vec{k}\cdot\vec{x} - ckt)\sin\theta, \tag{4}$$

while for $m = \pm 1$

$$E_\phi(\vec{x}, t) = -(2)^{-1/2} A \sin(\vec{k}\cdot\vec{x} - ckt + m\phi),$$
$$E_\theta(\vec{x}, t) = (2)^{-1/2} A \cos(\vec{k}\cdot\vec{x} - ckt + m\phi)\cos\theta. \tag{5}$$

For both $m = 0$ and $m = \pm 1$, the component of the electric field in the direction of propagation is zero, of course, because the wave is transverse. The polarization rules are thus the same as for the traditional treatments: For $m = 0$, the wave is plane polarized, while for $m = \pm 1$ the wave is elliptically polarized, the degree of ellipticity depending on the angle which the direction of propagation makes with the z axis. The amplitude A is proportional to the matrix element of Eq. (2a), with $j = 1$.

To obtain the permitted selection rule in the long-wavelength limit, one replaces $j_1(kr)$ by its value for which k is small, that is by $\frac{1}{3}kr$. One obtains formulas for the transition probabilities, which, we shall shortly show, are identical to the dipole approximations of Refs. 9–11. Then in the dipole approximation,

$$\langle 1|H_I|2\rangle \sim k\int_0^\infty R_1(r)^*\left(\frac{\partial}{\partial r}R_2(r)\right)r^2\,dr$$

for $j_1 = j_2 + 1$, for example. The integral is essentially the matrix element of the radial component of the momentum operator.

It is an easy matter to calculate the exact matrix elements in special cases. The matrix element which is important for the emission of Lyman-α radiation from hydrogen, where $n_1 = 2$, $j_1 = 1$, $m_1 = 0, \pm 1$, $n_2 = 1$, $j_2 = 0$, $m_2 = 0$, is

$$\langle 1|H_I|2\rangle = -(\tfrac{2}{3})^{7/2}(\pi)^{-1/2}\lambda i\alpha^{5/2}Mc^2 \times \frac{k/K}{[1+(k/K)^2]^2}\,\delta_{j,1}\delta_{m,m_1}, \quad (6)$$

where M is the mass of the electron and $K = 3/2a$. To obtain the dipole approximation one ignores k/K in comparison to 1. It is seen that the dipole approximation gives the wrong result for large k, and one expects divergent results when going to second-order processes. However, the exact result dies down very rapidly for large values of k, and one expects convergent results in many cases when the dipole approximation gives divergent answers. In later papers we show that when the two-level approximation is used, the expression for the frequency shift of the emitted radiation converges when the exact matrix elements are used, but that the expression diverges when the dipole approximation is used in the customary way. In Ref. 13 we show that the ultraviolet divergences in the contributions of each of the atomic states to the self-energy of the ground state of hydrogen are not present when the exact matrix elements are used.

A matrix element which is important for the calculation of the electromagnetic shift of the ground state of hydrogen is characterized by the atomic quantum numbers $n_1 = 1$, $j_1 = 0$, $m_1 = 0$, $n_2 = 2$, $j_2 = 1$, $m_2 = 0, \pm 1$:

$$\langle 1|H_I|2\rangle = (\tfrac{2}{3})^{7/2}(\pi)^{-1/2}\lambda i\alpha^{5/2}Mc^2 \times\frac{k/K}{[1+(k/K)^2]^2}\,(-1)^{m_2}\delta_{j,1}\delta_{m,-m_2}. \quad (7)$$

This matrix element differs from the previous one only in phase. The similarity between the two matrix elements illustrates the symmetry of the general matrix elements of Eqs. (2a) and (2b) in the atomic quantum numbers. This symmetry is quite different from that due to the Hermiticity of the operator H_I.

The matrix element which corresponds to the emission of Lyman-β radiation with a photon angular momentum of $j = 1$ has the atomic quantum numbers $n_1 = 3$, $j_1 = 1$, $m_1 = 0, \pm 1$, $n_2 = 1$, $j_2 = 0$, $m_2 = 0$. The matrix element is

$$\langle 1|H_I|2\rangle = -(96\pi)^{-1/2}\lambda i\alpha^{5/2}Mc^2 \times\frac{(k/W)[1+2(k/W)^2]}{[1+(k/W)^2]^3}\,\delta_{j,1}\delta_{m,m_1}, \quad (8)$$

where $W = 4/3a$. The related matrix element which is important for the calculation of the electromagnetic shift of the ground state has $n_1 = 1$, $j_1 = 0$, $m_1 = 0$, $n_2 = 3$, $j_2 = 1$, $m_2 = 0, \pm 1$. The element is

$$\langle 1|H_I|2\rangle = (96\pi)^{-1/2}\lambda i\alpha^{5/2}Mc^2 \times\frac{(k/W)[1+2(k/W)^2]}{[1+(k/W)^2]^3}(-1)^{m_2}\delta_{j,1}\delta_{m,-m_2}. \quad (9)$$

The transition probability for Lyman-α radiation using the matrix element Equation (6) is (on summing over both helicities and using the value of k obtained from the usual hydrogen energy-level formulas)

$$T = (\tfrac{2}{3})^8(\hbar)^{-1}\alpha^5(Mc^2)[1+(\tfrac{1}{4}\alpha)^2]^{-4}. \quad (10)$$

The entire effect of retardation is in the factor $[1+(\frac{1}{4}\alpha)^2]^{-4}$, which is unity to the fourth significant figure. Replacing this factor by unity gives the transition probability when retardation is ignored. When retardation is neglected, one obtains the same result for T as would be obtained using the dipole approximation in the traditional theory [use Eqs. (59.11) and (59.14) of Ref. 14 and the formula therein for the average oscillator strength on p. 263].

Our exact transition probability for Lyman-β radiation is (summing over λ)

$$T = (96\hbar)^{-1}\alpha^5(Mc^2)[1+2(\tfrac{1}{3}\alpha)^2]^2[1+(\tfrac{1}{3}\alpha)^2]^{-6}. \quad (11)$$

The effect of retardation is in the factor $[1+2(\frac{1}{3}\alpha)^2]^2[1+(\frac{1}{3}\alpha)^2]^{-6}$, which is unity to four significant figures. Replacing this factor by unity, one again obtains the result for the dipole approximation using traditional methods.

Thus in two cases where permitted transitions occur (that is, for which $j = 1$ for the photon), neglect of retardation is equivalent to the use of the dipole approximation in the standard derivation of transition probabilities. It seems likely that this result is general, though we have not had time to prove the general result.

II. ELECTROMAGNETIC THEORY IN TERMS OF IRREDUCIBLE REPRESENTATIONS OF THE POINCARÉ GROUP AND THE WAVE FUNCTION OF THE PHOTON

A. Irreducible Representations of the Poincaré Group and Wave Functions of the Photon

In relativistic quantum mechanics a particle is characterized by an irreducible representation of

the dynamical variables H, P_i, J_i, K_i, which satisfy the following commutation rules:

$$[P_i, P_j]=0, \quad [H, P_i]=0, \quad [J_i, H]=0, \quad [J_i, P_i]=0,$$
$$[J_i, K_i]=0, \quad [J_1, P_2]=[P_1, J_2]=i\hbar P_3(\text{cyc.}),$$
$$[J_1, K_2]=[K_1, J_2]=i\hbar K_3(\text{cyc.}), \quad [J_1, J_2]=i\hbar J_3(\text{cyc.}),$$
$$[K_j, H]=i\hbar c P_j, \quad [K_j, P_k]=i\hbar\delta_{jk}(H/c). \tag{12}$$

The operator H is the Hamiltonian, J_i $(i=1, 2, 3)$ the components of the angular momentum, P_i the components of the linear momentum, and K_i the space-time components of the relativistic angular-momentum tensor. In a covariant notation $P^0=-P_0=H/c$, $P^i=P_i$, P^μ is a four vector and $J_{\mu\nu}$ is the relativistic angular-momentum tensor with $J_{\mu\nu}=-J_{\nu\mu}$, $J_{23}=J_1$ (cyc.), $J_{0i}=K_i$.

Wigner (Ref. 15) has found all the irreducible representations of these dynamical variables. The representations with which we are concerned are the *mass-zero, positive-energy, finite-spin* representations. Each representation is characterized by a number λ, which can be any integer or half-odd integer of either sign. The number λ is called the helicity of the representation, while $|\lambda|$ is the spin of the representation. In Ref. 16 a form especially useful for our purpose is given. In this representation the carrier space is the Hilbert space of complex wave functions $\{g(\vec{p}, \lambda)\}$, where $\vec{p}=(p_1, p_2, p_3)$ covers the entire three-dimensional vector space and λ takes on only one value but is indicated explicitly for convenience. The inner product is chosen as

$$(f, g)=\int f^*(\vec{p}, \lambda)g(\vec{p}, \lambda)\frac{d\vec{p}}{cp}, \quad p=|\vec{p}| \tag{13}$$

and the dynamical variables are given by

$$\begin{aligned}
&Hg(\vec{p}, \lambda)=cpg(\vec{p}, \lambda),\\
&P_i g(\vec{p}, \lambda)=p_i g(\vec{p}, \lambda),\\
&J_1 g(\vec{p}, \lambda)=\hbar\left(-i(\vec{p}\times\vec{\nabla})_1+\frac{p_1}{p+p_3}\lambda\right)g(\vec{p}, \lambda),\\
&J_2 g(\vec{p}, \lambda)=\hbar\left(-i(\vec{p}\times\vec{\nabla})_2+\frac{p_2}{p+p_3}\lambda\right)g(\vec{p}, \lambda),\\
&J_3 g(\vec{p}, \lambda)=\hbar[-i(\vec{p}\times\vec{\nabla})_3+\lambda]g(\vec{p}, \lambda),\\
&K_1 g(\vec{p}, \lambda)=\hbar\left(ip\frac{\partial}{\partial p_1}+\frac{p_2}{p+p_3}\lambda\right)g(\vec{p}, \lambda),\\
&K_2 g(\vec{p}, \lambda)=\hbar\left(ip\frac{\partial}{\partial p_2}-\frac{p_1}{p+p_3}\lambda\right)g(\vec{p}, \lambda),\\
&K_3 g(\vec{p}, \lambda)=\hbar\left(ip\frac{\partial}{\partial p_3}\right)g(\vec{p}, \lambda).
\end{aligned} \tag{14}$$

We note that $(H/c)^2-P^2=0$, which is the zero-mass condition, the energy is positive, and that $(\vec{P}\cdot\vec{J})/P=\hbar\lambda$, where $P=(P^2)^{1/2}$. We shall now show how the wave functions $g(\vec{p}, \lambda)$ transform under the transformations of the Poincaré group. Define

$$x^0=-x_0=ct, \quad p^0=-p_0=p. \tag{15}$$

First consider the four-dimensional translation $T(a^\mu)$ in which the coordinates in the new frame are given in terms of those of the old by

$$x^{\mu\prime}=x^\mu-a^\mu. \tag{16a}$$

Denoting the wave function in the new frame by $g'(\vec{p}, \lambda)$

$$g'(\vec{p}, \lambda)=e^{i(a^\mu P_\mu)/\hbar}g(\vec{p}, \lambda). \tag{16b}$$

Consider a rotation of coordinates parametrized by $\vec{\theta}$ where $\theta=|\vec{\theta}|$ is the angle of rotation and $\vec{\theta}/\theta$ is the axis of rotation. Then

$$\begin{aligned}
&x^{0\prime}=x^0,\\
&\vec{x}'=\vec{x}\cos\theta+\frac{1-\cos\theta}{\theta^2}(\vec{\theta}\cdot\vec{x})\vec{\theta}-\frac{\sin\theta}{\theta}(\vec{\theta}\times\vec{x}).
\end{aligned} \tag{16c}$$

and

$$g'(\vec{p}, \lambda)=e^{i(\vec{\theta}\cdot\vec{J})/\hbar}g(\vec{p}, \lambda). \tag{16d}$$

Finally consider the pure Lorentz transformation $L(\vec{\beta})$, where $\beta=|\vec{\beta}|$ is given by $\cosh\beta=[1-(v/c)^2]^{-1/2}$ and where $\vec{\beta}/\beta$ points in the opposite direction to that of the moving frame as observed in the original frame. Then

$$\begin{aligned}
&x^{0\prime}=x^0\cosh\beta+\vec{\beta}\cdot\vec{x}(\sinh\beta)/\beta,\\
&\vec{x}'=\vec{x}+(\vec{\beta}\cdot\vec{x})\frac{\cosh\beta-1}{\beta^2}+\vec{\beta}x^0\frac{\sinh\beta}{\beta},
\end{aligned} \tag{16e}$$

and

$$g'(\vec{p}, \lambda)=e^{i(\vec{\beta}\cdot\vec{K})/\hbar}g(\vec{p}, \lambda). \tag{16f}$$

The explicit form of $g'(\vec{p}, \lambda)$ for each of the transformations is given in Ref. 17.

We shall define the dynamical system corresponding to a photon as being the direct sum of the representations for which $\lambda=1$ and $\lambda=-1$. The Hilbert space thus consists of functions $\{g(\vec{p}, \lambda)\}$, where $\vec{p}$ is defined over the entire vector space and λ takes on the two values ±1. The inner product is now defined by

$$(f, g)=\sum_{\lambda=\pm1}\int f^*(\vec{p}, \lambda)g(\vec{p}, \lambda)\frac{d\vec{p}}{cp}. \tag{17}$$

The quantity $\int_V[|g(\vec{p}, \lambda)|^2/cp]\,d\vec{p}$ gives the relative probability that a photon in a state given by $g(\vec{p}, \lambda)$ has its momentum in the volume V of momentum space and has the helicity λ. The norm of the wave function is defined, as usual, by

$$N(g)=[(g, g)]^{1/2}. \tag{18}$$

B. Expansion of Electromagnetic Field and Potentials in Irreducible Representations of Poincaré Group

In terms of cgs Gaussian units, Maxwell's equations in free space without sources are

$$\vec{\nabla}\times\vec{H}(\vec{x},t)=\frac{1}{c}\frac{\partial\vec{E}(\vec{x},t)}{\partial t},$$

$$\vec{\nabla}\times\vec{E}(\vec{x},t)=-\frac{1}{c}\frac{\partial\vec{B}(\vec{x},t)}{\partial t}, \tag{19}$$

$$\vec{\nabla}\cdot\vec{H}(\vec{x},t)=0,\quad \vec{\nabla}\cdot\vec{E}(\vec{x},t)=0.$$

In Ref. 18 eigenfunctions of the curl operator were introduced, and it was shown how the general initial value problem can be solved in terms of them. We first define the vector $\vec{Q}_\lambda(\vec{p})$ for $\lambda=0,\pm1$ by

$$\vec{Q}_0(\vec{p})=-(\vec{p}/p),$$

$$\vec{Q}_\lambda(\vec{p})=-\lambda(2)^{-1/2}\left(\frac{p_1(p_1+i\lambda p_2)}{p(p+p_3)}-1,\ \frac{p_2(p_1+i\lambda p_2)}{p(p+p_3)}-i\lambda,\ \frac{p_1+i\lambda p_2}{p}\right)\quad\text{for }\lambda=\pm1. \tag{20}$$

These vectors satisfy the following orthogonality and completeness relations:

$$\vec{Q}^*_\lambda(\vec{p})\cdot\vec{Q}_\mu(\vec{p})=\delta_{\lambda\mu},$$

$$\sum_\lambda Q^*_{i\lambda}(\vec{p})Q_{j\lambda}(\vec{p})=\delta_{ij}, \tag{21}$$

where $Q_{i\lambda}(\vec{p})$ is the ith component of $\vec{Q}_\lambda(\vec{p})$.

It is seen that the vectors $\vec{Q}_\lambda(\vec{p})e^{i\vec{p}\cdot\vec{x}}$ and their complex conjugates are eigenfunctions of the curl operator

$$\vec{\nabla}\times[\vec{Q}_\lambda(\vec{p})e^{i\vec{p}\cdot\vec{x}}]=p\lambda\vec{Q}_\lambda(\vec{p})e^{i\vec{p}\cdot\vec{x}}\quad\text{all }\lambda. \tag{22}$$

Furthermore,

$$\vec{\nabla}\cdot[\vec{Q}_\lambda(\vec{p})e^{i\vec{p}\cdot\vec{x}}]=-ipe^{i\vec{p}\cdot\vec{x}}\delta_{\lambda0}\quad\text{all }\lambda. \tag{23}$$

We can now state the following important theorems:

Theorem 1. The most general real solution in the infinite domain of Maxwell's equations (19) is

$$\vec{E}(\vec{x},t)=-\frac{i}{2\pi\hbar^{3/2}}\left(\sum_{\lambda=\pm1}\lambda\int\vec{Q}_\lambda(\vec{p})g(\vec{p},\lambda)e^{(i/\hbar)(\vec{p}\cdot\vec{x}-cpt)}d\vec{p}-\sum_{\lambda=\pm1}\lambda\int\vec{Q}^*_\lambda(\vec{p})g^*(\vec{p},\lambda)e^{-(i/\hbar)(\vec{p}\cdot\vec{x}-cpt)}d\vec{p}\right),$$

$$\vec{H}(\vec{x},t)=-\frac{1}{2\pi\hbar^{3/2}}\left(\sum_{\lambda=\pm1}\int\vec{Q}_\lambda(\vec{p})g(\vec{p},\lambda)e^{(i/\hbar)(\vec{p}\cdot\vec{x}-cpt)}d\vec{p}+\sum_{\lambda=\pm1}\int\vec{Q}^*_\lambda(\vec{p})g^*(\vec{p},\lambda)e^{-(i/\hbar)(\vec{p}\cdot\vec{x}-cpt)}d\vec{p}\right). \tag{24}$$

The two complex functions $g(\vec{p},\pm1)$ are uniquely given when $\vec{E}$ and $\vec{H}$ are prescribed at a time $t=t_0$.

Theorem 2. A necessary and sufficient condition that $\vec{E}(\vec{x},t)$ and $\vec{H}(\vec{x},t)$ transform under the Poincaré group in the usual relativistic fashion is that the amplitudes $g(\vec{p},\lambda)$ transform under the irreducible representations of the Poincaré group corresponding to zero mass, positive energy, and helicity λ, as in Eqs. (16a)–(16f).

The effect of these theorems, which are proved (with a somewhat different notation) in Ref. 2 and 4 is to state that the expansion equation (24) is the only solution of Maxwell's equations without sources that (within unitary transformations) transform appropriately. No other relativistic solution is possible. [It should be mentioned that the expansion equation (24) is actually invariant under a larger group than the Poincaré group, namely, the conformal group. We will not go into this matter further in the present paper, but we want to indicate that this larger invariance follows from Refs. 19–21.]

The expansion equation (24) is the same in all frames of reference obtained from the original frame by a transformation of the Poincaré group.

Let us define the vector and scalar potentials $\vec{A}(\vec{x},t)$ and $\Phi(\vec{x},t)$ in the usual fashion as being the solutions of the partial differential equations

$$\vec{H}(\vec{x},t)=\vec{\nabla}\times\vec{A}(\vec{x},t),$$

$$\vec{E}(\vec{x},t)=-\frac{1}{c}\frac{\partial\vec{A}(\vec{x},t)}{\partial t}-\nabla\Phi(\vec{x},t), \tag{25}$$

where $\vec{E}(\vec{x},t)$ and $\vec{H}(\vec{x},t)$ are solutions of Maxwell's equations.

Theorem 3. The most general form for the vector and scalar potentials for the case that currents and sources are not present is

$$\vec{A}(\vec{x},t)=-\frac{c}{2\pi\hbar^{1/2}}\left(\sum_{\lambda=\pm1}\lambda\int\vec{Q}_\lambda(\vec{p})g(\vec{p},\lambda)e^{(i/\hbar)(\vec{p}\cdot\vec{x}-cpt)}\frac{d\vec{p}}{cp}+\sum_{\lambda=\pm1}\lambda\int\vec{Q}^*_\lambda(\vec{p})g^*(\vec{p},\lambda)e^{-(i/\hbar)(\vec{p}\cdot\vec{x}-cpt)}\frac{d\vec{p}}{cp}\right)+\vec{\nabla}F(\vec{x},t),$$

$$\Phi(\vec{x},t)=-\frac{1}{c}\frac{\partial F(\vec{x},t)}{\partial t}+K, \tag{26}$$

where the functions $g(\vec{p}, \lambda)$ are the Poincaré amplitudes which occur in Eq. (24), $F(\vec{x}, t)$ is any real function of its arguments, and K is any real number.

Theorem 3 is extremely important because it resolves entirely the ambiguity in choosing potentials corresponding to a radiation field. The function $F(\vec{x}, t)$ and the constant K set the gauge completely. If $F(\vec{x}, t)$ satisfies Laplace's equation, the gauge is a radiation gauge, whereas if it satisfies the wave equation, the gauge is a Lorentz gauge. Radiation gauges are seen to be special cases of Lorentz gauges. If one is given an electromagnetic field $\vec{E}(\vec{x}, t)$ and $\vec{H}(\vec{x}, t)$, one can readily find $g(\vec{p}, \lambda)$ and thus $\vec{A}(\vec{x}, t)$ and $\Phi(\vec{x}, t)$ when one sets the gauge by choosing $F(\vec{x}, t)$ and K. Moreover, in Ref. 4 and later in Ref. 22, it is shown to be impossible to set the gauge in such a way that vector and scalar potentials satisfy the Lorentz condition and at the same time transform as a four-vector. In Ref. 4 it is shown that the closest approach is that the potentials $\vec{A}$ and Φ transform as a four-vector if the gauge is changed. The expansion equation (26) is nevertheless relativistic in the sense that this expansion is valid in all frames of reference.

Equation (26) is proved by expanding the vector potential in the eigenfunctions of the curl operator and taking the Fourier transform of the scalar potential. Substituting into Eq. (25) gives the result immediately.

Let us define the energy of the field E^f, the ith component of the linear momentum of the field P_i^f, and the ith component of the angular momentum of the field J_i^f in the usual way by

$$\begin{aligned} E^f &= (8\pi)^{-1} \int [\vec{E}^2(\vec{x}, t) + \vec{H}^2(\vec{x}, t)]\, d\vec{x}, \\ P_i^f &= (4\pi c)^{-1} \int [\vec{E}(\vec{x}, t) \times \vec{H}(\vec{x}, t)]_i\, d\vec{x}, \\ J_i^f &= (4\pi c)^{-1} \int \{\vec{x} \times [\vec{E}(\vec{x}, t) \times \vec{H}(\vec{x}, t)]\}_i\, d\vec{x}. \end{aligned} \tag{27}$$

These quantities can be obtained in terms of the Poincaré amplitudes $g(p, \lambda)$:

$$\begin{aligned} E^f &= \sum_{\lambda=\pm 1} \int g^*(\vec{p}, \lambda)[Hg(\vec{p}, \lambda)]\, \frac{d\vec{p}}{cp}, \\ P_i^f &= \sum_{\lambda=\pm 1} \int g^*(\vec{p}, \lambda)[P_i g(\vec{p}, \lambda)]\, \frac{d\vec{p}}{cp}, \\ J_i^f &= \sum_{\lambda=\pm 1} \int g^*(\vec{p}, \lambda)[J_i g(\vec{p}, \lambda)]\, \frac{d\vec{p}}{cp}, \end{aligned} \tag{28}$$

where $Hg(\vec{p}, \lambda)$, $P_i g(\vec{p}, \lambda)$, and $J_i g(\vec{p}, \lambda)$ are given by the first six parts of Eq. (14).

We shall interpret $g(\vec{p}, \lambda)$ [with the inner product Eq. (17)] as being the wave function of the photon associated with the electromagnetic field given by the expansion Eq. (26). That is, there will be a one-to-one correspondence between the wave function of the photon and the electromagnetic field.

The norm of the wave function $N(g)$ given by Eq. (18) is a measure of the strength of the electromagnetic field. If $\vec{E}(\vec{x}, t)$ and $\vec{H}(\vec{x}, t)$ of Eq. (26) were each multiplied by a real positive number k, $N(g)$ would be replaced by $kN(g)$. Furthermore, $N(g)$ is dimensionless and is invariant under changes of frame of reference. Thus we call $N(g)$ the (invariant) magnitude of the electromagnetic field.

We now have a relation between the field energy, linear-momentum components, and angular-momentum components E^f, P_i^f, and J_i^f, respectively, and the quantum-mechanical expectation values of the dynamical variables H, P_i, and J_i. From Eq. (28)

$$E^f/N(g) = \bar{H}, \quad P_i^f/N(g) = \bar{P}_i, \quad J_i^f/N(g) = \bar{J}_i, \tag{29}$$

where the bars mean the expectation value of the photon variables.

Another relation between the quantum-mechanical photon picture and the electromagnetic field picture is provided as follows:

Let us assume that the photon state is such that the wave function $g(\vec{p}, \lambda)$ vanishes for one value of λ ($= -\lambda_0$, say) and is very sharply peaked at $\vec{p} = \hat{p}$. One is then in a state in which the photon has the momentum $\hat{p}$ and helicity λ_0. Then from the expansion equation (26) it is seen that the electromagnetic field is a circularly polarized electromagnetic wave whose propagation vector is $\hat{p}/\hbar$, and which is left circularly polarized if $\lambda_0 = 1$ and is right circularly polarized if $\lambda_0 = 1$. This can be most simply seen by picking $\hat{p} = (0, 0, p)$.

We have thus shown how the photon or particle picture of radiation and the wave picture are related. An old dichotomy is thereby resolved. It should be noted that we have used positive-energy photons only. Furthermore, it is unnecessary and even incorrect to introduce timelike or longitudinal photons in a proper group-theoretical treatment of the source-free electromagnetic field.

C. Energy-Angular-Momentum Basis for Photons: Expansion of Vector Potential in Energy-Angular-Momentum Basis

We shall now introduce the angular-momentum basis for massless particles of finite spin and for photon wave functions, in particular. This basis is essential for obtaining the selection rules and matrix elements for atoms, for these quantities come from the conservation of total angular momentum. The angular-momentum basis for relativistic particles was derived in Ref. 23 from the commutation rules for the infinitesimal generators of the Poincaré group. The relation to the linear-momentum basis is given in Refs. 24–26. This re-

lation is most conveniently stated in terms of the generalized surface harmonics $Y_j^{m,n}(\theta,\phi)$, which were introduced in Ref. 27. For the purposes of the present paper, their properties are summarized in Appendix A of Ref. 28, which also has a table of these functions for $j=0,1,2$ in terms of trigonometric functions.

The functions $Y_j^{m,n}(\theta,\phi)$ are generalizations of the usual surface harmonics $Y_{jm}(\theta,\phi)$ in the sense that for j an integer

$$Y_j^{m,0}(\theta,\phi)=Y_{jm}(\theta,\phi), \tag{30}$$

where $Y_{jm}(\theta,\phi)$ are the usual surface harmonics in the notation, for example, of Ref. 12.

The Poincaré amplitudes $G(E,j,m,\lambda)$ in the energy–angular-momentum basis are defined by

$$g(\vec{p},\lambda)=\frac{c^{1/2}}{p}\sum_{j=1}^{\infty}\sum_{m=-j}^{j}Y_j^{m,\lambda}(\theta,\phi)G(cp,j,m,\lambda), \tag{31a}$$

where j goes through integer values only. The amplitude $G(E,j,m,\lambda)$ is found in terms of $g(\vec{p},\lambda)$ as follows:

$$G(E,j,m,\lambda)=\frac{E}{c^{3/2}}\int_0^{\pi}d\phi\int_0^{\pi}d\theta\sin\theta\,Y_j^{m,\lambda *}(\theta,\phi)g(\vec{p},\lambda), \tag{31b}$$

$$\vec{p}=(E/c)(\sin\theta\cos\phi,\ \sin\theta\sin\phi,\ \cos\theta).$$

The inner product in the new basis is (for the irreducible representations)

$$(f,g)=\int f^*(\vec{p},\lambda)g(\vec{p},\lambda)\frac{d\vec{p}}{cp}$$

$$=\sum_{j=1}^{\infty}\sum_{m=-j}^{j}\int_0^{\infty}F^*(E,j,m,\lambda)G(E,j,m,\lambda)\frac{dE}{E}, \tag{31c}$$

where $F(E,j,m,\lambda)$ is obtained from $f(\vec{p},\lambda)$ through Eq. (31a). Equation (31a) is the generalization of the expansion of a scalar function of $\vec{p}$ into spherical harmonics. [It should be mentioned that the function $G(E,j,m,\lambda)$ in the present paper differs from the corresponding function of Ref. 4 and 24 in phase, but agrees in phase with the function of Ref. 25].

One can obtain the dynamical variables in terms of the energy–angular-momentum basis. Of particular interest

$$\begin{aligned}
&HG(E,j,m,\lambda)=EG(E,j,m,\lambda),\\
&J_3G(E,j,m,\lambda)=\hbar mG(E,j,m,\lambda),\\
&(J_1\pm iJ_2)G(E,j,m,\lambda)=\hbar[(j\mp m+1)(j\pm m)]^{1/2}\\
&\qquad\times G(E,j,m\mp1,\lambda),\\
&\vec{J}^2G(E,j,m,\lambda)=\hbar^2j(j+1)G(E,j,m,\lambda),\\
&(\vec{P}\cdot\vec{J})G(E,j,m,\lambda)=\hbar(E/c)\lambda G(E,j,m,\lambda).
\end{aligned} \tag{32}$$

Thus the new basis is an angular-momentum basis in which $H, J_3, \vec{J}^2$ are diagonal, as is also the helicity.

The wave function of the photon in the energy–angular-momentum representation is denoted by $G(E,j,m,\lambda)$, where λ takes on the two values ±1. The inner product is

$$(f,g)=\sum_{\lambda=\pm1}\sum_{j=1}^{\infty}\sum_{m=-j}^{j}\int F^*(E,j,m,\lambda)G(E,j,m,\lambda)\frac{dE}{E}, \tag{31d}$$

instead of Eq. (31c). In terms of the angular-momentum representation the vector potential takes on the following form when $F(\vec{x},t)=0$:

$$\vec{A}(\vec{x},t)=\vec{A}_1(\vec{x},t)+\vec{A}_1^*(\vec{x},t), \tag{33a}$$

where

$$\begin{aligned}
\vec{A}_1(\vec{x},t)=-(2)^{1/2}\sum_{\lambda=\pm1}\sum_{k=1}^{\infty}\sum_{m=-k}^{k}(i)^k\{&\vec{Y}_{k,k,m}(\hat{\theta},\hat{\phi})A_{km\lambda,k}(r,t)-i\lambda[k/(2k+1)]^{1/2}\vec{Y}_{k,k-1,m}(\hat{\theta},\hat{\phi})A_{km\lambda,k+1}(r,t)\\
&+i\lambda[(k+1)/(2k+1)]^{1/2}\vec{Y}_{k,k-1,m}(\hat{\theta},\hat{\phi})A_{km\lambda,k-1}(r,t)\},
\end{aligned} \tag{33b}$$

where $r=|\vec{x}|$, $\hat{\theta}$ and $\hat{\phi}$ are the polar angles of $\vec{x}$ (not to be confused with θ and ϕ, which are the polar angles of $\vec{p}$), and $\vec{Y}_{j,k,m}$ are the vector spherical harmonics of Ref. 29 in the notation of Ref. 12. Finally

$$A_{km\lambda,k'}(r,t)=(\hbar c)^{-1/2}\int_0^{\infty}G(E,k,m,\lambda)\times j_k(Er/\hbar c)e^{-(i/\hbar)Et}dE, \tag{33c}$$

where $j_k(r)$ is the usual spherical Bessel function of order k.

The expression for the magnetic field $\vec{H}(\vec{x},t)$ in terms of the angular-momentum basis is identical to that of $\vec{A}(\vec{x},t)$, except that $G(E,j,m,\lambda)$ in Eq. (33c) is replaced by $(E/\hbar c)\lambda G(E,j,m,\lambda)$. The expression for the electric field $\vec{E}(\vec{x},t)$ is also the same, except that $G(E,j,m,\lambda)$ is replaced by $i(E/\hbar c)G(E,j,m,\lambda)$.

The decomposition of $\vec{A}(\vec{x},t)$ and $\vec{A}_1(\vec{x},t)$ as in Eqs. (33a) and (33b) also separates the vector potential into toroidal and poloidal modes which, in a sense, is complementary to the decomposition into the eigenfunctions of the curl operator.

Let us write

$$\vec{A}_1(\vec{x},t)=\vec{A}_T(\vec{x},t)+\vec{A}_P(\vec{x},t), \tag{33d}$$

where

$$\vec{A}_T(\vec{x},t)=-(2)^{1/2}\sum_{\lambda=\pm1}\sum_{k=1}^{\infty}\sum_{m=-k}^{k}(i)^k\vec{Y}_{k,k,m}(\hat{\theta},\hat{\phi})A_{km\lambda,k}(r,t),$$

$$\vec{A}_P(\vec{x},t)=(2)^{1/2}\sum_{\lambda=\pm1}\sum_{k=1}^{\infty}\sum_{m=-k}^{k}(i)^{k+1}\lambda\left[\left(\frac{k}{2k+1}\right)^{1/2}\vec{Y}_{k,k+1,m}(\hat{\theta},\hat{\phi})A_{km\lambda,k+1}(r,t)-\left(\frac{k+1}{2k+1}\right)^{1/2}\right.$$
$$\left.\times\vec{Y}_{k,k-1,m}(\hat{\theta},\hat{\phi})A_{km\lambda,k-1}(r,t)\right] \tag{33e}$$

Let us introduce the operator $\vec{L}=(L_1,L_2,L_3)$ by

$$\vec{L}=-i(\vec{x}\times\vec{\nabla}). \tag{33f}$$

Clearly the components of $\vec{L}$ are the components of the "orbital angular momentum" with $\hbar$ set equal to unity.

From the expressions on pp. 83–85 of Ref. 12

$$\vec{A}_T(\vec{x},t)=\vec{L}\tau(\vec{x},t),\quad \vec{A}_P(\vec{x},t)=\vec{\nabla}\times\vec{L}\psi(\vec{x},t), \tag{33g}$$

where $\tau(\vec{x},t)$ and $\psi(\vec{x},t)$ are potentials given by

$$\tau(\vec{x},t)=-(2)^{1/2}\sum_{\lambda=\pm1}\sum_{k=1}^{\infty}\sum_{m=-k}^{k}(i)^k[k(k+1)]^{-1/2}\times A_{km\lambda,k}(r,t)Y_k^{m,0}(\hat{\theta},\hat{\phi}),$$
$$\psi(\vec{x},t)=-(2)^{1/2}\sum_{\lambda=\pm1}\sum_{k=1}^{\infty}\sum_{m=-k}^{k}(i)^k\lambda[k(k+1)]^{-1/2}\times B_{km\lambda}(r,t)Y_k^{m,0}(\hat{\theta},\hat{\phi}), \tag{33h}$$

where

$$B_{km\lambda}(r,t)=(\hbar c)^{1/2}\int_0^{\infty}G(E,k,m,\lambda)j_k\left(\frac{Er}{\hbar c}\right)e^{-(i/\hbar)Et}\frac{dE}{E}. \tag{33i}$$

From Eq. (33g) it is seen that $\vec{A}_T$ is a toroidal vector and that $\vec{A}_P$ is a poloidal vector. For a discussion of such vectors see, for example, Appendix III of Ref. 30. As will be seen in the derivation of the selection rules, the rules split the contributions from the vector potential into its poloidal and toroidal parts.

From the earlier theorems it is seen that the method of introducing the angular-momentum basis for photons and the expansion of the vector potential in terms of the basis, which we have introduced, is the only proper method in terms of the Poincaré group. An example of an improper method is that of Ref. 31.

It is an easy matter to find the radiation pattern associated with photons of a given angular momentum. For example, let us derive the radiation pattern of Eqs. (3) and (4) for "permitted transitions," that is for $j=1$ in the matrix element of Eq. (2a). In Eq. (31a) we set $G(E,j,m,\lambda)=0$ for all $j>1$. Furthermore, from Eq. (2a)

$$G(E,1,m,\lambda)=\lambda B, \tag{34}$$

where B is independent of λ when we take into account that the wave function of the photon in the angular-momentum basis of the photon is proportional to the complex conjugate of the matrix element. Then

$$g(\vec{p},\lambda)=\lambda BY_1^{m,\lambda}(\theta,\phi). \tag{35}$$

When this $g(\vec{p},\lambda)$ is substituted into Eq. (25), the field equations (3) and (4) are obtained from the contribution of one value of the propagation vector $\vec{p}/\hbar$, where the explicit form of the surface harmonic is taken from Ref. 28. When one goes into the details of the calculation, one sees that a redefinition of B is needed so that it is proportional to the matrix element for all m. This is accomplished by replacing B by A in Eq. (4) and by $(2)^{-1/2}A$ in Eq. (5).

D. Quantization of Electromagnetic Field

1. *Annihilation and Creation Operators: Dynamical Variables*

It is seen that classical electromagnetic theory of radiation is already first-quantized. To second-quantize the theory we replace photon wave functions by annihilation operators and their complex conjugates by creation operators in the usual way. We shall first work in the linear-momentum basis. In the expansions equations (24) and (26) the quantities $g(\vec{p},\lambda)$ are now annihilation operators and the quantities $g^*(\vec{p},\lambda)$ are creation operators which are the Hermitian adjoints of $g(\vec{p},\lambda)$. The operators satisfy the following commutation relations:

$$[g(\vec{p},\lambda),g(\vec{p}',\lambda')]=[g^*(\vec{p},\lambda),g^*(\vec{p}',\lambda')]=0,$$
$$[g(\vec{p},\lambda),g^*(\vec{p}',\lambda')]=cp\delta_{\lambda,\lambda'}\delta(\vec{p}-\vec{p}'). \tag{36}$$

The second-quantized operators corresponding to the dynamical variables H, P_i, J_i, and K_i will be designated by $\hat{H}$, $\hat{P}_i$, $\hat{J}_i$, and $\hat{K}_i$, respectively. Then

$$\begin{aligned}
\hat{H} &= \sum_{\lambda=\pm 1} \int g^*(\vec{p},\lambda)[Hg(\vec{p},\lambda)]\frac{d\vec{p}}{cp}, \\
\hat{P}_i &= \sum_{\lambda=\pm 1} \int g^*(\vec{p},\lambda)[P_i g(\vec{p},\lambda)]\frac{d\vec{p}}{cp}, \\
\hat{J}_i &= \sum_{\lambda=\pm 1} \int g^*(\vec{p},\lambda)[J_i g(\vec{p},\lambda)]\frac{d\vec{p}}{cp}, \\
\hat{K}_i &= \sum_{\lambda=\pm 1} \int g^*(\vec{p},\lambda)[K_i g(\vec{p},\lambda)]\frac{d\vec{p}}{cp}.
\end{aligned} \tag{37}$$

In Eq. (37), $Hg(\vec{p},\lambda)$, $P_i g(\vec{p},\lambda)$, $J_i g(\vec{p},\lambda)$, and $K_i g(\vec{p},\lambda)$ are defined by the right-hand side of Eq. (14).

The following theorem is easily proved:

Theorem 4. The second-quantized operations $\hat{H}$, $\hat{P}_i$, $\hat{J}_i$, and $\hat{K}_i$ satisfy the commutation relations, Eqs. (12).

A consequence of Theorem 4 is that the second-quantized operators are dynamical variables of a relativistic system.

The number operator is defined by

$$N = \sum_{\lambda=\pm 1} \int g^*(\vec{p},\lambda) g(\vec{p},\lambda)\frac{d\vec{p}}{cp}. \tag{38}$$

The operator $\hat{H}$ is the Hamiltonian of the second-quantized field, and so on for the other second-quantized variables.

The electromagnetic fields which are expanded as in Eq. (24) are now Hermitian operators in the Heisenberg picture. They satisfy Maxwell's equations. The commutation rules for the components of the field are identical to those traditionally used. The vector potential is also a Hermitian operator in the Heisenberg picture.

The annihilation operators $g(\vec{p},\lambda)$ transform as the Poincaré wave functions in order that the quantized electromagnetic field transforms appropriately. It is readily shown that

$$\begin{aligned}
e^{-i(a^\mu \hat{P}_\mu)/\hbar} g(\vec{p},\lambda) e^{i(a^\mu \hat{P}_\mu)/\hbar} &= e^{i(a^\mu P_\mu)/\hbar} g(\vec{p},\lambda), \\
e^{-i(\vec{\theta}\cdot\hat{\vec{J}})/\hbar} g(\vec{p},\lambda) e^{i(\vec{\theta}\cdot\hat{\vec{J}})/\hbar} &= e^{i(\vec{\theta}\cdot\vec{J})/\hbar} g(\vec{p},\lambda), \\
e^{-i(\vec{\beta}\cdot\hat{\vec{K}})/\hbar} g(\vec{p},\lambda) e^{i(\vec{\beta}\cdot\hat{\vec{K}})/\hbar} &= e^{i(\vec{\beta}\cdot\vec{K})/\hbar} g(\vec{p},\lambda).
\end{aligned} \tag{39}$$

The following theorem is seen to hold:

Theorem 5. The set of annihilation and creation operators in two frames of reference related by a Poincaré transformation are unitarily equivalent to each other. Furthermore, the electromagnetic fields in the two frames are unitarily equivalent.

We now have a second-quantized Poincaré invariant theory with a positive definite metric for the Hilbert space that is completely free of the ambiguities of the usual treatments.

To obtain the second-quantized theory in an angular-momentum basis, we replace $G(E,j,m,\lambda)$ by an annihilation operator and its complex conjugate by a creation operator. The following commutation rules are satisfied:

$$\begin{aligned}
&[G(E,j,m,\lambda), G(E',j',m',\lambda')] \\
&\qquad = [G^*(E,j,m,\lambda), G^*(E',j',m',\lambda')] = 0, \\
&[G(E,j,m,\lambda), G^*(E',j',m',\lambda')] \\
&\qquad = E\delta(E-E')\delta_{j,j'}\delta_{m,m'}\delta_{\lambda,\lambda'}.
\end{aligned} \tag{40}$$

2. *Fock Representation*

We now give the usual realization for the annihilation and creation operators—namely, the Fock representation. This representation is characterized by the existence of a vacuum state $|V\rangle$ such that

$$\langle V|V\rangle = 1, \quad g(\vec{p},\lambda)|V\rangle = G(E,j,m,\lambda)|V\rangle = 0. \tag{41}$$

In the linear-momentum basis the n-particle ket is defined by

$$|\vec{p}_1,\lambda_1;\vec{p}_2,\lambda_2;\ldots;\vec{p}_n,\lambda_n\rangle = \prod_{i=1}^{n} g^*(\vec{p}_i,\lambda_i)|V\rangle. \tag{42}$$

The n-particle ket in the angular-momentum basis is defined analogously using G^*. In particular, the one-photon state is given by

$$|E,j,m,\lambda\rangle = G^*(E,j,m,\lambda)|V\rangle. \tag{43}$$

3. *Quantized Electromagnetic Fields with Infinite Numbers of Photons*

The Fock representation for the annihilation and creation operators is characterized by the existence of a vacuum state and by the fact that the number operator N is defined. There are, however, other realizations in which the number of particles is infinite. Such realizations have been introduced by Friedrichs in Ref. 32 who calls them "myriotic" because they correspond to an infinite number of particles. The occupation number operator is defined, however. The possibility of still other realizations is discussed in Ref. 33. More recently, Ref. 34 has introduced "coherent states" (which we believe to be special cases of Friedrichs' myriotic states) which also correspond to an infinite number of particles. Realizations other than the Fock representation are useful in statistical mechanics where an infinite number of photons are present (as in black-body radiation) and in the description of intense, coherent radiation. The introduction

of annihilation and creation operators in the manner of the present paper allows us to attach a relativistic photon interpretation to these infinite-particle quantizations of the electromagnetic fields. There is no difficulty whatever in computing matrix elements for the emission or absorption of photons by an atom when such infinite-number representations are used. However, we shall not pursue the problem in the present paper.

III. EVALUATION OF EXACT MATRIX ELEMENTS

A. Hilbert Space: Separation of Radial and Angular Integrations

The space in which the interaction

$$H_I = i(e\hbar/Mc)\vec{A}(\vec{x})\cdot\vec{\nabla} \tag{44}$$

is defined, is the direct product of the Hilbert spaces S_P and S_A, where S_P is the Hilbert space of the photons or second-quantized electromagnetic theory in the Fock representation, and S_A is the Hilbert space of atomic wave functions. Since we are working in the Schrödinger picture, the interaction is taken at time $t=0$ and the time variable is suppressed in the vector potential. The vector potential $\vec{A}(\vec{x})$ is taken with $F(\vec{x},t)\equiv 0$ and in the angular-momentum representation, as in Eqs. (33a) and (33b), with $G(E,j,m,\lambda)$ and $G^*(E,j,m,\lambda)$ as annihilation and creation operators, respectively.

In the space S_P we will be concerned primarily with the vacuum state $|V\rangle$ and the one-photon state $|E,j,m,\lambda\rangle$. In the space S_A we will be interested in the wave functions that correspond to the bound states of spinless hydrogenic atoms that also correspond to angular momentum eigenstates. Such states will be labeled by $|n,j,m\rangle$, where n is the principal quantum number, and j and m are the quantum numbers describing the total angular momentum and the z component of the angular momentum, respectively. In the $\vec{x}$ representation

$$\langle\vec{x}|n,j,m\rangle = R_{nj}(r)Y_j^{m,0}(\theta,\phi), \tag{45}$$

where r, θ, and ϕ are the polar coordinates of $\vec{x}$, and $R_{nj}(r)$ is the atomic radial wave function [see Eq. (30)]. In Eqs. (33b) and similar expressions we will drop the carats, since the polar coordinates of $\vec{p}$ will no longer play a role and the polar angles will thus henceforth refer to those of $\vec{x}$.

In the direct-product Hilbert space the state $|1\rangle$ is that corresponding to the case where there is no photon and where the atom is in the state described by the quantum numbers n_1, j_1, m_1. The state $|2\rangle$ is that for which the atom is in the state with quantum numbers n_2, j_2, m_2 and there is a photon with energy E, angular momentum given by j,m, and helicity given by λ. The energy E of the photon is the difference of the energies of the states, in the case that we are considering photon emission or absorption; but it is arbitrary in higher-order processes that do not conserve energy in the intermediate states.

Then

$$|1\rangle = |V\rangle\otimes|n_1,j_1,m_1\rangle, \quad |2\rangle = |E,j,m,\lambda\rangle\otimes|n_2,j_2,m_2\rangle. \tag{46}$$

Then

$$\begin{aligned}\langle 1|H_I|2\rangle = -(2\alpha)^{1/2}e^2ak(i)^{j+1}\int_0^\infty r^2\,dr\,R_1(r)\\ \times\{j_j(kr)O^{jjm}_{j_1m_1;j_2m_2} - i\lambda[j/(2j+1)]^{1/2}\\ \times j_{j+1}(kr)O^{j,j+1,m}_{j_1m_1;j_2m_2} + i\lambda[(j+1)/(2j+1)]^{1/2}\\ \times j_{j-1}(kr)O^{j,j-1,m}_{j_1m_1;j_2m_2}\}R_2(r),\end{aligned} \tag{47a}$$

where the operators

$$\begin{aligned}O^{JLM}_{j_1m_1;j_2m_2} = \int_0^{2\pi}d\phi\int_0^{2\pi}d\theta\sin\theta Y^*_{j_1m_1}(\theta,\phi)\\ \times[\vec{Y}_{JLM}(\theta,\phi)\cdot\vec{\nabla}]Y_{j_2m_2}(\theta,\phi)\end{aligned} \tag{47b}$$

operate on the r variable in the atomic radial functions. Furthermore, for simplicity we have written

$$R_1(r) = R_{n_1j_1}, \quad R_2(r)_{n_2j_2}. \tag{47c}$$

B. Evaluation of Operators $O^{JLM}_{j_1m_1;j_2m_2}$

We will first give the results and then sketch the derivations:

$$O^{jjm}_{j_1m_1;j_2m_2} = -(-1)^{m_1}\frac{1}{4}\left(\frac{(2j+1)(2j_1+1)(2j_2+1)}{\pi j(j+1)}\right)^{1/2}[(W-j)(W+j+2)(j+\Delta+1)(j-\Delta+1)]^{1/2}$$
$$\times\begin{pmatrix} j & j_1 & j_2\\ m & -m_1 & m_2\end{pmatrix}\begin{pmatrix} j+1 & j_1 & j_2\\ 0 & 0 & 0\end{pmatrix}\frac{1}{r}, \tag{48a}$$

$$O^{j,j+1,m}_{j_1m_1;j_2m_2} = -(-1)^{m_1}\frac{1}{4}\left(\frac{(2j_1+1)(2j_2+1)}{\pi(j+1)}\right)^{1/2}\begin{pmatrix} j & j_1 & j_2\\ m & -m_1 & m_2\end{pmatrix}\begin{pmatrix} j & j_1 & j_2\\ 0 & 0 & 0\end{pmatrix}\left(2(j+1)\frac{\partial}{\partial r}+[\Delta(W+1)-j(j+1)]\frac{1}{r}\right), \tag{48b}$$

$$O^{j,j-1,m}_{j_1m_1;j_2m_2} = (-1)^{m_1}\frac{1}{4}\left(\frac{(2j_1+1)(2j_2+1)}{\pi j}\right)^{1/2}\begin{pmatrix} j & j_1 & j_2 \\ m & -m_1 & m_2\end{pmatrix}\begin{pmatrix} j & j_1 & j_2 \\ 0 & 0 & 0\end{pmatrix}\left(2j\frac{\partial}{\partial r} - [\Delta(W+1) - j(j+1)]\frac{1}{r}\right). \tag{48c}$$

We will now sketch the derivation of Eq. (48). We use the notation and methods of Chap. 5 of Ref. 12. Accordingly, we introduce the vectors $\vec{e}_q$ for $q=0, \pm1$ by

$$\vec{e}_0 = (0,0,1), \quad \vec{e}_q = -q(2)^{-1/2}(1, iq, 0) \quad \text{for } q = \pm 1. \tag{49}$$

For any vector $\vec{A}$ we define A_q by

$$A_q = \vec{e}_q \cdot \vec{A}.$$

In particular

$$Y_{JLMq}(\theta,\phi) = \vec{e}_q \cdot \vec{Y}_{JLM}(\theta,\phi) = (-1)^q(L, M+q, 1, -q \mid L, 1, J, M)Y_{L,M+q}(\theta,\phi), \tag{50}$$

which follows from the definition of the vector surface harmonics.

Then also,

$$\vec{Y}_{JLM}(\theta,\phi)\cdot\vec{\nabla} = \sum_q (-1)^q Y_{JLM,-q}(\theta,\phi)\nabla_q. \tag{51}$$

The following rule for the product of two surface harmonics will be used:

$$Y^*_{jm}(\theta,\phi)Y_{JM}(\theta,\phi) = (-1)^M\sum_k\left(\frac{(2J+1)(2j+1)}{4\pi(2k+1)}\right)^{1/2}(j,-m,J,M\mid j,J,k,M-m)(j,0,J,0\mid j,J,k,0)Y^*_{k,m-M}(\theta,\phi). \tag{52}$$

Thus

$$O^{JLM}_{j_1m_1;j_2m_2} = \sum_{j,q}(-1)^{M-q}(L,M-q,1,q\mid L,1,J,M)(j_1,-m_1,L,M-q\mid j_1,L,j,M-q-m_1)(j_1,0,L,0\mid j_1,L,j,0)$$
$$\times\left(\frac{(2j_1+1)(2L+1)}{4\pi(2j+1)}\right)^{1/2}(j,m_1-m+q\mid\nabla_q\mid j_2,m_2), \tag{53a}$$

where the matrix elements defined by

$$(j_1,m_1\mid\nabla_q\mid j_2,m_2) = \int_0^{2\pi}d\phi\int_0^{\pi}d\theta\sin\theta\, Y^*_{j_1m_1}(\theta,\phi)\nabla_q Y_{j_2m_2}(\theta,\phi) \tag{53b}$$

are given in Ref. 12. The only nonvanishing elements are

$$(j+1,m+q\mid\nabla_q\mid j,m) = \left(\frac{j+1}{2j+3}\right)^{1/2}(j,m,1,q\mid j,1,j+1,m+q)\left(\frac{\partial}{\partial r} - \frac{j}{r}\right),$$
$$(j-1,m+q\mid\nabla_q\mid j,m) = -\left(\frac{j}{2j-1}\right)^{1/2}(j,m,1,q\mid j,1,j-1,m+q)\left(\frac{\partial}{\partial r} + \frac{j+1}{r}\right). \tag{53c}$$

The expression (53a) can be simplified greatly by noting that the operator $\vec{Y}_{JLM}(\theta,\phi)\cdot\vec{\nabla}$ acting on the Hilbert space of atomic states is an irreducible tensor of rank J. Therefore we can use the Wigner-Eckart theorem:

$$O^{JLM}_{j_1m_1;j_2m_2} = (j_2,m_2,J,M\mid j_2,J,j_1,m_1)f_L(j_1,j_2,J). \tag{54}$$

The function $f_L(j_1,j_2,j)$ is the reduced matrix element. It is obtained by evaluating $O^{JL,j_1-j_2}_{j_1j_1;j_2j_2}$ from Eq. (53a). In this case the various Clebsch-Gordan coefficients are relatively easy to compute explicitly and the reduced matrix elements can be found. Finally one replaces the Clebsch-Gordan coefficients $(j_2,m_2,J,M\mid j_2,J,j_1,m_1)$ and $(j_1,0,L,0\mid j_1,L,j,0)$ by the equivalent Wigner 3-j coefficients for greater symmetry to obtain Eq. (48).

C. Derivation of Matrix Elements

It is now a straightforward matter to evaluate the matrix elements Eqs. (2a) and (2b). The presence of the 3-j symbols

$$\begin{pmatrix} j+1 & j_1 & j_2 \\ 0 & 0 & 0\end{pmatrix}$$

in the expression for $O^{jjm}_{j_1m_1;j_2m_2}$ and

$$\begin{pmatrix} j & j_1 & j_2 \\ 0 & 0 & 0\end{pmatrix}$$

in the expression for $O^{j,j\pm1,m}_{j_1m_1;j_2m_2}$ splits the evaluation of the matrix elements into two cases, since

$$\begin{pmatrix} j & j_1 & j_2 \\ 0 & 0 & 0\end{pmatrix}$$

vanishes unless $j+j_1+j_2$ is even. Equation (2b) follows immediately from the use of Eq. (48) in Eq. (47a), in the case that $j+j_1+j_2$ is odd. It is seen that only the toroidal component of the vector potential contributes to the matrix element in this case. For the case where $j+j_1+j_2$ is even, the situation is somewhat more complicated. The expression in curly brackets in Eq. (47a) contains the expressions

$$[j_{j+1}(kr)+j_{j-1}(kr)]\frac{\partial}{\partial r}$$

and

$$[jj_{j+1}(kr)-(j+1)j_{j-1}(kr)].$$

But

$$[j_{j+1}(kr)+j_{j-1}(kr)]=\frac{2j+1}{kr}j_j(kr),$$

$$[jj_{j+1}(kr)-(j+1)j_{j-1}(kr)]=-\frac{2j+1}{kr}\frac{d}{dr}[rj_j(kr)]. \tag{55}$$

We then make the above substitutions into the expressions for the matrix elements. Finally, we integrate by parts to remove the derivative from the Bessel function. It is to be noted that only the poloidal part of the vector potential contributes to the matrix element of Eq. (2a).

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