Symmetries and polarization correlations in collision processes

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Abstract. A unified quantum collision theory for an elementary reaction is reviewed in the wave-packet approach. General kinematic analyses of various atomic collision processes by using the density-matrix and helicity formulations are presented. The rotation, parity, and time-reversal symmetries of the colliding system are considered. In addition to polarization and angular correlations in each collision process, correspondences among different collision processes are also studied. These symmetry studies in atomic collisions provide a great deal of valuable information about the colliding systems and enhances our knowledge on the collision dynamics.

1. Introduction

Atomic collisions have been the most fruitful probes of elementary interactions and atomic structure. Besides fundamental interests, atomic collisions have also important applications in astrophysics, plasma physics, and radiation physics. Most studies on atomic collisions are about cross sections, and not much attention has been paid to polarization and angular correlations in the collisions. As a consequence, significant achievements in understanding of the collision dynamics have been elusive. Polarization and angular correlations in atomic collisions can reveal a wealth of information about the collision dynamics and coherence. A notable application, for example, is the observation of parity nonconservation in inelastic scattering of longitudinal polarized electrons from unpolarized targets [1].

In this paper, quantum collision theory for an elementary reaction is reviewed in the wave-packet approach [2] which corresponds accurately to experimental conditions with no lapses in physical rigor. We will also present a brief account of polarization and angular correlations in atomic collisions. A relativistic helicity formulation is adopted such that the spin polarization of the electron and fine structure of the atom are built in from the outset. This approach is particularly suitable when colliding systems involve highly ionized ions.

A general description of collision processes to be treated in this paper is presented in Section II. A unified quantum collision theory in the wave-packet approach is reviewed in Section III. Photon and electron helicity states are presented in Section IV. Density matrix descriptions of polarization for the photon, electron, and atom are given in Section V. Section VI outlines the helicity formulation of atomic collisions employed in the present application. A general collision equation is introduced for collision processes in Section VII. Photoionization and electron-capture fluorescence are treated...
respectively in Sections VIII and IX. Roles played by the symmetry principle are demonstrated in Section X. Conclusions are made in Section XI.

2. General description of collision processes

Physicists study the nature and laws of the universe, and all beings in the universe are particles in nature but follow laws of waves. This is the so-called particle-wave duality. In this sense, we shall refer to any physical system, either elementary or composite, by the term particle; for examples, electron, photon, proton, atom, molecule, cluster, etc. are such systems. All physical and chemical phenomena are basically collision processes of particles. We shall be concerned with a single elementary reaction, namely,

\[ A + B + C + \cdots \rightarrow F + G + H + \cdots, \]

where we have \( \mu \) particles \( \{A, B, C, \cdots\} \) as the reactants and \( \nu \) particles \( \{F, G, H, \cdots\} \) as the products, shown schematically in Fig. 1. Specific examples are fluorescence, electron-impact ionization, charge exchange, chemical reaction, etc.

![Figure 1. Schematic diagram with the time scale for the reaction](image)

The state of a particle, referring to either one of the reactants or products, may be expressed generally by a density operator \( \rho \),

\[
\rho = \sum_{mn} \rho_{mn} |\phi_n\rangle \langle \phi_n|.
\]

Here \( \rho_{mn} \) are matrix elements of the density operator \( \rho \) in a complete orthonormal basis \( \{|\phi_n\rangle\} \). We shall refer to \( \rho \) either as the density operator or in a specific representation as the density matrix \( \rho \equiv (\rho_{mn}) \). The density-matrix description just-describes the state of a particle, whereas a single wave function over-describes the state on one hand by having a redundant over-all phase factor and under-describes the state on the other hand by leaving out the ensemble nature if the particle is in a mixed state. All measurable informations are given implicitly in the density matrix \( \rho \), no more and no less.

The specific representation we choose for the density matrix \( \rho \) will be in term of helicity eigenstates. The helicity formulation has the merits of being elegant in form for collisions involving spin, being applicable as well to particles of zero mass, such as photon, and having simple
transformation properties under Lorentz transformations, especially for high-energy collisions. For example, particle \( A \) in Fig. 1 is indicated with linear momentum \( p_a \) and helicity \( \lambda_a \), etc.

3. Quantum collision theory

We shall relate physical measurements made on colliding particles to the time-dependent wave function \( \Psi(t) \) which describes the entire colliding system composed of wave packets undergoing a reaction. In this way, our mathematical description of the collision process should correspond accurately to the real physical world with no lapses in physical rigor.

Consider a composite system initially prepared in \( \mu \) isolated parts, the so-called reactants, which later fuse into one as far as the interactions between these \( \mu \) parts are concerned. After a while, the composite system is again separated into \( \nu \) parts, the so-called products, and physical measurements carried out on these isolated parts will reflect the effects of mutual interactions between their constituents. This general collision process, or a reaction, which has been shown schematically in Fig. 1, certainly includes the situation in which an unstable system prepared at a certain instant of time decays at a subsequent time into two or more parts. A measurement of the decay products provides a means for studying the interactions which led to the decay of the initial system.

3.1. Time evolution of one isolated physical system

By definition, an isolated physical system is a physical system having no interaction with the rest of the universe. In practice, the system is confined in space such that it is outside the range of interactions with the rest of the universe. The natural description of a system confined in the position space is a wave packet. To study the time evolution, i.e., the dynamical behavior, of a wave packet we usually expend it in terms of basis states. Because eigenstates of the Hamiltonian \( K \) of the system evolve in time in a very simple manner, we choose the basis states to be energy eigenstates. In collision processes, we shall need wave packets in rectilinear motion. Therefore for convenience, we want the basis states also to be linear momentum eigenstates, and it is easy to show that the total linear momentum operator \( P \) and the total Hamiltonian \( K \) of the system are in fact compatible, i.e.,

\[
[K, P] = 0. \tag{3.1}
\]

To characterize each basis state distinctively, we shall adjoining other mutually commuting observables such that the basis states are simultaneous eigenstates of a complete set \( \{K, P, A\} \) of compatible observables, where \( A \) symbolically denotes all other observables. In the subsequent discussion, each isolated physical system will be referred to simply as a system or a particle.

3.1.1. Basis states. Choose the basis states of each isolated system as

\[
\chi_{q_0} = \chi_{q_0}(r) = \frac{1}{(2\pi)^{3/2}} e^{i\mathbf{q} \cdot \mathbf{r}} u_{q_0}, \tag{3.2}
\]

where \( q \) and \( r \) are respectively the total linear momentum and coordinate for the center-of-momentum (CM) frame of the system, \( a \) symbolically denotes eigenvalues corresponding to all the other observables \( A \) needed to specify the state. To be specific and for later convenience, we shall review the definition of the CM frame in Appendix A. For the ease of notations, we shall set the units such that \( \hbar = 1 \). Here the factor \( (2\pi)^{-3/2} \) is in accordance with the momentum-normalization convention, and \( u_{q_0} \) denotes the wave function describing the internal state of the system. For example, if the system is a molecule, \( u_{q_0} \) is the molecular wave function describing rotational, vibrational, and electronic states. If it is an atom, then \( u_{q_0} \) describes the atomic electronic state. If the system is an electron, \( u_{q_0} \) is the
spinor part of its wave function. Note that the internal state \( u_{q\alpha} \) is in general \( q \)-dependent and normalized as \( u_{q\alpha}^\dagger u_{q\alpha} = \delta_{\alpha\alpha} \). It is obvious that the basis states \( \chi_{q\alpha} \) satisfy the eigen-equations,

\[
K \chi_{q\alpha} = \varepsilon_{q\alpha} \chi_{q\alpha},
\]

\[
P \chi_{q\alpha} = q \chi_{q\alpha},
\]

and are normalized as

\[
\int d^3 r \chi_{q\alpha}^\dagger \chi_{q\alpha} = \delta^3 (q-q') \delta_{\alpha\alpha}.
\]

Here we note that the total energy \( \varepsilon_{q\alpha} \) and the total linear momentum \( q \) are related by the energy-momentum relation,

\[
\varepsilon_{q\alpha}^2 = M^2 c^4 + m^2 c^4 + q^2 c^2,
\]

where \( m \) is the effective mass of the system at rest, and \( M \) is the corresponding relativistic mass. If the system has internal structure, the mass \( m \) may include the internal energy depending on \( u_{q\alpha} \).

### 3.1.2. Particle confined in space and time

To localized a system with total linear momentum \( p \) within a volume \( V_0 \) centred about \( r = d \) in space, we assume its probability amplitude to be a wave packet of the form

\[
X_a = X_{rho}(r) = G(r) \chi_{rho},
\]

where \( G(r) \equiv G_d(r) \) is an envelope function centered about \( r = d \) and is approximately constant within \( V_0 \) and falls smoothly to zero outside, for which the Gaussian distribution function is a good example. Consequently the probability of finding the particle is confined within the volume \( V_0 \) about \( r = d \). We are concerned with wave packets which are large on a microscopic scale, or specifically the linear dimension \( W \) of the wave packet is large compared with the de Broglie-wave length \( \hbar |p| \) of the particle, \( i.e. \),

\[
W \gg \frac{\hbar}{|p|},
\]

where \( G(r) \) is characterized by the width \( W \) of the wave packet. We assume the wave-packet state \( X_a \) is normalized to unity such that

\[
\int d^3 r |G(r)|^2 = (2\pi)^3.
\]

By expanding the wave-packet state \( X_a \) in terms of the basis states \( \chi_{q\alpha} \), we have

\[
X_a = \int d^3 q A(q) \chi_{q\alpha},
\]

where the momentum-distribution function, or the wave function in the momentum space, \( A(q) \) can be evaluated as
\[ A(q) = A_p(q) = \int d^3r \chi^\dagger_{qa} \chi_{qa} = \frac{1}{(2\pi)^3} \int d^3r e^{-i(q-p)r} G(r)u^\dagger_{qa}u_{pa}, \] (3.11)

and is normalized as

\[ \int d^3q |A(q)|^2 = 1. \] (3.12)

If the internal state \( u_{qa} \) has a weak \( q \)-dependence or the spread of \( q \) about \( q = p \) is small such that \( u^\dagger_{qa}u_{pa} \approx u^\dagger_{pa}u_{pa} = 1 \), we would obtain the usual Fourier transform

\[ A(q) \approx \frac{1}{(2\pi)^3} \int d^3r e^{-i(q-p)r} G(r). \] (3.13)

This simple form is however not assumed in the present discussion.

In the momentum space, the wave function \( A(q) \) is a wave packet centered about \( q = p \) and has a linear dimension of \( h/W \) according to the indeterminacy relation, commonly known as the uncertainty relation. The width \( h/W \) of the wave packet \( A(q) \) in the momentum space characterizes its spread in \( q \)-values, \( |\Delta q| = h/W \). We have therefore

\[ |p| >> \frac{h}{W} = |\Delta q|, \] (3.14)

because the wave packet in the position space has been assumed to be large compared with the de Broglie-wave length \( h/|p| \) of the particle. This constraint in turn assures that under normal conditions that permit macroscopic observations, the variation in shape of the wave packet is ordinarily quite negligible.

3.1.3. Time-evolution of the wave packet. If the wave packet at \( t = 0 \) is given as \( \chi_{qa} \) for a system with Hamiltonian \( K \), then the wave packet \( \phi_a(t) \) at any time \( t \) is described by

\[ \phi_a(t) = e^{-iKt} \phi_a(0) = e^{-iKt} \chi_{qa} = \int d^3q A(q) e^{-i\epsilon_{qa}t} \chi_{qa}. \] (3.15)

We expand \( \epsilon_{qa} \) in a Taylor series about \( p \) as

\[ \epsilon_{qa} = \epsilon_{pa} + (q - p) \cdot v + \text{high-order terms}, \] (3.16)

where \( v \) is called the group velocity of the wave packet,

\[ v = \nabla_p \epsilon_{pa}, \] (3.17)

and the effect of high-order terms, which concerns the spreading or contraction of the wave packet with time, has been assumed to be negligible. We have therefore

\[ \phi_a(t) \approx e^{-i\epsilon_{pa}t} \int d^3q A(q) e^{-i(q-p)vt} \chi_{qa} = e^{-i\epsilon_{pa}t} G(r - vt) \chi_{pa}. \] (3.18)

We conclude that if the spreading or contraction of the wave packet is negligible, the envelope \( G(r - vt) \) of the wave packet moves with the group velocity \( v = p/M \), i.e., the region where we have
nonvanishing probabilities of finding the particle moves with the constant velocity \( v \). Consequently we have demonstrated that the wave packet given at \( t = 0 \) as \( X_a \) represents an isolated physical system moving approximately with velocity \( v \).

3.2. Time evolution of \( \mu \) wave packets

We shall now generalize our treatment for one wave packet to that for many wave packets. Assume there are \( \mu \) particles which are initially well-separated such that they effectively do not interact. The effective Hamiltonian for this system of well-separated particles is again denoted by \( K \). We may construct the wave-packet state for this \( \mu \)-particle system following the same procedure as that for the one-particle case. The same equations in the last subsection also apply in the \( \mu \)-particle case, so long as we adopt their \( \mu \)-particle interpretations:

\[
X_{\mu} = X_{\mu,0,1} \cdots X_{\mu,0,\mu},
\]

\[
\equiv \left[ \frac{1}{(2\pi)^{3/2}} e^{i\phi(r) u_{\mu,0}} \right] \cdots \left[ \frac{1}{(2\pi)^{3/2}} e^{i\phi(r) u_{\mu,\mu}} \right],
\]

\[
G(r) \equiv G_1(r_1) \cdots G_\mu(r_\mu),
\]

\[
\int d^3 r \equiv \int d^3 r_1 \cdots d^3 r_\mu,
\]

\[
A(q) \equiv A_1(q_1) \cdots A_\mu(q_\mu),
\]

\[
\int d^3 q \equiv \int d^3 q_1 \cdots d^3 q_\mu,
\]

\[
\delta^3(q' - q) \equiv \delta^3(q_1' - q_1) \cdots \delta^3(q_\mu' - q_\mu),
\]

and

\[
K X_{\mu} = E_{\mu} X_{\mu},
\]

\[
K \equiv K_1 + \cdots + K_\mu,
\]

\[
E_{\mu} \equiv E_{\mu,0} + \cdots + E_{\mu,\mu},
\]

\[
P X_{\mu} = P_{\mu} X_{\mu},
\]

\[
P \equiv P_1 + \cdots + P_\mu,
\]

\[
P \equiv q_1 + \cdots + q_\mu,
\]

such that

\[
\phi_a(t) = e^{-iKt} X_a
\]

\[
\equiv e^{-i(K_1 + \cdots + K_\mu)t} \left[ G_1(r_1) X_{\mu,0} \right] \cdots \left[ G_\mu(r_\mu) X_{\mu,\mu} \right]
\]

\[
\approx G(r - vt) X_{\mu}
\]

\[
\equiv G_1(r_1 - v_1 t) X_{\mu,0} \cdots G_\mu(r_\mu - v_\mu t) X_{\mu,\mu}.
\]
3.3. Collision of reactants
All μ particles would be supposed to come into simultaneous collision at time \( t = 0 \), i.e., the μ wave packets would overlap simultaneously to some extent at \( t = 0 \). The Hamiltonian for the entire reaction system of μ particles will be written as

\[
H = K + V, \tag{3.32}
\]

where the interaction \( V \) has a finite range \( R \) such that \( V \) leads to a null-state vector when operating on states which corresponding to particle separation large compared to \( R \). In other words, within the confined sub-Hilbert space, we have \( H = K \).

During time when wave packets were well-separated, the wave function evolves with time as

\[
\Psi(t) = e^{-iK(t-t_i)}\Psi(t_i), \tag{3.33}
\]

where \( t_i \) denotes any convenient reference time in this duration. To remove the time dependence of \( \Psi(t) \) associated with the \( K \) part of \( H \), we make a time-dependent unitary transformation to the Dirac picture, or commonly known as the interaction picture \( I \),

\[
\Psi_I(t) = e^{iKt}\Psi(t), \tag{3.34}
\]

which is time-independent as long as wave packets were well-separated. For convenience, we shall choose

\[
\Psi_I(t_i) = X_a. \tag{3.35}
\]

Subsequently, after particles come sufficiently close and within the range of mutual interactions, the time-evolution of \( \Psi_I(t) \) is governed by

\[
\Psi_I(t) = U(t,t_i)\Psi_I(t_i), \tag{3.36}
\]

where the time-evolution operator \( U(t,t_i) \) in the interaction picture may be written as

\[
U(t,t_i) = 1 + ie^{iKt}\int_{t_i}^{t} dt' e^{iHt'}V e^{-iKt'}. \tag{3.37}
\]

Because the time-evolution operator is intimately related to the Green operator, we shall summarize the Green operator technique in Appendix B. We can easily prove that for \( t_i \), long before the collision, we have

\[
\Psi_I(t) = U(t,t_i)X_a = U(t,-\infty)X_a. \tag{3.38}
\]

The wave function for the colliding system at time \( t = 0 \), when μ particles come into simultaneous collision, is given by

\[
\Psi_I(0) = U(0,-\infty)X_a = \int d^3q \ A(q) \ U(0,-\infty)\chi_{qa}. \tag{3.39}
\]

We define \( \psi_{qa}^{(+)} \) to be an eigenstate of \( H \) with the outgoing-wave boundary condition,

\[
H\psi_{qa}^{(+)} = E_a\psi_{qa}^{(+)} \tag{3.40}
\]

As shown in Appendix C, we can prove that

\[
\psi_{qa}^{(+)} = U(0,-\infty)\chi_{qa}. \tag{3.41}
\]

Therefore, we obtain
\[
\Psi_I(0) = \int d^3 q \, A(q) \, \psi_q^{(+)}.
\] (3.42)

Because \( \Psi(0) = \Psi_I(0) \) by definition, and \( \Psi(t) = e^{-iHt} \Psi(0) \), the wave function for the \( \mu \)-particle system at any time \( t \) may be expressed as
\[
\Psi(t) = e^{-iHt} \int d^3 q \, A(q) \, \psi_q^{(+)} = \int d^3 q \, A(q) \, e^{-iE_q t} \psi_q^{(+)}.
\] (3.43)

3.4. Emerging of reaction products
Assume the effective Hamiltonian for \( \nu \) reaction products to be \( K' \) when sufficiently separated in the position space, and \( V' \) denotes their mutual interactions with finite range. Consequently, the total Hamiltonian \( H \) for the entire reaction system, \( \mu \) particles, before and, \( \nu \) particles, after the collision can be split up as
\[
H = K + V = K' + V'.
\] (3.44)

Suppose that detectors are designed to detect long after the collision wave-packet states of the reaction products which have wave functions \( X_b' \) of the form
\[
X_b' = \int d^3 q \, B(q) \chi_q^{(b)}.
\] (3.45)
\[
K' \chi_q^{(b)} = E_b \chi_q^{(b)}.
\] (3.46)
\[
P_i \chi_q^{(b)} = P_b \chi_q^{(b)}.
\] (3.47)

The notations for emerging products are similarly described as those for incident reactants, except for a time-reversed scenario.

The detection of reaction products selects the quantum state \( \Psi'(t) \) of the entire reaction system. After the collision, we shall define a different interaction picture \( I' \) by
\[
\Psi_I'(t) = e^{iK't} \Psi'(t),
\] (3.48)
such that we have
\[
\Psi_I'(t) = U'(t,t_f) \Psi_I'(t_f),
\] (3.49)
where the time-evolution operators is given as
\[
U'(t,t_f) = 1 + i e^{iK't_f} e^{-iHt_f} \int_{t_f}^t dt' e^{iHt'} V e^{-iK't'}.
\] (3.50)

3.5. Scattering Matrix
Because we have chosen the interaction pictures \( I \) and \( I' \) respectively for the incident and emerging wave-packet states of the reaction such that
\[
\Psi(0) = \Psi_I(0) = U(0,-\infty) \Psi_I(-\infty) = U(0,-\infty) X_a,
\] (3.51)
\[
\Psi'(0) = \Psi_I'(0) = U'(0,\infty) \Psi_I'(\infty) = U'(0,\infty) X_b'.
\] (3.52)

The state \( \Psi(t) \) prepared initially and the state \( \Psi'(t) \) detected finally are given at any time \( t \) as
\[ \Psi(t) = e^{-i\hbar t} \Psi(0), \]  
\[ \Psi'(t) = e^{-i\hbar t} \Psi'(0). \]  

Therefore the scattering amplitude is given by
\[ \langle \Psi'(t) | \Psi(t) \rangle = \langle \Psi'(0) | \Psi(0) \rangle, \]  
which is constant in time and may in principle be evaluated at any convenient time \( t \), of course, with formally different but equivalent expressions. We present the following three forms of the scattering amplitude \( \langle \Psi'(t) | \Psi(t) \rangle \):

(i) Canonical-form:
\[ \langle \Psi'(t) | \Psi(t) \rangle_{\text{c}} = \langle \Psi'(0) | \Psi(0) \rangle = \langle X'_{h} | U'_{(\infty,0)} U(0,-\infty) | X_{a} \rangle. \]  

(ii) Prior-form:
\[ \langle \Psi'(t) | \Psi(t) \rangle_{\text{p}} = \langle \Psi'(\infty) | \Psi(\infty) \rangle = \langle X'_{h} | U'_{(\infty,0)} e^{i\hbar t} e^{-ik_{t}} | X_{a} \rangle_{t \to -\infty}. \]  

(iii) Post-form:
\[ \langle \Psi'(t) | \Psi(t) \rangle_{\text{p}} = \langle \Psi'(\infty) | \Psi(\infty) \rangle = \langle X'_{h} | e^{iK_{t}} e^{-i\hbar t} U(0,-\infty) | X_{a} \rangle_{t \to \infty}. \]  

Consider the canonical form of the scattering amplitude,
\[ \langle \Psi'(t) | \Psi(t) \rangle_{\text{c}} = \int d^{3}q' d^{3}q B^{*} (q') A(q) \langle X'_{q'} | U'_{(\infty,0)} U(0,-\infty) | X_{q} \rangle, \]  

Here we shall define the scattering operator \( S \) by
\[ S = U'_{(\infty,0)} U(0,-\infty), \]  
and the scattering matrix, or the \( S \)-matrix, \( \langle b | S | a \rangle \) by
\[ \langle b | S | a \rangle = \langle X_{q} | S | X_{q} \rangle, \]  
which will be discussed in some detail in Appendix D.

3.6. Detection of the Reaction
The transition probability \( P_{q'_{a}} \) of the entire reaction system from \( X_{a} \) to \( X'_{q} \) is given by
\[ P_{q'_{a}} = \left| \langle X_{q} | S | X_{a} \rangle \right|^{2}, \]  
which can be shown to be Lorentz invariant. Detection of the transition probability \( P_{q'_{a}} \) involves measurements of total and differential cross sections as well as polarizations of each particles. It can be shown [2] that under normal experimental conditions measured physical quantities are independent of specific envelope functions \( G_{r} (r_{e}) \) used for the wave packets and depend only on the \( S \)-matrices or \( T \)-matrices. The \( T \)-matrix is introduced in Appendix E, and its relation with the \( S \)-matrix is given in Appendix F. Theoretically, we would apply an appropriate dynamical theory for the particular reaction to evaluate the reduced \( T \)-matrices, which is defined in Appendix E. All physically measured quantities may be expressed in terms of the reduced \( T \)-matrices, which are finite. The kinematical structure of reduced \( T \)-matrices can also be separated out such that all measured physical quantities can now be expressed in terms of dynamical parameters, independent of collision geometry, and
angular functions, independent of dynamical theories. In this form, it would facilitate critical comparisons of different dynamical theories and interrelate various types of experiments which study the same dynamical effects.

4. Relativistic helicity states
The angular-momentum helicity state (or spherical-helicity state) \( |k; \lambda, j m\rangle \) with helicity \( \lambda \) can be constructed from the linear-momentum helicity state (or linear-helicity state) \( |k \lambda\rangle \), and vice versa. They are related by the following relations [3-5]:

\[
\int d\hat{k} D_{m\lambda}^{(j)}(\hat{k})^* \langle k; \lambda | k; \lambda, j m \rangle = \left( \frac{2j+1}{4\pi} \right)^{1/2} D_{m\lambda}^{(j)}(\hat{k}) \langle k; \lambda \rangle,
\]

and

\[
\langle k; \lambda \rangle = \sum_{jm} \left( \frac{2j+1}{4\pi} \right)^{1/2} D_{m\lambda}^{(j)}(\hat{k}) | k; \lambda, j m \rangle,
\]

where \( D_{m\lambda}^{(j)}(\hat{k}) \) are rotation matrices [6]. Here the helicity states are normalized such that

\[
\langle k; \lambda | k' \lambda' \rangle = \delta^3(k-k') \delta_{\lambda \lambda'},
\]

\[
\langle k; \lambda, j m | k' \lambda', J' m' \rangle = \frac{1}{k^2} \delta(k-k') \delta_{\lambda \lambda'} \delta_{j j'} \delta_{m m'}.
\]

4.1. Photon helicity states
The linear-helicity state of the photon is given as

\[
A_{kq} = (2\pi)^{-3/2} \hat{e}_q e^{ik \cdot r},
\]

where \( \hat{e}_q \) denotes the spherical unit vector [6]. The spherical-helicity state can be obtained by

\[
A_{kq; jm} = \left( \frac{2j+1}{4\pi} \right)^{1/2} \int d\hat{k} D_{mq}^{(j)}(\hat{k})^* A_{kq},
\]

In terms of the normalized electric, magnetic, and longitudinal multipole potentials we get [7]

\[
A_{k\pm; jm} = \mp(1/\sqrt{2}) (A_{jm}^{(M)} \pm i A_{jm}^{(E)}),
\]

\[
A_{k0; jm} = A_{jm}^{(L)},
\]

where \( A_{\pm; jm} \) correspond respectively to the positive and negative helicity states of the photon, and \( A_{k0; jm} \), however, is not a physical state of the photon.

4.2. Electron helicity states.
Polarization of the electron is described in some detail in Appendix F, according to which we have the linear-helicity state of the electron as
The spherical-helicity state can be obtained as [7]

\[
\langle r|E\mu\rangle = (2\pi)^{-3/2} e^{i k \cdot r} u_{E\mu},
\]

(4.9)

The spherical-helicity state can be obtained as [7]

\[
\langle r|k,\mu, j m \rangle = \left(\frac{2j+1}{4\pi}\right)^{1/2} \int d\hat{k} D_{\mu j}^{(*)\mu}(\hat{k})^* \langle r|k,\mu \rangle = \sum_i i^j \left(\frac{(2j+1)e^2}{kE(2j+1)}\right)^{1/2} \langle 0s\mu j \mu \rangle \langle r|\kappa m \rangle,
\]

(4.10)

where \( \langle r|\kappa m \rangle \) is the usual angular-momentum eigenstate normalized on the energy-scale,

\[
\langle r|\kappa m \rangle \equiv \psi_{\kappa m}(r) = \frac{1}{r} \left(\frac{G_{\kappa m}(r)}{iF_{\kappa m}(r)}\right) \Omega_{\kappa m},
\]

(4.11)

In the Pauli approximation, we have

\[
\langle r|\kappa m \rangle \equiv \langle r|(s) jm \rangle = \sum_{M_s} \langle s v jm \rangle \langle r|M \rangle \chi_v,
\]

(4.12)

where \( \chi_v \) is the spin eigenfunction with \( \nu = \pm 1/2 \).

5. Density matrix description of polarization

In the description of a physical system involved in the collision, a linear superposition of helicity states will suffice when the system is in a pure state. However, when the system is in a mixed state, the density matrix description is necessary.

5.1. Photon

Polarization of the photon is reviewed in some detail in Appendix G. One convenient description of the photon polarization is the density matrix \( \rho \) of the form [7]

\[
\rho \equiv \rho_{sv} = \begin{pmatrix}
\rho_{11} & \rho_{1-1} \\
\rho_{-11} & \rho_{-1-1}
\end{pmatrix} = \frac{1}{2} \begin{pmatrix}
1 + p \cos\theta & pe^{-i\varphi} \sin\theta \\
pe^{i\varphi} \sin\theta & 1 - p \cos\theta
\end{pmatrix}
\]

(5.1)

where we have

- \( I \) : intensity,
- \( p \) : degree of polarization, \( 0 \leq p \leq 1 \),
- \( \theta \) : type of polarization, \( 0 \leq \theta \leq \pi \),
- \( \varphi \) : orientation of polarization, \( 0 \leq \varphi < 2\pi \).

An equivalent description of the photon polarization is provided by Stokes vector \( S = (S_1, S_2, S_3) \).

Mathematically, we may expand the density matrix \( \rho \) in the complete basis set for \( 2 \times 2 \) matrices: the \( 2 \times 2 \) unit matrix together with the Pauli matrices \( \sigma \). The expansion is written as

\[
\rho = \frac{1}{2} I [1 + S \cdot \sigma],
\]

(5.2)

where the intensity \( I \) and Stokes vector \( S \) are thus defined as
\[ I = \text{tr} \{ \rho \}, \quad S = \frac{\text{tr} \{ \rho \overline{\sigma} \}}{\text{tr} \{ \rho \}}. \]  
\hfill (5.3)

For later convenience, we shall define a four-component tensor \( S_\mu \) and a \( 1 \times 4 \) matrix \( S \) formed by its components as

\[ S = (S_\mu) = \begin{pmatrix} S_0 \\ S_1 \\ S_2 \\ S_3 \end{pmatrix} \equiv \begin{pmatrix} 1 \\ S_x \\ S_y \\ S_z \end{pmatrix}. \]  
\hfill (5.4)

5.2. Electron

Polarization of the electron is reviewed in some detail in Appendix H. The spin-density matrix of the electron is given by

\[ \rho_e = (\rho_\rho_e) = \begin{pmatrix} \rho_{11} & \rho_{1-1} \\ \rho_{-11} & \rho_{-1-1} \end{pmatrix}. \]  
\hfill (5.5)

In terms of the intensity \( I_e \) and the polarization vector \( P \), we have [8]

\[ \rho_e = \frac{1}{2} I_e [1 + P \cdot \overline{\sigma}], \]  
\hfill (5.6)

\[ I_e = \text{tr} \{ \rho_e \}, \quad P = \frac{\text{tr} \{ \rho_e \overline{\sigma} \}}{\text{tr} \{ \rho_e \}}. \]  
\hfill (5.7)

Here we also define a four-component tensor \( P_\mu \) and a \( 1 \times 4 \) matrix \( P \) formed by its components as

\[ P = (P_\mu) = \begin{pmatrix} P_0 \\ P_1 \\ P_2 \\ P_3 \end{pmatrix} \equiv \begin{pmatrix} 1 \\ P_x \\ P_y \\ P_z \end{pmatrix}. \]  
\hfill (5.8)

5.3. Atom

The density matrix for the atom polarization may be expressed in the basis of total angular momentum eigenstates \( |JM \rangle \) as

\[ \rho_A = (\rho_{J'M,JM}) = (J'JM' | \rho_A | JM \rangle \langle JM |). \]  
\hfill (5.9)

It takes, in general, \( 4J(J+1) \) independent measurements to specify the polarization of state \( \rho_A \) with \( J' = J \). Define the spherical matrices, which are the generalization of Pauli matrices, as

\[ T_{lm}(J'M', JM) = \sqrt{2l+1} \begin{pmatrix} J' \\ M' \end{pmatrix} \begin{pmatrix} m \\ M \end{pmatrix}. \]  
\hfill (5.10)

Here we have used the Wigner 3-\( j \) coefficient in the covariant notation, called the 3-\( jm \) coefficient [5, 9]. By expanding the density matrix for the atom polarization in terms of spherical matrices, we obtain
\[ \rho_{JM',JM} = \sum_{lm} Q_{lm}(J'J) T_{lm}(J'M',JM), \]  

(5.11)

where the expansion coefficients \( Q_{lm}(J'J) \) are called the state multipoles of the atom [10].

6. Helicity formulation of atomic collisions

The helicity formulation of collision processes [3, 4] has the merits of being elegant in form for collisions involving spin, applicable as well to particles of zero mass, such as photon, and having simple transformation properties under Lorentz transformations. Consequently in the formulation of atomic collision processes, we shall describe physical systems generally by density matrices with relativistic helicity states as the basis.

To be specific, consider the general collision process where we have initially two colliding systems \( A \) and \( B \), each of which may be either an elementary particle or a composite particle, like atom or ion. After the collision, we have finally two departing systems \( C \) and \( D \), each of which may also be either an elementary particle or a composite particle. An elementary collision process, in which all systems involved are in linear helicity states in the laboratory (LAB) frame, is shown in Fig. 2. The \( S \)-matrix of this elementary collision process is expressed as

\[ \langle p_c \lambda_c ; p_d \lambda_d | S | p_a \lambda_a ; p_b \lambda_b \rangle, \]  

(6.1)

where \( p_\alpha \) and \( \lambda_\alpha \) are the momentum and helicity, respectively, of system \( \alpha \). Define the total 4-momenta of the colliding and departing systems as \( P \) and \( P' \), respectively,

\[ P = p_a + p_b, \]  

(6.2)

\[ P' = p_c + p_d, \]  

(6.3)

where \( p_\alpha \) denotes the 4-momentum of system \( \alpha \), and \( \alpha = a, b, c, d \). The same collision process in the CM frame is also shown in Fig. 2, where \( (\theta_0, \varphi_0) \) and \( (\theta, \varphi) \) are respectively scattering angles before and after the collision in the CM frame.

\[ \sum_{lm} Q_{lm}(J'J) T_{lm}(J'M',JM), \]  

Figure 2. Schematic diagram for the reaction: \( A + B \rightarrow C + D \). Here \( p_\alpha \) and \( \lambda_\alpha \) are respectively the momentum and helicity of system \( \alpha \) in the LAB frame, and \( (\theta_0, \varphi_0) \) and \( (\theta, \varphi) \) are respectively scattering angles before and after the collision in the CM frame.

The same collision process in the CM frame is also shown in Fig. 2, where \( (\theta_0, \varphi_0) \) and \( (\theta, \varphi) \) are scattering angles before and after the collision, respectively. The \( S \)-matrix \( \langle \theta_0 \varphi_0 \lambda_a \lambda_d | S(P') | \theta_0 \varphi_0 \lambda_a \lambda_b \rangle \) in the CM frame is related to the \( S \)-matrix in the LAB frame as

\[ \langle p_c \lambda_c ; p_d \lambda_d | S | p_a \lambda_a ; p_b \lambda_b \rangle = (2\pi)^6 \left( \frac{1}{pp'} \right) \sqrt{\sqrt{\Delta^4}} (P' - P) \langle \theta_0 \varphi_0 \lambda_a \lambda_d | S(P) | \theta_0 \varphi_0 \lambda_a \lambda_b \rangle. \]  

(6.4)
Here $p$ and $v$ are the magnitudes of the relative momentum and velocity, respectively, for the colliding systems, and $p'$ and $v'$ for the departing systems, defined in the CM frame. All the information about the collision dynamics is contained in the $S$-matrix in the CM frame, or equivalently in the reduced $T$-matrix which is related to the $S$-matrix as

$$S_{fi} = \delta_{fi} - 2\pi i \delta(P'_0 - P_0)T_{fi}, \quad \text{(6.5)}$$

where $P'_0$ and $P'_0$ denote the zeroth components of the 4-momenta $P'$ and $P$, respectively.

### 7. The collision equation

Denote symbolically the density matrices of the initial and final states of the colliding systems as $\rho_i$ and $\rho_f$, respectively. We have therefore the collision equation [7],

$$\rho_f = S_{fi}\rho_i S_{fi}^\dagger, \quad \text{(7.1)}$$

where $S_{fi}$ represents the appropriate $S$-matrix.

As a simple illustration, we consider photoemission from an excited atom. The elementary collision amplitude is given by [11]

$$S(q, J_f M_f; J, M) = \sqrt{\frac{\omega}{2\pi c}}J_f J M_f \sum_{\alpha} \langle \hat{\epsilon}_q^\dagger e^{i\mathbf{k}\cdot\mathbf{r}} | J, M, M' \rangle, \quad \text{(7.2)}$$

where $J_f M_f$ are the angular momentum quantum numbers of the de-excited atom, $N$ is the number of electrons in the atom, $\hat{\alpha}$ are the Dirac matrices, $\hat{\epsilon}_q$ and $\mathbf{k}$ are respectively the polarization vector and wavenumber vector of the emitted photon.

If the excited atom is initially described by the density matrix $\rho_{f|M_f;J,M}$, then the density matrix of the final state of the colliding systems, i.e., the departing systems, is given by

$$\rho_{f'|q',M'_f;J',M'} = \sum_{J_f|M_f;J,M} S(q, J_f M_f; J, M) \rho_{f|M_f;J,M} S^\dagger(q, J_f M_f; J, M). \quad \text{(7.3)}$$

Kinematical and dynamical effects are entangled together in the $S$-matrix especially when the collision processes involve composite particles, such as atoms or ions. The complexities in angular momentum couplings will be dealt with by a graphical approach [9].

The angular distribution and polarization of the photon, which leaves the atom in a definite angular momentum $J_f$ state, would be described by

$$P_{\phi q} = \sum_{M_f} \rho_{\phi q, J_f M_f; J_f M_f}. \quad \text{(7.4)}$$

Other atomic collision processes may be treated in a similar manner, and we will give only a few examples in the subsequent sections.

### 8. Photoionization

Consider the photoionization process in which initially a polarized photon with linear momentum $q$ is incident on an unpolarized target atom with total angular momentum $J_{\alpha}$. After the collision, an electron with linear momentum $k$ is emitted, and the residual ion is left with total angular momentum $J_f$. The process is described by the $S$-matrix.

$$S_{fi} = \delta_{fi} - 2\pi i \delta(P'_0 - P_0)T_{fi}, \quad \text{(6.5)}$$

where $P'_0$ and $P'_0$ denote the zeroth components of the 4-momenta $P'$ and $P$, respectively.
$J_\beta$. Two coordinate frames $XYZ$ and $xyz$, shown in Fig. 3, are employed respectively for the initial and final states with unit vectors defined as

\[ \hat{X} = (\hat{q} \times \hat{k}) \times \hat{q}, \quad \hat{Y} = \hat{q} \times \hat{k}, \quad \hat{Z} = \hat{q}, \]  
\[ \hat{x} = (\hat{q} \times \hat{k}) \times \hat{k}, \quad \hat{y} = \hat{q} \times \hat{k}, \quad \hat{z} = \hat{k}. \]  

(8.1)

(8.2)

where $\hat{q} \equiv q / |q|$ and $\hat{k} \equiv k / |k|$. When the polarization of the residual ion is not observed, the density matrix $\rho^{(e)}$ of the emerging electron is related to the density matrix $\rho^{(r)}$ of the incident photon by the collision equation as

\[ \rho^{(e)} = \frac{1}{2} \text{tr}_\beta \{ T (\rho^{(r)} \otimes 1^v) T^\dagger \}, \]  

(8.3)

where

\[ T \equiv T_{t_i} = V_i + V_f \frac{1}{E - H + i \eta} V_i, \]  

(8.4)

is the transition operator with $i$ and $f$ denoting, respectively, the entrance and exit channels of photoionization, $1^v \equiv 1_{(2J_z+1)}(2J_z+1)$ is the identity matrix in the subspace of the target atom, $\text{tr}_\beta \{ \}$ denotes the trace of the quantity within the curly brackets taken in the subspace of the residual ion.

In terms of the polarization vector of the emitted electron and the Stokes parameters of the incident photon, we may rewrite the collision equation as

\[ IP_{\mu} = \sum_{\nu=0}^3 \Lambda'_{\mu \nu} S_\nu, \]  

(8.5)

where we have defined the $4 \times 4$ correlation matrix $\Lambda' = (\Lambda'_{\mu \nu})$ of photoionization by

\[ \Lambda'_{\mu \nu} = \frac{1}{2} \text{tr} \{ (\sigma_\mu \otimes 1^\beta) T (\sigma_\nu \otimes 1^v) T^\dagger \}. \]  

(8.6)

Here the trace is now taken in both the spin space of the emitted electron and the subspace of the residual ion. Explicit formulas have been given previously [7].
9. Electron-capture fluorescence

Electron-capture fluorescence is the time-reversed process of photoionization. Consider initially an electron with linear momentum $k$ is incident upon an unpolarized ion with total angular momentum $J_\beta$ and is captured by the ion. After the collision, a photon with linear momentum $q$ is emitted while the atom system is left with total angular momentum $J_\alpha$. Two coordinate frames $x'y'z'$ and $X'Y'Z'$, shown in Fig. 4, are employed for the initial and final states, respectively, with unit vectors defined as

\begin{align}
\hat{x}' &= (\hat{k} \times \hat{q}) \times \hat{k}, \quad \hat{y}' = \hat{k} \times \hat{q}, \quad \hat{z}' = \hat{k}, \\
\hat{X}' &= (\hat{k} \times \hat{q}) \times \hat{q}, \quad \hat{Y}' = \hat{k} \times \hat{q}, \quad \hat{Z}' = \hat{q}.
\end{align}

Here a similar convention is adopted as the unprimed coordinate systems for photoionization. When the polarization of the final atomic state is not observed, we can derive the collision equation as

\begin{equation}
\rho^{(\nu)} = \frac{1}{2} tr_{\alpha} \{ T'(\rho^{(\nu)} \otimes 1^\alpha) T^{-1}' \},
\end{equation}

where $T'$ denotes the transition operator of the electron-capture fluorescence process, similarly defined as in the photoionization case. Again, this collision equation may be rewritten as

\begin{equation}
I S''_\mu = \sum_{\nu=0}^{3} \Lambda^F_{\mu\nu} P'_\nu,
\end{equation}

where we have defined the 4x4 correlation matrix $\Lambda^F = (\Lambda^F_{\mu\nu})$ of electron-capture fluorescence by

\begin{equation}
\Lambda^F_{\mu\nu} = \frac{1}{2} tr\{ (\sigma_\mu \otimes 1^\nu) T (\sigma_\nu \otimes 1^\beta) T^{-1} \}.
\end{equation}

Similar processes have been studied previously [12-14].

10. Rotation, space inversion, and time-reversal symmetries

By symmetry consideration, we may reduce the correlation matrix to a simpler form. We shall assume all interactions involved in the collision processes are invariant under rotation, space-inversion, and time-reversal transformations.
The time-reversal symmetry between photoabsorption and photoemission processes, as shown in Fig. 5, is one of the simple cases studied previously. A more interesting case is provided by the symmetry between photoionization ($I$) and electron-capture fluorescence ($F$). We can show that the rotation plus space-inversion invariance implies

$$
\Lambda^I = M^{(e)} \Lambda^I M^{(r)},
$$

(10.1)

$$
\Lambda^F = M^{(r)} \Lambda^F M^{(e)},
$$

(10.2)

where the transformation matrices $M^{(e)}$ and $M^{(r)}$ are

$$
M^{(e)} = \begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & -1 & 0 & 0 \\
0 & 0 & 1 & 0 \\
0 & 0 & 0 & -1
\end{pmatrix},
$$

(10.3)

$$
M^{(r)} = \begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & -1 & 0 \\
0 & 0 & 0 & -1
\end{pmatrix}.
$$

(10.4)

Consequently, the correlation matrices have the following simpler forms

$$
\Lambda^I = \begin{pmatrix}
\Lambda^I_{00} & \Lambda^I_{01} & 0 & 0 \\
0 & 0 & \Lambda^I_{12} & \Lambda^I_{13} \\
\Lambda^I_{20} & \Lambda^I_{21} & 0 & 0 \\
0 & 0 & \Lambda^I_{32} & \Lambda^I_{33}
\end{pmatrix},
$$

(10.5)
The rotation plus time-reversal invariance implies the symmetry between photoionization and 
electron-capture fluorescence,
\[ \Lambda^I = \Lambda^{(e)} \Lambda^F N^{(r)}, \]  
(10.7) 
or, equivalently
\[ \Lambda^F = N^{(r)} \Lambda^I N^{(e)}, \]  
(10.8) 
where the tilt above a matrix denotes the transpose of that matrix, and the transformation matrices 
\( N^{(e)} \) and \( N^{(r)} \) are
\[ \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \]  
(10.9) 
\[ \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \]  
(10.10) 

We have explicitly the relation between the correlation matrices \( \Lambda^I \) and \( \Lambda^F \),
\[ \begin{pmatrix} \Lambda^{F}_{00} & \Lambda^{F}_{10} & 0 & 0 \\ 0 & 0 & \Lambda^{F}_{21} & \Lambda^{F}_{31} \\ \Lambda^{F}_{02} & \Lambda^{F}_{12} & 0 & 0 \\ 0 & 0 & -\Lambda^{F}_{23} & \Lambda^{F}_{33} \end{pmatrix}, \]  
(10.11) 
\[ \begin{pmatrix} \Lambda^{I}_{00} & 0 & \Lambda^{I}_{10} & 0 \\ \Lambda^{I}_{01} & 0 & \Lambda^{I}_{11} & 0 \\ 0 & \Lambda^{I}_{12} & 0 & -\Lambda^{I}_{22} \\ 0 & -\Lambda^{I}_{13} & 0 & \Lambda^{I}_{23} \end{pmatrix}. \]  
(10.12) 

Additionally, scaling symmetry [15] and half-space symmetry [16] may also be considered for 
collision processes.

11. Conclusions
A unified quantum collision theory in the wave-packet approach for an elementary reaction has been 
reviewed to justify the formal treatment commonly in practice for various collision processes. We 
have considered four atomic collision processes to illustrate applications of the symmetry principle 
and the relativistic helicity formulation of atomic collisions. A detailed kinematic analysis has been
presented previously for each process. Polarization and angular correlations are given in concise parametrized forms in terms of known functions of angles. Angle-independent dynamic parameters in the formulas are expressible as sums of reduced matrix elements which reflect the interactions and target structure. Photoionization of polarized targets [17], coherent fluorescence radiation [18] and Auger transition [19] following photoexcitation and photoionization as well as other collision processes can also be treated similarly. These analyses bring to light the coherence and overall symmetry of the processes and facilitate comparison between theory and experiment.

The unraveling of all polarization and angular correlations in atomic collision processes would provide critical tests of many-body dynamic theories. The symmetry principle facilitates a comparison study of different collision processes. Because of difficulties in obtaining polarized electron beams and in detecting the polarization of outgoing electrons, only a limited number of experiments concern the polarization. Both theoretical and experimental efforts in this respect are needed toward a better understanding of the collision dynamics.

Appendix A: The center of momentum frame
The center of momentum (CM) frame of a \( \mu \)-particle system is defined to be the inertial frame in which the total linear momentum \( \mathbf{P}^{CM} \) of the system is zero. Take any particular inertial frame to be the laboratory (LAB) frame, then total energies and linear momenta in the LAB and CM frames are

\[
E^{LAB} = \sum_{i=1}^{\mu} E_i^{LAB}, \quad \mathbf{p}^{LAB} = \sum_{i=1}^{\mu} \mathbf{p}_i^{LAB},
\]

\[
E^{CM} = \sum_{i=1}^{\mu} E_i^{CM}, \quad \mathbf{p}^{CM} = \sum_{i=1}^{\mu} \mathbf{p}_i^{CM} = 0.
\]

The velocity \( \mathbf{v} \) of the CM frame in the LAB frame is given by

\[
\mathbf{v} = c^2 \frac{\mathbf{p}^{LAB}}{E^{LAB}}.
\]

Energy \( E \) and momentum \( \mathbf{p} \) in the LAB and CM frames are related as

\[
E^{CM} = \gamma (E^{LAB} - \mathbf{v} \cdot \mathbf{p}^{LAB}),
\]

\[
\mathbf{p}^{CM}_l = \gamma (\mathbf{p}_l^{LAB} - \frac{1}{c^2} \mathbf{v} E^{LAB}),
\]

\[
\mathbf{p}^{CM}_t = \mathbf{p}_t^{LAB},
\]

where \( \gamma = 1/\sqrt{1-v^2/c^2} \), and the subscripts \( l \) and \( t \) denote respectively the longitudinal (parallel) and transverse (perpendicular) components of a 3-vector with respect to the velocity \( \mathbf{v} \) of the CM frame.

Appendix B: Green operator technique
B.1. Green operator
To solve an inhomogeneous equation of the form

\[
(E - K)\psi = f,
\]

where \( E \) is real, and \( K \) is self-adjoint, we may first define the Green operator \( G_K \) for operator \( (E - K) \) by the operator equation

\[
(E - K)G_K = G_K (E - K) = I - P_K.
\]
Here $I$ denotes the identity operator, and $P_x$ is the projection operator onto the subspace of all $\chi$ which satisfy the homogeneous equation,

$$(E - K)\chi = 0 . \quad (B.3)$$

We can see that $G_k$ is almost the inverse operator to $(E - K)$ except in the subspace $P_x$.

We can easily prove that $G_k$ may be given in two linearly-independent forms as

$$G_k^{(\pm)} = \frac{1}{E - K \pm i\eta} \equiv \lim_{\eta \to 0} \frac{1}{E - K \pm i\eta} , \quad (B.4)$$

where $\eta$ is a positive real number, and the limit as $\eta \to 0$ is to be taken after the operation of the operator having been carried out. By using $G_k^{(\pm)}$, we obtain the general solution for $\psi$ as

$$\psi^{\pm} = \chi + G_k^{(\pm)} f , \quad (B.5)$$

where the superscripts $(\pm)$ and $(\mp)$ indicate the solutions $\psi^{(+)}$ and $\psi^{(-)}$ satisfy respectively the outgoing-wave and incoming-wave boundary conditions, when interpreted as wave functions with a time-evolution factor.

B.2. Solution of a homogeneous equation

The Green operator technique may be applied to solve a homogeneous equation of the form

$$(E - H)\psi = 0 . \quad (B.6)$$

We first rewrite the equation in the form of an inhomogeneous equation as

$$(E - K)\psi = f \equiv V\psi , \quad (B.7)$$

where $V = H - K$. The equation is thus transformed into

$$\psi^{(+)} = \chi + G_k^{(+)} V\psi . \quad (B.8)$$

We can prove that the Green operator $G_{H}^{(+)}$ for operator $(E - H)$ is related to $G_k^{(+)}$ by

$$(1 + G_{H}^{(+)} V)(1 - G_k^{(+)} V) = (1 - G_k^{(+)} V)(1 + G_{H}^{(+)} V) = 1 . \quad (B.9)$$

With the above relation, we can again transform the equation into

$$\chi = \psi^{(+)} - G_{H}^{(+)} V\chi , \quad (B.10)$$

which can also be obtained by exchange the roles played by $H$ and $K$. Therefore we can write $\psi^{(+)}$ in terms of $\chi$ as

$$\psi^{(+)} = (1 + G_{H}^{(+)} V)\chi . \quad (B.11)$$

Appendix C: Adiabatic evolution of states

The proof of $U((0,\infty))_\chi \psi^{(+)} = \psi^{(+)}$ should be treated in the context of approaching wave-packets which is an adiabatic process similar in essence to that considered in the Gell-Mann-Low Theorem [20].

We shall start with the state $\Psi(t)$ prepared initially at $t = t_i$ as $X_{\alpha}$. At time $t = 0$, we have
\[ \psi(0) = U(0,t_i)X_a = U(0,-\infty)X_a \]
\[ = X_a - i \int_{-\infty}^{0} dt e^{iBt} e^{-iKt} X_a. \]  
(C.1)

Consider the second term,
\[ -i \int_{-\infty}^{0} dt e^{iBt} e^{-iKt} X_a \]
\[ = -i \int d^3q A(q) \int_{-\infty}^{0} dt e^{iBt} e^{-iKt} \chi_{qa} \]
\[ = -i \int d^3q A(q) \int_{-\infty}^{0} dt e^{i(H-E_a)t} V \chi_{qa}, \]  
(C.2)

where the integration on \( t \) will give rise to undetermined quantities. To make the \( t \)-integration well-behaved and leading to solution with required asymptotic behavior upon integration across \( H = E_a \) over the momentum \( q \), we shall specify the integration path by adding a factor \( e^{+\eta} \) with positive real \( \eta \) to the mutual interaction \( V \). Because we will require \( \eta \to 0 \) at the end of derivation, no physics has been modified. Therefore, the \( \eta \)-procedure is simply a mathematical remedy when the conventional form used for \( U(0,\pm \infty) \) gives rise to undetermined mathematical manipulation. With this added factor \( e^{+\eta} \), we may carry out the \( t \)-integration as
\[ -i \int_{-\infty}^{0} dt e^{i(H-E_a)} e^{+\eta} \]
\[ = -i \int_{-\infty}^{0} dt e^{i(E_a-H+i\eta)t} \]
\[ = \frac{1}{E_a - H + i\eta}. \]  
(C.3)

Upon substituting this result, we obtain
\[ U(0,-\infty)X_a = \int d^3q A(q) \left[ 1 + \frac{1}{E_a - H + i\eta} V \right] \chi_{qa}. \]  
(C.4)

In Appendix B, we have proved that
\[ \psi_{qa}^{(+)} = \left[ 1 + \frac{1}{E_a - H + i\eta} V \right] \chi_{qa}. \]  
(C.5)

The case for \( U(0,\infty)X_a \) may similarly treated. In summary, we obtain
\[ U(0,\infty)X_a = \int d^3q A(q) U(0,\infty) \chi_{qa} \]
\[ = \int d^3q A(q) \left[ 1 + \frac{1}{E_a - H + i\eta} V \right] \chi_{qa} \]
\[ = \int d^3q A(q) \psi_{qa}^{(+)}. \]  
(C.6)

Therefore, under the \( \int d^3q A(q) \) integration, we have proved
\[ U(0,\infty) \chi_{qa} = \psi_{qa}^{(+)}. \]  
(C.7)
Appendix D: Scattering matrix

The scattering matrix, or the $S$-matrix, is commonly defined as

$$\langle b'|S|a \rangle = \langle \chi'_b|S|\chi'_a \rangle,$$

(D.1)

where the time-evolution operators $U(0, -\infty)$ and $U'(\infty, 0)$ have the following forms:

$$U(0, t_c) = e^{iHt} e^{-iKt},$$

(D.3)

$$U'(t_f, 0) = e^{iKt} e^{-i\beta},$$

(D.4)

The time scale has been shown in Fig. 1. Obviously, the order in which we take the limits $t_c \to -\infty$ and $t_f \to \infty$ in the $S$-matrix is immaterial. The $S$-matrix can be presented in three alternative forms:

(i) Canonical-form:

Because $\psi_{aq}^{(+)} = U(0, -\infty)\chi_{aq}$ and $\psi_{aq}^{(-)} = U'(0, \infty)\chi_{aq}$, we have

$$\langle b'|S|a \rangle_{t=0} = \langle \psi_{aq}^{(-)}| \psi_{aq}^{(+)} \rangle.$$

(D.5)

(ii) Prior-form:

By making use of $U(0, t) = e^{iHt} e^{-iKt}$, we obtain

$$\langle b'|S|a \rangle_{t=\infty} = \langle \psi_{aq}^{(+)}| e^{i(E_a - E_b)t} |\chi_{aq} \rangle_{t=\infty}.$$

(D.6)

(iii) Post-form:

By making use of $U'(t, 0) = e^{iKt} e^{-i\beta}$, we obtain

$$\langle b'|S|a \rangle_{t=\infty} = \langle \chi_{aq}'| e^{i(E_a - E_b)t} |\psi_{aq}^{(+)} \rangle_{t=\infty}.$$

(D.7)

Appendix E: Transition matrix

By using the operator identity

$$\frac{1}{A} = \frac{1}{B} \left[ 1 + (B - A) \frac{1}{A} \right],$$

(E.1)

we get

$$\frac{1}{E - H \pm i\eta} = \frac{1}{E - K' \pm i\eta} \left[ 1 + V' \frac{1}{E - H \pm i\eta} \right].$$

(E.2)

We have therefore
\[
\psi_{qa}^{(\pm)} = \left[ 1 + \frac{1}{E_a - H + i\eta} \right] \chi_{qa} = \left[ 1 + \frac{1}{E_a - K' + i\eta} \right] \chi_{qa},
\]
where we have defined the transition operator, or the \(T\)-operator, as

\[
T^{(\pm)} = T^{(\pm)}(E_a) = \left[ 1 + \frac{1}{E_a - H + i\eta} \right] V.
\]

Using the above result, we may expand \(\psi_{qa}^{(+)}\) in terms of \(\chi_{qb}'\) as

\[
\psi_{qa}^{(+)} = \chi_{qa} + \sum_{q,b} \chi_{qb}' \frac{1}{E_a - E_b + i\eta} \left< b' | T^{(+)} | a \right>,
\]

where the summation symbol \(\sum\) denotes implicitly both a summation over the discrete spectrum and an integration over the continuum spectrum, and the matrix element

\[
\left< b' | T^{(+)} | a \right> = \left< \chi_{qb}' | T_{vb}^{(+)}(E_a) | \chi_{qa} \right>,
\]

is called the \(T\)-matrix. Because the total momentum operator \(P\) commutes with the \(T\)-operator \(T^{(+)}\), we may assume the factorization,

\[
\left< b' | T^{(+)} | a \right> \equiv \delta^3(P_b - P_a)T_{ba}^{(+)},
\]

where we have removed the infinite quantity \(\delta^3(P_b - P_a)\) from \(\left< b' | T^{(+)} | a \right>\), which assures the momentum conservation of the reaction. Here \(T_{ba}^{(+)}\) is finite and is called the \(reduced T\)-matrix which is the quantity to be evaluated in dynamic theories.

Similarly, we have

\[
T^{(-)} = T^{(-)}(E_b) = \left[ 1 + \frac{1}{E_b - H - i\eta} \right] V',
\]

\[
\psi_{qb}^{(-)} = \chi_{qb} + \sum_{q,a} \chi_{qa} \frac{1}{E_b - E_a - i\eta} \left< a | T^{(-)} | b' \right>,
\]

\[
\left< b' | T^{(-)*} | a \right> = \left< \chi_{qb} | T_{vb}^{(-)*}(E_b) | \chi_{qa} \right> \equiv \delta^3(P_b - P_a)T_{ba}^{(-)},
\]

\[
T^{(-)*} = V' + \frac{1}{E_b - H + i\eta} V = V' - V + \frac{1}{E_a - H + i\eta} V,
\]

\[\text{for } E_a = E_b.\]

Appendix F: Relation between S-matrix and T-matrix
Consider the post-form of the \(S\)-matrix in Appendix D,
\[
\langle b'|S|a\rangle \big|_{\pm \infty} = \langle X^a_+ \rangle |\psi_{q_a}^{(+)}\rangle \big|_{i \rightarrow \pm \infty} .
\]  

(F.1)

By using the \(T\)-matrix expansion of \(\psi_{q_a}^{(+)}\) in Appendix D, we obtain

\[
\langle b'|S|a\rangle \big|_{\pm \infty} = \delta^3(q'-q)\delta_{ba} - \left[ \frac{e^{i(E_a - E_b)t}}{E_b - E_a - i\eta} \right]_{i \rightarrow \pm \infty} \langle b'|T^{(+)}|a\rangle .
\]  

(F.2)

where \(\delta_{ba}\) indicates that \(X_b' = X_a\) under the wave-packet interpretation. It can be shown that

\[
\lim_{t \rightarrow \pm \infty} \lim_{\eta \rightarrow 0} \left[ \frac{e^{ixt}}{x^2 + i\eta} \right] = \mp 2\pi i \delta(x) .
\]  

(F.3)

Therefore, we have

\[
\langle b'|S|a\rangle \big|_{\pm \infty} = \delta^3(q'-q)\delta_{ba} - 2\pi i \delta(E_b - E_a) \langle b'|T^{(+)}|a\rangle .
\]  

(F.4)

Similarly, by considering the prior-form of the \(S\)-matrix, we obtain

\[
\langle b'|S|a\rangle \big|_{\pm \infty} = \delta^3(q'-q)\delta_{ba} - 2\pi i \delta(E_b - E_a) \langle b'|T^{(-)}|a\rangle .
\]  

(F.5)

Consequently, by factoring \(\delta^3(P_b - P_a)\) out of \(\langle b'|T^{(+)}|a\rangle\) and \(\langle b'|T^{(-)}|a\rangle\), we have

\[
\langle b'|S|a\rangle \big|_{\pm \infty} = \delta^3(q'-q)\delta_{ba} - 2\pi i \delta(E_b - E_a) \delta^3(P_b - P_a) T^{(z)}_{ba} .
\]  

(F.6)

where we note particularly that because of the internal degrees of freedom of each particle the conservation of total energy \(\delta(E_b - E_a)\) and the conservation of total momentum \(\delta^3(P_b - P_a)\) are generally independent. Furthermore, we can prove that \(T^{(+)}_{ba} = T^{(-)}_{ba}\), and we may as well drop the superscripts \((+\) and \((-)\). Strictly speaking, however, this can only be justified in the context of approaching wave packets, \(i.e.,\) under the wave-packet integration \(\int d^3q\int d^3\eta\).

**Appendix G: Polarization of the photon**

G.1. Polarization vector of the photon

We define the polarization vector of the photon vector potential to be of the form

\[
\hat{e} = \hat{e}_{+1}e^{-i\phi/2} \cos(\theta/2) + \hat{e}_{-1}e^{i\phi/2} \sin(\theta/2) ,
\]  

(G.1)

where \(\hat{e}_{+1}\) and \(\hat{e}_{-1}\) are the spherical unit vectors [6] in a particular coordinate system XYZ and correspond to the positive and negative helicity states, respectively. In terms of parameters \((\theta,\phi)\), we obtain the spin-density matrix for a completely polarized photon as

\[
\rho_{pol} = \frac{1}{2} \begin{pmatrix} 1 + \cos \theta & e^{i\phi} \sin \theta \\ e^{-i\phi} \sin \theta & 1 - \cos \theta \end{pmatrix} .
\]  

(G.2)

The spin-density matrix for a completely unpolarized photon is given by

\[
\rho_{ unpol} = \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} .
\]  

(G.3)
The general spin state of the photon can be regarded as a mixture of completely polarized and completely unpolarized states. Assume the probability of complete polarization to be \( p \) \((0 \leq p \leq 1)\), referred to as the degree of polarization of the photon. With parameters \((p, \theta, \varphi)\), we may write the spin-density matrix for a generally polarized photon as

\[
\rho = p \rho_{pol} + (1 - p) \rho_{unpol}
\]

\[
= \frac{1}{2} \left[ \begin{array}{cc}
1 + p \cos \theta & pe^{-i\varphi} \sin \theta \\
pe^{i\varphi} \sin \theta & 1 - p \cos \theta 
\end{array} \right].
\]

(G.4)

For ease of notations, here the intensity \( I = tr\{\rho\} \) of the photon is normalized to 1. The parameters \((\theta, \varphi)\) are defined with the ranges: \(0 \leq \theta \leq \pi\) and \(0 \leq \varphi < 2\pi\). By inspecting the form of the polarization vector \( \hat{\epsilon} \), we find the parameter \( \theta \) indicates the type of polarization:

- \( \theta = 0 \), right circular polarization.
- \( 0 < \theta < \pi / 2 \), right elliptical polarization,
- \( \theta = \pi / 2 \), linear polarization,
- \( \pi / 2 < \theta < \pi \), left elliptical polarization,
- \( \theta = \pi \), left circular polarization.

Note that the right and left polarizations refer to positive and negative helicities, respectively, whereas in optics the converse definition is usually adopted. The parameter \( \varphi \) indicates the orientation of polarization. Specifically, the precession of the electric field at a given space point for an elliptically polarized photon traces out an ellipse with its major principle axis making an angle \( \varphi / 2 \) with the \( X \) axis.

G.2. Stokes vector

An equivalent description of a generally polarized photon is provided by Stokes parameters \((I, S_1, S_2, S_3)\), which are just the expansion coefficients of the spin-density matrix \( \rho \) in terms of the complete basis set of \( 2 \times 2 \) matrices, i.e., the \( 2 \times 2 \) unit matrix together with Pauli spin matrices \( \hat{\sigma} \):

\[
\rho = \frac{1}{2} I [1 + S \cdot \hat{\sigma}],
\]

(G.5)

\[
I = tr\{\rho\},
\]

(G.6)

\[
S = tr\{\rho \hat{\sigma} \} / tr\{\rho\}.
\]

(G.7)

By using the spin-density matrix \( \rho \) defined in terms of \((p, \theta, \varphi)\), we obtain the Stokes vector \( S = (S_1, S_2, S_3) \):

\[
S_1 = p \sin \theta \cos \varphi,
\]

(G.8)

\[
S_2 = p \sin \theta \sin \varphi,
\]

(G.9)

\[
S_3 = p \cos \theta.
\]

(G.10)

It is of interest to note that the polarization vector \( \hat{\epsilon} \) of the photon is so defined here such that the parameters \((p, \theta, \varphi)\) are just the radial length, the polar angle, and the azimuthal angle of the Stokes vector \( S \). We also note that the parametrization of the polarization vector \( \hat{\epsilon} \) here is an improved version of the one we adopted earlier [7].
Appendix H: Polarization of the electron

H.1. Spin operator of the electron

The spin operator of the electron may be defined in terms of the Dirac matrix as

\[ S = \frac{1}{2} \sum \right] \] (H.1)

In the representation in which \( \beta \) is diagonal, we have

\[ \beta = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}, \quad \tilde{\alpha} = \begin{pmatrix} 0 & \tilde{\sigma} \\ \tilde{\sigma} & 0 \end{pmatrix}, \quad \tilde{\Sigma} = \begin{pmatrix} \tilde{\sigma} & 0 \\ 0 & -\tilde{\sigma} \end{pmatrix} \] (H.2)

where \( I \) is the identity operator, and \( \tilde{\sigma} \) are the Pauli spin matrices.

H.2. Linear-helicity states of the electron

For an electron with definite energy and momentum \( \{E, \mathbf{p}\} \), we have two linearly independent states, called linear-helicity states, given by

\[ \langle r | \mathbf{E} p \mu \rangle = (2\pi)^{-3/2} e^{i \mathbf{p} \cdot \mathbf{r}} u_{\mathbf{E} p \mu}, \] (H.3)

\[ E = \sqrt{\mathbf{p}^2 c^2 + m^2 c^4} = Mc^2, \] (H.4)

where \( m \) and \( M \) are respectively the rest mass and relativistic mass of the electron, and we shall set the units such that \( \hbar = 1 \). Here \( \mu = \pm 1 \) is the helicity of the electron, and the Dirac spinor \( u_{\mathbf{E} p \mu} \) is given explicitly as

\[ u_{\mathbf{E} p \mu} = \begin{pmatrix} \sqrt{\frac{M + m}{2M}} \chi_{\mu/2} \\ \mu \sqrt{\frac{M - m}{2M}} \end{pmatrix}, \quad \text{for } \mu = \pm 1, \] (H.5)

where \( \chi_{\mu/2} \) is the spin eigenfunction with the quantization axis chosen in the \( \mathbf{p} \)-direction. The linear-helicity states are normalized as

\[ \langle E \mathbf{p} \mu' | E \mathbf{p} \mu \rangle = \delta^{\mu \mu'}, \] (H.6)

\[ u^\dagger_{\mathbf{E} p \mu} u_{\mathbf{E} p \mu'} = \delta_{\mu \mu'}, \] (H.7)

\[ \chi^\dagger_{\mu/2} \chi_{\mu/2} = \delta_{\mu \mu'}. \] (H.8)

A general mixed state of the electron with definite \( \{E, \mathbf{p}\} \) is given by the spin-density operator

\[ \rho = \sum_{\mu \nu} \rho_{\mu \nu} |E \mathbf{p} \mu\rangle \langle E \mathbf{p} \nu|, \] (H.9)

where we have chosen the linear-helicity states \( \{E \mathbf{p} \mu\} \) as the basis.
H.3. Polarization vector of the electron

The polarization vector \( P \) of the electron is defined as the expectation value of \( \Sigma \),

\[
P = \langle \Sigma \rangle = \frac{\text{tr}\{\rho \Sigma\}}{\text{tr}\{\rho\}}, \tag{H.10}
\]

where the notation \( \text{tr}\{\Omega\} \) denotes the trace of operator \( \Omega \) in any specific representation.

In the \( \{E\mu\} \) representation of the electron, both \( \rho \) and \( \Sigma \) are expressed as 2x2 matrices:

\[
\rho = (\rho_{\mu\nu}) \equiv \begin{pmatrix} \rho_{+1} & \rho_{+1-1} \\ \rho_{-1} & \rho_{-1-1} \end{pmatrix}, \tag{H.11}
\]

\[
\Sigma = (\Sigma_{\mu\nu}) \equiv \begin{pmatrix} \Sigma_{+1} & \Sigma_{+1-1} \\ \Sigma_{-1} & \Sigma_{-1-1} \end{pmatrix}. \tag{H.12}
\]

Here matrix elements \( \rho_{\mu\nu} \) are given or calculated for a specific collision process for the state of the electron, and matrix elements \( \Sigma_{\mu\nu} \) are evaluated by

\[
\Sigma_{\mu\nu} = \frac{\langle E\mu|\Sigma|E\nu\rangle}{\langle E\mu|E\nu\rangle}. \tag{H.13}
\]

Because we have chosen the linear-helicity states \( \{E\mu\} \) as our basis, the Pauli spin operators \( \vec{\sigma} \) are expressed in terms of eigenstates of \( \sigma_\mu \), i.e., we choose the quantization z-axis in the \( \mathbf{p} \)-direction. The polarization vector \( P \) so calculated is of course defined with the linear momentum \( p \) chosen as the z-axis.

For an electron with definite \( \{E, \mathbf{p}\} \), we need only to work in the spinor space \( \{u_{E\mu}\} \), i.e.,

\[
\Sigma_{\mu\nu} = u^\dagger_{E\mu} \Sigma u_{E\nu}.
\]

We obtain therefore the 2x2 matrix representation of the operator \( \Sigma \equiv \{\Sigma_x, \Sigma_y, \Sigma_z\} \) as

\[
\Sigma_x = \sigma_x (m/M) = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} (m/M), \tag{H.15}
\]
\[ \sum_x = \sigma_x (m/M) = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} (m/M), \]  
\[ \sum_z = \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \]  
where \( \vec{\sigma} = \{\sigma_x, \sigma_y, \sigma_z\} \) are in the standard representation, and

\[ m = \sqrt{1 - v^2 / c^2}. \]  

For an electron described by the spin-density matrix \( \rho \) with definite \( \{E, p\} \), we can always expand \( \rho \) in the form

\[ \rho = \begin{pmatrix} \rho_{11} & \rho_{1-1} \\ \rho_{-11} & \rho_{-1-1} \end{pmatrix} = \frac{1}{2} \text{tr} \{\rho\} \left[ I + \vec{P} \cdot \vec{\sigma} \right]. \]  

Now the polarization vector \( \vec{P} \) is calculated in the 2×2 matrix representation with the results:

\[ I = \text{tr} \{\rho\} = \rho_{11} + \rho_{-1-1}, \]  
\[ IP_x = (\rho_{1-1} + \rho_{-11}) (m/M), \]  
\[ IP_y = i(\rho_{1-1} - \rho_{-11}) (m/M), \]  
\[ IP_z = (\rho_{11} - \rho_{-1-1}). \]  

It is interesting to note that the longitudinal component \( P_z \) along the linear momentum \( p \) is independent of \( p \), while the transverse components \( \{P_x, P_y\} \) are contracted by a factor of \( m/M = \sqrt{1 - v^2 / c^2} \). Conventionally the polarization vector of the electron is defined in its rest frame, namely, without the factor \( (m/M) \) for the transverse components.

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