ICTS discussion meeting Structured Light and Spin-Orbit Photonics Spin-orbit interaction in atomic physics and optics Bimalendu Deb

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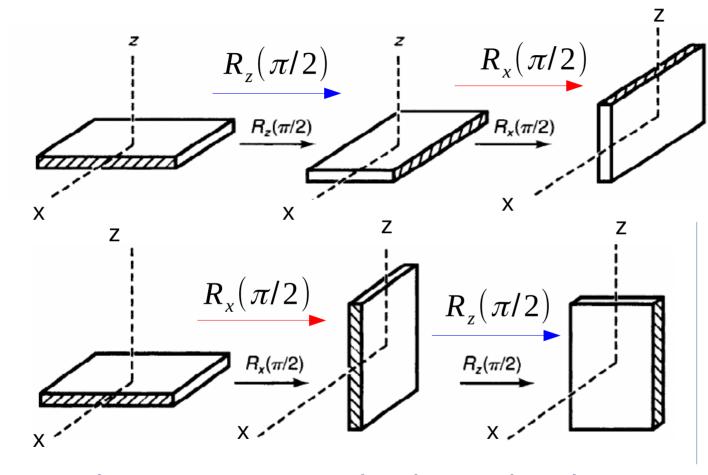
Part-1

- Classical concept of angular momentum
- Quantum concept of angular momentum
- Orbital and spin angular momentum
- Rotation matrices & rotation groups
- Spin-orbit interaction in atoms
- Relation to Berry phase

Part-2

- Optical angular momentum
- Orbital and "spin" angular momentum of light
- Spin-orbit interaction of light
- Relation to Berry phase

Classical concept of angular momentum



Modern Quantum Mechanics, Sakurai

Two alternative ways of viewing rotation: Active or passive

$$R_{_{X}}(\phi)$$
 , $R_{_{Z}}(\phi)$

Rotation matrices or operators

- What are their mathematical form?
- They act on what ?

Classical concept of angular momentum

Angular momentum is the generator of rotation: Prove this

$$G(q',p')=G(q,p)+\alpha \{G,F\}$$
Poisson bracket

F is called the generator of transformation $G(q, p) \rightarrow G(q', p')$

 α is an infinitesimally small change in the appropriate variable

Let
$$\Rightarrow F = L_z = [\vec{r} \times \vec{p}]_z = x p_y - y p_x$$
 $\alpha = \delta \phi$ (small angle)

$$x'=x-\alpha y$$
 $y'=y+\alpha x$ $z'=z$
 $p_x'=p_x-\alpha p_y$ $p_y'=p_y+\alpha p_x$ $p_z'=p_z$

Hamiltonian, Invariance, Symmetries & Conservation

Quantum concept of angular momentum

As in classical mechanics, angular momentum is the generator of rotation. However, the Poisson bracket is to be replaced by

$$\{G,F\} \rightarrow \frac{1}{i\hbar}[G,F]$$
, G and F are quantum mechanical operators

Orbital and spin angular momentum Orbital angular momentum is the generator of rotation in real space (x,y,z), spin is the generator of rotation in spinor domain. Spin is the intrinsic angular momentum of a particle in its rest frame.

Let the small rotation about z-axis be $\delta \phi \Rightarrow F = L_z$, $G \equiv A$

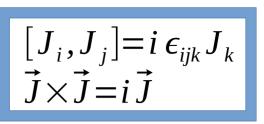
Frame transformation $\Rightarrow A' = A - \frac{i}{\hbar} \delta \phi [A, L_z] = A - \frac{i}{\hbar} \delta \phi [A L_z - L_z A]$

$$\simeq \left(1 + \frac{i}{\hbar} \delta \phi L_z\right) A \left(1 - \frac{i}{\hbar} \delta \phi\right) \Leftrightarrow D(R) = e^{-i\phi L_z/\hbar} = e^{-i\vec{L} \cdot \hat{z} \phi/\hbar} \Leftrightarrow D(R) = e^{-i\vec{L} \cdot \hat{n} \phi/\hbar}$$

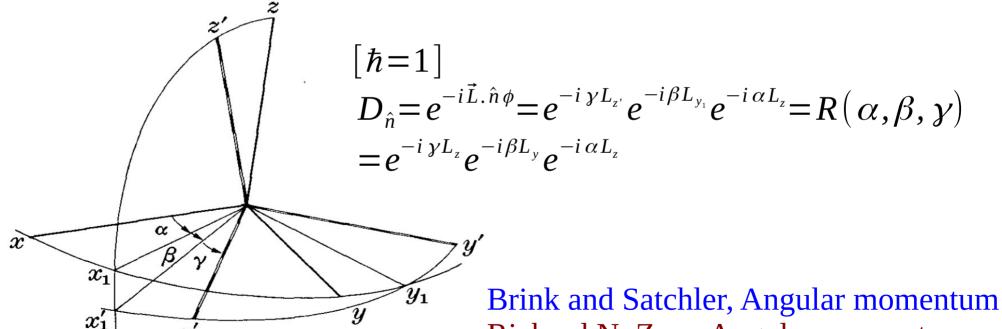
Rotation matrices & rotation groups

Commutation rules for J_x , J_y and $J_z \Rightarrow$

Derive using $D_z(R)$ acting on a vector operator \vec{A}



D(R) can be expressed in terms of Euler angles: Prove this



Richard N. Zare, Angular momentum

Rotation matrices & rotation groups

Rotation matrices satisfy all the group properties: prove this

- Rotation matrices describe transformation properies
- Spin rotation matrices describe transformation in spinor domain
- Spin operators obey similar commutation algebra as the orbital ones do
 Two or more angular momenta, including spin and orbital angular momenta
- can be added. Group theory is applied to get physical intuition.

Angular momentum of atoms and molecules

Eigen function of orbital angular momentum $\Rightarrow Y_{l.m}(\theta, \phi)$

- Simulatneous eigen function of \vec{L}^2 and L_z with eigen values l(l+1) and m Same applies to spin \vec{S}
- Structures of atoms or molecules <----> angular wave functions
- Spin-orbit interaction
- Spectra: Selection rules determined by angular momentum addition rules

Spin-orbit interaction (SOI) in atoms

SOI in atomic physics can be introduced in two ways:

- 1) By solving Dirac equation of an atomic electron in Coulomb potential, though perturbative, it is rigorous.
- 2) By considering interaction of electron's spin magnetic moment with the magnetic field produced by the electric field of the nucleus at the electron. This requires Lorentz transformation of the electric field.

These two ways are not equivalent as they yield quantitatively different results.

Relativistic quantum mechanics of a spin-1/2 particle in a central potential

Let us first consider Dirac equation of a free particle

For an atomic electron, $\frac{v}{c} \sim \alpha = \frac{1}{137}$

⇒ electrons in atoms move with relativistic speed

$$E^{2} = p^{2}c^{2} + m_{0}^{2}c^{4}, \quad p \rightarrow -i\hbar\nabla, \quad E \rightarrow i\hbar\frac{\partial}{\partial t} \Rightarrow \text{ relativistic wave equation}$$

$$E^{2}\psi = \left(p^{2}c^{2} + m_{0}^{2}c^{4}\right)\psi$$

$$E \psi - (p c + m_0 c) \psi$$

For spin-1/2 particles, the generators of rotation are Pauli operators σ

Coupling of spin with momentum

$$(\vec{\sigma}.\vec{A})(\vec{\sigma}.\vec{B}) = \vec{A}.\vec{B} + i\vec{\sigma}.(\vec{A} \times \vec{B}) \Rightarrow p^2 = (\vec{\sigma}.\vec{p})(\vec{\sigma}.\vec{p})$$

$$E^{2}\psi = \left(p^{2}c^{2} + m_{0}^{2}c^{4}\right)\psi \Rightarrow \frac{1}{m_{0}c^{2}}\left(E + c\vec{\sigma} \cdot \vec{p}\right)\left(E - c\vec{\sigma} \cdot \vec{p}\right)\psi = m_{0}c^{2}\psi$$

$$(E + c\vec{\sigma} \cdot \vec{p}) \left[\frac{1}{m_0 c^2} (E - c\vec{\sigma} \cdot \vec{p}) \psi \right] = m_0 c^2 \psi$$
Let
$$\frac{1}{m_0 c^2} (E - c\vec{\sigma} \cdot \vec{p}) \psi = \phi, \text{ then } (E + c\vec{\sigma} \cdot \vec{p}) \phi = m_0 c^2 \psi$$

A second order equation is split into two coupled first order equations

A second order equation is split into two coupled first order equations
$$(-E + c \vec{\sigma} \cdot \vec{p}) \psi = -m_0 c^2 \phi$$
$$(E + c \vec{\sigma} \cdot \vec{p}) \phi = m_0 c^2 \psi$$

Case-I: $m_0 = 0$, E = c p,

For
$$\psi$$
, $\vec{\sigma}$. $\hat{p} = \frac{E}{c p} = +1 \Rightarrow \psi$ has +ve helicity (spin is parallel to \vec{p})

For ϕ , $\vec{\sigma}$. $\hat{p} = -\frac{E}{c p} = -1 \Rightarrow \phi$ has -ve helicity (spin is anti-parallel to \vec{p})

$$(E + c\vec{\sigma} \cdot \vec{p}) \left[\frac{1}{m_0 c^2} (E - c\vec{\sigma} \cdot \vec{p}) \psi \right] = m_0 c^2 \psi$$
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Case-I: $m_0 \neq 0$, The state must be of mixed helicity

Let
$$\chi = \frac{1}{\sqrt{2}} (\psi + \phi)$$
, $\eta = \frac{1}{\sqrt{2}} (\psi - \phi)$ These are two-wave functions

These are two-component

$$\frac{(-E+c\vec{\sigma}.\vec{p})\psi=-m_0c^2\phi}{(E+c\vec{\sigma}.\vec{p})\phi=m_0c^2\psi} \longrightarrow \frac{c\vec{\sigma}.\vec{p}\chi-mc^2\eta=E\eta}{c\vec{\sigma}.\vec{p}\eta+mc^2\chi=E\chi}$$

$$\xi = \begin{pmatrix} \chi \\ \eta \end{pmatrix} = \begin{pmatrix} \chi_1 \\ \chi_2 \\ \eta_1 \\ \eta_2 \end{pmatrix} \longrightarrow c \vec{\sigma} \cdot \vec{p} \begin{pmatrix} \mathbf{1} & \mathbf{0} \\ \mathbf{0} & \mathbf{1} \end{pmatrix} \xi + m_0 c^2 \begin{pmatrix} \mathbf{0} & -\mathbf{1} \\ \mathbf{1} & \mathbf{0} \end{pmatrix} \xi = E \begin{pmatrix} \mathbf{0} & \mathbf{1} \\ \mathbf{1} & \mathbf{0} \end{pmatrix} \xi$$

$$\left[c\vec{\alpha}.\vec{p}+m_{0}c^{2}\beta_{4}\right]\xi=E\xi$$

$$\vec{\alpha} = \begin{pmatrix} 0 & \vec{\sigma} \\ \vec{\sigma} & 0 \end{pmatrix}$$

$$\vec{\alpha} = \begin{pmatrix} 0 & \vec{\sigma} \\ \vec{\sigma} & 0 \end{pmatrix} \quad \beta_4 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

For
$$\vec{p} = 0$$
, $m_0 \neq 0$

$$\left[c \vec{\alpha} \cdot \vec{p} + m_0 c^2 \beta_4 \right] \xi = E \xi$$

$$i \hbar \frac{\partial \xi}{\partial t} = m_0 c^2 \beta_4 \xi$$

$$\beta^2 = 1 \Rightarrow \beta_4^{-1} = \beta_4$$

$$\xi = \begin{pmatrix} \chi \\ \chi_2 \\ \chi_2 \\ \chi_3 \end{pmatrix}$$

$$\xi = \begin{pmatrix} \chi \\ \chi_2 \\ \chi_3 \\ \chi_4 \end{pmatrix}$$

 $i\hbar \beta_4 \frac{\partial \xi}{\partial t} = m_0 c^2 \xi$ $e^{\mp i m_0 c^2/\hbar t} \rightarrow + \text{ve and -ve energy states}$

 $\xi = \begin{pmatrix} \chi \\ \eta \end{pmatrix} \equiv \begin{pmatrix} \chi_1 \\ \chi_2 \\ \eta_1 \\ \chi_2 \end{pmatrix}$

$$\chi(t) = e^{-im_{0}c^{2}/\hbar t} \chi(0), \quad \chi(0) = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \quad \eta(0) = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} \Rightarrow \xi_{e, \uparrow}(t) = e^{-im_{0}c^{2}t/\hbar} \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \quad \xi_{p, \uparrow}(t) = e^{im_{0}c^{2}t/\hbar} \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}$$

$$\eta(t) = e^{im_{0}c^{2}/\hbar t} \chi(0), \quad \chi(0) = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \quad \chi(0) = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}, \quad \chi(0) = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$$

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Solution of Dirac equation with a central potential leads to SOI

$$\left[c\vec{\alpha}.\vec{p}+m_{0}c^{2}\beta_{4}\right]\xi=E\xi\Rightarrow\left[c\vec{\alpha}.\vec{p}+m_{0}c^{2}\beta_{4}+V(r)\mathbf{I}\right]\xi=E\xi$$

For an atomic electron
$$V(r) = -\frac{Ze^2}{4\pi \epsilon_0 r}$$

Let $E = m_0 c^2 + E'$ $E' \ll m_0 c^2$, perturbative solutions

perturbation parameter is fine structure constant $\alpha = \frac{v_{av}}{c} = \frac{e^2}{4\pi\epsilon_0\hbar c}$

SOI is one of the 3 terms which are of the order of α^2

Bransden & Joachain

$$H_{\rm so} = \frac{1}{2m_0^2c^2} \frac{1}{r} \frac{dV}{dr} L.S$$

$$S = \frac{1}{2} \hbar \sigma$$

Second method: Electron spin in internal magnetic field

Magnetic field **B** produced by moving nucleus as experienced by the electron

$$\mathbf{B} = -\frac{1}{c^2} \mathbf{v} \times \mathbf{E}, \quad \mathbf{E} = \frac{e}{4\pi \epsilon_0 r^2} \hat{r} = \frac{1}{e} \frac{dV}{dr} \hat{r}, \quad \mathbf{v} = \frac{\mathbf{p}}{m}$$

electron's spin magnetic moment $\mu = -g_s \frac{e}{2m} S$, $g_s = 2$

Classical electrodynamics Lorentz transformation

$$H' = -\mu \cdot \mathbf{B} = \frac{g_s}{2m^2c^2} \frac{1}{r} \frac{dV}{dr} \mathbf{L} \cdot \mathbf{S}$$

Earlier we have found

$$H_{\rm so} = \frac{1}{2m_{\rm o}^2c^2} \frac{1}{r} \frac{dV}{dr} \mathbf{L}.\mathbf{S}$$

 $H'=2\,H_{\rm so}$ \rightarrow due to Thomas precision What is Thomas precision ? What is its origin ? It is related to adibaticity and Berry phase

Berry phase connection to SOI

We have seen that spinor of electron at its rest frame oscillates at relativistic frequency mc^2/\hbar ($m=m_0$), [rest mass of electron $\simeq 0.5$ MeV]

Orbital motion of atomic electron (Bohr orbit) has characteristic frequency $\alpha^2 m c^2 / \hbar$ (13.6 eV), that is, orbital motion is slower than spin oscillations by 4 order of magnitude \Rightarrow clear separation of time scales

Thomas Precession, Spin-Orbit Interaction, and Berry's Phase

Harsh Mathur

Center for Theoretical Physics, Yale University, P.O. Box 6666, New Haven, Connecticut 06511 (Received 29 April 1991)

The spin-orbit interaction is shown to arise as a Berry phase term in the adiabatic effective Hamiltonian for the orbital motion of a Dirac electron. This approach makes explicit the intimate connection of the spin-orbit interaction and Thomas precession.

Pancharatnam-Berry phase: A brief introduction

- Adiabatic theorem
- Parallel transport of vectors on a sphere
- Slow vs. fast DOF: Born-Oppenheimer approximation
- Geometric phase: closed line integral of a vector in parameter space
- Vector function leads to Gauge structure
- Geometric phase is Gauge invariant
- Berry's connection: Curl of the vector or the curvature (field)

Part-2: Optical angular momentum

Contents

- Optical angular momentum
- Paraxial approximation
- Orbital and "spin" angular momentum of light
- Spin-orbit interaction of light

Angular momentum of light or of a massless particle photon Photon has no rest frame, the spin of photon is not well-defined, Only the total angular momentum of photon can be defined

The wavefunction of photon is $\vec{A}(\vec{r})$ or $\vec{A}(\vec{k})$

A *vector function* is equivalent to a spinor of rank 2

⇒ photon can behave like a spin-1 particle

- Spin and orbital angular momentum of a photon are defined to express transformation properties of the wave function under rotations.
- > S=1 implies that the wave function is a vector
- > *OAM=1* is the order of spherical harmonics

 $\hat{P}\vec{A}(\vec{k}) = -\vec{A}(-\vec{k}) \Rightarrow P = (-1)^{l+1}$

What are the possible states for a given i? $j \neq 0$, there are three states l=i, $P=(-1)^{l+1}=(-1)^{j+1}$

$$l=j\pm 1, \quad P=(-1)^{l+1}=(-1)^{j}$$

For $j=0$, there is only one state, with $l=1$ and $P=+1$

Because $\vec{A}(\vec{k})$ is a transverse vector, the states that correspond to a longitudinal vector are not allowed. Those states have $P = (-1)^{j}$

 \Rightarrow Photon has $i \neq 0$

Lorentz force
$$\Rightarrow \vec{F} = q(\vec{E} + \vec{v} \times \vec{B}) = \int dV (\rho \vec{E} + \vec{J} \times \vec{B})$$

Rate of doing work
$$\Rightarrow \vec{F} \cdot \vec{v} = q \vec{v} \cdot \vec{E} = \int dV \rho \vec{v} \cdot \vec{E} = \int dV \vec{J} \cdot \vec{E}$$

Maxwell equation
$$\Rightarrow \vec{\nabla} \times \vec{H} = \vec{J} + \frac{\partial \vec{D}}{\partial t} \Rightarrow \vec{\nabla} \times \vec{B} / \mu_0 = \vec{J} + \epsilon_0 \frac{\partial \vec{E}}{\partial t}$$

$$\Rightarrow \mu_0 \vec{J} = \vec{\nabla} \times \vec{B} - \mu_0 \epsilon_0 \frac{\partial \vec{E}}{\partial t} = \vec{\nabla} \times \vec{B} - \frac{1}{c^2} \frac{\partial \vec{E}}{\partial t}$$

$$\Rightarrow \vec{J} \cdot \vec{E} = \frac{1}{\mu_0} (\vec{\nabla} \times \vec{B}) \cdot \vec{E} - \epsilon_0 \frac{\partial \vec{E}}{\partial t} \cdot \vec{E}$$

$$\vec{J} \cdot \vec{E} = \frac{1}{\mu_0} (\vec{\nabla} \times \vec{B}) \cdot \vec{E} - \epsilon_0 \frac{\partial \vec{E}}{\partial t} \cdot \vec{E} = \frac{1}{\mu_0} \vec{E} \cdot (\vec{\nabla} \times \vec{B}) - \epsilon_0 \frac{\partial \vec{E}}{\partial t} \cdot \vec{E}$$

$$\vec{\nabla} \cdot (\vec{E} \times \vec{B}) = \vec{B} \cdot (\vec{\nabla} \times \vec{E}) - \vec{E} \cdot (\vec{\nabla} \times \vec{B}) \implies \vec{E} \cdot (\vec{\nabla} \times \vec{B}) = -\vec{\nabla} \cdot (\vec{E} \times \vec{B}) + \vec{B} \cdot (\vec{\nabla} \times \vec{E})$$

Maxwell equation
$$\vec{\nabla} \times \vec{E} = -\frac{\partial \vec{B}}{\partial t}$$

$$\vec{J} \cdot \vec{E} = -\vec{\nabla} \cdot \vec{S} - \frac{\partial u}{\partial t}, \quad \text{where} \quad \vec{S} = \frac{1}{\mu_0} (\vec{E} \times \vec{B}) = \vec{E} \times \vec{H}, \quad u = \frac{1}{2} \left[\epsilon_0 E^2 + \frac{1}{\mu_0} B^2 \right]$$
Rate of doing work $\Rightarrow \vec{F} \cdot \vec{v} = \frac{dE_{\text{mech}}}{dt} = \int dV \, \rho \, \vec{v} \cdot \vec{E} = \int dV \, \vec{J} \cdot \vec{E}$

$$\frac{d}{dt} \left(E_{\rm mech} + E_{\rm field} \right) = - \int dV \, \vec{\nabla} . \vec{S} = - \int ds \, \hat{n} . \left(\vec{\nabla} \times \vec{S} \right)$$

Momentum and momentum density of EM field

Lorentz force
$$\Rightarrow$$
 $\vec{F} = q(\vec{E} + \vec{v} \times \vec{B}) = \int dV (\rho \vec{E} + \vec{J} \times \vec{B}) = \frac{d\vec{P}_{\text{mech}}}{dt} = \int dV \frac{d\vec{p}_{\text{mech}}}{dt}$

Maxwell equations
$$\rho = \vec{\nabla} \cdot \vec{D} = \epsilon_0 \vec{\nabla} \cdot \vec{E}$$
, $\vec{J} = \vec{\nabla} \times \vec{H} - \frac{\partial \vec{D}}{\partial t} = \frac{1}{\mu_0} \vec{\nabla} \times \vec{B} - \epsilon_0 \frac{\partial \vec{E}}{\partial t}$

$$\vec{J} \times \vec{B} = \frac{1}{\mu_0} \left(\vec{\nabla} \times \vec{B} \right) \times \vec{B} - \epsilon_0 \frac{\partial \vec{E}}{\partial t} \times \vec{B} \quad \Leftrightarrow \quad \frac{\partial \vec{E}}{\partial t} \times \vec{B} = \frac{\partial}{\partial t} \left(\vec{E} \times \vec{B} \right) - \vec{E} \times \frac{\partial \vec{B}}{\partial t}$$

$$\frac{d \vec{P}_{\text{mech}}}{d t} + \frac{d}{d t} \int dV \, \epsilon_0 (\vec{E} \times \vec{B}) = \epsilon_0 \int dV \left[\left(\vec{\nabla} \cdot \vec{E} \right) \vec{E} + c^2 \left(\vec{\nabla} \times \vec{B} \right) \times \vec{B} + \vec{E} \times \frac{\partial \vec{B}}{\partial t} \right]$$

$$= \epsilon_0 \int dV \left[\vec{E} \left(\vec{\nabla} \cdot \vec{E} \right) - c^2 \vec{B} \times \left(\vec{\nabla} \times \vec{B} \right) - \vec{E} \times \left(\vec{\nabla} \times \vec{E} \right) \right]$$

$$\vec{P}_{\text{field}} = \int dV \, \epsilon_0 (\vec{E} \times \vec{B}) = \int dV \, c^2 \vec{S} \qquad \vec{J} \cdot \vec{E} = -\vec{\nabla} \cdot \vec{S} - \frac{\partial u}{\partial t},$$

$$\vec{S} - \frac{\partial u}{\partial t}$$

Total angular momentum of light

$$\vec{J}_{a} = \vec{r} \times \vec{P}_{field} = \int dV \, \epsilon_{0} \vec{r} \times (\vec{E} \times \vec{B}) = \int dV \, c^{2} \vec{r} \times \vec{S} \,, \qquad \vec{E} \times \vec{B} = \vec{E} \times (\vec{\nabla} \times \vec{A})$$

$$\vec{J}_{a} = \sum_{i} \epsilon_{0} \int dV \left[E_{i} (\vec{r} \times \vec{\nabla}) A_{i} + \vec{E} \times \vec{A} - \nabla_{i} (E_{i} \vec{r} \times \vec{A}) \right]$$

$$\simeq \sum_{i} \epsilon_{0} \int dV \left[E_{i} (\vec{r} \times \vec{\nabla}) A_{i} + \vec{E} \times \vec{A} \right] \quad \text{Andrews and Babiker (edt)}$$

$$\text{The Angular Momentum of Light}$$

$$\text{Orbital } \vec{L} \quad \text{Spin } \vec{S}$$

- Paraxial approximationSpin is associated with the polarization
- Vector ways equation reduces to scalar equation for constant polarization
- Vector wave equation reduces to scalar equation for constant polarization
- Orbital angular momentum is associated with azimuthal phase

Spin-orbit interaction of light

Orbital angular momentum of light arises due to slow $\,$ rotation of center of application of wave vectors \mathbf{k} (centroid)

Due to transversality condition, the rotation of \mathbf{k} vectors must influence the polarization state, leading to SOI of light.

Slow rotational motion of ${\bf k}$ vectors may be treated adiabatically while considering much faster spin (polarization) evolution, leading to Berry phase (Gauge) structure of SOI

Follow other lectures of SLSOP for details of SOI of light and its applications