

# 1 REVIEW OF QUANTUM MECHANICS

## 1.1 CLASSICAL MECHANICS

Classical mechanics is based on the assumption that any physically interesting variables connected with a system/particle, such as its position, velocity or its energy can be measured with arbitrary precision and without mutual interference from any other such measurement. Laws of classical mechanics can be expressed in various mathematical forms,

1. Newtonian mechanics
  2. Hamiltonian mechanics
- Hamiltonian of a physical system gives its total energy

$$H = T + V$$

Quantum mechanics is based on the realization that the measuring process may affect the physical system. It is therefore impossible to measure simultaneously certain pairs of variables with precision. In quantum mechanics physical system is described by a state vector or wave function, and variables are represented by operators.

- Quantum mechanics can be expressed by,
1. Wave mechanics
  2. Dirac's notation

## 1.2 WAVE MECHANICS:

A quantum mechanical system (such as atoms, molecules, ions etc.) are given by its wave function  $\psi(r, t)$ . Itself  $\psi(r, t)$  has no physical meaning but it allows to calculate the expectation values of all observables of interest.

Measurable quantities are called observables and are represented by hermitian operators  $\hat{O}$ . Expectation value is given by

$$\langle \hat{O} \rangle = \int d^3r \psi^*(r, t) \hat{O} \psi(r, t).$$

## 1.3 Probability:

The probability of finding the system in the volume element  $d^3r$  is

$$\psi^*(r, t) \hat{O} \psi(r, t).$$

As the system exist, its probability of being somewhere has to equal 1.

$$\begin{aligned} \int \psi^*(r, t) \psi(r, t) d^3r &= 1 \\ \int \psi_n^*(r, t) \psi_m(r, t) d^3r &= \delta_{nm}. \end{aligned}$$

The time development of wave function is determined by schrodinger equation,

$$i\hbar \frac{\partial}{\partial t} \psi(r, t) = H\psi(r, t),$$

where  $H$  is the Hamiltonian of the system. The energy of the unperturbed system for instance an atom not interacting with light is the sum of its potential and kinetic energies

$$H = \frac{p^2}{2m} + V(r).$$

#### 1.4 Stationary state:

Stationary states of schrodinger equation are those for which space and time dependence are separated,

$$\psi_n(r, t) = U_n(\vec{r})e^{-i\omega_n t}.$$

Time independent equation,

$$HU_n(\vec{r}) = E_n U_n(\vec{r}) = \hbar\omega_n U_n(\vec{r}),$$

where  $U_n(\vec{r})$  is an eigen function of  $H$  with eigen values  $E_n = \hbar\omega_n$ . The eigen values of hermitian operators are real numbers. The eigen functions of hermitian operators belonging to different eigen values are orthogonal, and eigen functions having same eigen values are normal.

$$\int U_n^*(r)U_m(r)d\vec{r} = \delta_{nm}$$

and complete

$$\sum_n U_n^*(r)U_n(r) = 1.$$

The completeness relation means that any function can be written as a linear combination of the  $U_n(r, t)$ . The wave function

$$\psi(r, t) = \sum_n \psi_n(r, t) = \sum_n C_n(t)U_n(\vec{r})e^{-i\omega_n t},$$

here  $C_n(t)$  are the expansion coefficients.

$C_n(t)$  - constant for problems related to free part of Hamiltonian

$C_n(t)$  - change in time if we include the interaction part of Hamiltonian.

Putting the values of  $\psi(r, t)$  in the normalization condition we get

$$\sum_n |C_n|^2 = 1,$$

gives the probability of finding the system in state  $n$ . The expectation value in terms of  $C_n$

$$\langle \hat{O} \rangle = \sum_{n,m} C_n C_m^* \hat{O}_{nm} e^{-i\omega_{nm} t},$$

Where

$$\hat{O}_{nm} = \int d^3r U_m^*(r) \hat{O} U_n(r),$$

and

$$\omega_{nm} = \omega_n - \omega_m.$$

## 1.5 DIRAC NOTATION:

The wave function of wave mechanics corresponds to the state vector in Dirac's formulation of quantum mechanics. The relation between state vector and wave function is analogous to using vectors instead of coordinates. A vector  $\vec{V}$  can be expanded as,

$$\vec{V} = V_x \hat{x} + V_y \hat{y}.$$

In Dirac's notation

$$|V\rangle = V_x |x\rangle + V_y |y\rangle.$$

x-component of a vector is obtained by

$$\vec{V} \cdot \hat{x} = V_x,$$

in Dirac's notation

$$\langle x|V\rangle = V_x \quad \text{and} \quad \langle y|V\rangle = V_y.$$

Using these Eqn's. we can write

$$\begin{aligned} |V\rangle &= |x\rangle \langle x|V\rangle + |y\rangle \langle y|V\rangle \\ &= (|x\rangle \langle x| + |y\rangle \langle y|) |V\rangle \end{aligned}$$

The identity diadic (outer product of two vectors)

$$|x\rangle \langle x| + |y\rangle \langle y| = 1$$

for  $n$  dimensions

$$\begin{aligned} |V\rangle &= \sum_n |n\rangle \langle n|V\rangle \\ \sum_n |n\rangle \langle n| &= I \end{aligned}$$

where  $\{ |n\rangle \}$  are complete set of vectors, i.e. a basis. The inner products  $\langle n|V\rangle$  are the expansion coefficients of the vector  $|V\rangle$  in this basis. Expansion coefficients are in general complex.

$$\langle k|V\rangle = \langle V|k\rangle^*$$

For continuous basis  $\{ |r\rangle \}$

$$I = \int d^3r |r\rangle \langle r|$$

The wave vector

$$|\psi(t)\rangle = \int d^3r |r\rangle \langle r|\psi\rangle$$

Where the wave function

$$\begin{aligned}\psi(r) &= \langle r|\psi\rangle \\ \psi(x) &= \langle x|\psi\rangle\end{aligned}$$

The expectation value of the operator  $\hat{O}$  is given by,

$$\langle \hat{O} \rangle = \langle \psi(t)|\hat{O}|\psi(t)\rangle$$

Hermitian

$$\begin{aligned}\langle \psi(t)|\hat{O}|\psi(t)\rangle &= \left[ \langle \psi(t)|\hat{O}^\dagger|\psi(t)\rangle \right]^* = \langle \psi(t)|\hat{O}|\psi(t)\rangle^* \\ \hat{O}^\dagger &= \hat{O}\end{aligned}$$

The set of eigen vectors of a hermitian operator is complete. This means that any arbitrary vector  $|\psi(t)\rangle$  can be expressed as a sum of orthogonal eigen vectors.

$$|\psi\rangle = \sum_{n=0}^{\infty} C_n |x_n\rangle$$

Eigen vectors are orthonormal

$$\begin{aligned}\langle X_n|X_m\rangle &= \delta_{nm} \\ \delta_{nm} &= 1 \text{ for } n = m \\ &= 0 \text{ for } n \neq m\end{aligned}$$

Completeness relation for discrete case is

$$\sum_n |X_n\rangle \langle X_n| = I$$

The state vector  $|\psi\rangle$  in terms of position eigen states (which are continuous).

$$\begin{aligned}|\psi(t)\rangle &= \int d\vec{x} |x\rangle \langle x|\psi\rangle \\ \int d\vec{x} |x\rangle \langle x| &= I\end{aligned}$$

The normalization of eigen vectors with a continuous set of eigen values must be normalized with the help of dirac delta function having properties,

$$\begin{aligned}\delta(x - x') &= 0 \quad \text{if } x \neq x' \\ \delta(x - x') &= \infty \quad \text{if } x = x' \\ \langle x|x'\rangle &= \delta(x - x')\end{aligned}$$

State vectors obey the Schrodinger's equation

$$\begin{aligned} i\hbar \left| \dot{\psi} \right\rangle &= H |\psi\rangle, \\ |\psi\rangle &= \sum_n C_n e^{-i\omega_n t} |n\rangle \end{aligned}$$

Expectation value can be written as

$$|\psi\rangle = \sum_{n,m} C_n^* C_m e^{-i(\omega_n - \omega_m)t} |n\rangle \hat{O}_{nm}$$

Where

$$\hat{O}_{nm} = \langle m | \hat{O} | n \rangle$$

### 1.6 Two level system:

Wave function for two level system is

$$\psi(r, t) = C_a U_a(\vec{r}) e^{-i\omega_a t} + C_b U_b(\vec{r}) e^{-i\omega_b t}$$

State vector

$$|\psi\rangle = C_a e^{-i\omega_a t} |a\rangle + C_b e^{-i\omega_b t} |b\rangle$$

### 1.7 SCHRODINGER, INTERACTION AND HEISENBERG PICTURES:

### 1.8 SCHRODINGER PICTURE:

The interaction of radiation with matter involves a hamiltonian.

$$H = H_o + V$$

$H_o$  - unperturbed energy

$V$  - Interaction energy

The corresponding Schrodinger equation

$$\begin{aligned} \left| \dot{\psi}(t) \right\rangle &= \frac{-i}{\hbar} H |\psi(t)\rangle \\ \left| \dot{\psi}(t) \right\rangle &= \frac{-i}{\hbar} (H_o + V) |\psi(t)\rangle, \\ |\psi(t)\rangle &= e^{\frac{-iHt}{\hbar}} |\psi(0)\rangle \end{aligned}$$

Expectation value of an operator  $\hat{O}$  which represents the observables.

$$\langle \hat{O} \rangle = \langle \psi(t) | \hat{O}(0) | \psi(t) \rangle$$

Operator  $\hat{O}$  is independent of time, but  $|\psi(t)\rangle$  is a function of time. This is the schrodinger picture way of writing the expectation value of an operator.

## 1.9 HEISENBERG PICTURE:

In Heisenberg picture total time dependence goes into operator, so state vector is independent of time, the expectation value of an operator in Schrodinger picture is,

$$\langle \hat{O} \rangle = \langle \psi(t) | \hat{O}(0) | \psi(t) \rangle$$

It can also be written as,

$$\langle \hat{O}(t) \rangle = \langle \psi(t) | e^{-\frac{iHt}{\hbar}} e^{\frac{+iHt}{\hbar}} \hat{O}(0) e^{-\frac{iHt}{\hbar}} e^{\frac{+iHt}{\hbar}} | \psi(t) \rangle$$

Where  $H$  is the total Hamiltonian. According to Schrodinger equation,

$$i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle = H |\psi(t)\rangle$$

Integrating

$$\begin{aligned} |\psi(t)\rangle &= e^{-\frac{iHt}{\hbar}} |\psi(0)\rangle \\ e^{\frac{+iHt}{\hbar}} |\psi(t)\rangle &= |\psi(0)\rangle \end{aligned}$$

Using this we can write

$$\langle \hat{O}(t) \rangle = \langle \psi(0) | e^{\frac{+iHt}{\hbar}} \hat{O}(0) e^{-\frac{iHt}{\hbar}} | \psi(0) \rangle$$

Define

$$\hat{O}(t) = e^{\frac{+iHt}{\hbar}} \hat{O}(0) e^{-\frac{iHt}{\hbar}}$$

Then

$$\langle \hat{O}(t) \rangle = \langle \psi(0) | \hat{O}(t) | \psi(0) \rangle$$

Which is called Heisenberg picture. In this all time dependence lies in operator.while wave function is independent of time.

### 1.9.1 Why called Heisenberg picture?

$$\begin{aligned} \hat{O}(t) &= e^{\frac{+iHt}{\hbar}} \hat{O}(0) e^{-\frac{iHt}{\hbar}} \\ \dot{\hat{O}}(t) &= \frac{i}{\hbar} H \hat{O} + \frac{-i}{\hbar} \hat{O} H \\ \dot{\hat{O}}(t) &= \frac{i}{\hbar} [H, \hat{O}] \end{aligned}$$

Which is Heisenberg equation of motion. That is why we call it Heisenberg picture. In between two extremes of Schrodinger and Heisenberg picture. There is an intermediate picture called interaction picture.

## 1.10 INTERACTION PICTURE:

Consider again the equation,

$$\langle \hat{O}(t) \rangle = \langle \psi(0) | e^{\frac{+iHt}{\hbar}} \hat{O}(0) e^{\frac{-iHt}{\hbar}} | \psi(0) \rangle$$

As

$$H = H_o + V$$

$H_o$ - free Hamiltonian,

$V$ - interaction part of Hamiltonian,

If the time dependence created by the interaction energy is only assigned to the state vector and rest of time dependence goes to the operator, then expectation value is written as,

$$\begin{aligned} \langle \hat{O}(t) \rangle &= \langle \psi(0) e^{\frac{+iVt}{\hbar}} | e^{\frac{+iH_o t}{\hbar}} \hat{O}(0) e^{\frac{-iH_o t}{\hbar}} | e^{\frac{-iVt}{\hbar}} \psi(0) \rangle \\ \langle \hat{O}(t) \rangle &= \langle \psi^I(t) | \hat{O}(t) | \psi^I(t) \rangle \end{aligned}$$

Interaction picture state vector

$$|\psi^I(t)\rangle = e^{\frac{-iVt}{\hbar}} |\psi(0)\rangle$$

Equation of motion

$$|\dot{\psi}^I(t)\rangle = \frac{-iV}{\hbar} |\psi^I(t)\rangle$$

This equation is simpler than ordinary schrodinger equation, but requires the calculation of  $\hat{O}^I(t)$ , where

$$\hat{O}^I(t) = e^{\frac{+iH_o t}{\hbar}} \hat{O}(0) e^{\frac{-iH_o t}{\hbar}}$$

In interaction picture both state vector and operator are time dependent. The interaction picture state vector,

$$|\psi^I(t)\rangle = \sum_n C_n(t) |n\rangle$$

The schrodinger picture state vector is

$$|\psi(t)\rangle = \sum_n c_n(t) |n\rangle = \sum_n C_n(t) e^{\frac{-i\omega_n t}{\hbar}} |n\rangle$$

Where

$$c_n(t) = C_n(t) e^{\frac{-i\omega_n t}{\hbar}}$$

The complete time dependence is given by  $c_n(t)$ , but due to interaction energy is given by  $C_n(t)$ .

### 1.11 PAULI SPIN MATRIX:

Another method to describe two- level atom is a use of  $2 \times 2$  matrix notation. The eigen function  $U_a$  and  $U_b$  or eigen vectors  $|a\rangle$  and  $|b\rangle$  can be represented by the column vectors

$$\begin{aligned}|a\rangle &= U_a \leftrightarrow \begin{pmatrix} 1 \\ 0 \end{pmatrix} \\ |b\rangle &= U_b \leftrightarrow \begin{pmatrix} 0 \\ 1 \end{pmatrix}\end{aligned}$$

And the wave function and wave vector by the column vectors

$$\psi(r, t) = \begin{bmatrix} C_a \\ C_b \end{bmatrix}$$

And

$$|\psi(r, t)\rangle = \begin{pmatrix} C_a \\ C_b \end{pmatrix}$$

The energy and electric- dipole operators are written in terms of the Pauli spin matrices as

$$\begin{aligned}\sigma_x &= \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \\ \sigma_y &= \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \\ \sigma_z &= \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\end{aligned}$$

These matrices are hermitian, but the spin- flip operators

$$\begin{aligned}\sigma_+ &= \frac{1}{2}(\sigma_x + i\sigma_y) = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \\ \text{and } \sigma_- &= \frac{1}{2}(\sigma_x - i\sigma_y) = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}\end{aligned}$$

are not hermitian,  $\sigma_-$  flips the system from upper- level to a lower- level

$$\sigma_- \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

While,  $\sigma_+$  flips the system from lower- level to the upper- level

$$\sigma_+ \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$



## 1.12 TWO LEVEL ATOMIC SYSTEM AND HAMILTONIAN IN TERMS OF MATRICES:

State vector of a system can be written as,

$$|\psi(r, t)\rangle = C_a e^{-i\omega_a t} |a\rangle + C_b e^{-i\omega_b t} |b\rangle,$$

Which corresponds to the wave function

$$\psi(r, t) = C_a U_a(\vec{r}) e^{-i\omega_a t} + C_b U_b(\vec{r}) e^{-i\omega_b t}$$

The matrix form from for the unit vectors (eigen vectors)  $|a\rangle$  and  $|b\rangle$  are

$$\psi(r, t) \leftrightarrow C_a e^{-i\omega_a t} \begin{pmatrix} 1 \\ 0 \end{pmatrix} + C_b e^{-i\omega_b t} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} C_a e^{-i\omega_a t} \\ C_b e^{-i\omega_b t} \end{pmatrix}$$

The two-level Hamiltonian of the semi-classical treatment is given as,

$$H = \hbar\omega_a |a\rangle\langle a| + V_{ab} |a\rangle\langle b| + V_{ba} |b\rangle\langle a| + \hbar\omega_b |b\rangle\langle b|$$

In matrix notation

$$H = \begin{pmatrix} H_{aa} & H_{ab} \\ H_{ba} & H_{bb} \end{pmatrix} = \begin{pmatrix} \hbar\omega_a & V_{ab} \\ V_{ba} & \hbar\omega_b \end{pmatrix}$$

Thus the matrix form of the schrodinger equation is

$$i\hbar \frac{d}{dt} \begin{pmatrix} C_a e^{-i\omega_a t} \\ C_b e^{-i\omega_b t} \end{pmatrix} = \begin{pmatrix} \hbar\omega_a & V_{ab} \\ V_{ba} & \hbar\omega_b \end{pmatrix} \begin{pmatrix} C_a e^{-i\omega_a t} \\ C_b e^{-i\omega_b t} \end{pmatrix}$$

### 1.13 EXPECTATION VALUE OF DIPOLE MOMENT OPERATOR FOR A TWO-LEVEL ATOM:

The expectation value of any operator is given by

$$\langle \psi | \hat{O} | \psi \rangle = C_a C_a^* \hat{O}_{aa} + C_b C_b^* \hat{O}_{bb} + \left\{ C_a C_b^* \hat{O}_{ab} e^{-i\omega_{ab}t} + c.c \right\}$$

The expectation value of “ $er$ ” is

$$\langle \psi | er | \psi \rangle = e C_a C_a^* \langle a | r | a \rangle + e C_b C_b^* \langle b | r | b \rangle + \left\{ e C_a C_b^* e^{-i(\omega_a - \omega_b)t} \langle b | r | a \rangle + c.c \right\}$$

As the diagonal matrix element of “ $er$ ” between eigen states of the Hamiltonian generally vanishes.

$$\begin{aligned} er_{aa} &= \langle a | er | a \rangle = e \int d^3r U_a^*(r) r U_a(r) = 0 \\ er_{bb} &= \langle b | er | b \rangle = e \int d^3r U_b^*(r) r U_b(r) = 0 \\ er_{ab} &= \langle a | er | b \rangle = e \int d^3r U_a^*(r) r U_b(r) \end{aligned}$$

In matrix form

$$\begin{aligned} \langle er \rangle &= e \begin{pmatrix} 0 & r_{ab} \\ r_{ba} & 0 \end{pmatrix} \\ \langle er \rangle &= e C_a C_b^* e^{-i(\omega_a - \omega_b)t} r_{ba} + c.c \end{aligned}$$

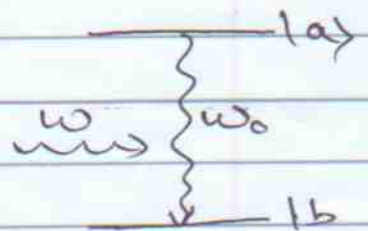
# ATOM - FIELD INTERACTION SEMICLASSICAL THEORY

$\Rightarrow$  Atom  $\rightarrow$  Quantum Mechanical

Field  $\rightarrow$  Classical

Two-level atomic system.

$$|\psi(t)\rangle = c_a(t)|a\rangle + c_b(t)|b\rangle$$



Hamiltonian of the system

$$H = H_0 + H'$$

$H_0$  — free part of Hamiltonian

$H'$  — perturbed part of Hamiltonian

Completeness relation for atomic system:

$$|a\rangle\langle a| + |b\rangle\langle b| = 1$$

$$\Rightarrow H_0 = \underbrace{(|a\rangle\langle a| + |b\rangle\langle b|)}_1 H_0 (|a\rangle\langle a| + |b\rangle\langle b|)$$

$$\text{As } H_0|a\rangle = E_a|a\rangle; H_0|b\rangle = E_b|b\rangle$$

$$\Rightarrow H_0 = E_a|a\rangle\langle a| + E_b|b\rangle\langle b|$$

$$\Rightarrow H_0 = \hbar\omega_a|a\rangle\langle a| + \hbar\omega_b|b\rangle\langle b|$$

Interaction part of Hamiltonian is written as.

$$H' = -er \cdot E(r,t)$$

under dipole approximation

$$E(r,t) = E(r,t) \approx E(t) \approx E_0 \cos \omega t$$

$$H' = -er \cdot E_0 \cos \omega t$$

$$H' = [|a\rangle\langle a| + |b\rangle\langle b|] H' [|a\rangle\langle a| + |b\rangle\langle b|]$$

$$= |a\rangle\langle a| \overset{\rightarrow 0}{H'|a\rangle} \langle a| + |b\rangle\langle b| \overset{\rightarrow 0}{H'|a\rangle} \langle a|$$

$$+ |a\rangle\langle a| \overset{\rightarrow 0}{H'|b\rangle} \langle b| + |b\rangle\langle b| \overset{\rightarrow 0}{H'|b\rangle} \langle b|$$

$$\text{As } H'_{aa} = 0 = H'_{bb}$$

$$H' = |a\rangle\langle b| H'_{ab} + |b\rangle\langle a| H'_{ba}$$

$$\begin{aligned} \text{Where } H'_{ab} &= \langle a | H' | b \rangle \\ &= -\langle a | er | b \rangle E_0 \cos \omega t \\ &= -p_{ab} E_0 \cos \omega t \end{aligned}$$

and

$$H'_{ba} = -p_{ba} E_0 \cos \omega t$$

$$\Rightarrow H' = - \left( p_{ab} |a\rangle\langle b| + p_{ba} |b\rangle\langle a| \right) E(t)$$

where

$p_{ab} = p_{ba}^* = e \langle a | r | b \rangle$  — matrix element of the electric dipole moment and  $E(t)$  is the field at the atom.

The time-development of the system is given by Schrodinger equation.

$$i\hbar \dot{|\psi(t)\rangle} = H |\psi(t)\rangle$$

Substitute values of state-vectors and Hamiltonian we get.



$$\dot{c}_a |a\rangle + \dot{c}_b |b\rangle = \frac{-i}{\hbar} [c_a \hbar \omega_a |a\rangle + c_b \hbar \omega_b |b\rangle + H'_{ab} c_b |a\rangle + H'_{ba} c_a |b\rangle]$$

Multiplying with  $\langle a|$  and using

$$\langle a|a\rangle = 1 \quad ; \quad \langle a|b\rangle = 0$$

$$\langle b|b\rangle = 1 \quad ; \quad \langle b|a\rangle = 0$$

$$\dot{c}_a = \frac{-i}{\hbar} [\hbar \omega_a c_a + H'_{ab} c_b]$$

and

$$\dot{c}_b = \frac{-i}{\hbar} [\hbar \omega_b c_b + H'_{ba} c_a]$$

Putting values of interaction Hamiltonian

$$\dot{c}_a = -i \omega_a c_a + \frac{i p_{ab}}{\hbar} \epsilon_0 \cos \omega t c_b$$

and

$$\dot{c}_b = -i \omega_b c_b + \frac{i p_{ba}}{\hbar} \epsilon_0 \cos \omega t c_a$$

Define

$$\Omega_R = \frac{|p_{ba}|}{\hbar} \epsilon_0 - \text{Rabi frequency}$$

$$P_{ba} = |P_{ba}| e^{i\phi}$$

$$\Rightarrow P_{ab} = P_{ba}^* = |P_{ba}| e^{-i\phi}$$

where  $\phi$  is the phase of the dipole matrix element.

$$\Rightarrow \dot{c}_a = -i\omega_a c_a + i\Omega_R e^{-i\phi} \cos\omega t c_b$$

$$\dot{c}_b = -i\omega_b c_b + i\Omega_R e^{i\phi} \cos\omega t c_a$$

Transform  $c_a$  &  $c_b$  (Sch. picture amplitudes)

into slowly varying interaction picture amplitudes

$$C_a = c_a e^{i\omega_a t}$$

$$C_b = c_b e^{i\omega_b t}$$

Differentiating above eqn's

$$\dot{C}_a = \dot{c}_a e^{i\omega_a t} + i\omega_a c_a e^{i\omega_a t}$$

$$\dot{C}_a = (-i\omega_a c_a + i\Omega_R e^{-i\phi} \cos\omega t c_b) e^{i\omega_a t} + i\omega_a c_a e^{i\omega_a t}$$

$$= i\Omega_R e^{-i\phi} \cos\omega t c_b e^{i\omega_a t}$$

$$= i\Omega_R e^{-i\phi} \cos\omega t e^{i\omega_a t} C_b$$

$$\omega_{ab} = \omega_a - \omega_b$$

Similarly.

$$\dot{C}_b = i\Omega_R e^{i\phi} \cos \omega t e^{-i\omega_{ab}t} C_a$$

$\omega_{ab} = \omega_0$  - transition frequency.

Expanding  $\cos \omega t$ .

$$\dot{C}_a = \frac{i\Omega_R}{2} e^{-i\phi} \left[ e^{i\omega t + i\omega_0 t} + e^{-i\omega t + i\omega_0 t} \right] C_b$$

Neglecting rapidly oscillating terms like  $e^{i(\omega + \omega_0)t}$

$$\dot{C}_a = \frac{i\Omega_R}{2} C_b e^{i(\omega_0 - \omega)t} e^{-i\phi}$$

Similarly.

$$\dot{C}_b = \frac{i\Omega_R}{2} C_a e^{-i(\omega_0 - \omega)t} e^{+i\phi}$$

where  $\Delta = \omega_0 - \omega$ . - detuning.

→ Consider atom initially in the excited state  $C_a(0) = 1$

$$C_b(0) = 0$$



Assume resonance  $\Delta = \omega_0 - \omega = 0$

$$C_a(t) = \cos \frac{\Omega R t}{2}$$

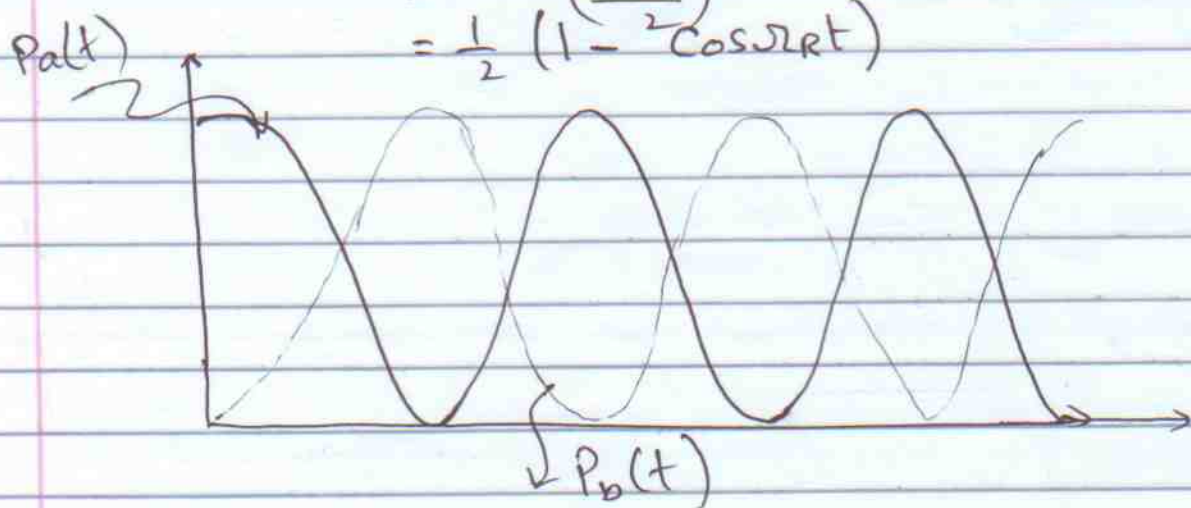
$$C_b(t) = i e^{i\phi} \sin \frac{\Omega R t}{2}$$

Probability of atom in state  $|a\rangle$   
at time  $t$

$$P_a(t) = |\langle \psi | a \rangle|^2 = |C_a(t)|^2 \\ = \cos^2 \left( \frac{\Omega R t}{2} \right) = \frac{1}{2} (1 + \cos \Omega R t)$$

and

$$P_b(t) = |C_b(t)|^2 = \text{Probability of atom} \\ \text{in state } |b\rangle \\ = \sin^2 \left( \frac{\Omega R t}{2} \right) \\ = \frac{1}{2} (1 - \cos \Omega R t)$$



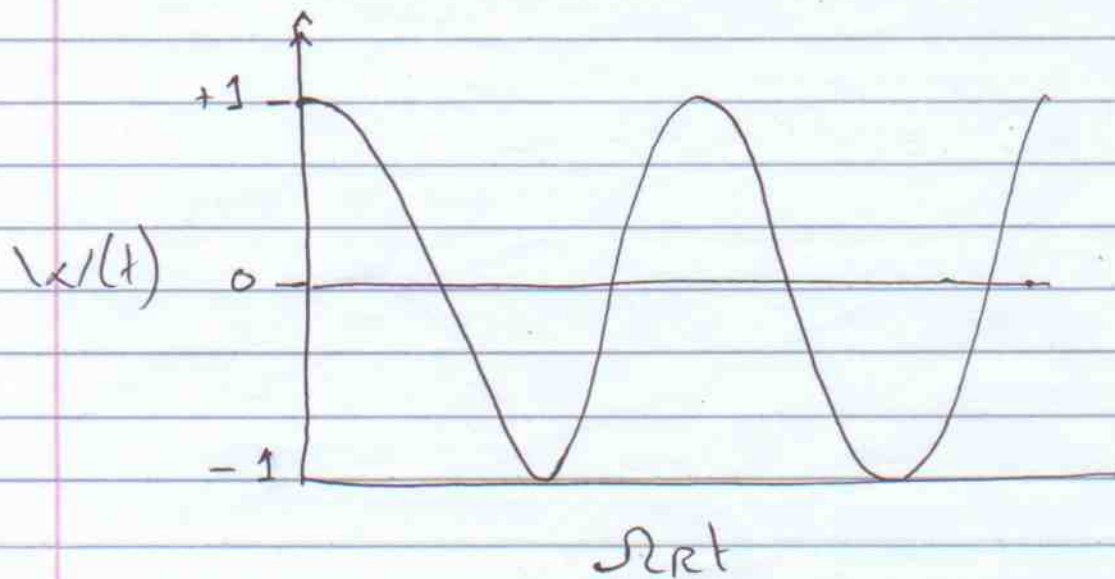
Atom oscillates with Rabi-freq.

## Population inversion

$$W(t) = P_a(t) - P_b(t) \quad \text{at } \Delta = 0$$

$$W(t) = \cos^2\left(\frac{\Omega_R t}{2}\right) - \sin^2\left(\frac{\Omega_R t}{2}\right) = \cos \Omega_R t$$

It oscillates between  $-1$  and  $+1$



There are three frequencies involved

1,  $\omega_0 = \omega_a - \omega_b = \frac{E_a - E_b}{\hbar}$  — Transition frequency

2,  $\omega$  frequency of the field

3, Rabi frequency  $\Omega_R = \frac{|P_{ab}| E}{\hbar}$

## 1.14 DENSITY OPERATOR

For a given physical system there exist a state vector  $|\psi\rangle$  which contain all possible information about the system. If we want to extract a piece of information about the system we must calculate the expectation value of the corresponding operator  $\hat{O}$

$$\langle \hat{O} \rangle_{Q M} = \langle \psi | \hat{O} | \psi \rangle$$

In many situations we do not know  $|\psi\rangle$  but we know  $P_\psi$ , probability of finding the system in  $|\psi\rangle$ . For such a situation we not only need to take quantum mechanical average but also the ensemble average over many identical systems that have been similarly prepared

$$\langle \langle \hat{O} \rangle_{Q M} \rangle_{ensemble} = \sum_{\psi} P_{\psi} \langle \psi | \hat{O} | \psi \rangle$$

It is called a quantum statistical system.

$$\begin{aligned} \sum_n |n\rangle \langle n| &= 1 \\ \langle \langle \hat{O} \rangle_{Q M} \rangle_{ensemble} &= \sum_n \sum_{\psi} P_{\psi} \langle \psi | n \rangle \langle n | \hat{O} | \psi \rangle \\ &= \sum_n \sum_{\psi} P_{\psi} \langle n | \hat{O} | \psi \rangle \langle \psi | n \rangle \\ &= \sum_n \langle n | \hat{O} \left[ \sum_{\psi} P_{\psi} |\psi\rangle \langle \psi| \right] | n \rangle \\ &= \sum_n \langle n | \hat{O} \rho | n \rangle = \sum_n (\hat{O} \rho)_{nn} \end{aligned}$$

where

$$\rho = \sum_{\psi} P_{\psi} |\psi\rangle \langle \psi|$$

The sum of diagonal elements gives

$$\langle \langle \hat{O} \rangle_{Q M} \rangle_{ensemble} = Tr(\hat{O} \rho) = Tr(\rho \hat{O})$$

where

$$\rho = \sum_{\psi} P_{\psi} |\psi\rangle \langle \psi|$$

is called density operator. In a particular case where all  $P_{\psi}$  are zero except the one for a state  $|\psi_0\rangle$  then

$$\rho = |\psi_0\rangle \langle \psi_0|$$

and state is called a Pure state. It follows from the conservation of probability that  $Tr(\rho) = 1$ . For a pure state

$$Tr(\rho^2) = 1$$

For mixed case

$$Tr(\rho^2) < 1$$

### 1.15 EQUATION OF MOTION FOR DENSITY OPERATOR

$$\begin{aligned}\rho &= \sum_{\psi} P_{\psi} |\psi\rangle \langle \psi| \\ \dot{\rho} &= \sum_{\psi} P_{\psi} [|\dot{\psi}\rangle \langle \psi| + |\psi\rangle \langle \dot{\psi}|]\end{aligned}$$

From Schrodinger equation, we know that

$$|\dot{\psi}\rangle = \frac{1}{i\hbar} H|\psi\rangle$$

Also

$$\langle \dot{\psi}| = -\frac{1}{i\hbar} \langle \psi| H$$

Using these values, we get

$$\begin{aligned}\dot{\rho} &= \frac{1}{i\hbar} \sum_{\psi} P_{\psi} [H|\psi\rangle \langle \psi| - |\psi\rangle \langle \psi| H] \\ &= \frac{1}{i\hbar} [H\rho - \rho H]\end{aligned}$$

where  $\rho$  and  $H$  are operators.

$$\dot{\rho} = \frac{1}{i\hbar} [H, \rho]$$

It is called “Liouville equation” or “von Neumann equation” and it is equivalent to Schrodinger , but more general (because it has quantum mechanical as well as statistical aspect). In the above equation we have not included the decay of atomic levels due spontaneous emission. The excited atomic levels can also decay because of collision and other phenomena. The finite life time of the atomic level can be dicribed by adding phenominalogical decay terms to the density operator.

The decay rates can be incorporated in equation by a relaxation matrix  $\Gamma$ , which is defined by the equation

$$\Gamma_{nm} = \langle n | \Gamma | m \rangle = \gamma_n \delta_{nm}$$

$$\dot{\rho} = -\frac{i}{\hbar} [H, \rho] - \frac{1}{2} \{\Gamma, \rho\}; \quad \{\Gamma \rho + \rho \Gamma\} = \{\Gamma, \rho\}$$

Equation of motion for the density matrix elements is

$$\dot{\rho}_{ij} = \frac{1}{i\hbar} \sum_k [H_{ik} \rho_{kj} - \rho_{ik} H_{kj}] - \frac{1}{2} \sum_k [\Gamma_{ik} \rho_{kj} + \rho_{ik} \Gamma_{kj}]$$

## 1.16 TWO LEVEL ATOM

$$\begin{aligned} |\psi\rangle &= c_a(t) |a\rangle + c_b(t) |b\rangle \\ \rho &= |\psi\rangle \langle\psi| \\ \langle\psi| &= c_a^*(t) \langle a| + c_b^*(t) \langle b| \\ \rho &= |\psi\rangle \langle\psi| = |c_a(t)|^2 |a\rangle \langle a| + c_a(t) c_b^*(t) |a\rangle \langle b| + c_a^*(t) c_b(t) |b\rangle \langle a| + |c_b(t)|^2 |b\rangle \langle b| \\ \rho_{aa} &= \langle a | \rho | a \rangle = |c_a|^2 \quad \text{probability of upper state} \\ \rho_{bb} &= \langle b | \rho | b \rangle = |c_b|^2 \quad \text{probability of lower state} \\ \rho_{ab} &= c_a c_b^* \quad \text{is propotional to dipole moment} \\ \rho_{ba} &= c_b c_a^* = \rho_{ab}^* \end{aligned}$$

In matrix form

$$\rho = \begin{pmatrix} |c_a|^2 & c_a c_b^* \\ c_a^* c_b & |c_b|^2 \end{pmatrix}$$

$$P(z, t) = c_a c_b^* p_{ba} + c.c = \rho_{ab}(z, t) p_{ba} + c.c$$

In spiner notation,

$$\begin{aligned} |\psi\rangle &= \begin{pmatrix} c_a \\ c_b \end{pmatrix} & \langle\psi| &= \begin{pmatrix} c_a^* & c_b^* \end{pmatrix} \\ \rho &= \begin{pmatrix} c_a \\ c_b \end{pmatrix} \begin{pmatrix} c_a^* & c_b^* \end{pmatrix} = \begin{pmatrix} |c_a|^2 & c_a c_b^* \\ c_a^* c_b & |c_b|^2 \end{pmatrix} \end{aligned}$$

## 1.17 EQUATION OF MOTION FOR DENSITY MATIRX ELEMENTS

Consider  $i = a, j = a$

$$\dot{\rho}_{aa} = \frac{1}{i\hbar} \sum_{k=a,b} [H_{ak} \rho_{ka} - \rho_{ak} H_{ka}] - \frac{1}{2} \sum_{k=a,b} [\Gamma_{ak} \rho_{ka} + \rho_{ak} \Gamma_{ka}]$$

using this

$$\begin{aligned}
\Gamma_{nm} &= \langle n|\Gamma|m\rangle = \gamma_n \delta_{nm} \quad \text{and} \\
H &= H_o + \gamma \\
\dot{\rho}_{aa} &= \frac{1}{i\hbar} \sum_{k=a,b} [(H_o)_{ak} \rho_{ka} - \rho_{ak} (H_o)_{ka}] - \frac{1}{2} [\gamma_a \rho_{aa} + \rho_{aa} \gamma_a] \\
&\quad + \frac{1}{i\hbar} \sum_{k=a,b} [V_{ak} \rho_{ka} - \rho_{ak} V_{ka}] \\
(H_o)_{ab} &= \langle a|H_o|b\rangle = E_b \langle a|b\rangle = 0 \\
(H_o)_{aa} &= \langle a|H_o|a\rangle = E_a \quad \text{and} \quad V_{aa}=V_{bb}=0 \\
\dot{\rho}_{aa} &= -\gamma_a \delta_{aa} + \frac{1}{i\hbar} \sum_{k=a,b} [V_{ab} \rho_{ba} - \rho_{ab} V_{ba}] \\
\dot{\rho}_{bb} &= -\gamma_b \delta_{bb} + \frac{1}{i\hbar} [V_{ba} \rho_{ab} - \rho_{ba} V_{ab}] \\
\dot{\rho}_{ab} &= -(i\omega_o + \gamma_{ab}) \delta_{ab} + \frac{1}{i\hbar} [V_{ab} \rho_{bb} - \rho_{aa} V_{ab}] \\
&\quad \text{where} \\
\gamma_{ab} &= \frac{1}{2} (\gamma_a + \gamma_b) \quad \text{and} \quad \omega_o = \frac{1}{\hbar} (E_a - E_b)
\end{aligned}$$

The population of excited level decays in time because of spontaneous emission. In soome cases the upper level decays to ground state lower level then

$$\dot{\rho}_{aa} = -\Gamma \rho_{aa} + \frac{1}{i\hbar} [V_{ab} \rho_{ba} - \rho_{ab} V_{ba}]$$

and

$$\dot{\rho}_{bb} = \Gamma \rho_{bb} + \frac{1}{i\hbar} [V_{ba} \rho_{ab} - \rho_{ba} V_{ab}]$$

Where  $\Gamma$  is the upper-to-lower level decay constant.