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Density operator.

⇒ For a given physical system there exists a state vector $|\psi\rangle$ which contains 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 $\hat{O}$

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

In many situation, we dont know $|\psi\rangle$ but we know P_ψ i,e the probability of finding the system in $|\psi\rangle$. For such situations

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

It is called Quantum statistical system.

Using the completeness relation.

$$\sum_n |n\rangle\langle n| = 1$$

$$\langle\langle \hat{O}\rangle_{QM}\rangle_{em} = \sum_n \sum_\psi P_\psi \langle\psi|n\rangle\langle n|\hat{O}|\psi\rangle$$

$$= \sum_n \sum_\psi P_\psi \langle n|\hat{O}|\psi\rangle\langle\psi|n\rangle$$

$$= \sum_n \langle n|\hat{O}\sum_\psi P_\psi|\psi\rangle\langle\psi|n\rangle$$

$$= \sum_n \langle n|\hat{O}\rho|n\rangle$$

$$= \sum_n (\hat{O}\rho)_{nn} = \text{Sum of diagonal elements}$$

where

$$\rho = \sum_\psi P_\psi |\psi\rangle\langle\psi| \quad \text{density operator}$$

$$\Rightarrow \langle\langle \hat{O}\rangle_{QM}\rangle_{em} = \mathrm{Tr}(\hat{O}\rho) = \mathrm{Tr}(\rho\hat{O})$$

In a particular case where all P_ψ's are zero except the one for state $|\psi_0\rangle$, then we have a pure state i.e

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

From conservation of probability

$$\mathrm{Tr}(\rho) = 1$$

For pure state

$$\mathrm{Tr}(\rho) = \langle\psi_0|\psi_0\rangle = 1$$

$$\rho^2 = |\psi_0\rangle\langle\psi_0|\psi_0\rangle\langle\psi_0|$$
$$= |\psi_0\rangle\langle\psi_0|$$

$\Rightarrow$

$$\mathrm{Tr}\,\rho^2 = \langle\psi_0|\psi_0\rangle = 1$$

For mixed state.

$$\rho^2 = \sum_\psi P_\psi |\psi\rangle\langle\psi| \sum_\phi P_\phi |\phi\rangle\langle\phi|$$

$$= \sum_\psi \sum_\phi P_\psi P_\phi |\psi\rangle\underbrace{\langle\psi|\phi\rangle}_{\delta_{\psi,\phi}}\langle\phi|$$

$$= \sum_\psi P_\psi^2 |\psi\rangle\langle\psi|$$

$$\Rightarrow \mathrm{Tr}\,\rho^2 = \sum_\psi P_\psi^2 |\psi\rangle\langle\psi|$$

$$= \sum_\psi P_\psi^2 < 1$$

2) $\rho = |\psi_0\rangle\langle\psi_0|$ Pure state

$\Rightarrow$ $\rho = \sum_\psi P_\psi |\psi\rangle\langle\psi|$ Mixed case.

$Tr(\rho^2) = 1$ for pure state

$Tr(\rho^2) < 1$ mixed state.

<u>Equation of Motion for the density matrix</u>

As $\rho = \sum_\psi P_\psi |\psi\rangle\langle\psi|$

$$\dot{\rho} = \sum_\psi P_\psi \left[|\dot{\psi}\rangle\langle\psi| + |\psi\rangle\langle\dot{\psi}| \right]$$

From Schrodinger equation.

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

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

$$\Rightarrow \dot{\rho} = \sum_\psi P_\psi \left[-\frac{i}{\hbar} H |\psi\rangle\langle\psi| + |\psi\rangle \frac{i}{\hbar} \langle\psi| H \right]$$

Rearranging

$$\dot{\rho} = -\frac{i}{\hbar} H \sum_\psi P_\psi |\psi\rangle\langle\psi| + \frac{i}{\hbar} \sum_\psi P_\psi |\psi\rangle\langle\psi| H$$

$$\Rightarrow \quad \dot{\rho} = -\frac{i}{\hbar}\left[H\rho - \rho H\right] = -\frac{i}{\hbar}\left[H, \rho\right]$$

The finite life time of the atomic levels due to spontaneous emission, collisions and other phenomena can be described by adding phenomenological decay terms to the density operator.

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

where Γ = relaxation matrix

$$\dot{\rho} = -\frac{i}{\hbar}\left[H, \rho\right] - \frac{1}{2}\{\Gamma, \rho\}$$

$$\langle i|\dot{\rho}|j\rangle = -\frac{i}{\hbar}\langle i|[H,\rho]|j\rangle - \frac{1}{2}\langle i|\{\Gamma,\rho\}|j\rangle$$

$$= -\frac{i}{\hbar}\langle i|H\rho - \rho H|j\rangle - \frac{1}{2}\langle i|\Gamma\rho + \rho\Gamma|j\rangle$$

$$= -\frac{i}{\hbar}\langle i|H\rho|j\rangle + \frac{i}{\hbar}\langle i|\rho H|j\rangle - \frac{1}{2}\langle i|\Gamma\rho|j\rangle$$

$$- \frac{1}{2}\langle i|\rho\Gamma|j\rangle$$

using $\sum_k |k\rangle\langle k| = 1$

$$\langle i|\dot{\rho}|j\rangle = \sum_k \frac{-i}{\hbar}\left[\langle i|H|k\rangle\langle k|\rho|j\rangle - \langle i|\rho|k\rangle\langle k|H|j\rangle\right] - \frac{1}{2}\sum_k\left[\langle i|\Gamma|k\rangle\langle k|\rho|j\rangle + \langle i|\rho|k\rangle\langle k|\Gamma|j\rangle\right]$$

$\Rightarrow$

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

We use this formula in the treatment of many level systems.

<u>Two-level atom:</u>

$$|\psi\rangle = C_a(t)\,|a\rangle + C_b(t)\,|b\rangle$$

$$\langle\psi| = C_a^*(t)\langle a| + C_b^*(t)\langle b|$$

$$\rho = |\psi\rangle\langle\psi|$$

$$= \left(C_a(t)|a\rangle + C_b(t)|b\rangle\right)\left(C_a^*(t)\langle a| + C_b^*(t)\langle b|\right)$$

$$= C_a(t)\,C_a^*(t)\,|a\rangle\langle a| + C_a(t)\,C_b^*(t)\,|a\rangle\langle b| +$$

$$+ C_b(t)\,C_a^*(t)\,|b\rangle\langle a| + C_b(t)\,C_b^*(t)\,|b\rangle\langle b|$$

$$\Rightarrow \rho = |C_a(t)|^2 |a\rangle\langle a| + C_a(t) C_b^*(t) |a\rangle\langle b| +$$

$$+ C_b(t) C_a^*(t) |b\rangle\langle a| + |C_b(t)|^2 |b\rangle\langle b|$$

$\rho_{aa} = \langle a|\rho|a\rangle = |C_a(t)|^2 \Rightarrow$ Probability of state $|a\rangle$

$\rho_{bb} = \langle b|\rho|b\rangle = |C_b(t)|^2 \rightarrow$ " " " $|b\rangle$

$\rho_{ab} = \langle a|\rho|b\rangle = C_a C_b^* \rightarrow$ Proportional to dipole moment.

$\rho_{ba} = \langle b|\rho|a\rangle = C_b C_a^* = \rho_{ab}^*$

In matrix form.

$$\rho = \begin{pmatrix} |C_a(t)|^2 & C_a C_b^* \\ C_b C_a^* & |C_b|^2 \end{pmatrix} = \begin{pmatrix} \rho_{aa} & \rho_{ab} \\ \rho_{ba} & \rho_{bb} \end{pmatrix}$$

Expectation value of dipole moment

$$\langle P\rangle = \langle \psi | er | \psi\rangle$$

$$= \left(C_a^* \langle a| + C_b^* \langle b| \right) er \left(C_a |a\rangle + C_b |b\rangle \right)$$

$$= |C_a|^2 \overset{0}{\cancel{\langle a|er|a\rangle}} + C_a^* C_b \langle a|er|b\rangle +$$

$$+ C_b^* C_a \langle b|er|a\rangle + |C_b|^2 \overset{0}{\cancel{\langle b|er|b\rangle}}$$

$$= C_a^* C_b P_{ab} + C_b^* C_a P_{ba}$$

$\Rightarrow \mathbb{P}(z,t) = C_a C_b^* P_{ba} + c.c$

where $P(z,t) \Rightarrow$ Atomic Polarization.

$P(z,t) = \rho_{ab}(z,t) P_{ab} + \rho_{ba} P_{ba}$

In spinor notation:

$$|\psi\rangle = \begin{pmatrix} C_a \\ C_b \end{pmatrix} \qquad \langle\psi| = (C_a^* \quad C_b^*)$$

$$\rho = |\psi\rangle\langle\psi| = \begin{pmatrix} C_a \\ C_b \end{pmatrix} (C_a^* , C_b^*)$$

$$\rho = \begin{pmatrix} |C_a|^2 & C_a C_b^* \\ C_b C_a^* & |C_b|^2 \end{pmatrix}$$

Now consider equation of motion for density Matrix for two-level atom.

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

For $i = a$; $j = a$ and $k = a, b$.

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

$$\dot{\rho}_{aa} = \frac{-i}{\hbar}\sum_k \left[H_{ak}\rho_{ka} - \rho_{ak}H_{ka}\right] - \frac{1}{2}\left[\Gamma_{aa}\rho_{aa} + \rho_{aa}\Gamma_{aa} + \Gamma_{ab}\rho_{ba} + \rho_{ab}\Gamma_{ba}\right]$$

As $\Gamma_{nm} = \gamma_n \delta_{nm}$.

$$\Rightarrow \dot{\rho}_{aa} = \frac{-i}{\hbar}\sum_{k=a,b}\left[H_{ak}\rho_{ka} - \rho_{ak}H_{ka}\right] - \frac{1}{2}\left(\gamma_a\rho_{aa} + \gamma_a\rho_{aa}\right)$$

As

$$H = H_0 + V$$

$$\dot{\rho}_{aa} = -\gamma_a\rho_{aa} - \frac{i}{\hbar}\sum_{k=a,b}\left[H_{0_{ak}}\rho_{ka} - \rho_{ak}H_{0_{ak}}\right] + \cancel{\frac{A}{\hbar}}$$

$$- \frac{i}{\hbar}\sum_{k=a,b}\left[V_{ak}\rho_{ka} - \rho_{ak}V_{ka}\right]$$

$$= -\gamma_a\rho_{aa} - \frac{i}{\hbar}\left[H_{0_{aa}}\rho_{aa} + H_{0_{ab}}\rho_{ba} - \rho_{aa}H_{0_{aa}} - \rho_{ab}H_{0_{ab}}\right]$$

$$- \frac{i}{\hbar}\left[V_{aa}\rho_{aa} + V_{ab}\rho_{ba} - \rho_{aa}V_{aa} - \rho_{ab}V_{ba}\right]$$

$$= -\gamma_a\rho_{aa} - \frac{i}{\hbar}\left(E_a\rho_{aa} - E_a\rho_{aa}\right) - \frac{i}{\hbar}\left(V_{ab}\rho_{ba} - \rho_{ab}V_{ba}\right)$$

$$= -\gamma_a\rho_{aa} - \frac{i}{\hbar}\left(V_{ab}\rho_{ba} - \rho_{ab}V_{ba}\right) \qquad a)$$

Similary.

$$\dot{\rho}_{bb} = -\gamma_b\rho_{bb} - \frac{i}{\hbar}\left(V_{ba}\rho_{ab} - \rho_{ba}V_{ab}\right) \qquad b)$$

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

$$= -\frac{i}{\hbar}\sum_{k=a,b}\left[H_{ak}\rho_{kb} - \rho_{ak}H_{kb}\right] - \frac{1}{2}\left[\Gamma_{aa}\rho_{ab} + \Gamma_{ab}\rho_{bb} + \rho_{aa}\Gamma_{ab} + \rho_{ab}\Gamma_{bb}\right]$$

$$= -\frac{i}{\hbar}\sum_{k}\left[H_{ak}\rho_{kb} - \rho_{ak}H_{kb}\right] - \frac{1}{2}\left(\gamma_a\rho_{ab} + \gamma_b\rho_{ab}\right)$$

$$= -\frac{1}{2}\rho_{ab}(\gamma_a+\gamma_b) - \frac{i}{\hbar}\sum_{k=a,b}\left[H_{0ak}\rho_{kb} - \rho_{ak}H_{0kb}\right] - \frac{i}{\hbar}\sum_{k=a,b}\left[V_{ak}\rho_{kb} - \rho_{ak}V_{kb}\right]$$

$$= -\frac{1}{2}\rho_{ab}(\gamma_a+\gamma_b) - \frac{i}{\hbar}\left[(H_0)_{aa}\rho_{ab} + H_{0_{ab}}\rho_{bb} - \rho_{aa}H_{0_{ab}} - \rho_{ab}H_{0_{bb}}\right] - \frac{i}{\hbar}\left[V_{aa}\rho_{ab} + V_{ab}\rho_{bb} - \rho_{aa}V_{ab} - \rho_{ab}V_{bb}\right]$$

$$= -\frac{1}{2}\rho_{ab}(\gamma_a+\gamma_b) - \frac{i}{\hbar}\left[E_a\rho_{ab} - E_b\rho_{ab}\right] - \frac{i}{\hbar}\left(V_{ab}\rho_{bb} - \rho_{aa}V_{ab}\right)$$

Since $\gamma_{ab} = \dfrac{\gamma_a+\gamma_b}{2}$ and $\omega_0 = \dfrac{E_a - E_b}{\hbar}$

$$\Rightarrow \dot{\rho}_{ab} = -\gamma_{ab}\rho_{ab} - i\omega_0\rho_{ab} + \frac{i}{\hbar}\left[V_{ab}\rho_{aa} - V_{ab}\rho_{bb}\right]$$

As $V = -e r\cdot E \Rightarrow V_{ab} = -P_{ab}E$

& $V_{ba} = -P_{ba}E$

Putting this in equations ⓐ, ⓑ & ⓒ

$$\Rightarrow \dot{\rho}_{aa} = -\gamma_a \rho_{aa} - \frac{i}{\hbar}\left[-P_{ab} E \rho_{ba} + \rho_{ab} P_{ba} E\right]$$

$$= -\gamma_a \rho_{aa} + \frac{i}{\hbar}\left[P_{ab} E \rho_{ba} + c.c\right]$$

$$\dot{\rho}_{bb} = -\gamma_b \rho_{bb} + \frac{i}{\hbar}\left[P_{ab} E \rho_{ba} + c.c\right]$$

&

$$\dot{\rho}_{ab} = -(i\omega_0 + \gamma_{ab})\rho_{ab} - \frac{i}{\hbar}(\rho_{aa} - \rho_{bb}) P_{ab} E$$

These are the equations of motion for the density matrix elements of a two-level atom.

Population Matrix and it's equations of motion.

⇒ The interaction of a single atom with the single-mode field represents a simple but idealizied system.

⇒ Interaction of radiation field with a large number of atoms.

⇒ Consider the interaction of an E.M.F with a medium which consists of two-level atoms.

Density operator for an atom is written as:

$$\rho(z,t,t_0) = \sum_{\alpha,\beta} \rho_{\alpha,\beta}(z,t,t_0)\, |\alpha\rangle\langle\beta|$$

⇒ Shows that an atom excited to the state $\alpha,\beta = (a,b)$, at time 't_0' is described by $\rho(z,t,t_0)$ at time t and place z, that start interacting with field at an initial time t_0.

$\Rightarrow$ The state of the atom at the time of injection is described by.

$$\rho(z,t_0,t_0) = \sum_{\alpha,\beta} \rho_{\alpha\beta}^{(0)} |\alpha\rangle\langle\beta|$$

$$\Rightarrow \quad \rho_{\alpha\beta}(z,t_0,t_0) = \rho_{\alpha\beta}^{(0)}$$

Population Matrix

The effect of all the atoms which are pumped at the rate $r_a(z,t_0)$ atoms per second per unit volume is obtain by summing over initial times.

$$\tilde{\rho}(z,t) = \int_{-\infty}^{t} dt_0 \; r_a(z,t_0) \; \rho(z,t,t_0)$$

putting value of $\rho(z,t,t_0)$ we get.

$$\tilde{\rho}(z,t) = \sum_{\alpha,\beta} \int_{-\infty}^{t} dt_0 \; r_a(z,t_0)\, \rho_{\alpha\beta}(z,t,t_0) \times |\alpha\rangle\langle\beta|$$

Assume:

i, $r_a(z,t_0) = r_a$ — uniform rate of pumping.

ii, Atoms are pumped in level $|a\rangle$ & $|b\rangle$

The macroscopic polarization of the medium $P(z,t)$ will be.

$$P(z,t) = \int_{-\infty}^{t} dt_0 \; r_a \, Tr\left[er\, \rho(z,t,t_0)\right]$$

putting value of $\rho(z,t,t_0)$ and performing trace.

$$P(z,t) = \sum_{\alpha,\beta} \int_{-\infty}^{t} dt_0 \; r_a \; \rho_{\alpha\beta}(z,t,t_0) \langle\beta|er|\alpha\rangle$$

For a two-level atom with

$$p_{ab} = p_{ba} = p = er$$

we get.

$$P(z,t) = p\left[\tilde{\rho}_{ab}(z,t) + c.c\right]$$

where

$$\tilde{\rho}_{ab}(z,t) = \int_{-\infty}^{t} dt_0 \, r_a \, \rho_{ab}(z,t,t_0)$$

The off-diagonal elements of the population matrix determine the macro-scopic Polarization.

The equations of motion for the elements of the population matrix can be obtained by taking the time derivative of population matrix

As $p(t) = \int_0^t q(t')\,dt' \Rightarrow \dot{p}(t) = q(t')\Big]_{t'=t} + \int_0^t \frac{\dot{q}(t')}{dt}$

we get

$$\dot{\rho}(z,t) = \sum_{\alpha,\beta} r_a \rho_{\alpha,\beta}(z,t,t)|\alpha\rangle\langle\beta| + \sum_{\alpha,\beta}\int_{-\infty}^{t} dt_0 \times$$
$$\times\, r_a(z,t_0)\, \dot{\rho}_{\alpha\beta}(z,t,t_0)\, |\alpha\rangle\langle\beta|$$

→ As we assumed no off-diagonal excitation

$$\Rightarrow \rho_{ij}(z,t,t) = \delta_{i\alpha}\delta_{j\alpha}$$

$\rho_{aa}(z) = \delta_{a\alpha}\delta_{a\alpha}$

$\rho_{bb} = \delta_{b\alpha}\delta_{b\alpha}$

that is if atoms are incoherently excited to level $|a\rangle$ and $|b\rangle$ at a constt. rate r_a $\left(\rho_{ab}^{(0)} = \rho_{ba}^{(0)} = 0\right)$

The equations of motion for the elements of the population matrix

$$\dot{\tilde{\rho}}_{aa} = \sum_{\alpha,\beta} r_a \rho_{\alpha,\beta}\langle a|\alpha\rangle\langle\beta|a\rangle + \sum_{\alpha,\beta}\int_{-\infty}^{t} dt_0\, r_a\, \dot{\rho}_{\alpha\beta}(z,t,t_0) \times \langle a|\alpha\rangle\langle\beta|a\rangle$$

$$\dot{\tilde{\rho}} = r_a \rho_{aa} + \int_{-\infty}^{t} dt_0\, r_a\, \dot{\rho}_{aa}(z,t_0,t)$$ putting $\dot{\rho}_{aa}$

⇒ from Last Lecture

$$\dot{\tilde{\rho}}_{aa} = r_a \rho_{aa} - \gamma_a \tilde{\rho}_{aa} - \frac{i}{\hbar}\left[V_{ab}\tilde{\rho}_{ba} - c.c\right]$$

where

$$\tilde{\rho}_{aa} = \int_{-\infty}^{t} dt_0 \, r_a \, \rho_{aa}(z,t,t_0)$$

Define $\lambda_a = r_a \rho_{aa}^{(0)}$

$\lambda_b = r_a \rho_{bb}^{(0)}$

$\Rightarrow$

$$\dot{\rho}_{aa} = \lambda_a - \gamma_a \rho_{aa} - \frac{i}{\hbar}\left[V_{ab}\rho_{ba} - c.c\right]$$

$$\dot{\rho}_{bb} = \lambda_b - \gamma_b \rho_{bb} + \frac{i}{\hbar}\left[V_{ab}\rho_{ba} - c.c\right]$$

$$\dot{\rho}_{ab} = -\left(i\omega_0 + \gamma\right)\rho_{ab} + \frac{i}{\hbar} V_{ab}\left[\rho_{aa} - \rho_{bb}\right]$$