# Density Matrix Description of 2-Level Atoms

## More about the Density Matrix

Let $|\psi\rangle = \sum_j c_j |u_j\rangle$ , where $\{|u_j\rangle\}$ is a basis and the index $k$ labels members of the ensemble

**Populations:** (real-valued) $\quad \rho_{nn} = \langle c_n^{(k)} c_n^{(k)*} \rangle_k = \langle |c_j^{(k)}|^2 \rangle_k$

**Bayesianist:**
Single system: $\rho_{nn}$ is prob of observing the state $|u_n\rangle$

**Frequentist:**
Ensemble: The state $|u_n\rangle$ occurs with frequency $\rho_{nn}$

**Coherences:** (complex-valued) $\quad \rho_{np} = \langle c_n^{(k)} c_p^{(k)*} \rangle_k \qquad \rho_{pn} = \rho_{pn}^*$

**Note:** Defining $c_q = |c_q| e^{i\theta_q}$ we have

$$|\langle c_n^{(k)} c_p^{(k)*} \rangle_k| = |\langle |c_n^{(k)}||c_p^{(k)}| e^{i(\theta_n^{k} - \theta_p^{(k)})} \rangle_k| \le |\langle |c_n^{(k)}||c_p^{(k)*}| \rangle_k|$$

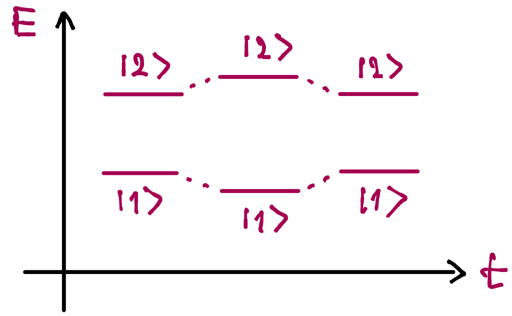
It follows that

$\rho_{np}\rho_{pn} \le \rho_{nn}\rho_{pp}$

with = for pure states

$$\rho = \begin{pmatrix} \rho_{nn} & \cdots & \rho_{np} \\ \vdots & \ddots & \vdots \\ \rho_{pn} & \cdots & \rho_{pp} \end{pmatrix}$$

**Example:** 2-level atom w/random perturbations




Perturbing events cause random phase shifts $e^{i\theta}$ between states.

The ensemble average $\quad \rho_{np} = \langle c_n c_p^* e^{i\theta} \rangle_k$

is reduced by the randomly fluctuating phase

**Dipole Radiation:**

$$\langle \hat{\vec{p}} \rangle = Tr[\rho \hat{\vec{p}}] = Tr\left[\begin{pmatrix} \rho_{11} & \rho_{12} \\ \rho_{21} & \rho_{22} \end{pmatrix}\begin{pmatrix} 0 & \vec{p}_{12} \\ \vec{p}_{21} & 0 \end{pmatrix}\right]$$

$$= \rho_{12}\vec{p}_{21} + \rho_{21}\vec{p}_{12} = 2Re[\rho_{12}\vec{p}_{21}]$$

For an ensemble of pure states w/different $\theta$

$$\langle \hat{\vec{p}} \rangle = 2\sum_k p_k \underbrace{Re[\rho_{12}^{(k)} \vec{p}_{21}]}$$

Oscillating dipole w/phase that varies between atoms with different perturbation history

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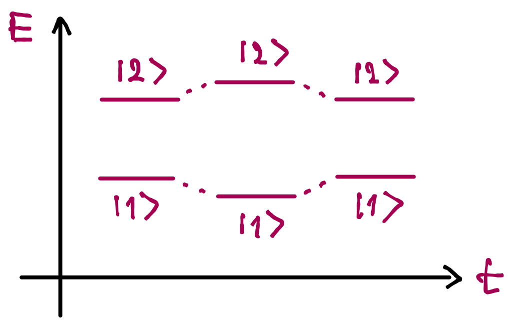


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## Time Evolution of the Density Matrix

**Challenge**: We need "equations of motion" that combine the Schrödinger Equation with the effect of processes that can change $Tr\,\rho^2$ (measure of purity)

**Approach**: We do not have time for a rigorous derivation, so will rely on plausible arguments to justify the equations

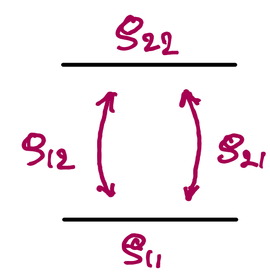
**Schrödinger Evolution**: In general, we have

$$\dot{\rho} = -\frac{i}{\hbar}[H, \rho] = -\frac{i}{\hbar}(H\rho - \rho H)$$

matrix elements

$$\dot{\rho}_{nm} = -\frac{i}{\hbar} \sum_{k=1,2} (H_{nk} \rho_{km} - \rho_{nk} H_{km})$$

2-Level Atom ⇨ { 2 populations, 2 coherences }



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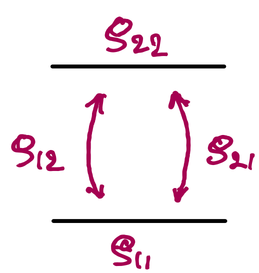


## Consider the 2-Level Rabi problem with

$$H = H_0 + V \quad \& \quad V_{12} = \frac{1}{2}\hbar\chi_{12}e^{-i\omega t} + c.c.$$

$$H = \hbar\begin{pmatrix} 0 & \frac{1}{2}(\chi_{12}e^{-i\omega t} + \chi_{12}^* e^{i\omega t}) \\ \frac{1}{2}(\chi_{21}e^{-i\omega t} + \chi_{21}^* e^{i\omega t}) & \omega_{21} \end{pmatrix}$$

Set $\chi_{12} = \chi,\ \chi_{21} = \chi^*$, substitute $\rho_{12} = \tilde{\rho}_{12}e^{i\omega t}$

slow variable

(Pure state ⇒ $\rho_{12} = a_1 a_2^* = c_1(c_2 e^{-i\omega t})$)

Substitute in $(*)$, make RWA, and drop $\sim$

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Rabi Eqs. for pure and mixed states

End 02-13-2024

Begin 02-15-2024

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Types of events

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## Simple Model of Elastic Collisions

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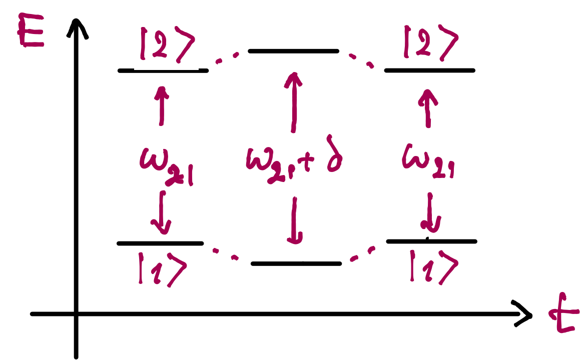


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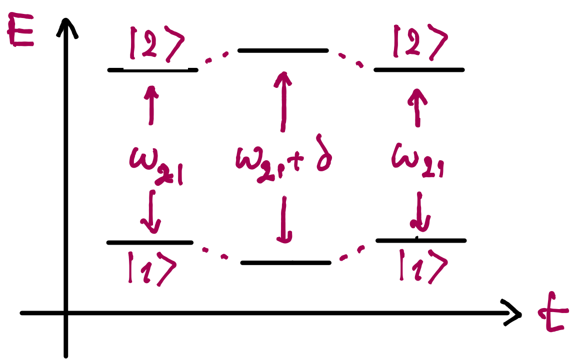


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## Evolution of coherence (fast variables)

$$\dot{\rho}_{12} = -i\left[\omega_{21} + \delta\omega(t)\right]\rho_{12}$$

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$$\Rightarrow \rho_{12}(t) = \rho_{12}(0)\, e^{-i\omega_{21}t}\, e^{-i\int_0^t dt'\,\delta\omega(t')}$$

We need the <u>ensemble average of</u> $\rho_{12}(t)$

<u>Assumptions</u>:

- From atom to atom $\delta\omega(t)$ is a Gaussian Random Variable
- Averaged over the ensemble $\langle \delta\omega(t)\rangle_{\mathcal{E}} = 0$
- Collisions have no memory over time,

$$\langle \delta\omega(t)\,\delta\omega(t')\rangle_t = \frac{2}{\tau}\,\delta(t-t')$$

⬇

Can show that, averaged over time and the ensemble

$$\left\langle e^{-i\int_0^t dt'\,\delta\omega(t')}\right\rangle_{\mathcal{E}} = e^{-t/\tau}$$

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It follows that: $\rho_{12}(t) = \rho_{12}(0)\, e^{-i\omega_{21}t}\, e^{-t/\tau}$

Add this decay to the equation of motion to get

$$\boxed{\dot{\rho}_{12} = (\dot{\rho}_{12})_{S.E.} + (\dot{\rho}_{12})_{E.C.} = -(i\omega_{21} - 1/\tau)\rho_{12}}$$

## Simple Model of Inelastic Collisions

As modeled by, e. g., Milloni & Eberly, this is a steady loss of atoms

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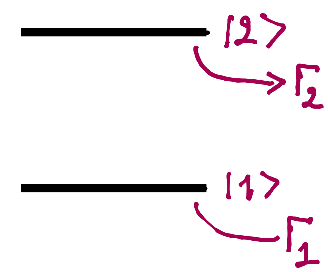


This is strange because $Tr\,\rho(t)$ is not preserved

Convenient when working with quantities

$$N\langle \vec{\mu}\rangle \propto N(\vec{\mu}_{12}\rho_{21} + \vec{\mu}_{21}\rho_{12})$$

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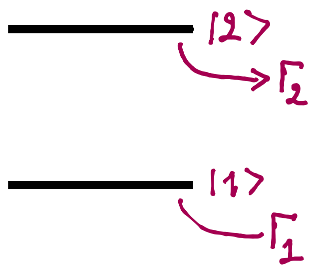


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## Effect on probability amplitudes

**Populations are ensemble averages of the type**

$$\rho_{11}(t) = \langle |a_1(t)|^2 \rangle = \langle |a_1(0)|^2 \rangle e^{-\Gamma_1 t}$$

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**When the populations decay, the averages of the probability amplitudes must decay accordingly,**

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**Thus, for the coherences**

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**This gives us**

$$\boxed{\dot{\rho}_{12} = (\dot{\rho}_{22})_{S.E.} \underbrace{- 1/\tau\, \rho_{12}}_{\text{elastic}} \underbrace{- \frac{\Gamma_1 + \Gamma_2}{2} \rho_{12}}_{\text{inelastic}}}$$

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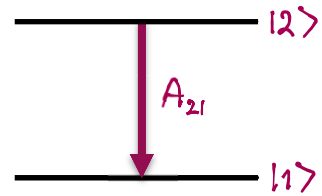
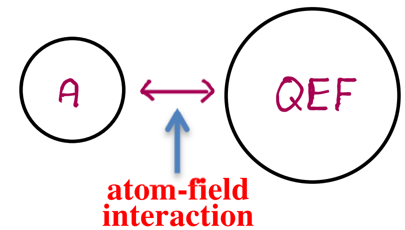
## Spontaneous Decay

This process occurs due to interaction between the Atom and the Quantized Electromagnetic Field




## Warm-up: A Bayesian recipe for Mixed States

Alice has two 2-level atoms in the ground state.

**Step (1)** She applies a Hamiltonian that drives the evolution

$$|1\rangle_A |1\rangle_B \rightarrow a_1 |1\rangle_A |1\rangle_B + a_2 |2\rangle_A |2\rangle_B$$

**Step (2)** She gives atom B to Bob and asks him to measure if it is in $|1\rangle_B$ or $|2\rangle_B$ and keep the result secret forever.

**Result:** Alice now has a 2-level atom in the state

$$\rho = |a_1|^2 |1\rangle_{BB}\langle 1| + |a_2|^2 |2\rangle_{BB}\langle 2|$$

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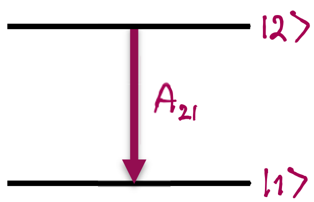


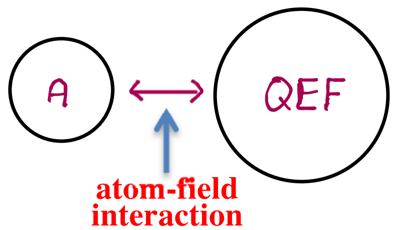


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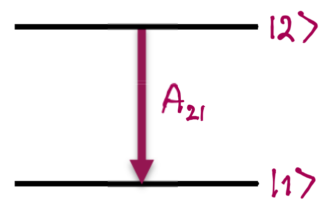


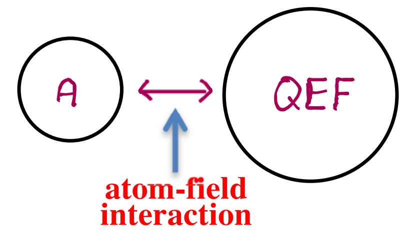


## Final OPTI 544 Lectures:

$|\psi(0)\rangle = |2\rangle_A |vac\rangle_{QEF}$ ⇨ evolution over time $t$

$$|\psi(t)\rangle = C_{2,0}(t)|2\rangle_A|vac\rangle_{QEF} + \sum_k C_{1,1k}(t)|1\rangle_A|n_k=1\rangle_{QEF}$$

photon "in the atom" photon in field mode $k$

Cannot recover info in continuum of field modes

Probability $|C_{2,0}(t)|^2$ of having no decay

Probability $\sum_k |C_{1,1k}(t)|^2$ of having decay

No Coherence established between states $|1\rangle, |2\rangle$

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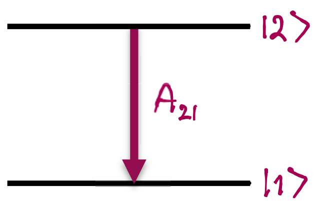


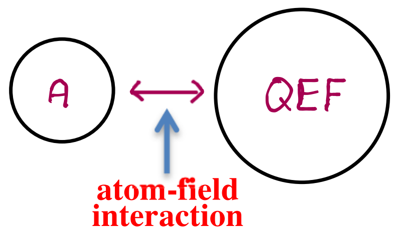


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**Conclusion: Decay moves population $|2\rangle \to |1\rangle$ at rate $A_{21}$, damps coherence at rate $A_{21}/2$**

$$\dot{\rho}_{11} = A_{21}\rho_{22}\,, \quad \dot{\rho}_{22} = -A_{21}\rho_{11}$$

$$\dot{\rho}_{12} = -\frac{A_{21}}{2}\rho_{12} = \dot{\rho}_{21}^*$$

### Putting it all together:

$$\dot{\rho}_{11} = -\Gamma_1\rho_{11} + A_{21}\rho_{22} - \frac{i}{2}(\chi\rho_{12} - \chi^*\rho_{21})$$

$$\dot{\rho}_{22} = -\Gamma_2\rho_{22} - A_{21}\rho_{22} + \frac{i}{2}(\chi\rho_{12} - \chi^*\rho_{21})$$

$$\dot{\rho}_{12} = (i\Delta - \beta)\rho_{12} + \frac{i\chi^*}{2}(\rho_{22} - \rho_{11}) = \dot{\rho}_{21}^*$$

where $\beta = \frac{1}{\tau} + \frac{A_{21}}{2} + \frac{\Gamma_1 + \Gamma_2}{2}$

**These are our desired Density Matrix Equations of Motion**

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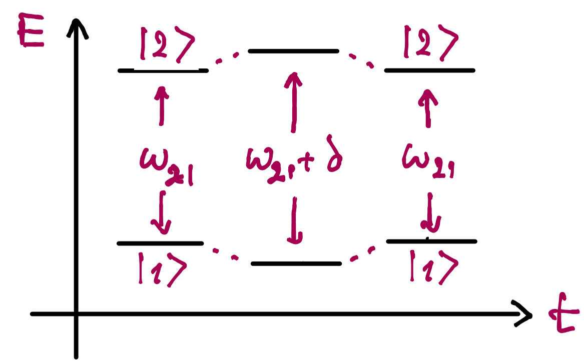


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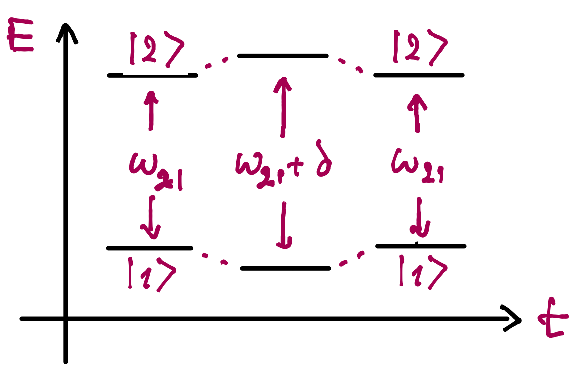


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**Assumptions**:

- From atom to atom $\delta\omega(t)$ is a Gaussian Random Variable
- Averaged over the ensemble $\langle\delta\omega(t)\rangle_{\mathcal{E}} = 0$
- Collisions have no memory over time,

$$\langle\delta\omega(t)\,\delta\omega(t')\rangle_t = \frac{2}{\tau}\,\delta(t-t')$$

Can show that, averaged over time and the ensemble

$$\left\langle e^{-i\int_0^t dt'\,\delta\omega(t')}\right\rangle_{\mathcal{E}} = e^{-t/\tau}$$

# Density Matrix Description of 2-Level Atoms

## Evolution of coherence (fast variables)

$$\dot\rho_{12} = -i\left[\omega_{21} + \delta\omega(t)\right]\rho_{12}$$

collisional history

$$\Rightarrow \rho_{12}(t) = \rho_{12}(0)\, e^{-i\omega_{21}t}\, e^{-i\int_0^t dt'\,\delta\omega(t')}$$

We need the <u>ensemble average of</u> $\rho_{12}(t)$

<u>Assumptions</u>:

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It follows that: $\rho_{12}(t) = \rho_{12}(0)\, e^{-i\omega_{21}t}\, e^{-t/\tau}$

Add this decay to the equation of motion to get

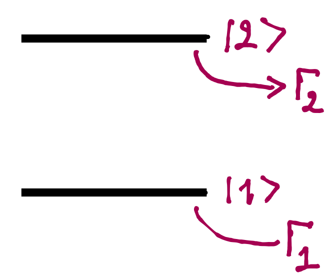
$$\boxed{\dot\rho_{12} = (\dot\rho_{12})_{S.E.} + (\dot\rho_{12})_{E.C.} = -(i\omega_{21} - 1/\tau)\rho_{12}}$$

## Simple Model of Inelastic Collisions

As modeled by, e. g., Milloni & Eberly, this is a steady loss of atoms

$$\dot\rho_{11} = (\dot\rho_{11})_{S.E.} - \Gamma_1\rho_{11}$$

$$\dot\rho_{22} = (\dot\rho_{22})_{S.E.} - \Gamma_2\rho_{22}$$




This is strange because $Tr\,\rho(t)$ is not preserved

Convenient when working with quantities

$$N\langle\vec\mu\rangle \propto N(\vec\mu_{12}\rho_{21} + \vec\mu_{21}\rho_{12})$$

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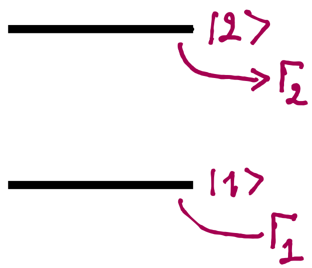


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$$N\langle \vec{p} \rangle \propto N(\vec{p}_{12}\rho_{21} + \vec{p}_{21}\rho_{12})$$

## Effect on probability amplitudes

Populations are ensemble averages of the type

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When the populations decay, the averages of the probability amplitudes must decay accordingly,

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Thus, for the coherences

$$\rho_{12}(t) = \langle a_1(t) a_2(t)^* \rangle = \langle a_1(0) a_2(0)^* \rangle e^{-\Gamma_1/2\, t} e^{-\Gamma_2/2\, t}$$

This gives us

$$\boxed{\dot{\rho}_{12} = (\dot{\rho}_{22})_{S.E.} \underbrace{- 1/\tau\, \rho_{12}}_{\text{elastic}} \underbrace{- \frac{\Gamma_1 + \Gamma_2}{2} \rho_{12}}_{\text{inelastic}}}$$

# Density Matrix Description of 2-Level Atoms

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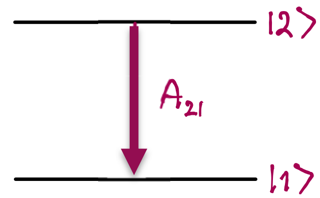
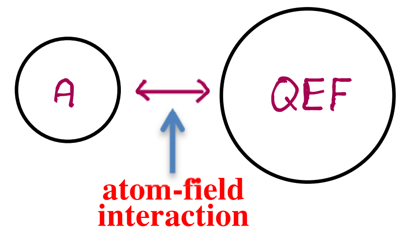
## Spontaneous Decay

This process occurs due to interaction between the Atom and the Quantized Electromagnetic Field




## Warm-up: A Bayesian recipe for Mixed States

Alice has two 2-level atoms in the ground state.

**Step (1)** She applies a Hamiltonian that drives the evolution

$$|1\rangle_A |1\rangle_B \rightarrow a_1 |1\rangle_A |1\rangle_B + a_2 |2\rangle_A |2\rangle_B$$

**Step (2)** She gives atom B to Bob and asks him to measure if it is in $|1\rangle_B$ or $|2\rangle_B$ and keep the result secret forever.

**Result:** Alice now has a 2-level atom in the state

$$\rho = |a_1|^2 |1\rangle_{BB}\langle 1| + |a_2|^2 |2\rangle_{BB}\langle 2|$$

# Density Matrix Description of 2-Level Atoms

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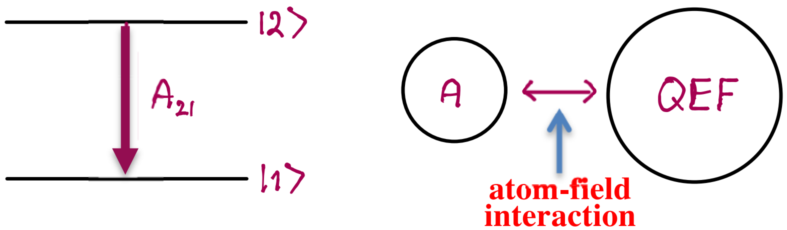


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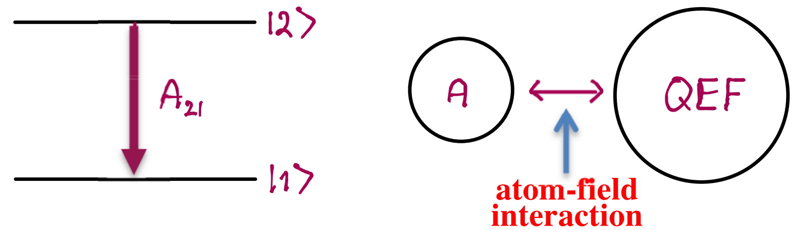



### Final OPTI 544 Lectures:

$|\psi(0)\rangle = |2\rangle_A |vac\rangle_{QEF}$ ⇨ evolution over time *t*

$$|\psi(t)\rangle = C_{2,0}(t)\,|2\rangle_A |vac\rangle_{QEF} + \sum_k C_{1,1k}(t)\,|1\rangle_A |n_k = 1\rangle_{QEF}$$

photon "in the atom" — photon in field mode *k*

Cannot recover info in continuum of field modes

Probability $|C_{2,0}(t)|^2$ of having **no decay**

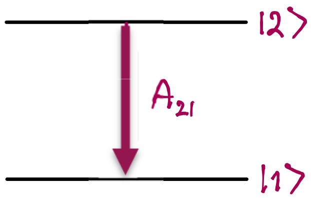
Probability $\sum_k |C_{1,1k}(t)|^2$ of having **decay**

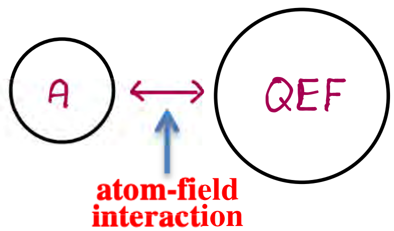
<u>No Coherence</u> established between states $|1\rangle, |2\rangle$

# Density Matrix Description of 2-Level Atoms

## Spontaneous Decay

**This process occurs due to interaction between the Atom and the Quantized Electromagnetic Field**

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excitation in the atom — excitation in field mode $k$

**Cannot recover info in continuum of field modes**

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<u>No Coherence</u> established between states $|1\rangle, |2\rangle$

**Conclusion: Decay moves population $|2\rangle \rightarrow |1\rangle$ at rate $A_{21}$, damps coherence at rate $A_{21}/2$**

$$\dot{\rho}_{11} = A_{21}\rho_{22}, \quad \dot{\rho}_{22} = -A_{21}\rho_{22}$$

$$\dot{\rho}_{12} = -\frac{A_{21}}{2}\rho_{12} = \dot{\rho}_{21}^*$$

**Putting it all together:**

$$\dot{\rho}_{11} = -\Gamma_1 \rho_{11} + A_{21}\rho_{22} - \frac{i}{2}(\chi\rho_{12} - \chi^*\rho_{21})$$

$$\dot{\rho}_{22} = -\Gamma_2 \rho_{22} - A_{21}\rho_{22} + \frac{i}{2}(\chi\rho_{12} - \chi^*\rho_{21})$$

$$\dot{\rho}_{12} = (i\Delta - \beta)\rho_{12} + \frac{i\chi^*}{2}(\rho_{22} - \rho_{11}) = \dot{\rho}_{21}^*$$

where $\beta = \frac{1}{\tau} + \frac{A_{21}}{2} + \frac{\Gamma_1 + \Gamma_2}{2}$

**These are our desired Density Matrix Equations of Motion**

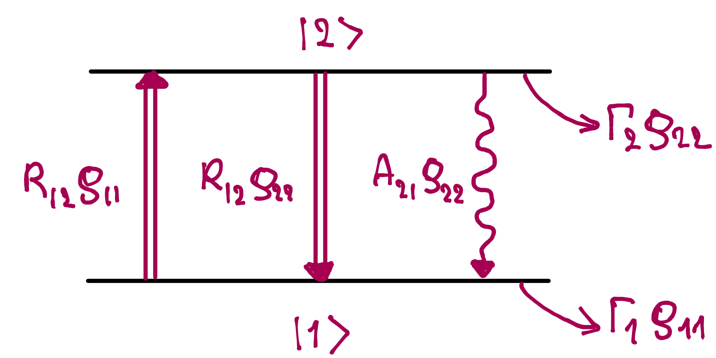
# Emission and Absorption – Population Rate Equations

**Note: The terms remaining after elimination of $\rho_{12}, \rho_{21}$ are commonly identified with induced or stimulated processes. They are proportional to $|X|^2, |E_0|^2$ and thus the intensity of the light field.**

**Def: Absorption Rate = Stimulated Emission Rate**

$$R_{12} = \frac{|X|^2 \beta/2}{\Delta^2 + \beta^2} = \frac{|\vec{r}_{12} \cdot \vec{\varepsilon} E_0/\hbar|^2 \beta/2}{(\omega_{21} - \omega)^2 + \beta^2}$$

**Schematic:**



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