

Tuesday, October 7, 2025

Density Matrix for modeling coherent & incoherent quantum dynamics

Definitions: $\rho = |\psi\rangle\langle\psi|$ for a wavefunction $|\psi\rangle$

$\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|$ for a statistical mixture of $|\psi_i\rangle$ states with probabilities p_i

Expectation value: $\langle A \rangle = \langle \psi | A | \psi \rangle = \text{Tr}(\rho A)$

Time evolution:

$$i\hbar \frac{d\rho}{dt} = [H, \rho]$$

notation:

$$\rho = \begin{pmatrix} \rho_{gg} & \rho_{ge} \\ \rho_{eg} & \rho_{ee} \end{pmatrix} = \begin{pmatrix} c_g c_g^* & c_g c_e^* \\ c_e c_g^* & c_e c_e^* \end{pmatrix}$$

Resonance Fluorescence - Optical Bloch Equations

The great advantage of the density matrix approach is that the decoherence that accompanies spontaneous emission can be easily added in:

Coherent evolution: $i\hbar \frac{d\rho}{dt} = [H, \rho]$

with $H = \begin{bmatrix} E_g & \frac{\hbar\Omega}{2} \cos(\omega_L t) \\ \frac{\hbar\Omega^*}{2} \cos(\omega_L t) & E_e \end{bmatrix}$ + RWA
+ rotating frame

or $H = H_{\text{dressed}} = \begin{bmatrix} \delta & \Omega/2 \\ \Omega^*/2 & 0 \end{bmatrix}$

Next, add in decoherence / spontaneous emission (decay rate γ),

$$\left\{ \begin{array}{l} \frac{d}{dt} \rho_{ee} = -\frac{i}{\hbar} [H, \rho]_{ee} - \gamma \rho_{ee} \\ \frac{d}{dt} \rho_{gg} = -\frac{i}{\hbar} [H, \rho]_{gg} + \gamma \rho_{ee} \\ \frac{d}{dt} \rho_{eg} = -\frac{i}{\hbar} [H, \rho]_{eg} - \frac{1}{2} \gamma \rho_{eg} \\ \frac{d}{dt} \rho_{ge} = -\frac{i}{\hbar} [H, \rho]_{ge} - \frac{1}{2} \gamma \rho_{ge} \end{array} \right. \quad \begin{array}{l} \text{Optical Bloch} \\ \text{equations} \end{array}$$

these equations are equivalent

$\Rightarrow$ Solve for $\rho_{gg}, \rho_{ee}, \rho_{eg}$ $\rightarrow$ all continuous quantities
↗ $\rho_{|g\rangle}$ ↗ $\rho_{|e\rangle}$ $\rightarrow$ wavefunction collapse is already included (due to decoherence)
 $\rightarrow$ average output of many measurements

For generalization to multi-level atoms and multiple lasers see: Margardt, Robinson, Hallberg JOSA B, 13, 1384 (1996).

We are interested in the steady state scattering rate:

$$\rightarrow \text{set } \frac{d}{dt} \rho_{ij} = 0 = \frac{-i}{\hbar} [H, \rho]_{ij} + \gamma \rho_{ij} \left(\frac{1}{2}\right)$$

choose appropriately

$\Rightarrow$ solve for ρ_{ij} .

$$\text{Scattering rate} = \gamma_{\text{scattering}} = \gamma \rho_e = \gamma \rho_{ee}$$

some work
(1 page-ish)

probability to be in the
excited state

$$\rho_g = |\langle g | \rho | g \rangle = \rho_{gg}$$

$$\rho_e = |\langle e | \rho | e \rangle = \rho_{ee}$$

$$= \frac{\rho_0}{1 + \rho_0 + \left(\frac{2\delta}{\gamma}\right)^2} \frac{\gamma}{2} = \gamma_{\text{scattering}}$$

where $\left\{ \begin{array}{l} \rho_0 = \text{saturation parameter} = \frac{\hbar^2}{I_{\text{sat}}} = \frac{2 |\Omega|^2}{\gamma^2} \\ I_{\text{sat}} = \frac{\pi \hbar c}{3 \lambda^2 \tau} = 1.6 \text{ mW/cm}^2 \text{ for } ^{87}\text{Rb (D}_2 \text{ line)} \\ \quad \quad \quad 780 \text{ nm} \end{array} \right.$

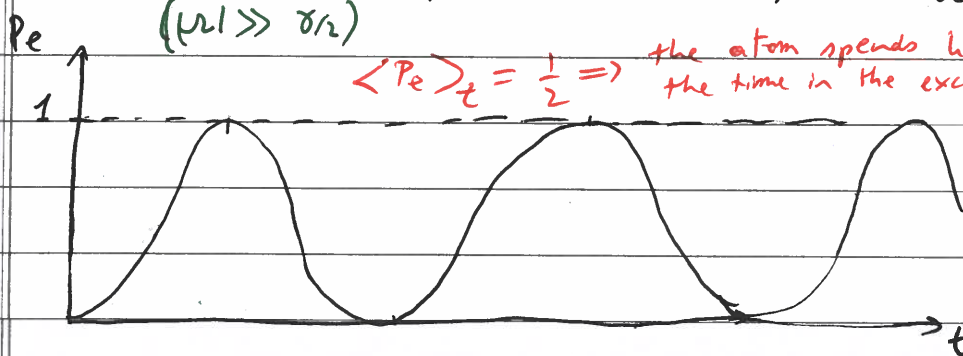
= intensity required to reach half of the maximum
average upper state population in steady state (i.e. $\frac{1}{4}$)

On Resonance: $\delta = 0$

Case I $\gg I_{\text{sat}}$, i.e. $\rho_0 \rightarrow +\infty$, then $\gamma_{\text{scattering}} = \frac{\gamma}{2} = 1.9 \times 10^6 \frac{\text{photons}}{\text{s}}$
($|\Omega| \gg \delta/2$)

$\langle \rho_e \rangle_t = \frac{1}{2} \Rightarrow$ the atom spends half
the time in the excited state.

rubidium



↑
agrees well
with experiment

(disagrees with
classical prediction)

Case: $I \ll I_{\text{sat}}$, i.e. $\rho_0 \rightarrow 0$, then $\sigma_{\text{scattering}} \approx \rho_0 \frac{\sigma}{2} \propto$ incident intensity
 $(|\Omega| \ll \gamma/2)$

good qualitative agreement with classical physics.

OFF - Resonance

Linewidth for $\rho_0 \rightarrow 0$: $\sigma_s = \frac{1}{1 + \left(\frac{2\delta}{\gamma}\right)^2} \rho_0 \frac{\sigma}{2}$
 (low intensity limit)

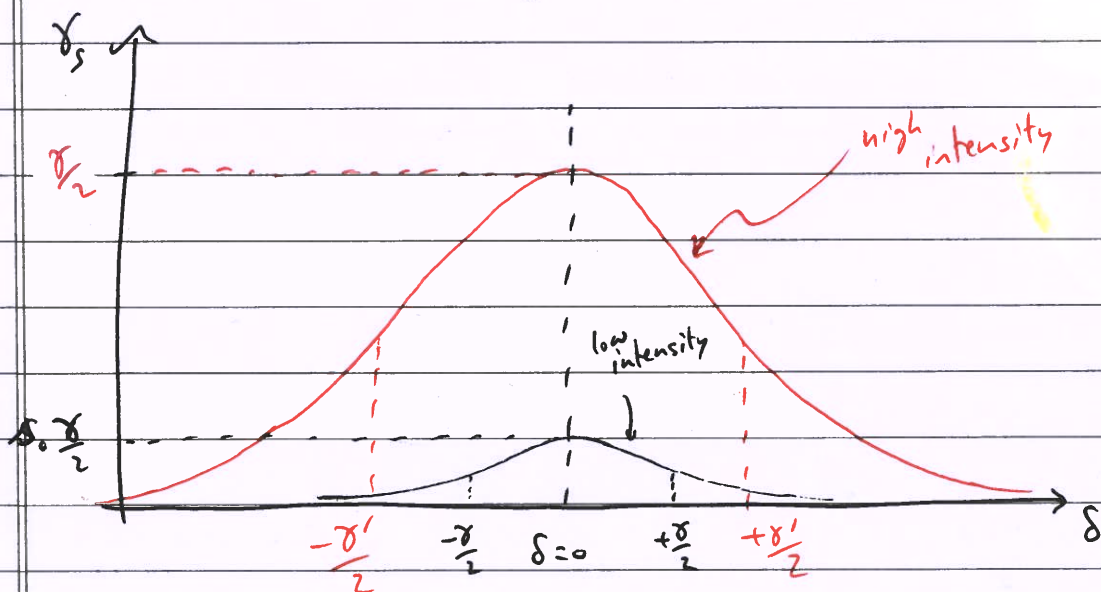
$\Rightarrow$ Lorentzian with FWHM = γ

Linewidth for $\rho_0 \rightarrow +\infty$
 (high intensity limit)

"power broadening"

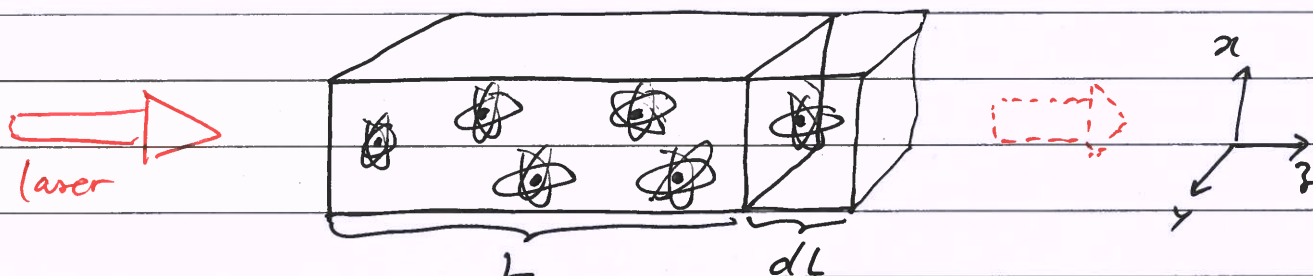
$$\sigma_s = \frac{\rho_0}{1 + \rho_0} \frac{1}{1 + \left(\frac{2\delta}{\gamma\sqrt{1+\rho_0}}\right)^2} \frac{\sigma}{2} \approx \frac{1}{1 + \left(\frac{2\delta}{\gamma'}\right)^2} \frac{\sigma}{2}$$

$\Rightarrow$ Lorentzian with FWHM = $\gamma' = \gamma\sqrt{1+\rho_0}$



Beer's law : Absorption in atomic vapor

Q: How is a laser attenuated as it travels through a gas of resonant atoms?



$$\text{gas density} = n = \frac{N_{\text{atoms}}}{\text{Volume}}$$

$$\text{Change in intensity} = dI = \frac{d\text{Power}}{\text{Area}} = - \frac{\hbar \omega_L \gamma_s}{A} n A dL$$

Area of laser beam (cross-section)

photons per atom
of atoms in "dL" volume

$$\Rightarrow \frac{dI}{dL} = -\hbar \omega_L \gamma_s n$$

$$\text{In the weak intensity limit: } \gamma_s = \frac{I}{I_{\text{sat}}} \cdot \frac{\gamma}{2} \quad (\text{on resonance})$$

$$\Rightarrow \frac{dI}{dL} = -\hbar \omega_L \frac{\gamma}{2} \frac{n}{I_{\text{sat}}} \cdot I = - \frac{3 \lambda^2}{2\pi} n I \quad (\text{on resonance})$$

$$= -\sigma_{\text{eg}} n I$$

σ_{eg} = cross-section on resonance

$$\Rightarrow I(z) = I_0 e^{-\sigma_{eg} n z}$$

Beer's law

note: optical depth = $\sigma_{eg} n z$

$$\hookrightarrow I = I_0 e^{-\text{optical depth}}$$

Application: Absorption imaging of cold atoms