APPPHYS383 Thursday 18 February 2010

Bloch Equations for a two-level atom

Recall the general relation between spin-1/2 operators and the Pauli matrices,

$$S_z = \frac{\hbar}{2}\sigma_z = \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad S_x = \frac{\hbar}{2}\sigma_x = \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad S_y = \frac{\hbar}{2}\sigma_y = \frac{\hbar}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

Here the matrix forms of the spin operators are written in a basis in which

$$|-_{z}\rangle \leftrightarrow \begin{pmatrix} 0\\1 \end{pmatrix}, |+_{z}\rangle \leftrightarrow \begin{pmatrix} 1\\0 \end{pmatrix},$$

where

$$S_{z}|-_{z}\rangle = -\frac{\hbar}{2}|-_{z}\rangle, \quad S_{z}|+_{z}\rangle = +\frac{\hbar}{2}|+_{z}\rangle.$$

The dimensionless matrices $\sigma_x, \sigma_y, \sigma_z$ satisfy the commutation relations

$$[\sigma_x, \sigma_y] = 2i\sigma_z, \quad [\sigma_y, \sigma_z] = 2i\sigma_x, \quad [\sigma_z, \sigma_x] = 2i\sigma_y.$$

In addition,

$$\mathrm{Tr}[\sigma_i \sigma_j] = 2\delta_{ij}$$

and

$$\sigma_x^2 = \sigma_y^2 = \sigma_z^2 = 1.$$

The Pauli matrices are both Hermitian and unitary.

If we switch now to considering a two-level atom whose pure states live in the Hilbert space spanned by orthonormal basis kets representing a ground state and excited state,

 $|\Psi\rangle \in \operatorname{span}\{|g\rangle, |e\rangle\},\$

we can use the matrix notation corresponding to

$$|g\rangle \leftrightarrow \begin{pmatrix} 0\\1 \end{pmatrix}, |e\rangle \leftrightarrow \begin{pmatrix} 1\\0 \end{pmatrix},$$

in which case we have

$$|e\rangle\langle e| \leftrightarrow \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \leftrightarrow \frac{1}{2}(1+\sigma_z), \quad \sigma \equiv |g\rangle\langle e| \leftrightarrow \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \leftrightarrow \frac{1}{2}(\sigma_x - i\sigma_y),$$

and so for example we can equate the usual Hamiltonian for the atomic internal state

$$H_{\rm atom} = \hbar \omega_{\rm at} |e\rangle \langle e|,$$

which is equivalent (by change of the origin of the energy scale) to

$$H_{\text{atom}} = \frac{1}{2}\hbar\omega_{\text{at}}(|e\rangle\langle e| - |g\rangle\langle g|) \leftrightarrow \frac{1}{2}\hbar\omega_{\text{at}}\sigma_z$$

This is then formally equivalent to the Hamiltonian for a spin-1/2 particle in a static field along the z-axis,

$$H = -\gamma S_z B_z = \omega_L S_z = \frac{1}{2} \hbar \omega_L \sigma_z$$

with the simple correspondence $\omega_L \leftrightarrow \omega_{at}$. Furthermore, for a rotating transverse magnetic field

$$\vec{B}_{\perp}(t) = b_1(\hat{x}\cos(\omega t) + \hat{y}\sin(\omega t))$$

the corresponding spin Hamiltonian can be written in the form

$$H = -\gamma b_1 (S_x \cos(\omega t) + S_y \sin(\omega t)) = \frac{1}{2} \hbar \Omega_1 (\sigma_x \cos(\omega t) + \sigma_y \sin(\omega_t))$$

$$\leftrightarrow \frac{1}{2} \hbar \Omega_1 \begin{pmatrix} 0 & \cos(\omega t) - i \sin(\omega t) \\ \cos(\omega t) + i \sin(\omega t) & 0 \end{pmatrix}$$

$$\leftrightarrow \frac{1}{2} \hbar \Omega_1 (e^{+i\omega t} \sigma + e^{-i\omega t} \sigma^{\dagger}),$$

which is identical in form to the usual Hamiltonian used to describe the response of a two-level atom to a harmonic driving field in the RWA.

It thus follows that the Bloch Equations that arise in the context of magnetic resonance can equally well be used to describe the response of a two-level atom to harmonic driving fields. When using the spin language and the Bloch sphere in reference to a two-level atom, one often speaks of the dimensionless version of the Bloch vector.

$$\vec{v} \equiv \langle \vec{\mathbf{\sigma}} \rangle = \frac{2}{\hbar} \langle \vec{\mathbf{S}} \rangle = \langle \sigma_x \rangle \hat{x} + \langle \sigma_y \rangle \hat{y} + \langle \sigma_z \rangle \hat{z},$$

as representing the state of a 'pseudo-spin' associated with the mapping

$$|-_z\rangle \leftrightarrow |g\rangle, |+_z\rangle \leftrightarrow |e\rangle$$

Rotating frame as a unitary transformation of the state space

In this section we will revisit the idea of transformation to a rotating frame and show how it can be performed via unitary transformation of the Hilbert space. We will have in mind a general scenario for a harmonically driven two-level system,

$$H = H_0 + H_1,$$

$$H_0 = \frac{1}{2}\hbar\omega_0\sigma_z, \quad H_1 = \frac{1}{2}\hbar\Omega_1 \left(e^{+i\omega t}\sigma + e^{-i\omega t}\sigma^{\dagger}\right).$$

Consider a general unitary transformation acting on the entire state space,

$$|\Psi'(t)\rangle \equiv U|\Psi(t)\rangle.$$

We can start from the Schrödinger Equation

$$i\hbar \frac{d}{dt} |\Psi(t)\rangle = H |\Psi(t)\rangle = H U^{-1} |\Psi'(t)\rangle$$

and simply apply the chain rule on the left-hand side to yield

$$\begin{split} i\hbar\frac{d}{dt}|\Psi(t)\rangle &= i\hbar\frac{d}{dt}(U^{-1}|\Psi'(t)\rangle) = i\hbar\left(\frac{dU^{-1}}{dt}|\Psi'(t)\rangle + U^{-1}\frac{d}{dt}|\Psi'(t)\rangle\right)\\ i\hbar U^{-1}\frac{d}{dt}|\Psi'(t)\rangle &= i\hbar\frac{d}{dt}|\Psi(t)\rangle - i\hbar\frac{dU^{-1}}{dt}|\Psi'(t)\rangle. \end{split}$$

Hence, combining the two expressions and multiplying through from the left by U, we obtain

$$i\hbar\frac{d}{dt}|\Psi'(t)\rangle = \left(UHU^{-1} - i\hbar U\frac{dU^{-1}}{dt}\right)|\Psi'(t)\rangle$$
$$\equiv H'|\Psi'(t)\rangle.$$

Recall that since U is unitary, $U^{-1} = U^{\dagger}$. Hence if we now specialize to the case U

$$= \exp(+i\omega\sigma_z t/2), \quad U^{\dagger} = \exp(-i\omega\sigma_z t/2),$$

we have

$$-i\hbar U \frac{dU^{-1}}{dt} = -i\hbar \exp(+i\omega\sigma_z t/2) \frac{d}{dt} \exp(-i\omega\sigma_z t/2) = -\frac{\hbar\omega}{2}\sigma_z,$$

where the final step follows from a power-series expansion of the operator exponential. Noting the commutation relations

$$\begin{bmatrix} \sigma^{\dagger}, \sigma_z \end{bmatrix} = \frac{1}{2} ([\sigma_x, \sigma_z] + i[\sigma_y, \sigma_z]) = \frac{1}{2} (-2i\sigma_y - 2\sigma_x) = -2\sigma^{\dagger},$$

$$[\sigma, \sigma_z] = \frac{1}{2} ([\sigma_x, \sigma_z] - i[\sigma_y, \sigma_z]) = \frac{1}{2} (-2i\sigma_y + 2\sigma_x) = 2\sigma,$$

we have

$$\begin{aligned} H' &= UHU^{-1} - i\hbar U \frac{dU^{-1}}{dt} \\ &= U(H_0 + H_1)U^{-1} - \frac{\hbar\omega}{2}\sigma_z \\ &= U\left(\frac{1}{2}\hbar\omega_0\sigma_z + \frac{1}{2}\hbar\Omega_1\left(e^{+i\omega t}\sigma + e^{-i\omega t}\sigma^{\dagger}\right)\right)U^{-1} - \frac{\hbar\omega}{2}\sigma_z \\ &= \frac{1}{2}\hbar\Delta\sigma_z + \frac{1}{2}\hbar\Omega_1\exp(+i\omega\sigma_z t/2)\left(e^{+i\omega t}\sigma + e^{-i\omega t}\sigma^{\dagger}\right)\exp(-i\omega\sigma_z t/2), \end{aligned}$$

where $\Delta \equiv \omega_0 - \omega$ and we have used the fact that $[\sigma_z, U^{-1}] = [\sigma_z, \exp(-i\omega\sigma_z t/2)] = 0$. Next we need to compute

$$\sigma^{\dagger} \exp(-i\omega\sigma_z t/2) = \sigma^{\dagger} \sum_{n=0}^{\infty} \frac{1}{n!} (-i\omega\sigma_z t/2)^n$$
$$= \sum_{n=0}^{\infty} \frac{1}{n!} (-i\omega t/2)^n (\sigma^{\dagger}\sigma_z^n)$$
$$= \sum_{n=0}^{\infty} \frac{1}{n!} (-i\omega t/2)^n (-1)^n \sigma^{\dagger}$$

 $= \exp(+i\omega t/2)\sigma^{\dagger},$

where in going from the second to the third line we have used the fact that

$$\sigma^{\dagger}\sigma_{z} = |e\rangle\langle g|(|e\rangle\langle e| - |g\rangle\langle g|) = -|e\rangle\langle g| = -\sigma^{\dagger}$$

Similarly,

$$\exp(+i\omega\sigma_z t/2)\sigma^{\mathsf{T}} = \exp(+i\omega t/2)\sigma^{\mathsf{T}},$$

$$\sigma \exp(-i\omega\sigma_z t/2) = \exp(-i\omega t/2)\sigma,$$

$$\exp(-i\omega\sigma_z t/2)\sigma = \exp(+i\omega t/2)\sigma,$$

and we finally arrive at

$$H' = \frac{1}{2}\hbar\Delta\sigma_z + \frac{1}{2}\hbar\Omega_1(\sigma + \sigma^{\dagger}) = \frac{1}{2}\hbar\Delta\sigma_z + \frac{1}{2}\hbar\Omega_1\sigma_x.$$

In the case where we are considering magnetic resonance, we see that

$$\begin{split} H' &= -\gamma \mathbf{S} \cdot \dot{B}_{eff}, \\ \vec{B}_{eff} &= \left(B_0 + \frac{\omega}{\gamma} \right) \hat{z} - \frac{\Omega_1}{\gamma} \hat{x}, \end{split}$$

and we recover the simple idea that if $\omega = -\gamma B_0$ the \hat{z} component of \vec{B}_{eff} vanishes.

Density matrices and the Bloch vector

When working with density operators, the dimensionless Bloch vector is given by

$$\vec{v} \equiv \langle \vec{\sigma} \rangle = \langle \sigma_x \rangle \hat{x} + \langle \sigma_y \rangle \hat{y} + \langle \sigma_z \rangle \hat{z},$$

$$v_x = \operatorname{Tr}[\sigma_x \rho], \quad v_y = \operatorname{Tr}[\sigma_y \rho], \quad v_z = \operatorname{Tr}[\sigma_z \rho].$$

It is worth noting that for a pure state $|\vec{v}|^2 = 1$ while for a mixed state, $|\vec{v}|^2 \le 1$. For example, if $\rho = \frac{1}{2}$ then $\vec{v} = 0$ since the Pauli matrices are all traceless (Tr[σ_i] = 0).

In cases where ρ corresponds to a known ensemble

$$\rho = \sum_{j} p_{j} |\Psi_{j}\rangle \langle \Psi_{j}|,$$

then

$$\vec{v} = \operatorname{Tr}[\vec{\sigma}\rho] = \operatorname{Tr}\left[\vec{\sigma}\sum_{j} p_{j}|\Psi_{j}\rangle\langle\Psi_{j}|\right]$$
$$= \sum_{j} p_{j}\operatorname{Tr}[|\Psi_{j}\rangle\langle\Psi_{j}|\vec{\sigma}|\Psi_{j}\rangle\langle\Psi_{j}|] = \sum_{j} p_{j}\langle\Psi_{j}|\vec{\sigma}|\Psi_{j}\rangle\operatorname{Tr}[|\Psi_{j}\rangle\langle\Psi_{j}|] = \sum_{j} p_{j}\vec{v}_{j}.$$

where $\vec{v}_j = \langle \Psi_j | \vec{\sigma} | \Psi_j \rangle$ and the summation is a vector sum. In other words, the Bloch vector corresponding to an ensemble of pure states is the *weighted* vector sum of the Bloch vectors representing the members of the ensemble. Hence we find that for any equally-weighted two-member ensemble with $\langle \Psi_1 | \Psi_2 \rangle = 0$, the ensemble Bloch vector will be zero since $|\Psi_1\rangle$ and $|\Psi_2\rangle$ correspond to antipodal points. Indeed, we know that $\rho = \frac{1}{2}(|\Psi_1\rangle\langle\Psi_1| + |\Psi_2\rangle\langle\Psi_2|) = \frac{1}{2}$ for any such ensemble. Similarly, we see that the generalized Bloch vector corresponding to

$$\begin{aligned} |\Psi_1\rangle &= |+_x\rangle, \quad p_1 = \alpha, \\ |\Psi_2\rangle &= |-_x\rangle, \quad p_2 = \alpha, \\ |\Psi_3\rangle &= |+_z\rangle, \quad p_3 = 1 - 2\alpha, \end{aligned}$$

will simply be $(v_x, v_y, v_z) = (0, 0, 1 - 2\alpha)$. Hence the Bloch vector (now using the spin form with units of angular momentum)

$$\langle \vec{S} \rangle = \frac{\hbar}{2} (\operatorname{Tr}[\sigma_x \rho] \hat{x} + \operatorname{Tr}[\sigma_y \rho] \hat{y} + \operatorname{Tr}[\sigma_z \rho] \hat{z}),$$

can clearly be used to compute the net magnetization of an ensemble of spins,

$$\vec{M} \equiv -N\gamma \langle \vec{S} \rangle,$$

assuming the ensemble density operator ρ is used in computing the Bloch vector.

It is worth noting that any density operator may be expressed in the form

$$\rho = \frac{1}{2}(1 + \vec{v} \cdot \vec{\sigma}),$$

by virtue of the trace orthogonality of the Pauli matrices noted above. Thus \vec{v} is just as general as ρ for the purpose of specifying mixed quantum states. The Bloch vector \vec{v} has only three real parameters v_x, v_y, v_z (or $\theta, \varphi, |\vec{v}|$), but the same is true for ρ since Hermiticity ($\rho = \rho^{\dagger}$) fixes

Im
$$[\rho_{11}] = \text{Im} [\rho_{22}] = 0$$
, Re $[\rho_{21}] = \text{Re} [\rho_{12}]$, Im $[\rho_{21}] = -\text{Im} [\rho_{12}]$

and normalization $(Tr[\rho] = 1)$ gives us $Re[\rho_{22}] = 1 - Re[\rho_{11}]$. Hence $Re[\rho_{11}]$, $Re[\rho_{12}]$, and $Im[\rho_{12}]$ are the only real degrees of freedom for a density operator on a two-dimensional Hilbert space. Furthermore,

 $\mathrm{Tr}[\rho^{2}] = \frac{1}{4} \mathrm{Tr}\left[(1 + \vec{v} \cdot \vec{\sigma})^{2} \right] = \frac{1}{4} \mathrm{Tr}\left[(1 + v_{x}^{2} \sigma_{x}^{2} + v_{y}^{2} \sigma_{y}^{2} + v_{z}^{2} \sigma_{z}^{2}) \right] = \frac{1}{2} \left(1 + |\vec{v}|^{2} \right).$

Hence the length of the Bloch vector is directly related to the *purity* of ρ .

Derivation of Bloch damping terms from a Master Equation

If we consider the Master Equation

$$\dot{\rho} = -\frac{i}{\hbar} [H, \rho] + \gamma_{\perp} \Big(2\sigma \rho \sigma^{\dagger} - \sigma^{\dagger} \sigma \rho - \rho \sigma^{\dagger} \sigma \Big)$$

using

$$\rho = \frac{1}{2}(1 + \vec{v} \cdot \vec{\sigma}),$$

we see that the decay terms produce

$$\begin{aligned} \frac{dv_{i}}{dt} &= \gamma_{\perp} \operatorname{Tr} \Big[\sigma_{i} \Big(2\sigma\rho\sigma^{\dagger} - \sigma^{\dagger}\sigma\rho - \rho\sigma^{\dagger}\sigma \Big) \Big] \\ &= \frac{\gamma_{\perp}}{2} \operatorname{Tr} \Big[\sigma_{i} \Big(2\sigma(1 + \vec{v} \cdot \vec{\sigma})\sigma^{\dagger} - \sigma^{\dagger}\sigma(1 + \vec{v} \cdot \vec{\sigma}) - (1 + \vec{v} \cdot \vec{\sigma})\sigma^{\dagger}\sigma \Big) \Big] \\ &= \frac{\gamma_{\perp}}{2} \operatorname{Tr} \Big[\sigma_{i} \Big(2\sigma\sigma^{\dagger} + 2\sigma(\vec{v} \cdot \vec{\sigma})\sigma^{\dagger} - 2\sigma^{\dagger}\sigma - \sigma^{\dagger}\sigma(\vec{v} \cdot \vec{\sigma}) - (\vec{v} \cdot \vec{\sigma})\sigma^{\dagger}\sigma \Big) \Big] \\ &= \frac{\gamma_{\perp}}{2} \operatorname{Tr} \Big[\sigma_{i} \Big(-2\sigma_{z} + 2\sigma(\vec{v} \cdot \vec{\sigma})\sigma^{\dagger} - \sigma^{\dagger}\sigma(\vec{v} \cdot \vec{\sigma}) - (\vec{v} \cdot \vec{\sigma})\sigma^{\dagger}\sigma \Big) \Big] \\ &= \frac{\gamma_{\perp}}{2} \Big(-2\operatorname{Tr} \big[\sigma_{i}\sigma_{z} \big] + 2\operatorname{Tr} \Big[\sigma^{\dagger}\sigma_{i}\sigma(\vec{v} \cdot \vec{\sigma}) \Big] - \operatorname{Tr} \Big[\sigma_{i}\sigma(\vec{v} \cdot \vec{\sigma}) \Big] - \operatorname{Tr} \Big[\sigma_{i}(\vec{v} \cdot \vec{\sigma})\sigma^{\dagger}\sigma \Big] \Big) \end{aligned}$$

From the relations

$$\begin{aligned} \sigma_x \sigma^{\dagger} \sigma + \sigma^{\dagger} \sigma \sigma_x &= (|g\rangle\langle e| + |e\rangle\langle g|)|e\rangle\langle e| + |e\rangle\langle e|(|g\rangle\langle e| + |e\rangle\langle g|) &= |g\rangle\langle e| + |e\rangle\langle g| = \sigma_x, \\ \sigma_y \sigma^{\dagger} \sigma + \sigma^{\dagger} \sigma \sigma_y &= (i|g\rangle\langle e| - i|e\rangle\langle g|)|e\rangle\langle e| + |e\rangle\langle e|(i|g\rangle\langle e| - i|e\rangle\langle g|) &= i|g\rangle\langle e| - i|e\rangle\langle g| = \sigma_y, \\ \sigma_z \sigma^{\dagger} \sigma + \sigma^{\dagger} \sigma \sigma_z &= (|e\rangle\langle e| - |g\rangle\langle g|)|e\rangle\langle e| + |e\rangle\langle e|(|e\rangle\langle e| - |g\rangle\langle g|) &= 2|e\rangle\langle e| = 1 + \sigma_z, \end{aligned}$$

and

$$\sigma^{\dagger}\sigma_{x}\sigma = |e\rangle\langle g|(|g\rangle\langle e| + |e\rangle\langle g|)|g\rangle\langle e| = |e\rangle\langle e||g\rangle\langle e| = 0,$$

$$\sigma^{\dagger}\sigma_{y}\sigma = |e\rangle\langle g|(i|g\rangle\langle e| - i|e\rangle\langle g|)|g\rangle\langle e| = i|e\rangle\langle e||g\rangle\langle e| = 0,$$

$$\sigma^{\dagger}\sigma_{z}\sigma = |e\rangle\langle g|(|e\rangle\langle e| - |g\rangle\langle g|)|g\rangle\langle e| = -|e\rangle\langle g||g\rangle\langle e| = -|e\rangle\langle e|,$$

and

$$|e\rangle\langle e|\sigma_{x} = |e\rangle\langle e|(|g\rangle\langle e| + |e\rangle\langle g|) = |e\rangle\langle g|,$$

$$|e\rangle\langle e|\sigma_{y} = |e\rangle\langle e|(i|g\rangle\langle e| - i|e\rangle\langle g|) = -i|e\rangle\langle g|,$$

$$|e\rangle\langle e|\sigma_{z} = |e\rangle\langle e|(|e\rangle\langle e| - |g\rangle\langle g|) = |e\rangle\langle e|,$$

we have

$$\begin{aligned} \frac{dv_x}{dt} &= -\gamma_{\perp} v_x, \\ \frac{dv_y}{dt} &= -\gamma_{\perp} v_y, \\ \frac{dv_z}{dt} &= \frac{\gamma_{\perp}}{2} (-4 - 2 \mathbf{Tr} [|e\rangle \langle e|(\vec{v} \cdot \vec{\sigma})] - 2v_z) = -2\gamma_{\perp} - 2\gamma_{\perp} v_z \end{aligned}$$

We see that this reproduces the decay terms in the 'zero-temperature' Bloch Equations, with $\gamma_{\perp} \equiv \Gamma/2$. In your

homework this week you will show that the Hamiltonian part of the above Master Equation reproduces the remaining 'torque' terms in the Bloch Equations.

The full zero-temperature Bloch Equations resulting from the above Master Equation are thus found to be

$$\dot{v}_x = -\Delta v_y - \frac{\Gamma}{2} v_x,$$

$$\dot{v}_y = \Delta v_x - \Omega_1 v_z - \frac{\Gamma}{2} v_y,$$

$$\dot{v}_z = \Omega_1 v_y - \Gamma v_z - \Gamma.$$

The following figure will give you an idea of the effect of damping on the dynamics of the two level system.



The oscillations between the ground and excited state are damped and for large enough Γ they disappear altogether. The excited state population settles down to a steady state value which depends Ω_1, Γ, Δ so long as $\Gamma \neq 0$. We see from the graph (which is computed with $\Delta = 0$) that the excited state population at long times is higher for larger Ω_1 or lower Γ .

It is enlightening to consider the 'quantum trajectory' picture of spontaneous emission interrupting Larmor/Rabi oscillations to produce dephasing in the above plots.