Quantum two-level systems and density matrices

PHYS514

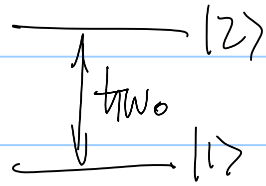
Note Title 2/21/2005

We need the density matrix formalism to deal with quantum systems where we don't measure everything

$$\rho = \sum_i w_i |\psi_i\rangle\langle\psi_i|$$ ← definition of density matrix for an ensemble

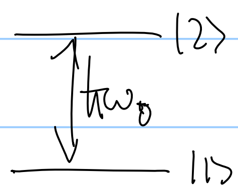
note: $|\psi_i\rangle$s are not necessarily an orthonormal basis

Examples of ensembles

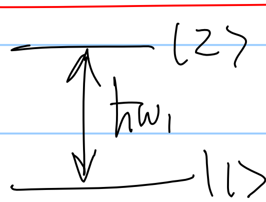


$|\psi_i\rangle = a|1\rangle + b|2\rangle$

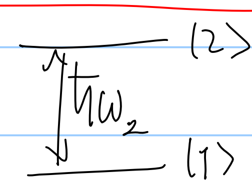
could be a single spin



$|\psi_1\rangle = e^{-i\hbar\omega_0 t/2}|2\rangle + e^{i\hbar\omega_0 t/2}|1\rangle$

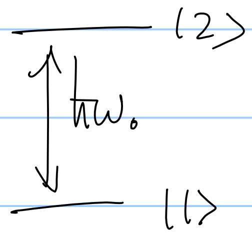


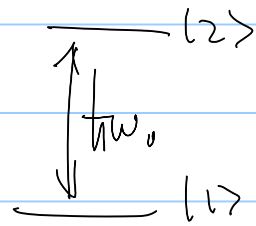
$|\psi_2\rangle = e^{-i\hbar\omega_1 t/2}|2\rangle + e^{i\hbar\omega_1 t/2}|1\rangle$



$|\psi_3\rangle = \ldots$

Or a bunch of spins in a superposition state but with different Larmor frequencies





$|\psi_1\rangle = a_1|1\rangle + b_1|2\rangle \qquad |\psi_2\rangle = a_2|1\rangle + b_2|2\rangle \quad \ldots$

Or a bunch of spins with the same Larmor frequency but different coefficients!

The $|\psi_i\rangle$'s are different possibilities in the ensemble, which occur with probabilities w_i

What do density matrices look like?

Single spin-½

$$|\psi\rangle = \cos\theta/2\,|1\rangle + \sin\theta/2\; e^{i\varphi}|2\rangle$$

Get matrix elements: $\rho_{11} = \langle 1|\psi\rangle\langle\psi|1\rangle$, $\rho_{12} = \langle 1|\psi\rangle\langle\psi|2\rangle$ etc.

$$\rho = \begin{pmatrix} \cos^2\theta/2 & \sin\theta/2 \cos\theta/2\, e^{i\varphi} \\ \sin\theta/2 \cos\theta/2\, e^{-i\varphi} & \sin^2\theta/2 \end{pmatrix}$$

What about an ensemble?

N spin-1/2's, where Bloch vector points randomly on the sphere

$$|\psi_i\rangle = \cos\frac{\theta_i}{2}|1\rangle + \sin\frac{\theta_i}{2} e^{i\varphi_i}|2\rangle$$

$$\rho = \frac{1}{N}\sum_{i=1}^{N} |\psi_i\rangle\langle\psi_i| = \frac{1}{N}\sum_{i=1}^{N} \begin{pmatrix} \cos^2\frac{\theta_i}{2} & \sin\theta_i/2 \cos\theta_i/2\, e^{i\varphi_i} \\ \sin\theta_i/2 \cos\theta_i/2\, e^{-i\varphi_i} & \sin^2\theta_i/2 \end{pmatrix}$$

in the limit $N \to \infty$

$$\rho = \frac{1}{4\pi}\int d\Omega \begin{pmatrix} \cos^2\theta/2 & \sin\theta/2 \cos\theta/2\, e^{i\varphi} \\ \sin\theta/2 \cos\theta/2\, e^{-i\varphi} & \sin^2\theta/2 \end{pmatrix}$$

$$\rho = \begin{pmatrix} 1/2 & 0 \\ 0 & 1/2 \end{pmatrix}$$

Look at what's different! The off-diagonal terms are new!

Generic features / language:

$$\rho = \begin{pmatrix} \rho_{11} & \rho_{12} \\ \rho_{21} & \rho_{22} \end{pmatrix}$$

"coherences"

"populations" — probabilities to be found in different basis states

If ρ represents a pure quantum state — $\rho^2 = \rho$, and the coherences are as large as possible

"Mixed states" $\rho^2 \neq \rho$ — no longer a pure quantum state, coherences are smaller

Classical states — coherences are zero!

When you use density matrices, you have to take expectation values in a funny way:

$$\boxed{\langle A\rangle = tr(\rho A)}$$

Examples: 1

$$\rho = \begin{pmatrix} 1/2 & 1/2 \\ 1/2 & 1/2 \end{pmatrix} \qquad |\psi\rangle = 1/\sqrt{2}\left(|1\rangle + |2\rangle\right)$$

$$\langle \sigma_x\rangle = tr \begin{pmatrix} 1/2 & 1/2 \\ 1/2 & 1/2 \end{pmatrix}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} =$$

$$tr \begin{pmatrix} 1/2 & 1/2 \\ 1/2 & 1/2 \end{pmatrix} = 1$$

but: $\langle \sigma_y\rangle = \langle \sigma_z\rangle = 0$

There is a basis where $\langle \sigma_i\rangle \neq 0$

2

$$\rho = \begin{pmatrix} 1/2 & 0 \\ 0 & 1/2 \end{pmatrix}$$

$$\langle \sigma_x\rangle = tr \begin{pmatrix} 1/2 & 0 \\ 0 & 1/2 \end{pmatrix}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = 0 = \langle \sigma_z\rangle = \langle \sigma_y\rangle$$

No basis where $\langle \sigma_i\rangle = 0$

Also: Consider $|\psi\rangle = \frac{1}{\sqrt{2}}\left(|1\rangle_a |1\rangle_b + |2\rangle_a |2\rangle_b\right)$

$$\rho = \begin{array}{c|cccc} & |1\rangle|1\rangle & |1\rangle|2\rangle & |2\rangle|1\rangle & |2\rangle|2\rangle \\ \hline |1\rangle|1\rangle & \frac{1}{2} & 0 & 0 & \frac{1}{2} \\ |1\rangle|2\rangle & 0 & 0 & 0 & 0 \\ |2\rangle|1\rangle & 0 & 0 & 0 & 0 \\ |2\rangle|2\rangle & \frac{1}{2} & 0 & 0 & \frac{1}{2} \end{array}$$

an entangled state

partial trace

If we look only at particle a, then we to construct the reduced density matrix:

$$\rho^a = tr_b(\rho)$$ "partial trace"; ρ^a is the "reduced density matrix"

Mathematically: $tr_b\left(|x\rangle_a |t\rangle_b \langle y|_a \langle s|_a\right)$

$$|x\rangle_a \langle y|_a \, tr\left(|t\rangle_b \langle s|_b\right) =$$

$$|x\rangle_a \langle y|_a \langle t|s\rangle$$

For this example: $\rho^a = \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{pmatrix}$ this looks like a mixed state!

Why use this funny partial trace?

→ If you don't observe one variable, but you could then you miss out on all of the coherent information in that variable

→ You must: incoherently sum up the populations & coherences in the variable you care about, weighted by the probability of finding the unobserved variable in a given state

Some Math from Nielsen and Chuang:

M is an observable on system a, measured using some device

$\tilde{M}$ same observable on ab, measured using the same device

if $|\psi\rangle = |m\rangle_a |\phi\rangle_b \qquad M|m\rangle_a = m|m\rangle_a$

and $\tilde{M}|\psi\rangle = m|\psi\rangle$

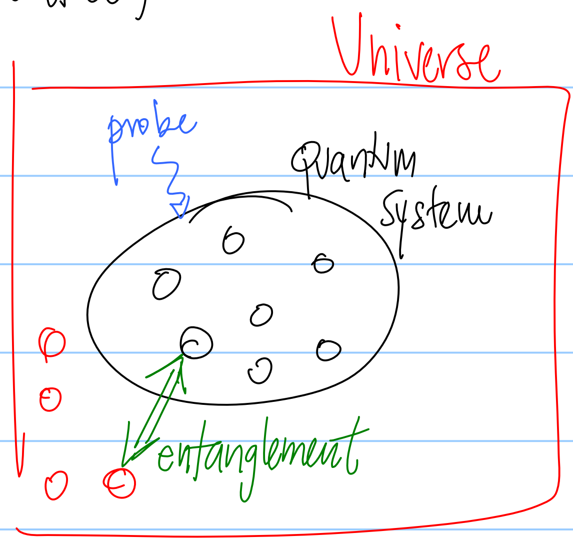
So, $\tilde{M} = M \otimes \mathbb{1}_b$

measurement averages must be the same whether we use ρ^a or ρ

$$\mathrm{tr}(M\rho^a) = \mathrm{tr}(\tilde{M}\rho) = \mathrm{tr}\left[(M \otimes \mathbb{1}_b)\rho\right]$$

<u>choose:</u> $\rho^a = \mathrm{tr}_b\, \rho$ this works, and is unique (N & C, p107)

This is the basis for our current understanding of decoherence (which we do not believe is fundamental)



Because we don't measure everything, we see quantum states that become entangled with "environmental" degrees of freedom behaving classically

If we make the "Quantum System" big enough, then we don't see much decoherence — the goal of Quantum Computing!

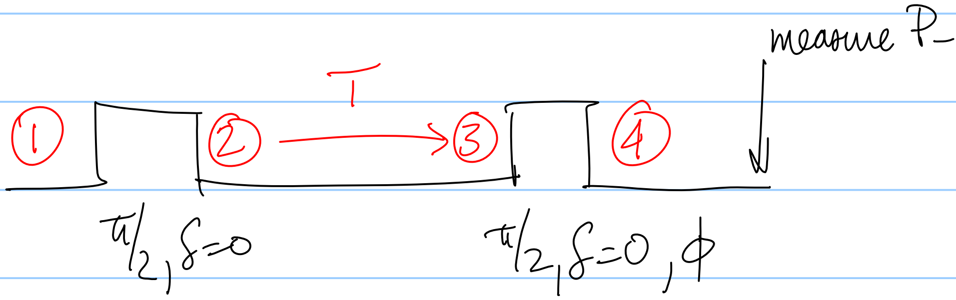
We say that the density matrix contains all of the physically relevant information about our system

Back to something practical...

$\boxed{\text{Coherences control the degree of interference effects}}$

Huh? What?

Let's think about our Ramsey experiment:



perfect world:

(in the rotating frame)

$$|\psi\rangle^{(1)} = |+\rangle$$

$$|\psi\rangle^{(2)} = \frac{1}{\sqrt{2}}\left(|+\rangle - i|-\rangle\right)$$

(assuming $\gamma<0$, spin is along $-\hat{y}$)

$$|\psi\rangle^{(3)} = \frac{1}{\sqrt{2}}\left(|+\rangle - i|-\rangle\right)$$

$$|\psi\rangle^{(4)} = \frac{1}{2}\left[\left(1-e^{-i\varphi}\right)|+\rangle - i\left(1+e^{i\varphi}\right)|-\rangle\right]$$

$$P_- = \left|\langle -|\psi\rangle^{(4)}\right|^2 = \frac{1}{2}\left(1+\cos\varphi\right)$$

In density matrices:

$$\rho^{(1)} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \qquad \rho^{(2)} = \rho^{(3)} = \begin{pmatrix} 1/2 & -i/2 \\ i/2 & 1/2 \end{pmatrix}$$

$$\rho^{(4)} = \begin{pmatrix} 1/2(1-\cos\varphi) & -i(1+e^{i\varphi})(1-e^{-i\varphi}) \\ i(1+e^{-i\varphi})(1-e^{i\varphi}) & 1/2(1+\cos\varphi) \end{pmatrix}$$

Now, what about that fluctuating magnetic field?

Larmor frequency changes, Bloch vector rotates in the rotating frame:

$$|\psi\rangle^{(3)} \rightarrow 1/\sqrt{2}\left(|+\rangle - i e^{i\alpha} |-\rangle\right)$$

where $\alpha = \dfrac{\mu \Delta B T}{\hbar}$

If we make measurements on an ensemble, where α is not fixed but is random, then we should take:

$$\rho = \frac{1}{2\pi}\int_0^{2\pi} \frac{1}{2}\left(|+\rangle - ie^{i\alpha}|-\rangle\right)\left(ie^{-i\alpha}\langle -| + \langle +|\right) d\alpha$$

if α is equally spread out between 0 and 2π (T long enough, fluctuations in B big enough)

$$\rho^{(3)} \longrightarrow \begin{pmatrix} 1/2 & 0 \\ 0 & 1/2 \end{pmatrix}$$

now a mixed state! coherences have disappeared

What happen at the second pulse? What is $\rho^{(4)}$?

<u>Need:</u> $\dot{\rho} = -\frac{i}{\hbar}[H, \rho]$

"Liouville equation"

"von Neumann - Liouville equation"

This can be proven using Schrödinger's equation

For a two-level system in the rotating frame:

$$\begin{cases} \dot{\rho}_{++} = -i\Omega \left(\rho_{-+} e^{-i\varphi} - \rho_{+-} e^{i\varphi} \right) \\ \dot{\rho}_{--} = i\Omega \left(\rho_{-+} e^{-i\varphi} - \rho_{+-} e^{i\varphi} \right) \\ \dot{\rho}_{+-} = i\delta \rho_{+-} + i\Omega e^{-i\varphi} \left(\rho_{++} - \rho_{--} \right) \end{cases}$$ and c.c.

So, if $\rho = \begin{pmatrix} 1/2 & 0 \\ 0 & 1/2 \end{pmatrix}$, nothing happens after the 2^{nd} π-pulse, and $P_- = 1/2$ regardless of φ (note: $\dot{\rho}_{++} = \dot{\rho}_{--} = \dot{\rho}_{+-} = \dot{\rho}_{-+} = 0$)

Look - without coherences, populations do not change, and phase sensitivity / interference is lost

Can create a Bloch-vector like picture based on the density matrix

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slightly different rotating frame definition (see Meystre and Sargent)

start from Schrödinger picture, take $\tilde{\rho}_{ab} = \rho_{ab} e^{i\omega t}$

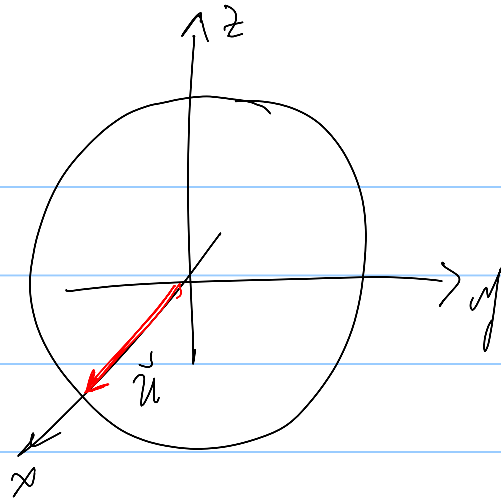
$$U = \tilde{\rho}_{+-} + \tilde{\rho}_{-+}$$
$$V = i(\tilde{\rho}_{+-} - \tilde{\rho}_{-+})$$
$$W = \rho_{++} - \rho_{--} \qquad \text{"inversion"}$$

$\vec{U} = U\hat{x} + V\hat{y} + W\hat{z}$ $\qquad \dot{\vec{U}} = \vec{U} \times \vec{R}$ $\qquad$ Bloch vector

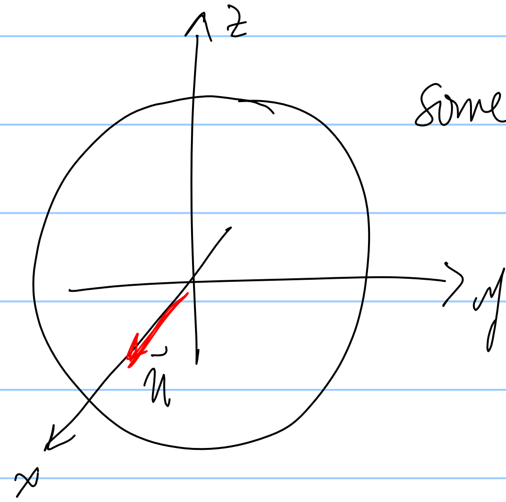
$\vec{R} = \Omega\hat{x} - \delta\hat{z}$ $\qquad$ effective torque

Same equations of motion, except $|\vec{U}|$ can change if decoherence sets in!

$$\tilde{\rho} = \begin{pmatrix} 1/2 & 1/2 \\ 1/2 & 1/2 \end{pmatrix}$$



$$\tilde{\rho} = \begin{pmatrix} 1/2 & 1/4 \\ 1/4 & 1/2 \end{pmatrix}$$

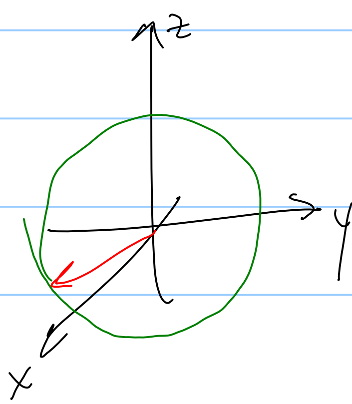


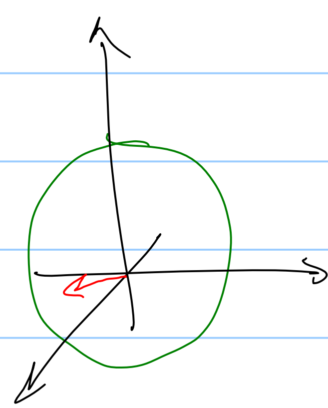
some coherence lost

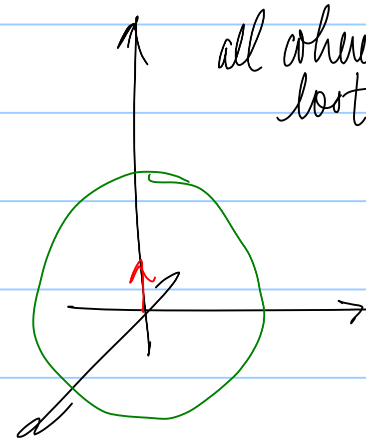
$$\xrightarrow{\text{decoherence}}$$

$$\tilde{\rho} = \begin{pmatrix} 2/3 & \sqrt{2}/3 \\ \sqrt{2}/3 & 1/3 \end{pmatrix} \longrightarrow \begin{pmatrix} 2/3 & 1/3 \\ 1/3 & 1/3 \end{pmatrix} \longrightarrow \begin{pmatrix} 2/3 & 0 \\ 0 & 1/3 \end{pmatrix}$$

$$|\psi\rangle = \sqrt{2/3}\,|+\rangle + \sqrt{1/3}\,|-\rangle$$







all coherence lost

How do we describe decoherence?

Basically, add it in phenomenologically to the equation of motion for the density matrix

This can be motivated physically, but there are only 2 things that can happen:

$$\dot{\rho} = -i/\hbar \, [H, \rho] - \begin{pmatrix} (\rho_{11} - \rho_{11}')/T_1 & \rho_{12}/T_2 \\ \rho_{21}/T_2 & (\rho_{22} - \rho_{22}')/T_1 \end{pmatrix}$$

sidenote: T_1 processes, in this form, are not like spontaneous emission. It is driven by a bath – ρ_{11} relaxes to ρ_{11}' regardless of what ρ_{22} is doing (and vice-versa)

simplest thing we can write down, consistent with Hamiltonian evolution, and conserves probability (iff $\rho_{22}' + \rho_{11}' = 1$)

What does this do to the equation of motion?

there are additional decay terms:

$$\dot{\rho}_{12} = \ldots - \rho_{12}/T_2$$ exponential decay to 0

$$\dot{\rho}_{22} = \ldots - (\rho_{22} - \rho_{22}')/T_1$$ exponential decay to ρ_{22}'

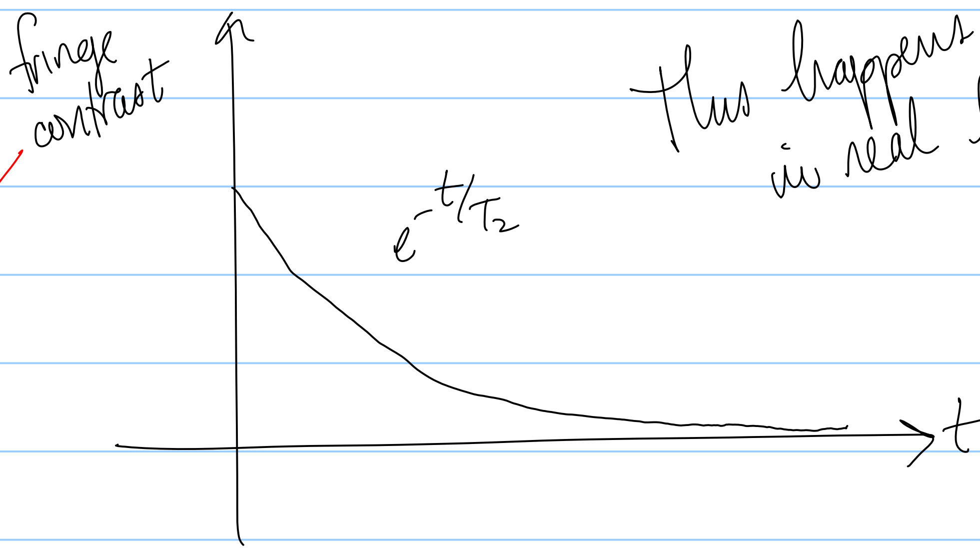
$$\dot{\rho}_{11} = \ldots - (\rho_{11} - \rho_{11}')/T_1 \quad \text{exponential decay to } \rho_{11}'$$

populations: relax at T_1
coherences: relax at T_2

Bloch vector equations of motion:

$$\begin{cases} \dot{u} = -\delta v - u/T_2 \\ \dot{v} = \delta u - v/T_2 + \Omega w \\ \dot{w} = -(\rho_{11}' - \rho_{22}')/T_1 - \Omega v \end{cases}$$

So, in the Ramsey experiment, we are sensitive to the coherences (u and v), which decay exponentially!

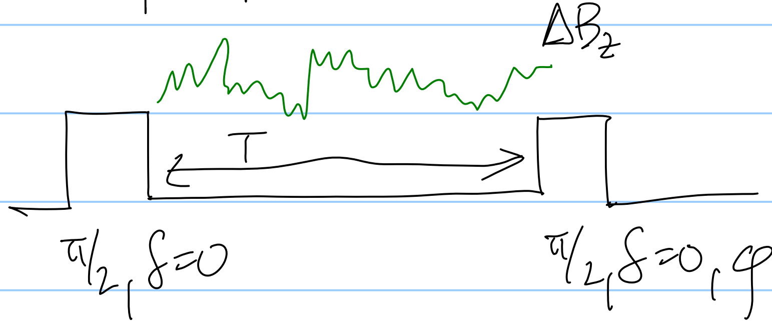


$\frac{\text{max} - \text{min}}{\text{max} + \text{min}}$

This happens in real life!

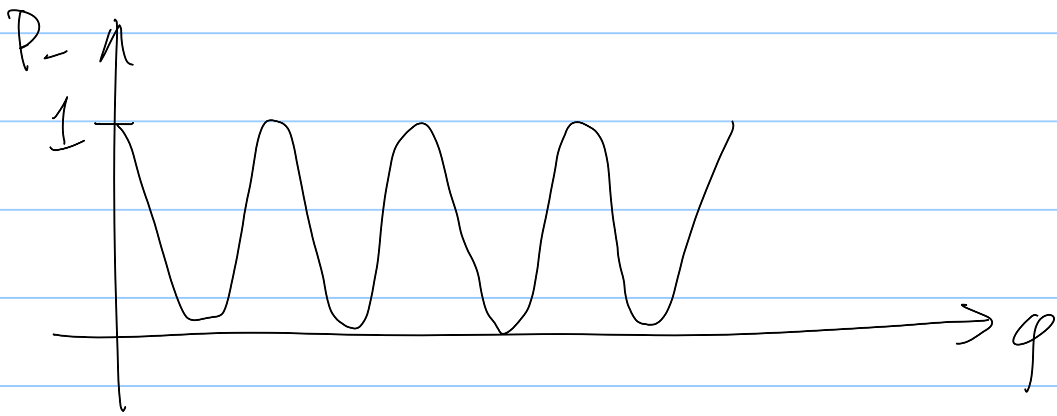
Explicit example of T_2 process:

Ramsey experiment



rapidly fluctuating magnetic field present along $\hat{z}$

without ΔB_z:



What happens with ΔB_z present?

- equivalent to inhomogeneous broadening (see Meystre and Sargent, Ch 4)

Start with our ensemble as one spin:

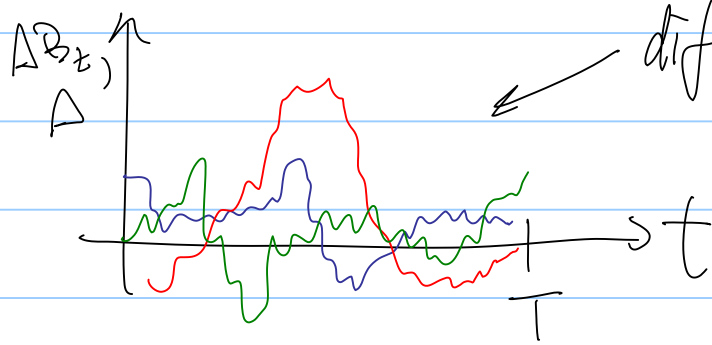
$$\dot{\rho}_{-+} = -i\delta\rho_{-+} - i\Delta\rho_{-+}$$

add in the effect of ΔB_z as a change in defining — this is pure Hamiltonian evolution!

$$\rho_{-+}(t) = \rho_{-+}(0)\, e^{-i\delta t - i\int_0^t dt'\Delta(t')}$$

just formal integration

Now, let's expand our ensemble to include all possible experiments. That means we're averaging over all possible variations in ΔB_z:



different possibilities in our ensemble

Start by expanding:

$$e^{-i\int_0^t dt'\Delta(t')} = 1 - i\int_0^t dt'\Delta(t') - \tfrac{1}{2}\int_0^t dt'\int_0^t dt''\Delta(t')\Delta(t'') + \dots$$

For truly random variation in ΔB_z,

$\langle \Delta(t) \rangle = 0$ since Δ is equally likely to be >0 and <0

$\langle \Delta(t)\Delta(t') \rangle = 0$ unless $t=t'$, then

$\langle \Delta(t)\Delta(t') \rangle > 0$ ($\Delta(t)^2 > 0$ always!)

just define: $\langle \Delta(t)\Delta(t') \rangle = 2/T_2 \, \delta(t-t')$

This is the Markov approximation – people like to say that the system has an "infinitely short memory"

after some hard math (summing a series where only even powers of Δ contribute):

$$\left\langle e^{-i\int_0^t dt' \Delta(t')} \right\rangle = e^{-t/T_2}$$

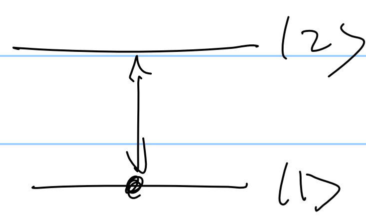
and $\rho_{-+} = \rho_{-+}(0)\, e^{-i\delta - t/T_2}$ *this is for an ensemble which includes all possibilities of ΔB_z

Voila! Pure Hamiltonian evolution + ensemble $\longrightarrow$ decoherence

What if we have T_1 and T_2 processes present?

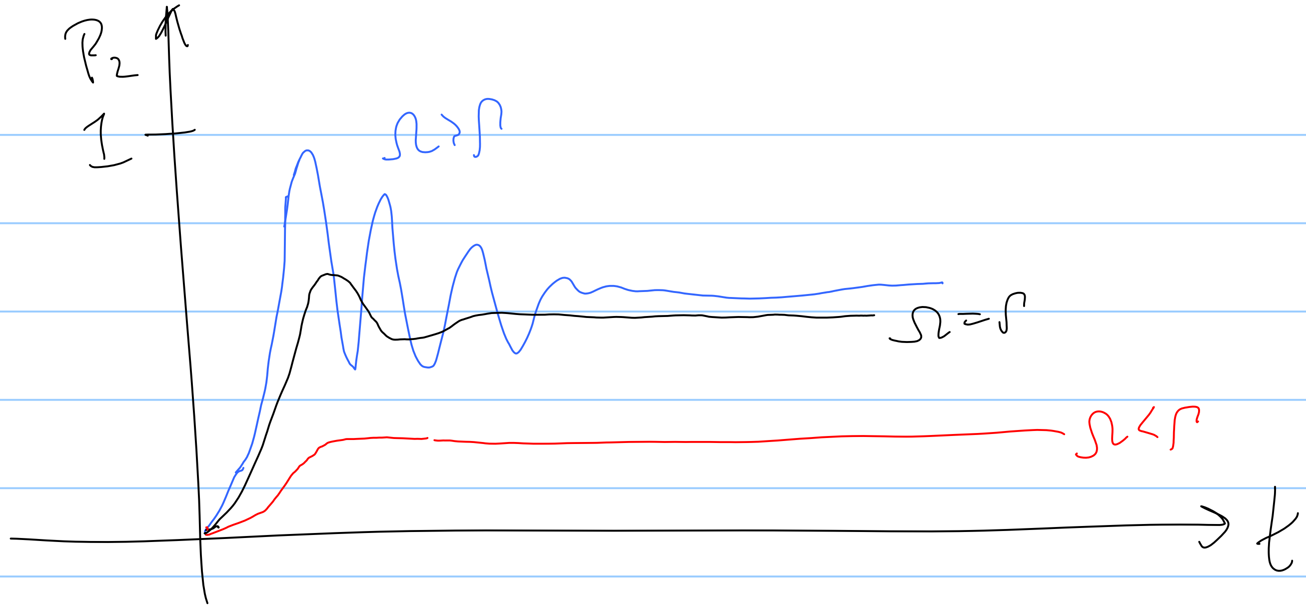
*Note: just T_1 gives unphysical results! (doesn't make much sense either)

$$\Gamma = 1/T_1 = 1/T_2$$



$$P_2 = \rho_{22} = \frac{2\Omega^2}{\delta^2 + \Gamma^2 + 4\Omega^2}\left\{1 - e^{-\Gamma t}\left[\cos(\Omega' t) + \frac{\sin(\Omega' t)}{\Omega'}\right]\right\}$$

where $\Omega' = \sqrt{4\Omega^2 + \delta^2}$



P_2
1
$\Omega > \Gamma$
$\Omega = \Gamma$
$\Omega < \Gamma$
t