"When you see a car lifted by a huge magnet, remember that magnetism of solids is a purely quantum effect"

M. I. Kaganov



## What is this course about?

Modern approaches to describing, analysing, and controlling spin/qubit dynamics.
Approaches that are actually used in most laboratories right now. Not only for spin qubits but also for Josephson junction qubits, trapped ions, cavity-QED qubits, etc.

Many things you have already seen or heard about.
Our goal - to set up a framework for your knowledge, organize it, and look at old things in a new way.
To give you a set of very general concepts and ideas, applicable to many experimental situations.

We will try not to use much math, work mostly with simple examples to introduce and illustrate ideas and concepts

## Brief history of spins in solids



First study of spins in solids: 400 years old
First modern scientific book:
W. Gilbert and A. Dowling, De Magnete, (1600)

## Modern times

W. Pauli

1924
A. Kronig 1925

Studying spectra of alkali atoms conjectured a two-valued internal degree of freedom

Internal rotation of the electron
Objection from Pauli: No, rotation is too fast
G.Uhlenbeck (TU Delft, Chem. Eng.) and S. Goudsmit, 1925

## Brief reminder - quantum mechanical systems

State of a quantum system: wave function
A vector in many-dimensional (d-dimensional) space (Hilbert space)
Our "usual" 3D space:
choose a basis, i.e. any three orthonormal vectors $\vec{e}_{1}, \vec{e}_{2}$, and $\vec{e}_{3}$
$\vec{a}=a_{1} \cdot \vec{e}_{1}+a_{2} \cdot \vec{e}_{2}+a_{3} \cdot \vec{e}_{3} \quad$ or $\quad \vec{a}=\left[\begin{array}{l}a_{1} \\ a_{2} \\ a_{3}\end{array}\right] \quad a_{1}, a_{2}, a_{3} \in \mathbb{R}$
> Quantum state vector in a Hilbert space
$d$-dimensional basis, i.e. $d$ orthonormal vectors $\vec{e}_{1}, \vec{e}_{2}, \ldots \vec{e}_{d}$
$\vec{\psi}=\psi_{1} \cdot \vec{e}_{1}+\psi_{2} \cdot \vec{e}_{2}+\cdots+\psi_{d} \cdot \vec{e}_{d} \quad$ or $\vec{\psi}=\left[\begin{array}{c}\psi_{1} \\ \ldots \\ \psi_{d}\end{array}\right] \quad \psi_{1}, \ldots, \psi_{d} \in \mathbb{C}$
Dirac's notations (bra/ket formalism): basis vectors $\left|e_{1}\right\rangle, \ldots,\left|e_{d}\right\rangle$
$|\psi\rangle=\psi_{1} \cdot\left|e_{1}\right\rangle+\cdots+\psi_{d} \cdot\left|e_{d}\right\rangle \quad$ with the requirement $\quad\left|\psi_{1}\right|^{2}+\cdots+\left|\psi_{d}\right|^{2}=1$

## $>$ Scalar (inner) product and dual vectors

$(\vec{a}, \vec{b})=\left[a_{1}, a_{2}, a_{3}\right] \cdot\left[\begin{array}{l}b_{1} \\ b_{2} \\ b_{3}\end{array}\right]=\sum_{k=1}^{3} a_{k} \cdot b_{k} ; \quad\left[a_{1}, a_{2}, a_{3}\right]-$ dual of $\vec{a}=\left[\begin{array}{l}a_{1} \\ a_{2} \\ a_{3}\end{array}\right]$
Bra-ket form: $|\varphi\rangle=\left[\begin{array}{c}\varphi_{1} \\ \ldots \\ \varphi_{d}\end{array}\right]$, its dual $\langle\varphi|=\left[\varphi_{1}^{*}, \varphi_{2}^{*}, \varphi_{3}^{*}\right]$, and $\langle\varphi \mid \psi\rangle=\sum_{k=1}^{d} \varphi_{k}^{*} \cdot \psi_{k}$
$>$ Changing the quantum state. Linear operators

$$
\hat{A}:|\psi\rangle \rightarrow|\varphi\rangle=\hat{A}|\psi\rangle \equiv|\hat{A} \psi\rangle \quad \hat{A}[a|\psi\rangle+b|\phi\rangle] \equiv a|\hat{A} \psi\rangle+b|\hat{A} \phi\rangle
$$

With a given basis, the operator $\hat{A}$ is a matrix, i.e. $\hat{A}=\sum_{j, k=1}^{d} A_{j k}\left|e_{j}\right\rangle\left\langle e_{k}\right|$
Why? Because each $\varphi_{k}=\left\langle e_{k} \mid \varphi\right\rangle=\left\langle e_{k} \mid \hat{A} \psi\right\rangle=\left\langle e_{k}\right| \hat{A}|\psi\rangle$ is linear in $|\psi\rangle$.
Riesz theorem: any continuous linear function $f$ of $|\psi\rangle$ has a form $f=\langle\alpha \mid \psi\rangle$
For "good" quantum systems $\hat{A}|\psi\rangle$ is a matrix-vector multiplication

## Our main character: spin 1/2 (qubit)

$d=2$ : two basis states, $|\uparrow\rangle$ and $|\downarrow\rangle$, or $|0\rangle$ and $|1\rangle$
$|\psi\rangle=\alpha|\uparrow\rangle+\beta|\downarrow\rangle \quad \rho=|\psi\rangle\langle\psi|=\left[\begin{array}{cc}|\alpha|^{2} & \beta^{*} \alpha \\ \alpha^{*} \beta & |\beta|^{2}\end{array}\right]$
All operators are linear combinations of Pauli matrices:
$\sigma_{0} \equiv 1=\left(\begin{array}{ll}1 & 0 \\ 0 & 1\end{array}\right), \quad \sigma_{x}=\left(\begin{array}{ll}0 & 1 \\ 1 & 0\end{array}\right), \quad \sigma_{y}=\left(\begin{array}{cc}0 & -i \\ i & 0\end{array}\right), \quad \sigma_{z}=\left(\begin{array}{cc}1 & 0 \\ 0 & -1\end{array}\right)$
Spin operators (observables): $S_{\mu}=\frac{1}{2} \sigma_{\mu}$

Bloch sphere mapping:


$$
\begin{aligned}
& \left\langle S_{z}\right\rangle=\frac{1}{2}\left(\rho_{00}-\rho_{11}\right) \\
& \left\langle S_{x}\right\rangle=\frac{1}{2}\left(\rho_{01}+\rho_{10}\right) \\
& \left\langle S_{y}\right\rangle=\frac{i}{2}\left(\rho_{01}-\rho_{10}\right)
\end{aligned}
$$

## Brief reminder - quantum mechanical averages

What are the quantities $\left\langle S_{x}\right\rangle,\left\langle S_{y}\right\rangle$, and $\left\langle S_{z}\right\rangle$ ?
$>$ Hermitian operators - observables. Describe physically observable quantities
Diagonal form: $\hat{O}=\sum_{n} O_{n} \cdot\left|\omega_{n}\right\rangle\left\langle\omega_{n}\right|$

- eigenvectors $\left|\omega_{n}\right\rangle$ form a complete orthonormal basis
- eigenvalues $O_{n}$ are real

Born's postulate: if the quantum state vector $|\psi\rangle$ is a superposition,

$$
|\psi\rangle=\sum_{k} \psi_{k}\left|\omega_{k}\right\rangle, \quad \psi_{k}=\left\langle\omega_{k} \mid \psi\right\rangle
$$

then by measuring the quantity $O$ on this quantum system we will:

- with the probability $w_{n}=\left|\psi_{n}\right|^{2}=\left|\left\langle\omega_{n} \mid \psi\right\rangle\right|^{2}$ obtain the value $O_{n}$
- and simultaneously change the state of the system to $\left|\omega_{n}\right\rangle$

The measurement outcome is random, cannot be predicted in principle
E.g., one spin, unknown state: measure $S_{z}$, obtain the value $+1 / 2$

This is it. Nothing more can be done/learned.
Ensemble of "similar" (?) spins: only then we can estimate $\left\langle S_{z}\right\rangle$ (average) and can learn something useful.

## Spins and magnetic fields

Spin dynamics are controlled by magnetic fields (external or internal)

$$
H=g \mu \vec{B}(t) \cdot \vec{S}=\gamma \hbar \vec{B}(t) \cdot \vec{S}
$$

Almost everywhere below:

- set $\hbar=1$ : measure energy in rad/s or Hz
E.g., $E=1 \mathrm{~J} \rightarrow \omega \approx 10^{34} \mathrm{rad} / \mathrm{s}$ or $v \approx 1.5 \cdot 10^{33} \mathrm{~Hz}$

Usually, in spin physics we deal with $v$ in $\mathrm{kHz}-\mathrm{GHz}$ range

- set $\gamma=1$ : measure magnetic fields in $\mathrm{rad} / \mathrm{s}$ or Hz This is spin-dependent!
Electron spin: $B=1 \mathrm{~T}$ corresponds to $v \approx 30 \mathrm{GHz}$
Nuclear ${ }^{13} \mathrm{C}$ spin: $B=1 \mathrm{~T} \rightarrow v \approx 11 \mathrm{MHz}$
Important: $\omega \cdot t$ is dimensionless, while $v \cdot t$ is not Indeed: $\sin \omega t$, not $\sin v t$ !


## How to think of real spin/qubit (say, spin 1/2):



Static noise:

random $B$ : ensemble of possible level positions

Dynamic noise:
$B(t)$

Relaxation:
energy of the upper level is not well defined:

$$
\Delta E \sim 1 / \tau_{\text {relax }}
$$


level positions randomly vary in time
Seen e.g. in spectroscopic experiment: levels with finite width

but


## Preliminaries are over

## Now let's actually work on spins

## Choice of the basis: quantization axis

Basis states: $|\uparrow\rangle$ and $|\downarrow\rangle$. But where is "up"? And why not left/right?
Different quantization axis - different basis : unitary transformation

$$
|\uparrow\rangle,|\downarrow\rangle \mapsto \quad\left|\varphi_{\uparrow}\right\rangle=W|\uparrow\rangle, \quad\left|\varphi_{\downarrow}\right\rangle=W|\downarrow\rangle
$$

At home: what is the most general form of $W$ for $\operatorname{spin} 1 / 2 ?$
Any choice of $U$ is equally good (unitary equivalence) If the spin coupled to magnetic field or other spins : $H_{\varphi}=W W^{\dagger}$ Home: describe Larmor precession with $\vec{B}=B \vec{e}_{z}$ and with $\vec{B}=B \vec{e}_{x}$, show equivalence

Formally the same, but in practice? Time-dependent field along $x$ :

$$
\begin{array}{ccc}
H=B(t) \cdot S_{x} & i|\dot{\psi}\rangle=B(t) S_{x}|\psi\rangle & |\psi\rangle=\alpha|\uparrow\rangle+\beta|\downarrow\rangle \\
i \dot{\alpha}=\frac{1}{2} h(t) \beta & \ddot{\alpha}=\dot{\alpha} \frac{\dot{h}}{h}-\frac{h(t)^{2}}{4} \alpha & \text { Oops... }
\end{array}
$$

Now choose different quantization axis. New basis: eigenvectors of $S_{x}$

$$
\left|\varphi_{\uparrow}\right\rangle=\frac{1}{\sqrt{2}}\binom{1}{1}, \quad\left|\varphi_{\downarrow}\right\rangle=\frac{1}{\sqrt{2}}\binom{-1}{1}, \quad W=\frac{1}{\sqrt{2}}\left(\begin{array}{cc}
1 & -1 \\
1 & 1
\end{array}\right)
$$

$H_{\varphi}=B(t) \cdot \frac{1}{2}\left(\begin{array}{cc}1 & 0 \\ 0 & -1\end{array}\right)=B(t) \cdot S_{z}-$ just another coordinate frame in the new basis !

$$
\begin{gathered}
|\psi\rangle=a|\uparrow\rangle+b|\downarrow\rangle \quad i \dot{a}=\frac{1}{2} B(t) a, \quad i \dot{b}=\frac{1}{2} B(t) b \\
a(t)=a_{0} \exp [-i \Phi(t) / 2], \quad b(t)=b_{0} \exp [i \Phi(t) / 2]
\end{gathered}
$$

$$
\Phi(t)=\int_{0}^{t} B(s) d s
$$

Regular Larmor precession, but in a time-varying field

$$
\begin{gathered}
\left\langle S_{x}\right\rangle(t)=\left\langle S_{x}^{0}\right\rangle \cos \Phi-\left\langle S_{y}^{0}\right\rangle \sin \Phi \\
\left\langle S_{y}\right\rangle(t)=\left\langle S_{y}^{0}\right\rangle \cos \Phi+\left\langle S_{x}^{0}\right\rangle \sin \Phi \\
\left\langle S_{z}\right\rangle(t)=\left\langle S_{z}^{0}\right\rangle \\
\left\langle S_{x, y, z}^{0}\right\rangle \equiv\left\langle S_{x, y, z}\right\rangle(0) \text { (in the new basis!) }
\end{gathered}
$$

Choice of the quantization axis is the key to success in science!
But there is much more to it ...

But first, as a preparatory step, let us solve some problems
Heisenberg representation: matrices of operators with time-dependent entries

$$
\begin{aligned}
\hat{S}_{x}(t) & =\left(\begin{array}{ll}
s_{00}(t) & s_{01}(t) \\
s_{10}(t) & s_{11}(t)
\end{array}\right) \\
\left\langle S_{x}\right\rangle(t) & =\langle\psi(0)| \hat{S}_{x}(t)|\psi(0)\rangle
\end{aligned}
$$

Heisenberg equations of motion $\quad \dot{\hat{S}}_{\mu}(t)=i\left[\hat{H}, \hat{S}_{\mu}(t)\right]$
Use the operators

$$
\hat{S}^{+}=\hat{S}_{x}+i \hat{S}_{y}, \quad \hat{S}^{-}=\hat{S}_{x}-i \hat{S}_{y}
$$

Repeat the same calculation, but now via evolution operator
Static field - static Hamiltonian: $\widehat{U}=\exp (-i \widehat{H} t)$
Time-dep Hamiltonian: $i \dot{\widehat{U}}=\widehat{H}(t) \widehat{U}$

## Larmor precession with noise: dephasing

Important: experiments are never perfect $B=B_{0}+\beta: \widehat{H}=\left(B_{0}+\beta\right) \cdot \hat{S}_{z}, \quad \beta-$ noise, assume (quasi)static

$\begin{aligned} & \hat{S}^{+}(t)=\hat{S}^{+} \mathrm{e}^{i\left(B_{0}+\beta\right) t} \\ & \hat{S}^{-}(t)=\hat{S}^{-} \mathrm{e}^{-i\left(B_{0}+\beta\right) t}\end{aligned} \rightarrow\left\langle\hat{S}^{+}(t)\right\rangle_{\beta}=\hat{S}^{+} \cdot \mathrm{e}^{i B_{0} t} \int_{-\infty}^{\infty} P(\beta) \mathrm{e}^{i t \beta} d \beta$
and similar for $\left\langle S^{-}(t)\right\rangle_{\beta}$

$$
\int_{-\infty}^{\infty} P(\beta) \mathrm{e}^{i t \beta} d \beta=\exp \left[-b^{2} t^{2} / 2\right]
$$

Average operators $\left\langle\hat{S}^{ \pm}(t)\right\rangle_{\beta} \rightarrow 0$ as $t \rightarrow \infty$, so that average values

$$
\begin{aligned}
& \left\langle\left\langle S_{x, y}\right\rangle(t)\right\rangle_{\beta}=\left\langle\operatorname{Tr} \rho(0) \hat{S}_{x, y}(t)\right\rangle_{\beta} \rightarrow 0 \\
& \text { and only }\left\langle\left\langle S_{z}\right\rangle(t)\right\rangle_{\beta}=\left\langle S_{z}\right\rangle(0)=\mathrm{const}
\end{aligned}
$$

## A few comments on theory of dephasing (and decoherence in general)

$>$ Can use either noise-averaged operators or noise-averaged density matrix:

$$
\begin{gathered}
\left\langle\left\langle S_{x}\right\rangle(t)\right\rangle_{\beta}=\left\langle\operatorname{Tr} \rho(0) \hat{S}_{x}(t)\right\rangle_{\beta}=\left\langle\operatorname{Tr} \rho(0) \widehat{U}_{\beta}^{\dagger}(t) \hat{S}_{x} \widehat{U}_{\beta}(t)\right\rangle_{\beta}= \\
=\left\langle\operatorname{Tr} \widehat{U}_{\beta}(t) \rho(0) \widehat{U}_{\beta}^{\dagger}(t) \hat{S}_{x}\right\rangle_{\beta}=\left\langle\operatorname{Tr} \rho_{\beta}(t) \hat{S}_{x}\right\rangle_{\beta}
\end{gathered}
$$

But cannot use noise-averaged ev.op. $\langle\widehat{U}(t)\rangle_{\beta}$ or $\langle\psi(t)\rangle_{\beta}=\left\langle\widehat{U}_{\beta}(t) \psi(0)\right\rangle_{\beta}$

$$
\begin{aligned}
\text { Indeed: }\left\langle\left\langle S_{x}\right\rangle(t)\right\rangle_{\beta}= & \operatorname{Tr}\left\langle\widehat{U}_{\beta}(t) \rho(0) \widehat{U}_{\beta}^{\dagger}(t)\right\rangle_{\beta} \hat{S}_{x} \\
& \text { but } \\
\left\langle\widehat{U}_{\beta}(t) \rho(0) \widehat{U}_{\beta}^{\dagger}(t)\right\rangle_{\beta}= & \left.\langle\mid \psi(t)\rangle\langle\psi(t) \mid\rangle_{\beta} \neq\langle\mid \psi(t)\rangle\right\rangle_{\beta} \cdot\left\langle\langle\psi(t) \mid\rangle_{\beta}\right.
\end{aligned}
$$

$>\mathrm{QM}$ : need to repeat experiment many times. If there is no control over noise then QM averaging includes the noise averaging. But this depends on specific experimental settings - be careful! For that reason, below we omit the symbol $\langle\ldots\rangle_{\beta}$ when possible.

## General quasistatic noise: FT spectroscopy

$\widehat{H}=\left(B_{0}+\beta\right) \cdot \hat{S}_{z}, \quad \beta-($ quasi $)$ static noise, some general $P(\beta)$

$$
\begin{gathered}
\begin{array}{c}
\hat{S}^{+}(t)=\hat{S}^{+} \mathrm{e}^{i\left(B_{0}+\beta\right) t} \\
\hat{S}^{-}(t)=\hat{S}^{-} \mathrm{e}^{-i\left(B_{0}+\beta\right) t}
\end{array} \rightarrow \begin{array}{c}
\left\langle\hat{S}^{+}(t)\right\rangle_{\beta}=\hat{S}^{+} \cdot \mathrm{e}^{i B_{0} t} \int_{-\infty}^{\infty} P(\beta) \mathrm{e}^{i t \beta} d \beta \\
\text { and similar for }\left\langle S^{-}(t)\right\rangle_{\beta}
\end{array} \\
f(t)=\int_{-\infty}^{\infty} P(\beta) \mathrm{e}^{i t \beta} d \beta: \text { characteristic function of a } \\
\text { random variable }
\end{gathered}
$$

Experiment:

1) Prepare spin in a state $\psi=\frac{1}{\sqrt{2}}(|\uparrow\rangle+|\downarrow\rangle)$ with $\left\langle S_{x}^{0}\right\rangle=\frac{1}{2},\left\langle S_{y, z}^{0}\right\rangle=0$
2) Measure $\left\langle S_{x}\right\rangle(t)$ and $\left\langle S_{y}\right\rangle(t)$ : determine $f(t)$
3) Do inverse Fourier transform of $f(t)$ - find $P(\beta)$

FT spectroscopy: by knowing the noise properties we can learn a lot about its origin (interaction with other spins/systems, etc.)

## Dephasing and pointer states

$|\psi\rangle=\alpha|\uparrow\rangle+\beta|\downarrow\rangle$. Fix global phase: $|\psi\rangle=u|\uparrow\rangle+v e^{i \varphi}|\downarrow\rangle, u, v \in \mathbb{R}$

$$
\begin{gathered}
\rho=|\psi\rangle\langle\psi|=\left[\begin{array}{cc}
u^{2} & u v e^{-i \phi} \\
u v e^{i \phi} & v^{2}
\end{array}\right], \phi-\text { quantum phase } \\
\rho(t)=\left(\begin{array}{cc}
u^{2} & u v e^{-i\left(\phi+B_{0} t\right)} \mathrm{e}^{-\frac{b^{2} t^{2}}{2}} \\
u v e^{i\left(\phi+B_{0} t\right)} \mathrm{e}^{-\frac{b^{2} t^{2}}{2}} & v^{2}
\end{array}\right) \xrightarrow{t \rightarrow \infty}\left(\begin{array}{cc}
u^{2} & 0 \\
0 & v^{2}
\end{array}\right)
\end{gathered}
$$

Purely classical spin - phase is randomized, quantumness gone Besides, a special set of states is selected : $|\uparrow\rangle$ and $|\downarrow\rangle$

Quantum spin - all basis sets are the same (unitarily equivalent) Decohered spin - some states are special, survive dephasing (although their superpositions do not)
$\underline{\text { Pointer states }}$

## Dephasing and the choice of quantization axis

$H=B S_{z}+h S_{x}=\frac{1}{2} B \sigma_{z}+\frac{1}{2} h \sigma_{x}$ - static field

$$
\begin{gathered}
U=\mathrm{e}^{-i H t}=\exp \left[-i\left(n_{x} \sigma_{x}+n_{z} \sigma_{z}\right) \varphi / 2\right] \\
\exp [-i(\vec{\sigma} \vec{n}) \varphi / 2]=\cos \varphi / 2-i(\vec{\sigma} \vec{n}) \sin \varphi / 2
\end{gathered}
$$


$\varphi=\Omega t, \quad \Omega=\sqrt{B^{2}+h^{2}}, \quad n_{x}=h / \Omega, n_{z}=B / \Omega$

Add weak static noise : $B=B_{0}+\beta$

$$
\begin{aligned}
P(\beta)=\frac{1}{\sqrt{2 \pi b^{2}}} & \exp \left(-\frac{\beta^{2}}{2 b^{2}}\right) \\
b & \ll h, B_{0}
\end{aligned}
$$

How do we solve this problem?
Can try to use exact solution, but it is quite complicated, and provides limited info.
Another powerful idea: Secular and non-secular terms

## Secular and non-secular terms

$$
\Omega=\sqrt{B^{2}+h^{2}} \equiv \sqrt{\left(B_{0}+\beta\right)^{2}+h^{2}} \approx \sqrt{B_{0}^{2}+h^{2}} \equiv \Omega_{0}
$$

This is a good approximation for $\Omega$ : look at the expansion

$$
\Omega=\Omega_{0}+B_{0} \cdot\left(\beta / \Omega_{0}\right)+\left[h^{2} / 2 \Omega_{0}\right] \cdot\left(\beta / \Omega_{0}\right)^{2}+\cdots
$$

and when averaging $\quad \int P(\beta) d \beta\left(\beta / \Omega_{0}\right)^{n} \propto\left(b / \Omega_{0}\right)^{n} \ll 1$

But is it also good for $\varphi$ ? Emphatic NO!

$$
\begin{gathered}
\varphi=\Omega t=\Omega_{0} t+\varepsilon t+\cdots, \quad \text { where } \varepsilon=\left(B_{0} / \Omega_{0}\right) \beta \ll \Omega_{0} \\
\cos \varphi \approx \cos \left[\Omega_{0} t+\varepsilon t\right]=\cos \Omega_{0} t \cdot \cos \varepsilon t-\sin \Omega_{0} t \cdot \sin \varepsilon t
\end{gathered}
$$

If $t$ is large then $\varepsilon t \sim 1$, and $\sin \varepsilon t$ can be as large as $\sin \Omega_{0} t$ Small corrections accumulate with time! These are secular terms

Brief quiz: is it ok to approximate $n_{x}=h / \Omega$ as $n_{x}^{0}=h / \Omega_{0}$ ?

## Dephasing and the choice of quantization axis

Careful analysis (simple but omitted to save time) shows: in the leading order

$$
U \approx U_{0}=\exp \left[-i\left(n_{x}^{0} \sigma_{x}+n_{z}^{0} \sigma_{z}\right) \Omega^{\prime} t / 2\right], \quad \Omega^{\prime}=\Omega_{0}+B_{0} \cdot\left(\beta / \Omega_{0}\right)
$$

$$
\begin{aligned}
& S_{z}(t)=n_{z}^{0} \cdot\left(S_{z} n_{z}^{0}+S_{x} n_{x}^{0}\right)+\{\text { osc.terms }\} \\
& S_{x}(t)=n_{x}^{0} \cdot\left(S_{z} n_{z}^{0}+S_{x} n_{x}^{0}\right)+\{\text { osc.terms }\} \\
& S_{y}(t)=\{\text { osc.terms }\}
\end{aligned}
$$



At long times $S_{z}(t) \rightarrow n_{z}^{0} S_{n 0}$ and $S_{x}(t) \rightarrow n_{x}^{0} S_{n 0}$
The state decays into mixture of eigenstates of $S_{n 0}=S_{z} n_{z}^{0}+S_{x} n_{x}^{0}$
These are pointer states, defined by the "real" quantization axis $\vec{n}_{0}$
I.e. quantization axis is not about math: physical processes give objective preference to certain quantization axes

## Dynamics of dephasing

$$
S_{z}(t)=n_{z}^{0} S_{n 0}+\{\text { osc. terms }\}, S_{x}(t)=n_{x}^{0} S_{n 0}+\{\text { osc. terms }\}, \text { etc. }
$$

Oscillating terms: some combinations of $\sigma_{x, y, z}$ (i.e. some $2 \times 2$ matrices) multiplied by $\cos \Omega^{\prime} t$ and $\sin \Omega^{\prime} t$, where $\Omega^{\prime}=\Omega_{0}+B_{0} \cdot\left(\beta / \Omega_{0}\right)$ Averaging over noise:

$$
\begin{gathered}
\int P(\beta) d \beta\left\{\begin{array}{c}
\cos \left[\Omega_{0} t+t B_{0} \beta / \Omega_{0}\right] \\
\sin \left[\Omega_{0} t+t B_{0} \beta / \Omega_{0}\right]
\end{array}\right\}=\left\{\begin{array}{l}
\mathrm{Re} \\
\operatorname{Im}
\end{array}\right\} \int P(\beta) d \beta \mathrm{e}^{i \Omega_{0} t} \mathrm{e}^{i t \beta B_{0} / \Omega_{0}} \\
\int P(\beta) d \beta \mathrm{e}^{i t \beta B_{0} / \Omega_{0}}=\frac{1}{\sqrt{2 \pi b^{2}}} \int \mathrm{e}^{i t \beta B_{0} / \Omega_{0}} \mathrm{e}^{-\frac{\beta^{2}}{2 b^{2}}} d \beta=\mathrm{e}^{-\frac{B_{0}^{2}}{\Omega_{0}^{2} t^{2}} \frac{2}{2}} \\
\text { I.e. oscillating terms lead to Gaussian decay: } \exp \left[-\frac{1}{2}\left(\frac{t}{T_{2}^{*}}\right)^{2}\right]
\end{gathered}
$$

Coherence time depends on situation! $T_{2}^{*}=b^{-1}$ for $B_{0} \gg h$ but becomes much longer when $B_{0} \ll h: T_{2}^{*}=b^{-1}\left(h / B_{0}\right)$

## Secular / non-secular terms: comments

$>$ Arise in many areas of many-body theory and solid state physics. E.g., using perturbation theory with $\varepsilon \ll 1$, but the result includes $\varepsilon \cdot N$ with $N \rightarrow \infty$ (number of atoms in a macroscopic crystal)
$>$ Expansion in terms of $\beta / \Omega_{0}$ requires well-behaved noise, with $\operatorname{good} P(\beta)$ to ensure that $\int P(\beta) d \beta\left(\beta / \Omega_{0}\right)^{n} \alpha\left(b / \Omega_{0}\right)^{n} \ll 1$ May not work otherwise: e.g. for Lorentzian distribution

$$
P_{L}(\beta)=(b / \pi) \cdot\left[\beta^{2}+b^{2}\right]^{-1}
$$

the integrals $\int P_{L}(\beta) d \beta\left(\beta / \Omega_{0}\right)^{n}$ diverge for $n=2,4, \ldots$ although $b / \Omega_{0} \ll 1$. Same problem: accumulation of small terms.
$>$ Closely related to the notion of absolute convergence and uniform convergence of series and integrals.
> Secular: siècle (Fr.) - century. Accumulates over long times.

## Decoherence, pointer states, quantum superpositions: comments

$>$ Pointer states do not always form an orthonormal basis.
> May be very complex entangled states of many spins.
I.e. entanglement by itself is not a big deal - can be formed spontaneously. It is time evolution that is important in quantum science and technology.
$>$ Can be different on different time scales: e.g. in NV centers: $T_{1}$ (days) vs $T_{2}^{*}(\mu \mathrm{~s})$. Analogy: thermal equilibrium.
What we have considered (dephasing by static noise) is called $T_{2}^{*}$ or inhomogeneous broadening.
> Often hear that decoherence destroys superpositions. But superpositions of what? Any state is a superposition of some other states. Answer: superpositions of pointer states (but remember: pointer states can be nontrivial !)

## Possible projects.

1) For mathematically inclined: consider $H=B S_{z}+h S_{x}$, with

$$
B=B_{0}+\beta \text {, where } P(\beta)=\frac{1}{\sqrt{2 \pi b^{2}}} \exp \left(-\frac{\beta^{2}}{2 b^{2}}\right) \text {, and } b \ll h, B_{0}
$$

Expansion of the evolution operator (or time-dependent operators, or density matrix) in terms of small $\beta$ is not formally justified: averaging involves integration over all $\beta \in(-\infty,+\infty)$.

Can you justify in a more rigorous way that at long times

$$
S_{z}(t) \rightarrow n_{z}^{0} S_{n 0} \text { and } S_{x}(t) \rightarrow n_{x}^{0} S_{n 0} ?
$$

(Hint: start by looking up Lebesgue-Riemann lemma)
2) Consider the same situation, $H=B S_{z}+h S_{x}$, with $B=B_{0}+\beta$, but with Lorentzian noise: $P_{L}(\beta)=(b / \pi)\left[\beta^{2}+b^{2}\right]^{-1}, b \ll h, B_{0}$
Can you justify that $S_{z}(t) \rightarrow n_{z}^{0} S_{n 0}$ and $S_{x}(t) \rightarrow n_{x}^{0} S_{n 0}$ at $t \rightarrow \infty$ ?
(Hint: start by looking up Lebesgue-Riemann lemma)

Take-home messages:

1. All choices of the quantization axes are formally equivalent.

The same as the choice of the representation
But some choices are convenient - can be important
2. Some choices of quantization axis are objectively special, correspond to pointer states. However, these states may not be always obvious, esp. in many-spin systems.
3. Averaging density matrix - ok, time-dep observables - ok. Wavefunction of evolution operator - not ok!
4. Dynamics of dephasing: Fourier-transform spectroscopy
5. Secular terms - small corrections may accumulate. Carefully separate them from those which stay small.
6. Both pointer states and the decoherence dynamics/rates depend on experimental situation.

## Pauli matrices

$$
\sigma_{x} \equiv \sigma_{1}=\left(\begin{array}{cc}
0 & 1 \\
1 & 0
\end{array}\right) \quad \sigma_{y} \equiv \sigma_{2}=\left(\begin{array}{cc}
0 & -i \\
i & 0
\end{array}\right) \quad \sigma_{z} \equiv \sigma_{3}=\left(\begin{array}{cc}
1 & 0 \\
0 & -1
\end{array}\right)
$$

Very convenient for calculations:

$$
\sigma_{\alpha}{ }^{2}=\hat{1} \quad \sigma_{\alpha} \sigma_{\beta}=-\sigma_{\beta} \sigma_{\alpha} \text { for } \alpha \neq \beta
$$

$$
\sigma_{x} \sigma_{y}=i \sigma_{z} \text { and similar for circular permutations }
$$

Therefore $\sigma_{\alpha} \sigma_{\beta} \sigma_{\alpha}=\sigma_{\beta}$ for $\alpha=\beta$ and $\sigma_{\alpha} \sigma_{\beta} \sigma_{\alpha}=-\sigma_{\beta}$ for $\alpha \neq \beta$

$$
\operatorname{Tr} \sigma_{\alpha}=0 \text { and therefore } \operatorname{Tr} \sigma_{\alpha} \sigma_{\beta}=2 \cdot \delta_{\alpha \beta}
$$

Consider projection of Pauli vector on any unit vector $\vec{n}$

$$
\sigma_{n}=(\vec{\sigma} \cdot \vec{n})=\sigma_{x} n_{x}+\sigma_{y} n_{y}+\sigma_{z} n_{z}
$$

where $|\vec{n}|^{2}=n_{x}^{2}+n_{x}^{2}+n_{x}^{2}=1$
Show that $\sigma_{n}{ }^{2}=\hat{1}$ and $\operatorname{Tr} \sigma_{n}=0$

## How to deal with the exponentials of operators

## Way 1. Use the definition. Example: spin $\mathbf{1 / 2}$ operators

Consider rotation by $\alpha=2 \beta$ around the $x$-axis, i.e. $\boldsymbol{u}=\boldsymbol{e}_{x}$
$e^{-i \cdot \alpha \cdot \hat{S}_{x}}=e^{-i \beta \sigma_{x}}=\sum_{k=0}^{\infty} \frac{(-i \beta)^{k}}{k!}\left(\sigma_{x}\right)^{k}=\hat{1}-i \beta \sigma_{x}-\frac{\beta^{2}}{2!} \sigma_{x}^{2}+\cdots$
But $\sigma_{x}^{2}=\hat{1}$, so $\sigma_{x}^{k}=\hat{1}$ for even $k$, and $\sigma_{x}^{k}=\sigma_{x}$ for odd $k$
$e^{-i \beta \sigma_{x}}=\sum_{\text {even } k}^{\infty} \frac{(-i \beta)^{k}}{k!} \cdot \hat{1}+\sum_{\text {odd } k}^{\infty} \frac{(-i \beta)^{k}}{k!} \cdot \sigma_{x}=\begin{gathered}\text { This is only for spin } 1 / 2! \\ \cos \beta \cdot \hat{1}-i \sigma_{x} \sin \beta=e^{-i \beta \sigma_{x}}\end{gathered}$

Taylor expansion of sin and cos:
$\sum_{\text {even } k}^{\infty} \frac{(-i \beta)^{k}}{k!}=\sum_{m=0}^{\infty} \frac{(-1)^{m}}{(2 m)!} \cdot \beta^{2 m}=\cos \beta$
$\sum_{\text {odd } k}^{\infty} \frac{(-i \beta)^{k}}{k!}=-i \cdot \sum_{m=0}^{\infty} \frac{(-1)^{m}}{(2 m)!} \cdot \beta^{2 m+1}=-i \cdot \sin \beta$

Same calculation can be repeated for any

$$
\sigma_{n}=(\vec{\sigma} \cdot \vec{n}), \text { i.e. }
$$

$$
e^{-i \beta \sigma_{n}}=\cos \beta \cdot \hat{1}-i \sigma_{n} \sin \beta
$$

## How to deal with the exponentials of operators

## Way 2. Diagonal form: use eigenfunctions and eigenvalues.

$\hat{A}-$ Hermitian operator, $\hat{A}^{\dagger}=\hat{A} \quad$ Diagonal form: $\hat{A}=\sum_{n} a_{n} \cdot\left|\alpha_{n}\right\rangle\left\langle\alpha_{n}\right|$
Consider a function $f(x)$, with Taylor series expansion $f(x)=\sum_{k=0}^{\infty} f_{k} \cdot x^{k}$ $\hat{F}=f(\hat{A})=\sum_{k=0}^{\infty} f_{k} \cdot \hat{A}^{k} \quad$ but $\quad \hat{A}^{k}=\sum_{n}\left(a_{n}\right)^{k} \cdot\left|\alpha_{n}\right\rangle\left\langle\alpha_{n}\right|$

$$
\widehat{F}=f(\hat{A})=\sum_{n} f\left(a_{n}\right) \cdot\left|\alpha_{n}\right\rangle\left\langle\alpha_{n}\right|
$$

Note: we can define many functions, not just exp

Example: spin $\mathbf{1 / 2}$ operators $\quad$ Rotation by $\alpha=2 \beta$ around the $z$-axis

$$
\begin{gathered}
\hat{S}_{z}=\frac{1}{2} \cdot\left(\begin{array}{cc}
1 & 0 \\
0 & -1
\end{array}\right)=\frac{1}{2} \cdot|\uparrow\rangle\langle\uparrow|-\frac{1}{2} \cdot|\downarrow\rangle\langle\downarrow|=\frac{1}{2} \cdot\left(\begin{array}{cc}
1 & 0 \\
0 & 0
\end{array}\right)-\frac{1}{2} \cdot\left(\begin{array}{ll}
0 & 0 \\
0 & 1
\end{array}\right) \\
e^{-i \alpha \hat{S}_{z}}=e^{-i \alpha / 2} \cdot|\uparrow\rangle\langle\uparrow|+e^{i \alpha / 2} \cdot|\downarrow\rangle\langle\downarrow|=\left(\begin{array}{cc}
e^{-i \beta} & 0 \\
0 & e^{i \beta}
\end{array}\right)
\end{gathered}
$$

