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

M. I. Kaganov

Quantum spins

What is this course about?

Modern approaches to describing, analysing, and controlling spin/qubit dynamics.

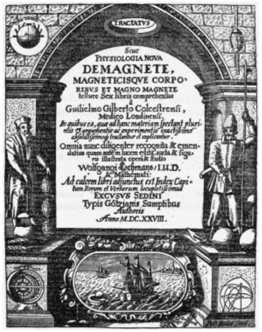
Approaches that are actually used in most laboratories right now. Not only for spin qubits but also for Josephson junction qubits, trapped ions, cavity-QED qubits, etc.

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

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

A. Kronig
1925

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)

<u>Our "usual" 3D space:</u>
choose a basis, i.e. any three orthonormal vectors $\vec{e}_1$, $\vec{e}_2$, and $\vec{e}_3$

$$\vec{a} = a_1 \cdot \vec{e}_1 + a_2 \cdot \vec{e}_2 + a_3 \cdot \vec{e}_3 \quad \text{or} \quad \vec{a} = \begin{bmatrix} a_1 \\ a_2 \\ a_3 \end{bmatrix} \qquad a_1, a_2, a_3 \in \mathbb{R}$$

- **<u>Quantum state vector in a Hilbert space</u>**

d-dimensional basis, i.e. d orthonormal vectors $\vec{e}_1$, $\vec{e}_2$, … $\vec{e}_d$

$$\vec{\psi} = \psi_1 \cdot \vec{e}_1 + \psi_2 \cdot \vec{e}_2 + \cdots + \psi_d \cdot \vec{e}_d \quad \text{or} \quad \vec{\psi} = \begin{bmatrix} \psi_1 \\ \ldots \\ \psi_d \end{bmatrix} \qquad \psi_1, \ldots, \psi_d \in \mathbb{C}$$

Dirac's notations (bra/ket formalism): basis vectors $|e_1\rangle, \ldots, |e_d\rangle$

$$|\psi\rangle = \psi_1 \cdot |e_1\rangle + \cdots + \psi_d \cdot |e_d\rangle \quad \text{with the requirement} \quad |\psi_1|^2 + \cdots + |\psi_d|^2 = 1$$

- **<u>Scalar (inner) product and dual vectors</u>**

$$\left(\vec{a},\vec{b}\right) = [a_1\,, a_2\,, a_3] \cdot \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix} = \sum_{k=1}^{3} a_k \cdot b_k \quad ; \qquad [a_1\,, a_2\,, a_3] \text{ - dual of } \vec{a} = \begin{bmatrix} a_1 \\ a_2 \\ a_3 \end{bmatrix}$$

Bra-ket form: $|\varphi\rangle = \begin{bmatrix} \varphi_1 \\ \cdots \\ \varphi_d \end{bmatrix}$, its dual $\langle\varphi| = [\varphi_1^*\,, \varphi_2^*\,, \varphi_3^*]$, and $\langle\varphi|\psi\rangle = \sum_{k=1}^{d} \varphi_k^* \cdot \psi_k$

- Changing the quantum state. **<u>Linear operators</u>**

$$\hat{A} : |\psi\rangle \to |\varphi\rangle = \hat{A}|\psi\rangle \equiv |\hat{A}\,\psi\rangle \qquad\qquad \hat{A}\,[a|\psi\rangle + b|\phi\rangle] \equiv a\big|\hat{A}\psi\big\rangle + b\big|\hat{A}\phi\big\rangle$$

With a given basis, the operator $\hat{A}$ is a matrix, i.e. $\hat{A} = \sum_{j,k=1}^{d} A_{jk}|e_j\rangle\langle e_k|$

Why? Because each $\varphi_k = \langle e_k|\varphi\rangle = \langle e_k|\hat{A}\psi\rangle = \langle e_k|\hat{A}|\psi\rangle$ is linear in $|\psi\rangle$.
Riesz theorem: **<u>any</u>** continuous linear function f of $|\psi\rangle$ has a form $f = \langle\alpha|\psi\rangle$

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 $|1\rangle$

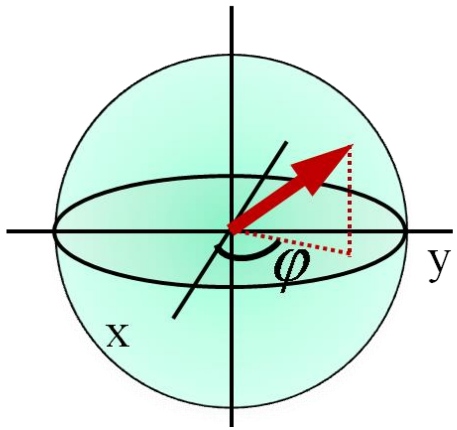
$$|\psi\rangle = \alpha|\uparrow\rangle + \beta|\downarrow\rangle \qquad \rho = |\psi\rangle\langle\psi| = \begin{bmatrix} |\alpha|^2 & \beta^*\alpha \\ \alpha^*\beta & |\beta|^2 \end{bmatrix}$$

All operators are linear combinations of Pauli matrices:

$$\sigma_0 \equiv 1 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Spin operators (observables): $S_\mu = \frac{1}{2}\sigma_\mu$

Bloch sphere mapping:



$$\langle S_z \rangle = \frac{1}{2}(\rho_{00} - \rho_{11})$$

$$\langle S_x \rangle = \frac{1}{2}(\rho_{01} + \rho_{10})$$

$$\langle S_y \rangle = \frac{i}{2}(\rho_{01} - \rho_{10})$$

Brief reminder – quantum mechanical averages

What are the quantities $\langle S_x \rangle$, $\langle S_y \rangle$, and $\langle S_z \rangle$?

➢ <u>Hermitian operators – observables.</u> Describe physically observable quantities

Diagonal form: $\hat{O} = \sum_n O_n \cdot |\omega_n\rangle\langle\omega_n|$

- eigenvectors $|\omega_n\rangle$ form a complete orthonormal basis
- eigenvalues O_n are real

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

$$|\psi\rangle = \sum_k \psi_k\, |\omega_k\rangle\ , \qquad \psi_k = \langle\omega_k|\psi\rangle$$

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

- with the probability $w_n = |\psi_n|^2 = |\langle\omega_n|\psi\rangle|^2$ obtain the value O_n
- and simultaneously change the state of the system to $|\omega_n\rangle$

The measurement outcome is <u>random</u>, 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 $\langle S_z \rangle$ (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., $E = 1$ J $\rightarrow$ $\omega \approx 10^{34}$ rad/s or $\nu \approx 1.5\cdot 10^{33}$ Hz
  Usually, in spin physics we deal with ν in kHz–GHz range

- set $\gamma = 1$: measure magnetic fields in rad/s or Hz
  This is spin-dependent !
  Electron spin: $B = 1$ T corresponds to $\nu \approx 30$ GHz
  Nuclear ^{13}C spin: $B = 1$ T $\rightarrow$ $\nu \approx 11$ MHz

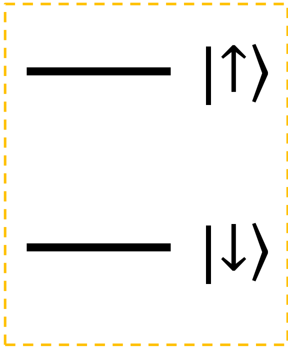
Important: $\omega\cdot t$ is dimensionless, while $\nu\cdot t$ is not

Indeed: $\sin\omega t$, not $\sin\nu t$!

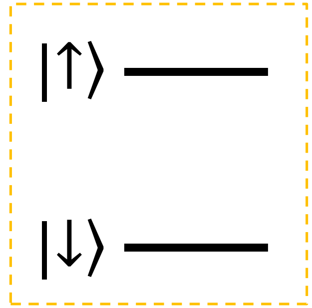
How to think of real spin/qubit (say, spin 1/2):

Ideal:

$\hat{H} = B\hat{S}_z$



Static noise:



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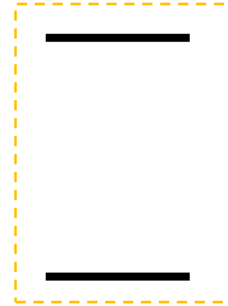

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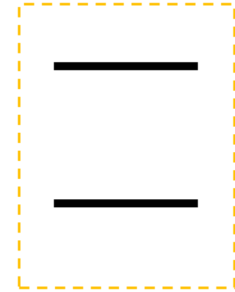
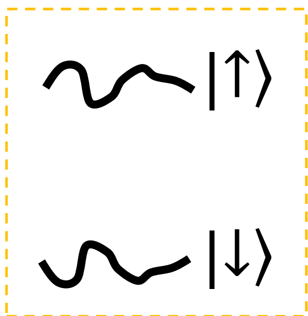


…

random B: ensemble of possible level positions

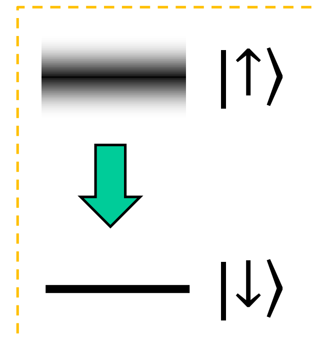
Dynamic noise: $B(t)$



level positions randomly vary in time

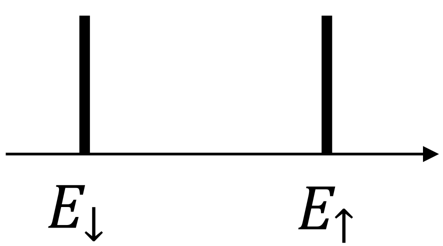
Relaxation:

energy of the upper level is not well defined: $\Delta E \sim 1/\tau_{\mathrm{relax}}$

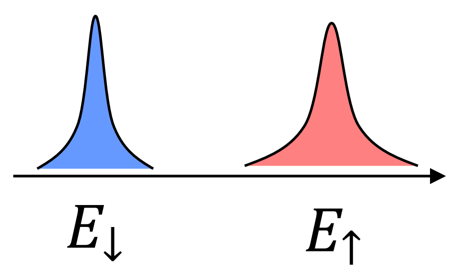


Seen e.g. in spectroscopic experiment: <u>levels with finite width</u>

not



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

$$|\uparrow\rangle\,,|\downarrow\rangle \quad \mapsto \quad |\varphi_\uparrow\rangle = W\,|\uparrow\rangle\,, \quad |\varphi_\downarrow\rangle = W\,|\downarrow\rangle$$

At home: what is the most general form of W for spin $1/2$?

Any choice of U is equally good (unitary equivalence)

If the spin coupled to magnetic field or other spins : $H_\varphi = W\,H\,W^\dagger$

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:

$$H = B(t)\cdot S_x \qquad i\,|\dot{\psi}\rangle = B(t)\,S_x\,|\psi\rangle \qquad |\psi\rangle = \alpha|\uparrow\rangle + \beta|\downarrow\rangle$$

$$i\,\dot{\alpha} = \tfrac{1}{2}h(t)\,\beta \qquad \ddot{\alpha} = \dot{\alpha}\,\frac{\dot{h}}{h} - \frac{h(t)^2}{4}\alpha \qquad \text{Oops...}$$
$$i\,\dot{\beta} = \tfrac{1}{2}h(t)\,\alpha$$

Now choose <u>different quantization axis</u>. New basis: eigenvectors of S_x

$$|\varphi_\uparrow\rangle = \tfrac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix}, \quad |\varphi_\downarrow\rangle = \tfrac{1}{\sqrt{2}}\begin{pmatrix}-1\\1\end{pmatrix}, \quad W = \tfrac{1}{\sqrt{2}}\begin{pmatrix}1 & -1\\1 & 1\end{pmatrix}$$

$$H_\varphi = B(t)\cdot\tfrac{1}{2}\begin{pmatrix}1 & 0\\0 & -1\end{pmatrix} = B(t)\cdot S_z$$ – just another coordinate frame

in the new basis !

$$|\psi\rangle = a|\uparrow\rangle + b|\downarrow\rangle \qquad i\dot{a} = \tfrac{1}{2}B(t)\,a\;,\quad i\dot{b} = \tfrac{1}{2}B(t)\,b$$

$$a(t) = a_0\exp[-i\Phi(t)/2]\;,\quad b(t) = b_0\exp[i\Phi(t)/2]$$

$$\Phi(t) = \int_0^t B(s)\,ds$$

$$\langle S_x\rangle(t) = \langle S_x^0\rangle\cos\Phi - \langle S_y^0\rangle\sin\Phi$$
$$\langle S_y\rangle(t) = \langle S_y^0\rangle\cos\Phi + \langle S_x^0\rangle\sin\Phi$$
$$\langle S_z\rangle(t) = \langle S_z^0\rangle$$

Regular Larmor precession,
but in a time-varying field

$\langle S_{x,y,z}^0\rangle \equiv \langle S_{x,y,z}\rangle(0)$ **(in the new basis!)**

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

$$\hat{S}_x(t) = \begin{pmatrix} s_{00}(t) & s_{01}(t) \\ s_{10}(t) & s_{11}(t) \end{pmatrix}$$

$$\langle S_x \rangle(t) = \left\langle \psi(0) \middle| \hat{S}_x(t) \middle| \psi(0) \right\rangle$$

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

Use the operators $\hat{S}^+ = \hat{S}_x + i\hat{S}_y$, $\hat{S}^- = \hat{S}_x - i\hat{S}_y$

Repeat the same calculation, but now via evolution operator

Static field – static Hamiltonian: $\hat{U} = \exp\left(-i\hat{H}t\right)$

Time-dep Hamiltonian: $i\,\dot{\hat{U}} = \hat{H}(t)\,\hat{U}$

Larmor precession with noise: dephasing

Important: experiments are never perfect

$B = B_0 + \beta$: $\hat{H} = (B_0 + \beta) \cdot \hat{S}_z$, β – noise, assume (quasi)static

Also assume it is Gaussian :
(e.g. central limit theorem)

$$P(\beta) = \frac{1}{\sqrt{2\pi b^2}} \exp\left(-\frac{\beta^2}{2b^2}\right)$$

$$\hat{S}^+(t) = \hat{S}^+ \, \mathrm{e}^{i(B_0+\beta)t}$$
$$\hat{S}^-(t) = \hat{S}^- \, \mathrm{e}^{-i(B_0+\beta)t}$$
$$\longrightarrow \left\langle \hat{S}^+(t) \right\rangle_\beta = \hat{S}^+ \cdot \mathrm{e}^{iB_0 t} \int_{-\infty}^{\infty} P(\beta) \, \mathrm{e}^{it\beta} \, d\beta$$

and similar for $\langle S^-(t) \rangle_\beta$

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

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

$$\left\langle \langle S_{x,y} \rangle(t) \right\rangle_\beta = \left\langle \mathrm{Tr}\, \rho(0) \, \hat{S}_{x,y}(t) \right\rangle_\beta \to 0$$

and only $\left\langle \langle S_z \rangle(t) \right\rangle_\beta = \langle S_z \rangle(0) = \mathrm{const}$

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

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

$$\left\langle \langle S_x \rangle (t) \right\rangle_\beta = \left\langle \mathrm{Tr}\, \rho(0)\, \hat{S}_x(t) \right\rangle_\beta = \left\langle \mathrm{Tr}\, \rho(0)\, \hat{U}_\beta^\dagger(t)\, \hat{S}_x\, \hat{U}_\beta(t) \right\rangle_\beta =$$

$$= \left\langle \mathrm{Tr}\;\; \hat{U}_\beta(t)\, \rho(0)\, \hat{U}_\beta^\dagger(t)\, \hat{S}_x \right\rangle_\beta = \left\langle \mathrm{Tr}\;\; \rho_\beta(t)\, \hat{S}_x \right\rangle_\beta$$

But **<u>cannot use</u>** noise-averaged ev.op. $\left\langle \hat{U}(t) \right\rangle_\beta$ or $\langle \psi(t) \rangle_\beta = \left\langle \hat{U}_\beta(t)\, \psi(0) \right\rangle_\beta$

Indeed: $\left\langle \langle S_x \rangle (t) \right\rangle_\beta = \mathrm{Tr}\; \left\langle \hat{U}_\beta(t)\, \rho(0)\, \hat{U}_\beta^\dagger(t) \right\rangle_\beta \hat{S}_x$

but

$$\left\langle \hat{U}_\beta(t)\, \rho(0)\, \hat{U}_\beta^\dagger(t) \right\rangle_\beta = \langle |\psi(t)\rangle\langle\psi(t)| \rangle_\beta \neq \left\langle |\psi(t)\rangle \right\rangle_\beta \cdot \left\langle \langle\psi(t)| \right\rangle_\beta$$

- 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 $\langle \dots \rangle_\beta$ when possible.

General quasistatic noise: FT spectroscopy

$\widehat{H} = (B_0 + \beta) \cdot \hat{S}_z$, β – (quasi)static noise, some general $P(\beta)$

$$\hat{S}^+(t) = \hat{S}^+ \, \mathrm{e}^{i(B_0+\beta)t}$$
$$\hat{S}^-(t) = \hat{S}^- \, \mathrm{e}^{-i(B_0+\beta)t}$$

$$\rightarrow \quad \left\langle \hat{S}^+(t) \right\rangle_\beta = \hat{S}^+ \cdot \mathrm{e}^{iB_0 t} \int_{-\infty}^{\infty} P(\beta) \, \mathrm{e}^{it\beta} \, d\beta$$

and similar for $\langle S^-(t) \rangle_\beta$

$f(t) = \int_{-\infty}^{\infty} P(\beta) \, \mathrm{e}^{it\beta} \, d\beta$: characteristic function of a random variable

Experiment:

1) Prepare spin in a state $\psi = \frac{1}{\sqrt{2}}(|\uparrow\rangle + |\downarrow\rangle)$ with $\langle S_x^0 \rangle = \frac{1}{2}$, $\left\langle S_{y,z}^0 \right\rangle = 0$

2) Measure $\langle S_x \rangle(t)$ 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: $|\psi\rangle = u|\uparrow\rangle + ve^{i\varphi}|\downarrow\rangle\,,\ u, v \in \mathbb{R}$

$$\rho = |\psi\rangle\langle\psi| = \begin{bmatrix} u^2 & uv\,e^{-i\phi} \\ uv\,e^{i\phi} & v^2 \end{bmatrix}\,, \quad \phi \text{ – quantum phase}$$

$$\rho(t) = \begin{pmatrix} u^2 & uv\,e^{-i(\phi+B_0 t)}\mathrm{e}^{-\frac{b^2t^2}{2}} \\ uv\,e^{i(\phi+B_0 t)}\mathrm{e}^{-\frac{b^2t^2}{2}} & v^2 \end{pmatrix} \xrightarrow{t\to\infty} \begin{pmatrix} u^2 & 0 \\ 0 & v^2 \end{pmatrix}$$

Purely classical spin – phase is randomized, quantumness gone

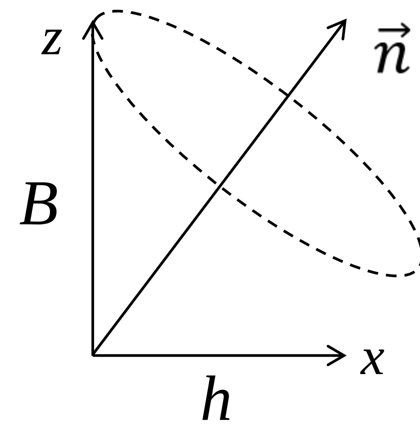
<u>Besides, a special set of states is selected</u> : $|\uparrow\rangle$ and $|\downarrow\rangle$

Quantum spin – all basis sets are the same (unitarily equivalent)
Decohered spin – some states are special, survive dephasing
(although their superpositions do not)

<u>**Pointer states**</u>

Dephasing and the choice of quantization axis

$$H = B\,S_z + h\,S_x = \tfrac{1}{2}B\,\sigma_z + \tfrac{1}{2}\,h\,\sigma_x$$ - static field



$$U = \mathrm{e}^{-iHt} = \exp[-i\,(n_x\sigma_x + n_z\sigma_z)\,\varphi/2]$$

$$\exp[-i\,(\vec{\sigma}\vec{n})\,\varphi/2] = \cos\varphi/2 - i(\vec{\sigma}\vec{n})\sin\varphi/2$$

$$\varphi = \Omega t\,,\quad \Omega = \sqrt{B^2 + h^2}\,,\quad n_x = h/\Omega\,,\quad n_z = B/\Omega$$

Add weak static noise : $B = B_0 + \beta$ $\qquad P(\beta) = \frac{1}{\sqrt{2\pi b^2}}\exp\left(-\frac{\beta^2}{2b^2}\right)$

$$b \ll h, B_0$$

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

$$\Omega = \sqrt{B^2 + h^2} \equiv \sqrt{(B_0 + \beta)^2 + h^2} \approx \sqrt{B_0^2 + h^2} \equiv \Omega_0$$

This is a good approximation for Ω : look at the expansion

$$\Omega = \Omega_0 + B_0 \cdot (\beta/\Omega_0) + [h^2/2\Omega_0] \cdot (\beta/\Omega_0)^2 + \cdots$$

and when averaging $\int P(\beta) d\beta \, (\beta/\Omega_0)^n \propto (b/\Omega_0)^n \ll 1$

But is it also good for φ ? Emphatic **<u>NO</u>** !

$$\varphi = \Omega t = \Omega_0 t + \varepsilon t + \cdots , \quad \text{where } \varepsilon = (B_0/\Omega_0)\, \beta \ll \Omega_0$$

$$\cos\varphi \approx \cos[\Omega_0 t + \varepsilon t] = \cos\Omega_0 t \cdot \cos\varepsilon t - \sin\Omega_0 t \cdot \sin\varepsilon t$$

If t is large then $\varepsilon t \sim 1$, and $\sin\varepsilon t$ can be as large as $\sin\Omega_0 t$

Small corrections <u>accumulate with time</u>! These are **<u>secular terms</u>**

<u>Brief quiz</u>: is it ok to approximate $n_x = h/\Omega$ as $n_x^0 = h/\Omega_0$?

Dephasing and the choice of quantization axis

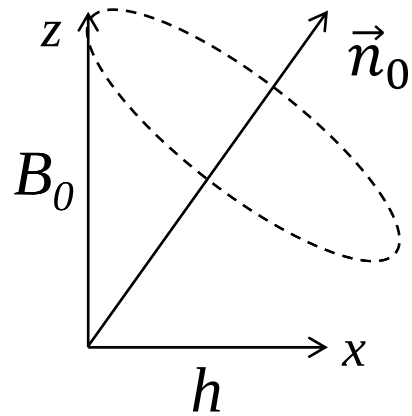
Careful analysis (simple but omitted to save time) shows: in the leading order

$$U \approx U_0 = \exp[-i\,(n_x^0\,\sigma_x + n_z^0\,\sigma_z)\,\Omega' t/2]\,, \quad \Omega' = \Omega_0 + B_0 \cdot (\beta/\Omega_0)$$

$$S_z(t) = n_z^0 \cdot (S_z\, n_z^0 + S_x\, n_x^0) \; + \{\text{osc. terms}\}$$

$$S_x(t) = n_x^0 \cdot (S_z\, n_z^0 + S_x\, n_x^0) \; + \{\text{osc. terms}\}$$

$$S_y(t) = \{\text{osc. terms}\}$$



At long times $S_z(t) \to n_z^0\, S_{n0}$ and $S_x(t) \to n_x^0\, S_{n0}$

The state decays into mixture of eigenstates of $S_{n0} = S_z\, n_z^0 + S_x\, n_x^0$

These are **<u>pointer states</u>**, defined by the "real" quantization axis $\vec{n}_0$

I.e. quantization axis is not about math: physical processes give <u>objective preference</u> to certain quantization axes

Dynamics of dephasing

$$S_z(t) = n_z^0\, S_{n0} + \{\text{osc. terms}\}\,,\ S_x(t) = n_x^0\, S_{n0} + \{\text{osc. terms}\}\,, \text{etc.}$$

Oscillating terms: some combinations of $\sigma_{x,y,z}$ (i.e. some 2x2 matrices) multiplied by $\cos\Omega' t$ and $\sin\Omega' t$, where $\Omega' = \Omega_0 + B_0 \cdot (\beta/\Omega_0)$

Averaging over noise:

$$\int P(\beta) d\beta \begin{Bmatrix} \cos[\Omega_0 t + t\, B_0 \beta/\Omega_0] \\ \sin[\Omega_0 t + t\, B_0 \beta/\Omega_0] \end{Bmatrix} = \begin{Bmatrix} \mathrm{Re} \\ \mathrm{Im} \end{Bmatrix} \int P(\beta) d\beta\, \mathrm{e}^{i\Omega_0 t} \mathrm{e}^{it\beta B_0/\Omega_0}$$

$$\int P(\beta) d\beta\, \mathrm{e}^{it\beta B_0/\Omega_0} = \frac{1}{\sqrt{2\pi b^2}} \int \mathrm{e}^{it\beta B_0/\Omega_0}\, \mathrm{e}^{-\frac{\beta^2}{2b^2}}\, d\beta = \mathrm{e}^{-\frac{B_0^2}{\Omega_0^2}\frac{b^2 t^2}{2}}$$

I.e. oscillating terms lead to <u>Gaussian decay</u>: $\exp\left[-\frac{1}{2}\left(\frac{t}{T_2^*}\right)^2\right]$

<u>Coherence time depends on situation</u>! $T_2^* = b^{-1}$ for $B_0 \gg h$

but becomes **much longer** when $B_0 \ll h$: $T_2^* = b^{-1}(h/B_0)$

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 $N \to \infty$ (number of atoms in a macroscopic crystal)

- Expansion in terms of β/Ω_0 requires well-behaved noise, with good $P(\beta)$ to ensure that $\int P(\beta) d\beta \, (\beta/\Omega_0)^n \propto (b/\Omega_0)^n \ll 1$

  May not work otherwise: e.g. for Lorentzian distribution

$$P_L(\beta) = (b/\pi) \cdot [\beta^2 + b^2]^{-1}$$

  the integrals $\int P_L(\beta) d\beta \, (\beta/\Omega_0)^n$ 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 <u>time evolution</u> 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^* (μs) . 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. <u>Answer</u>: 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

$$B = B_0 + \beta, \text{ where } P(\beta) = \frac{1}{\sqrt{2\pi b^2}} \exp\left(-\frac{\beta^2}{2b^2}\right), \text{ and } b \ll h, B_0$$

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

Can you justify in a more rigorous way that at long times $S_z(t) \to n_z^0\, S_{n0}$ and $S_x(t) \to n_x^0\, S_{n0}$?

(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: $P_L(\beta) = (b/\pi)[\beta^2 + b^2]^{-1}$, $b \ll h, B_0$

Can you justify that $S_z(t) \to n_z^0\, S_{n0}$ and $S_x(t) \to n_x^0\, S_{n0}$ at $t \to \infty$?

(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

$$\sigma_x \equiv \sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \sigma_y \equiv \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \qquad \sigma_z \equiv \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Very convenient for calculations:

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

$\sigma_x \sigma_y = i\sigma_z$ 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 $\alpha \neq \beta$

$\mathrm{Tr}\, \sigma_\alpha = 0$ and therefore $\mathrm{Tr}\, \sigma_\alpha \sigma_\beta = 2 \cdot \delta_{\alpha\beta}$

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 $\mathrm{Tr}\, \sigma_n = 0$

How to deal with the exponentials of operators

Way 1. Use the definition. **Example: spin 1/2 operators**

Consider rotation by $\alpha = 2\beta$ around the x-axis, i.e. $\boldsymbol{u} = \boldsymbol{e}_x$

$$e^{-i\cdot\alpha\cdot\hat{S}_x} = e^{-i\beta\sigma_x} = \sum_{k=0}^{\infty} \frac{(-i\beta)^k}{k!} (\sigma_x)^k = \hat{1} - i\beta\sigma_x - \frac{\beta^2}{2!}\sigma_x^2 + \cdots$$

But $\sigma_x^2 = \hat{1}$, so $\sigma_x^k = \hat{1}$ for even k, and $\sigma_x^k = \sigma_x$ for odd k

This is only for spin 1/2 !

$$e^{-i\beta\sigma_x} = \sum_{\text{even } k}^{\infty} \frac{(-i\beta)^k}{k!} \cdot \hat{1} + \sum_{\text{odd } k}^{\infty} \frac{(-i\beta)^k}{k!} \cdot \sigma_x = \boxed{\cos\beta \cdot \hat{1} - i\,\sigma_x \sin\beta = e^{-i\beta\sigma_x}}$$

Taylor expansion of sin and cos:

$$\sum_{\text{even } k}^{\infty} \frac{(-i\beta)^k}{k!} = \sum_{m=0}^{\infty} \frac{(-1)^m}{(2m)!} \cdot \beta^{2m} = \cos\beta$$

$$\sum_{\text{odd } k}^{\infty} \frac{(-i\beta)^k}{k!} = -i \cdot \sum_{m=0}^{\infty} \frac{(-1)^m}{(2m)!} \cdot \beta^{2m+1} = -i \cdot \sin\beta$$

Same calculation can be repeated for any

$\sigma_n = (\vec{\sigma} \cdot \vec{n})$, 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, $\hat{A}^\dagger = \hat{A}$ Diagonal form: $\hat{A} = \sum_n a_n \cdot |\alpha_n\rangle\langle\alpha_n|$

Consider a function $f(x)$, with Taylor series expansion $f(x) = \sum_{k=0}^{\infty} f_k \cdot x^k$

$$\hat{F} = f(\hat{A}) = \sum_{k=0}^{\infty} f_k \cdot \hat{A}^k \quad \text{but} \quad \hat{A}^k = \sum_n (a_n)^k \cdot |\alpha_n\rangle\langle\alpha_n|$$

$$\boxed{\hat{F} = f(\hat{A}) = \sum_n f(a_n) \cdot |\alpha_n\rangle\langle\alpha_n|}$$

Note: we can define many functions, not just exp

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

$$\hat{S}_z = \tfrac{1}{2} \cdot \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \tfrac{1}{2} \cdot |\uparrow\rangle\langle\uparrow| - \tfrac{1}{2} \cdot |\downarrow\rangle\langle\downarrow| = \tfrac{1}{2} \cdot \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} - \tfrac{1}{2} \cdot \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$$

$$e^{-i\alpha\hat{S}_z} = e^{-i\alpha/2} \cdot |\uparrow\rangle\langle\uparrow| + e^{i\alpha/2} \cdot |\downarrow\rangle\langle\downarrow| = \begin{pmatrix} e^{-i\beta} & 0 \\ 0 & e^{i\beta} \end{pmatrix}$$