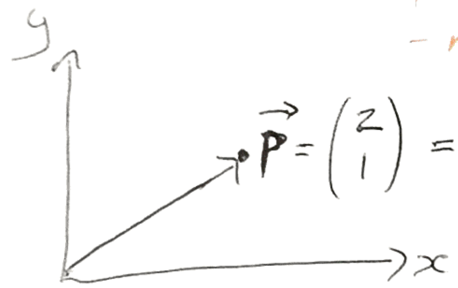
Vectors

$|p\rangle$ is a "superposition" of $|x\rangle$ and $|y\rangle$
– no mystery or "quantum weirdness" about this!



$$\vec{p} = \begin{pmatrix} 2 \\ 1 \end{pmatrix} = 2\hat{\imath} + \hat{\jmath} = \begin{pmatrix} 2 \\ 0 \end{pmatrix} + \begin{pmatrix} 0 \\ 1 \end{pmatrix} = 2\begin{pmatrix} 1 \\ 0 \end{pmatrix} + \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$|p\rangle = 2|x\rangle + |y\rangle, \quad |x\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad |y\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$= \begin{pmatrix} 2 \\ 1 \end{pmatrix}$$

"Dual vector" or Hermitian conjugate: $\langle p| = (2 \;\; 1) = 2\langle x| + \langle y|$

Magnitude of P, $|p|^2 = 2^2 + 1^2$ (Pythagoras)

$$= (2 \;\; 1)\cdot\begin{pmatrix} 2 \\ 1 \end{pmatrix} = \langle p|p\rangle \quad \text{"inner product"}$$

NB. $|p\rangle\langle p| = \begin{pmatrix} 2 \\ 1 \end{pmatrix}\cdot(2 \;\; 1) = \begin{pmatrix} 4 & 2 \\ 2 & 1 \end{pmatrix}$ is not equal to $\langle p|p\rangle$!

"outer product"

Othogonal basis: $\langle x|y\rangle = \langle y|x\rangle = 0$

Normal basis: $\langle x|x\rangle = \langle y|y\rangle = 1$

together $\Rightarrow$ "orthonormal"

For basis vectors $\{|i\rangle\}$, $\sum_i |i\rangle\langle i| = I$ (identity matrix)

Change of basis

$$|p\rangle = 2|x\rangle + |y\rangle$$

projection of $|x\rangle$ onto $|a\rangle$ = length of $|x\rangle$ along $|a\rangle$ direction times $|a\rangle$

$$= (|a\rangle\langle a| + |b\rangle\langle b|)\,(2|x\rangle + |y\rangle)$$

$$= 2\,|a\rangle\langle a|x\rangle + |a\rangle\langle a|y\rangle$$

$$+ 2\,|b\rangle\langle b|x\rangle + |b\rangle\langle b|y\rangle$$

$$= \left(2\cdot\tfrac{1}{\sqrt{2}} + \tfrac{1}{\sqrt{2}}\right)|a\rangle + \left(2\cdot\tfrac{-1}{\sqrt{2}} + \tfrac{1}{\sqrt{2}}\right)|b\rangle$$

$$= \tfrac{3}{\sqrt{2}}|a\rangle - \tfrac{1}{\sqrt{2}}|b\rangle$$

$$|a\rangle = \tfrac{1}{\sqrt{2}}|x\rangle + \tfrac{1}{\sqrt{2}}|y\rangle$$

$$|b\rangle = -\tfrac{1}{\sqrt{2}}|x\rangle + \tfrac{1}{\sqrt{2}}|y\rangle$$

$$\langle a|x\rangle = \left(\tfrac{1}{\sqrt{2}} \;\; \tfrac{1}{\sqrt{2}}\right)\cdot\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \tfrac{1}{\sqrt{2}} \qquad \langle b|x\rangle = -1/\sqrt{2}$$

$$\langle a|y\rangle = 1/\sqrt{2} \qquad \langle b|y\rangle = 1/\sqrt{2}$$

Sanity check: $\langle p|p\rangle = 5$ in both bases!

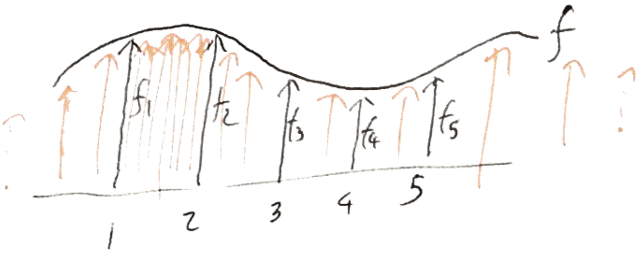
Vectors and functions

There is a <u>deep</u> connection between vectors and functions:

Imagine 5dimensional vectors $|f\rangle$ and $|g\rangle$:

$$|f\rangle = \begin{pmatrix} f_1 \\ f_2 \\ f_3 \\ f_4 \\ f_5 \end{pmatrix} = \begin{pmatrix} f(1) \\ f(2) \\ f(3) \\ f(4) \\ f(5) \end{pmatrix} \qquad |g\rangle = \begin{pmatrix} g_1 \\ g_2 \\ g_3 \\ g_4 \\ g_5 \end{pmatrix} = \begin{pmatrix} g(1) \\ g(2) \\ g(3) \\ g(4) \\ g(5) \end{pmatrix}$$

We can represent a function's values through the components of the vector



Now imagine including more points (dimensions) in $|f\rangle$ ...

Ultimately they become completely indistinguishable.

Take home message: functions are "just" infinite-dimensional vectors! $\langle f|g\rangle = \int f^*(x)g(x)dx = \vec{f}\cdot\vec{g}$

What does this mean for QM / NMR? Don't get too hung up on difference between wavefunctions, wavevectors, eigenfunctions, eigenvectors... it's all the same in the end! Can use whatever approach is most useful – for NMR, this is usually the vector picture.

Introducing QM: wavefunctions and complex vector spaces

Wavefunction $|\Psi\rangle = \begin{pmatrix} c_1 \\ c_2 \end{pmatrix}$ represents a spin-½ nucleus

Only difference to before: complex numbers in vector.

$$|\Psi\rangle = \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = \begin{pmatrix} a_1 + ib_1 \\ a_2 + ib_2 \end{pmatrix}$$

Components are written in some basis space, but the wavefunction itself doesn't depend on this choice

eg. previously $|p\rangle$ is same whether written in terms of $|x\rangle$ and $|y\rangle$ or $|a\rangle$ and $|b\rangle$

Measurements

THIS is where QM gets weird!

Observable quantities $\hat{Q}$ are operators, $\hat{Q} \cdot f(x) = g(x)$

or equivalently, matrices: $\hat{Q} \cdot \vec{x} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \cdot \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \vec{y}$

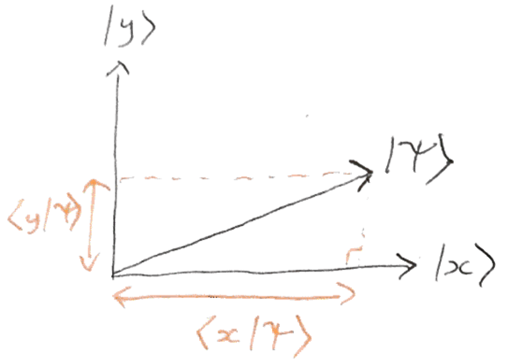
Dirac notation: $\hat{Q}\,|f\rangle = a \cdot |g\rangle$

For some combinations, $\hat{Q} \cdot |x\rangle = \lambda\,|x\rangle$ → $|x\rangle$ is eigenstate/eigenvector/...
→ λ is eigenvalue of $|x\rangle$

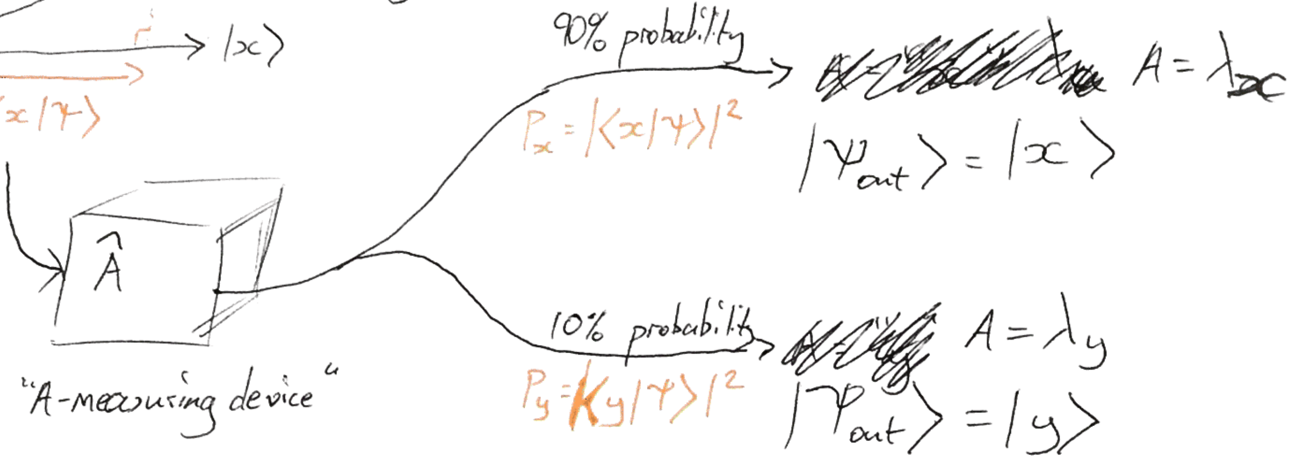
Eigenstates of observable operators form complete basis sets.

WHATEVER the wavefunction before a measurement of operator $\hat{Q}$, afterwards the wavefunction will ALWAYS be in an eigenstate of $\hat{Q}$!

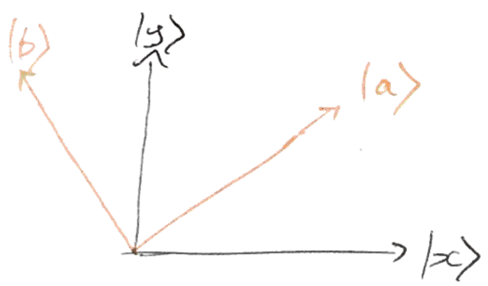
Measurements change the wavefunction!

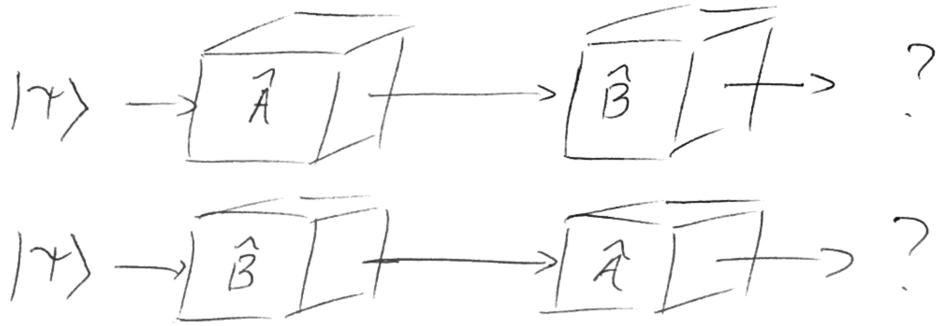


Suppose $|x\rangle$ and $|y\rangle$ are the eigenstates of some observable, $\hat{A}$, with eigenvalues λ_x and λ_y:



Repeated measurements of $\hat{A}$ will give the same result.
What about a 2nd observable, $\hat{B}$, with eigenstates $|a\rangle$ and $|b\rangle$?





All very weird and interesting – but for NMR we don't actually need to worry about the measurement problem! We only need to care about averages over lots of spins.

QM description of spin-½ nucleus

spin $\frac{1}{2}$ $\Rightarrow$ $2 \times \frac{1}{2} + 1 = 2$ energy levels

= 2 eigenstates of Hamiltonian

$\Longrightarrow$ 2 dimensional system

$$|\psi\rangle = \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = c_\alpha \begin{pmatrix} 1 \\ 0 \end{pmatrix} + c_\beta \begin{pmatrix} 0 \\ 1 \end{pmatrix} = c_\alpha |\alpha\rangle + c_\beta |\beta\rangle$$

$$= c_\alpha |\uparrow\rangle + c_\beta |\downarrow\rangle$$

NB. $|\uparrow\rangle$ is NOT equal to $-|\downarrow\rangle$

$\langle\downarrow|\uparrow\rangle = 0$ $\Rightarrow$ $|\uparrow\rangle$ and $|\downarrow\rangle$ are at RIGHT ANGLES!

How many dof needed to describe a spin?

How many dof are available?