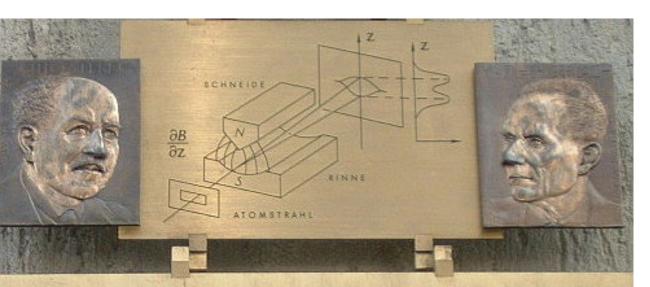
# An Important 2-State System: Spin 1/2



IM FEBRUAR 1922 WURDE IN DIESEM GEBÄUDE DES PHYSIKALISCHEN VEREINS, FRANKFURT AM MAIN, VON OTTO STERN UND WALTHER GERLACH DIE FUNDAMENTALE ENTDECKUNG DER RAUMQUANTISIERUNG DER MAGNETISCHEN MOMENTE IN ATOMEN GEMACHT. AUF DEM STERN-GERLACH-EXPERIMENT BERUHEN WICHTIGE PHYSIKALISCH-TECHNISCHE ENTWICKLUNGEN DES 20. JHDTS., WIE KERNSPINRESONANZMETHODE, ATOMUHR ODER LASER. OTTO STERN WURDE 1943 FÜR DIESE ENTDECKUNG DER NOBELPREIS VERLIEHEN.

# Energy of magnet in a magnetic field

 $U = -\boldsymbol{\mu} \cdot \boldsymbol{B}$ 

Force on the magnet

 $F = -\frac{\partial U}{\partial z} = -\boldsymbol{\mu} \cdot \frac{\partial \boldsymbol{B}}{\partial z}$ 

Particles deflection determined by  $\mu_z$ . In other words, the S-G apparatus measures  $\mu_z$ .

# Stern-Gerlach Experiment

Watch the animation at http://en.wikipedia.org/wiki/Stern%E2%80%93Gerlach\_experiment

Quantum mechanical interpretation of the S-G experiment

Spin angular momentum S is intrinsic to the electron. The associated magnetic momentum  $\mu \propto -S$ .

The S-G apparatus measures the projection of S in a direction, say, along the *z* axis. There can only be two outcomes,  $+\hbar/2$  and  $-\hbar/2$ , called the eigenvalues. Each of them corresponds to an eigenstate.

These are fundamental concepts of quantum mechanics.

The two states are said to be orthogonal, as they are exclusive to each other. We labeled  $|\uparrow\rangle$  and  $|\downarrow\rangle$  in Dirac notation. Or, we may label them  $|0\rangle$  and  $|1\rangle$  in the context of quantum computing.

Orthogonality does *not* mean the electron can only be in these two states! Actually, superposition is among the most important concepts.

The electron's spin state is described by  $|\chi\rangle = c_{\uparrow}|\uparrow\rangle + c_{\downarrow}|\downarrow\rangle$ , where  $c_{\uparrow}$  and  $c_{\downarrow}$  are *complex* numbers, called "amplitudes". When the  $\mu_z$  of an electron in this state is measured, the electron "collapses" to one of the eigenstates; the *probability* of collapsing onto  $|\uparrow\rangle$  is  $c_{\uparrow}$  while that onto  $|\downarrow\rangle$  is  $c_{\downarrow}$ . Therefore, we have normalization  $|c_{\uparrow}|^2 + |c_{\downarrow}|^2 = 1$ .

#### Mathematical description of electron spin states

The state is described by  $|\chi\rangle = c_{\uparrow}|\uparrow\rangle + c_{\downarrow}|\downarrow\rangle$ , where the *complex* amplitudes satisfy  $|c_{\uparrow}|^2 + |c_{\downarrow}|^2 = 1$ .

Such a state is represented by a vector in a 2D space, with two basis states  $|\uparrow\rangle$  and  $|\downarrow\rangle$ .

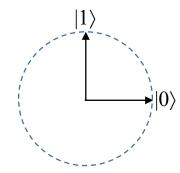
This space is different from the one we live in, since the projections (amplitudes) are *complex*. It is a Hilbert space.

The phase of the *complex* amplitude has profound ramifications!

In the basis of  $|\uparrow\rangle$  and  $|\downarrow\rangle$  (or  $|0\rangle$  and  $|1\rangle$ ),

$$|\uparrow\rangle = |0\rangle = {1 \choose 0}, \quad |\downarrow\rangle = |1\rangle = {0 \choose 1}, \text{ and } |\chi\rangle = {c_\uparrow \choose c_\downarrow}.$$

We say that  $|\uparrow\rangle$  and  $|\downarrow\rangle$  form an orthonormal basis set. The electron spin is a 2-state system. Any possible spin state is in the 2D Hilbert space defined by  $|\uparrow\rangle$  and  $|\downarrow\rangle$ . Therefore,  $|\uparrow\rangle$  and  $|\downarrow\rangle$  form a complete basis set.



Not exactly representing a spin state, since the amplitudes are in general *complex*.

(There is a better visualization.)

An electron spin can be made a **qubit**. Different from a classical bit: The states of a classical bit can only be at two points in a 2D state space. The states of a qubit are richer than the blue dashed circle, since the **amplitudes** are **complex**. Phase matters! A measurement of a physical quantity only results in eigenvalues. That is, any arbitrary state of a quantum system "collapses" onto an eigenstate upon measurement.

#### An important hypothesis of quantum mechanics:

A physical quantity Q is represented by an operator, which is a matrix Q.

A matrix turns a vector into another vector.  $Q|\chi_1\rangle = |\chi_2\rangle$ .

In *N*-dimensional Hilbert space (for an *N*-state system), *Q* has eigenvalues  $q_0, q_1, ..., q_n, ..., q_{N-1}$ , corresponding to eigenstates  $|0\rangle, |1\rangle, ..., |n\rangle, ..., |N-1\rangle$ .

$$\mathbf{Q}|n\rangle = q_n|n\rangle.$$

Confused? The simple 2-state spin makes it easy to understand.

Here, the physical quantity is the projection of the spin angular momentum on the *z* axis,  $S_z$ , represented by operator  $S_z$ . The eigenvalues are  $+\hbar/2$  and  $-\hbar/2$ , corresponding to eigenstates  $|\uparrow\rangle$  and  $|\downarrow\rangle$ .

$$S_{z}|\uparrow\rangle = (+\hbar/2)|\uparrow\rangle$$
 and  $S_{z}|\downarrow\rangle = (-\hbar/2)|\downarrow\rangle$ 

Given  $|\uparrow\rangle = |0\rangle = {1 \choose 0}$  and  $|\downarrow\rangle = |1\rangle = {0 \choose 1}$ , we immediately see

$$S_{z} = \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$S_{z}|\uparrow\rangle = (+\hbar/2)|\uparrow\rangle \quad \text{and} \quad S_{z}|\downarrow\rangle = (-\hbar/2)|\downarrow\rangle$$
$$|\uparrow\rangle = |0\rangle = \begin{pmatrix}1\\0\end{pmatrix} \text{ and } |\downarrow\rangle = |1\rangle = \begin{pmatrix}0\\1\end{pmatrix}, \qquad S_{z} = \frac{\hbar}{2} \begin{pmatrix}1&0\\0&-1\end{pmatrix}$$

For convenience, we love dimensionless, integer numbers. We define  $S_z = s_z(\hbar/2)$ .

Thus the dimensionless quantity  $s_z$  has integer eigenvalues +1 and -1, eigenstates  $|\uparrow\rangle$  and  $|\downarrow\rangle$ , and operator

$$\sigma_{\rm z} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

 $\sigma_z$  is the Pauli matrix for  $s_z$ .

$$\sigma_z |\uparrow\rangle = |\uparrow\rangle$$
 and  $\sigma_z |\downarrow\rangle = -|\downarrow\rangle$ 

Before moving further forward, we need to play with the notation and math.

Given 
$$|\uparrow\rangle = |0\rangle = \begin{pmatrix} 1\\0 \end{pmatrix}$$
,  $|\downarrow\rangle = |1\rangle = \begin{pmatrix} 0\\1 \end{pmatrix}$ , and  $|\chi\rangle = \begin{pmatrix} c_{\uparrow}\\c_{\downarrow} \end{pmatrix}$ , we can find the projection  $|\chi\rangle$  on  $|\uparrow\rangle$  and  $|\downarrow\rangle$  by calculating inner products:

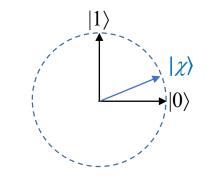
$$c_{\uparrow} = (1 \quad 0) \begin{pmatrix} c_{\uparrow} \\ c_{\downarrow} \end{pmatrix}$$
  $c_{\downarrow} = (0 \quad 1) \begin{pmatrix} c_{\uparrow} \\ c_{\downarrow} \end{pmatrix}$   
Transposed conjugate matrices

We defined the kets:  $|\uparrow\rangle = |0\rangle = {1 \choose 0}$ ,  $|\downarrow\rangle = |1\rangle = {0 \choose 1}$ , and  $|\chi\rangle = {c_\uparrow \choose c_\downarrow}$ . Now, we define their corresponding bras:

$$\langle \uparrow | = \langle 0 | = (1 \quad 0) \qquad \langle \downarrow | = \langle 1 | = (0 \quad 1) \qquad \langle \chi | = (c_{\uparrow}^* \quad c_{\downarrow}^*)$$

Then we can express the ideas in a concise way:

Projection  $\langle \uparrow | \chi \rangle = c_{\uparrow}$   $\langle \downarrow | \chi \rangle = c_{\downarrow}$   $| \chi \rangle = c_{\uparrow} | \uparrow \rangle + c_{\downarrow} | \downarrow \rangle = | \uparrow \rangle (\langle \uparrow | \chi \rangle) + | \downarrow \rangle (\langle \downarrow | \chi \rangle)$   $= | \uparrow \rangle \langle \uparrow | \chi \rangle + | \downarrow \rangle \langle \downarrow | \chi \rangle = (| \uparrow \rangle \langle \uparrow | + | \downarrow \rangle \langle \uparrow |) | \chi \rangle$   $\implies | \uparrow \rangle \langle \uparrow | + | \downarrow \rangle \langle \uparrow | = 1$  Completeness Orthogonality  $\langle \uparrow | \downarrow \rangle = 0$   $\langle \downarrow | \uparrow \rangle = 0$ 



Commental

Not exactly representing a spin state, since the amplitudes are in general *complex*.

(There is a better visualization.)

Normalization

$$\langle \uparrow | \uparrow \rangle = 1 \qquad \quad \langle \downarrow | \downarrow \rangle = 1 \\ \langle \chi | \chi \rangle = (c_{\uparrow}^{*} \quad c_{\downarrow}^{*}) \begin{pmatrix} c_{\uparrow} \\ c_{\downarrow} \end{pmatrix} = c_{\uparrow}^{*} c_{\uparrow} + c_{\downarrow}^{*} c_{\downarrow} = |c_{\uparrow}|^{2} + |c_{\downarrow}|^{2} = 1$$

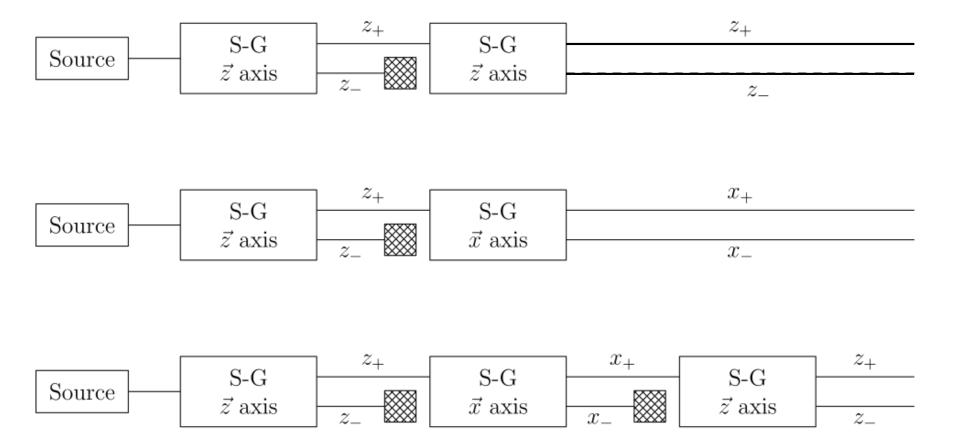
For any real phase  $\varphi$ ,  $e^{i\varphi}|\chi\rangle$  and  $|\chi\rangle$  describe the same physical state.

An overall phase has no physical consequence. What matters is the phase difference between  $c_{\uparrow}$  and  $c_{\downarrow}$ .

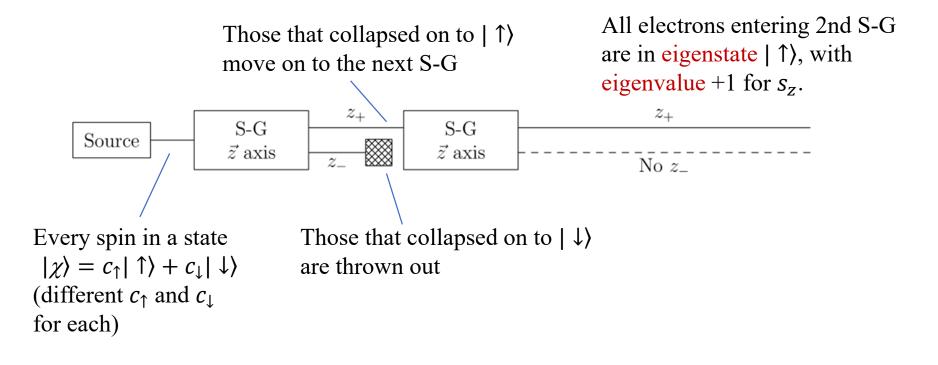
Amplitudes can never be directly measured!

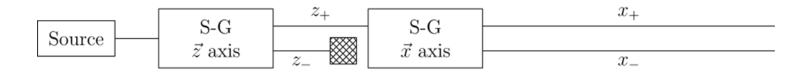
#### Sequential Stern-Gerlach (S-G) experiments

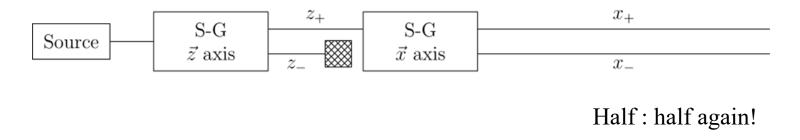
Don't be shy, guess the results!



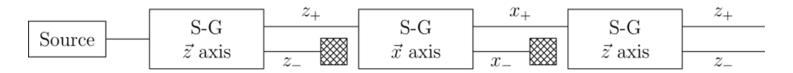
We already know enough to understand the first experiment:







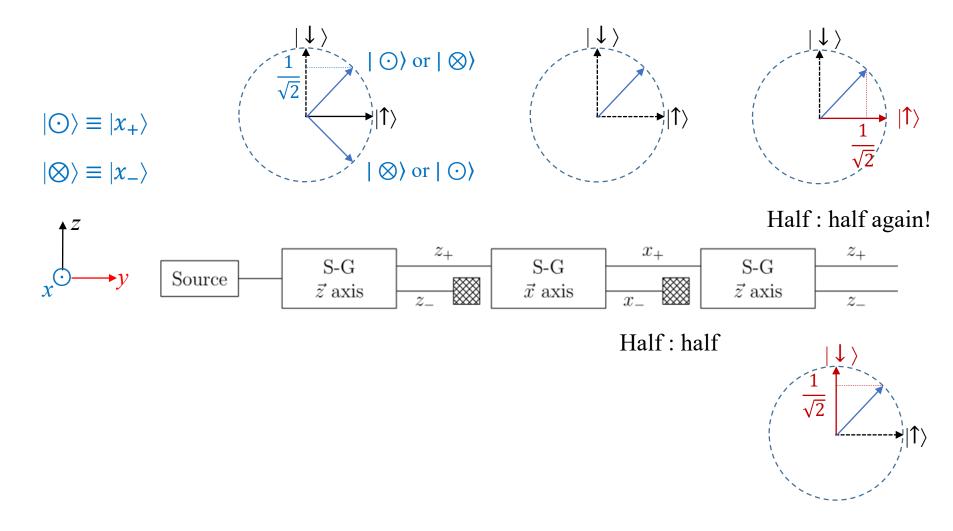
The outcome of a 3rd S-G is also half : half!



These results are the same as light polarization experiments, which give us clues.

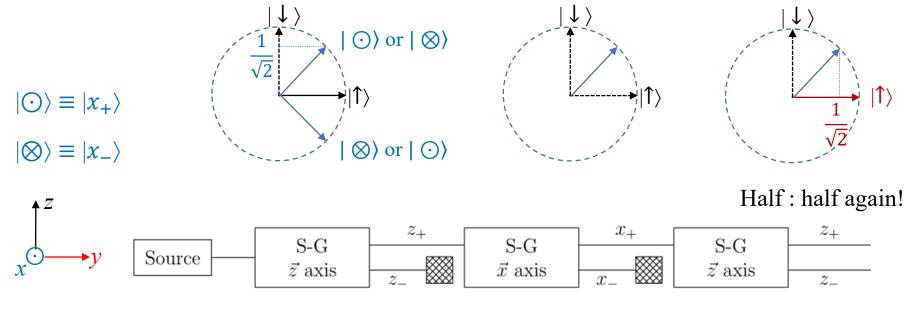
The outcome of a 3rd S-G is also half : half!

These results are the same as light polarization experiments, which give us clues.



The outcome of a 3rd S-G is also half : half!

These results are the same as light polarization experiments, which give us clues.



Half: half

 $\sqrt{2}$ 

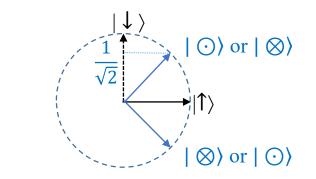
From the results, we infer:

$$|\langle \uparrow | \odot \rangle| = \frac{1}{\sqrt{2}} \iff |\langle \uparrow | \odot \rangle|^2 = \frac{1}{2}$$
$$|\langle \downarrow | \otimes \rangle| = \frac{1}{\sqrt{2}} \iff |\langle \downarrow | \otimes \rangle|^2 = \frac{1}{2}$$

$$|\langle \uparrow | \odot \rangle| = \frac{1}{\sqrt{2}} \iff |\langle \uparrow | \odot \rangle|^2 = \frac{1}{2}$$
$$|\langle \downarrow | \otimes \rangle| = \frac{1}{\sqrt{2}} \iff |\langle \downarrow | \otimes \rangle|^2 = \frac{1}{2}$$

Keep in mind that the overall phase has no physical consequences and only the phase difference matters. Let

$$|\odot\rangle = \frac{|\uparrow\rangle + e^{i\Delta\varphi_{\chi}}|\downarrow\rangle}{\sqrt{2}}$$



Not exactly representing spin states, since the amplitudes are in general *complex*.

(There is a better visualization.)

Then, 
$$|\otimes\rangle = \frac{|\uparrow\rangle - e^{i\Delta\varphi_x}|\downarrow\rangle}{\sqrt{2}}$$
 (required by orthogonality)

We could turn the S-Gs by 90°, and repeat all the experiments for the y projection of spin.

Define  $| \rightarrow \rangle \equiv | y_+ \rangle$  and  $| \leftarrow \rangle \equiv | y_- \rangle$ 

Then, 
$$| \rightarrow \rangle = \frac{|\uparrow\rangle + e^{i\Delta\varphi_y}|\downarrow\rangle}{\sqrt{2}}$$
  $|\leftarrow\rangle = \frac{|\uparrow\rangle - e^{i\Delta\varphi_y}|\downarrow\rangle}{\sqrt{2}}$ 

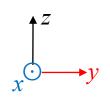
Assuming God is fair to all directions, we must have  $|\langle \rightarrow | \odot \rangle|^2 = 1/2$ .

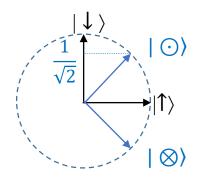
$$|\odot\rangle = \frac{|\uparrow\rangle + e^{i\Delta\varphi_{\chi}}|\downarrow\rangle}{\sqrt{2}} \qquad |\rightarrow\rangle = \frac{|\uparrow\rangle + e^{i\Delta\varphi_{y}}|\downarrow\rangle}{\sqrt{2}}$$
$$\langle\rightarrow|\odot\rangle = \frac{1 + e^{i(\Delta\varphi_{\chi} - \Delta\varphi_{y})}}{2}$$

$$|\langle \rightarrow | \odot \rangle|^2 = \frac{1 + \cos(\Delta \varphi_x - \Delta \varphi_y)}{2} \qquad \Longrightarrow \qquad \Delta \varphi_x - \Delta \varphi_y = \pm \frac{\pi}{2}$$

This is all we *can* know. *By convention*, we set  $\Delta \varphi_x = 0$ . Thus,

$$|\odot\rangle = \frac{|\uparrow\rangle + |\downarrow\rangle}{\sqrt{2}} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1\\1 \end{pmatrix} \qquad |\otimes\rangle = \frac{|\uparrow\rangle - |\downarrow\rangle}{\sqrt{2}} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1\\-1 \end{pmatrix}$$





Now we can find the operator  $\sigma_x$  for  $s_x$  such that

$$\sigma_{x} | \odot \rangle = \frac{1}{\sqrt{2}} \sigma_{x} \begin{pmatrix} 1 \\ 1 \end{pmatrix} = \frac{+1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} = (+1) | \odot \rangle \qquad \qquad \sigma_{x} | \otimes \rangle = \frac{-1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix} = (-1) | \odot \rangle$$
  
It turns out that 
$$\sigma_{x} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

**Exercise**: Verify the above.

**Exercise**: Given the above  $\sigma_x$ , find the eigenvalues and eigenstates. Expected answer: The eigenvalues are +1 and -1, and the corresponding eigenstates in the basis of  $|\uparrow\rangle$  and  $|\downarrow\rangle$  are

$$|\odot\rangle = |x_+\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1\\1 \end{pmatrix} = \frac{1}{\sqrt{2}} (|\uparrow\rangle + |\downarrow\rangle) \text{ and } |\otimes\rangle = |x_-\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1\\-1 \end{pmatrix} = \frac{-1}{\sqrt{2}} (|\uparrow\rangle - |\downarrow\rangle).$$

Do not forget the original physical quantity  $S_x$ . Its operator is  $S_x = (\hbar/2)\sigma_x$ . The eigenvalues of  $S_x$  are indeed  $+\hbar/2$  and  $-\hbar/2$ , corresponding to eigenstates  $|\odot\rangle$  and  $|\otimes\rangle$  in the basis of  $|\uparrow\rangle$  and  $|\downarrow\rangle$ .

The Thu 1/26/2023 class ended here.

Let's now turn to the operator  $S_y = (\hbar/2)\sigma_y$ .

$$|\odot\rangle = \frac{|\uparrow\rangle + e^{i\Delta\varphi_{x}}|\downarrow\rangle}{\sqrt{2}} \qquad |\rightarrow\rangle = \frac{|\uparrow\rangle + e^{i\Delta\varphi_{y}}|\downarrow\rangle}{\sqrt{2}} \qquad |\leftarrow\rangle = \frac{|\uparrow\rangle - e^{i\Delta\varphi_{y}}|\downarrow\rangle}{\sqrt{2}}$$
$$\Delta\varphi_{x} - \Delta\varphi_{y} = \pm \frac{\pi}{2}$$

**By convention**, we set  $\Delta \varphi_x = 0$ . Thus,  $\Delta \varphi_y = \mp \frac{\pi}{2}$ . Let's choose  $\Delta \varphi_y = \pm \frac{\pi}{2}$ . Then,

$$| \rightarrow \rangle = \frac{|\uparrow\rangle + i|\downarrow\rangle}{\sqrt{2}} = \frac{1}{\sqrt{2}} \binom{1}{i} \qquad \qquad | \leftarrow \rangle = \frac{|\uparrow\rangle - i|\downarrow\rangle}{\sqrt{2}} = \frac{1}{\sqrt{2}} \binom{1}{-i} = \frac{-i}{\sqrt{2}} \binom{i}{1}$$

Therefore, alternatively,  $| \leftarrow \rangle = \frac{1}{\sqrt{2}} {i \choose 1}$ 

(The factor  $-i = e^{-i(\pi/2)}$  has no physical consequences.)

()\_\_\_

We then fin that the operator for  $s_y$  is  $\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$ .

Note: You are encouraged to do the exercise as done with  $\sigma_x$ , thus to verify *consistency*. Our form of  $\sigma_y$  under our choice of  $\Delta \varphi_y = +\frac{\pi}{2}$  achieves the

consistency in our right-hand coordinate system.

Before moving further, a few words on *notations*.

We use *bold italic* for vector quantities, e.g., spin angular momentum *S*.

We use *non-bold italic* for scalar quantities, e.g., the magnitude S and projection  $S_z$  of **S**.

We use **bold non-italic** for vector **operators**, e.g., the operator **S** for **S**.

In many textbooks (e.g. Townsend),  $\hat{Q}$  is the operator for quantity Q ( $\hat{Q}$  for vector Q). We reserve the "hat" for unit vectors, e.g.  $\hat{z}$ . We distinguish operators from the corresponding quantities only by font.

We use non-bold non-italic for scalar operators, e.g., the operator S for S,  $S_z$  for  $S_z$ , etc.

For spin quantities (in uppercase letters), we define the corresponding dimensionless quantities (in lower case letters):

$$\boldsymbol{S} = S_{x} \widehat{\boldsymbol{x}} + S_{y} \widehat{\boldsymbol{y}} + S_{z} \widehat{\boldsymbol{z}} = \boldsymbol{S} \left(\frac{\hbar}{2}\right) = s_{x} \left(\frac{\hbar}{2}\right) \widehat{\boldsymbol{x}} + s_{y} \left(\frac{\hbar}{2}\right) \widehat{\boldsymbol{y}} + s_{z} \left(\frac{\hbar}{2}\right) \widehat{\boldsymbol{z}}.$$

The operators for  $s_x$ ,  $s_y$ , and  $s_z$  are Pauli matrices  $\sigma_x$ ,  $\sigma_x$ , and  $\sigma_z$ .

The operator for  $\boldsymbol{s}$  is Pauli matrix  $\boldsymbol{\sigma} = \sigma_x \hat{\boldsymbol{x}} + \sigma_y \hat{\boldsymbol{y}} + \sigma_z \hat{\boldsymbol{z}}$ .

$$\mathbf{S} = S_{\chi}\widehat{\mathbf{x}} + S_{y}\widehat{\mathbf{y}} + S_{z}\widehat{\mathbf{z}} = \mathbf{\sigma}\left(\frac{\hbar}{2}\right) = \sigma_{\chi}\left(\frac{\hbar}{2}\right)\widehat{\mathbf{x}} + \sigma_{y}\left(\frac{\hbar}{2}\right)\widehat{\mathbf{y}} + \sigma_{z}\left(\frac{\hbar}{2}\right)\widehat{\mathbf{z}}.$$

#### Operator of a derived quantity

Given operator Q for physical quantity Q, the operator for derived quantity f(Q) is f(Q).

Simple example:

The electron's magnetic moment

$$\boldsymbol{\mu} = -\frac{e}{m}\boldsymbol{S}$$

$$\mu_z = -\frac{e}{m}S_z = -\frac{e\hbar}{2m}s_z = -\mu_B s_z = \mp \mu_B$$

⇒ The magnetic moment operator

$$\mu_z = -\frac{e}{m}S_z = -\frac{e\hbar}{2m}\sigma_z = -\mu_B\sigma_z$$

The S-G actually measures  $\mu_z$ .

Another example:

$$S_{z} = \frac{\hbar}{2} s_{z} \qquad S_{z}^{2} = \frac{\hbar^{2}}{4} s_{z}^{2}$$
  
The operators 
$$S_{z}^{2} = \frac{\hbar^{2}}{4} \sigma_{z}^{2}$$

Side note:  
Define the Bohr magneton  
Electron charge  
$$\mu_B \equiv \frac{e\hbar}{2m}$$
  
Electron mass  
Notice that s\_ is dimensionless

Notice that  $s_z$  is dimensionless, with eigenvalues  $\pm 1$ .

 $s_z = \pm 1$  but  $s_z^2$  has only one possible value!

More generally, relations between operators in quantum mechanics follow those between physical quantities known in classical physics.

Take-home exercise: Use matrix multiplication to show  $\sigma_x^2 = \sigma_y^2 = \sigma_z^2 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = I$ . The unit matrix I can be written as simply 1.

$$\sigma_x^2 = \sigma_y^2 = \sigma_z^2 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = I \implies S_x^2 = S_y^2 = S_z^2 = \hbar^2/4$$

$$\sigma^2 = \sigma_x^2 + \sigma_y^2 + \sigma_z^2 = 3$$

$$S^2 = S_x^2 + S_y^2 + S_z^2 = \frac{3}{4}\hbar^2$$

While  $S_z$ ,  $S_x$ , and  $S_y$  cannot be determined at the same time,  $S_x^2 = S_y^2 = S_z^2 = \hbar^2/4$  and  $S^2 = S_x^2 + S_y^2 + S_z^2 = \frac{3}{4}\hbar^2$  always hold, i.e., they are always determined.

Since  $\sigma_z^2 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = I$ , any  $|\chi\rangle$  satisfies  $\sigma_z^2 |\chi\rangle = |\chi\rangle$ . Therefore, any  $|\chi\rangle$ , including  $|\uparrow\rangle$  and  $|\downarrow\rangle$ , is an eigenstate of  $\sigma_z^2$  with eigenvalue 1. Thus  $|\uparrow\rangle$  and  $|\downarrow\rangle$  are common eigenstates of  $\sigma_z$  and  $\sigma_z^2$ .

The same is true for any  $\sigma_i$  and  $\sigma_i^2$  as well as  $\sigma^2$ .

Common (or simultaneous) eigenstates

Since 
$$\sigma_z^2 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = I$$
, any  $|\chi\rangle$  satisfies  $\sigma_z^2 |\chi\rangle = |\chi\rangle$ .

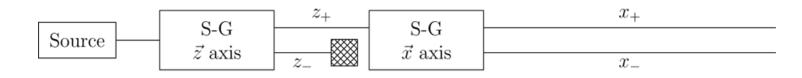
Therefore, any  $|\chi\rangle$ , including  $|\uparrow\rangle$  and  $|\downarrow\rangle$ , is an eigenstate of  $\sigma_z^2$  with eigenvalue 1. Thus  $|\uparrow\rangle$  and  $|\downarrow\rangle$  are common eigenstates of  $\sigma_z$  and  $\sigma_z^2$ .

 $\sigma_{z} | \uparrow \rangle = | \uparrow \rangle \qquad \qquad \sigma_{z}^{2} | \uparrow \rangle = | \uparrow \rangle$   $\implies \sigma_{z}^{2} \sigma_{z} | \uparrow \rangle = \sigma_{z}^{2} | \uparrow \rangle = | \uparrow \rangle \qquad \qquad \sigma_{z} \sigma_{z}^{2} | \uparrow \rangle = \sigma_{z} | \uparrow \rangle = | \uparrow \rangle$ 

$$\implies \qquad \sigma_z^2 \sigma_z = \sigma_z \sigma_z^2$$

For two physical quantities P and Q to have common eigenstates, the operators must satisfy PQ = QP.

#### Common (or simultaneous) eigenstates



For an electron in  $|\uparrow\rangle$ ,  $\sigma_z|\uparrow\rangle = |\uparrow\rangle$ . From  $\sigma_x|\uparrow\rangle = |\downarrow\rangle = \frac{1}{\sqrt{2}}(|x_+\rangle - |x_-\rangle)$ , which is neither  $|x_+\rangle$  nor  $|x_-\rangle$ , we see that the eigenstate  $|\uparrow\rangle$  of  $\sigma_z$  is not an eigenstate of  $\sigma_x$ . Therefore,  $S_z$  and  $S_x$  cannot be determined at the same time.  $S_z$  and  $S_x$  do not have common (or simultaneous) eigenstates.

Since  $\sigma_z |\uparrow\rangle = |\uparrow\rangle$ , we can write  $\sigma_x |\uparrow\rangle = |\downarrow\rangle = \sigma_x (\sigma_z |\uparrow\rangle) = (\sigma_x \sigma_z) |\uparrow\rangle$ , therefore  $\sigma_x \sigma_z |\uparrow\rangle = |\downarrow\rangle$ . On the other hand,  $\sigma_z \sigma_x |\uparrow\rangle = \sigma_z (\sigma_x |\uparrow\rangle) = \sigma_z |\downarrow\rangle = -|\downarrow\rangle$ .

Apparently,  $\sigma_x \sigma_z \neq \sigma_z \sigma_x$ . It appears that  $\sigma_x \sigma_z = -\sigma_z \sigma_x$ .

**Exercise**: Use matrix multiplication to show  $\sigma_x \sigma_z = -\sigma_z \sigma_x$  is generally true.

## Energy and time evolution of a quantum system

An isolated electron in free space will remain in a quantum state forever.

Quite boring and not useful.

We can turn some dynamics by just apply a magnetic field.

Energy of a magnetic moment :

$$E = -\boldsymbol{\mu} \cdot \boldsymbol{B} = -\mu_z(-B) = \mu_z B = -\mu_B s_z B$$

In this system (an isolated electron in **B**), E,  $\mu_z$ , and  $s_z$  have common eigenstates.

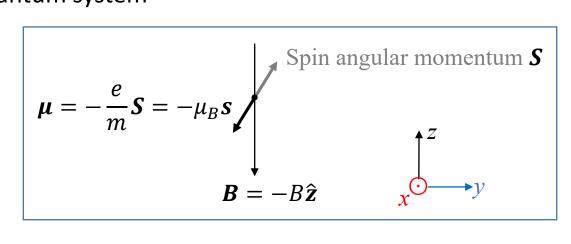
$$E_{\uparrow} = -\mu_B B$$
 and  $E_{\downarrow} = \mu_B B$ 

The energy of a system is so important, that we give its operator a special name: the Hamiltonian, H.

The dynamics of the system is described by the Schrödinger equation  $i\hbar \frac{d}{dt} |\psi(t)\rangle = H |\psi(t)\rangle$ 

This would be a familiar type of differential equation, if H were a constant (instead of an operator). The steady-state or stationary solution would be  $|\psi(t)\rangle = e^{-i\frac{H}{\hbar}t}|\psi(0)\rangle$ .

In the 2-state system, a common eigenstate of E,  $\mu_z$ , and  $s_z$  is a steady-state solution to this equation, which we call a stationary state.



By definition, the *n*-th eigenstate,  $|n\rangle$ , of H satisfies  $H|n\rangle = E_n|n\rangle$ .

Now we show that  $|\psi_n(t)\rangle = e^{-i\frac{E_n}{\hbar}t}|n\rangle$ 

are solutions to the Schrödinger equation  $i\hbar \frac{d}{dt} |\psi(t)\rangle = H |\psi(t)\rangle$ 

$$i\hbar \frac{d}{dt} |\psi_{n}(t)\rangle = i\hbar \left(-i\frac{E_{n}}{\hbar}\right) e^{-i\frac{E_{n}}{\hbar}t} |n\rangle = e^{-i\frac{E_{n}}{\hbar}t} E_{n} |n\rangle = e^{-i\frac{E_{n}}{\hbar}t} H|n\rangle = He^{-i\frac{E_{n}}{\hbar}t} |n\rangle = H|\psi_{n}(t)\rangle$$

$$\uparrow \text{ insert} \qquad \uparrow \text{ insert}$$

$$|\psi_{n}(t)\rangle = e^{-i\frac{E_{n}}{\hbar}t} |n\rangle \qquad H|n\rangle = E_{n}|n\rangle \qquad |\psi_{n}(t)\rangle = e^{-i\frac{E_{n}}{\hbar}t} |n\rangle$$

For the stationary state, the phase factor has no physical consequences!

 $|\psi_n(t)\rangle$  and  $|n\rangle$  describe *exactly the same* state.

Once in a stationary state, stay in a stationary state (as long as H is *t*-independent).

These terms mean the same thing:

A steady-state solution to the Schrödinger equation, a stationary state, an eigenstate of the Hamiltonian

But, a general state  $|\psi(t)\rangle = \sum_{n} c_n(t) |n\rangle$  evolves in time!! Next we exemplify this with a spin.

Time evolution of a spin state

 $|\chi(t)\rangle = c_{\uparrow}(t)|\uparrow\rangle + c_{\downarrow}(t)|\downarrow\rangle \xrightarrow{\text{insert}} i\hbar \frac{d}{dt} |\chi(t)\rangle = H|\chi(t)\rangle$  $i\hbar \frac{d}{dt} |\chi(t)\rangle = i\hbar \left\{ \left[ \frac{d}{dt} c_{\uparrow}(t) \right] |\uparrow\rangle + \left[ \frac{d}{dt} c_{\downarrow}(t) \right] |\downarrow\rangle \right\}$  $) = c_{\uparrow}(t)H|\uparrow\rangle + c_{\downarrow}(t)H|\downarrow\rangle = \left[ -\mu_{B}Bc_{\uparrow}(t) \right]|\uparrow\rangle + \left[ \mu_{B}Bc_{\downarrow}(t) \right]|\downarrow\rangle$ insert  $E_{\uparrow} = -\mu_B B$  and  $E_{\downarrow} = \mu_B B$  $\frac{d}{dt}c_{\uparrow}(t) = i\frac{\mu_{B}B}{\hbar}c_{\uparrow}(t) = i\frac{\omega}{2}c_{\uparrow}(t) \quad \text{and} \quad \frac{d}{dt}c_{\downarrow}(t) = -i\frac{\mu_{B}B}{\hbar}c_{\downarrow}(t) = -i\frac{\omega}{2}c_{\downarrow}(t)$ Define  $\omega = \frac{2\mu_B B}{\hbar}$  $c_{\uparrow}(t) = c_{\uparrow}(0)e^{i\frac{\omega}{2}t}$  and  $c_{\downarrow}(t) = c_{\downarrow}(0)e^{-i\frac{\omega}{2}t}$ 

Time evolution of a spin state

$$\begin{aligned} |\chi(t)\rangle &= c_{\uparrow}(t)|\uparrow\rangle + c_{\downarrow}(t)|\downarrow\rangle \\ c_{\uparrow}(t) &= c_{\uparrow}(0)e^{i\frac{\omega}{2}t} \qquad c_{\downarrow}(t) = c_{\downarrow}(0)e^{-i\frac{\omega}{2}t} \qquad \omega = \frac{2\mu_{B}B}{\hbar} \end{aligned}$$

Define  $|\chi\rangle \equiv |\chi(0)\rangle = c_{\uparrow}(0)|\uparrow\rangle + c_{\downarrow}(0)|\downarrow\rangle \equiv c_{\uparrow}|\uparrow\rangle + c_{\downarrow}|\downarrow\rangle$ . In the matrix form, we have

$$|\chi(0)\rangle = \begin{pmatrix} c_{\uparrow} \\ c_{\downarrow} \end{pmatrix}$$
  
and  $|\chi(t)\rangle = \begin{pmatrix} c_{\uparrow}e^{i\frac{\omega}{2}t} \\ c_{\downarrow}e^{-i\frac{\omega}{2}t} \end{pmatrix}$ .

We immediately see

$$\chi(t)\rangle = \begin{pmatrix} e^{i\frac{\omega}{2}t} & 0\\ 0 & e^{-i\frac{\omega}{2}t} \end{pmatrix} \begin{pmatrix} c_{\uparrow}\\ c_{\downarrow} \end{pmatrix} = \begin{pmatrix} e^{i\frac{\omega}{2}t} & 0\\ 0 & e^{-i\frac{\omega}{2}t} \end{pmatrix} |\chi(0)\rangle$$

This time evolution is vividly visualized with the Bloch sphere.

## The Bloch Sphere: visualizing a 2-level system state

We used a not-so-good visualization:

 $\frac{1}{\sqrt{2}}$ 

Not exactly representing a spin state, since the amplitudes are in general *complex*. (There is a better visualization.)

Here comes the better visualization.  $\checkmark$ 

Define real 
$$c_{\uparrow} = \cos\frac{\theta}{2}$$
 and  $c_{\downarrow} = \sin\frac{\theta}{2}$   
 $|\chi\rangle = c_{\uparrow}|\uparrow\rangle + c_{\downarrow}|\downarrow\rangle = \left(\cos\frac{\theta}{2}\right)|\uparrow\rangle + \left(e^{i\varphi}\sin\frac{\theta}{2}\right)|\downarrow\rangle = \left(\frac{\cos\frac{\theta}{2}}{e^{i\varphi}\sin\frac{\theta}{2}}\right)$ 

0)

θ

|1>

 $|\Psi\rangle$ 

٧

- Normalization condition automatically satisfied.
- Phase difference between  $c_{\uparrow}$  and  $c_{\downarrow}$  is  $\varphi$ . (Overall phase meaningless)
- Any possible |χ⟩ is represented by a point on the sphere. A complete visualization of 2D Hilbert space.

Visualize the time evolution of a spin state with Bloch sphere

$$|\chi(t)\rangle = \begin{pmatrix} c_{\uparrow} e^{i\frac{\omega}{2}t} \\ c_{\downarrow} e^{-i\frac{\omega}{2}t} \end{pmatrix} \qquad \omega = \frac{2\mu_B B}{\hbar}$$

Define  $|\chi\rangle \equiv |\chi(0)\rangle = c_{\uparrow}(0)|\uparrow\rangle + c_{\downarrow}(0)|\downarrow\rangle \equiv c_{\uparrow}|\uparrow\rangle + c_{\downarrow}|\downarrow\rangle$  with real  $c_{\uparrow}$  and  $c_{\downarrow}$ .

$$c_{\uparrow} = \cos\frac{\theta}{2} \text{ and } c_{\downarrow} = \sin\frac{\theta}{2}$$
$$|\chi(t)\rangle = \begin{pmatrix} e^{i\frac{\omega}{2}t}\cos\frac{\theta}{2}\\ e^{-i\frac{\omega}{2}t}\sin\frac{\theta}{2} \end{pmatrix} = e^{i\frac{\omega}{2}t} \begin{pmatrix} \cos\frac{\theta}{2}\\ e^{-i\omega t}\sin\frac{\theta}{2} \end{pmatrix}$$

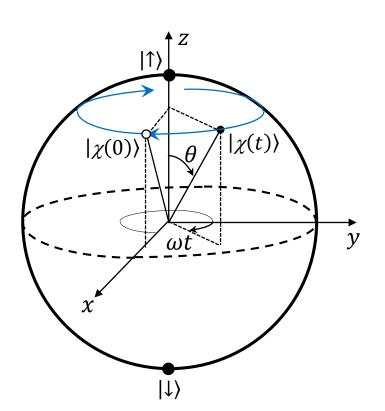
Physically meaningless; thrown away.

We immediately see  $\varphi(t) = -\omega t$ . By defining real  $c_{\uparrow}$  and  $c_{\downarrow}$ , we set  $\varphi(0) = 0$ .

#### Note

A point on the Bloch sphere represents a state, *not* the spin angular momentum **S**.

But the rotation at  $\omega = 2\mu_B B/\hbar$  is reminiscent of a semi-classical picture of the spin in a magnetic field!



# A semi-classical picture of the spin

Recall the following:

$$\sigma_x^2 = \sigma_y^2 = \sigma_z^2 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = I \implies S_x^2 = S_y^2 = S_z^2 = \hbar^2/4$$
$$\sigma^2 = \sigma_x^2 + \sigma_y^2 + \sigma_z^2 = 3 \qquad \qquad S^2 = S_x^2 + S_y^2 + S_z^2 = \frac{3}{4}\hbar^2$$

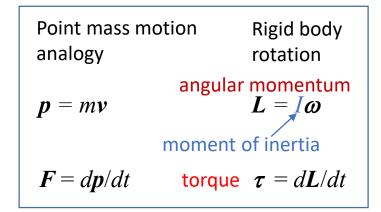
The total spin angular momentum always satisfies  $S^2 = S_x^2 + S_y^2 + S_z^2 = 3\hbar^2/4$ . This can be *loosely* interpreted as the magnitude of the total spin angular momentum is always  $S = |\mathbf{S}| = \frac{\sqrt{3}}{2}\hbar$ . A *semi-classical* picture of spin thus emerges: In DC magnetic field  $\mathbf{B} = -B\hat{\mathbf{z}}$ ,  $|\uparrow\rangle$  and  $|\downarrow\rangle$  are the low- and highenergy states, respectively.  $|\chi(t)\rangle$  $|\chi(0)\rangle$ ħ/2 But, field **B** does not ħ/2 align the spins with it; ωt spins precess around **B**. Without disturbance from the environment, В х an electron stays forever is a state  $(|\uparrow\rangle \text{ or } |\downarrow\rangle)$ .

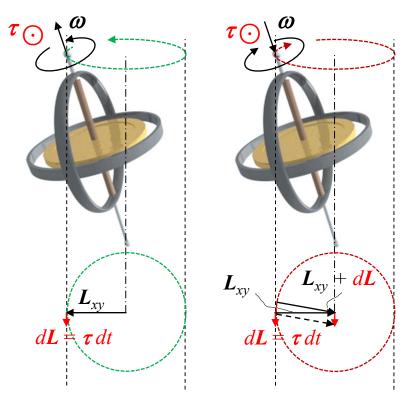
y

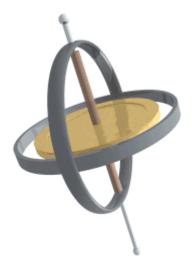
The vector for state  $|\chi(t)\rangle$  in the Bloch sphere visualization  $\langle \mathcal{S} \rangle$  is somehow related to S.

A semi-classical picture of the spin

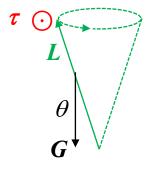
First, the classical spin.







A precessing gyroscope. See animation at <u>https://en.wikipedia.org/wiki/Top</u>. The gyro is "spinning down" in the animation.



#### The Tue 1/31/2023 class ended here.

A second classical example: an orbiting *classical* electron in magnetic field

$$\boldsymbol{\mu} = -(e/2m)\boldsymbol{L} \qquad \boldsymbol{\tau} = \boldsymbol{\mu} \times \boldsymbol{B} \quad \boldsymbol{\Box} > \boldsymbol{\tau} = (e/2m)\boldsymbol{L}\boldsymbol{B}\boldsymbol{\sin}\boldsymbol{\theta}$$

Notice that  $\tau \propto L$  here, unlike the gravitation case.

Without external disturbance, field *B* cannot change  $L_z$  or  $L_{xy}$ . *L* (and  $\mu$ ) precesses around *B*. The field *B* alone does not align *L* (or  $\mu$ ) to itself.

Unlike the gyro in gravitational field, the orbit precesses in the same direction for both  $L \cdot B > 0$  and  $L \cdot B < 0$  cases.

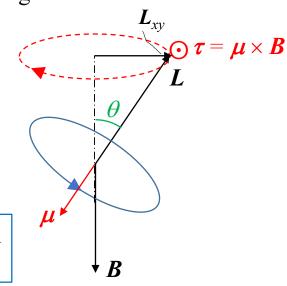
The precession frequency

$$\omega_{p} = \frac{dL/L_{xy}}{dt} = \frac{dL}{dt} \left( \frac{1}{L \sin \theta} \right) = \frac{\tau}{L \sin \theta} = \left( \frac{e}{2m} \right) \frac{L \operatorname{Bsin} \theta}{L \sin \theta} = \left( \frac{e}{2m} \right) B = \frac{1}{\hbar} \mu_{B} B$$

$$\mu_{B} \equiv \frac{e\hbar}{2m}$$

$$\mu_{B} \equiv \frac{e\hbar}{2m}$$

$$\mu_{B} \equiv \frac{e\hbar}{2m}$$
Orbit radius
Orbit radius
Orbit ing angular frequency
By definition, the magnetic moment
$$\mu = \pi R^{2} \left( -e \frac{\omega_{0}}{2\pi} \right) = -\frac{e}{2} R^{2} \frac{L}{mR^{2}} = -\frac{e}{2m} L$$
current



## The semi-classical picture of electron spin

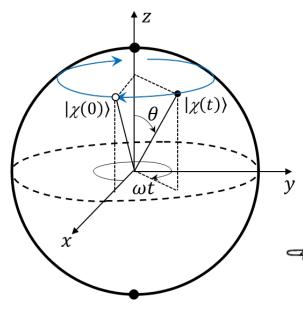
Unlike the orbit magnetic moment  $\mu = -(e/2m)L$ , the electron's spin magnetic moment is

$$\boldsymbol{\mu} = -\frac{e}{m}\boldsymbol{S}$$

Following the same procedure as for the orbit moment, the precession frequency

$$\omega_p = \left(\frac{e}{m}\right)B = \frac{2}{\hbar}\mu_B B \qquad \mu_B \equiv \frac{e\hbar}{2m}$$

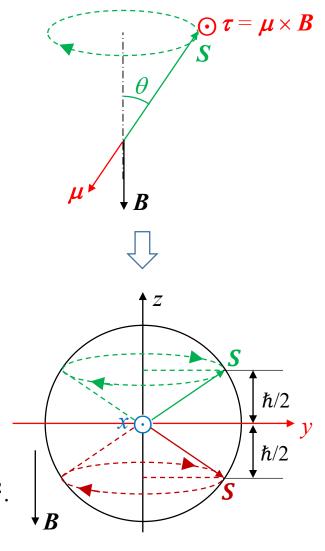
Precession direction same for  $S \cdot B > 0$  and  $S \cdot B < 0$ .



We have just arrived at the semi-classical picture:  $S^2 = S_x^2 + S_y^2 + S_z^2 = 3(\hbar/2)^2$ . Loosely,  $S = |S| = \frac{\sqrt{3}}{2}\hbar$ . Only two possible states: up and down.

*S* precesses around -B at angular frequency  $\omega = 2\mu_B B/\hbar$ , same as the spin state rotates on the Bloch sphere.

Can the vector there represent the spin itself?



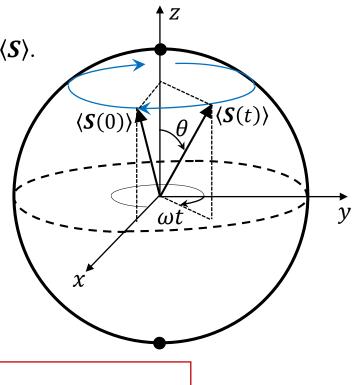
Bloch sphere visualization of the spin: a *better* semi-classical picture

First, we give the conclusions, to be rationalized later.

The state vector can represent the average value of spin,  $\langle S \rangle$ .

Interpretation of "average" of something of a single electron: averaged over many, many measurements of electrons in the same state, or manifested by some macroscopic quantity of a system made of many, many electrons in the same spin state.

We have defined a set of dimensionless quantities, such that:  $S = s(\hbar/2)$ ,  $S = s(\hbar/2)$ ,  $S_z = s_z(\hbar/2)$ , and so on.



 $\frac{dS}{dt} = \boldsymbol{\mu} \times \boldsymbol{B} \qquad \Longrightarrow$   $\uparrow$   $\boldsymbol{\mu} = -\frac{e}{m}\boldsymbol{S}$ 

$$\frac{d\mathbf{S}}{dt} = -\frac{e}{m}\mathbf{S} \times \mathbf{B}$$

$$\Box$$

$$\frac{d\boldsymbol{\mu}}{dt} = -\frac{e}{m}\boldsymbol{\mu} \times \mathbf{B}$$

$$\frac{d\langle \mathbf{S} \rangle}{dt} = -\frac{e}{m} \langle \mathbf{S} \rangle \times \mathbf{B}$$
$$\frac{d\langle \mathbf{\mu} \rangle}{dt} = -\frac{e}{m} \langle \mathbf{\mu} \rangle \times \mathbf{B}$$

The Landau–Lifshitz–Gilbert (LLG) equation for a single electron or non-interacting electrons in the same spin state under magnetic field B.

Bloch sphere visualization of the spin: a *better* semi-classical picture

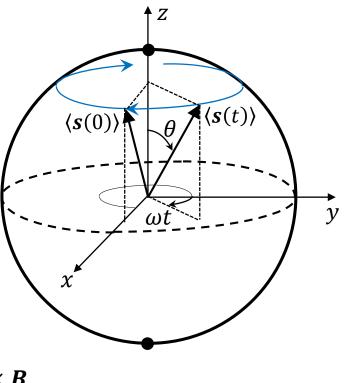
With the radius of the Bloch sphere set to 1, the vector represents the dimensionless spin  $\langle s(t) \rangle$ .

We may also set the radius to  $\hbar/2$ , thus the vector represents  $\langle S(t) \rangle$ .

$$S(t) = s(t)(\hbar/2)$$
  
 $\langle S(t) \rangle = \langle s(t) \rangle(\hbar/2)$ 

Both  $\langle S(t) \rangle$  and the corresponding magnetic moment  $\langle \mu(t) \rangle$  follow the same differential equation:

$$\frac{d\langle S\rangle}{dt} = -\frac{e}{m}\langle S\rangle \times B \qquad \qquad \frac{d\langle \mu\rangle}{dt} = -\frac{e}{m}\langle \mu\rangle \times B$$



The Landau–Lifshitz–Gilbert (LLG) equation for <u>a single electron</u> or <u>non-interacting electrons in the same spin state</u>, under magnetic field  $\boldsymbol{B}$  but otherwise isolated (no other interaction with the world).

To rationalize this graphical representation of  $\langle S \rangle$  or  $\langle S \rangle$ , we need to understand the average.

# Homework 1

Now we have learned that the vector in the Bloch sphere chart visualizing spin state

$$|\chi\rangle = \begin{pmatrix} \cos\frac{\theta}{2} \\ e^{i\varphi}\sin\frac{\theta}{2} \end{pmatrix}$$

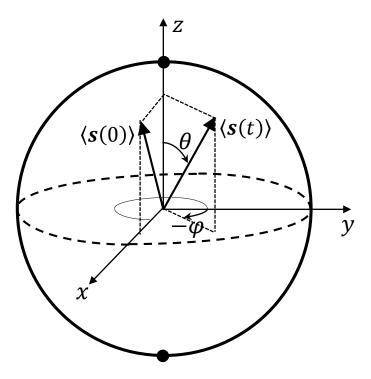
also represents the average value of the spin of this state. From the figure to the right, we see

 $\langle s \rangle = \hat{x} \sin \theta \cos \varphi + \hat{y} \sin \theta \sin \varphi + \hat{z} \cos \theta$ 

Obviously, the projection of  $\langle s \rangle$  onto  $\hat{z}$  is  $\langle s_z \rangle = \cos \theta$ .

You see,  $-1 \le \langle s_z \rangle \le 1$  while  $s_z = \pm 1$ .

Pretend that you have not been taught about the above. Prove that  $\langle s_z \rangle = \cos \theta$  for spin state  $|\chi\rangle$  characterized by  $\theta$  and  $\varphi$ .



#### Average values

Example: Find the average value  $\langle s_z \rangle$  of a spin state  $|\chi\rangle = c_{\uparrow}|\uparrow\rangle + c_{\downarrow}|\downarrow\rangle$ .

Obviously,  $\langle s_z \rangle = |c_{\uparrow}|^2 (+1) + |c_{\downarrow}|^2 (-1) = |c_{\uparrow}|^2 - |c_{\downarrow}|^2$ 

In general, the average (expected) value of Q,  $\langle Q \rangle = \langle \chi | Q | \chi \rangle$ . We now show the special example  $\langle s_z \rangle = \langle \chi | \sigma_z | \chi \rangle$ :

$$\langle \chi | \sigma_z | \chi \rangle = (\langle \uparrow | c_{\uparrow}^* + \langle \downarrow | c_{\downarrow}^* \rangle [(+1)c_{\uparrow} | \uparrow \rangle + (-1)c_{\downarrow} | \downarrow \rangle ]$$
$$= (+1)c_{\uparrow}^* c_{\uparrow} + (-1)c_{\downarrow}^* c_{\downarrow} = |c_{\uparrow}|^2 - |c_{\downarrow}|^2 = \langle s_z \rangle$$

This is obvious only in a special case, where we seek  $\langle s_z \rangle$  in the basis made of the eigenstates of  $s_z$ .

In general, we calculate  $\langle Q \rangle = \langle \chi | Q | \chi \rangle$  not in the basis of eigenstates of Q. For example, we may calculate  $\langle Q \rangle$  in the basis set  $|\uparrow\rangle$  and  $|\downarrow\rangle$ , i.e. eigenstates of  $s_z$ .

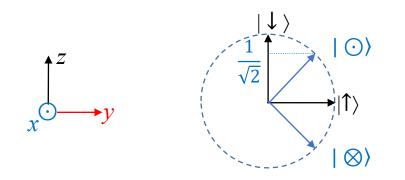
To show the general applicability of  $\langle Q \rangle = \langle \chi | Q | \chi \rangle$ , we need to talk about basis changes.

Basis change

$$|\odot\rangle = \frac{|\uparrow\rangle + |\downarrow\rangle}{\sqrt{2}} = \frac{1}{\sqrt{2}} \begin{pmatrix}1\\1\end{pmatrix}$$

$$|\uparrow\rangle = \frac{|\odot\rangle + |\otimes\rangle}{\sqrt{2}} = \frac{1}{\sqrt{2}} \begin{pmatrix}1\\0\end{pmatrix}$$

$$|\uparrow\rangle = \frac{|\odot\rangle - |\otimes\rangle}{\sqrt{2}} = \frac{1}{\sqrt{2}} \begin{pmatrix}0\\1\end{pmatrix}$$



In-class exercise

$$\sigma_{z}|\odot\rangle = \frac{\sigma_{z}|\uparrow\rangle + \sigma_{z}|\downarrow\rangle}{\sqrt{2}} = \frac{|\uparrow\rangle - |\downarrow\rangle}{\sqrt{2}} = |\otimes\rangle$$

$$\sigma_{z} | \otimes \rangle = \frac{\sigma_{z} | \uparrow \rangle - \sigma_{z} | \downarrow \rangle}{\sqrt{2}} = \frac{| \uparrow \rangle + | \downarrow \rangle}{\sqrt{2}} = | \odot \rangle$$

$$\sigma_{z}|\odot\rangle = \frac{\sigma_{z}|\uparrow\rangle + \sigma_{z}|\downarrow\rangle}{\sqrt{2}} = \frac{|\uparrow\rangle - |\downarrow\rangle}{\sqrt{2}}$$

$$(\bigcirc |\sigma_{z}|\odot\rangle = \left(\frac{\langle\uparrow| + \langle\downarrow|}{\sqrt{2}}\right) \left(\frac{|\uparrow\rangle - |\downarrow\rangle}{\sqrt{2}}\right) = \frac{\langle\uparrow| \uparrow\rangle + \langle\downarrow| \uparrow\rangle - \langle\uparrow| \downarrow\rangle - \langle\downarrow| \downarrow\rangle}{\sqrt{2}} = 0$$

 $\langle \otimes |\sigma_z| \otimes \rangle = ?$ 

What do the above mean?

Similarly,  $\langle \uparrow | \sigma_x | \uparrow \rangle = ?$  And, in general,  $\langle \chi | \sigma_x | \chi \rangle = ?$ 

We can find  $\langle \chi | \sigma_{\chi} | \chi \rangle$  in the basis of  $| \odot \rangle$  and  $| \otimes \rangle$ , where

$$|\chi\rangle = c_{\odot}|\odot\rangle + c_{\otimes}|\otimes\rangle$$

Following the same procedure as finding  $\langle \chi | \sigma_z | \chi \rangle$  in the basis of  $|\uparrow\rangle$  and  $|\downarrow\rangle$ , we immediately see  $\langle s_x \rangle = \langle \chi | \sigma_x | \chi \rangle$  for arbitrary  $|\chi\rangle$ .

For physical quantity Q, there exist two eigenstates  $|q_1\rangle$  and  $|q_2\rangle$ , corresponding to eigenvalues  $q_1$  and  $q_2$ , respectively. Thus,

$$|\chi\rangle = c_1 |q_1\rangle + c_2 |q_2\rangle$$

Following the same procedure as finding  $\langle \chi | \sigma_z | \chi \rangle$  in the basis of  $|\uparrow\rangle$  and  $|\downarrow\rangle$ , we see  $\langle Q \rangle = \langle \chi | Q | \chi \rangle$  for arbitrary  $|\chi\rangle$  by finding  $\langle \chi | Q | \chi \rangle$  in the basis of  $|q_1\rangle$  and  $|q_2\rangle$ :

$$\langle \chi | Q | \chi \rangle = (\langle q_1 | c_1^* + \langle q_2 | c_2^*)(q_1 c_1 | q_1 \rangle + q_2 c_2 | q_2 \rangle) = |c_1|^2 q_1 + |c_2|^2 q_2 = \langle Q \rangle$$

# Read offline

Proof that the vector in the Bloch sphere chart visualizing spin state  $|\chi\rangle$  also represents the average value of the spin of this state,  $\langle s \rangle$ .

$$\langle s \rangle = \langle \chi | \sigma | \chi \rangle = \langle \chi | (\sigma_x \hat{\chi} + \sigma_y \hat{y} + \sigma_z \hat{z}) | \chi \rangle$$

$$= \hat{\chi} \left( \cos \frac{\theta}{2} - e^{-i\varphi} \sin \frac{\theta}{2} \right) \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \cos \frac{\theta}{2} \\ e^{i\varphi} \sin \frac{\theta}{2} \end{pmatrix}$$

$$+ \hat{y} \left( \cos \frac{\theta}{2} - e^{-i\varphi} \sin \frac{\theta}{2} \right) \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \begin{pmatrix} \cos \frac{\theta}{2} \\ e^{i\varphi} \sin \frac{\theta}{2} \end{pmatrix} + \hat{z} \left( \cos \frac{\theta}{2} - e^{-i\varphi} \sin \frac{\theta}{2} \right) \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} \cos \frac{\theta}{2} \\ e^{i\varphi} \sin \frac{\theta}{2} \end{pmatrix}$$

Ζ

 $\langle s \rangle$ 

$$= \widehat{x} \left( \cos \frac{\theta}{2} - e^{-i\varphi} \sin \frac{\theta}{2} \right) \begin{pmatrix} e^{i\varphi} \sin \frac{\theta}{2} \\ \cos \frac{\theta}{2} \end{pmatrix} + \widehat{y} \left( \cos \frac{\theta}{2} - e^{-i\varphi} \sin \frac{\theta}{2} \right) \begin{pmatrix} -ie^{i\varphi} \sin \frac{\theta}{2} \\ i\cos \frac{\theta}{2} \end{pmatrix} + \widehat{z} \left( \cos \frac{\theta}{2} - e^{-i\varphi} \sin \frac{\theta}{2} \right) \begin{pmatrix} \cos \frac{\theta}{2} \\ -e^{i\varphi} \sin \frac{\theta}{2} \end{pmatrix}$$

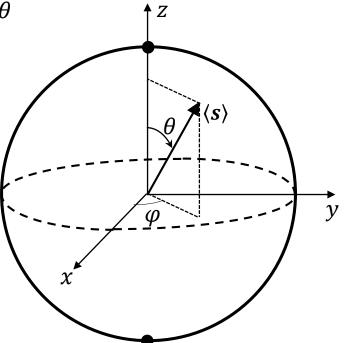
$$= \hat{x} \left( \cos \frac{\theta}{2} e^{-i\varphi} \sin \frac{\theta}{2} \right) \begin{pmatrix} e^{i\varphi} \sin \frac{\theta}{2} \\ \cos \frac{\theta}{2} \end{pmatrix} + \hat{y} \left( \cos \frac{\theta}{2} e^{-i\varphi} \sin \frac{\theta}{2} \right) \begin{pmatrix} -i e^{i\varphi} \sin \frac{\theta}{2} \\ i \cos \frac{\theta}{2} \end{pmatrix}$$
  
(this step copied from last page) 
$$+ \hat{z} \left( \cos \frac{\theta}{2} e^{-i\varphi} \sin \frac{\theta}{2} \right) \begin{pmatrix} \cos \frac{\theta}{2} \\ -e^{i\varphi} \sin \frac{\theta}{2} \end{pmatrix}$$
$$= \hat{x} \left( e^{i\varphi} + e^{-i\varphi} \right) \cos \frac{\theta}{2} \sin \frac{\theta}{2} + \hat{y} \left( -i e^{i\varphi} + i e^{-i\varphi} \right) \cos \frac{\theta}{2} \sin \frac{\theta}{2} + \hat{z} \left( \cos^2 \frac{\theta}{2} - \sin^2 \frac{\theta}{2} \right)$$

$$= \hat{x}(2\cos\varphi)\frac{1}{2}\sin\theta + \hat{y}(-i)(2i\sin\varphi)\frac{1}{2}\sin\theta + \hat{z}\cos\theta$$
$$= \hat{x}\sin\theta\cos\varphi + \hat{y}\sin\theta\sin\varphi + \hat{z}\cos\theta$$

This means that the average spin,  $\langle s \rangle = \langle \chi | \sigma | \chi \rangle$ , of a spin state

$$|\chi\rangle = \begin{pmatrix} \cos\frac{\theta}{2} \\ e^{i\varphi}\sin\frac{\theta}{2} \end{pmatrix}$$

is a unit vector of polar angle  $\theta$  and azimuthal angle  $\varphi$ . QED.



Time evolution revisited

$$\begin{aligned} |\chi(t)\rangle &= \begin{pmatrix} e^{i\frac{\omega}{2}t} & 0\\ 0 & e^{-i\frac{\omega}{2}t} \end{pmatrix} \begin{pmatrix} c_{\uparrow} \\ c_{\downarrow} \end{pmatrix} = \begin{pmatrix} e^{i\frac{\omega}{2}t} & 0\\ 0 & e^{-i\frac{\omega}{2}t} \end{pmatrix} |\chi(0)\rangle = e^{i\frac{\omega}{2}t} \begin{pmatrix} 1 & 0\\ 0 & e^{-i\omega t} \end{pmatrix} |\chi(0)\rangle \\ &= \begin{pmatrix} e^{i\frac{\omega}{2}t}\cos\frac{\theta}{2}\\ e^{-i\frac{\omega}{2}t}\sin\frac{\theta}{2} \end{pmatrix} = e^{i\frac{\omega}{2}t} \begin{pmatrix} \cos\frac{\theta}{2}\\ e^{-i\omega t}\sin\frac{\theta}{2} \end{pmatrix} \end{aligned}$$

Physically insignificant.

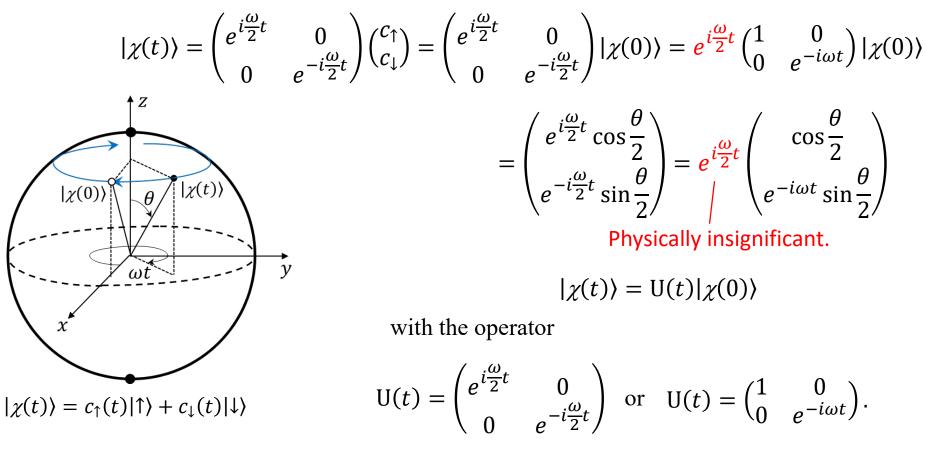
ħω

Whether or not the physically insignificant factor  $e^{i\frac{\omega}{2}t}$  is thrown out, we can write  $|\chi(t)\rangle = U(t)|\chi(0)\rangle$ 

with the operator

$$U(t) = \begin{pmatrix} e^{i\frac{\omega}{2}t} & 0\\ 0 & e^{-i\frac{\omega}{2}t} \end{pmatrix} \text{ or } U(t) = \begin{pmatrix} 1 & 0\\ 0 & e^{-i\omega t} \end{pmatrix}.$$

In the former,  $c_{\uparrow}(t)$  and  $c_{\downarrow}(t)$  rotate at angular frequencies  $\frac{\omega}{2}$  and  $-\frac{\omega}{2}$ , respectively. In the latter,  $c_{\uparrow}(t)$  is fixed while  $c_{\downarrow}(t)$  rotates at angular frequency  $\omega$ . Either way,  $c_{\downarrow}(t)$  rotates at angular frequency  $\omega$  with regard to  $c_{\downarrow}(t)$ , and  $\hbar\omega$  is the difference between the two energy eigenvalues (levels).  $\frac{\hbar\omega}{2} = \frac{\frac{\hbar\omega}{2}}{\frac{\hbar\omega}{2}}$ 



Either way,  $c_{\downarrow}(t)$  rotates at angular frequency  $\omega$  with regard to  $c_{\downarrow}(t)$ , thus  $|\chi(t)\rangle$  rotates at  $\omega$  around  $\hat{z}$ , as visualized in the Bloch sphere chart.

The time evolution is said to be a unitary transformation, since  $\langle \chi(t) | \chi(t) \rangle = 1$  always holds. The operator U(t) is a unitary matrix.

Furthermore,  $U(t + \Delta t) = U(\Delta t)U(t)$ .

The unitary transformation  $|\chi(t)\rangle = U(t)|\chi(0)\rangle$  is naturally expected from the Schrödinger equation:

$$i\hbar \frac{d}{dt} |\psi(t)\rangle = \mathbf{H} |\psi(t)\rangle \qquad \qquad \frac{d}{dt} |\psi(t)\rangle = -i\frac{1}{\hbar}\mathbf{H} |\psi(t)\rangle \qquad \qquad |\psi(t)\rangle = e^{-i\frac{t}{\hbar}\mathbf{H}} |\psi(t)\rangle$$

Keeping in mind that  $e^{-i\frac{\tau}{\hbar}H}$  is an operator, we immediately see

$$U(t) = e^{-i\frac{t}{\hbar}H}$$

But, what does the exponential function of an operator mean? This is to be explained later, when we go beyond 2-state systems. You may want to figure this out. Here are two hints:

1. Consider 
$$|\psi(t)\rangle = \sum_{n} c_n(t) |n\rangle$$
.

2. Use  $e^{-i\frac{t}{\hbar}H} = 1 + (-i\frac{t}{\hbar}H) + \frac{1}{2}(-i\frac{t}{\hbar}H)^2 + \cdots$  Apply this operator to each term in the above expansion.

# A bit of digression: gate-based quantum computing

Having understood time evolution, we are now able to understand the very basic ideas of gate-based quantum computing and the single-qubit gates.

- A 2-state system can be a qubit.
- A gate is a unitary transformation of the qubit.

One example is the quantum counterpart of the classical NOT gate.

A classical bit can only be two states:  $|0\rangle$  and  $|1\rangle$ . The NOT gate is the operator  $X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ . Obviously,  $X|0\rangle = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix} = |1\rangle$  and  $X|1\rangle = |0\rangle$ . The quantum NOT gate is a generalization, which operates on a qubit  $|\psi\rangle$ .

An electron spin can be made a qubit. Here,  $|\psi\rangle = \alpha |0\rangle + \beta |1\rangle$ 

$$= |\chi\rangle = c_{\uparrow}|\uparrow\rangle + c_{\downarrow}|\downarrow\rangle.$$

$$X|\psi\rangle = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \begin{pmatrix} \beta \\ \alpha \end{pmatrix}$$

Not all quantum gates have classical counterparts. For example, the Z gate:

$$Z|\psi\rangle = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \begin{pmatrix} \alpha \\ -\beta \end{pmatrix}$$

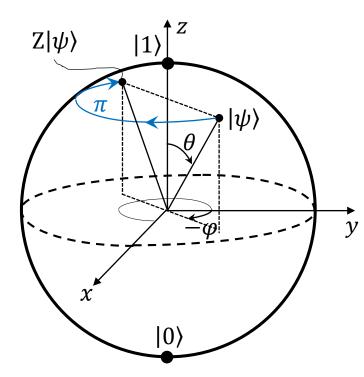
We now consider the implementation of the Z gate.

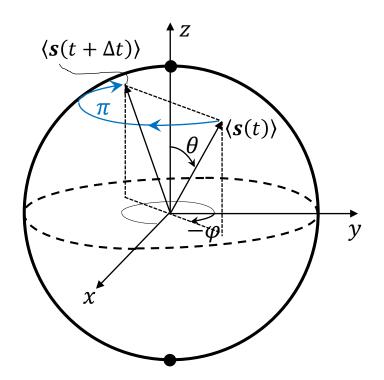
$$\mathbf{Z} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & e^{-i\pi} \end{pmatrix}$$

Recall that if we apply a magnetic field  $\mathbf{B} = -B\hat{\mathbf{z}}$ , the qubit will undergo unitary transformation

$$\mathbf{U}(t) = \begin{pmatrix} 1 & 0 \\ 0 & e^{-i\omega t} \end{pmatrix}$$

So, we can apply a magnetic field pulse, with a pulse width  $\Delta t$ , such that  $\omega \Delta t = \pi$ , i.e.,  $\Delta t$  is half a precession period. This operation is a Z gate:  $U(\Delta t) = Z$ .

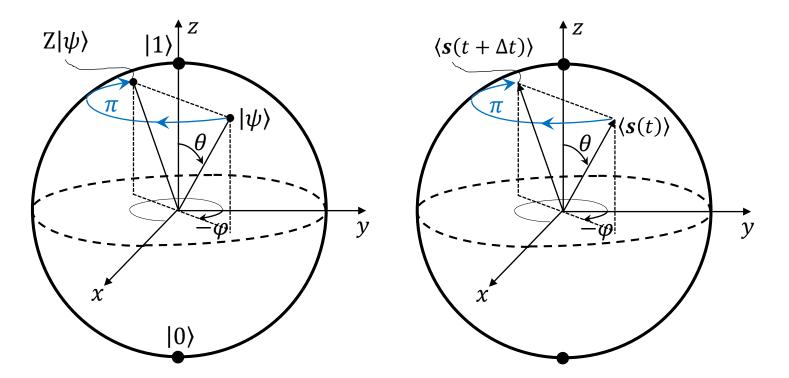




$$Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & e^{-i\pi} \end{pmatrix} \implies Z |\psi\rangle = \begin{pmatrix} 1 & 0 \\ 0 & e^{-i\pi} \end{pmatrix} \begin{pmatrix} \cos\frac{\theta}{2} \\ e^{i\varphi}\sin\frac{\theta}{2} \end{pmatrix} = \begin{pmatrix} \cos\frac{\theta}{2} \\ e^{i(\varphi-\pi)}\sin\frac{\theta}{2} \end{pmatrix}$$
  
BTW, notice that Z is formally the same as  $\sigma_z$ .

The Z gate operation:  $(\theta, \varphi - \pi) \rightarrow (\theta, \varphi - \pi)$ . Visualized by the two charts below:

 $|\psi\rangle \rightarrow \mathbf{Z}|\psi\rangle \qquad \langle \mathbf{s}(t)\rangle \rightarrow \langle \mathbf{s}(t+\Delta t)\rangle; \omega\Delta t = \pi$ 



# Homework 2

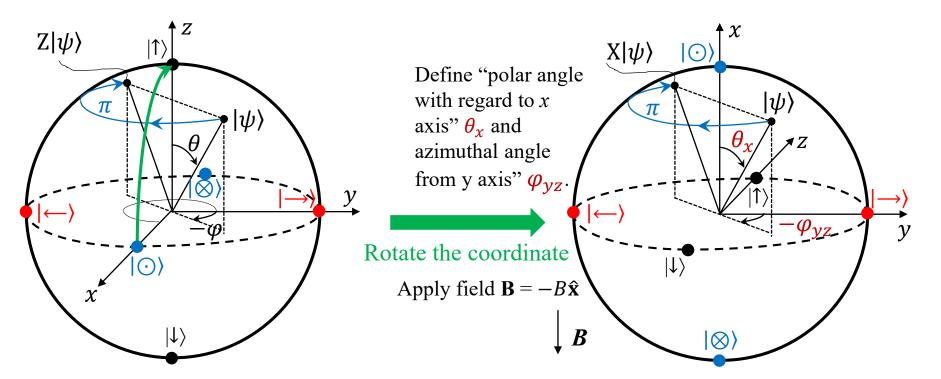
Find an implementation of the X gate. Visualize the relation between  $|\psi\rangle$  and  $X|\psi\rangle$ .

Hint: We figured out how to implement the Z gate. We assume God is fair and does not favor a particular direction.

Note: There is also a Y gate,  $Y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$ , which is formally the same as Pauli matrix  $\sigma_y$ .

 $|\psi\rangle \rightarrow Z|\psi\rangle$ 

 $|\psi\rangle \rightarrow X|\psi\rangle$ 



Matrix elements

Earlier we found  $\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$  by finding the four matrix elements that satisfy  $\sigma_x | \odot \rangle = \frac{1}{\sqrt{2}} \sigma_x \begin{pmatrix} 1 \\ 1 \end{pmatrix} = \frac{+1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} = (+1) | \odot \rangle$   $\sigma_x | \otimes \rangle = \frac{-1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix} = (-1) | \odot \rangle$ 

Now, we introduce the general formulation for the matrix elements of a general operator Q.

Let 
$$Q = \begin{pmatrix} Q_{\uparrow\uparrow} & Q_{\uparrow\downarrow} \\ Q_{\downarrow\uparrow} & Q_{\downarrow\downarrow} \end{pmatrix}$$
 in the basis of  $|\uparrow\rangle$  and  $|\downarrow\rangle$ .  
 $Q|\uparrow\rangle = \begin{pmatrix} Q_{\uparrow\uparrow} & Q_{\uparrow\downarrow} \\ Q_{\downarrow\uparrow} & Q_{\downarrow\downarrow} \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} Q_{\uparrow\uparrow} \\ Q_{\downarrow\uparrow} \end{pmatrix} \implies \begin{pmatrix} \uparrow |Q|\uparrow\rangle = (1 & 0) \begin{pmatrix} Q_{\uparrow\uparrow} \\ Q_{\downarrow\uparrow} \end{pmatrix} = Q_{\uparrow\uparrow} \\ \langle\downarrow |Q|\uparrow\rangle = (0 & 1) \begin{pmatrix} Q_{\uparrow\uparrow} \\ Q_{\downarrow\uparrow} \end{pmatrix} = Q_{\downarrow\uparrow} \\ \langle\downarrow |Q|\downarrow\rangle = (0 & 1) \begin{pmatrix} Q_{\uparrow\uparrow} \\ Q_{\downarrow\uparrow} \end{pmatrix} = Q_{\downarrow\downarrow} \\ \langle\uparrow |Q|\downarrow\rangle = (1 & 0) \begin{pmatrix} Q_{\uparrow\uparrow} \\ Q_{\downarrow\uparrow} \end{pmatrix} = Q_{\uparrow\downarrow} \\ \langle\downarrow |Q|\downarrow\rangle = (1 & 0) \begin{pmatrix} Q_{\uparrow\uparrow} \\ Q_{\downarrow\uparrow} \end{pmatrix} = Q_{\uparrow\downarrow} \\ \langle\downarrow |Q|\downarrow\rangle = (0 & 1) \begin{pmatrix} Q_{\uparrow\uparrow} \\ Q_{\downarrow\uparrow} \end{pmatrix} = Q_{\downarrow\downarrow} \end{cases}$ 

We finished this slide on Thu 2/2/2023.

# **Quantum Mechanics Primer Part I Highlights**

1. The electron spin is used as the simplest example to illustrate the most basic concepts of quantum mechanics:

Eigenstates, eigenvalues, measurements;

A measurement projects the system's state onto one of the system's eigenstates for the measured quantity, i.e., the system collapses onto an eigenstate upon measurement.

Amplitudes, superposition, statistical interpretation of amplitudes;

Eigenstates as vectors in Hilbert space, orthogonality, normalization, completeness; Dirac notations;

Physical quantities and their operators, eigenvalue equations;

Common (simultaneous) eigenstates:

Operators P and Q have common eigenstates  $\Leftrightarrow$  PQ = QP

Time evolution and Schrödinger equation

The Hamiltonian H is the operator of the energy of a quantum system;

The eigenstates of H are steady-state solutions to the Schrödinger equation, and are referred to as stationary states;

An arbitrary state  $|\psi\rangle$  undergoes unitary transformation determined by H:

$$|\psi(t)\rangle = U(t)|\psi(0)\rangle$$
 where  $U(t) = e^{-i\frac{t}{\hbar}H}$ 

2. Features of the electron spin as a 2-state quantum system: An electron spin state  $|\chi\rangle$  resides in a 2D Hilbert space;

The projection of the spin angular momentum in an *arbitrary* direction has two eigenvalues, +1 and -1 in the unit of  $\hbar/2$ , corresponding to two eigenstates;

Take 3 *arbitrary* directions to form a right-hand Cartesian coordinate system, then the operators for the 3 projections are the Pauli matrices  $\sigma_x$ ,  $\sigma_y$ ,  $\sigma_z$ ;

No two Pauli matrices have common (simultaneous) eigenstates,

Therefore  $\boldsymbol{\sigma} = \sigma_x \hat{\boldsymbol{x}} + \sigma_y \hat{\boldsymbol{y}} + \sigma_z \hat{\boldsymbol{z}}$  has *no eigenvalues* and *no eigenstates*! Interestingly,  $\sigma_x^2 = \sigma_y^2 = \sigma_z^2 = 1$  thus  $\sigma^2 = \sigma_x^2 + \sigma_y^2 + \sigma_z^2 = 3$ ,

which means  $S_x^2 = S_y^2 = S_z^2 = \hbar^2/4$  and  $S^2 = S_x^2 + S_y^2 + S_z^2 = \frac{3}{4}\hbar^2$ .

Applying a constant magnetic field makes the direction of the field *special*:

By convention, 
$$\mathbf{B} = -B\hat{\mathbf{z}}$$
 thus, with  $\mu_B \equiv \frac{e\hbar}{2m}$ , we have  $\mathbf{H} = \begin{pmatrix} -\mu_B B & 0\\ 0 & \mu_B B \end{pmatrix}$ ;

 $\sigma_z$  and H have common eigenstates  $|\uparrow\rangle$  and  $|\downarrow\rangle$  (neither  $\sigma_x$  nor  $\sigma_y$  has common eigenstate with H);

An arbitrary spin state  $|\chi\rangle$  rotates *clockwise* around  $\hat{z}$ , as visualized by the Bloch sphere;

The vector for the spin state  $|\chi\rangle$  in the Bloch sphere chart also represents  $\langle s \rangle$ , which is well-defined although *s* has no eigenvalues,

thus  $\langle s \rangle$  precesses around  $\hat{z}$  at  $\omega = 2\mu_B B/\hbar$ .

3. Concepts alluded to but not sufficiently stressed:

Diagonalizing matrix Q finds the eigenvalues and eigenstates.

Degeneracy: Same eigenvalue for multiple eigenstates.

Within the subspace of the degenerate states, any linear combination of degenerate states is a degenerate state.

For 2D Hilbert space, a degenerate subspace is the *entire* 2D Hilbert space, that is, any arbitrary state is an eigenstate of an operator with degeneracy. For the electron spin,  $\sigma_x^2 = \sigma_y^2 = \sigma_z^2 = 1$  and  $\sigma^2 = \sigma_x^2 + \sigma_y^2 + \sigma_z^2 = 3$ .

## 4. Scope and *Limitations* of **Part I**:

Focused on isolated single-particle systems.

The *only* interaction discussed was the electron spin with an constant external magnetic field.

Without any disturbance from the surroundings or interaction with other electrons, an electron spin state will rotate around  $\hat{z}$  forever, and its  $\langle s \rangle$  precesses around  $\hat{z}$  forever; in other words, the precession is not damped, and the polar angle  $\theta$  of  $\langle s \rangle$  will never change.

Moving forward, **Part II** will extend to many-state (including infinite) systems while remaining within the single particle systems (i.e. not considering *many-body interactions*, which is to be discussed in **Part III**).

5. Generalization from spin ½ to general 2-state systems (not discussed until now)
All 2-state systems follow the same math (Pauli matrices), despite different physics.
Examples: H<sub>2</sub><sup>+</sup>, NH<sub>3</sub>, qubits not based on spin.

Other 2-state systems are often described using the language of spin 1/2.

6. Gate- (or circuit-) based quantum computing was touched upon

A 2-state system *may* make a qubit.

Not necessarily a spin ½, but the non-spin-based are often discussed in the language of spin and are sometimes referred to as artificial spin.

A gate is an operation on a qubit or qubits. The operation is a unitary transformation that can be described by a *unitary* operator.

As we are so far limited to single-particle systems, our digression to qubits and gates are limited to single-qubit gates, and important concepts like entanglement have not been mentioned.

FYI, further reading on quantum computing: <u>https://doi.org/10.1145/3517340</u>

Footnotes: In discussing spin, we touched upon magnetism. We (largely) use SI units in this course. Notice that equations in electromagnetism may look quite different in different unit systems. For example, the proportional constant in  $\mu \propto S$ .

## Offline exercise 1

Find  $\langle \uparrow | \odot \rangle$  and  $\langle \uparrow | \otimes \rangle$ , and think about a sequential S-G measurements in which the first S-G apparatus measures  $S_x$  and the second measures  $S_z$ .



Comments

$$\langle a|b\rangle = (a_0^* \quad a_1^*) \begin{pmatrix} b_0 \\ b_1 \end{pmatrix} = a_0^* b_0 + a_1^* b_1$$
 is the inner product of the two vectors  $|a\rangle = \begin{pmatrix} a_0 \\ a_1 \end{pmatrix}$  and  $|b\rangle = \begin{pmatrix} b_0 \\ b_1 \end{pmatrix}$ 

Notice that the elements of the bra are complex conjugates of the corresponding ones in the ket.

Recall that the inner product  $\langle a|b\rangle$  is the projection of  $|b\rangle$  onto  $|a\rangle$ . When projecting a vector onto a basis vector, you get the amplitudes: For arbitrary  $|\chi\rangle = c_{\uparrow}|\uparrow\rangle + c_{\downarrow}|\downarrow\rangle$ , we have  $\langle\uparrow|\chi\rangle = c_{\uparrow}$  and  $\langle\downarrow|\chi\rangle = c_{\downarrow}$ .

#### Offline exercise 2

An electron spin is initially in the state  $|\chi(0)\rangle = |\odot\rangle = |x_+\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle + |\downarrow\rangle)$  at t = 0 under an applied magnetic field  $\mathbf{B} = -B\hat{\mathbf{z}}$ . We also define  $|\otimes\rangle = |x_-\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle - |\downarrow\rangle)$ . Let's follow the time evolution of this electron:

$$|\chi(t)\rangle = \frac{1}{\sqrt{2}} \left( e^{i\frac{\omega}{2}t} |\uparrow\rangle + e^{-i\frac{\omega}{2}t} |\downarrow\rangle \right).$$

Write  $|\chi(t)\rangle$  in the basis of  $|\odot\rangle$  and  $|\otimes\rangle$ .

If we measure electron spin in *z*-direction at time *t*, what are the probabilities of getting  $+\hbar/2$  and  $-\hbar/2$ ? If we measure electron spin in *x*-direction at time *t*, what are the probabilities of getting  $+\hbar/2$  and  $-\hbar/2$ ?

(Answer the questions *first and then* check the answers below.)

Answers & comments

Inserting  $|\uparrow\rangle = \frac{1}{\sqrt{2}} (|\odot\rangle + |\otimes\rangle)$  and  $|\downarrow\rangle = \frac{1}{\sqrt{2}} (|\odot\rangle - |\otimes\rangle)$  leads to

$$\begin{aligned} |\chi(t)\rangle &= \frac{1}{\sqrt{2}} \left( e^{i\frac{\omega}{2}t} \frac{|\odot\rangle + |\otimes\rangle}{\sqrt{2}} + e^{-i\frac{\omega}{2}t} \frac{|\odot\rangle - |\otimes\rangle}{\sqrt{2}} \right) = \frac{1}{2} \left[ \left( e^{i\frac{\omega}{2}t} + e^{-i\frac{\omega}{2}t} \right) |\odot\rangle + \left( e^{i\frac{\omega}{2}t} - e^{-i\frac{\omega}{2}t} \right) |\otimes\rangle \right] \\ &= \left( \cos\frac{\omega}{2}t \right) |\odot\rangle + \left( \sin\frac{\omega}{2}t \right) |\otimes\rangle \end{aligned}$$

When  $S_z$  is measured, the probabilities for obtaining  $+\hbar/2$  and  $-\hbar/2$  are both 1/2 at any time t.

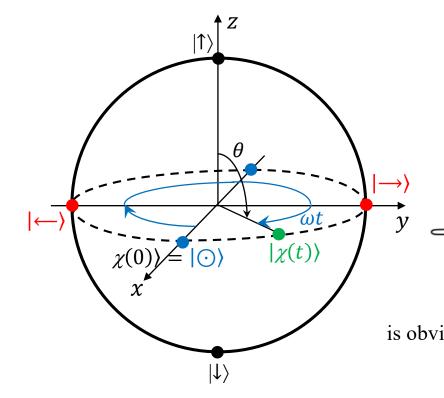
When  $S_x$  is measured, the probabilities for obtaining  $+\hbar/2$  and  $-\hbar/2$  are both 1/2 at time t is  $\cos^2 \frac{\omega}{2}t = \frac{1}{2}(1 + \cos \omega t)$  and  $\sin^2 \frac{\omega}{2}t = \frac{1}{2}(1 - \cos \omega t)$ , respectively.

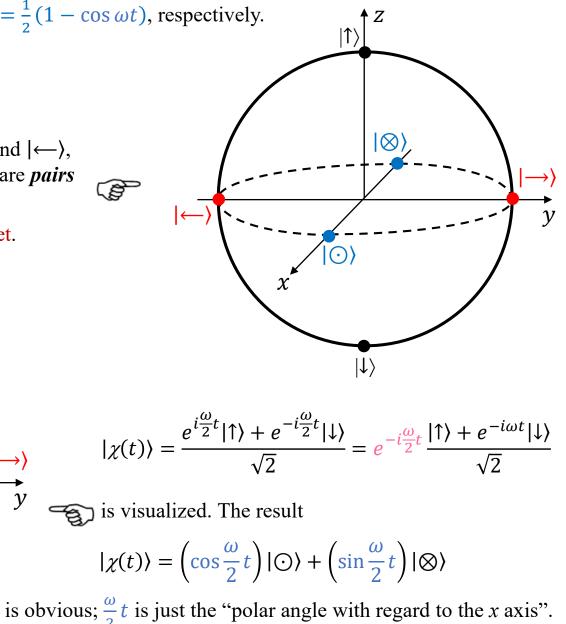
#### Comments

Bloch sphere visualization:

States  $|\odot\rangle$  and  $|\otimes\rangle$ , as well as  $|\rightarrow\rangle$  and  $|\leftarrow\rangle$ , are shown on the Bloch sphere. They are *pairs of poles*, as are  $|\uparrow\rangle$  and  $|\downarrow\rangle$ .

Moreover, any pair of poles is basis set.





In this case where  $|\bigcirc\rangle = \frac{1}{\sqrt{2}} (|\uparrow\rangle + |\downarrow\rangle)$  at t = 0, it is said that the system is prepared in an initial state  $|\bigcirc\rangle$ . Since  $\mathbf{B} = -B\hat{\mathbf{z}}$ ,  $|\odot\rangle$  is *not* an eigenstate of H, i.e., the system does not have a definitive energy. The prepared initial state is a superposition of the ground and excited states (spin-up and -down states). In such cases, beating happens -- the spin state oscillates between  $|\odot\rangle$  and  $|\otimes\rangle$  at the resonance frequency  $\frac{\omega}{2}$ .

The same underlying math describes many similar physical phenomena:

A classical example is a system of two symmetric coupled harmonic oscillators, which has two eigenmodes with frequencies  $\omega_0$  and  $\omega_1$ . Let  $\omega_1 - \omega_0 = \omega > 0$ , then  $\frac{\omega_1 + \omega_0}{2} = \omega_0 + \frac{\omega_1 - \omega_0}{2} = \omega_0$ 

 $\omega_0 + \frac{\omega}{2}$ . The lower- and higher-frequency modes are just in-phase and out-of-phase superpositions of oscillations of the two oscillators.

×

For visualization, see

https://www.youtube.com/watch?v=x\_ZkKPtgTeA and https://en.wikipedia.org/wiki/Oscillation#Coupled\_oscillations.  $\bigcirc$ With the coupling, the oscillation of each individual oscillator is *not* an eigenmode. The oscillation must transfer back and forth between the two oscillators (see animation at Wikipedia page), even if starting out at t = 0 with all energy at one oscillator. In this example, the  $\omega_0$  and  $\omega_1$  eigenmodes are analogies of stationary states  $|\uparrow\rangle$  and  $|\downarrow\rangle$ . Quantum examples are plenty: In  $H_2^+$ , the electron oscillates between two states – being with the two protons, each equivalent to the  $|\odot\rangle$  aor  $|\otimes\rangle$  state whereas the bonding (ground) and the antibonding (excited) states correspond to  $|\uparrow\rangle$  and  $|\downarrow\rangle$ , respectively. The NH<sub>3</sub> oscillates between two opposite orientations.

## Further questions

If the system is prepared in an initial state  $|\uparrow\rangle$ , everything else the same as in the above case, how do the probabilities of measuring spin up and spin down change with time? Will there be beating between  $|\uparrow\rangle$  and  $|\downarrow\rangle$ ?

#### Answers & comments:

The probabilities of measuring spin up and spin down will remain 1 and 0, respectively. There is no beating between stationary states  $|\uparrow\rangle$  and  $|\downarrow\rangle$ .

The reason is that  $|\uparrow\rangle$  is an eigenstate of H, i.e., with a definitive energy, and therefore a definitive rate of phase evolution,  $\omega_0$ . We often set  $\omega_0 = 0$  for the ground state in quantum mechanics An energy eigenstate is said to be a stationary state.

Will the electron remain in  $|\uparrow\rangle$  forever?

Yes and No. If H  $\propto -B\sigma_z$  indeed, without any other contributions (as in this problem), then yes.

There will always be disturbance from the environment, which add to the Hamiltonian of a real system.

## Offline exercise 3

Problem 1. (a) Find the eigenvalues and the corresponding eigenstates of  $\sigma_x \sigma_z$ . (b) Find the eigenvalues and the corresponding eigenstates of  $\sigma_z \sigma_x$ . (c) Compare your results with the eigenvalues and the corresponding eigenstates of  $\sigma_y$ . Explain your observations.

Problem 2. Find a relation between  $\sigma_y$  and  $\sigma_z$ , which is similar to  $\sigma_x \sigma_z = -\sigma_z \sigma_x$ .

#### Hints & comments

Applying matrix multiplication to matrices  $\sigma_x$  and  $\sigma_z$ , we get  $\sigma_x \sigma_z = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$  and  $\sigma_z \sigma_x = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$ . Therefore  $\sigma_x \sigma_z = -\sigma_z \sigma_x$ .