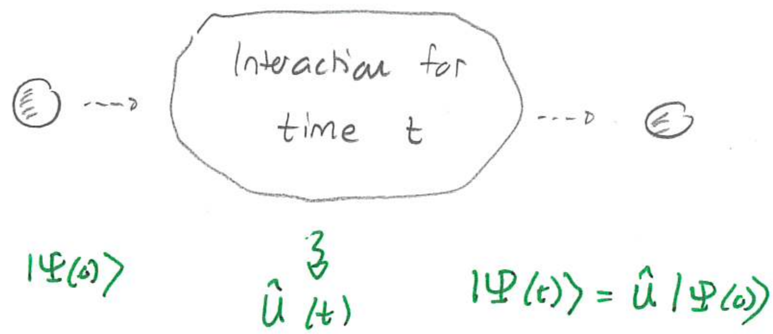
Thurs

Fri: HW by 5pm

## Schrödinger equation

The general framework for evolution of a quantum system is that the state evolves via a unitary transformation. Sometimes this depends on time and




$$|\Psi(t)\rangle = \hat{U}(t)\,|\Psi(0)\rangle$$

In such cases an additional axiom for evolution is that

> The state of the system satisfies:
>
> $$i\hbar \frac{d}{dt}|\Psi(t)\rangle = \hat{H}\,|\Psi(t)\rangle$$
>
> where $\hat{H}$ is the Hamiltonian (energy observable)

This is the Schrödinger equation. We can often construct the Hamiltonian by extending a classical energy function to an observable. This is then inserted into the Schrödinger equation to produce a set of differential equations.

# Evolution for spin-1/2 particle in a magnetic field

Consider the general case of a spin-1/2 particle in a magnetic field that could be time-dependent. Then the process for describing the evolution is:

Given $\vec{B}$, construct classical energy $\longrightarrow$

$$\vec{B} = B_x(t)\,\hat{x} + B_y(t)\,\hat{y} + B_z(t)\,\hat{z}$$

Classical

$$E = -\frac{gq}{2m}\,\vec{B}\cdot\vec{S}$$

$$E = -\frac{gq}{2m}\left[B_x(t)S_x + B_y(t)S_y + B_z(t)S_z\right]$$

$\downarrow$

Construct Hamiltonian by replacing measurable quantities for the system by observables $\longrightarrow$

$$\hat{H} = -\frac{gq}{2m}\left[B_x(t)\,\hat{S}_x + B_y(t)\,\hat{S}_y + B_z(t)\,\hat{S}_z\right]$$

$\downarrow$

Represent state of system ket by a vector and insert into Schrödinger equation $\longrightarrow$

$$|\Psi(t)\rangle = \begin{pmatrix} C_+(t) \\ C_-(t) \end{pmatrix}$$

$$\hat{H} = -\frac{gq}{2m}\frac{\hbar}{2}\left[B_x(t)\,\hat{\sigma}_x + B_y(t)\,\hat{\sigma}_y + B_z(t)\,\hat{\sigma}_z\right]$$

$$= -\frac{gq}{2m}\frac{\hbar}{2}\begin{pmatrix} B_z(t) & B_x(t) - iB_y(t) \\ B_x(t) + iB_y(t) & -B_z(t) \end{pmatrix}$$

Then

$$i\hbar \frac{d|\Psi\rangle}{dt} = \hat{H}\,|\Psi\rangle$$

$$\Rightarrow \quad i\hbar \begin{pmatrix} \dfrac{dc_+}{dt} \\[2ex] \dfrac{dc_-}{dt} \end{pmatrix} = -\frac{gq}{2m}\frac{\hbar}{2} \begin{pmatrix} B_z(t) & B_x(t) - iB_y(t) \\ B_x(t) + iB_y(t) & -B_z(t) \end{pmatrix} \begin{pmatrix} c_+ \\ c_- \end{pmatrix}$$

Gives coupled differential equations:

$$\frac{dc_+}{dt} = \frac{igq}{4m}\left[ B_z c_+ + (B_x - iB_y) c_- \right]$$

$$\frac{dc_-}{dt} = \frac{igq}{4m}\left[ (B_x + iB_y) c_+ - B_z c_+ \right]$$

Solve differential equations to get $c_+, c_-$ and construct

$$|\Psi(t)\rangle = c_+(t)\,|+\hat{z}\rangle + c_-(t)\,|-\hat{z}\rangle$$

this depends on the initial state (linearly)

$$|\Psi(0)\rangle = c_+(c)\,|+\hat{z}\rangle + c_-(t)\,|-\hat{z}\rangle$$

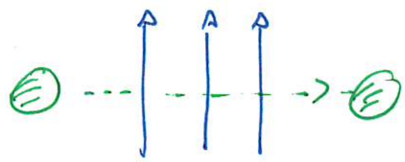
Extract the unitary evolution operator $\hat{U}(t)$ s.t.

$$|\Psi(t)\rangle = \hat{U}\,|\Psi(0)\rangle$$

e.g. $U_{++} = \langle +\hat{z}|\hat{U}|+\hat{z}\rangle \rightsquigarrow$ set $\left.\begin{matrix} c_+(0)=1 \\ c_-(0)=1 \end{matrix}\right\}$ find $c_+(t), c_-(t) \ldots$

## Time-independent Hamiltonians

Consider the case where the magnetic field is time-independent. Then the Hamiltonian will also be time-independent.



$$\vec{B} = B_0 \hat{z}$$

constant.

In this case a general mathematical result gives:

> If $\hat{H}$ is <u>time-independent</u> then
>
> $$i\hbar \frac{d}{dt} |\Psi(t)\rangle = \hat{H} |\Psi(t)\rangle$$
>
> has solution
>
> $$|\Psi(t)\rangle = \hat{U}(t) |\Psi(0)\rangle$$
>
> where
>
> $$\hat{U} = e^{-i\hat{H}t/\hbar}$$

## 1 Spin-1/2 particle in a constant magnetic field

Suppose that a spin-1/2 particle of mass $m$, charge $q$ and g-factor, $g$ in the magnetic field

$$\mathbf{B} = B_0\hat{\mathbf{z}}$$

Determine the evolution operator and show that it is a rotation. Find the axis and angle of rotation.

Answer: $\hat{H} = -\frac{gq}{2m}\frac{\hbar}{2}B_0\hat{\sigma}_z$

$$\hat{U}(t) = e^{-i\hat{H}t/\hbar} = e^{i\frac{gq}{4m}B_0 t\hat{\sigma}_z}$$

$$= e^{-i\left(-\frac{gqB_0}{2m}t\right)\hat{\sigma}_z/2}$$

This is a rotation about $\hat{z}$ through $\varphi = -\frac{gqB_0t}{2m} = \omega t$

where $\omega = -\frac{gqB_0}{2m}$. $\blacksquare$

Thus for any constant magnetic field

Given a constant field $\vec{B} = B\hat{n}$ then the evolution operator is a rotation about $\hat{n}$ through angle $\omega t$ where

$$\omega = -\frac{gqB}{2M}$$

This is a clockwise rotation at angular rate $\omega$.

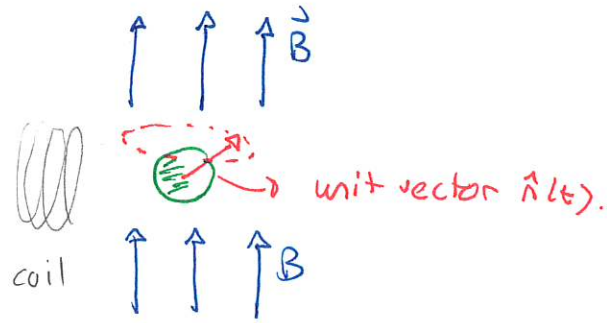
## Application to magnetic resonance

In nuclear magnetic resonance (NMe) and magnetic resonance imaging appartus, spin-$\frac{1}{2}$ particles are placed in magnetic fields. There are usually two:

1) a strong constant magnetic field
2) weaker time-varying fields that are turned on and off

When only the strong field is present then the evolution is a rotation about the field direction.

Thus the state has form




$$|+\hat{n}(t)\rangle$$

where

$$\hat{n}(t)$$

is a unit vector rotating about $\vec{B}$ with angular frequency $\frac{gq}{2M}B$

This motion is called Larmor precession and the frequency is the Larmor frequency.

The rotating magnetic dipole generates its own field and this can be detected in nearby coils.

## Evolution in terms of energy eigenstates

The Hamiltonian is an observable and thus has eigenstates with real eigenvalues. These satisfy:

$$\hat{H}|\phi_i\rangle = E_i|\phi_i\rangle$$

where $i$ is an index and $E_i$ is the energy eigenvalue. In general any state of a system can be expressed as a superposition of energy eigenstates. So for a spin-½ system there are at most two energy eigenstates $|\phi_1\rangle, |\phi_2\rangle$. Then

$$|\Psi\rangle = c_1|\phi_1\rangle + c_2|\phi_2\rangle$$

It will emerge that this is a convenient form for determining the evolution of the state. Suppose that at $t=0$

$$|\Psi(0)\rangle = c_1|\phi_1\rangle + c_2|\phi_2\rangle.$$

Then by linearity, at a later time,

$$|\Psi(t)\rangle = c_1|\phi_1(t)\rangle + c_2|\phi_2(t)\rangle$$

and we need to find $|\phi_i(t)\rangle$.

## 2 Energy eigenstate evolution

Suppose that the Hamiltonian for a spin-1/2 system is

$$\hat{H} = \frac{\hbar\omega}{2}\hat{\sigma}_x$$

where $\omega$ has units of frequency.

a) Show that $|+\hat{x}\rangle$ and $|-\hat{x}\rangle$ are eigenstates of the Hamiltonian.

b) Suppose that a spin-1/2 particle is initially in the state $|+\hat{x}\rangle$. Determine its state at any later time.

c) If the spin-1/2 particle is initially in the state $|+\hat{x}\rangle$ will the measurement statistics at any later time be any different than at the initial instant?

Answer: a)

$$|+\hat{x}\rangle = \frac{1}{\sqrt{2}}|+\hat{z}\rangle + \frac{1}{\sqrt{2}}|-\hat{z}\rangle$$

$$|-\hat{x}\rangle = \frac{1}{\sqrt{2}}|+\hat{z}\rangle - \frac{1}{\sqrt{2}}|-\hat{z}\rangle$$

$$\hat{H}|+\hat{x}\rangle = \frac{\hbar\omega}{2}\begin{pmatrix}0&1\\1&0\end{pmatrix}\frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix} = \frac{\hbar\omega}{2}\frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix} = \frac{\hbar\omega}{2}|+\hat{x}\rangle$$

$$\hat{H}|-\hat{x}\rangle = \frac{\hbar\omega}{2}\begin{pmatrix}0&1\\1&0\end{pmatrix}\frac{1}{\sqrt{2}}\begin{pmatrix}1\\-1\end{pmatrix} = \frac{\hbar\omega}{2}\frac{1}{\sqrt{2}}\begin{pmatrix}-1\\1\end{pmatrix} = -\frac{\hbar\omega}{2}|-\hat{x}\rangle.$$

Thus

$\hat{H}|+x\rangle = \frac{\hbar\omega}{2}|+\hat{x}\rangle$ eigenvalue $+\frac{\hbar\omega}{2}$

$\hat{H}|-\hat{x}\rangle = -\frac{\hbar\omega}{2}|-\hat{x}\rangle$ eigenvalue $-\frac{\hbar\omega}{2}$

b)

$$|\Psi(t)\rangle = \hat{U}|\Psi(0)\rangle$$

$$= e^{-i\hat{H}t/\hbar}|\Psi(0)\rangle$$

$$= e^{-i\omega t\hat{\sigma}_x/2}|\Psi(0)\rangle.$$

Then $e^{-i\omega t \hat{\sigma}_x/2} = \hat{I} + \left(-\frac{i\omega t}{2}\hat{\sigma}_x\right) + \frac{1}{2!}\left(-\frac{i\omega t}{2}\hat{\sigma}_x\right)^2 + \frac{1}{3!}\left(-\frac{i\omega t}{2}\right)^3 \hat{\sigma}_x^3$

$$= \hat{I} + \left(-\frac{i\omega t}{2}\right)\hat{\sigma}_x + \frac{1}{2!}\left(-\frac{i\omega t}{2}\right)^2 \hat{\sigma}_x^2 + \frac{1}{3!}\left(-\frac{i\omega t}{2}\right)^3 \hat{\sigma}_x^3 + \dots$$

Then $\hat{\sigma}_x\hat{\sigma}_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \hat{I}$. Thus

$$e^{-i\omega t \hat{\sigma}_x/2} = \left[1 + \frac{1}{2!}\left(-\frac{i\omega t}{2}\right)^2 + \frac{1}{4!}\left(-\frac{i\omega t}{2}\right)^4 + \dots\right]\hat{I}$$

$$+ \left[\left(-\frac{i\omega t}{2}\right) + \frac{1}{3!}\left(-\frac{i\omega t}{2}\right)^3 + \dots\right]\hat{\sigma}_x$$

$$= \left[1 - \frac{1}{2!}\left(\frac{\omega t}{2}\right)^2 + \frac{1}{4!}\left(\frac{\omega t}{2}\right)^4 + \dots\right]\hat{I}$$

$$-i\left[\frac{\omega t}{2} - \frac{1}{3!}\left(\frac{\omega t}{2}\right)^3 + \dots\right]\hat{\sigma}_x$$

$$= \cos\left(\frac{\omega t}{2}\right)\hat{I} - i\sin\left(\frac{\omega t}{2}\right)\hat{\sigma}_x$$

$$= \begin{pmatrix} \cos\frac{\omega t}{2} & -i\sin\frac{\omega t}{2} \\ -i\sin\frac{\omega t}{2} & \cos\frac{\omega t}{2} \end{pmatrix}$$

Thus $|\Psi(t)\rangle = \begin{pmatrix} \cos\frac{\omega t}{2} & -i\sin\frac{\omega t}{2} \\ -i\sin\frac{\omega t}{2} & \cos\frac{\omega t}{2} \end{pmatrix} \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}$

$$= \frac{1}{\sqrt{2}}\begin{pmatrix} \cos\frac{\omega t}{2} - i\sin\frac{\omega t}{2} \\ \cos\frac{\omega t}{2} - i\sin\frac{\omega t}{2} \end{pmatrix} = \frac{1}{\sqrt{2}} e^{-i\omega t/2}\begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

$\Rightarrow |\Psi(t)\rangle = e^{-i\omega t/2}\hat{\sigma}_x$

c) No $e^{-i\omega t/2}$ contributes a global phase. This can be ignored.

This is an example of a general rule:

Suppose $|\phi_j\rangle$ is an energy eigenstate with eigenvalue $E_j$.
Then if

$$|\Psi(0)\rangle = |\phi_j\rangle$$

the state at a later time will be

$$|\Psi(t)\rangle = e^{-iE_j t/\hbar}\,|\phi_j\rangle.$$

It follows that if

$$|\Psi(0)\rangle = c_1|\phi_1\rangle + c_2|\phi_2\rangle$$

then

$$|\Psi(t)\rangle = c_1 e^{-iE_1 t/\hbar}|\phi_1\rangle + c_2 e^{-iE_2 t/\hbar}|\phi_2\rangle.$$

and this completely describes the state of the system at later times (for a time-independent Hamiltonian)