Thurs: Exam I Covers * all material up to Fri Feb 24

* lectures 1 → 10
* HW 1 → 10

Study: Previous exams

2007 Q1, Q2, Q3 (challenging)

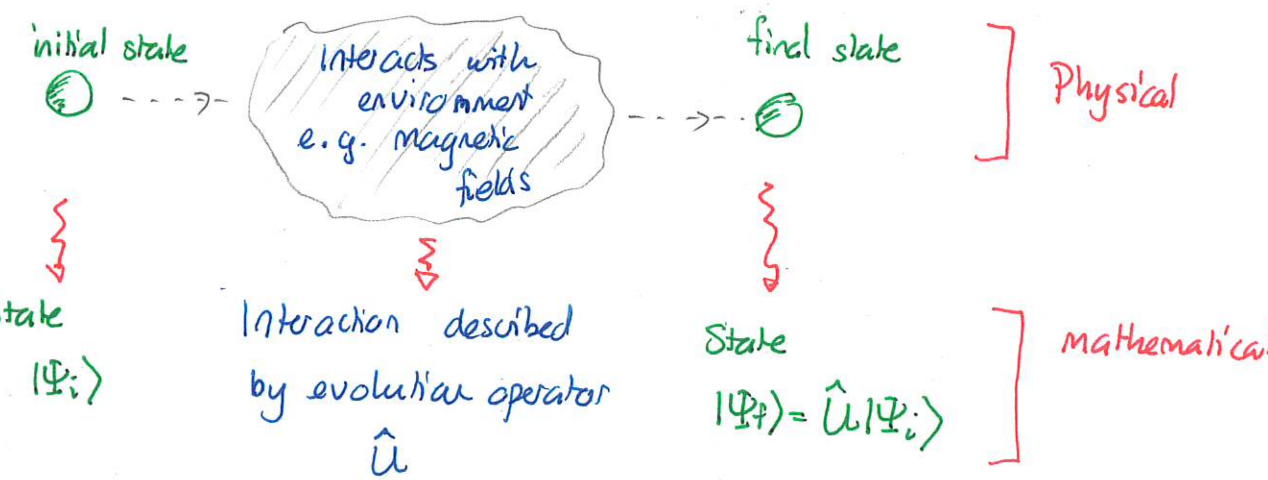
2022 Q1 → Q5

Formulas: Some given – see 2022 exam

– bring half letter sheet - single side.

Evolution of spin-1/2 quantum systems

The general framework for evolution of a system is



The evolution operator satisfies:

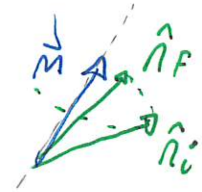
1) it is linear

2) it is unitary ⇒ $\boxed{\hat{U}^\dagger \hat{U} = \hat{I}}$

A series of mathematical theorems and derivations gives:

> Any unitary evolution operator for a spin-½ system is equivalent to a rotation operator.

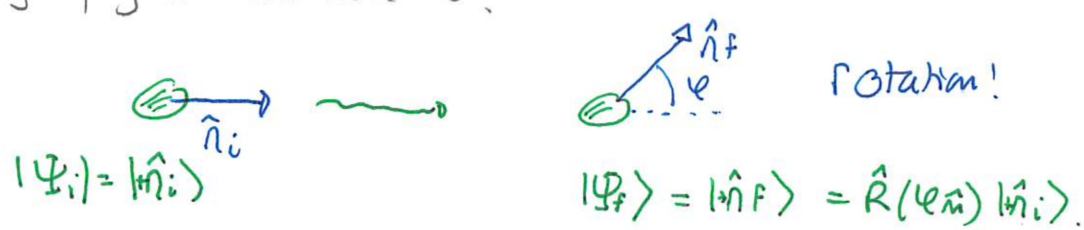
To make this concrete note that

> A rotation about axis $\hat{m}$ through angle φ:
>
> 1) maps
>
> $$|+\hat{n}_i\rangle \to |+\hat{n}_F\rangle$$
>
> where $\hat{n}_F$ is obtained by rotating $\hat{n}_i$ through angle φ about $\hat{m}$.
>
> 
>
>
> 2) is constructed as:
>
> $$\hat{R}(\varphi\hat{m}) = e^{-i\varphi/2}|+\hat{m}\rangle\langle+\hat{m}| + e^{i\varphi/2}|-\hat{m}\rangle\langle-\hat{m}|.$$

Then one can show that

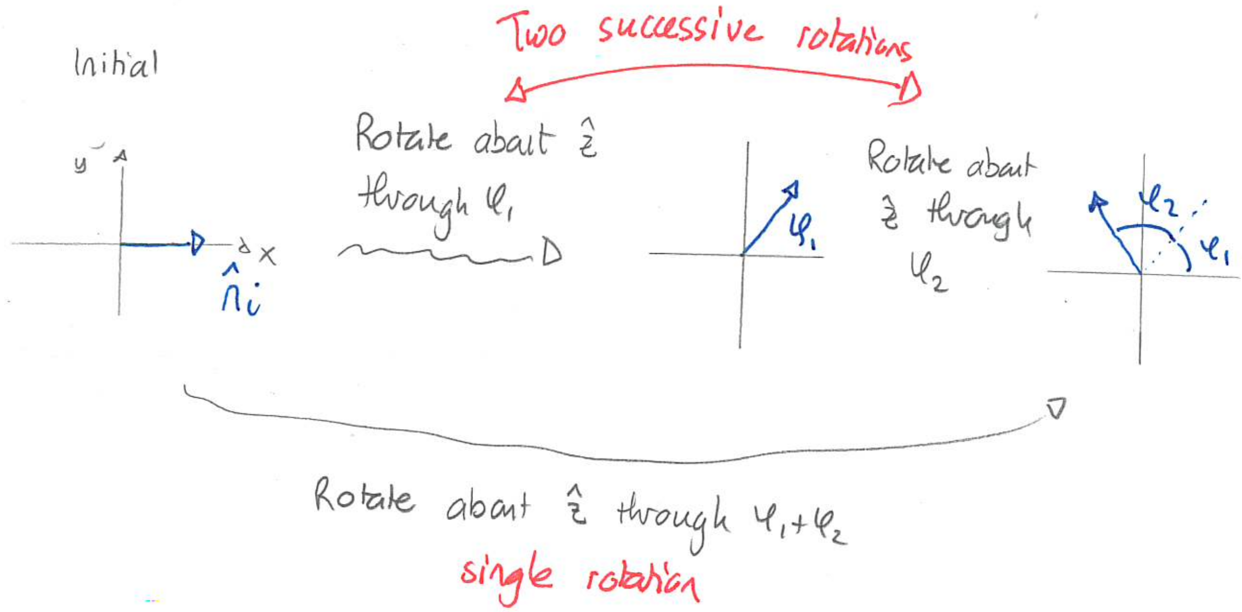
> For any unitary $\hat{U}$ there is a rotation and $\alpha > 0$ s.t.
>
> $$\hat{U} = e^{i\alpha}\hat{R}(\varphi\hat{m})$$

The $e^{i\alpha}$ contributes a global phase to the state. Thus we can picture any physical evolution as.



Generating rotations

General considerations about rotations show that a sequence of two or more rotations is itself a (new) single rotation. For example



This can extend to an arbitrary number of rotations applied successively. Then we can ask whether any given rotation can be constructed, in a compact form, as a sequence of small basic rotations. So we might hope

$$\hat{R}(\varphi\hat{z}) = \hat{R}\left(\frac{\varphi}{N}\hat{z}\right)\hat{R}\left(\frac{\varphi}{N}\hat{z}\right)\ldots\ldots\hat{R}\left(\frac{\varphi}{N}\hat{z}\right) \qquad (N \text{ factors})$$

$$= \left[R\left(\frac{\varphi}{N}\hat{z}\right)\right]^N$$

$$= \left[\hat{I} + \frac{\varphi}{N}\text{ operator}\right]^N$$

This resembles an exponential

$$e^X = \lim_{N\to\infty}\left(1+\frac{X}{N}\right)^N$$

So we seek a notation of matrix exponentiation.

We would like to define

$$e^{\hat{A}}$$

for any operator $\hat{A}$. To do this note that for any real number x

$$e^x = 1 + \frac{x}{1!} + \frac{x^2}{2!} + \frac{x^3}{3!} + \dots = \sum \frac{x^n}{n!} = \sum_{n=0}^{\infty} \frac{1}{n!} x^n$$

Thus we define:

$$\boxed{\begin{array}{l} e^{\hat{A}} := \hat{I} + \frac{1}{1!}\hat{A} + \frac{1}{2!}\hat{A}^2 + \frac{1}{3!}\hat{A}^3 + \dots = \displaystyle\sum_{n=0}^{\infty} \frac{1}{n!}\hat{A}^n \\ \text{where } \hat{A}^0 := \hat{I} \end{array}}$$

We will see that any rotation can be constructed via exponentiation

1 Operator exponentiation

a) Determine the operator

$$\hat{U} = e^{-i\varphi\hat{\sigma}_z/2}$$

where

$$\hat{\sigma}_z \leftrightarrow \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

b) Verify that $\hat{U}$ is unitary.

c) Check that

$$\hat{R}(\varphi\hat{\mathbf{z}}) = e^{-i\varphi\hat{\sigma}_z/2}.$$

Answer: a) Use $\hat{A} = \frac{-i\varphi\hat{\sigma}_z}{2}$

$$e^{\hat{A}} = \hat{I} + \hat{A} + \frac{1}{2!}\hat{A}^2 + \frac{1}{3!}\hat{A}^3 + \dots$$

Now

$$\hat{A}^2 = \left(\frac{-i\varphi}{2}\hat{\sigma}_z\right)\left(\frac{-i\varphi}{2}\hat{\sigma}_z\right)$$

$$= -\left(\frac{\varphi}{2}\right)^2 \hat{\sigma}_z\hat{\sigma}_z = -\left(\frac{\varphi}{2}\right)^2\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = -\left(\frac{\varphi}{2}\right)^2\hat{I}$$

$$\hat{A}^3 = \left(-\frac{i\varphi}{2}\right)^3 \underbrace{\hat{\sigma}_z\hat{\sigma}_z}_{\hat{I}}\hat{\sigma}_z = +i\left(\frac{\varphi}{2}\right)^3\hat{\sigma}_z$$

$$\hat{A}^4 = \left(\frac{-i\varphi}{2}\right)^4 \underbrace{\hat{\sigma}_z\hat{\sigma}_z}_{\hat{I}}\underbrace{\hat{\sigma}_z\hat{\sigma}_z}_{\hat{I}} \qquad \left(\frac{\varphi}{2}\right)^4\hat{I}$$

Thus

$$e^{\hat{A}} = \hat{I} + \left(\frac{-i\varphi}{2}\right)\hat{\sigma}_z + \frac{1}{2!}\left(\frac{-i\varphi}{2}\right)^2\hat{I} + \frac{1}{3!}\left(\frac{-i\varphi}{2}\right)^3\hat{\sigma}_z + \frac{1}{4!}\left(\frac{-i\varphi}{2}\right)^4\hat{I} + \dots$$

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

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

So

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

$$-i\left[\left(\frac{\varphi}{2}\right) - \frac{1}{3!}\left(\frac{\varphi}{2}\right)^3 + \frac{1}{5!}\left(\frac{\varphi}{2}\right)^5 + \dots\right]\hat{\sigma}_z$$

$$= \cos\left(\frac{\varphi}{2}\right)\hat{I} - i\sin\frac{\varphi}{2}\,\hat{\sigma}_z$$

Thus

$$\hat{U} = \cos\frac{\varphi}{2}\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix} - i\sin\frac{\varphi}{2}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}$$

$$= \begin{pmatrix}\cos\frac{\varphi}{2} - i\sin\varphi/2 & 0\\ 0 & \cos\varphi/2 + i\sin\varphi/2\end{pmatrix} = \begin{pmatrix}e^{-i\varphi/2} & 0\\ 0 & e^{i\varphi/2}\end{pmatrix}$$

b) $$\hat{U}^\dagger\hat{U} = \begin{pmatrix}e^{i\varphi/2} & 0\\ 0 & e^{-i\varphi/2}\end{pmatrix}\begin{pmatrix}e^{-i\varphi/2} & 0\\ 0 & e^{i\varphi/2}\end{pmatrix} = \begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix} = \hat{I}$$

This is unitary.

c) $$\hat{R}(\varphi\hat{z}) = e^{-i\varphi/2}\,|+\hat{z}\rangle\langle+\hat{z}| + e^{i\varphi/2}\,|-\hat{z}\rangle\langle-\hat{z}|$$

$$\to e^{-i\varphi/2}\begin{pmatrix}1\\ 0\end{pmatrix}(1\ 0) + e^{i\varphi/2}\begin{pmatrix}0\\ 1\end{pmatrix}(0\ 1)$$

$$= e^{-i\varphi/2}\begin{pmatrix}1 & 0\\ 0 & 0\end{pmatrix} + e^{i\varphi/2}\begin{pmatrix}0 & 0\\ 0 & 1\end{pmatrix}$$

$$= \begin{pmatrix}e^{-i\varphi/2} & 0\\ 0 & e^{i\varphi/2}\end{pmatrix} = \hat{U}.$$

The exercise demonstrates that

$$\hat{R}(\varphi\hat{z}) = e^{-i\varphi\hat{\sigma}_z/2}$$

This is an example of a general rule

$$\boxed{\begin{array}{l}\text{Any rotation can be generated by exponentiation:} \\ \qquad \hat{R}(\varphi\hat{m}) = e^{-i\varphi\hat{\sigma}_m/2} \\ \text{where} \\ \qquad \hat{\sigma}_m = |+\hat{m}\rangle\langle+\hat{m}| - |-\hat{m}\rangle\langle-\hat{m}|\end{array}}$$

In the conventional $\{|\pm\hat{z}\rangle\}$ basis, there are three special <u>Pauli operators</u>:

$$\hat{\sigma}_x \leadsto \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \hat{\sigma}_y \leadsto \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \qquad \hat{\sigma}_z \leadsto \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

In general

$$\boxed{\begin{array}{l}\text{If } \hat{m} = m_x\hat{x} + m_y\hat{y} + m_z\hat{z} \text{ then} \\ \qquad \hat{\sigma}_m = m_x\hat{\sigma}_x + m_y\hat{\sigma}_y + m_z\hat{\sigma}_z\end{array}}$$

<u>Properties of matrix exponentiation</u>

It can be shown that:

1) $e^{\alpha\hat{A}}e^{\beta\hat{A}} = e^{(\alpha+\beta)\hat{A}}$ for any complex α, β

2) $\left(e^{\alpha\hat{A}}\right)^{\beta} = e^{\alpha\beta\hat{A}}$ " " " α, β

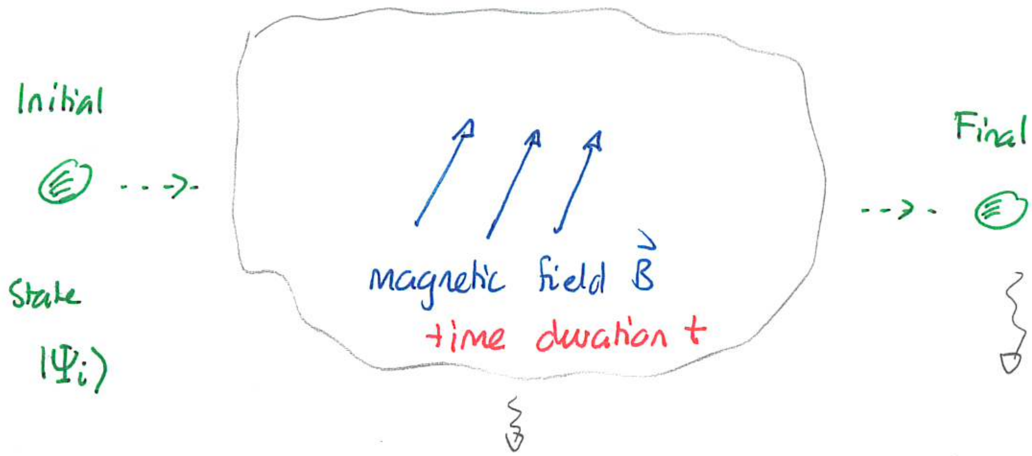
3) $\frac{d}{d\alpha}e^{\alpha\hat{A}} = \hat{A}e^{\alpha\hat{A}}$ " " " α

But unless $\hat{A}, \hat{B}$ commute

$$e^{\hat{A}}e^{\hat{B}} \neq e^{\hat{A}+\hat{B}}.$$

Time dependent evolution

The evolution of a system will often depend on time.



evolution operator depends on t : $\hat{U}(t)$

final state depends on t $|\Psi_F(t)\rangle = \hat{U}(t)|\Psi_i\rangle$

Then: using $|\Psi(t)\rangle$ rather than the subscripts, we get

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

We now consider:

1) What equation should the evolution operator satisfy? How is this related to $\vec{B}$, t, ...

2) What equation should $|\Psi(t)\rangle$ satisfy. How is this related to $\vec{B}$, t, ...

2 Time-dependent evolution

Consider a situation where the evolution operator is a rotation about the z axis through a time dependent angle ωt where ω is a constant. Determine the matrix that represents the operator $\hat{R}((\omega t)z)$. Suppose that the initial state of the spin-1/2 particle is $|+\hat{x}\rangle$. Determine the state at time t and describe the direction of the component of spin whose measurement will yield $+\hbar/2$ with certainty.

Answer:

$$\hat{R}\left((\omega t)\hat{z}\right) = e^{-i\omega t/2}|+\hat{z}\rangle\langle+\hat{z}| + e^{i\omega t/2}|-\hat{z}\rangle\langle-\hat{z}|$$

$$\rightsquigarrow e^{-i\omega t/2}\begin{pmatrix}1\\0\end{pmatrix}\begin{pmatrix}1 & 0\end{pmatrix} + e^{i\omega t/2}\begin{pmatrix}0\\1\end{pmatrix}\begin{pmatrix}0 & 1\end{pmatrix}$$

$$= e^{-i\omega t/2}\begin{pmatrix}1 & 0\\0 & 0\end{pmatrix} + e^{i\omega t/2}\begin{pmatrix}0 & 0\\0 & 1\end{pmatrix}$$

$$= \begin{pmatrix}e^{-i\omega t/2} & 0\\0 & e^{i\omega t/2}\end{pmatrix}$$

The initial state is $|\Psi(0)\rangle = |+\hat{x}\rangle = \frac{1}{\sqrt{2}}|+\hat{z}\rangle + \frac{1}{\sqrt{2}}|-\hat{z}\rangle$

$$\rightsquigarrow \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix}$$

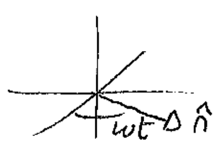
Then

$$|\Psi(t)\rangle = \hat{U}(t)|\Psi(0)\rangle \rightsquigarrow \begin{pmatrix}e^{-i\omega t/2} & 0\\0 & e^{i\omega t/2}\end{pmatrix}\frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix}$$

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

$$\Rightarrow |\Psi(t)\rangle = e^{-i\omega t/2}\frac{1}{\sqrt{2}}|+\hat{z}\rangle + e^{i\omega t/2}\frac{1}{\sqrt{2}}|-\hat{z}\rangle$$

$$= \underbrace{e^{-i\omega t/2}}_{\text{global phase}}\underbrace{\left[\frac{1}{\sqrt{2}}|+\hat{z}\rangle + e^{i\omega t}\frac{1}{\sqrt{2}}|-\hat{z}\rangle\right]}_{|+\hat{n}\rangle \text{ where } \hat{n} \text{ has } \theta=\pi/2 \;\; \phi=\omega t}$$



$\rightsquigarrow$ Measure at angle ωt in xy plane.

In terms of matrix / vector operations,

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

$$|\Psi(0)\rangle = C_+(0)|+\hat{z}\rangle + C_-(0)|-\hat{z}\rangle \rightsquigarrow \begin{pmatrix} C_+(0) \\ C_-(0) \end{pmatrix}$$

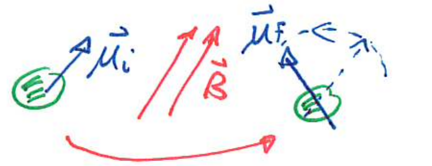
and

$$\hat{U}(t) \rightsquigarrow \begin{pmatrix} U_{++}(t) & U_{+-}(t) \\ U_{-+}(t) & U_{--}(t) \end{pmatrix}$$

This gives:

$$|\Psi(t)\rangle = \hat{U}(t)|\Psi(0)\rangle \rightsquigarrow \begin{pmatrix} C_+(t) \\ C_-(t) \end{pmatrix} = \begin{pmatrix} U_{++}(t) & U_{+-}(t) \\ U_{-+}(t) & U_{--}(t) \end{pmatrix} \begin{pmatrix} C_+(0) \\ C_-(0) \end{pmatrix}$$

This describes the mathematics of time evolution. Then it remains to connect this to the physical situation. For spin-½ particles that are also magnetic dipoles, we know that the magnetic field determines how the dipole moment and spin evolve.



magnetic field relates $\vec{\mu}_f$ to $\vec{\mu}_i$

So we want:

Given known magnetic field $\vec{B}$ and duration in field

get $\hat{U}$ →

← determine what $\vec{B}, t$ were...

Unitary evolution operator $\hat{U}(t)$

We can attempt a differential equation for $|\Psi(t)\rangle$. We find

$$i\hbar \frac{d|\Psi(t)\rangle}{dt} = i\hbar \frac{d\hat{U}}{dt} \hat{U}^{+} |\Psi(t)\rangle$$

and

$$i\hbar \frac{d\hat{U}}{dt} \hat{U}^{+}$$

is a Hermitian operator with units of energy.

Proof: $|\Psi(t)\rangle = \hat{U}(t)|\Psi(0)\rangle$ $\quad \begin{pmatrix} C_+(t) \\ C_-(t) \end{pmatrix} = \begin{pmatrix} U_{++} & U_{+-} \\ U_{-+} & U_{--} \end{pmatrix} \begin{pmatrix} C_+(0) \\ C_-(0) \end{pmatrix}$

$$\frac{d|\Psi(t)\rangle}{dt} = \frac{d\hat{U}}{dt}|\Psi(0)\rangle \qquad \begin{pmatrix} \frac{dC_+}{dt} \\ \frac{dC_-}{dt} \end{pmatrix} = \begin{pmatrix} \frac{dU_{++}}{dt} & \frac{dU_{+-}}{dt} \\ \frac{dU_{-+}}{dt} & \frac{dU_{--}}{dt} \end{pmatrix} \begin{pmatrix} C_+(0) \\ C_-(0) \end{pmatrix}$$

$$\Rightarrow \frac{d|\Psi(t)\rangle}{dt} = \frac{d\hat{U}}{dt} \underbrace{\hat{U}^{+}\hat{U}}_{\hat{I}} |\Psi(0)\rangle$$

$\leftarrow$ insert identity

$$= \frac{d\hat{U}}{dt} \hat{U}^{+} |\Psi(t)\rangle$$

Thus

$$i\hbar \frac{d|\Psi(t)\rangle}{dt} = i\hbar \frac{d\hat{U}}{dt} \hat{U}^{+} |\Psi(t)\rangle$$

Now consider where $i\hbar \frac{d\hat{U}}{dt}\hat{U}^{+}$ is Hermitian. To prove this

$$\hat{U}^{+}\hat{U} = \hat{I} \Rightarrow \hat{U}\hat{U}^{+} = \hat{I} \Rightarrow \frac{d\hat{U}}{dt}\hat{U}^{+} + \hat{U}\frac{d\hat{U}^{+}}{dt} = 0. \Rightarrow \hat{U}\frac{d\hat{U}^{+}}{dt} = -\frac{d\hat{U}}{dt}\hat{U}^{+}$$

so

$$\left(i\hbar \frac{dU}{dt}\hat{U}^{+}\right)^{+} = -i\hbar\left(\hat{U}^{+}\right)^{+}\left(\frac{d\hat{U}}{dt}\right)^{+} = -i\hbar\,\hat{U}\,\frac{d\hat{U}^{+}}{dt} = i\hbar\frac{d\hat{U}}{dt}\hat{U}^{+}$$

Finally $\frac{dU}{dt}\hat{U}^{+}$ has units of s^{-1} and $\hbar$ units of Js $\Rightarrow$ units of energy ∎

We then postulate that $i\hbar \frac{d\hat{U}}{dt}\hat{U}^{+}$ is exactly the energy observable for the system. Then the energy observable for the system is called the Hamiltonian, $\hat{H}$.

Thus

> Any state of a spin-½ system satisfies:
>
> $$i\hbar \frac{d|\Psi(t)\rangle}{dt} = \hat{H}\,|\Psi(t)\rangle$$
>
> where $\hat{H}$ is the Hamiltonian (energy observable) that describes the system and its interaction with its surroundings.

This is the <u>Schrödinger equation</u>