Time evolution
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Here we discuss the time evolution operator. There are three kinds of pictures; Schrödinger picture, Heisenberg picture, and Dirac picture. In the Schrodinger picture, the eigenket depends on time, while the operator is independent of time. The Schrodinger equation indicates how the eigenket (wave function) changes with time. For simplicity, we discuss mainly the case when the Hamiltonian is independent of time *t*. In the Heisenberg picture, the eigenket is independent of time. The operator changes with time *t* according to the Heisenberg's equation of motion. This equation of motion is similar to the corresponding equation in the classical mechanics. The Dirac picture is used when the Hamiltonian includes the interacting Hamiltonian as a perturbation. Both the eigenket and operator depends on time *t*. We will use this picture for the discussion of the time-dependent perturbation theory.

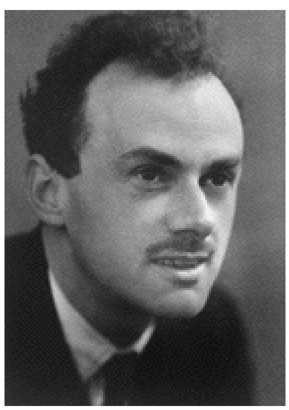
Erwin Rudolf Josef Alexander Schrödinger (12 August 1887– 4 January 1961) was an Austrian theoretical physicist who was one of the fathers of quantum mechanics, and is famed for a number of important contributions to physics, especially the Schrödinger equation, for which he received the Nobel Prize in Physics in 1933. In 1935, after extensive correspondence with personal friend Albert Einstein, he proposed the Schrödinger's cat thought experiment.

http://en.wikipedia.org/wiki/Erwin_Schr%C3%B6dinger

Werner Heisenberg (5 December 1901– 1 February 1976) was a German theoretical physicist who made foundational contributions to quantum mechanics and is best known for asserting the uncertainty principle of quantum theory. In addition, he made important contributions to nuclear physics, quantum field theory, and particle physics. Heisenberg, along with Max Born and Pascual Jordan, set forth the matrix formulation of quantum mechanics in 1925. Heisenberg was awarded the 1932 Nobel Prize in Physics for the creation of quantum mechanics, and its application especially to the discovery of the allotropic forms of hydrogen.

http://en.wikipedia.org/wiki/Werner_Heisenberg

Paul Adrien Maurice Dirac (8 August 1902 – 20 October 1984) was a British theoretical physicist. Dirac made fundamental contributions to the early development of both quantum mechanics and quantum electrodynamics. He held the Lucasian Chair of Mathematics at the University of Cambridge and spent the last fourteen years of his life at Florida State University. Among other discoveries, he formulated the Dirac equation, which describes the behavior of fermions. This led to a prediction of the existence of antimatter. Dirac shared the Nobel Prize in physics for 1933 with Erwin Schrödinger, "for the discovery of new productive forms of atomic theory."



http://en.wikipedia.org/wiki/Paul_Dirac

1 Time evolution operator

We define the Unitary operator as

$$|\psi(t)\rangle = \hat{U}(t,t_0)|\psi(t_0)\rangle,$$

$$\langle\psi(t)| = \langle\psi(t_0)|\hat{U}^+(t,t_0).$$

Normalization

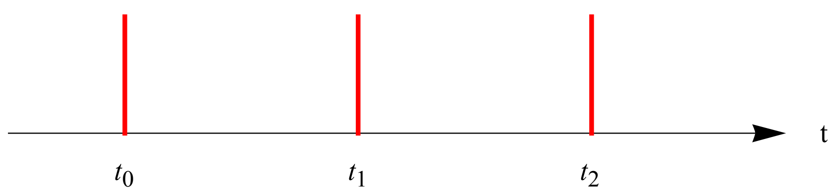
$$\langle\psi(t)|\psi(t)\rangle = \langle\psi(t_0)|\psi(t_0)\rangle = 1.$$

Then

$$\langle\psi(t_0)|\hat{U}^+(t,t_0)\hat{U}(t,t_0)|\psi(t_0)\rangle = \langle\psi(t_0)|\psi(t_0)\rangle,$$

or

$\hat{U}^+(t,t_0)\hat{U}(t,t_0) = \hat{1}$ (unitary operator),



We note that

$$|\psi(t_2)\rangle = \hat{U}(t_2,t_1)|\psi(t_1)\rangle = \hat{U}(t_2,t_1)\hat{U}(t_1,t_0)|\psi(t_0)\rangle.$$

This should be

$$\hat{U}(t_2,t_0) = \hat{U}(t_2,t_1)\hat{U}(t_1,t_0).$$

It is easy to generalize this procedure

$$\hat{U}(t_n,t_1) = \hat{U}(t_n,t_{n-1})\hat{U}(t_{n-1},t_{n-2})......\hat{U}(t_3,t_2)\hat{U}(t_2,t_1).$$

where t_1, t_2, ..., t_n are arbitrary. If we assume that $t_1<t_2<t_3<...<t_n$, this formula is simple to interpret: to go from t_1 to t_n, the system progresses from t_1 to t_2, then from t_2 to t_3, ... , then finally from t_{n-1} to t_n.

2 Infinitesimal time-evolution operator

We consider the infinitesimal time evolution operator

$$\left|\psi(t_0+dt)\right\rangle = \hat{U}(t_0+dt,t_0)\left|\psi(t_0)\right\rangle ,$$

with

$$\lim_{dt\to 0}\hat{U}(t_0+dt,t_0)=\hat{1} .$$

We assert that all these requirements are satisfied by

$$\hat{U}(t_0+dt,t_0)=\hat{1}-i\hat{\Omega}dt .$$

The dimension of $\hat{\Omega}$ is a frequency or inverse time.

$$\begin{aligned}\hat{U}^+(t_0+dt,t_0)\hat{U}(t_0+dt,t_0) &= (\hat{1}-i\hat{\Omega}dt)^+(\hat{1}-i\hat{\Omega}dt)\\ &= (\hat{1}+i\hat{\Omega}^+dt)(\hat{1}-i\hat{\Omega}dt)\\ &= \hat{1}+i(\hat{\Omega}^+-\hat{\Omega})dt\\ &= \hat{1}\end{aligned}$$

or

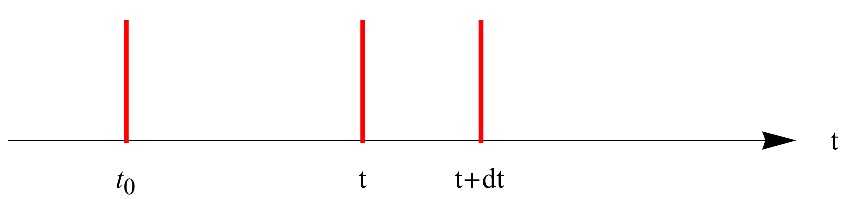
$$\hat{\Omega}^+=\hat{\Omega} \qquad \text{(Hermitian).}$$

We assume that

$$\hat{\Omega}=\frac{\hat{H}}{\hbar},$$

where $\hat{H}$ is a Hamiltonian.

3 Schrödinger equation



$$\hat{U}(t+dt,t_0)=\hat{U}(t+dt,t)\hat{U}(t,t_0)$$
$$=(\hat{1}-i\frac{\hat{H}}{\hbar}dt)\hat{U}(t,t_0),$$

or

$$\hat{U}(t+dt,t_0)-\hat{U}(t,t_0)=-i\frac{\hat{H}}{\hbar}dt\hat{U}(t,t_0),$$

$$\lim_{dt\to 0}\frac{\hat{U}(t+dt,t_0)-\hat{U}(t,t_0)}{dt}=-i\frac{\hat{H}}{\hbar}\hat{U}(t,t_0),$$

or

$$\frac{\partial}{\partial t}\hat{U}(t,t_0)=-i\frac{\hat{H}}{\hbar}\hat{U}(t,t_0),$$

or

$$i\hbar\frac{\partial}{\partial t}\hat{U}(t,t_0)=\hat{H}\hat{U}(t,t_0).$$

Since $\hat{U}(t_0,t_0)=\hat{1}$, we get a formal solution for $\hat{U}(t,t_0)$ as

$$\hat{U}(t,t_0)=\hat{1}-\frac{i}{\hbar}\int_{t_0}^{t}\hat{H}(t')\hat{U}(t',t_0)dt',$$

when $\hat{H}$ is dependent on *t*. This is the Schrödinger equation for the time-evolution operator.

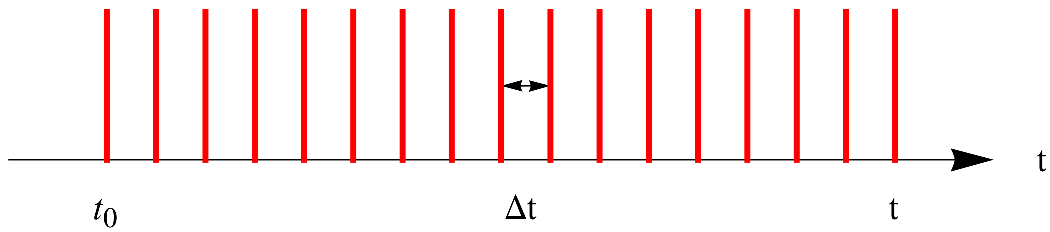
$$i\hbar\frac{\partial}{\partial t}\hat{U}(t,t_0)|\psi(t_0)\rangle=\hat{H}\hat{U}(t,t_0)|\psi(t_0)\rangle,$$

or

$$i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle=\hat{H}|\psi(t)\rangle.$$

4 Unitary operator for time independent $\hat{H}$

What is the form of $\hat{U}(t,t_0)$ when $\hat{H}$ is independent of *t*?



$$\Delta t = \frac{t - t_0}{N},$$

$$\lim_{N \to \infty} [\hat{1} - \frac{i\hat{H}}{\hbar}(\frac{t - t_0}{N})]^N = \exp[-\frac{i\hat{H}}{\hbar}(t - t_0)],$$

from the definition of the mathematical constant *e*, or

$$\hat{U}(t, t_0) = \exp[-\frac{i\hat{H}}{\hbar}(t - t_0)].$$

Using this, we have

$$|\psi(t)\rangle = \exp[-\frac{i}{\hbar}\hat{H}(t - t_0)]|\psi(t_0)\rangle,$$

or simply, we have

$$|\psi(t)\rangle = \exp[-\frac{i}{\hbar}\hat{H}t]|\psi(0)\rangle,$$

for $t_0 = 0$.

5. Time evolution (general case)

Suppose that the Hamiltonian is time dependent. We consider the state is given by

$$|\psi(t)\rangle = \sum_n C_n(t)|\phi_n\rangle,$$

where $C_n(t)$ is a time-dependent coefficient and $|\phi_n\rangle$ is the orthonormal set of eigenfunctions, where

$$\langle\phi_n|\phi_m\rangle = \delta_{nm}.$$

The Schrodinger equation:

$$i\hbar \frac{\partial}{\partial t}\left|\psi(t)\right\rangle = \hat{H}(t)\left|\psi(t)\right\rangle,$$

or

$$\sum_m i\hbar \frac{dC_m(t)}{dt}\left|\phi_m\right\rangle = \sum_m C_m(t)\hat{H}(t)\left|\phi_m\right\rangle.$$

Multiplying $\left\langle\phi_n\right|$, we get

$$\sum_m i\hbar \frac{dC_m(t)}{dt}\left\langle\phi_n|\phi_m\right\rangle = \sum_m C_m(t)\left\langle\phi_n\right|\hat{H}(t)\left|\phi_m\right\rangle,$$

or

$$\sum_m i\hbar \frac{dC_m(t)}{dt}\delta_{nm} = \sum_m C_m(t)\left\langle\phi_n\right|\hat{H}(t)\left|\phi_m\right\rangle,$$

or

$$i\hbar \frac{dC_n(t)}{dt} = \sum_m \left\langle\phi_n\right|\hat{H}(t)\left|\phi_m\right\rangle C_m(t).$$

For the system with only $n = 1$ and 2

$$i\hbar \frac{dC_1(t)}{dt} = H_{11}(t)C_1(t) + H_{12}(t)C_2(t),$$

$$i\hbar \frac{dC_2(t)}{dt} = H_{21}(t)C_1(t) + H_{22}(t)C_2(t),$$

or

$$i\hbar \frac{d}{dt}\begin{pmatrix} C_1(t) \\ C_2(t) \end{pmatrix} = \begin{pmatrix} H_{11}(t) & H_{12}(t) \\ H_{21}(t) & H_{22}(t) \end{pmatrix}\begin{pmatrix} C_1(t) \\ C_2(t) \end{pmatrix}.$$

This equation is a fundamental one for the maser with two energy levels.

6. Example-I

We start with

$$\left|\psi(t)\right\rangle = \exp(-\frac{i}{\hbar}\hat{H}t)\left|\psi(=0)\right\rangle.$$

When $\left|\psi(=0)\right\rangle$ is described by the combination of the eigenkets of $\hat{H}$

$$\left|\psi(=0)\right\rangle = \sum_n c_n\left|\phi_n\right\rangle,$$

then we have

$$\left|\psi(t)\right\rangle = \sum_n \exp(-\frac{i}{\hbar}\hat{H}t)c_n\left|\phi_n\right\rangle = \sum_n \exp(-\frac{i}{\hbar}\varepsilon_n t)c_n\left|\phi_n\right\rangle,$$

where

$$H\left|\phi_n\right\rangle = \varepsilon_n\left|\phi_n\right\rangle.$$

We consider the particle in the one-dimensional box with the potential V=0 for 0<x<a and V= infinity for x<0 and x>a. The initial state is described by

$$\left|\psi(0)\right\rangle = \frac{1}{\sqrt{6}}[\left|\phi_3\right\rangle + 2\left|\phi_2\right\rangle + \left|\phi_1\right\rangle],$$

with

$$\left\langle x\middle|\phi_n\right\rangle = \sqrt{\frac{2}{a}}\sin(\frac{n\pi x}{a}),$$

$$\varepsilon_n = \frac{\hbar^2}{2m}(\frac{\pi}{a})^2 n^2 = E_1 n^2,$$

$$\begin{aligned}\left|\psi(t)\right\rangle &= \exp(-\frac{i}{\hbar}\hat{H}t)\left|\psi(=0)\right\rangle \\ &= \exp(-\frac{i}{\hbar}\hat{H}t)\frac{1}{\sqrt{6}}[\left|\phi_3\right\rangle + 2\left|\phi_2\right\rangle + \left|\phi_1\right\rangle] \\ &= e^{-\frac{i}{\hbar}\varepsilon_3 t}\frac{1}{\sqrt{6}}\left|\phi_3\right\rangle + e^{-\frac{i}{\hbar}\varepsilon_2 t}\frac{2}{\sqrt{6}}\left|\phi_2\right\rangle + e^{-\frac{i}{\hbar}\varepsilon_1 t}\frac{1}{\sqrt{6}}\left|\phi_1\right\rangle]\end{aligned}$$

or

$$\langle x|\psi(t)\rangle = e^{-\frac{i}{\hbar}\varepsilon_3 t}\frac{1}{\sqrt{6}}\langle x|\phi_3\rangle + e^{-\frac{i}{\hbar}\varepsilon_2 t}\frac{1}{\sqrt{6}}\langle x|\phi_2\rangle + e^{-\frac{i}{\hbar}\varepsilon_1 t}\frac{2}{\sqrt{6}}\langle x|\phi_1\rangle,$$

$$P(x,t) = \left|\langle x|\psi(t)\rangle\right|^2.$$

It is interesting to make a plot of $P(x, t)$ as a function of x at various t using Mathematica'

((Mathematica))

Wave function in the One dimensional box ; time dependence of the wav e function

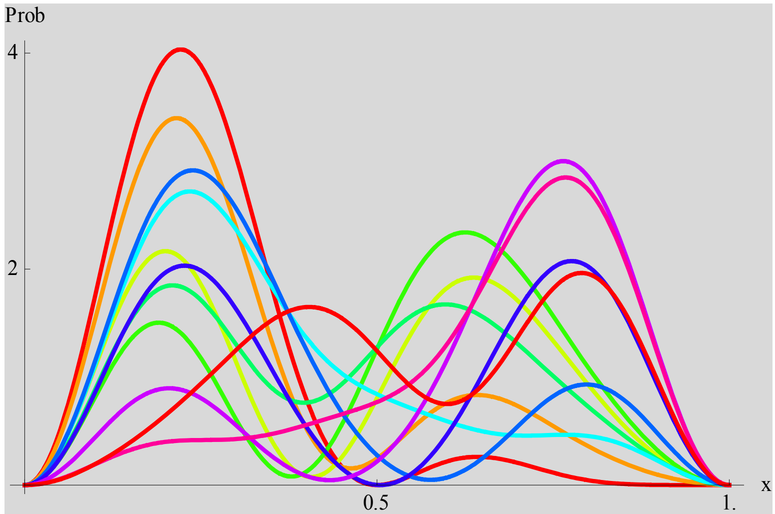
```
ψ[x_, n_] := Sqrt[2/a] Sin[n π x/a];

ε[k_] := ħ^2/(2 m) (k π/a)^2;

Φ = 1/Sqrt[6] (E^(-I ε[3] t/ħ) ψ[x, 3] + 2 E^(-I ε[2] t/ħ) ψ[x, 2] + E^(-I ε[1] t/ħ) ψ[x, 1]);

rule1 = {m → 1, ħ → 1, a → 1}; Φ1 = Φ /. rule1 // Simplify;
Φ2 = Abs[Φ1]^2;

R1 = Plot[Evaluate[Table[Φ2, {t, 0, 5, 0.5}]], {x, 0, 1},
  PlotStyle → Table[{Thick, Hue[0.1 i]}, {i, 0, 10}],
  Background → LightGray, AxesLabel → {"x", "Prob"},
  Ticks → {Range[0, 1, 0.5], Range[0, 4, 2]}]
```

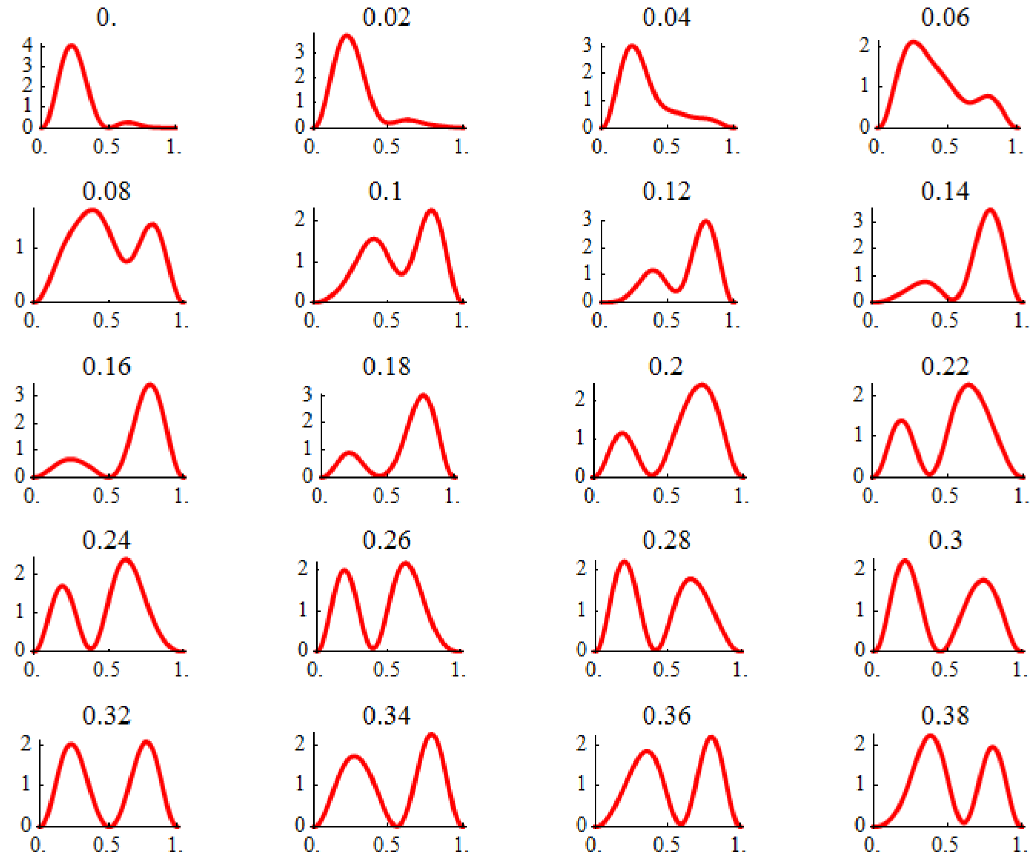


Time dependence of the probability

```
Γ[n_] := Φ2 /. t → n/50 ; x[n_] = n / 50 // N
```

0.02 n

```
G[n_] := Plot[Γ[n], {x, 0, 1}, DisplayFunction → Identity,
  PlotLabel → x[n ], Ticks → {Range[0, 1, 0.5], Range[0, 4, 1]},
  PlotStyle → {Red, Thick}];
pt2 = Evaluate[Table[G[n], {n, 0, 50}]];
Show[GraphicsGrid[Partition[pt2, 4],
  DisplayFunction → $DisplayFunction]]
```


0.
0.02
0.04
0.06
0.08
0.1
0.12
0.14
0.16
0.18
0.2
0.22
0.24
0.26
0.28
0.3
0.32
0.34
0.36
0.38

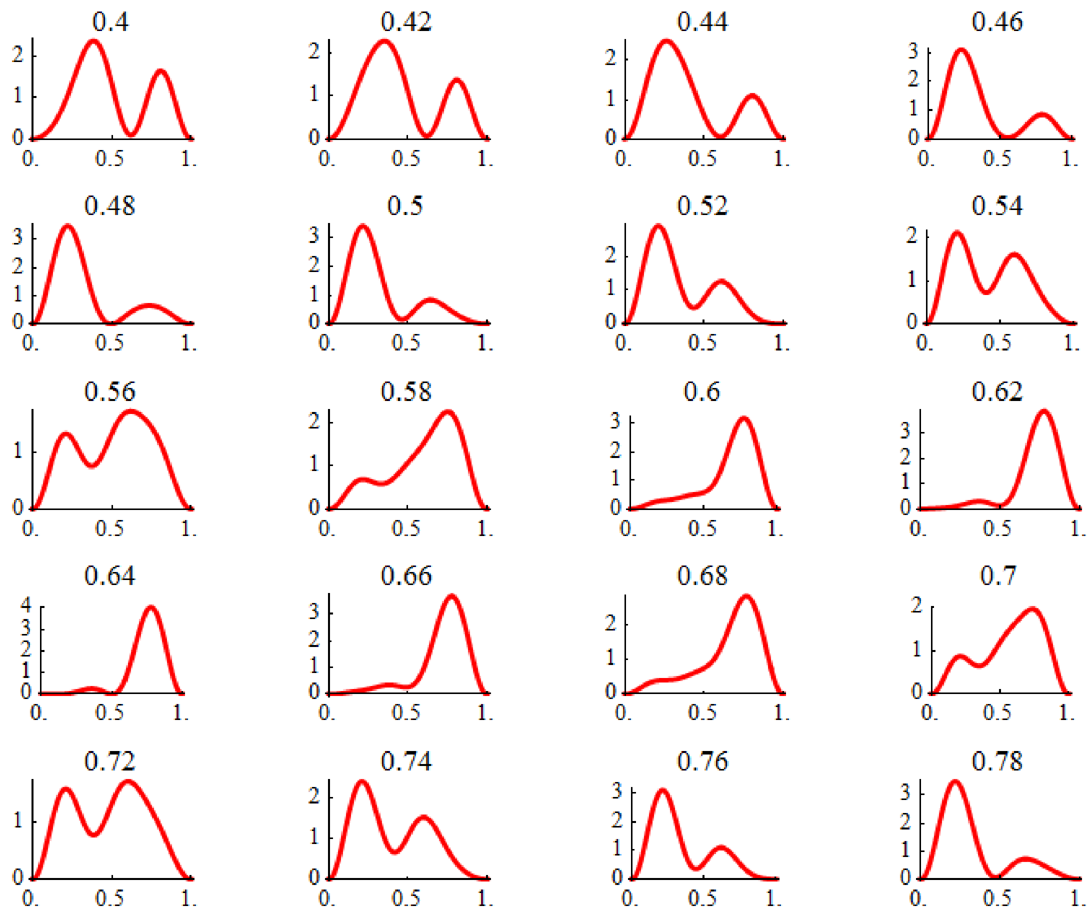


Fig. Time dependence of $P(t)$ as a function of x, at $t = 0 - 0.78$.

7. Example-II

Suppose that the Hamiltonian operator $\hat{H}$ is given by the matrix element of the basis $\{|b_n\rangle\}$. We assume the unitary operator $\hat{U}$ such that

$$|\phi_n\rangle = \hat{U}|b_n\rangle .$$

We consider the eigenvalue problem;

$$\hat{H}|\phi_n\rangle = \varepsilon_n|\phi_n\rangle ,$$

or

$$\hat{H}\hat{U}|b_n\rangle = \varepsilon_n\hat{U}|b_n\rangle ,$$

or

$$\hat{U}^+\hat{H}\hat{U}\left|b_n\right\rangle = \varepsilon_n\left|b_n\right\rangle .$$

Thus the matrix form of $\hat{U}^+\hat{H}\hat{U}$ is given by the diagonal matrix with the diagonal element of the eigenvalues.

$$\hat{U}^+\hat{H}\hat{U} = \begin{pmatrix} \varepsilon_1 & 0 & 0 & 0 \\ 0 & \varepsilon_2 & 0 & 0 \\ 0 & 0 & . & 0 \\ 0 & 0 & 0 & \varepsilon_n \end{pmatrix}.$$

Similary,

$$\hat{U}^+\hat{H}^2\hat{U} = \begin{pmatrix} \varepsilon_1{}^2 & 0 & 0 & 0 \\ 0 & . & 0 & 0 \\ 0 & 0 & . & 0 \\ 0 & 0 & 0 & \varepsilon_n{}^2 \end{pmatrix},$$

$$\hat{U}^+\exp(-\frac{i}{\hbar}\hat{H}t)\hat{U} = \begin{pmatrix} e^{-\frac{i}{\hbar}\varepsilon_1 t} & 0 & 0 & 0 \\ 0 & . & 0 & 0 \\ 0 & 0 & . & 0 \\ 0 & 0 & 0 & e^{-\frac{i}{\hbar}\varepsilon_n t} \end{pmatrix}.$$

Thus we have

$$\exp(-\frac{i}{\hbar}\hat{H}t) = \hat{U}\begin{pmatrix} e^{-\frac{i}{\hbar}\varepsilon_1 t} & 0 & 0 & 0 \\ 0 & . & 0 & 0 \\ 0 & 0 & . & 0 \\ 0 & 0 & 0 & e^{-\frac{i}{\hbar}\varepsilon_n t} \end{pmatrix}\hat{U}^+ .$$

Once one can determine the matrix element of $\exp(-\frac{i}{\hbar}\hat{H}t)$, one can calculate the time dependence of wavefunction $\left|\psi(t)\right\rangle$ in the basis of $\{\left|b_n\right\rangle\}$.

8. Calculation of exponential of matrix

Here we calculate the matrix $\exp(-\frac{i}{\hbar}\hat{H}t)$ (see also the APPENDIX for the derivation detail) with

$$\hat{H} = \begin{pmatrix} 1 & 2 \\ 2 & 1 \end{pmatrix},$$

in the basis of $|1\rangle, |2\rangle$.

Eigensystem[$\hat{H}$].

$$|\psi_1\rangle = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix}, \qquad \text{for the eigenvalue } \lambda = 3$$

$$|\psi_2\rangle = \begin{pmatrix} -\frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix}. \qquad \text{for the eigenvalue } \lambda = -1$$

The unitary operator is

$$\hat{U} = \begin{pmatrix} \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix},$$

$$\hat{U}^{+} = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix},$$

$$\begin{aligned} \hat{U}^{+} \exp(-\frac{i}{\hbar}\hat{H}t)\hat{U} &= \exp(-\frac{i}{\hbar}\hat{U}^{+}\hat{H}\hat{U}t) \\ &= \begin{pmatrix} e^{-\frac{i}{\hbar}3t} & 0 \\ 0 & e^{\frac{i}{\hbar}t} \end{pmatrix} \end{aligned},$$

or

$$\exp(-\frac{i}{\hbar}\hat{H}t) = \hat{U}\begin{pmatrix} e^{-\frac{i}{\hbar}3t} & 0 \\ 0 & e^{\frac{i}{\hbar}t} \end{pmatrix}\hat{U}^{+} = e^{-\frac{i}{\hbar}t}\begin{pmatrix} \cos(\frac{2t}{\hbar}) & -i\sin(\frac{2t}{\hbar}) \\ -i\sin(\frac{2t}{\hbar}) & \cos(\frac{2t}{\hbar}) \end{pmatrix}.$$

Note that using the Mathematica, one can directly calculate the exponential of the matrix, even if the matrix is a diagonal one. We need to use

MatrixExp[A],

where *A* is an arbitrary matrix.

((**Mathematica**))

```
Clear["Global`*"]; exp_* := exp /. {Complex[re_, im_] :→ Complex[re, -im]};

H = {{1, 2}, {2, 1}}; eq1 = Eigensystem[H]
{{3, -1}, {{1, 1}, {-1, 1}}}

ψ1 = Normalize[eq1[[2, 1]]]; ψ2 = Normalize[eq1[[2, 2]]]; a1 = eq1[[1, 1]];
a2 = eq1[[1, 2]];

ψ1*.ψ2
0

UT = {ψ1, ψ2}
```

$\left\{\left\{\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}\right\}, \left\{-\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}\right\}\right\}$

```
U = Transpose[UT]; UH = UT*; H1 = UH.H.U // Simplify

{{3, 0}, {0, -1}}
```

$\text{K1} = \left\{\left\{\text{Exp}\left[-\frac{i}{\hbar}\, t\, \text{a1}\right], 0\right\}, \left\{0, \text{Exp}\left[-\frac{i}{\hbar}\, t\, \text{a2}\right]\right\}\right\}$ `// Simplify`

$\left\{\left\{e^{-\frac{3 i t}{\hbar}}, 0\right\}, \left\{0, e^{\frac{i t}{\hbar}}\right\}\right\}$

```
p1 = U.K1.UH // Expand
```

$\left\{\left\{\frac{1}{2} e^{\frac{i t}{\hbar}} + \frac{1}{2} e^{-\frac{3 i t}{\hbar}}, -\frac{1}{2} e^{\frac{i t}{\hbar}} + \frac{1}{2} e^{-\frac{3 i t}{\hbar}}\right\}, \left\{-\frac{1}{2} e^{\frac{i t}{\hbar}} + \frac{1}{2} e^{-\frac{3 i t}{\hbar}}, \frac{1}{2} e^{\frac{i t}{\hbar}} + \frac{1}{2} e^{-\frac{3 i t}{\hbar}}\right\}\right\}$

Direct calculation for comparison

$\text{p2} = \text{MatrixExp}\left[-\frac{i}{\hbar}\, t\, H\right]$ `// FullSimplify`

$\left\{\left\{e^{-\frac{i t}{\hbar}} \text{Cos}\left[\frac{2 t}{\hbar}\right], -i\, e^{-\frac{i t}{\hbar}} \text{Sin}\left[\frac{2 t}{\hbar}\right]\right\}, \left\{-i\, e^{-\frac{i t}{\hbar}} \text{Sin}\left[\frac{2 t}{\hbar}\right], e^{-\frac{i t}{\hbar}} \text{Cos}\left[\frac{2 t}{\hbar}\right]\right\}\right\}$

```
p1 - p2 // Simplify
{{0, 0}, {0, 0}}
```

9. Spin precession

We consider the motion of spin *S* (=1/2) in the presence of an external magnetic field *B* along the *z* axis. The magnetic moment of spin is given by

$$\hat{\mu}_z = -\frac{2\mu_B \hat{S}_z}{\hbar} = -\mu_B \hat{\sigma}_z .$$

Then the spin Hamiltonian (Zeeman energy) is described by

$$\hat{H} = -\hat{\mu}_z B = -(-\frac{2\mu_B \hat{S}_z}{\hbar})B = \mu_B \hat{\sigma}_z B.$$

Since the Bohr magneton μ_B is given by $\mu_B = \frac{e\hbar}{2mc}$,

$$\mu_B B = \frac{eB\hbar}{2mc} = \frac{\hbar}{2}\frac{eB}{mc} = \frac{\hbar}{2}\omega_0 \qquad (e>0).$$

or

$$\omega_0 = \frac{eB}{mc}, \qquad \text{(angular frequency of the Larmor precession)}$$

Thus the Hamiltonian can be rewritten as

$$\hat{H} = \frac{\hbar}{2}\omega_0 \hat{\sigma}_z.$$

Thus the Schrödinger equation is obtained as

$$|\psi(t)\rangle = \exp[-\frac{i}{\hbar}\hat{H}t]|\psi(t=0)\rangle = \exp[-\frac{i}{2}\omega_0\hat{\sigma}_z t]|\psi(t=0)\rangle.$$

Note that the time evolution operator coincides with the rotation operator

$$\hat{R}_z(\omega_0 t) = \exp[-\frac{i}{2}\omega_0 \hat{\sigma}_z t].$$

((**Note**)) Classical physics

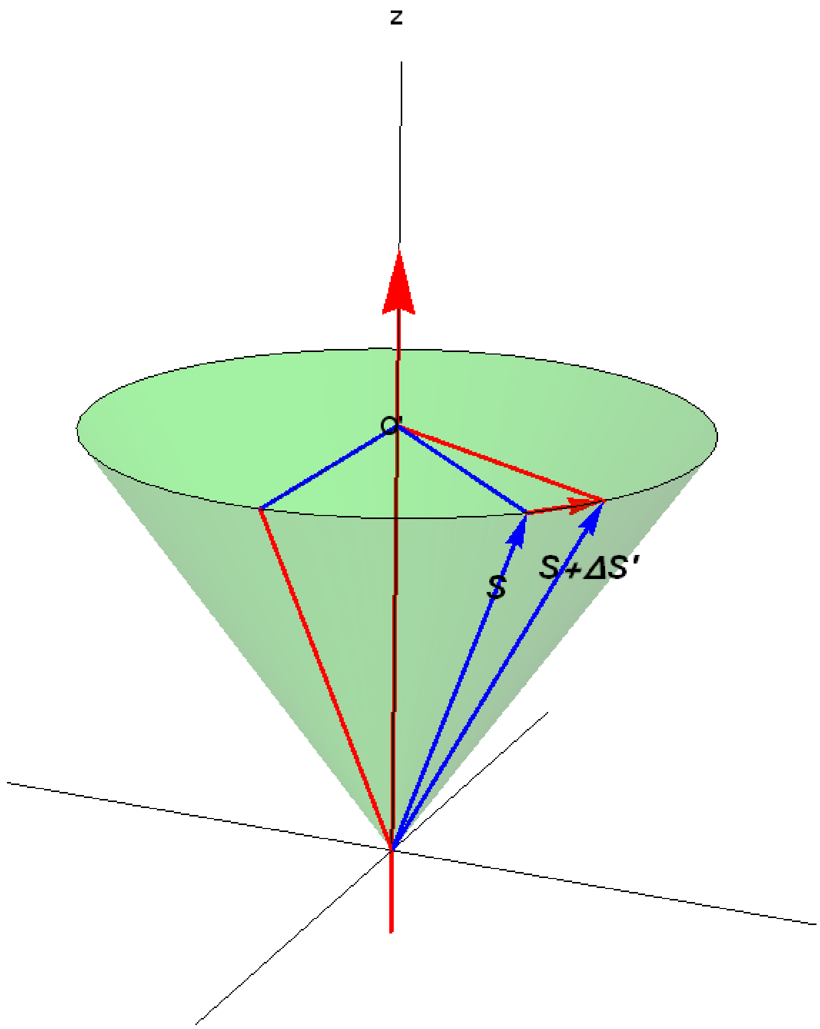


Fig. Precession motion of spin around the *z* axis, where the magnetic field ***B*** is applied along the *z* axis.

The torque is exerted on the magnetic moment $\boldsymbol{\mu} = -\frac{2\mu_B \boldsymbol{S}}{\hbar}$, in the form

$$\boldsymbol{\tau} = \boldsymbol{\mu} \times \boldsymbol{B} = (-\frac{2\mu_B \boldsymbol{S}}{\hbar}) \times \boldsymbol{B} .$$

So the spin vector ***S*** rotates around the *z* axis in counter-clock wise.

We assume that

$$\left|\psi(t=0)\right\rangle = \left|+\boldsymbol{n}\right\rangle = \exp[-\frac{i}{2}\hat{\sigma}_z\phi]\exp[-\frac{i}{2}\hat{\sigma}_y\theta]\left|+z\right\rangle = \begin{pmatrix} e^{-\frac{i\phi}{2}}\cos(\frac{\theta}{2}) \\ e^{\frac{i\phi}{2}}\sin(\frac{\theta}{2}) \end{pmatrix},$$

$$\hat{R}_z(\omega_0 t) = \exp[-\frac{i}{2}\omega_0\hat{\sigma}_z t],$$

The average

$$\left\langle S_x\right\rangle_t = \left\langle\psi(t)\right|\hat{S}_x\left|\psi(t)\right\rangle = \frac{\hbar}{2}\left\langle+\boldsymbol{n}\right|\exp[\frac{i}{2}\omega_0\hat{\sigma}_z t]\sigma_x\exp[-\frac{i}{2}\omega_0\hat{\sigma}_z t]\left|+\boldsymbol{n}\right\rangle,$$

$$\left\langle S_y\right\rangle_t = \left\langle\psi(t)\right|\hat{S}_y\left|\psi(t)\right\rangle = \frac{\hbar}{2}\left\langle+\boldsymbol{n}\right|\exp[\frac{i}{2}\omega_0\hat{\sigma}_z t]\sigma_y\exp[-\frac{i}{2}\omega_0\hat{\sigma}_z t]\left|+\boldsymbol{n}\right\rangle,$$

$$\left\langle S_z\right\rangle_t = \left\langle\psi(t)\right|\hat{S}_z\left|\psi(t)\right\rangle = \frac{\hbar}{2}\left\langle+\boldsymbol{n}\right|\exp[\frac{i}{2}\omega_0\hat{\sigma}_z t]\sigma_z\exp[-\frac{i}{2}\omega_0\hat{\sigma}_z t]\left|+\boldsymbol{n}\right\rangle.$$

Here we have

$$\exp[\frac{i}{2}\omega_0\hat{\sigma}_z t]\sigma_x\exp[-\frac{i}{2}\omega_0\hat{\sigma}_z t] = \begin{pmatrix} e^{\frac{it\omega_0}{2}} & 0 \\ 0 & e^{-\frac{it\omega_0}{2}} \end{pmatrix}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} e^{-\frac{it\omega_0}{2}} & 0 \\ 0 & e^{\frac{it\omega_0}{2}} \end{pmatrix} = \begin{pmatrix} 0 & e^{it\omega_0} \\ e^{-it\omega_0} & 0 \end{pmatrix}$$

$$\exp[\frac{i}{2}\omega_0\hat{\sigma}_z t]\sigma_y\exp[-\frac{i}{2}\omega_0\hat{\sigma}_z t] = \begin{pmatrix} e^{\frac{it\omega_0}{2}} & 0 \\ 0 & e^{-\frac{it\omega_0}{2}} \end{pmatrix}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}\begin{pmatrix} e^{-\frac{it\omega_0}{2}} & 0 \\ 0 & e^{\frac{it\omega_0}{2}} \end{pmatrix} = \begin{pmatrix} 0 & -ie^{it\omega_0} \\ ie^{-it\omega_0} & 0 \end{pmatrix}$$

$$\exp[\frac{i}{2}\omega_0\hat{\sigma}_z t]\sigma_z\exp[-\frac{i}{2}\omega_0\hat{\sigma}_z t] = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},$$

Thus we have

$$\langle S_x \rangle_t = \frac{\hbar}{2}\sin\theta\cos(\omega_0 t+\phi)$$
$$= \frac{\hbar}{2}\sin\theta[\cos(\omega_0 t)\cos\phi - \sin(\omega_0 t)\sin\phi]$$

$$\langle S_y \rangle_t = \frac{\hbar}{2}\sin\theta[\sin(\omega_0 t+\phi)$$
$$= \frac{\hbar}{2}\sin\theta[\sin(\omega_0 t)\cos\phi + \cos(\omega_0 t)\sin\phi]$$

$$\langle S_z \rangle_t = \frac{\hbar}{2}\cos\theta .$$

At $t = 0$,

$$\langle S_x \rangle_0 = \frac{\hbar}{2}\sin\theta\cos\phi ,$$

$$\langle S_y \rangle_0 = \frac{\hbar}{2}\sin\theta\sin\phi ,$$

$$\langle S_z \rangle_0 = \frac{\hbar}{2}\cos\theta .$$

Using this we have

$$\langle S_x \rangle_t = \langle S_x \rangle_0 \cos(\omega_0 t) - \langle S_y \rangle_0 \sin(\omega_0 t) ,$$

$$\langle S_y \rangle_t = \langle S_x \rangle_0 \sin(\omega_0 t) + \langle S_y \rangle_0 \cos(\omega_0 t) ,$$

$$\langle S_z \rangle_t = \langle S_z \rangle_0 = \frac{\hbar}{2}\cos\theta .$$

Note that

$$\langle S_x \rangle_t + i\langle S_y \rangle_t = e^{i\omega_0 t}(\langle S_x \rangle_0 + i\langle S_y \rangle_0) ,$$

$$\begin{aligned}\langle S_x \rangle_t &= \langle \psi(t)|\hat{S}_x|\psi(t)\rangle = \frac{\hbar}{2}\langle +\boldsymbol{n}|\exp[\frac{i}{2}\omega_0\hat{\sigma}_z t]\hat{\sigma}_x \exp[-\frac{i}{2}\omega_0\hat{\sigma}_z t]|+\boldsymbol{n}\rangle \\ &= \frac{\hbar}{2}\langle +\boldsymbol{n}|\hat{\sigma}_x\cos(\omega_0 t) - \hat{\sigma}_y\sin(\omega_0 t)|+\boldsymbol{n}\rangle\end{aligned},$$

where

$$\langle S_x \rangle_0 = \frac{\hbar}{2}\langle +\boldsymbol{n}|\hat{\sigma}_x|+\boldsymbol{n}\rangle .$$

We also get

$$\begin{aligned}\langle S_y \rangle_t &= \langle \psi(t)|\hat{S}_y|\psi(t)\rangle = \frac{\hbar}{2}\langle +\boldsymbol{n}|\exp[\frac{i}{2}\omega_0\hat{\sigma}_z t]\hat{\sigma}_y \exp[-\frac{i}{2}\omega_0\hat{\sigma}_z t]|+\boldsymbol{n}\rangle \\ &= \frac{\hbar}{2}\langle +\boldsymbol{n}|\hat{\sigma}_x \sin(\omega_0 t) + \hat{\sigma}_y \cos(\omega_0 t)|+\boldsymbol{n}\rangle\end{aligned}$$

by using the Baker-Hausdorf lemma,

$$\langle S_y \rangle_0 = \frac{\hbar}{2}\langle +\boldsymbol{n}|\hat{\sigma}_y|+\boldsymbol{n}\rangle ,$$

and

$$\begin{aligned}\langle S_z \rangle_t &= \langle \psi(t)|\hat{S}_z|\psi(t)\rangle \\ &= \frac{\hbar}{2}\langle +\boldsymbol{n}|\exp[\frac{i}{2}\omega_0\hat{\sigma}_z t]\hat{\sigma}_z \exp[-\frac{i}{2}\omega_0\hat{\sigma}_z t]|+\boldsymbol{n}\rangle \\ &= \frac{\hbar}{2}\langle +\boldsymbol{n}|\hat{\sigma}_z|+\boldsymbol{n}\rangle = \langle S_z \rangle_0\end{aligned}$$

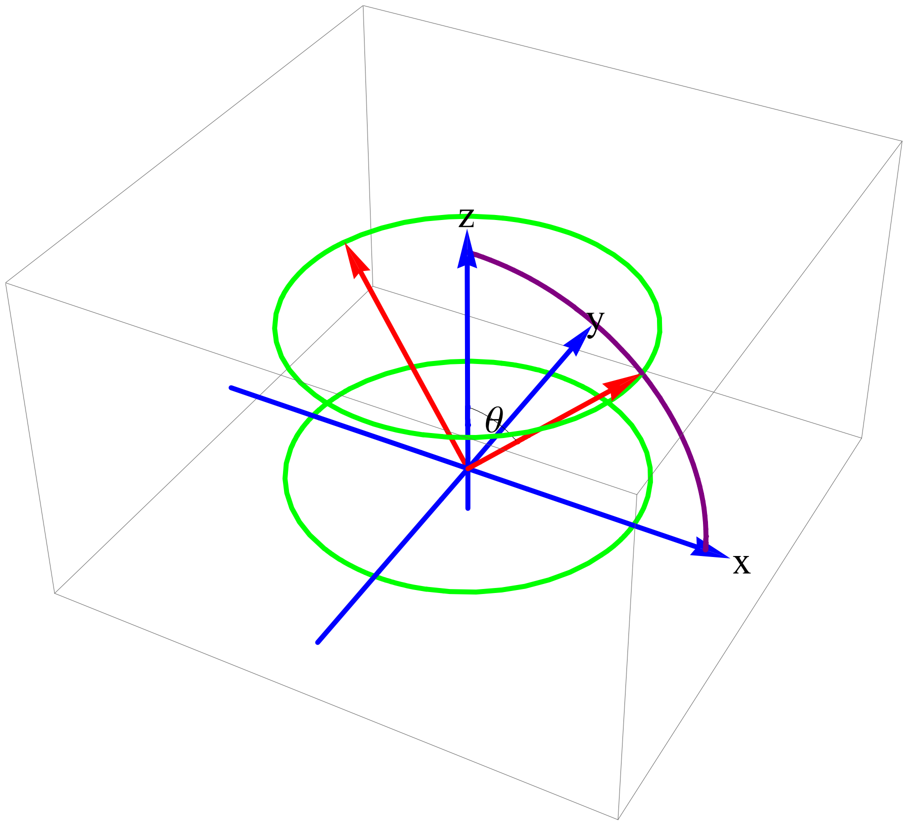
Then

$$\langle S_x \rangle_t = \langle S_x \rangle_0 \cos(\omega_0 t) - \langle S_y \rangle_0 \sin(\omega_0 t) ,$$

$$\langle S_y \rangle_t = \langle S_x \rangle_0 \sin(\omega_0 t) + \langle S_y \rangle_0 \cos(\omega_0 t) ,$$

and

$$\langle S_z \rangle_t = \langle S_z \rangle_0 .$$



10 Baker- Hausdorff lemma

Baker-Campbell-Hausdorff Theorem

Henry Frederick Baker,
John Edward Campbell,
Felix Hausdorff.

(We will discuss this theorem in the topics of coherent state and squeezed state later).

In the commutation relations, $[\hat{J}_z, \hat{J}_x] = i\hbar \hat{J}_y$, we put $\hat{J}_z = \frac{\hbar}{2}\hat{\sigma}_z$ and $\hat{J}_x = \frac{\hbar}{2}\hat{\sigma}_x$

Then we have

$$[\frac{\hbar}{2}\hat{\sigma}_z, \frac{\hbar}{2}\hat{\sigma}_x] = i\hbar\frac{\hbar}{2}\hat{\sigma}_y \qquad \text{or} \qquad [\hat{\sigma}_z, \hat{\sigma}_x] = 2i\hat{\sigma}_y .$$

Similarly, we have

$$[\hat{\sigma}_x, \hat{\sigma}_y] = 2i\hat{\sigma}_z , \qquad [\hat{\sigma}_y, \hat{\sigma}_z] = 2i\hat{\sigma}_x .$$

We notice the following relations which can be derived from the Baker-Hausdorf lemma:

$$\exp(\hat{A}x)\hat{B}\exp(-\hat{A}x) = \hat{B} + \frac{x}{1!}[\hat{A},\hat{B}] + \frac{x^2}{2!}[\hat{A},[\hat{A},\hat{B}]] + \frac{x^3}{3!}[\hat{A},[\hat{A},[\hat{A},\hat{B}]]] + ...$$

$$\exp[i\frac{\theta}{2}\hat{\sigma}_z]\hat{\sigma}_x\exp[-i\frac{\theta}{2}\hat{\sigma}_z] = \hat{\sigma}_x\cos\theta - \hat{\sigma}_y\sin\theta\,,$$

$$\exp[i\frac{\theta}{2}\hat{\sigma}_z]\hat{\sigma}_y\exp[-i\frac{\theta}{2}\hat{\sigma}_z] = \hat{\sigma}_x\sin\theta + \hat{\sigma}_y\cos\theta.$$

((**Proof**))

We note that

$$x = \frac{i\theta}{2}, \qquad \hat{A} = \hat{\sigma}_z, \qquad \text{and} \qquad \hat{B} = \hat{\sigma}_x\,.$$

$$[\hat{A},\hat{B}] = [\hat{\sigma}_z,\hat{\sigma}_x] = 2i\hat{\sigma}_y$$

Then we have

$$\begin{aligned} I &= \exp[x\hat{\sigma}_z]\hat{\sigma}_x\exp[-x\hat{\sigma}_z] \\ &= \hat{\sigma}_x + \frac{x}{1!}[\hat{\sigma}_z,\hat{\sigma}_x] + \frac{x^2}{2!}[\hat{\sigma}_z,[\hat{\sigma}_z,\hat{\sigma}_x]] + \frac{x^3}{3!}[\hat{\sigma}_z,[\hat{\sigma}_z,[\hat{\sigma}_z,\hat{\sigma}_x]]] \\ &\qquad + \frac{x^4}{4!}[\hat{\sigma}_z,[\hat{\sigma}_z,[\hat{\sigma}_z,[\hat{\sigma}_z,\hat{\sigma}_x]]]] + ... \end{aligned}$$

$$\begin{aligned} I &= \hat{\sigma}_x + \frac{1}{1!}\frac{i\theta}{2}2i\hat{\sigma}_y + \frac{1}{2!}\left(\frac{i\theta}{2}\right)^2[\hat{\sigma}_z,2i\hat{\sigma}_y] + \frac{1}{3!}\left(\frac{i\theta}{2}\right)^3[\hat{\sigma}_z,[\hat{\sigma}_z,2i\hat{\sigma}_y]] \\ &\quad + \frac{1}{4!}\left(\frac{i\theta}{2}\right)^4[\hat{\sigma}_z,[\hat{\sigma}_z,[\hat{\sigma}_z,2i\hat{\sigma}_y]]] + . \end{aligned}$$

or

$$I = \hat{\sigma}_x - \theta\hat{\sigma}_y + i\frac{\theta^2}{2^2}[\hat{\sigma}_y, \hat{\sigma}_z] - \frac{i}{3!}\frac{\theta^3}{2^3}(-2i)[\hat{\sigma}_z, [\hat{\sigma}_y, \hat{\sigma}_z]]$$
$$+ \frac{1}{4!}\frac{\theta^4}{2^4}(-2i)[\hat{\sigma}_z, [\hat{\sigma}_z, [\hat{\sigma}_y, \hat{\sigma}_z]]].....$$
$$= \hat{\sigma}_x - \theta\hat{\sigma}_y + i\frac{\theta^2}{2^2}2i\hat{\sigma}_x - \frac{i}{3!}\frac{\theta^3}{2^3}(-2i)(2i)[\hat{\sigma}_z, \hat{\sigma}_x]$$
$$+ \frac{1}{4!}\frac{\theta^4}{2^4}(-2i)(2i)[\hat{\sigma}_z, [\hat{\sigma}_z, \hat{\sigma}_x]] + ...$$

or

$$I = \hat{\sigma}_x - \theta\hat{\sigma}_y - \frac{\theta^2}{2}\hat{\sigma}_x - \frac{i}{3!}\frac{\theta^3}{2^3}(-2i)(2i)^2\hat{\sigma}_y + \frac{1}{4!}\frac{\theta^4}{2^4}(-2i)(2i)(2i)(-2i)\hat{\sigma}_x + ...$$
$$= \hat{\sigma}_x - \theta\hat{\sigma}_y - \frac{\theta^2}{2}\hat{\sigma}_x + \frac{\theta^3}{3!}\hat{\sigma}_y + \frac{\theta^4}{4!}\hat{\sigma}_x + ...$$
$$= \hat{\sigma}_x(1 - \frac{\theta^2}{2} + \frac{\theta^4}{4!}...) - \hat{\sigma}_y(1 - \frac{\theta^3}{3!} + ...)$$
$$= \hat{\sigma}_x \cos\theta - \hat{\sigma}_y \cos\theta$$

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11 Schrödinger picture

The Schrödinger equation

$$|\psi(t)\rangle = |\psi_s(t)\rangle,$$

$$|\psi_s(t)\rangle = \hat{U}(t, t_0)|\psi_s(t_0)\rangle,$$

where $\hat{U}(t, t_0)$ is the time evolution operator;

$$\hat{U}^{+}(t, t_0) = \hat{U}^{-1}(t, t_0).$$

In the Schrodinger picture, the average of the operator $\hat{A}_s$ in the state $|\psi_s(t)\rangle$ is defined by

$$\langle\psi_s(t)|\hat{A}_s|\psi_s(t)\rangle.$$

12 Heisenberg picture

The state vector, which is constant, is equal to

$$|\psi_H(t)\rangle = |\psi_s(t_0)\rangle.$$

From the definition

$$\langle \psi_H | \hat{A}_H(t) | \psi_H \rangle = \langle \psi_s | \hat{A}_s(t) | \psi_s \rangle ,$$

or

$$\hat{A}_H(t) = \hat{U}^+(t,t_0)\hat{A}_s(t)\hat{U}(t,t_0).$$

In general, $\hat{A}_H(t)$ depends on time, even if $\hat{A}_s(t)$ does not.

13 Heisenberg's equation of motion

The Schrödinger equation can be described in the Schrödinger picture

$$i\hbar \frac{\partial}{\partial t} |\psi_s(t)\rangle = \hat{H}_s(t) |\psi_s(t)\rangle ,$$

or

$$i\hbar \frac{d}{dt} \hat{U}(t,t_0) |\psi_s(t_0)\rangle = \hat{H}_s(t)\hat{U}(t,t_0) |\psi_s(t_0)\rangle ,$$

or

$$i\hbar \frac{d}{dt} \hat{U}(t,t_0) = \hat{H}_s(t)\hat{U}(t,t_0) ,$$

or

$$\frac{d}{dt} \hat{U}(t,t_0) = -\frac{i}{\hbar} \hat{H}_s(t)\hat{U}(t,t_0) ,$$

and

$$\frac{d}{dt} \hat{U}^+(t,t_0) = \frac{i}{\hbar} \hat{U}^+(t,t_0)\hat{H}_s(t) ,$$

where $\hat{H}_s^+(t) = \hat{H}_s(t)$. Therefore

$$\begin{aligned}\frac{d\hat{A}_H(t)}{dt} &= \frac{d\hat{U}^+(t,t_0)}{dt}\hat{A}_s(t)\hat{U}(t,t_0) + \hat{U}^+(t,t_0)\hat{A}_s(t)\frac{d\hat{U}(t,t_0)}{dt} + \hat{U}^+(t,t_0)\frac{d\hat{A}_s(t)}{dt}\hat{U}(t,t_0)\\ &= \frac{i}{\hbar}\hat{U}^+(t,t_0)\hat{H}_s(t)\hat{A}_s(t)\hat{U}(t,t_0) - \hat{U}^+(t,t_0)\hat{A}_s(t)\frac{i}{\hbar}\hat{H}_s(t)\hat{U}(t,t_0) + \hat{U}^+(t,t_0)\frac{d\hat{A}_s(t)}{dt}\hat{U}(t,t_0)\\ &= \frac{i}{\hbar}\hat{U}^+(t,t_0)[\hat{H}_s(t),\hat{A}_s(t)]\hat{U}(t,t_0) + \hat{U}^+(t,t_0)\frac{d\hat{A}_s(t)}{dt}\hat{U}(t,t_0)\\ &= \frac{i}{\hbar}[\hat{H}_H(t),\hat{A}_H(t)] + (\frac{d\hat{A}_s(t)}{dt})_H\end{aligned}$$

where

$$\hat{H}_H(t) = \hat{U}^+(t,t_0)\hat{H}_s(t)\hat{U}(t,t_0).$$

Finally we obtain the Heisenberg's equation of motion

$$i\hbar\frac{d}{dt}\hat{A}_H(t) = [\hat{A}_H(t),\hat{H}_H(t)] + i\hbar(\frac{d\hat{A}_s(t)}{dt})_H$$

14 Simple example for the Heisenberg picture

$$\hat{H}_s(t) = \hat{H}, \qquad \hat{A}_s(t) = \hat{A},$$

$t_0 = 0$

$$\hat{U} = e^{-\frac{i}{\hbar}\hat{H}t},$$

$$\hat{A}_H = \hat{U}^+\hat{A}_s\hat{U} = e^{\frac{i}{\hbar}\hat{H}t}\hat{A}_s e^{-\frac{i}{\hbar}\hat{H}t},$$

$$\hat{H}_H = \hat{H}_s.$$

Then we have the Heisenberg's equation of motion:

$$i\hbar\frac{d}{dt}\hat{A}_H = [\hat{A}_H,\hat{H}_H].$$

We get an analogy between the classical equations of motion in the Hamiltonian form and the quantum equations of motion in the Heisenberg's form. $\hat{A}_H$ is called a constant of the motion, when $[\hat{A}_H,\hat{H}_H]$=0 at all times.

$$[\hat{A}_H, \hat{H}_H] = \hat{U}^+ \hat{A}_S \hat{U} \hat{U}^+ \hat{H}_S \hat{U} - \hat{U}^+ \hat{H}_S \hat{U} \hat{U}^+ \hat{A}_S \hat{U}$$
$$= \hat{U}^+ [\hat{A}_S, \hat{H}_S] \hat{U}$$

Therefore $[\hat{A}_H, \hat{H}_H]$ means $[\hat{A}_S, \hat{H}_S] = 0$

15. Ehrenfest's theorem: Schrodinger picture

Paul Ehrenfest (January 18, 1880 – September 25, 1933) was an Austrian and Dutch physicist and mathematician, who made major contributions to the field of statistical mechanics and its relations with quantum mechanics, including the theory of phase transition and the Ehrenfest theorem.

http://en.wikipedia.org/wiki/Paul_Ehrenfest

Schrödinger equation:

$$i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle = \hat{H} |\psi(t)\rangle \qquad \text{or} \qquad \frac{\partial}{\partial t} |\psi(t)\rangle = -\frac{i}{\hbar} \hat{H} |\psi(t)\rangle .$$

Taking the Hermitian conjugate of both sides,

$$-i\hbar \frac{\partial}{\partial t} \langle\psi(t)| = \langle\psi(t)| \hat{H}^+ = \langle\psi(t)| \hat{H} ,$$

or

$$\frac{\partial}{\partial t} \langle\psi(t)| = \frac{i}{\hbar} \langle\psi(t)| \hat{H}^+ = \frac{i}{\hbar} \langle\psi(t)| \hat{H} .$$

We now consider the time dependence of the average defined by $\langle\psi(t)|\hat{A}|\psi(t)\rangle$

$$\frac{d}{dt}\langle\psi(t)|\hat{A}(t)|\psi(t)\rangle = (\frac{\partial}{\partial t}\langle\psi(t)|)\hat{A}|\psi(t)\rangle + \langle\psi(t)|\frac{\partial\hat{A}}{\partial t}|\psi(t)\rangle + \langle\psi(t)|\hat{A}(\frac{\partial}{\partial t}|\psi(t)\rangle)$$

$$= \frac{i}{\hbar}\langle\psi(t)|\hat{H}\hat{A}|\psi(t)\rangle + \langle\psi(t)|\frac{\partial\hat{A}}{\partial t}|\psi(t)\rangle + \langle\psi(t)|\hat{A}(-\frac{i}{\hbar})|\psi(t)\rangle$$

$$= -\frac{i}{\hbar}\langle\psi(t)|[\hat{A},\hat{H}]|\psi(t)\rangle + \langle\psi(t)|\frac{\partial\hat{A}}{\partial t}|\psi(t)\rangle$$

or

$$\frac{d}{dt}\langle\psi(t)|\hat{A}|\psi(t)\rangle = -\frac{i}{\hbar}\langle\psi(t)|[\hat{A},\hat{H}]|\psi(t)\rangle + \langle\psi(t)|\frac{\partial\hat{A}}{\partial t}|\psi(t)\rangle.$$

When $\frac{\partial\hat{A}}{\partial t} = 0$, we have

$$\frac{d}{dt}\langle\psi(t)|\hat{A}|\psi(t)\rangle = -\frac{i}{\hbar}\langle\psi(t)|[\hat{A},\hat{H}]|\psi(t)\rangle,$$

where

$$[\hat{A},\hat{H}] = \hat{A}\hat{H} - \hat{H}\hat{A}.$$

When $[\hat{A},\hat{H}] = 0$, we get

$$\langle\psi(t)|\hat{A}|\psi(t)\rangle = const.$$

16. Heisenberg's principle of uncertainty

((Messiah, Quantum mechanics, Townsend problem (4-15) first edition of Quantum Mechanics))

Consider any observable $\hat{A}$ associated with the state of the system in quantum mechanics. Show that there is an uncertainty relation of the form

$$(\Delta E)\frac{(\Delta A)}{|\frac{d}{dt}\langle A\rangle|} \geq \frac{\hbar}{2},$$

provided the operator $\hat{A}$ does not depend on explicitly on time. The quantity $(\Delta A)/|\frac{d}{dt}\langle A\rangle|$ is a time we may call *Δt*. What is the physical significance of *Δt*.?

((**Solution**))
We recall that

$$[\hat{A},\hat{B}] = i\hat{C}\ ,$$

implies that

$$(\Delta A)(\Delta B) \geq \frac{|\langle C\rangle|}{2}.$$

We start with the commutator $[\hat{A},\hat{H}]$; then

$$(\Delta A)(\Delta E) \geq \frac{1}{2}|\langle[\hat{A},\hat{H}]\rangle|.$$

But since

$$\frac{d}{dt}\langle\hat{A}\rangle = \frac{i}{\hbar}\langle[\hat{A},\hat{H}]\rangle,$$

then we get

$$(\Delta A)(\Delta E) \geq \frac{\hbar}{2}|\frac{d}{dt}\langle A\rangle|,$$

or

$$(\Delta E)\frac{(\Delta A)}{|\frac{d}{dt}\langle A\rangle|} \geq \frac{\hbar}{2}.$$

If we define

$$\Delta t = \frac{(\Delta A)}{|\frac{d}{dt}\langle A\rangle|},$$

then

$$\Delta E\Delta t \geq \frac{\hbar}{2}.$$

For example, for position, if *Δx* = 1 cm and $\frac{d}{dt}\langle x\rangle = 0.1 cm/s$. then we have

$$\frac{\Delta x}{\frac{d\langle x\rangle}{dt}} = 10 \text{ s},$$

which is the time necessary for $\langle x\rangle$ to shift by an amount *Δx*.

17. Example for the Ehrenfest theorem

We consider a particle in a stationary potential.

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{x}).$$

So that we can write

$$\begin{aligned}
\frac{d}{dt}\langle\psi(t)|\hat{x}|\psi(t)\rangle &= -\frac{i}{\hbar}\langle\psi(t)|[\hat{x},\hat{H}]|\psi(t)\rangle \\
&= -\frac{i}{\hbar}\langle\psi(t)|[\hat{x},\frac{\hat{p}^2}{2m}]|\psi(t)\rangle \\
&= -\frac{i}{\hbar}i\hbar\langle\psi(t)|\frac{\hat{p}}{m}]|\psi(t)\rangle
\end{aligned}$$

or

$$\frac{d}{dt}\langle\psi(t)|\hat{x}|\psi(t)\rangle = \langle\psi(t)|\frac{\hat{p}}{m}]|\psi(t)\rangle,$$

or

$$\frac{d}{dt}\langle x\rangle = \frac{1}{m}\langle p\rangle.$$

Similarly

$$\begin{aligned}
\frac{d}{dt}\langle\psi(t)|\hat{p}|\psi(t)\rangle &= -\frac{i}{\hbar}\langle\psi(t)|[\hat{p},\hat{H}]|\psi(t)\rangle \\
&= -\frac{i}{\hbar}\langle\psi(t)|[\hat{p},V(\hat{x})]|\psi(t)\rangle \\
&= -\frac{i}{\hbar}\frac{\hbar}{i}\langle\psi(t)|\frac{\partial}{\partial\hat{x}}V(\hat{x})]|\psi(t)\rangle
\end{aligned}$$

or

$$\frac{d}{dt}\langle\psi(t)|\hat{p}|\psi(t)\rangle = -\langle\psi(t)|\frac{\partial}{\partial\hat{x}}V(\hat{x})]|\psi(t)\rangle,$$

or

$$\frac{d}{dt}\langle p\rangle = -\left\langle\frac{dV}{dx}\right\rangle,$$

The equations

$$\frac{d}{dt}\langle x\rangle = \frac{1}{m}\langle p\rangle,$$

and

$$\frac{d}{dt}\langle p\rangle = -\left\langle\frac{dV}{dx}\right\rangle$$

express the Ehrenfest's theorem. These forms recall that of classical Hamiltonian-Jacobi equations for a particle.

18 The same example in the Heisenberg picture

$$H_S = \frac{1}{2m}\hat{p}_S{}^2 + V(\hat{x}_S), \qquad \text{(Schrödinger picture)}$$

$$H_H = \frac{1}{2m}\hat{p}_H{}^2 + V(\hat{x}_H), \qquad \text{(Heisenberg's picture)}$$

$$\begin{aligned}[\hat{x}_H, \hat{p}_H] &= \hat{x}_H\hat{p}_H - \hat{p}_H\hat{x}_H \\ &= \hat{U}^+\hat{x}\hat{U}\hat{U}^+\hat{p}\hat{U} - \hat{U}^+\hat{p}\hat{U}\hat{U}^+\hat{x}\hat{U} \\ &= \hat{U}^+[\hat{x},\hat{p}]\hat{U} = i\hbar\hat{U}^+\hat{U} = i\hbar\hat{1}\end{aligned}$$

$$\begin{aligned}[\hat{x}_H, \hat{p}_H{}^2] &= \hat{U}^+[\hat{x},\hat{p}^2]\hat{U} \\ &= 2i\hbar\hat{U}^+\hat{p}\hat{U} \\ &= 2i\hbar\hat{p}_H\end{aligned}$$

Heisenberg's equation for the free particles,

$$i\hbar\frac{d}{dt}\hat{x}_H = [\hat{x}_H, \hat{H}_H] = \frac{1}{2m}[\hat{x}_H, \hat{p}_H{}^2] = \frac{1}{2m}i\hbar\frac{\partial}{\partial\hat{p}_H}\hat{p}_H{}^2 = \frac{2}{2m}i\hbar\hat{p}_H,$$

or

$$\frac{d}{dt}\hat{x}_H = [\hat{x}_H, \hat{H}_H] = \frac{1}{m}\hat{p}_H.$$

Similarly

$$i\hbar\frac{d}{dt}\hat{p}_H = [\hat{p}_H, \hat{H}_H] = \hat{U}^+[\hat{p}, \hat{H}]\hat{U} = \hat{U}^+[\hat{p}, \hat{V}(\hat{x})]\hat{U} = (-i\hbar)\frac{\partial}{\partial\hat{x}_H}V(\hat{x}_H),$$

or

$$\frac{d}{dt}\hat{p}_H = (-)\frac{\partial V(\hat{x}_H)}{\partial\hat{x}_H}.$$

We consider a simple harmonics.

$$V(\hat{x}_H) = \frac{1}{2}m\omega^2\hat{x}_H{}^2,$$

$$\frac{d}{dt}\hat{p}_H = -m\omega^2\hat{x}_H.$$

Now consider the linear combination,

$$\frac{d}{dt}(\hat{x}_H + \frac{i}{m\omega}\hat{p}_H) = -i\omega(\hat{x}_H + \frac{i}{m\omega}\hat{p}_H),$$

$$(\hat{x}_H + \frac{i}{m\omega}\hat{p}_H) = \hat{A}_H e^{-i\omega t},$$

or

$$\frac{d}{dt}(\hat{x}_H - \frac{i}{m\omega}\hat{p}_H) = i\omega(\hat{x}_H - \frac{i}{m\omega}),$$

$$(\hat{x}_H - \frac{i}{m\omega}\hat{p}_H) = \hat{B}_H e^{i\omega t}.$$

where $\hat{A}_H$ and $\hat{B}_H$ are time-independent operators:

$$\hat{A}_H = \hat{x}_H(0) + \frac{i}{m\omega}\hat{p}_H(0) ,$$

$$\hat{B}_H = \hat{x}_H(0) - \frac{i}{m\omega}\hat{p}_H(0) .$$

Note that $\hat{x}_H(0)$ and $\hat{p}_H(0)$ correspond to the operators in the Schrödinger picture. From these equations, we get final results

$$\hat{x}_H = \hat{x}_H(0)\cos\omega t + \frac{1}{m\omega}\hat{p}_H(0)\sin\omega t ,$$

$$\hat{p}_H = \hat{p}_H(0)\cos\omega t - m\omega\hat{x}_H(0)\sin\omega t .$$

These look to the same as the classical equation of motion. We see that $\hat{x}_H$ and $\hat{p}_H$ operators oscillate just like their classical analogue.

An advantage of the Heisenberg picture is therefore that it leads to equations which are formally similar to those of classical mechanics.

((**Note**))

$$i\hbar\frac{d^2}{dt^2}\hat{x}_H = [\frac{d\hat{x}_H}{dt},\hat{H}_H] = [\frac{\hat{p}_H}{m},\hat{H}_H] = \frac{1}{m}[\hat{p}_H,\frac{m\omega^2}{2}\hat{x}_H{}^2] = \frac{\omega^2}{2}[\hat{p}_H,\hat{x}_H{}^2] = \frac{\omega^2}{2}\frac{\hbar}{i}2\hat{x}_H ,$$

or

$$\frac{d^2}{dt^2}\hat{x}_H = -\omega^2\hat{x}_H ,$$

with the initial condition

$$\frac{d}{dt}\hat{x}_H|_{t=0} = \frac{1}{m}\hat{p}_H(0) , \qquad \hat{x}_H|_{t=0} = \hat{x}_H(0) .$$

The solution is

$$\hat{x}_H = \hat{C}_1\cos(\omega t) + \hat{C}_2\sin(\omega t) ,$$

$$\hat{x}_H(0) = \hat{C}_1 ,$$

$$\frac{d\hat{x}_H}{dt}\Big|_{t=0} = [-\omega\hat{C}_1\sin(\omega t) + \omega\hat{C}_2\cos n(\omega t)]_{t=0} = \omega\hat{C}_2 = \frac{\hat{p}_H(0)}{m}.$$

Thus we have

$$\hat{C}_2 = \frac{\hat{p}_H(0)}{m\omega},$$

and

$$\hat{x}_H = \hat{x}_H(0)\cos(\omega t) + \frac{\hat{p}_H(0)}{m\omega}\sin(\omega t).$$

19 Analogy with classical mechanics

In the classical mechanics, dynamical variables vary with time according to the Hamilton's equations of motion,

$$\frac{dq_j}{dt} = \frac{\partial H}{\partial p_j},$$

where q_j and p_j are a set of canonical co-ordinate and momentum, and H is the Hamiltonian expressed as a function of them,

$$H = H(q_1, q_2, q_3, ..., q_n, p_1, p_2, p_3, ...p_n).$$

where n is the degree of freedom.

For a given variable $A = v(q_1, q_2, q_3, ..., q_n, p_1, p_2, p_3, ... p_n)$,

$$\frac{dA}{dt} = \sum_j \left(\frac{\partial A}{\partial q_j}\frac{dq_j}{dt} + \frac{\partial A}{\partial p_j}\frac{dp_j}{dt} \right)$$
$$= \sum_j \left(\frac{\partial A}{\partial q_j}\frac{\partial H}{\partial p_j} - \frac{\partial A}{\partial p_j}\frac{\partial H}{\partial q_j} \right)$$
$$= [A, H]_{classical}$$

$[\ ]_{classical}$:a classical definition of a Poisson bracket.

20 Dirac picture (Interaction picture)

$$\hat{H} = \hat{H}_0 + \hat{V}_s(t),$$

where $\hat{H}_0$ is independent of *t*.

$$\left|\psi_s(t)\right\rangle = e^{-\frac{i}{\hbar}\hat{H}_0 t}\left|\psi_I(t)\right\rangle,$$

or

$$\left|\psi_I(t)\right\rangle = e^{\frac{i}{\hbar}\hat{H}_0 t}\left|\psi_s(t)\right\rangle.$$

We assume that

$$\left\langle\psi_I(t)\right|\hat{A}_I(t)\left|\psi_I(t)\right\rangle = \left\langle\psi_s(t)\right|\hat{A}_s\left|\psi_s(t)\right\rangle.$$

For convenience, $\hat{A}_s$ is independent of *t*.

or

$$\left\langle\psi_s(t)\right|e^{-\frac{i}{\hbar}\hat{H}_0 t}\hat{A}_I(t)e^{\frac{i}{\hbar}\hat{H}_0 t}\left|\psi_s(t)\right\rangle = \left\langle\psi_s(t)\right|\hat{A}_s\left|\psi_s(t)\right\rangle,$$

or

$$e^{-\frac{i}{\hbar}\hat{H}_0 t}\hat{A}_I(t)e^{\frac{i}{\hbar}\hat{H}_0 t} = \hat{A}_s,$$

or

$$\hat{A}_I(t) = e^{\frac{i}{\hbar}\hat{H}_0 t}\hat{A}_s e^{-\frac{i}{\hbar}\hat{H}_0 t},$$

or

$$\begin{aligned} i\hbar\frac{d}{dt}\hat{A}_I(t) &= i\hbar\frac{i}{\hbar}[\hat{H}_0 e^{\frac{i}{\hbar}\hat{H}_0 t}\hat{A}_s e^{-\frac{i}{\hbar}\hat{H}_0 t} - e^{\frac{i}{\hbar}\hat{H}_0 t}\hat{A}_s e^{-\frac{i}{\hbar}\hat{H}_0 t}\hat{H}_0] \\ &= [\hat{A}_I(t), \hat{H}_0] \end{aligned}.$$

Thus every operator behaves as if it would in the Heisenberg representation for a non-interacting system.

$$i\hbar\frac{\partial}{\partial t}\left|\psi_I(t)\right\rangle = i\hbar\frac{\partial}{\partial t}e^{\frac{i}{\hbar}\hat{H}_0 t}\left|\psi_s(t)\right\rangle$$

$$= -\hat{H}_0 e^{\frac{i}{\hbar}\hat{H}_0 t}\left|\psi_s(t)\right\rangle + e^{\frac{i}{\hbar}\hat{H}_0 t} i\hbar\frac{\partial}{\partial t}\left|\psi_s(t)\right\rangle$$

Since

$$i\hbar\frac{\partial}{\partial t}\left|\psi_s(t)\right\rangle = [\hat{H}_0 + \hat{V}_s(t)]\left|\psi_s(t)\right\rangle,$$

$$i\hbar\frac{\partial}{\partial t}\left|\psi_I(t)\right\rangle = i\hbar\frac{\partial}{\partial t}e^{\frac{i}{\hbar}\hat{H}_0 t}\left|\psi_s(t)\right\rangle = -\hat{H}_0 e^{\frac{i}{\hbar}\hat{H}_0 t}\left|\psi_s(t)\right\rangle + e^{\frac{i}{\hbar}\hat{H}_0 t}[\hat{H}_0 + \hat{V}(t)]\left|\psi_s(t)\right\rangle,$$

or

$$i\hbar\frac{\partial}{\partial t}\left|\psi_I(t)\right\rangle = e^{\frac{i}{\hbar}\hat{H}_0 t}\hat{V}(t)e^{-\frac{i}{\hbar}\hat{H}_0 t}\left|\psi_I(t)\right\rangle = \hat{V}_I(t)\left|\psi_I(t)\right\rangle,$$

or

$$i\hbar\frac{\partial}{\partial t}\left|\psi_I(t)\right\rangle = \hat{V}_I(t)\left|\psi_I(t)\right\rangle,$$

where

$$\hat{V}_I(t) = e^{\frac{i}{\hbar}\hat{H}_0 t}\,\hat{V}_s(t)e^{-\frac{i}{\hbar}\hat{H}_0 t} \qquad \text{(Schrödinger-like)}$$

which is a Schrödinger equation with the total $\hat{H}$ replaced by $\hat{V}_I$.

We assume that

$$\left|\psi_I(t)\right\rangle = \hat{U}_I(t,t_0)\left|\psi_I(t_0)\right\rangle,$$

satisfies the equation

$$i\hbar\frac{\partial}{\partial t}\left|\psi_I(t)\right\rangle = \hat{V}_I(t)\left|\psi_I(t)\right\rangle.$$

Then we have the following relation.

$$i\hbar\frac{\partial}{\partial t}\hat{U}_I(t,t_0) = \hat{V}_I(t)\hat{U}_I(t,t_0),$$

with the initial condition

$$\hat{U}_I(t,t_0) = 1 - \frac{i}{\hbar}\int_{t_0}^{t} \hat{V}_I(t')\hat{U}_I(t',t_0)dt' .$$

We can obtain an approximate solution to this equation [Dyson series].

$$\hat{U}_I(t,t_0) = 1 - \frac{i}{\hbar}\int_{t_0}^{t} \hat{V}_I(t')[1 - \frac{i}{\hbar}\int_{t_0}^{t'} \hat{V}_I(t'')\hat{U}_I(t'',t_0)dt'']dt'$$

$$= 1 + (-\frac{i}{\hbar})\int_{t_0}^{t} \hat{V}_I(t')dt' + (-\frac{i}{\hbar})^2\int_{t_0}^{t} dt'\int_{t_0}^{t'} dt''\hat{V}_I(t')\hat{V}_I(t'') + ...$$

21 Transition probability

Once $\hat{U}_I(t,t_0)$ is given we have

$$|\psi_I(t)\rangle = \hat{U}_I(t,t_0)|\psi_I(t_0)\rangle ,$$

where

$$|\psi_s(t)\rangle = e^{-\frac{i}{\hbar}\hat{H}_0 t}|\psi_I(t)\rangle , \qquad \text{or} \qquad |\psi_I(t)\rangle = e^{\frac{i}{\hbar}\hat{H}_0 t}|\psi_s(t)\rangle ,$$

and

$$|\psi_s(t)\rangle = \hat{U}(t,t_0)|\psi_s(t_0)\rangle ,$$

$$|\psi_I(t)\rangle = e^{\frac{i}{\hbar}\hat{H}_0 t}\hat{U}_s(t,t_0)|\psi_s(t_0)\rangle$$

$$= e^{\frac{i}{\hbar}\hat{H}_0 t}\hat{U}_s(t,t_0)e^{-\frac{i}{\hbar}\hat{H}_0 t_0}|\psi_I(t_0)\rangle$$

Then we have

$$\hat{U}_I(t,t_0) = e^{\frac{i}{\hbar}\hat{H}_0 t}\hat{U}_s(t,t_0)e^{-\frac{i}{\hbar}\hat{H}_0 t_0} .$$

Let us now look at the matrix element of $\hat{U}_I(t,t_0)$

$$\hat{H}_0|n\rangle = E_n|n\rangle ,$$

$$\langle n|\hat{U}_I(t,t_0)|m\rangle = e^{\frac{i}{\hbar}(E_n t - E_m t_0)}\langle n|\hat{U}_s(t,t_0)|m\rangle,$$

$$\left|\langle n|\hat{U}_I(t,t_0)|m\rangle\right|^2 = \left|\langle n|\hat{U}_s(t,t_0)|m\rangle\right|^2.$$

((**Remark**))

When

$$[\hat{H}_0,\hat{A}]\neq 0 \quad \text{and} \quad [\hat{H}_0,\hat{B}]\neq 0,$$

$$\hat{A}|a'\rangle = a'|a'\rangle \quad \text{and} \quad \hat{B}|b'\rangle = b'|b'\rangle,$$

in general,

$$\left|\langle b'|\hat{U}_I(t,t_0)|a'\rangle\right|^2 \neq \left|\langle b'|\hat{U}_s(t,t_0)||a'\rangle\rangle\right|^2.$$

Because

$$\begin{aligned}\langle b'|\hat{U}_I(t,t_0)|a'\rangle &= \sum_{n,m}\langle b'|e^{\frac{i}{\hbar}\hat{H}_0 t}|n\rangle\langle n|\hat{U}_s(t,t_0)e^{-\frac{i}{\hbar}\hat{H}_0 t_0}|a'\rangle \\ &= \sum_{n,m} e^{\frac{i}{\hbar}(E_n t - E_m t_0)}\langle b'|n\rangle\langle n|\hat{U}_s(t,t_0)|m\rangle\langle m|a'\rangle\end{aligned}$$

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22. Application of Schrödinger and Heisenberg pictures to simple harmonics

$$\hat{U} = e^{-\frac{i}{\hbar}\hat{H}t}.$$

The operator in the Heisenberg picture is defined by

$$\hat{A}_H = \hat{U}^+\hat{A}_s\hat{U} = e^{\frac{i}{\hbar}\hat{H}t}\hat{A}_s e^{-\frac{i}{\hbar}\hat{H}t},$$

where $\hat{H}$ is the Hamiltonian

$$\hat{H} = \frac{1}{2m}\hat{p}^2 + \frac{m\omega_0^2}{2}\hat{x}^2.$$

Using the equation of Heisenberg picture, we obtain

$$\hat{x}_H = \hat{x}\cos\omega t + \frac{1}{m\omega}\hat{p}\sin\omega t ,$$

and

$$\hat{p}_H = \hat{p}\cos\omega t - m\omega\hat{x}\sin\omega t .$$

The matrix of $\hat{x}$ and $\hat{p}$ are given by

$$\hat{x} = \frac{1}{\sqrt{2}\beta}\begin{pmatrix} 0 & \sqrt{1} & 0 & 0 & 0 & \\ \sqrt{1} & 0 & \sqrt{2} & 0 & 0 & \\ 0 & \sqrt{2} & 0 & \sqrt{3} & 0 & \cdots \\ 0 & 0 & \sqrt{3} & 0 & \sqrt{4} & \\ 0 & 0 & 0 & \sqrt{4} & 0 & \\ & & \vdots & & & \end{pmatrix},$$

and

$$\hat{p} = \frac{m\omega_0}{\sqrt{2}i\beta}\begin{pmatrix} 0 & \sqrt{1} & 0 & 0 & 0 & \\ -\sqrt{1} & 0 & \sqrt{2} & 0 & 0 & \\ 0 & -\sqrt{2} & 0 & \sqrt{3} & 0 & \cdots \\ 0 & 0 & -\sqrt{3} & 0 & \sqrt{4} & \\ 0 & 0 & 0 & -\sqrt{4} & 0 & \\ & & \vdots & & & \end{pmatrix},$$

((**Discussion**))

What are the expectation values $\langle\psi(t)|\hat{x}|\psi(t)\rangle$ and $\langle\psi(t)|\hat{p}|\psi(t)\rangle$?

$$\begin{aligned}\langle\psi(t)|\hat{x}|\psi(t)\rangle &= \langle\psi(0)|\hat{x}_H|\psi(0)\rangle \\ &= \langle\psi(0)|\hat{x}\cos\omega t + \frac{1}{m\omega}\hat{p}\sin\omega t|\psi(0)\rangle \\ &= \langle\psi(0)|\hat{x}|\psi(0)\rangle\cos\omega t + \frac{1}{m\omega}\langle\psi(0)|\hat{p}|\psi(0)\rangle\sin\omega t\end{aligned}$$

$$\langle\psi(t)|\hat{p}|\psi(t)\rangle = \langle\psi(0)|\hat{p}_H|\psi(0)\rangle$$
$$= \langle\psi(0)|\hat{p}\cos\omega t - m\omega\hat{x}\sin\omega t|\psi(0)\rangle$$
$$= \langle\psi(0)|\hat{p}|\psi(0)\rangle\cos\omega t - m\omega\langle\psi(0)|\hat{x}|\psi(0)\rangle\sin\omega t$$

Suppose that

(1) $$|\psi(0)\rangle = \frac{1}{\sqrt{6}}(|0\rangle + 2|1\rangle + |2\rangle).$$

we can calculate the matrix elements $\langle\psi(0)|\hat{x}|\psi(0)\rangle$ and $\langle\psi(0)|\hat{p}|\psi(0)\rangle$ as follows.

$$\langle\psi(0)|\hat{x}|\psi(0)\rangle = \begin{pmatrix} \frac{1}{\sqrt{6}} & \frac{2}{\sqrt{6}} & \frac{1}{\sqrt{6}} \end{pmatrix} \frac{1}{\sqrt{2}\beta} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & \sqrt{2} \\ 0 & \sqrt{2} & 0 \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{6}} \\ \frac{2}{\sqrt{6}} \\ \frac{1}{\sqrt{6}} \end{pmatrix}$$

$$= \frac{1}{\sqrt{2}\beta}\frac{2}{3}(1+\sqrt{2})$$

$$\langle\psi(0)|\hat{p}|\psi(0)\rangle = \begin{pmatrix} \frac{1}{\sqrt{6}} & \frac{2}{\sqrt{6}} & \frac{1}{\sqrt{6}} \end{pmatrix} \frac{m\omega_0}{\sqrt{2}\beta i} \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & \sqrt{2} \\ 0 & -\sqrt{2} & 0 \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{6}} \\ \frac{2}{\sqrt{6}} \\ \frac{1}{\sqrt{6}} \end{pmatrix} = 0,$$

(2) $$|\psi(0)\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle),$$

$$\langle\psi(0)|\hat{x}|\psi(0)\rangle = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix} \frac{1}{\sqrt{2}\beta} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix} = \frac{1}{\sqrt{2}\beta},$$

$$\langle\psi(0)|\hat{p}|\psi(0)\rangle = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix} \frac{1}{\sqrt{2}\beta} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix} = 0,$$

$$\langle \psi(t)|\hat{x}|\psi(t)\rangle = \frac{1}{\sqrt{2}\beta}\cos\omega t\,,$$

and

$$\langle \psi(t)|\hat{p}|\psi(t)\rangle = -\frac{m\omega}{\sqrt{2}\beta}\sin\omega t\,.$$

((**Another method, Schrödinger picture)**)

$$\begin{aligned}|\psi(t)\rangle &= e^{-i\hat{H}t/\hbar}\frac{1}{\sqrt{2}}\left(|0\rangle + |1\rangle\right)\\ &= \frac{1}{\sqrt{2}}\left(e^{-iE_0t/\hbar}|0\rangle + e^{-iE_1t/\hbar}|1\rangle\right)\\ &= \frac{1}{\sqrt{2}}\begin{pmatrix} e^{-iE_0t/\hbar}\\ e^{-iE_1t/\hbar}\end{pmatrix}\end{aligned}$$

$$\langle \psi(t)| = \frac{1}{\sqrt{2}}\begin{pmatrix} e^{iE_0t/\hbar} & {}^{iE_1t/\hbar}\end{pmatrix},$$

$$\begin{aligned}\langle \psi(t)|\hat{x}|\psi(t)\rangle &= \left(\frac{1}{\sqrt{2}}\right)^2\frac{1}{\sqrt{2}\beta}\begin{pmatrix} e^{iE_0t/\hbar} & {}^{iE_1t/\hbar}\end{pmatrix}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\begin{pmatrix} e^{-iE_0t/\hbar}\\ e^{-iE_1t/\hbar}\end{pmatrix}\\ &= \frac{1}{2}\frac{1}{\sqrt{2}\beta}\begin{pmatrix} e^{iE_0t/\hbar} & {}^{iE_1t/\hbar}\end{pmatrix}\begin{pmatrix} e^{-iE_1t/\hbar}\\ e^{-iE_0t/\hbar}\end{pmatrix}\\ &= \frac{1}{2}\frac{1}{\sqrt{2}\beta}(e^{i\omega_0t} + e^{-i\omega_0t}) = \frac{1}{\sqrt{2}\beta}\cos\omega_0 t\end{aligned}$$

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23. Example-1

A spin 1/2 particles in a eigenstate of S_x, with eigenvalue $\hbar/2$ at time $t = 0$. At that time it is placed in a magnetic field of magnitude B pointing in the z direction, in which it is allowed to precess for a time T. At that instant, the magnetic field is rotated very rapidly, so that it is now points in the y direction. After another time interval T, a measurement of S_x is carried. What is the probability that the value $\hbar/2$ will be found?

((**Solution**))

The spin has a spin magnetic moment.

$$\hat{\boldsymbol{\mu}} = -\frac{2\mu_B}{\hbar}\hat{\boldsymbol{S}} = -\frac{2\mu_B}{\hbar}\frac{\hbar}{2}\hat{\boldsymbol{\sigma}} = -\mu_B\hat{\boldsymbol{\sigma}} .$$

The spin Hamiltonian in the presence of the magnetic field ***B***,

$$\hat{H} = -\hat{\boldsymbol{\mu}} \cdot \boldsymbol{B} = \mu_B\hat{\boldsymbol{\sigma}} \cdot \boldsymbol{B} = \frac{e\hbar B}{2mc}\hat{\boldsymbol{\sigma}} \cdot \boldsymbol{n} = \frac{1}{2}\hbar\left(\frac{eB}{mc}\right)\hat{\boldsymbol{\sigma}} \cdot \boldsymbol{n} = \frac{1}{2}\hbar\omega_0\hat{\boldsymbol{\sigma}} \cdot \boldsymbol{n} ,$$

where ***n*** is the unit vector along the direction of ***B***, and ω_0 is the Larmor angular frequency. Note that the period T_0 is expressed by $T_0 = \frac{2\pi}{\omega_0}$

At $t = 0$, we have $\left|\psi(t=0)\right\rangle = \left|+x\right\rangle$.

For $0 \le t \le T$, the magnetic field is applied along the z direction.

$$\hat{H} = \frac{1}{2}\hbar\omega_0\hat{\sigma}_z$$

we have

$$\left|\psi(t)\right\rangle = \exp(-\frac{it\hat{H}}{\hbar})\left|\psi(t=0)\right\rangle = \exp(-\frac{i\omega_0 t}{2}\hat{\sigma}_z)\left|\psi(t=0)\right\rangle ,$$

and

$$\left|\psi(t=T)\right\rangle = \exp(-\frac{i\omega_0 T}{2}\hat{\sigma}_z)\left|\psi(t=0)\right\rangle = \exp(-i\pi\frac{T}{T_0}\hat{\sigma}_z)\left|+x\right\rangle = \hat{R}_z(2\pi\frac{T}{T_0})\left|+x\right\rangle .$$

where $\hat{R}_z(\phi)$ is the rotation operator around the z axis by the angle ϕ.

For $T \le t \le 2T$, the magnetic field is applied along the y direction.

$$\hat{H} = \frac{1}{2}\hbar\omega_0\hat{\sigma}_y$$

we have

$$\begin{aligned}\left|\psi(t)\right\rangle &= \exp(-\frac{i(t-T)\hat{H}}{\hbar})\left|\psi(t=T)\right\rangle \\ &= \exp(-\frac{i\omega_0(t-T)}{2}\hat{\sigma}_y)\left|\psi(t=T)\right\rangle\end{aligned}$$

$$\left|\psi(t=2T)\right\rangle = \exp(-\frac{i\omega_0 T}{2}\hat{\sigma}_y)\left|\psi(t=T)\right\rangle$$
$$= \exp(-i\pi\frac{T}{T_0}\hat{\sigma}_y)\left|\psi(t=T)\right\rangle$$
$$= \hat{R}_y(2\pi\frac{T}{T_0})\hat{R}_z(2\pi\frac{T}{T_0})\left|+x\right\rangle$$

Now we calculate

$$\left\langle +x\middle|\psi(t=2T)\right\rangle = \left\langle +x\right|\hat{R}_y(2\pi\frac{T}{T_0})\hat{R}_z(2\pi\frac{T}{T_0})\left|+x\right\rangle$$
$$= \left\langle +x\right|\hat{R}_y(\theta)\hat{R}_z(\theta)\left|+x\right\rangle$$

where

$$\theta = 2\pi\frac{T}{T_0}.$$

Using the formula

$$\hat{R}_{\boldsymbol{n}}(\theta) = \exp(-i\frac{\theta}{2}\boldsymbol{n}\cdot\hat{\sigma}) = \cos(\frac{\theta}{2})\hat{1} - i(\boldsymbol{n}\cdot\hat{\sigma})\sin(\frac{\theta}{2}),$$

$$\hat{R}_z(\theta) = \cos(\frac{\theta}{2})\hat{1} - i\hat{\sigma}_z\sin(\frac{\theta}{2}) = \begin{pmatrix} e^{-i\frac{\theta}{2}} & 0 \\ 0 & e^{i\frac{\theta}{2}} \end{pmatrix},$$

$$\hat{R}_y(\theta) = \cos(\frac{\theta}{2})\hat{1} - i\hat{\sigma}_y\sin(\frac{\theta}{2}) = \begin{pmatrix} \cos\frac{\theta}{2} & -\sin\frac{\theta}{2} \\ \sin\frac{\theta}{2} & \cos\frac{\theta}{2} \end{pmatrix}.$$

Note that

$$\left|+x\right\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

$$\langle +x|\psi(t=2T)\rangle = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} \cos\frac{\theta}{2} & -\sin\frac{\theta}{2} \\ \sin\frac{\theta}{2} & \cos\frac{\theta}{2} \end{pmatrix} \begin{pmatrix} e^{-i\frac{\theta}{2}} & 0 \\ 0 & e^{i\frac{\theta}{2}} \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix}$$

or

$$\langle +x|\psi(t=2T)\rangle = \frac{1+i}{4}(2\cos\theta - 2i)$$

Then the probability is given by

$$P(\theta = 2\pi\frac{T}{T_0}) = \left|\frac{1+i}{4}(2\cos\theta - 2i)\right|^2 = \frac{1}{2}[1+\cos^2\theta] = \frac{1}{2}[1+\cos^2(2\pi\frac{T}{T_0})]$$

24. Example-2

A particle with intrinsic spin one is placed in a constant external magnetic field B_0 in the x direction. The initial spin state of the particle is $|\psi(0)\rangle = |l=1, m=1\rangle = |1,1\rangle$, that is, a state with $S_z = \hbar$. Take the spin Hamiltonian to be

$$\hat{H} = \omega_0 \hat{J}_x,$$

and determine the probability $P(t)$ that the particle is in the state $|1,-1\rangle$ at time t. Make a plot of $P(t)$ as a function of time t ($0 \le \omega_0 t \le 2\pi$). Hint: $|1,1\rangle_x$, $|1,0\rangle_x$, and $|1,-1\rangle_x$ are the eigenket of $\hat{H}$.

((**Solution**))

$$|\psi(t)\rangle = \exp(-\frac{i}{\hbar}\hat{H}t)|\psi(0)\rangle = \exp(-i\frac{\omega_0 t}{\hbar}\hat{J}_x)|1,1\rangle_z$$

For simplicity, hereaftre we use

$$|1,1\rangle_z = |1,1\rangle.$$

Noting that

$$|1,1\rangle = \frac{1}{2}|1,1\rangle_x + \frac{1}{\sqrt{2}}|1,0\rangle_x + \frac{1}{2}|1,-1\rangle_x$$

we get

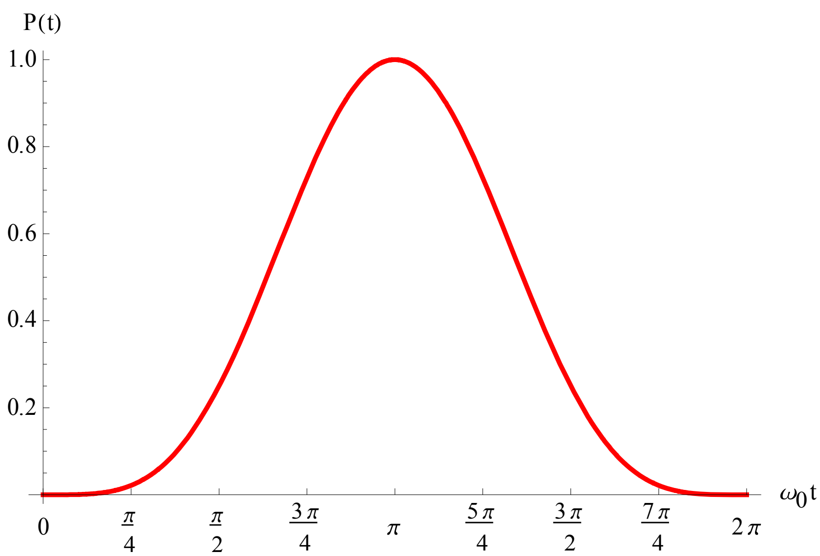
$$|\psi(t)\rangle = \exp(-i\frac{\omega_0 t}{\hbar}\hat{J}_x)|1,1\rangle$$
$$= \exp(-i\frac{\omega_0 t}{\hbar}\hat{J}_x)[\frac{1}{2}|1,1\rangle_x + \frac{1}{\sqrt{2}}|1,0\rangle_x + \frac{1}{2}|1,-1\rangle_x]$$
$$= \frac{1}{2}\exp(-i\omega_0 t)|1,1\rangle_x + \frac{1}{\sqrt{2}}|1,0\rangle_x + \frac{1}{2}\exp(i\omega_0 t)|1,-1\rangle_x$$

The probability $P(t)$ is given by

$$P(t) = |\langle 1,-1|\psi(t)\rangle|^2 = \left|\frac{1}{2}\exp(-i\omega_0 t)\langle 1,-1|1,1\rangle_x + \frac{1}{\sqrt{2}}\langle 1,-1|1,0\rangle_x + \frac{1}{2}\exp(i\omega_0 t)\langle 1,-1|1,-1\rangle_x\right|^2$$

Then we have

$$P(t) = |\langle 1,-1|\psi(t)\rangle|^2$$
$$= \left|\frac{1}{4}\exp(-i\omega_0 t) - \frac{1}{2} + \frac{1}{4}\exp(i\omega_0 t)\right|^2$$
$$= \frac{1}{4}(1-\cos\omega_0 t)^2 = \sin^4\left(\frac{\omega_0 t}{2}\right)$$



((**Note**))

$$|1,1\rangle = \hat{U}^{+}|1,1\rangle_x = \begin{pmatrix} \frac{1}{2} & \frac{1}{\sqrt{2}} & \frac{1}{2} \\ \frac{1}{\sqrt{2}} & 0 & -\frac{1}{\sqrt{2}} \\ \frac{1}{2} & -\frac{1}{\sqrt{2}} & \frac{1}{2} \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} \frac{1}{2} \\ \frac{1}{\sqrt{2}} \\ \frac{1}{2} \end{pmatrix} = \frac{1}{2}|1,1\rangle_x + \frac{1}{\sqrt{2}}|1,0\rangle_x + \frac{1}{2}|1,-1\rangle_x$$

$$|1,1\rangle_z = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \quad |1,0\rangle_z = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \quad |1,-1\rangle_z = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

$$|1,1\rangle_x = \frac{1}{2}\begin{pmatrix} 1 \\ \sqrt{2} \\ 1 \end{pmatrix}, \qquad |1,0\rangle_x = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix},$$

$$|1,-1\rangle_x = \frac{1}{2}\begin{pmatrix} 1 \\ -\sqrt{2} \\ 1 \end{pmatrix}$$

with the unitary operator,

$$\hat{U}_x = \begin{pmatrix} \frac{1}{2} & \frac{1}{\sqrt{2}} & \frac{1}{2} \\ \frac{1}{\sqrt{2}} & 0 & -\frac{1}{\sqrt{2}} \\ \frac{1}{2} & -\frac{1}{\sqrt{2}} & \frac{1}{2} \end{pmatrix}, \qquad \hat{U}_x^{+} = \begin{pmatrix} \frac{1}{2} & \frac{1}{\sqrt{2}} & \frac{1}{2} \\ \frac{1}{\sqrt{2}} & 0 & -\frac{1}{\sqrt{2}} \\ \frac{1}{2} & -\frac{1}{\sqrt{2}} & \frac{1}{2} \end{pmatrix}$$

25. Example-3

Let |1> and |2> be eigenstates of a Hermitian operator $\hat{A}$ with eigenvalues a_1 and a_2, respectively ($a_1 \neq a_2$). The Hamiltonian operator is given by

$$\hat{H} = \delta|1\rangle\langle 2| + \delta|2\rangle\langle 1|$$

or

$$\hat{H} = \begin{pmatrix} 0 & \delta \\ \delta & 0 \end{pmatrix} = \delta\hat{\sigma}_x$$

where δ is just a real number.

(a) Clearly, |1> and |2> are not eigenstate of the Hamiltonian. Write down the eigenstates of the Hamiltonian. What are their energy eigenvalues?

(b) Suppose that the system is known to be in the state |2> at t = 0. Write down the state vector at t>0.

(c) What is the probability for finding the system in |1> for t>0 if the system is known to be in state |2> at t = 0?

((**Solution**))

(a)

Eigenvalue problem

$$\hat{H}\left|+x\right\rangle = \delta\hat{\sigma}_x\left|+x\right\rangle = \delta\left|+x\right\rangle$$

$$\hat{H}\left|-x\right\rangle = \delta\hat{\sigma}_x\left|-x\right\rangle = -\delta\left|-x\right\rangle$$

under the basis of $\{\left|1\right\rangle, \left|2\right\rangle\}$, where

$$\left|+x\right\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix} = \frac{1}{\sqrt{2}}[\left|1\right\rangle + \left|2\right\rangle], \qquad \text{for} \qquad E_1 = \delta,$$

$$\left|-x\right\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\-1\end{pmatrix} = \frac{1}{\sqrt{2}}[\left|1\right\rangle - \left|2\right\rangle], \qquad \text{for} \qquad E_2 = -\delta,$$

(b)

$$\left|\psi(t)\right\rangle = \exp(-\frac{i}{\hbar}\hat{H}t)\left|2\right\rangle$$

$$= \frac{1}{\sqrt{2}}\exp(-\frac{i}{\hbar}\hat{H}t)[\left|+x\right\rangle - \left|-x\right\rangle]$$

$$= \frac{1}{\sqrt{2}}[e^{-\frac{i}{\hbar}E_1 t}\left|+x\right\rangle - e^{-\frac{i}{\hbar}E_2 t}\left|-x\right\rangle]$$

or

$$\left|\psi(t)\right\rangle = \frac{1}{\sqrt{2}}[e^{-\frac{i}{\hbar}E_1 t}\frac{1}{\sqrt{2}}(\left|1\right\rangle + \left|2\right\rangle) - e^{-\frac{i}{\hbar}E_2 t}(\frac{1}{\sqrt{2}}(\left|1\right\rangle - \left|2\right\rangle)],$$

or

$$|\psi(t)\rangle = \frac{1}{2}[e^{-\frac{i}{\hbar}E_1 t}(|1\rangle + |2\rangle) - e^{-\frac{i}{\hbar}E_2 t}(|1\rangle - |2\rangle)]$$

$$= \frac{1}{2}(e^{-\frac{i}{\hbar}E_1 t} - e^{-\frac{i}{\hbar}E_2 t})|1\rangle + \frac{1}{2}(e^{-\frac{i}{\hbar}E_1 t} + e^{-\frac{i}{\hbar}E_2 t})|2\rangle$$

(c)

$$P(t) = |\langle 1|\psi(t)\rangle|^2 = \frac{1}{4}(e^{-\frac{i}{\hbar}E_1 t} - e^{-\frac{i}{\hbar}E_2 t})(e^{\frac{i}{\hbar}E_1 t} - e^{\frac{i}{\hbar}E_2 t})$$

$$= \frac{1}{4}[2 - e^{\frac{i}{\hbar}(E_2 - E_1)t} - e^{-\frac{i}{\hbar}(E_2 - E_1)t}]$$

or

$$P(t) = \frac{1}{4}\{2 - 2\cos[\frac{1}{\hbar}(E_2 - E_1)t]\} = \sin^2\left(\frac{1}{2\hbar}(E_2 - E_1)t\right).$$

26. Example-4

Consider a simple harmonic oscillator in the superposition state. Given that at t = 0 the particle is in a state given by

$$|\psi(0)\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle),$$

where $|n\rangle$ is the eigenket of a one-dimensional harmonic oscillator with a mass m and an angular frequency ω_0: $\hat{H}|n\rangle = E_n|n\rangle$ with $E_n = (n + \frac{1}{2})\hbar\omega_0$. $\beta = \sqrt{\frac{m\omega_0}{\hbar}}$

(a) Calculate

$$|\psi(t)\rangle = \exp(-\frac{i}{\hbar}\hat{H}t)|\psi(t=0)\rangle.$$

(b) Calculate the expectation value defined by

$$\langle\psi(t)|\hat{x}|\psi(t)\rangle = \langle\psi(0)|\hat{x}_H|\psi(0)\rangle,$$

$$\langle\psi(t)|\hat{x}^2|\psi(t)\rangle = \langle\psi(0)|\hat{x}_H{}^2|\psi(0)\rangle.$$

$\hat{x}_H$ is the operator in the Heisenberg picture

$$\hat{x}_H = \hat{x}\cos\omega_0 t + \frac{1}{m\omega_0}\hat{p}\sin\omega_0 t .$$

$$\hat{x} = \frac{1}{\sqrt{2}\beta}\begin{pmatrix} 0 & \sqrt{1} & 0 & 0 & 0 & \\ \sqrt{1} & 0 & \sqrt{2} & 0 & 0 & \\ 0 & \sqrt{2} & 0 & \sqrt{3} & 0 & \cdots \\ 0 & 0 & \sqrt{3} & 0 & \sqrt{4} & \\ 0 & 0 & 0 & \sqrt{4} & 0 & \\ & & \vdots & & & \end{pmatrix},$$

$$\hat{p} = \frac{m\omega_0}{\sqrt{2}i\beta}\begin{pmatrix} 0 & \sqrt{1} & 0 & 0 & 0 & \\ -\sqrt{1} & 0 & \sqrt{2} & 0 & 0 & \\ 0 & -\sqrt{2} & 0 & \sqrt{3} & 0 & \cdots \\ 0 & 0 & -\sqrt{3} & 0 & \sqrt{4} & \\ 0 & 0 & 0 & -\sqrt{4} & 0 & \\ & & \vdots & & & \end{pmatrix}$$

((**Heisenberg picture**))
Simple harmonics

$$\hat{U} = e^{-\frac{i}{\hbar}\hat{H}t} .$$

The operator in the Heisenberg picture is defined by

$$\hat{A}_H = \hat{U}^+ \hat{A}_s \hat{U} = e^{\frac{i}{\hbar}\hat{H}t}\hat{A}_s e^{-\frac{i}{\hbar}\hat{H}t},$$

where $\hat{H}$ is the Hamiltonian

$$\hat{H} = \frac{1}{2m}\hat{p}^2 + \frac{m\omega_0^2}{2}\hat{x}^2 .$$

Using the equation of Heisenberg picture, we obtain

$$\hat{x}_H = \hat{x}\cos\omega_0 t + \frac{1}{m\omega}\hat{p}\sin\omega_0 t ,$$

and

$$\hat{p}_H = \hat{p}\cos\omega_0 t - m\omega\hat{x}\sin\omega_0 t .$$

What are the expectation values $\langle\psi(t)|\hat{x}|\psi(t)\rangle$ and $\langle\psi(t)|\hat{p}|\psi(t)\rangle$?

$$\begin{aligned}\langle\psi(t)|\hat{x}|\psi(t)\rangle &= \langle\psi(0)|\hat{x}_H|\psi(0)\rangle \\ &= \langle\psi(0)|\hat{x}\cos\omega_0 t + \frac{1}{m\omega_0}\hat{p}\sin\omega_0 t|\psi(0)\rangle \\ &= \langle\psi(0)|\hat{x}|\psi(0)\rangle\cos\omega_0 t + \frac{1}{m\omega_0}\langle\psi(0)|\hat{p}|\psi(0)\rangle\sin\omega_0 t\end{aligned}$$

$$\begin{aligned}\langle\psi(t)|\hat{p}|\psi(t)\rangle &= \langle\psi(0)|\hat{p}_H|\psi(0)\rangle \\ &= \langle\psi(0)|\hat{p}\cos\omega_0 t - m\omega_0\hat{x}\sin\omega_0 t|\psi(0)\rangle \\ &= \langle\psi(0)|\hat{p}|\psi(0)\rangle\cos\omega_0 t - m\omega_0\langle\psi(0)|\hat{x}|\psi(0)\rangle\sin\omega_0 t\end{aligned}$$

At $t = 0$,

$$|\psi(0)\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle).$$

The average values of $\hat{x}$ and $\hat{p}$ at $t = 0$ is obtained as

$$\langle\psi(0)|\hat{x}|\psi(0)\rangle = \begin{pmatrix}\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}}\end{pmatrix}\frac{1}{\sqrt{2}\beta}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\begin{pmatrix}\frac{1}{\sqrt{2}}\\ \frac{1}{\sqrt{2}}\end{pmatrix} = \frac{1}{\sqrt{2}\beta},$$

and

$$\langle\psi(0)|\hat{p}|\psi(0)\rangle = \begin{pmatrix}\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}}\end{pmatrix}\frac{1}{\sqrt{2}\beta}\begin{pmatrix}0 & 1\\ -1 & 0\end{pmatrix}\begin{pmatrix}\frac{1}{\sqrt{2}}\\ \frac{1}{\sqrt{2}}\end{pmatrix} = 0.$$

The average values of $\hat{x}$ and $\hat{p}$ at the time t is obtained as

$$\langle\psi(t)|\hat{x}|\psi(t)\rangle = \frac{1}{\sqrt{2}\beta}\cos\omega_0 t.$$

and

$$\langle\psi(t)|\hat{p}|\psi(t)\rangle = -\frac{m\omega_0}{\sqrt{2}\beta}\sin\omega_0 t.$$

((**Schrödinger picture**))

In this picture $|\psi(t)\rangle$ is obtained as

$$|\psi(t)\rangle = e^{-i\hat{H}t/\hbar}\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) = \frac{1}{\sqrt{2}}(e^{-iE_0t/\hbar}|0\rangle + e^{-iE_1t/\hbar}|1\rangle) = \frac{1}{\sqrt{2}}\begin{pmatrix} e^{-iE_0t/\hbar} \\ e^{-iE_1t/\hbar} \end{pmatrix}.$$

Since

$$\langle\psi(t)| = \frac{1}{\sqrt{2}}\begin{pmatrix} e^{iE_0t/\hbar} & e^{iE_1t/\hbar} \end{pmatrix},$$

we have

$$\begin{aligned}
\langle\psi(t)|\hat{x}|\psi(t)\rangle &= \left(\frac{1}{\sqrt{2}}\right)^2 \frac{1}{\sqrt{2}\beta}\begin{pmatrix} e^{iE_0t/\hbar} & e^{iE_1t/\hbar} \end{pmatrix}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} e^{-iE_0t/\hbar} \\ e^{-iE_1t/\hbar} \end{pmatrix} \\
&= \frac{1}{2}\frac{1}{\sqrt{2}\beta}\begin{pmatrix} e^{iE_0t/\hbar} & e^{iE_1t/\hbar} \end{pmatrix}\begin{pmatrix} e^{-iE_1t/\hbar} \\ e^{-iE_0t/\hbar} \end{pmatrix} \\
&= \frac{1}{2}\frac{1}{\sqrt{2}\beta}(e^{i\omega_0t} + e^{-i\omega_0t}) = \frac{1}{\sqrt{2}\beta}\cos\omega_0 t
\end{aligned}$$

$$\begin{aligned}
\langle\psi(t)|\hat{p}|\psi(t)\rangle &= \left(\frac{1}{\sqrt{2}}\right)^2 \frac{m\omega_0}{\sqrt{2}\beta i}\begin{pmatrix} e^{iE_0t/\hbar} & e^{iE_1t/\hbar} \end{pmatrix}\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}\begin{pmatrix} e^{-iE_0t/\hbar} \\ e^{-iE_1t/\hbar} \end{pmatrix} \\
&= \frac{1}{2}\frac{m\omega_0}{\sqrt{2}\beta i}\begin{pmatrix} e^{iE_0t/\hbar} & e^{iE_1t/\hbar} \end{pmatrix}\begin{pmatrix} e^{-iE_1t/\hbar} \\ -e^{-iE_0t/\hbar} \end{pmatrix} \\
&= \frac{1}{2}\frac{m\omega_0}{\sqrt{2}\beta i}(e^{-i\omega_0t} - e^{i\omega_0t}) \\
&= -\frac{m\omega_0}{\sqrt{2}\beta}\sin\omega_0 t
\end{aligned}$$

---

27. Example-5: Cohen-Tannoudji (4-2)

Consider a spin 1/2 particle.

a. At time t = 0, we measure S_y and find $+\hbar/2$. What is the state vector $|\psi(0)\rangle$ immediately after the measurement?

b. Immediately after this measurement, we apply a uniform time-dependent field parallel to the z axis. The Hamiltonian operator of the spin $\hat{H}(t)$ is then written:

$$\hat{H}(t) = \omega_0(t)\hat{S}_z .$$

Assume that $\omega_0(t)$ is zero for $t<0$ and $t>T$ and increases linearly from 0 to ω_0 when $0 \le t \le T$ (T is a given parameter whose dimensions are those of time). Show that at time t the state vector can be written as

$$\left|\psi(t)\right\rangle = \frac{1}{\sqrt{2}}[e^{i\theta(t)}\left|+z\right\rangle + ie^{-i\theta(t)}\left|-z\right\rangle],$$

where $\theta(t)$ is a real function of t.

c. At a time $t = \tau > T$. we measure S_y. What results can we find, and with what probabilities? Determine the relation which must exist between ω_0 and T in order for us to be sure of the result. Give the physical interpretation.

((**Solution**))

(a)

$$\left|\psi(t=0)\right\rangle = \left|+y\right\rangle = \frac{1}{\sqrt{2}}[\left|+z\right\rangle + i\left|-z\right\rangle] .$$

(b)

$$\hat{H}(t) = \omega_0(t)\hat{S}_z .$$

Schrodinger equation

$$i\hbar\frac{\partial}{\partial t}\left|\psi(t)\right\rangle = \hat{H}(t)\left|\psi(t)\right\rangle = \omega_0(t)\hat{S}_z\left|\psi(t)\right\rangle .$$

Suppose that

$$\left|\psi(t)\right\rangle = \hat{U}(t)\left|\psi(t=0)\right\rangle .$$

$\hat{U}(t)$ satisfies the differential equation

$$i\hbar\frac{\partial}{\partial t}\hat{U}(t) = \hat{H}(t)\hat{U}(t) = \omega(t)\hat{S}_z\hat{U}(t) .$$

The solution is

$$\hat{U}(t) = \exp(-\frac{i}{\hbar}\int_0^t \hat{H}(t')dt') .$$

$\hat{H}(t)$ is time-dependent but $\hat{H}(t)$'s at different times commute.

$$\hat{U}(t) = \exp[-i\hat{S}_z \frac{1}{\hbar}\int_0^t \omega_0(t')dt'] = \exp[-i\frac{1}{\hbar}\theta_0(t)\hat{S}_z],$$

where

$$\theta_0(t) = \int_0^t \omega_0(t')dt'.$$

Then we get

$$\begin{aligned}
|\psi(t)\rangle &= \exp[-i\frac{1}{\hbar}\theta_0(t)\hat{S}_z]|\psi(t=0)\rangle \\
&= \exp[-i\frac{1}{\hbar}\theta_0(t)\hat{S}_z]|+y\rangle \\
&= \frac{1}{\sqrt{2}}\exp[-i\frac{1}{\hbar}\theta_0(t)\hat{S}_z][|+z\rangle + i|-z\rangle] \\
&= \frac{1}{\sqrt{2}}[e^{-i\frac{1}{2}\theta_0(t)}|+z\rangle + ie^{i\frac{1}{2}\theta_0(t)}|-z\rangle] \\
&= \frac{1}{\sqrt{2}}[e^{i\theta(t)}|+z\rangle + ie^{-i\theta(t)}|-z\rangle]
\end{aligned}$$

where

$$\theta(t) = -\frac{1}{2}\theta_0(t) = -\frac{1}{2}\int_0^t \omega_0(t')dt'.$$

$$\omega_0(t') = \frac{\omega_0}{T}t' \quad \text{for } 0 < t' < T,$$

$$\omega_0(t') = 0. \qquad \text{for } t'<0 \text{ and } t'>T.$$

(c)

At $t = \tau > T$,

$$\theta(t) = -\frac{1}{2}\int_0^T \omega_0(t')dt' = -\frac{1}{2}\int_0^T \frac{\omega_0}{T}t'\,dt' = -\frac{1}{4}\omega_0 T.$$

Now we measure $\hat{S}_y$ at *t*.

$$\langle \pm y | \psi(t) \rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & \mp i \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{2}} e^{i\theta(t)} \\ \frac{i}{\sqrt{2}} e^{-i\theta(t)} \end{pmatrix} = \frac{1}{2} e^{i\theta(t)} \pm \frac{1}{2} e^{-i\theta(t)}.$$

The probability

$$P_+ = \left| \langle + y | \psi(t) \rangle \right|^2 = \frac{1}{2}[1 + \cos(2\theta(t))] = \frac{1}{2}[1 + \cos(\frac{\omega_0 T}{2}))].$$

$$P_- = \left| \langle - y | \psi(t) \rangle \right|^2 = \frac{1}{2}[1 - \cos(2\theta(t))] = \frac{1}{2}[1 - \cos(\frac{\omega_0 T}{2})].$$

When $\omega_0 T = 2\pi$, $P_+ = 0$, $P_- = 1$.

When $\omega_0 T = 4\pi$, $P_+ = 1$, $P_- = 0$.

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APPENDIX-I

Calculation of exponential of matrix

A.1 Example-1

Calculate $\exp(\frac{\pi i\hat{A}}{2})$,

where

$$\hat{A}=\begin{pmatrix} 0 & -\frac{i}{\sqrt{2}} & 0 \\ \frac{i}{\sqrt{2}} & 0 & -\frac{i}{\sqrt{2}} \\ 0 & \frac{i}{\sqrt{2}} & 0 \end{pmatrix},$$

in the basis of $|1\rangle, |2\rangle, |3\rangle$.

We use the Mathematica to calculate the eigenvaluse and eigenvectors of $\hat{A}$.

Eigensystem[$\hat{A}$]

The eigenvalues and eigenkets are obtained as

$$|\psi_1\rangle = \hat{U}|1\rangle = \begin{pmatrix} \frac{1}{2} \\ \frac{i}{\sqrt{2}} \\ -\frac{1}{2} \end{pmatrix} \quad \text{for the eigenvalue } \lambda = 1$$

$$|\psi_0\rangle = \hat{U}|2\rangle = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ 0 \\ \frac{1}{\sqrt{2}} \end{pmatrix} \quad \text{for the eigenvalue } \lambda = 0$$

$$|\psi_{-1}\rangle = \hat{U}|3\rangle = \begin{pmatrix} \frac{1}{2} \\ -\frac{i}{\sqrt{2}} \\ -\frac{1}{2} \end{pmatrix} \quad \text{for the eigenvalue } \lambda = \text{-1}$$

$$\hat{U} = \begin{pmatrix} \frac{1}{2} & \frac{1}{\sqrt{2}} & \frac{1}{2} \\ \frac{i}{\sqrt{2}} & 0 & -\frac{i}{\sqrt{2}} \\ -\frac{1}{2} & \frac{1}{\sqrt{2}} & -\frac{1}{2} \end{pmatrix},$$

$$\hat{U}^{+} = \begin{pmatrix} \frac{1}{2} & -\frac{i}{\sqrt{2}} & -\frac{1}{2} \\ \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \\ \frac{1}{2} & \frac{i}{\sqrt{2}} & -\frac{1}{2} \end{pmatrix}.$$

The calculation is as follows.

$$\begin{aligned}
\exp(\frac{\pi i\hat{A}}{2}) &= \exp(\frac{\pi i\hat{A}}{2})(|\psi_1\rangle\langle\psi_1| + |\psi_0\rangle\langle\psi_0| + |\psi_{-1}\rangle\langle\psi_{-1}|) \\
&= \exp(\frac{\pi i}{2})|\psi_1\rangle\langle\psi_1| + \exp(\frac{\pi i}{2}0)|\psi_2\rangle\langle\psi_2| + \exp(-\frac{\pi i}{2})|\psi_3\rangle\langle\psi_3| \\
&= \hat{U}[\exp(\frac{\pi i}{2})|1\rangle\langle 1| + \exp(\frac{\pi i}{2}0)|2\rangle\langle 2| + \exp(-\frac{\pi i}{2})|3\rangle\langle 3|\hat{U} \\
&= \hat{U}\begin{pmatrix} e^{\pi i/2} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & e^{-\pi i/2} \end{pmatrix}\hat{U} = \begin{pmatrix} \frac{1}{2} & \frac{1}{\sqrt{2}} & \frac{1}{2} \\ -\frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \\ \frac{1}{2} & -\frac{1}{\sqrt{2}} & \frac{1}{2} \end{pmatrix}
\end{aligned}$$

since

$$A|\psi_1\rangle = 1|\psi_1\rangle, \qquad A|\psi_2\rangle = 0|\psi_2\rangle, \qquad A|\psi_3\rangle = (-1)|\psi_3\rangle.$$

The above result can be also obtained using the Mathematica.

((**Mathematica**))

Calculate the exponent of the Matrix

```
Clear["Global`*"];
exp_* := exp /. {Complex[re_, im_] :> Complex[re, -im]};
```

$$A = \frac{1}{\sqrt{2}} \{\{0, -i, 0\}, \{i, 0, -i\}, \{0, i, 0\}\};$$

```
eq1 = Eigensystem[A]
```

$$\{\{-1, 1, 0\}, \{\{-1, i\sqrt{2}, 1\}, \{-1, -i\sqrt{2}, 1\}, \{1, 0, 1\}\}\}$$

```
a1 = eq1[[1, 2]]; a2 = eq1[[1, 3]]; a3 = eq1[[1, 1]];
ψ1 = -Normalize[eq1[[2, 2]]]
```

$$\left\{\frac{1}{2}, \frac{i}{\sqrt{2}}, -\frac{1}{2}\right\}$$

```
ψ2 = Normalize[eq1[[2, 3]]]
```

$$\left\{\frac{1}{\sqrt{2}}, 0, \frac{1}{\sqrt{2}}\right\}$$

```
ψ3 = -Normalize[eq1[[2, 1]]]
```

$$\left\{\frac{1}{2}, -\frac{i}{\sqrt{2}}, -\frac{1}{2}\right\}$$

```
eq2 = {ψ1*.ψ2, ψ2*.ψ3 , ψ3*.ψ2} // Simplify
```

{0, 0, 0}

```
UT = {ψ1, ψ2, ψ3}; U = Transpose[UT]; UH = UT*;
A1 = UH.A.U
```

{{1, 0, 0}, {0, 0, 0}, {0, 0, -1}}

$$R = \left\{\left\{\text{Exp}\left[\frac{\pi\, i\, a1}{2}\right], 0, 0\right\}, \left\{0, \text{Exp}\left[\frac{\pi\, i\, a2}{2}\right], 0\right\}, \left\{0, 0, \text{Exp}\left[\frac{\pi\, i\, a3}{2}\right]\right\}\right\} // \text{Simplify}$$

{{i, 0, 0}, {0, 1, 0}, {0, 0, -i}}

```
A1 = U.R.UH // Simplify; A1 // MatrixForm
```

$$\begin{pmatrix} \frac{1}{2} & \frac{1}{\sqrt{2}} & \frac{1}{2} \\ -\frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \\ \frac{1}{2} & -\frac{1}{\sqrt{2}} & \frac{1}{2} \end{pmatrix}$$

Direct calculation for comparison

```
A2 = MatrixExp[π ⅈ A / 2] // Simplify; A2 // MatrixForm
```

$$\begin{pmatrix} \frac{1}{2} & \frac{1}{\sqrt{2}} & \frac{1}{2} \\ -\frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \\ \frac{1}{2} & -\frac{1}{\sqrt{2}} & \frac{1}{2} \end{pmatrix}$$

A.2 Example-2

Calculate the matrix $\exp(\frac{i\phi}{2}\hat{\sigma}_x)$

with

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

Eigensystem[$\hat{\sigma}_x$]

$$|\psi_1\rangle = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix}$$ for the eigenvalue $\lambda = 1$

$$|\psi_{-1}\rangle = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} \end{pmatrix}$$ for the eigenvalue $\lambda = -1$

The unitary operator is

$$\hat{U} = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{pmatrix},$$

$$\hat{U}^{+} = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{pmatrix},$$

$$\hat{U}^{+} \exp(\frac{i\phi}{2}\hat{\sigma}_x)\hat{U} = \exp(\frac{i\phi}{2}\hat{U}^{+}\hat{\sigma}_x\hat{U}) = \begin{pmatrix} e^{\frac{i\phi}{2}} & 0 \\ 0 & e^{-\frac{i\phi}{2}} \end{pmatrix},$$

or

$$\exp(\frac{i\phi}{2}\hat{\sigma}_x) = \hat{U}\begin{pmatrix} e^{\frac{i\phi}{2}} & 0 \\ 0 & e^{-\frac{i\phi}{2}} \end{pmatrix}\hat{U}^{+} = \begin{pmatrix} \cos(\frac{\phi}{2}) & i\sin(\frac{\phi}{2}) \\ i\sin(\frac{\phi}{2}) & \cos(\frac{\phi}{2}) \end{pmatrix}.$$

((**Mathematica**)) Example-2

```
Clear["Global`*"];

exp_* := exp /. {Complex[re_, im_] :> Complex[re, -im]};

σx = {{0, 1}, {1, 0}};

eq1 = Eigensystem[σx]

{{-1, 1}, {{-1, 1}, {1, 1}}}

a1 = eq1[[1, 2]]; a2 = eq1[[1, 1]]; ψ1 = Normalize[eq1[[2, 2]]];
ψ2 = -Normalize[eq1[[2, 1]]];
ψ1*.ψ2

0

UT = {ψ1, ψ2}; U = Transpose[UT]; UH = UT*;

W1 = UH.σx.U

{{1, 0}, {0, -1}}
```

$$A1 = \left\{\left\{\text{Exp}\left[a1\, i\, \frac{\phi}{2}\right], 0\right\}, \left\{0, \text{Exp}\left[a2\, i\, \frac{\phi}{2}\right]\right\}\right\} \text{ // Simplify;}$$

A1 // MatrixForm

$$\begin{pmatrix} e^{\frac{i\phi}{2}} & 0 \\ 0 & e^{-\frac{i\phi}{2}} \end{pmatrix}$$

A2 = U.A1.UH // ExpToTrig // Simplify; A2 // MatrixForm

$$\begin{pmatrix} \text{Cos}\left[\frac{\phi}{2}\right] & i\,\text{Sin}\left[\frac{\phi}{2}\right] \\ i\,\text{Sin}\left[\frac{\phi}{2}\right] & \text{Cos}\left[\frac{\phi}{2}\right] \end{pmatrix}$$

Direct cxalculation for comparison

$$A3 = \text{MatrixExp}\left[i\, \frac{\phi}{2}\, \sigma x\right] \text{ // Simplify; A3 // MatrixForm}$$

$$\begin{pmatrix} \text{Cos}\left[\frac{\phi}{2}\right] & i\,\text{Sin}\left[\frac{\phi}{2}\right] \\ i\,\text{Sin}\left[\frac{\phi}{2}\right] & \text{Cos}\left[\frac{\phi}{2}\right] \end{pmatrix}$$