Stern-Gerlach experiments

Masatsugu Sei Suzuki
Department of Physics, SUNY at Binghamton
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The existence of a spin magnetic moment for the electron was first demonstrated in 1921 in a classic experiment performed by Otto Stern and Walter Gerlach. The Stern–Gerlach experiment was originally assumed to demonstrate the space quantization of the orbital magnetic moment associated with the orbital motion of electrons in silver atoms. In their experiment, a beam of silver atoms was passed through a non-uniform magnetic field along the *z* axis. Such a non-uniform field exerts a force on any magnetic moment, so that each atom is deflected by an amount governed by the orientation of its magnetic moment (the *z*-axis). So the silver atomic beam should split into a number of discrete components. Experimentally the silver atomic beam was clearly split—but into only *two* components, not the odd number ($2l+1$) which is expected from the space quantization of orbital magnetic moments. It was realized that silver atoms in their ground state has no orbital angular momentum ($l = 0$) with *s* state. In 1927, T. E. Phipps and J. B. Taylor had the same experiment with a beam of hydrogen atoms replacing silver, where the ground state has no orbital angular momentum. The result for hydrogen atom was the same as that by Stern and Gerlach for silver atom. From these experiments, it was concluded that there is some contribution to the spin magnetic moment other than the orbital motion of electrons. The origin of the spin magnetic moment is due to the spinning motion of electrons. The spin angular momentum obeys the same quantization rules as orbital angular momentum.

In conclusion, the magnetic moment observed in the Stern–Gerlach experiment is attributed to the spin of the outermost electron in silver. Because all allowed orientations of the spin moment should be represented in the atomic beam, the observed splitting presents a dramatic confirmation of space quantization as applied to electron spin, with the number of components ($2s + 1 = 2$) indicating the value of the spin quantum number s ($= ½$).

Here we discuss the Stern-Gerlach experiment which is a simple experiment that demonstrates the basic principles of quantum mechanics. The measurement of the Stern-Gerlach experiment is equivalent to solving the eigenvalue problems of spin matrices. For simplicity, we use the Dirac notation.

1. Fundamentals

A. Angular momentum and magnetic momentum of one electron

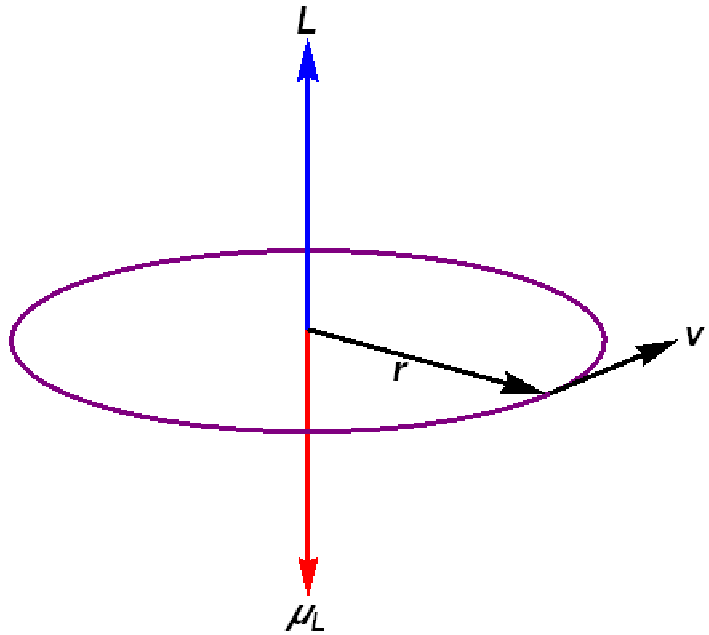


Fig. Orbital (circular) motion of electron with mass *m* and a charge –*e*. The direction of orbital angular momentum *L* is perpendicular to the plane of the motion (*x*-*y* plane).

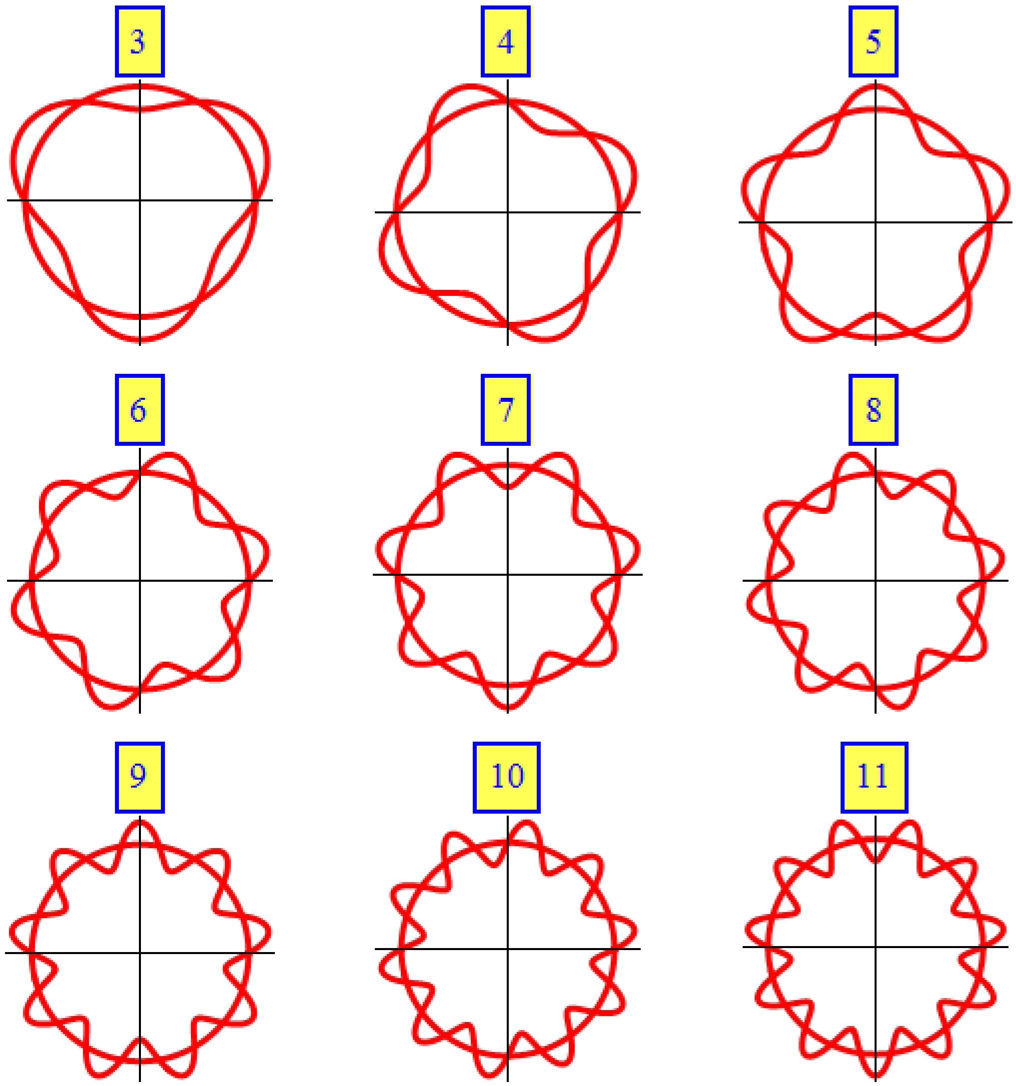
The orbital angular momentum of an electron (charge –*e* and mass *m*) *L* is defined by

$$\boldsymbol{L} = \boldsymbol{r} \times \boldsymbol{p} = \boldsymbol{r} \times (m\boldsymbol{v}), \qquad \text{or} \qquad L_z = mvr. \qquad (1)$$

According to the de Broglie relation, we have

$$p(2\pi r) = \frac{h}{\lambda} 2\pi r = nh, \qquad (2)$$

where p (= mv) is the momentum ($p = \frac{h}{\lambda}$), n is integer, h is the Planck constant, and λ is the wavelength.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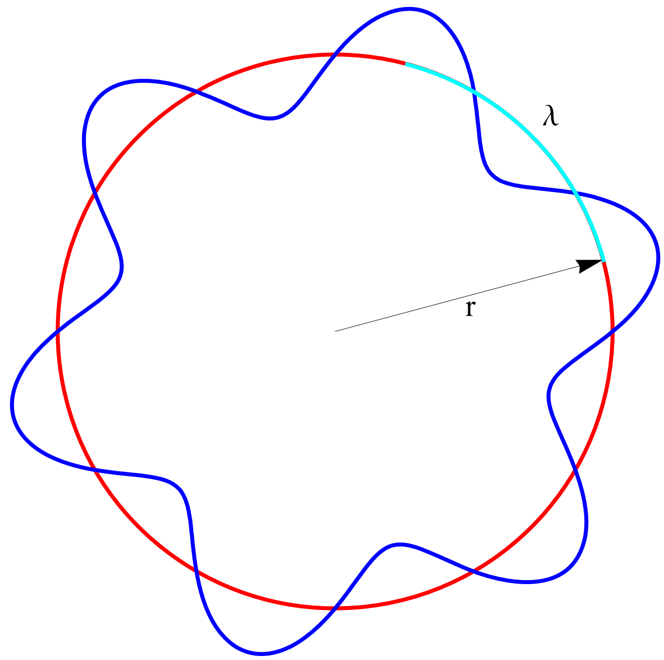

Fig. Acceptable wave on the ring (circular orbit). The circumference should be equal to the integer n (=1, 2, 3,…) times the de Broglie wavelength λ. The picture of fitting the de Broglie waves onto a circle makes clear the reason why the orbital angular momentum is quantized. Only integral numbers of wavelengths can be fitted. Otherwise, there would be destructive interference between waves on successive cycles of the ring.

Then the angular momentum L_z is described by

$$L_z = pr = mvr = \frac{nh}{2\pi} = n\hbar\,. \tag{3}$$

The magnetic moment of the electron is given by

$$\mu_z = \frac{1}{c} I_\theta A\,, \tag{4}$$

where c is the velocity of light, $A = \pi r^2$ is the area of the electron orbit, and I_θ is the current due to the circular motion of the electron. Note that the direction of the current is opposite to that of the velocity because of the negative charge of the electron. The current I_θ is given by

$$I_\theta = -\frac{e}{T} = -\frac{e}{(2\pi r / v)} = -\frac{ev}{2\pi r}\,, \tag{5}$$

where T is the period of the circular motion. Then the magnetic moment is derived as

$$\mu_z = \frac{1}{c} I_\theta A = -\frac{evr}{2c} = -\frac{e}{2mc} L_z = -\frac{e\hbar}{2mc}\frac{L_z}{\hbar} = -\frac{\mu_B}{\hbar} L_z \;\; (e > 0), \tag{6}$$

where μ_B (= $\frac{e\hbar}{2mc}$) is the Bohr magneton.

μ_B = 9.27400915 x 10^{-21} emu (emu=erg/Oe).

Since $L_z = n\hbar$, the magnitude of orbital magnetic moment is $n\mu_B$. The spin magnetic moment is given by

$$\boldsymbol{\mu}_S = -\frac{2\mu_B}{\hbar}\boldsymbol{S}, \tag{7}$$

where $\boldsymbol{S}$ is the spin angular momentum. In quantum mechanics, the above equation is described by

$$\hat{\mu} = -\frac{2\mu_B}{\hbar}\hat{S}, \tag{8}$$

using operators (Dirac). When $\hat{S} = \frac{\hbar}{2}\hat{\sigma}$, we have $\hat{\mu} = -\mu_B\hat{\sigma}$. The spin angular momentum is described by the Pauli matrices (operators)

$$\hat{S}_x = \frac{\hbar}{2}\hat{\sigma}_x,\ \hat{S}_y = \frac{\hbar}{2}\hat{\sigma}_y\ \hat{S}_z = \frac{\hbar}{2}\hat{\sigma}_z. \tag{9}$$

Using the basis,

$$|+z\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix},$$

$$|-z\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \tag{10}$$

we have

$$\hat{\sigma}_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \hat{\sigma}_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \hat{\sigma}_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{11}$$

The commutation relations are valid;

$$[\hat{\sigma}_x, \hat{\sigma}_y] = 2i\hat{\sigma}_z,\ [\hat{\sigma}_y, \hat{\sigma}_z] = 2i\hat{\sigma}_x,\ [\hat{\sigma}_z, \hat{\sigma}_x] = 2i\hat{\sigma}_y. \tag{12}$$

B. Magnetic moment of atom

We consider an isolated atom with incomplete shell of electrons. The orbital angular momentum $\boldsymbol{L}$ and spin angular momentum $\boldsymbol{S}$ are given by

$$\boldsymbol{L} = \boldsymbol{L}_1 + \boldsymbol{L}_2 + \boldsymbol{L}_3 + \ldots, \qquad \boldsymbol{S} = \boldsymbol{S}_1 + \boldsymbol{S}_2 + \boldsymbol{S}_3 + \ldots \tag{13}$$

The total angular momentum $\boldsymbol{J}$ is defined by

$$\boldsymbol{J} = \boldsymbol{L} + \boldsymbol{S}. \tag{14}$$

The total magnetic moment $\boldsymbol{\mu}$ is given by

$$\boldsymbol{\mu} = -\frac{\mu_B}{\hbar}(\boldsymbol{L} + 2\boldsymbol{S}). \tag{15}$$

The Landé g-factor is defined by

$$\boldsymbol{\mu}_J = -\frac{g_J \mu_B}{\hbar}\boldsymbol{J}, \tag{16}$$

where

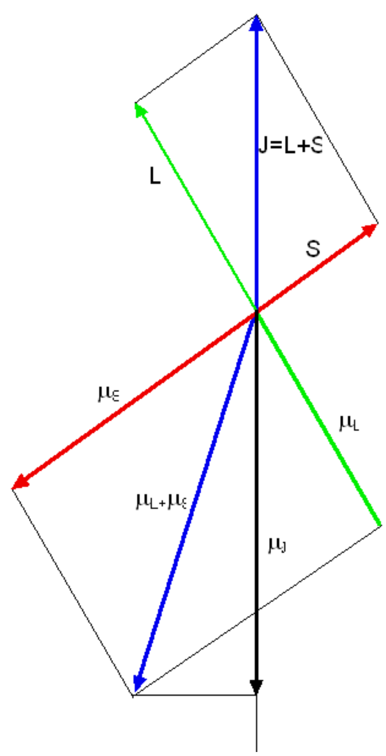

Fig. Basic classical vector model of orbital angular momentum ($\boldsymbol{L}$), spin angular momentum ($\boldsymbol{S}$), orbital magnetic moment ($\boldsymbol{\mu}_L$), and spin magnetic moment ($\boldsymbol{\mu}_S$). $\boldsymbol{J}$ (= $\boldsymbol{L}$ + $\boldsymbol{S}$) is the total angular momentum. $\boldsymbol{\mu}_J$ is the component of the total magnetic moment ($\boldsymbol{\mu}_L$ + $\boldsymbol{\mu}_S$) along the direction ($-J$).

Suppose that

$$\boldsymbol{L} = a\boldsymbol{J} + \boldsymbol{L}_\perp \text{ and } \boldsymbol{S} = b\boldsymbol{J} + \boldsymbol{S}_\perp, \tag{17}$$

where a and b are constants, and the vectors $\boldsymbol{S}_\perp$ and $\boldsymbol{L}_\perp$ are perpendicular to $\boldsymbol{J}$.

Here we have the relation $a + b = 1$, and $\boldsymbol{L}_\perp + \boldsymbol{S}_\perp = 0$. The values of a and b are determined as follows.

$$a = \frac{\boldsymbol{J}\cdot\boldsymbol{L}}{\boldsymbol{J}^2}, \qquad b = \frac{\boldsymbol{J}\cdot\boldsymbol{S}}{\boldsymbol{J}^2}. \tag{18}$$

Here we note that

$$\boldsymbol{J}\cdot\boldsymbol{S} = (\boldsymbol{L}+\boldsymbol{S})\cdot\boldsymbol{S} = \boldsymbol{S}^2 + \boldsymbol{L}\cdot\boldsymbol{S} = \boldsymbol{S}^2 + \frac{\boldsymbol{J}^2 - \boldsymbol{L}^2 - \boldsymbol{S}^2}{2} = \frac{\boldsymbol{J}^2 - \boldsymbol{L}^2 + \boldsymbol{S}^2}{2}, \tag{19}$$

or

$$\boldsymbol{J}\cdot\boldsymbol{S} = \frac{\boldsymbol{J}^2 - \boldsymbol{L}^2 + \boldsymbol{S}^2}{2} = \frac{\hbar^2}{2}[J(J+1) - L(L+1) + S(S+1)], \tag{20}$$

using the average in quantum mechanics. The total magnetic moment $\boldsymbol{\mu}$ is

$$\boldsymbol{\mu} = -\frac{\mu_B}{\hbar}(\boldsymbol{L} + 2\boldsymbol{S}) = -\frac{\mu_B}{\hbar}[(a+2b)\boldsymbol{J} + (L_\perp + 2S_\perp)]. \tag{21}$$

Thus we have

$$\boldsymbol{\mu}_J = -\frac{\mu_B}{\hbar}(a+2b)\boldsymbol{J} = -\frac{\mu_B}{\hbar}(1+b)\boldsymbol{J} = -\frac{g_J\mu_B}{\hbar}\boldsymbol{J}, \tag{22}$$

with

$$g_J = 1 + b = 1 + \frac{\boldsymbol{J}\cdot\boldsymbol{S}}{\boldsymbol{J}^2} = \frac{3}{2} + \frac{S(S+1) - L(L+1)}{2J(J+1)}. \tag{23}$$

((Note))
The spin component is given by

$$\boldsymbol{S} = b\boldsymbol{J} + \boldsymbol{S}_\perp = (g_J - 1)\boldsymbol{J} + \boldsymbol{S}_\perp, \tag{24}$$

with $b = g_J - 1$. The de Gennes factor is defined by

$$\frac{(g_J - 1)^2 \boldsymbol{J}^2}{\hbar^2} = (g_J - 1)^2 J(J+1)\,. \qquad (25)$$

In ions with strong spin-orbit coupling the spin is not a good quantum number, but rather the total angular momentum , $\boldsymbol{J} = \boldsymbol{L}+\boldsymbol{S}$. The spin operator is described by

$$\boldsymbol{S} = (g_J - 1)\boldsymbol{J}\,. \qquad (26)$$

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2 Stern-Gerlach (SG) experiment

We consider the Stern-Gerlach experiment, which provides a direct evidence of the quantization of magnetic moment and angular momentum. One way of measuring the angular momentum is by means of a Stern-Gerlach experiment. Suppose that we want to measure the angular momentum of the electrons in a given type of atom. A beam of these atoms is prepared by evaporation from the solid, and passing the evaporated atoms through a set of collimating slits. This beam then enters a region in which there is an inhomogeneous magnetic field that is normal to the direction of motion of atoms. The apparatus is shown schematically in Fig. The angular magnetic moment is related to the orbital angular momentum as

$$\boldsymbol{\mu}_L = -\frac{e}{2mc}\boldsymbol{L}\,,$$

where e>0. In an inhomogeneous magnetic field, we have an interaction energy called the Zeeman energy,

$$V = -\boldsymbol{\mu}_L \cdot \boldsymbol{B}\,.$$

The atoms experience a force given by

$$\boldsymbol{F} = -\nabla V = -\nabla(-\boldsymbol{\mu}_L \cdot \boldsymbol{B}) = \nabla(\boldsymbol{\mu}_L \cdot \boldsymbol{B})\,.$$

We consider the case when the magnetic field $\mathbf{B} = B_z \mathbf{e}_z$ is applied along the z axis. Then we have the force along the z axis,

$$F_z = \mu_{Lz}\frac{\partial B_z}{\partial z} = -\frac{e\hbar}{2mc}\frac{L_z}{\hbar}\frac{\partial B_z}{\partial z} = -\mu_B \frac{L_z}{\hbar}\frac{\partial B_z}{\partial z}\,,$$

where μ_B $(= e\hbar/2mc)$ is the Bohr magneton. Thus, each atom experiences a force which is proportional to the z component of the orbital angular momentum. The beam is collected some distance from the magnet at a point that is far enough away so that atoms of different L_z is separated. By measuring the deflection one can calculate L_z.

$$\hat{L}_z |l,m\rangle = m\hbar |l,m\rangle\,,$$

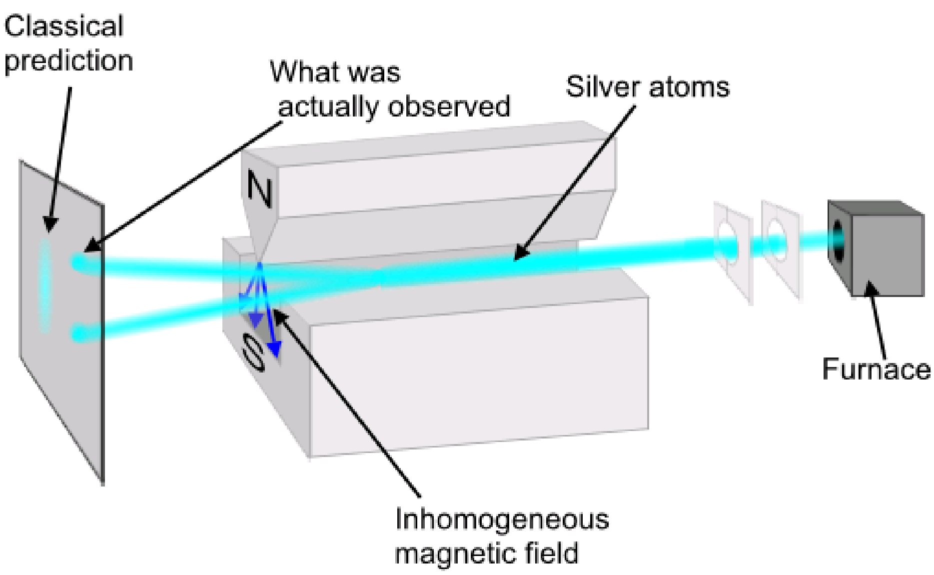
where $m = -l, -l+1, \ldots, l$.

The experiment can also be used to reveal the existence of electron spin. For example, if we send a beam of hydrogen atoms in their ground state, the beam split into two parts. Note that the spin magnetic moment is related to the spin angular momentum as

$$\boldsymbol{\mu}_S = -2\mu_B \frac{\boldsymbol{S}}{\hbar},$$

where $\boldsymbol{\mu}_S$ is the spin magnetic moment and $\boldsymbol{S}$ ($= \frac{\hbar}{2}\boldsymbol{\sigma}$) is the spin angular momentum, and

$$\hat{S}_z|+z\rangle = \frac{\hbar}{2}|+z\rangle, \qquad \hat{S}_z|-z\rangle = -\frac{\hbar}{2}|-z\rangle.$$



http://en.wikipedia.org/wiki/Stern%E2%80%93Gerlach_experiment

Fig. Stern-Gerlach (SG) apparatus. A beam of particles with magnetic moment enters the inhomogeneous magnetic field. Classically, the beam is expected to fan out and a produce a continuous trace. In fact, the atomic beam is split into two beams, indicating that the magnetic moments of the atoms are quantized to two orientations in space.

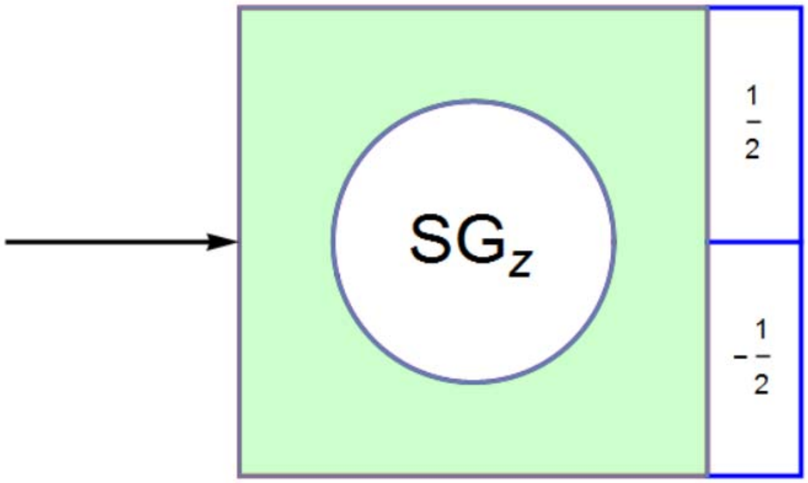


Fig. Schematic diagram for the Stern-Gerlach experiment in the presence of a magnetic field along the *z* axis.

3 Stern-Gerlach for *S* = 1/2 with the magnetic field along the *z* axis

Spin angular momentum is related to the Pauli matrices as

$$\hat{S}_x = \frac{\hbar}{2}\hat{\sigma}_x, \qquad \hat{S}_y = \frac{\hbar}{2}\hat{\sigma}_y \qquad \hat{S}_z = \frac{\hbar}{2}\hat{\sigma}_z$$

The eigenkets of $\hat{S}_z$ are given by

$$|+z\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \qquad |-z\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$ (the column vector, 2 x 1 matrix)

The Pauli matrices are defined as

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

The commutation relations

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

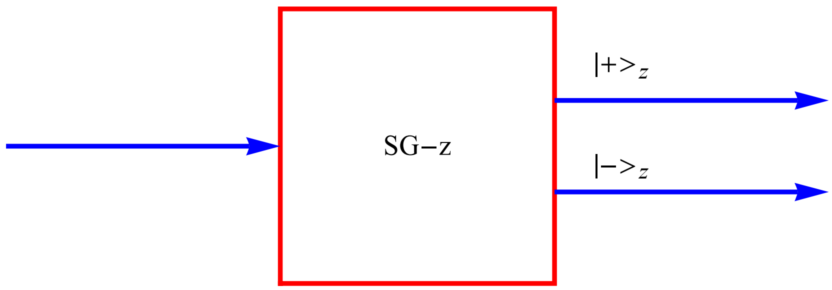
SG$_z$ stands for an apparatus with the inhomogeneous magnetic field along the *z* direction. We assume that $\frac{\partial B_z}{\partial z} > 0$. The atom with $\mu_z > 0$ ($S_z < 0$) experiences a downward force, while the atom with $\mu_z < 0$ ($S_z > 0$) experiences a upward force, where the force F_z along the *z* axis is given by

$$F_z = 2\mu_B \frac{S_z}{\hbar}\frac{\partial B_z}{\partial z},$$

where

$$\boldsymbol{\mu} = -2\mu_B \frac{\boldsymbol{S}}{\hbar},$$

where μ_B is the Bohr magneton, and the magnetic moment $\boldsymbol{\mu}$ is antiparallel to the spin angular momentum $\boldsymbol{S}$.



The beam is then expected to get slit according to the values of μ (or S_z). In other words, the SG apparatus measures the z-component of $\boldsymbol{\mu}$, or equivalently, the z-component of $\boldsymbol{S}$.

$$\hat{S}_z|+z\rangle = \frac{\hbar}{2}\hat{\sigma}_z|+z\rangle = \frac{\hbar}{2}|+z\rangle, \qquad \text{or} \qquad \hat{\sigma}_z|+z\rangle = |+z\rangle.$$

$$\hat{S}_z|-\rangle z = \frac{\hbar}{2}\hat{\sigma}_z|-z\rangle = -\frac{\hbar}{2}|-z\rangle, \qquad \text{or} \qquad \hat{\sigma}_z|-z\rangle = -|-z\rangle.$$

where

$$\hat{\sigma}_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \qquad |+z\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |-z\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

We use the Dirac notation; the ket vector and the bra vector.

$|+z\rangle$, $|-z\rangle$ (the ket vectors, we use these as basis)

$\langle +z| = (1 \quad 0)$, $\langle -z| = (0 \quad 1)$ (the bra vector, the row vector, 1 x 2 matrix)

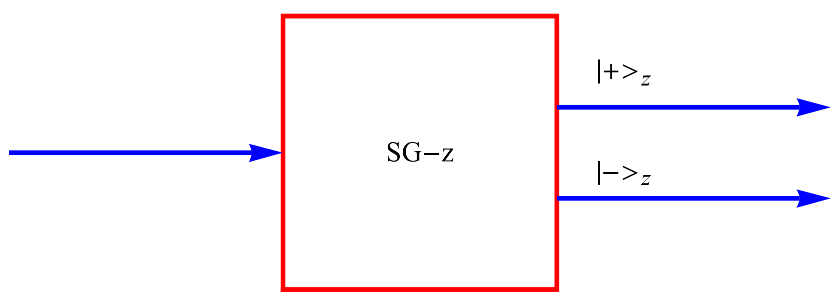
The denotations of bra and ket vectors are from the words, "bra(c)ket.

((**Note**))

The notations of kets for the eigenstates of $\hat{S}_x$, $\hat{S}_y$, and $\hat{S}_z$ are different for different standard textbooks of quantum mechanics. Here we use the notations used by Townsend.

Townsend	Sakurai	McinTyre
$\|+z\rangle$	$\|+\rangle$	$\|+\rangle$
$\|-z\rangle$	$\|-\rangle$	$\|-\rangle$
$\|+x\rangle$	$\|S_x;+\rangle$	$\|+\rangle_x$
$\|-x\rangle$	$\|S_x;-\rangle$	$\|-\rangle_x$
$\|+y\rangle$	$\|S_y;+\rangle$	$\|+\rangle_y$
$\|-y\rangle$	$\|S_y;-\rangle$	$\|-\rangle_y$
$\|+\boldsymbol{n}\rangle$	$\|\hat{\boldsymbol{n}},+\rangle$	$\|+\rangle_{\boldsymbol{n}}$
$\|-\boldsymbol{n}\rangle$	$\|\hat{\boldsymbol{n}},-\rangle$	$\|-\rangle_{\boldsymbol{n}}$

4. Eigenvalue and eigenkets: $\hat{\sigma}_z$



The eigenkets:

$$\hat{\sigma}_z|+z\rangle = |+z\rangle, \qquad \hat{\sigma}_z|-z\rangle = -|-z\rangle$$

with

$$|+z\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |-z\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

We note that

$$\hat{\sigma}_z|+z\rangle = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} = |+z\rangle, \qquad \hat{\sigma}_z|-z\rangle = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ -1 \end{pmatrix} = -|-z\rangle$$

(a) The inner product

We define the inner product as

$$\langle +z|+z\rangle = (1 \quad 0)^* \begin{pmatrix} 1 \\ 0 \end{pmatrix} = (1 \quad 0)\begin{pmatrix} 1 \\ 0 \end{pmatrix} = 1,$$

$$\langle -z|+z\rangle = (0 \quad 1)^* \begin{pmatrix} 1 \\ 0 \end{pmatrix} = (0 \quad 1)\begin{pmatrix} 1 \\ 0 \end{pmatrix} = 0,$$

$$\langle -z|-z\rangle = (0 \quad 1)^* \begin{pmatrix} 0 \\ 1 \end{pmatrix} = (0 \quad 1)\begin{pmatrix} 0 \\ 1 \end{pmatrix} = 1$$

(b) The Closure relation (completeness)

$$|+z\rangle\langle +z| = \begin{pmatrix} 1 \\ 0 \end{pmatrix}(1 \quad 0) = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \qquad |-z\rangle\langle -z| = \begin{pmatrix} 0 \\ 1 \end{pmatrix}(0 \quad 1) = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$$

Thus we have

$$|+z\rangle\langle +z| + |-z\rangle\langle -z| = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \hat{1}, \qquad \text{(identity matrix)}$$

(d) Spin operator $\hat{S}_z$

The operator $\hat{S}_z$ can be written as

$$\hat{S}_z = \hat{S}_z(|+z\rangle\langle+z| + |-z\rangle\langle-z|)$$
$$= \frac{\hbar}{2}(|+z\rangle\langle+z| - |-z\rangle\langle-z|) \,.$$

(e) The rotation matrix

The rotation matrix is defined by

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

5. Probability, average value, and uncertainty

Suppose that the state of the system before entering the SG-z device is given by the superposition of $|+z\rangle$ and $|-z\rangle$,

$$|\psi\rangle = \alpha|+z\rangle + \beta|-z\rangle = \begin{pmatrix} \alpha \\ \beta \end{pmatrix},$$

where α and β are complex numbers, and

$$|\alpha|^2 + |\beta|^2 = 1 \,.$$

$$\langle +z|\psi\rangle = \alpha\langle +z|+z\rangle + \beta\langle +z|-z\rangle = \alpha \,,$$

$$\langle -z|\psi\rangle = \alpha\langle -z|+z\rangle + \beta\langle -z|-z\rangle = \beta \,.$$

The state is normalized such that the inner product is equal to 1;

$$\langle\psi|\psi\rangle = 1 = \begin{pmatrix} \alpha^* & \beta^* \end{pmatrix}\begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \alpha\alpha^* + \beta\beta^* = |\alpha|^2 + |\beta|^2 = 1 \,,$$

where

$$\langle\psi| = \alpha^*\langle +z| + \beta^*\langle -z| = \begin{pmatrix} \alpha^* & \beta^* \end{pmatrix},$$

where "*" denotes the complex conjugate; $(1+i)^* = 1-i$.

$$\langle\psi|+z\rangle = \alpha^* = \langle +z|\psi\rangle^*, \qquad \langle\psi|-z\rangle = \beta^* = \langle -z|\psi\rangle^*.$$

(a) Probability

The probability of finding the system in the state $|+z\rangle$ is defined by

$$P_+ = |\langle +z|\psi\rangle|^2 = |\alpha|^2,$$

since

$$\langle +z|\psi\rangle = \begin{pmatrix} 1 & 0 \end{pmatrix}\begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \alpha .$$

The probability of finding the system in the state $|-z\rangle$ is defined by

$$P_- = |\langle -z|\psi\rangle|^2 = |\beta|^2,$$

since

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

(b) Expectation value $\langle\psi|\hat{S}_z|\psi\rangle = \langle \hat{S}_z \rangle$

The expectation value (average value) is given by

$$\langle\psi|\hat{S}_z|\psi\rangle = \frac{\hbar}{2}\begin{pmatrix} \alpha^* & \beta^* \end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \frac{\hbar}{2}(|\alpha|^2 - |\beta|^2) .$$

This form can be also derived from

$$\langle\psi|\hat{S}_z|\psi\rangle = \frac{\hbar}{2}P_+ + (-\frac{\hbar}{2})P_- = \frac{\hbar}{2}|\alpha|^2 - \frac{\hbar}{2}|\beta|^2 .$$

(c) Uncertainty $\Delta S_z = \sqrt{\langle\psi|\hat{S}_z{}^2|\psi\rangle - \langle\psi|\hat{S}_z|\psi\rangle^2}$

$$\langle\psi|\hat{S}_z{}^2|\psi\rangle = \frac{\hbar^2}{4}\begin{pmatrix}\alpha^* & \beta^*\end{pmatrix}\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}\begin{pmatrix}\alpha\\ \beta\end{pmatrix} = \frac{\hbar^2}{4}(|\alpha|^2 + |\beta|^2) = 1 .$$

since

$$\hat{S}_z{}^2 = \frac{\hbar^2}{4}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix} = \frac{\hbar^2}{4}\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix} = \frac{\hbar^2}{4}\hat{1} .$$

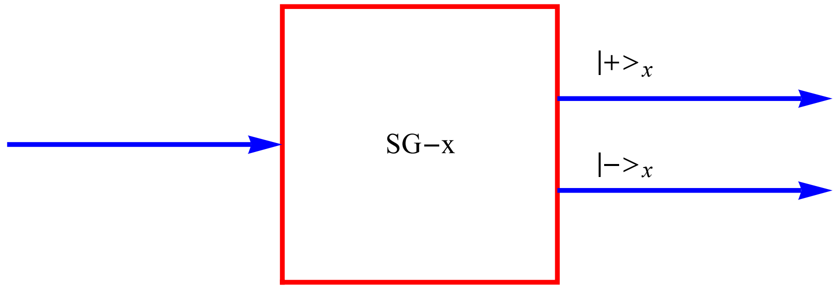
$\langle\psi|\hat{S}_z{}^2|\psi\rangle$ can be also determined from

$$\langle\psi|\hat{S}_z{}^2|\psi\rangle = (\frac{\hbar}{2})^2 P_+ + (-\frac{\hbar}{2})^2 P_- = \frac{\hbar^2}{4}(|\alpha|^2 + |\beta|^2) = \frac{\hbar^2}{4} .$$

Then the uncertainty ΔS_z is obtained as

$$\begin{aligned}\Delta S_z &= \sqrt{\langle\psi|\hat{S}_z{}^2|\psi\rangle - \langle\psi|\hat{S}_z|\psi\rangle^2}\\ &= \frac{\hbar}{2}\sqrt{1 - (|\alpha|^2 - |\beta|^2)^2}\\ &= \frac{\hbar}{2}\sqrt{(1 - |\alpha|^2 + |\beta|^2)(1 + |\alpha|^2 - |\beta|^2)}\\ &= \frac{\hbar}{2}\sqrt{4|\alpha|^2|\beta|^2} = \hbar|\alpha||\beta|\end{aligned}$$

5. Stern-Gerlach for $S = 1/2$ with the magnetic field along the x axis



Here we discuss the expression for $|\pm x\rangle$

$$\hat{\sigma}_x|\pm x\rangle = \pm|\pm x\rangle, \qquad \text{(eigenvalue problem)}$$

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

This matrix form of $\hat{\sigma}_x$ will be derived later.

$$|+x\rangle = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix} = \frac{1}{\sqrt{2}}(|+z\rangle + |-z\rangle),$$

$$|-x\rangle = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} \end{pmatrix} = \frac{1}{\sqrt{2}}(|+z\rangle - |-z\rangle).$$

The bra vector (the row vector)

$$\langle +x| = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix}, \qquad \langle -x| = \begin{pmatrix} \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{pmatrix}$$

The closure relation:

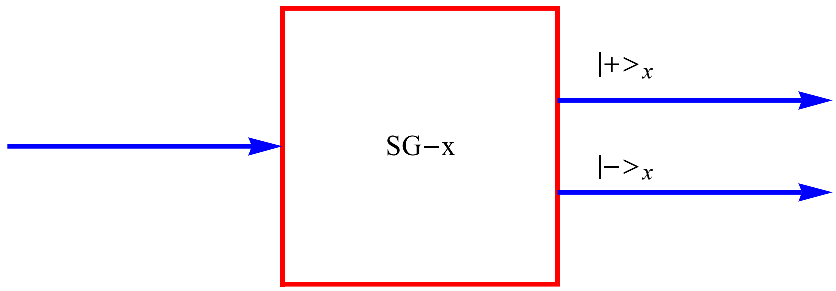
$$|+x\rangle\langle +x| = \frac{1}{2}\begin{pmatrix} 1 \\ 1 \end{pmatrix}\begin{pmatrix} 1 & 1 \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix},$$

$$|-x\rangle\langle -x| = \frac{1}{2}\begin{pmatrix} 1 \\ -1 \end{pmatrix}(1 \quad -1) = \frac{1}{2}\begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}.$$

Then we have

$$|+x\rangle\langle +x| + |-x\rangle\langle -x| = \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} + \frac{1}{2}\begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \hat{1}.$$

6. Eigenvalue and eigenkets: $\hat{\sigma}_x$



The eigenkets:

$\hat{\sigma}_x|+x\rangle = |+x\rangle$, $\hat{\sigma}_x|-x\rangle = -|-x\rangle$, (eigenvalue problem)

Note that

$$\hat{\sigma}_x|+x\rangle = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 1 \\ 1 \end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix} = |+x\rangle,$$

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

The operator $\hat{S}_x$ is expressed by

$$\begin{aligned}\hat{S}_x &= \hat{S}_x(|+x\rangle\langle+x| + |-x\rangle\langle-x|) \\ &= \frac{\hbar}{2}(|+x\rangle\langle+x| - |-x\rangle\langle-x|)\end{aligned}.$$

The rotation matrix is given by

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

((**Eigenvalue problem**))

$$\hat{\sigma}_x|+z\rangle = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix} = |-z\rangle,$$

$$\hat{\sigma}_x|-z\rangle = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} = |+z\rangle$$

Thus $|+z\rangle$ and $|-z\rangle$ are not the eigenkets of $\hat{\sigma}_x$. However, we ahve

$$\hat{\sigma}_x\frac{1}{\sqrt{2}}(|+z\rangle + |-z\rangle) = \frac{1}{\sqrt{2}}(|+z\rangle + |-z\rangle) \qquad \text{(eigenvalue +1)}$$

$$\hat{\sigma}_x\frac{1}{\sqrt{2}}(|+z\rangle - |-z\rangle) = -\frac{1}{\sqrt{2}}(|+z\rangle - |-z\rangle) \qquad \text{(eigenvalue -1)}$$

This means that

$$|+x\rangle = \frac{1}{\sqrt{2}}(|+z\rangle + |-z\rangle), \qquad |-x\rangle = \frac{1}{\sqrt{2}}(|+z\rangle - |-z\rangle).$$

((**Probability and expectation**))

Suppose that the state of the system before entering the SG-*x* device is given by the superposition of $|+z\rangle$ and $|-z\rangle$,

$$|\psi\rangle = \alpha|+z\rangle + \beta|-z\rangle = \begin{pmatrix} \alpha \\ \beta \end{pmatrix},$$

where α and β are complex numbers, and

$$|\alpha|^2 + |\beta|^2 = 1 .$$

The probability of finding the system in the state $|+x\rangle$ is defined by

$$\begin{aligned} P_+ &= |\langle +x|\psi\rangle|^2 \\ &= \frac{1}{2}|\alpha+\beta|^2 \\ &= \frac{1}{2}(\alpha+\beta)(\alpha^*+\beta^*) \\ &= \frac{1}{2}(|\alpha|^2+|\beta|^2+\alpha^*\beta+\alpha\beta^*) \end{aligned},$$

since

$$\langle +x|\psi\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \end{pmatrix}\begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \frac{1}{\sqrt{2}}(\alpha+\beta) .$$

The probability of finding the system in the state $|-x\rangle$ is defined by

$$
\begin{aligned}
P_- &= \left|\langle -x|\psi\rangle\right|^2 \\
&= \frac{1}{2}|\alpha-\beta|^2 \\
&= \frac{1}{2}(\alpha-\beta)(\alpha^*-\beta^*) \\
&= \frac{1}{2}(|\alpha|^2+|\beta|^2-\alpha^{*2}\beta-\alpha\beta^*)
\end{aligned}
$$

since

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

The expectation value $\langle\psi|\hat{S}_x|\psi\rangle$ is

$$
\begin{aligned}
\langle\psi|\hat{S}_x|\psi\rangle &= \begin{pmatrix}\alpha^* & \beta^*\end{pmatrix}\begin{pmatrix}0 & 1 \\ 1 & 0\end{pmatrix}\begin{pmatrix}\alpha \\ \beta\end{pmatrix} \\
&= \begin{pmatrix}\alpha^* & \beta^*\end{pmatrix}\begin{pmatrix}\beta \\ \alpha\end{pmatrix} \\
&= \alpha^*\beta+\alpha\beta^*
\end{aligned}
$$

This expectation value can be also obtained as

$$
\begin{aligned}
\langle\psi|\hat{S}_x|\psi\rangle &= \frac{\hbar}{2}P_+ + (-\frac{\hbar}{2})P_- \\
&= \frac{\hbar}{4}(|\alpha|^2+|\beta|^2+\alpha^*\beta+\alpha\beta^*) - \frac{\hbar}{4}(|\alpha|^2+|\beta|^2-\alpha^*\beta-\alpha\beta^*) \\
&= \frac{\hbar}{2}(\alpha^*\beta+\alpha\beta^*)
\end{aligned}
$$

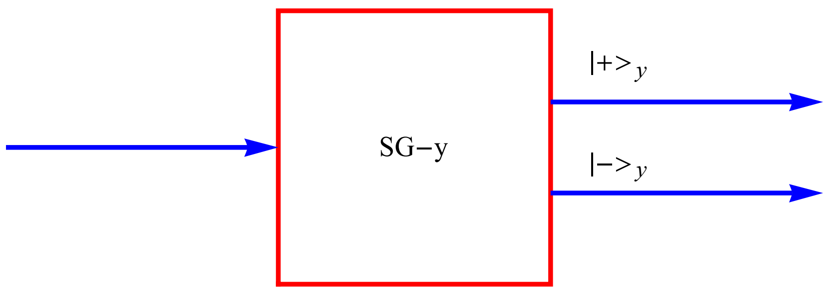
Note that

$$\langle\psi|\hat{S}_x^{\ 2}|\psi\rangle = (\frac{\hbar}{2})^2 P_+ + (-\frac{\hbar}{2})^2 P_-$$
$$= \frac{\hbar^2}{4}$$

The uncertainty is evaluated as

$$\Delta S_x = \frac{\hbar}{2}\sqrt{1-(\alpha^*\beta+\alpha\beta^*)^2}$$

7. Eigenvalue and eigenkets: $\hat{\sigma}_y$



$$\hat{\sigma}_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}.$$

The eigenkets:

$$\hat{\sigma}_y|+y\rangle = |+y\rangle, \qquad \hat{\sigma}_y|-y\rangle = -|-y\rangle, \qquad \text{(eigenvalue problem)}$$

with

$$|+y\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ i \end{pmatrix} = \frac{1}{\sqrt{2}}(|+z\rangle + i|-z\rangle), \quad |-y\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -i \end{pmatrix} = \frac{1}{\sqrt{2}}(|+z\rangle - i|-z\rangle).$$

Note that

$$\hat{\sigma}_y\left|+y\right\rangle = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ i \end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}\begin{pmatrix} 1 \\ i \end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix} -i^2 \\ i \end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ i \end{pmatrix} = \left|+y\right\rangle,$$

$$\hat{\sigma}_y\left|-y\right\rangle = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -i \end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}\begin{pmatrix} 1 \\ -i \end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix} i^2 \\ i \end{pmatrix} = -\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -i \end{pmatrix} = -\left|-y\right\rangle,$$

The bra vector (the row vector)

$$\left\langle +y\right| = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{i}{\sqrt{2}} \end{pmatrix}^* = \begin{pmatrix} \frac{1}{\sqrt{2}} & -\frac{i}{\sqrt{2}} \end{pmatrix},$$

$$\left\langle -y\right| = \begin{pmatrix} \frac{1}{\sqrt{2}} & -\frac{i}{\sqrt{2}} \end{pmatrix}^* = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{i}{\sqrt{2}} \end{pmatrix}.$$

The closure relation:

$$\left|+y\right\rangle\left\langle +y\right| = \frac{1}{2}\begin{pmatrix} 1 \\ i \end{pmatrix}\begin{pmatrix} 1 & -i \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 1 & -i \\ i & 1 \end{pmatrix},$$

$$\left|-y\right\rangle\left\langle -y\right| = \frac{1}{2}\begin{pmatrix} 1 \\ -i \end{pmatrix}\begin{pmatrix} 1 & i \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 1 & i \\ -i & 1 \end{pmatrix}.$$

Then we have

$$\left|+y\right\rangle\left\langle +y\right| + \left|-y\right\rangle\left\langle -y\right| = \frac{1}{2}\begin{pmatrix} 1 & -i \\ i & 1 \end{pmatrix} + \frac{1}{2}\begin{pmatrix} 1 & i \\ -i & 1 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \hat{1}.$$

The operator $\hat{S}_y$ is expressed by

$$\begin{aligned} \hat{S}_y &= \hat{S}_y(\left|+y\right\rangle\left\langle +y\right| + \left|-y\right\rangle\left\langle -y\right|) \\ &= \frac{\hbar}{2}(\left|+y\right\rangle\left\langle +y\right| - \left|-y\right\rangle\left\langle -y\right|) \end{aligned}.$$

The rotation matrix is given by

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

((**Eigenvalue problem**))

$$\hat{\sigma}_y |+z\rangle = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ i \end{pmatrix} = i|-z\rangle ,$$

$$\hat{\sigma}_y |-z\rangle = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} -i \\ 0 \end{pmatrix} = -i|+z\rangle .$$

Thus $|+z\rangle$ and $|-z\rangle$ are not the eigenkets of $\hat{\sigma}_y$. However, we ahve

$$\hat{\sigma}_y \frac{1}{\sqrt{2}}(|+z\rangle + i|-z\rangle) = \frac{1}{\sqrt{2}}(|+z\rangle + i|-z\rangle), \quad \text{(eigenvalue +1)}$$

$$\hat{\sigma}_y \frac{1}{\sqrt{2}}(|+z\rangle - i|-z\rangle) = -\frac{1}{\sqrt{2}}(|+z\rangle - i|-z\rangle), \quad \text{(eigenvalue -1)}$$

This means that

$$|+y\rangle = \frac{1}{\sqrt{2}}(|+z\rangle + i|-z\rangle),$$

$$|-y\rangle = \frac{1}{\sqrt{2}}(|+z\rangle - i|-z\rangle).$$

((**Probability and expectation**))

Suppose that the state of the system before entering the SG-y device is given by the superposition of $\left|+z\right\rangle$ and $\left|-z\right\rangle$,

$$\left|\psi\right\rangle = \alpha\left|+z\right\rangle + \beta\left|-z\right\rangle = \begin{pmatrix}\alpha \\ \beta\end{pmatrix}.$$

where α and β are complex numbers, and

$$\left|\alpha\right|^2 + \left|\beta\right|^2 = 1.$$

The probability of finding the system in the state $\left|+y\right\rangle$ is defined by

$$\begin{aligned}P_+ &= \left|\left\langle +y\middle|\psi\right\rangle\right|^2 \\ &= \frac{1}{2}\left|\alpha - i\beta\right|^2 \\ &= \frac{1}{2}(\alpha - i\beta)(\alpha^* + i\beta^*) \\ &= \frac{1}{2}(\left|\alpha\right|^2 + \left|\beta\right|^2 - i\alpha^*\beta + i\alpha\beta^*)\end{aligned},$$

since

$$\left\langle +y\middle|\psi\right\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1 & -i\end{pmatrix}\begin{pmatrix}\alpha \\ \beta\end{pmatrix} = \frac{1}{\sqrt{2}}(\alpha - i\beta).$$

The probability of finding the system in the state $\left|-y\right\rangle$ is defined by

$$\begin{aligned}P_- &= \left|\left\langle -y\middle|\psi\right\rangle\right|^2 \\ &= \frac{1}{2}\left|\alpha + i\beta\right|^2 \\ &= \frac{1}{2}(\alpha + i\beta)(\alpha^* - i\beta^*) \\ &= \frac{1}{2}(\left|\alpha\right|^2 + \left|\beta\right|^2 + i\alpha^*\beta - i\alpha\beta^*)\end{aligned}$$

since

$$\langle -y|\psi\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1 & i\end{pmatrix}\begin{pmatrix}\alpha \\ \beta\end{pmatrix} = \frac{1}{\sqrt{2}}(\alpha + i\beta)\ .$$

The expectation value $\langle\psi|\hat{S}_x|\psi\rangle$ is

$$\begin{aligned}\langle\psi|\hat{S}_y|\psi\rangle &= \frac{\hbar}{2}\begin{pmatrix}\alpha^* & \beta^*\end{pmatrix}\begin{pmatrix}0 & -i \\ i & 0\end{pmatrix}\begin{pmatrix}\alpha \\ \beta\end{pmatrix} \\ &= \frac{\hbar}{2}\begin{pmatrix}\alpha^* & \beta^*\end{pmatrix}\begin{pmatrix}-i\beta \\ i\alpha\end{pmatrix} \\ &= \frac{\hbar}{2}i(-\alpha^*\beta + \alpha\beta^*)\end{aligned}$$

This expectation value can be also obtained as

$$\begin{aligned}\langle\psi|\hat{S}_y|\psi\rangle &= \frac{\hbar}{2}P_+ + (-\frac{\hbar}{2})P_- \\ &= \frac{\hbar}{4}(|\alpha|^2 + |\beta|^2 - i\alpha^*\beta + i\alpha\beta^*) - \frac{\hbar}{4}(|\alpha|^2 + |\beta|^2 + i\alpha^*\beta - i\alpha\beta^*) \\ &= i\frac{\hbar}{2}(-\alpha^*\beta + \alpha\beta^*)\end{aligned}$$

8. Properties of Pauli matrix

The Pauli matrices are defined as

$$\hat{1} = \begin{pmatrix}1 & 0 \\ 0 & 1\end{pmatrix}, \qquad \hat{\sigma}_1 = \hat{\sigma}_x = \begin{pmatrix}0 & 1 \\ 1 & 0\end{pmatrix},$$

$$\hat{\sigma}_2 = \hat{\sigma}_y = \begin{pmatrix}0 & -i \\ i & 0\end{pmatrix}, \qquad \hat{\sigma}_3 = \hat{\sigma}_z = \begin{pmatrix}1 & 0 \\ 0 & -1\end{pmatrix}$$

(a) Commutation relations

$$\hat{\sigma}_1\hat{\sigma}_2 = -\hat{\sigma}_2\hat{\sigma}_1 = i\hat{\sigma}_3,$$

$$\hat{\sigma}_2\hat{\sigma}_3 = -\hat{\sigma}_3\hat{\sigma}_2 = i\hat{\sigma}_1,$$

$$\hat{\sigma}_3\hat{\sigma}_1 = -\hat{\sigma}_1\hat{\sigma}_3 = i\hat{\sigma}_2,$$

$$\hat{\sigma}_1^2 = \hat{\sigma}_2^2 = \hat{\sigma}_3^2.$$

Solution: see any textbook for the solution.

$$\hat{\sigma}_1\hat{\sigma}_2 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = \begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix} = i\hat{\sigma}_3,$$

$$\hat{\sigma}_2\hat{\sigma}_1 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} -i & 0 \\ 0 & i \end{pmatrix} = -i\hat{\sigma}_3,$$

$$\hat{\sigma}_1\hat{\sigma}_1 = \hat{\sigma}_1{}^2 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \hat{1},$$

$$\hat{\sigma}_2\hat{\sigma}_2 = \hat{\sigma}_2{}^2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \hat{1},$$

$$\hat{\sigma}_3\hat{\sigma}_3 = \hat{\sigma}_3{}^2 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \hat{1}.$$

(b)

$$Tr(\hat{\sigma}_1) = Tr(\hat{\sigma}_2) = Tr(\hat{\sigma}_3) = 0,$$

$$\det(\hat{\sigma}_1) = \det(\hat{\sigma}_2) = \det(\hat{\sigma}_3) = -1$$

where Tr denotes a trace and det denotes a determinant.

(c)

For two arbitrary vectors ***A*** and ***B***,

$$(\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{A})(\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{B}) = (\boldsymbol{A}\cdot\boldsymbol{B})\hat{1} + i\hat{\boldsymbol{\sigma}}\cdot(\boldsymbol{A}\times\boldsymbol{B}),$$

where

$$\boldsymbol{A} = (A_x, A_y, A_z) \text{ and } \boldsymbol{B} = (B_x, B_y, B_z).$$

(d) ((Mathematica)) Schaum's problem 7-11

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

expr_* := expr /. {Complex[a_, b_] :> Complex[a, -b]}

σx = {{0, 1}, {1, 0}}; σy = {{0, -ⅈ}, {ⅈ, 0}}; σz = {{1, 0}, {0, -1}}; II = {{1, 0}, {0, 1}}
{{1, 0}, {0, 1}}

fA = σx Ax + σy Ay + σz Az
{{Az, Ax - ⅈ Ay}, {Ax + ⅈ Ay, -Az}}

fB = σx Bx + σy By + σz Bz
{{Bz, Bx - ⅈ By}, {Bx + ⅈ By, -Bz}}

eq1 = fA.fB // Expand // Simplify
{{Ax (Bx + ⅈ By) + Ay (-ⅈ Bx + By) + Az Bz, Az Bx - ⅈ Az By - Ax Bz + ⅈ Ay Bz},
 {-Az (Bx + ⅈ By) + (Ax + ⅈ Ay) Bz, Ax (Bx - ⅈ By) + Ay (ⅈ Bx + By) + Az Bz}}

A = {Ax, Ay, Az}; B = {Bx, By, Bz}; AB = Cross[A, B]
{-Az By + Ay Bz, Az Bx - Ax Bz, -Ay Bx + Ax By}

σAB = σx AB[[1]] + σy AB[[2]] + σz AB[[3]];

eq2 = A.B II + ⅈ σAB // Simplify
{{Ax (Bx + ⅈ By) + Ay (-ⅈ Bx + By) + Az Bz, Az Bx - ⅈ Az By - Ax Bz + ⅈ Ay Bz},
 {-Az (Bx + ⅈ By) + (Ax + ⅈ Ay) Bz, Ax (Bx - ⅈ By) + Ay (ⅈ Bx + By) + Az Bz}}

eq1 - eq2
{{0, 0}, {0, 0}}
```

(e)

When ***A*** = ***B*** = ***n*** (unit vector)

$$(\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{n})(\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{n}) = \hat{1}.$$

(f)

Suppose a 2x2 matrix $\hat{X}$ (not necessarily Hermitian, nor unitary) is

$$\hat{X} = a_0\hat{1} + \hat{\sigma}_1 a_1 + \hat{\sigma}_2 a_2 + \hat{\sigma}_3 a_3 = \begin{pmatrix} a_0 + a_3 & a_1 - ia_2 \\ a_1 + ia_2 & a_0 - a_3 \end{pmatrix} = \begin{pmatrix} X_{11} & X_{12} \\ X_{21} & X_{22} \end{pmatrix},$$

with

$$X_{11} = a_0 + a_3,\ X_{12} = a_1 - ia_2,\ X_{21} = a_1 + ia_2, \text{ and } X_{22} = a_0 - a_3.$$

We show that

$$Tr(\hat{1}) = 2,\ Tr(\hat{\sigma}_1) = Tr(\hat{\sigma}_2) = Tr(\hat{\sigma}_3) = 0$$

$$Tr(\hat{X}) = 2a_0$$

$$Tr(\hat{\sigma}_1\hat{X}) = 2a_1$$

$$Tr(\hat{\sigma}_2\hat{X}) = 2a_2$$

$$Tr(\hat{\sigma}_3\hat{X}) = 2a_3$$

((**Proof**))

$$Tr(\hat{1}) = 2,\ Tr(\hat{\sigma}_1) = Tr(\hat{\sigma}_2) = Tr(\hat{\sigma}_3) = 0,$$

$$Tr(\hat{X}) = Tr(a_0\hat{I} + \hat{\sigma}_1 a_1 + \hat{\sigma}_2 a_2 + \hat{\sigma}_3 a_3) = 2a_0.$$

Using the relations

$$\hat{\sigma}_1\hat{\sigma}_2 = -\hat{\sigma}_2\hat{\sigma}_1 = i\hat{\sigma}_3$$

$$\hat{\sigma}_2\hat{\sigma}_3 = -\hat{\sigma}_3\hat{\sigma}_2 = i\hat{\sigma}_1$$

$$\hat{\sigma}_3\hat{\sigma}_1 = -\hat{\sigma}_1\hat{\sigma}_3 = i\hat{\sigma}_2$$

$$\hat{\sigma}_1^2 = \hat{\sigma}_2^2 = \hat{\sigma}_3^2$$

$$\begin{aligned} Tr(\hat{\sigma}_1\hat{X}) &= Tr[\hat{\sigma}_1(a_0\hat{1} + \hat{\sigma}_1 a_1 + \hat{\sigma}_2 a_2 + \hat{\sigma}_3 a_3)] \\ &= Tr(\hat{\sigma}_1 a_0 + \hat{\sigma}_1^2 a_1 + \hat{\sigma}_1\hat{\sigma}_2 a_2 + \hat{\sigma}_1\hat{\sigma}_3 a_3) \\ &= Tr(\hat{\sigma}_1 a_0 + \hat{\sigma}_1^2 a_1 + i\hat{\sigma}_3 a_2 - i\hat{\sigma}_2 a_3) \\ &= 2a_1 \end{aligned}$$

Similarly, we have

$$Tr(\hat{\sigma}_2\hat{X}) = 2a_2, \qquad Tr(\hat{\sigma}_3\hat{X}) = 2a_3,$$

$$\hat{\sigma}_1\hat{X} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} X_{11} & X_{12} \\ X_{21} & X_{22} \end{pmatrix} = \begin{pmatrix} X_{21} & X_{22} \\ X_{11} & X_{12} \end{pmatrix},$$

$$\hat{\sigma}_2\hat{X} = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}\begin{pmatrix} X_{11} & X_{12} \\ X_{21} & X_{22} \end{pmatrix} = \begin{pmatrix} -iX_{21} & -iX_{22} \\ iX_{11} & iX_{12} \end{pmatrix},$$

$$\hat{\sigma}_3\hat{X} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\begin{pmatrix} X_{11} & X_{12} \\ X_{21} & X_{22} \end{pmatrix} = \begin{pmatrix} X_{11} & X_{12} \\ -X_{21} & -X_{22} \end{pmatrix},$$

$$a_0 = \frac{Tr(\hat{X})}{2} = \frac{X_{11} + X_{22}}{2}, \qquad a_1 = \frac{Tr(\hat{\sigma}_1\hat{X})}{2} = \frac{X_{21} + X_{12}}{2},$$

$$a_2 = \frac{Tr(\hat{\sigma}_2\hat{X})}{2} = \frac{-iX_{21} + iX_{12}}{2} = \frac{i}{2}(X_{12} - X_{21}),$$

$$a_3 = \frac{Tr(\hat{\sigma}_3\hat{X})}{2} = \frac{X_{11} - X_{22}}{2}.$$

((**Mathematica**))

```
(*Sakurai 1-2*)

Clear["Global`*"];

SuperStar /: expr_* := expr /. {Complex[a_, b_] :> Complex[a, -b]};

σ1 = {{0, 1}, {1, 0}}; σ2 = {{0, -ⅈ}, {ⅈ, 0}}; σ3 = {{1, 0}, {0, -1}};
ϵ = {{1, 0}, {0, 1}}

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

X = a0 ϵ + σ1 a1 + σ2 a2 + σ3 a3; X // MatrixForm

( a0 + a3    a1 - ⅈ a2 )
( a1 + ⅈ a2  a0 - a3   )

{Tr[ϵ], Tr[σ1], Tr[σ2], Tr[σ3]}

{2, 0, 0, 0}

{Tr[X], Tr[σ1.X], Tr[σ2.X], Tr[σ3.X]}

{2 a0, 2 a1, ⅈ (a1 - ⅈ a2) - ⅈ (a1 + ⅈ a2), 2 a3}

σ1.X // MatrixForm

( a1 + ⅈ a2  a0 - a3   )
( a0 + a3    a1 - ⅈ a2 )

σ2.X // MatrixForm

( -ⅈ (a1 + ⅈ a2)  -ⅈ (a0 - a3)  )
( ⅈ (a0 + a3)     ⅈ (a1 - ⅈ a2) )

σ3.X // MatrixForm

( a0 + a3     a1 - ⅈ a2 )
( -a1 - ⅈ a2  -a0 + a3  )
```

9. Rotation operator

The rotation operator [rotation around the unit vector $\boldsymbol{u}$ in the 3D space by an angle α] is

$$\hat{R}_u(\alpha) = \exp[-\frac{i\alpha}{2}(\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{u})] = \cos(\frac{\alpha}{2})\hat{1} - i(\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{u})\sin(\frac{\alpha}{2})$$

((proof))

Taylor expansion:

$$\hat{R}_u(\alpha) = \hat{1} + \frac{(-i\frac{\alpha}{2})}{1!}(\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{u}) + \frac{(-i\frac{\alpha}{2})^2}{2!}(\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{u})^2 + \frac{(-i\frac{\alpha}{2})^3}{3!}(\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{u})^3$$
$$+\frac{(-i\frac{\alpha}{2})^4}{4!}(\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{u})^4 + \frac{(-i\frac{\alpha}{2})^5}{5!}(\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{u})^5 + \frac{(-i\frac{\alpha}{2})^6}{6!}(\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{u})^6 + .$$

Here we use

$$(\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{u})^2 = \boldsymbol{u}^2 = 1$$

$$(\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{A})(\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{B}) = \boldsymbol{A}\cdot\boldsymbol{B} + i\hat{\sigma}\cdot(\boldsymbol{A}\times\boldsymbol{B})$$

which leads to

$$(\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{u})^n = 1 \qquad \text{for even } n$$

$$(\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{u})^n = \hat{\sigma}\cdot\boldsymbol{u} \qquad \text{for odd } n$$

Then we have

$$\hat{R}_u(\alpha) = [1 - \frac{(\frac{\alpha}{2})^2}{2!} + \frac{(\frac{\alpha}{2})^4}{4!} - \frac{(\frac{\alpha}{2})^6}{6!} + ...]\hat{1} + [\frac{(\frac{\alpha}{2})}{1!} - \frac{(\frac{\alpha}{2})^3}{3!} + \frac{(\frac{\alpha}{2})^5}{5!} + ...](-i\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{u})$$
$$= \cos(\frac{\alpha}{2})\hat{1} - i(\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{u})\sin(\frac{\alpha}{2})$$

or

$$\hat{R}_u(\alpha) = \cos(\frac{\alpha}{2})\hat{1} - i(\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{u})\sin(\frac{\alpha}{2})$$

10. Rotation matrix (another derivation)

(a)

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

since

$$\hat{R}_z(\theta)(|+z\rangle\langle+z| + |-z\rangle\langle-z|) = \exp(-i\hat{\sigma}_z \frac{\theta}{2})(|+z\rangle\langle+z| + |-z\rangle\langle-z|$$
$$= e^{-i\theta/2}|+z\rangle\langle+z| + e^{i\theta/2}|-z\rangle\langle-z|$$
$$= e^{-i\theta/2}\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} + e^{i\theta/2}\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$$
$$= \begin{pmatrix} e^{-i\theta/2} & 0 \\ 0 & e^{i\theta/2} \end{pmatrix}$$

(b)

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

since

$$\hat{R}_x(\theta)(|+x\rangle\langle+x|+|-x\rangle\langle-x|) = \exp(-i\hat{\sigma}_x\frac{\theta}{2})(|+x\rangle\langle+x|+|-x\rangle\langle-x|$$

$$= e^{-i\theta/2}|+x\rangle\langle+x| + e^{i\theta/2}|-x\rangle\langle-x|$$

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

$$= \begin{pmatrix}\frac{e^{i\theta/2}+e^{-i\theta/2}}{2} & \frac{-(e^{i\theta/2}-e^{-i\theta/2})}{2}\\ \frac{-(e^{i\theta/2}-e^{-i\theta/2})}{2} & \frac{e^{i\theta/2}+e^{-i\theta/2}}{2}\end{pmatrix}$$

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

where

$$|+x\rangle\langle+x| = \frac{1}{2}\begin{pmatrix}1\\ 1\end{pmatrix}\begin{pmatrix}1 & 1\end{pmatrix} = \frac{1}{2}\begin{pmatrix}1 & 1\\ 1 & 1\end{pmatrix}, \qquad |-x\rangle\langle-x| = \frac{1}{2}\begin{pmatrix}1\\ -1\end{pmatrix}\begin{pmatrix}1 & -1\end{pmatrix} = \frac{1}{2}\begin{pmatrix}1 & -1\\ -1 & 1\end{pmatrix}.$$

(c)

$$\hat{R}_y(\theta) = \exp(-i\hat{\sigma}_y\frac{\theta}{2})$$

$$= \cos\frac{\theta}{2}\hat{1} - i\hat{\sigma}_y\sin\frac{\theta}{2}$$

$$= \begin{pmatrix}\cos\frac{\theta}{2} & -\sin\frac{\theta}{2}\\ \sin\frac{\theta}{2} & \cos\frac{\theta}{2}\end{pmatrix}$$

$$
\begin{aligned}
\hat{R}_y(\theta)(|+y\rangle\langle+y|+|-y\rangle\langle-y|) &= \exp(-i\hat{\sigma}_y\frac{\theta}{2})(|+y\rangle\langle+y|+|-y\rangle\langle-y| \\
&= e^{-i\theta/2}|+y\rangle\langle+y|+e^{i\theta/2}|-y\rangle\langle-y| \\
&= e^{-i\theta/2}\frac{1}{2}\begin{pmatrix}1 & -i\\ i & 1\end{pmatrix}+e^{i\theta/2}\frac{1}{2}\begin{pmatrix}1 & i\\ -i & 1\end{pmatrix} \\
&= \begin{pmatrix}\frac{e^{i\theta/2}+e^{-i\theta/2}}{2} & \frac{i(e^{i\theta/2}-e^{-i\theta/2})}{2}\\ -\frac{i(e^{i\theta/2}-e^{-i\theta/2})}{2} & \frac{e^{i\theta/2}+e^{-i\theta/2}}{2}\end{pmatrix} \\
&== \begin{pmatrix}\cos\frac{\theta}{2} & -\sin\frac{\theta}{2}\\ \sin\frac{\theta}{2} & \cos\frac{\theta}{2}\end{pmatrix}
\end{aligned}
$$

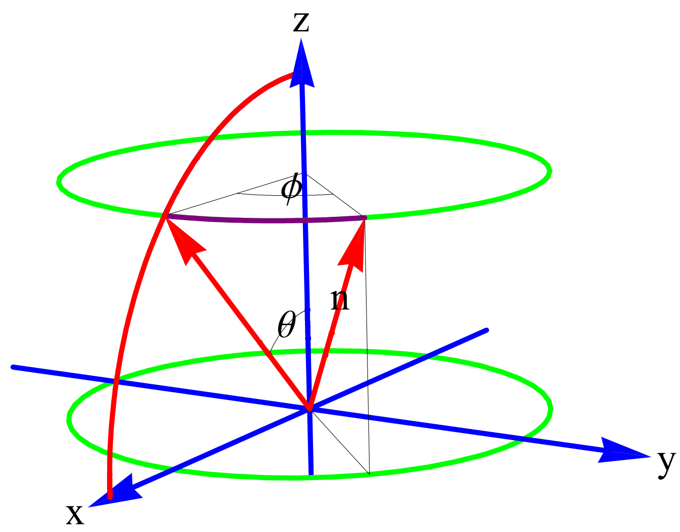
where

$$|+y\rangle\langle+y| = \frac{1}{2}\begin{pmatrix}1\\ i\end{pmatrix}\begin{pmatrix}1 & -i\end{pmatrix} = \frac{1}{2}\begin{pmatrix}1 & -i\\ i & 1\end{pmatrix},$$

$$|-y\rangle\langle-y| = \frac{1}{2}\begin{pmatrix}1\\ -i\end{pmatrix}\begin{pmatrix}1 & i\end{pmatrix} = \frac{1}{2}\begin{pmatrix}1 & i\\ -i & 1\end{pmatrix}.$$

11. Representation of rotation (general case)

Let the polar and the azimuthal angles that characterize ***n*** (the unit vector) be θ and ϕ, respectively. We first rotate about the y axis by angle θ. We subsequently rotate by ϕ about the z axis.



$$\boldsymbol{e}_z \to \boldsymbol{n} : \boldsymbol{n} = \Re_z(\phi)\Re_y(\theta)\boldsymbol{e}_z ,$$

$$\boldsymbol{n} = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta) ,$$

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

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

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

Thus

$$\hat{R}_z(\phi)\hat{R}_y(\theta)\left|+z\right\rangle = \begin{pmatrix} e^{-i\frac{\phi}{2}}\cos(\frac{\theta}{2}) & -e^{-i\frac{\phi}{2}}\sin(\frac{\theta}{2}) \\ e^{i\frac{\phi}{2}}\sin(\frac{\theta}{2}) & e^{i\frac{\phi}{2}}\cos(\frac{\theta}{2}) \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} e^{-i\frac{\phi}{2}}\cos(\frac{\theta}{2}) \\ e^{i\frac{\phi}{2}}\sin(\frac{\theta}{2}) \end{pmatrix} = \left|+\boldsymbol{n}\right\rangle$$

$$\hat{R}_z(\phi)\hat{R}_y(\theta)\left|-z\right\rangle = \begin{pmatrix} e^{-i\frac{\phi}{2}}\cos(\frac{\theta}{2}) & -e^{-i\frac{\phi}{2}}\sin(\frac{\theta}{2}) \\ e^{i\frac{\phi}{2}}\sin(\frac{\theta}{2}) & e^{i\frac{\phi}{2}}\cos(\frac{\theta}{2}) \end{pmatrix}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} -e^{-i\frac{\phi}{2}}\sin(\frac{\theta}{2}) \\ e^{i\frac{\phi}{2}}\cos(\frac{\theta}{2}) \end{pmatrix} = \left|-\boldsymbol{n}\right\rangle$$

((**Note**)) Relation between $\left|+\boldsymbol{n}\right\rangle$ and $\left|-\boldsymbol{n}\right\rangle$

In the notation of the ket vector $\left|+\boldsymbol{n}\right\rangle$, we replace the variables, $\theta \to \pi - \theta$, and $\phi \to \phi + \pi$

$$\begin{aligned} \left|+\boldsymbol{n}\right\rangle &\to \begin{pmatrix} e^{-i\frac{\phi}{2}}e^{-i\frac{\pi}{2}}\cos(\frac{\pi-\theta}{2}) \\ e^{i\frac{\phi}{2}}e^{i\frac{\pi}{2}}\sin(\frac{\pi-\theta}{2}) \end{pmatrix} \\ &= \begin{pmatrix} -ie^{-i\frac{\phi}{2}}\cos(\frac{\pi-\theta}{2}) \\ e^{i\frac{\phi}{2}}i\sin(\frac{\pi-\theta}{2}) \end{pmatrix} \\ &= i\begin{pmatrix} -e^{-i\frac{\phi}{2}}\sin(\frac{\theta}{2}) \\ e^{i\frac{\phi}{2}}i\cos(\frac{\theta}{2}) \end{pmatrix} = i\left|-\boldsymbol{n}\right\rangle \end{aligned}$$

We note that

$$\hat{R}_z(\phi)\left|+z\right\rangle = \begin{pmatrix} e^{-i\frac{\phi}{2}} & 0 \\ 0 & e^{i\frac{\phi}{2}} \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} e^{-i\frac{\phi}{2}} \\ 0 \end{pmatrix} = e^{-i\frac{\phi}{2}}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = e^{-i\frac{\phi}{2}}\left|+z\right\rangle.$$

Similarly we have

$$\hat{R}_z(\phi)\left|-z\right\rangle = \begin{pmatrix} e^{-i\frac{\phi}{2}} & 0 \\ 0 & e^{i\frac{\phi}{2}} \end{pmatrix}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ e^{i\frac{\phi}{2}} \end{pmatrix} = e^{i\frac{\phi}{2}}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = e^{i\frac{\phi}{2}}\left|-z\right\rangle.$$

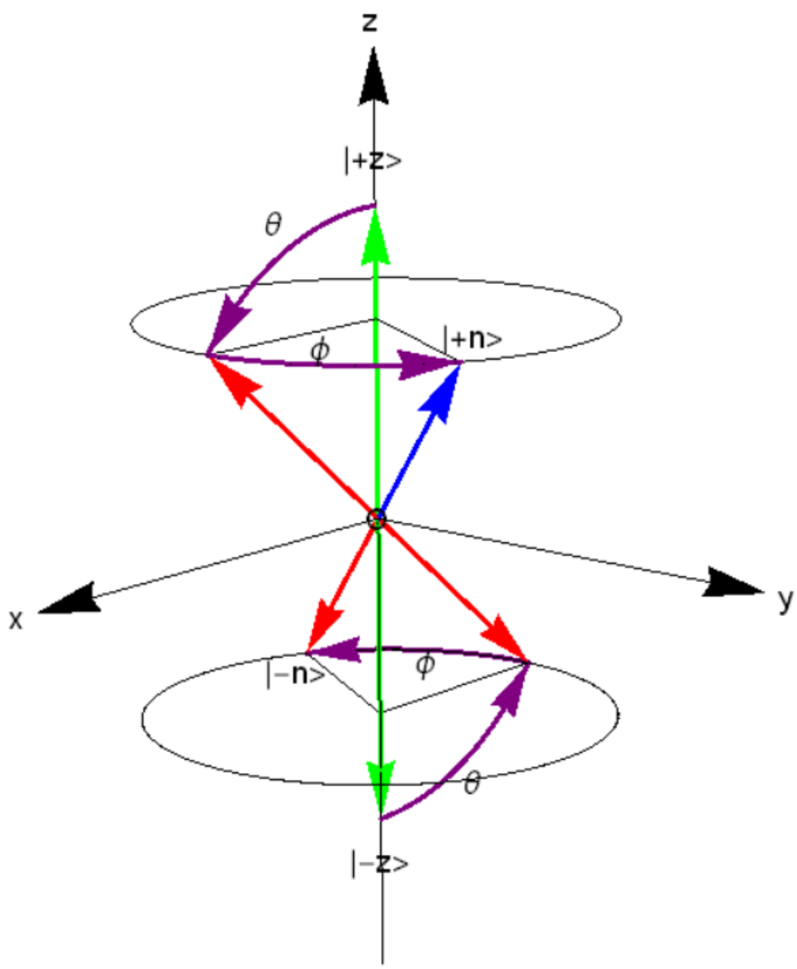


Fig. Schematic diagram for the rotation process of $|+\boldsymbol{n}\rangle = \hat{R}_z(\phi)\hat{R}_y(\theta)|+z\rangle$ and $|-\boldsymbol{n}\rangle = \hat{R}_z(\phi)\hat{R}_y(\theta)|-z\rangle$ during the rotation with angle θ around the y axis and rotation with the angle ϕ around the z axis, sequantially.

12. Eigenstates of the operator $\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{n}$

Here we show that $\hat{R}_z(\phi)\hat{R}_y(\theta)|+z\rangle$ and $\hat{R}_z(\phi)\hat{R}_y(\theta)|-z\rangle$ are the eigenkets of the operator $\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{n}$ with the eigenvalues +1, and -1, respectively, by using the Mathematica. In other words, we can say that

$$(\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{n})\hat{R}_z(\phi)\hat{R}_y(\theta)|+z\rangle = \hat{R}_z(\phi)\hat{R}_y(\theta)|+z\rangle,$$

$$(\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{n})\hat{R}_z(\phi)\hat{R}_y(\theta)|-z\rangle = -\hat{R}_z(\phi)\hat{R}_y(\theta)|-z\rangle.$$

where

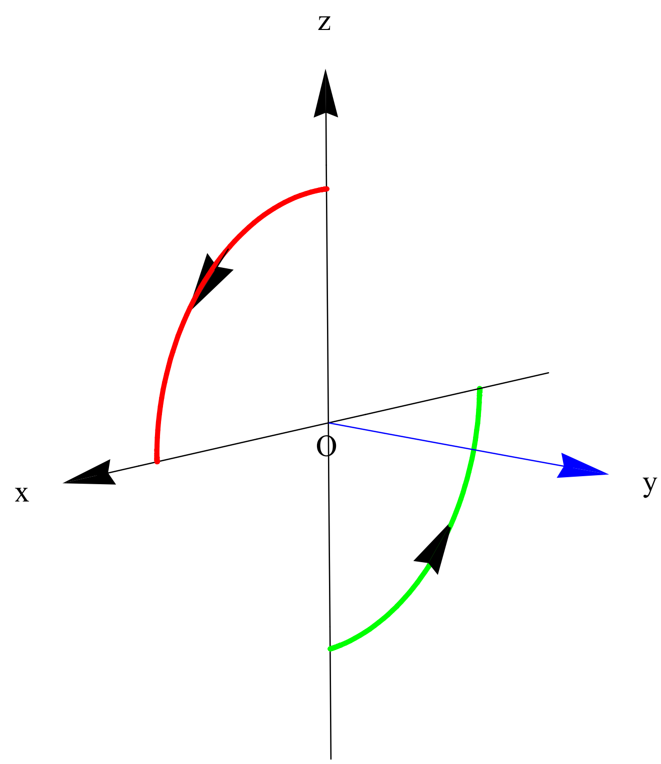
$$\boldsymbol{n} = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$$

((**Mathematica**))

```
Clear["Global`*"]; ψ1 = (1
                         0); ψ2 = (0
                                   1);

σx = PauliMatrix[1]; σy = PauliMatrix[2];
σz = PauliMatrix[3]; Ry = MatrixExp[-ⅈ/2 σy θ];
Rz = MatrixExp[-ⅈ/2 σz ϕ]; R = Rz.Ry;
n1 = {Sin[θ] Cos[ϕ], Sin[θ] Sin[ϕ], Cos[θ]};

σn = σx n1[[1]] + σy n1[[2]] + σz n1[[3]] // Simplify;

σn.(R.ψ1) - R.ψ1 // Simplify
{{0}, {0}}

σn.(R.ψ2) + R.ψ2 // Simplify
{{0}, {0}}
```

13. Example-1

Rotation around the *y* axis by the angle π/2: $\boldsymbol{e}_z \rightarrow \boldsymbol{e}_x : \boldsymbol{e}_x = \Re_y(\frac{\pi}{2})\boldsymbol{e}_z$

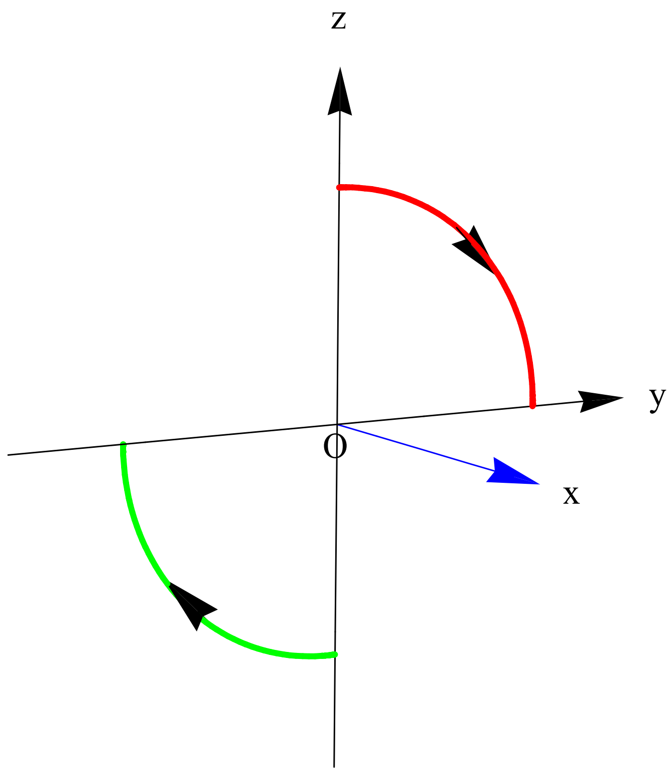


$$\hat{R}_y(\frac{\pi}{2})|+z\rangle = \begin{pmatrix} \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix} = |+x\rangle,$$

$$\hat{R}_y(\frac{\pi}{2})|-z\rangle = \begin{pmatrix} \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} -\frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix} = -|-x\rangle.$$

14. Example-2

Rotation around the x axis by the angle -π/2: $\boldsymbol{e}_z \to \boldsymbol{e}_y : \boldsymbol{e}_y = \Re_x(-\frac{\pi}{2})\boldsymbol{e}_z$

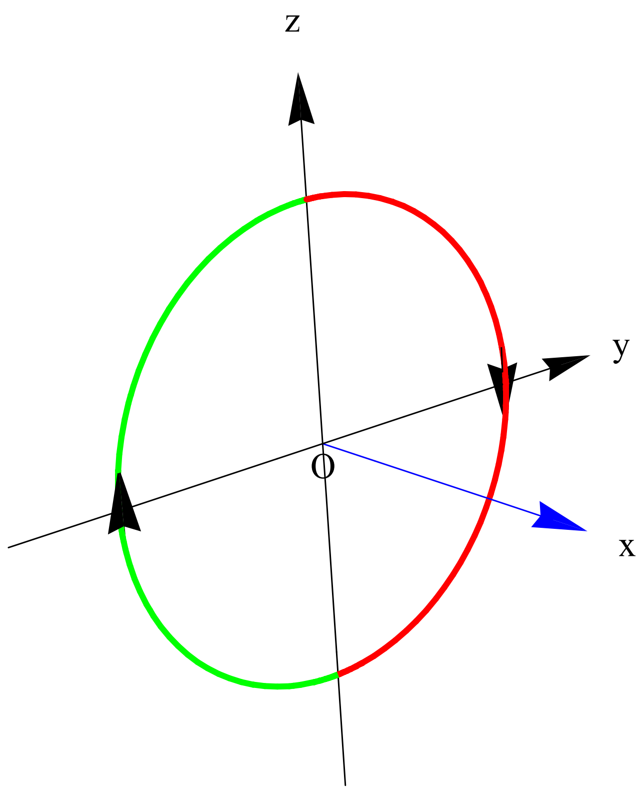


$$\hat{R}_x(-\frac{\pi}{2})|+z\rangle = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{i}{\sqrt{2}} \\ \frac{i}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{i}{\sqrt{2}} \end{pmatrix} = |+y\rangle,$$

$$\hat{R}_x(-\frac{\pi}{2})|-z\rangle = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{i}{\sqrt{2}} \\ \frac{i}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} \frac{i}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix} = i|-y\rangle.$$

15. Example-3

Rotation around the y axis by the angle π: $\boldsymbol{e}_z \rightarrow -\boldsymbol{e}_z : -\boldsymbol{e}_z = \Re_y(\pi)\boldsymbol{e}_z$



$$\hat{R}_y(\pi)\left|+z\right\rangle = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \left|-z\right\rangle,$$

$$\hat{R}_y(\pi)\left|-z\right\rangle = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} -1 \\ 0 \end{pmatrix} = -\left|+z\right\rangle.$$

16. Example-4

Rotation around the y axis by the angle $2n\pi$: $\boldsymbol{e}_z \to \boldsymbol{e}_z : \boldsymbol{e}_z = \Re_y(2n\pi)\boldsymbol{e}_z$

$$\hat{R}_y(2n\pi)\left|+z\right\rangle = \begin{pmatrix} (-1)^n & 0 \\ 0 & (-1)^n \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} (-1)^n \\ 0 \end{pmatrix} = (-1)^n\left|+z\right\rangle,$$

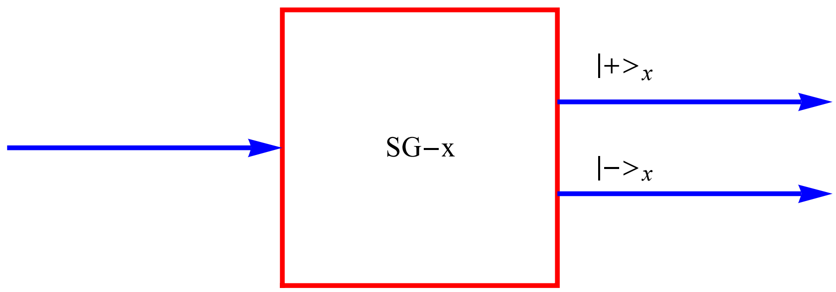
$$\hat{R}_y(2n\pi)\left|-z\right\rangle = \begin{pmatrix} (-1)^n & 0 \\ 0 & (-1)^n \end{pmatrix}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ (-1)^n \end{pmatrix} = (-1)^n\left|-z\right\rangle .$$

We have a closure relation.

$$\left|+z\right\rangle\left\langle+z\right| + \left|-z\right\rangle\left\langle-z\right| = \hat{1}$$

$$\hat{S}_z = \hat{S}_z(\left|+z\right\rangle\left\langle+z\right| + \left|-z\right\rangle\left\langle-z\right|) = \frac{\hbar}{2}\left|+z\right\rangle\left\langle+z\right| - \frac{\hbar}{2}\left|-z\right\rangle\left\langle-z\right|$$

17. Eigenvalue problem-I: Stern-Gerlach for *S* = 1/2 with the magnetic field along the *x* axis



Here we discuss the expression for $\left|\pm x\right\rangle$

$$\hat{\sigma}_x\left|\pm x\right\rangle = \pm\left|\pm x\right\rangle ,$$

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

$$\left|+x\right\rangle = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix} = \frac{1}{\sqrt{2}}(\left|+z\right\rangle + \left|-z\right\rangle),$$

$$\left|-x\right\rangle = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} \end{pmatrix} = \frac{1}{\sqrt{2}}(\left|+z\right\rangle - \left|-z\right\rangle).$$

((Mathematica))

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

SuperStar /: expr_* := expr /. {Complex[a_, b_] :→ Complex[a, -b]};

σx = {{0, 1}, {1, 0}};

eq1 = Eigensystem[σx]
```

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

```
ψ2 = -Normalize[eq1[[2, 1]]]
```

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

```
ψ1 = Normalize[eq1[[2, 2]]]
```

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

```
UT = {ψ1, ψ2}
```

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

Unitary operator U

```
U = Transpose[UT]
```

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

```
U // MatrixForm
```

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

Hermite conjugate of U

```
UH = UT*
```

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

```
UH // MatrixForm
```

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

```
UH.U
```

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

```
U.UH
```

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

18. Unitary operator

Eigenvalues: ±1

$$|\pm x\rangle = \hat{U}|\pm z\rangle,$$

where

$$\hat{U} = \begin{pmatrix} U_{11} & U_{12} \\ U_{21} & U_{22} \end{pmatrix},$$

under the basis of $\{|+z\rangle, |-z\rangle\}$.
Eigenkets:

$$|+x\rangle = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix} = \hat{U}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} U_{11} \\ U_{21} \end{pmatrix}, \qquad |-x\rangle = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} \end{pmatrix} = \hat{U}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} U_{12} \\ U_{22} \end{pmatrix}.$$

The unitary operator:

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

((**Another method**))

$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = \lambda\begin{pmatrix} c_1 \\ c_2 \end{pmatrix},$$

or

$$\begin{pmatrix} -\lambda & 1 \\ 1 & -\lambda \end{pmatrix}\begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix},$$

$$\det = \begin{vmatrix} -\lambda & 1 \\ 1 & -\lambda \end{vmatrix} = \lambda^2 - 1 = 0.$$

$$\lambda = \pm 1.$$

For $\lambda = 1$,

$$\begin{pmatrix} -1 & 1 \\ 1 & -1 \end{pmatrix}\begin{pmatrix} c_{1+} \\ c_{2+} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix},$$

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

Similarly,

For $\lambda = -1$,

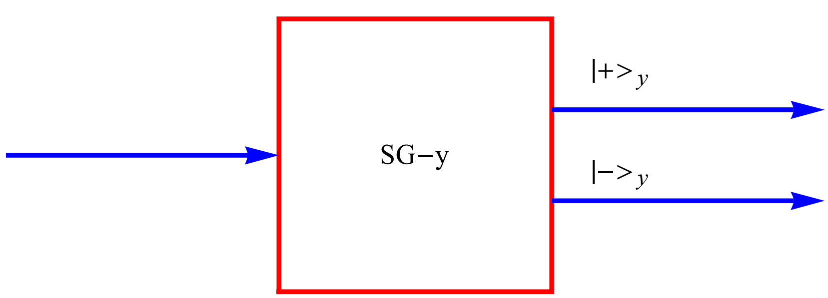
$$\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}\begin{pmatrix} c_{1-} \\ c_{2-} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix},$$

$$|-x\rangle = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} \end{pmatrix}.$$

Then we have the unitary matrix as

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

19. Eigenvalue problem-II: Stern-Gerlach for S = 1/2 with the magnetic field along the *y* axis



Expression for $|\pm y\rangle$

$$\hat{\sigma}_y|\pm y\rangle = \pm|\pm y\rangle ,$$

$$\hat{\sigma}_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix},$$

$$|+y\rangle = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{i}{\sqrt{2}} \end{pmatrix} = \frac{1}{\sqrt{2}}(|+z\rangle + i|-z\rangle) ,$$

$$|-y\rangle = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} \end{pmatrix} = \frac{1}{\sqrt{2}}(|+z\rangle - i|-z\rangle).$$

((**Mathematica**))

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

SuperStar /: expr_* := expr /. {Complex[a_, b_] :→ Complex[a, -b]};

σy = {{0, -ⅈ}, {ⅈ, 0}};

eq1 = Eigensystem[σy]
```

{{-1, 1}, {{ⅈ, 1}, {-ⅈ, 1}}}

```
ψ2 = (-ⅈ) Normalize[eq1[[2, 1]]]
```

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

```
ψ1 = ⅈ Normalize[eq1[[2, 2]]]
```

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

```
UT = {ψ1, ψ2}
```

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

Unitary operator U

```
U = Transpose[UT]
```

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

```
U // MatrixForm
```

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

Hermite conjugate of U

```
UH = UT*
```

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

```
UH // MatrixForm
```

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

```
UH.U
```

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

```
U.UH
```

20. Summary

The eigenkets:

$$|+y\rangle = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{i}{\sqrt{2}} \end{pmatrix} = \hat{U}\begin{pmatrix} 1 \\ 0 \end{pmatrix},$$

$$|-y\rangle = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} \end{pmatrix} = \hat{U}\begin{pmatrix} 0 \\ 1 \end{pmatrix},$$

The Unitary operator:

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

((**Another method**))

Expression for $|\pm y\rangle$

$$\hat{\sigma}_y|\pm y\rangle = \pm|\pm y\rangle,$$

$$\hat{\sigma}_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}.$$

We assume that

$$|\pm y\rangle = \begin{pmatrix} C_1 \\ C_2 \end{pmatrix}.$$

We solve the eigenvalue problem

$$\hat{\sigma}_y|\pm y\rangle = \lambda|\pm y\rangle,$$

where λ is an eigenvalue.

$$\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}\begin{pmatrix} C_1 \\ C_2 \end{pmatrix} = \lambda \begin{pmatrix} C_1 \\ C_2 \end{pmatrix},$$

or

$$\begin{pmatrix} -\lambda & -i \\ i & -\lambda \end{pmatrix}\begin{pmatrix} C_1 \\ C_2 \end{pmatrix} = 0,$$

$$M = \begin{pmatrix} -\lambda & -i \\ i & -\lambda \end{pmatrix},$$

$$\det M = \begin{vmatrix} -\lambda & -i \\ i & -\lambda \end{vmatrix} = \lambda^2 - 1 = 0,$$

or

$$\lambda = \pm 1.$$

For $\lambda = 1$

$$\begin{pmatrix} -1 & -i \\ i & -1 \end{pmatrix}\begin{pmatrix} C_1 \\ C_2 \end{pmatrix} = 0,$$

or

$$C_1 = -iC_2,$$

The normalization condition: $|C_1|^2 + |C_2|^2 = 1$. We choose $C_1 = -iC_2 = \frac{1}{\sqrt{2}}$. Then we have

$$|+y\rangle = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{i}{\sqrt{2}} \end{pmatrix} = \frac{1}{\sqrt{2}}(|+\rangle + i|-\rangle).$$

Similarly, for $\lambda = -1$

$$\begin{pmatrix} 1 & -i \\ i & 1 \end{pmatrix}\begin{pmatrix} C_1 \\ C_2 \end{pmatrix} = 0,$$

or

$C_1 = iC_2$.

The normalization condition: $|C_1|^2 + |C_2|^2 = 1$. We choose $C_1 = iC_2 = \frac{1}{\sqrt{2}}$. Then we have

$$|-y\rangle = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ -i\frac{i}{\sqrt{2}} \end{pmatrix} = \frac{1}{\sqrt{2}}(|+z\rangle - i|-z\rangle).$$

Unitary operator $\hat{U}$

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

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

21. General case

$$\hat{U}^+\hat{\sigma}_y\hat{U} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},$$

$$\hat{U}^+\hat{\sigma}_y{}^2\hat{U} = \hat{U}^+\hat{\sigma}_y\hat{U}\hat{U}^+\hat{\sigma}_y\hat{U} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix},$$

$$\hat{U}^+\hat{\sigma}_y{}^3\hat{U} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

In general

$$\hat{U}^+\hat{\sigma}_y{}^n\hat{U} = \begin{pmatrix} 1^n & 0 \\ 0 & (-1)^n \end{pmatrix},$$

$$\hat{U}^{+}\exp(-\frac{i\theta}{2}\hat{\sigma}_y)\hat{U}=\begin{pmatrix} e^{-i\theta/2} & 0 \\ 0 & e^{i\theta/2}\end{pmatrix}.$$

From this we can calculate the matrix of $\hat{\sigma}_y$; $\exp(-\frac{i\theta}{2}\hat{\sigma}_y)$,

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

22. Mathematica: MatrixPower

$$\sigma_x{}^n,\quad \sigma_y{}^n,\quad \sigma_z{}^n\ (n = 1, 2, 3,...).$$

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

σx = {{0, 1}, {1, 0}}; σy = {{0, -ⅈ}, {ⅈ, 0}}; σz = {{1, 0}, {0, -1}};

K1 =
 Prepend[Table[{n, MatrixPower[σx, n], MatrixPower[σy, n],
     MatrixPower[σz, n]}, {n, 1, 12}], {"n", " σx^n ", " σy^n ", " σz^n "}] //
  TableForm
```

n	$\sigma_x{}^n$	$\sigma_y{}^n$	$\sigma_z{}^n$
1	0 1 1 0	0 −ⅈ ⅈ 0	1 0 0 −1
2	1 0 0 1	1 0 0 1	1 0 0 1
3	0 1 1 0	0 −ⅈ ⅈ 0	1 0 0 −1
4	1 0 0 1	1 0 0 1	1 0 0 1
5	0 1 1 0	0 −ⅈ ⅈ 0	1 0 0 −1
6	1 0 0 1	1 0 0 1	1 0 0 1
7	0 1 1 0	0 −ⅈ ⅈ 0	1 0 0 −1
8	1 0 0 1	1 0 0 1	1 0 0 1
9	0 1 1 0	0 −ⅈ ⅈ 0	1 0 0 −1
10	1 0 0 1	1 0 0 1	1 0 0 1
11	0 1 1 0	0 −ⅈ ⅈ 0	1 0 0 −1
12	1 0 0 1	1 0 0 1	1 0 0 1

23. Mathematica: MatrixExp

```
A1 = MatrixExp[-ⅈ σx α/2]
```

$$\left\{\left\{\text{Cos}\left[\frac{\alpha}{2}\right], -i\,\text{Sin}\left[\frac{\alpha}{2}\right]\right\}, \left\{-i\,\text{Sin}\left[\frac{\alpha}{2}\right], \text{Cos}\left[\frac{\alpha}{2}\right]\right\}\right\}$$

```
A2 = MatrixExp[-ⅈ σy θ/2]
```

$$\left\{\left\{\text{Cos}\left[\frac{\theta}{2}\right], -\text{Sin}\left[\frac{\theta}{2}\right]\right\}, \left\{\text{Sin}\left[\frac{\theta}{2}\right], \text{Cos}\left[\frac{\theta}{2}\right]\right\}\right\}$$

```
A3 = MatrixExp[-ⅈ σz ϕ/2]
```

$$\left\{\left\{e^{-\frac{i\phi}{2}}, 0\right\}, \left\{0, e^{\frac{i\phi}{2}}\right\}\right\}$$

```
R = A3.A2 // Simplify
```

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

```
R // MatrixForm
```

$$\begin{pmatrix} e^{-\frac{i\phi}{2}}\text{Cos}\left[\frac{\theta}{2}\right] & -e^{-\frac{i\phi}{2}}\text{Sin}\left[\frac{\theta}{2}\right] \\ e^{\frac{i\phi}{2}}\text{Sin}\left[\frac{\theta}{2}\right] & e^{\frac{i\phi}{2}}\text{Cos}\left[\frac{\theta}{2}\right] \end{pmatrix}$$

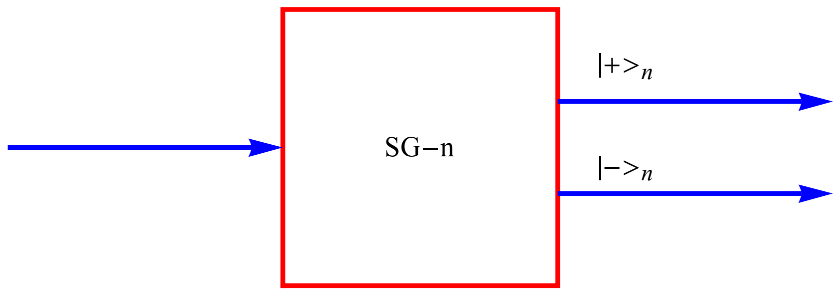
```
R.{1, 0}
```

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

```
R.{0, 1}
```

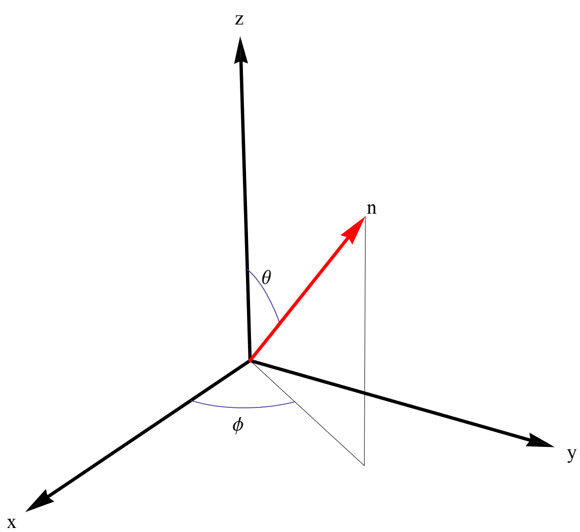
$$\left\{-e^{-\frac{i\phi}{2}}\text{Sin}\left[\frac{\theta}{2}\right], e^{\frac{i\phi}{2}}\text{Cos}\left[\frac{\theta}{2}\right]\right\}$$

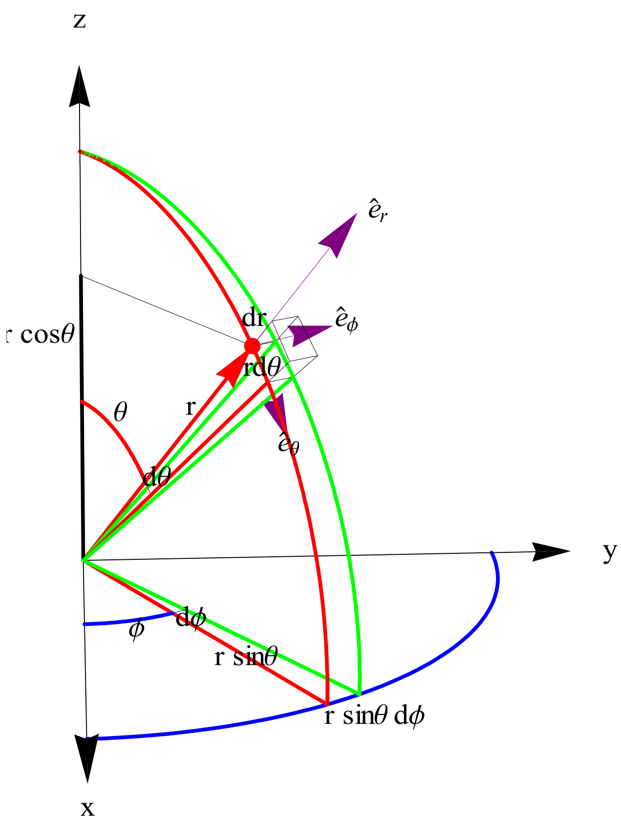
24. Eigenvalue problem-IV: Stern-Gerlach for S = 1/2 with the magnetic field along the *n* direction



$$\boldsymbol{n} = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta),$$

$$\hat{\sigma}_{\boldsymbol{n}} = \hat{\sigma}\cdot\boldsymbol{n} = \begin{pmatrix} \cos\theta & \sin\theta e^{-i\phi} \\ \sin\theta e^{i\phi} & -\cos\theta \end{pmatrix},$$





(a) **Eigenvalue problem**

Here we use the rotation operator for $j = 1/2$.

$$\hat{\sigma}_{\boldsymbol{n}}\left|+\boldsymbol{n}\right\rangle = \left|+\boldsymbol{n}\right\rangle, \qquad \hat{\sigma}_{\boldsymbol{n}}\left|-\boldsymbol{n}\right\rangle = -\left|-\boldsymbol{n}\right\rangle.$$

Unitary operator $\hat{U}$ is given by the rotation operator for $j = 1/2$.

$$\hat{U} = R(\theta,\phi) = D^{(1/2)}(\theta,\phi) = \begin{pmatrix} e^{-i\frac{\phi}{2}}\cos(\frac{\theta}{2}) & -e^{-i\frac{\phi}{2}}\sin(\frac{\theta}{2}) \\ e^{i\frac{\phi}{2}}\sin(\frac{\theta}{2}) & e^{i\frac{\phi}{2}}\cos(\frac{\theta}{2}) \end{pmatrix}.$$

The eigenkets $\left|+\boldsymbol{n}\right\rangle$ and $\left|-\boldsymbol{n}\right\rangle$ are obtained as

$$\left|+\boldsymbol{n}\right\rangle = \hat{U}\left|+z\right\rangle = \begin{pmatrix} e^{-i\frac{\phi}{2}}\cos(\frac{\theta}{2}) \\ e^{i\frac{\phi}{2}}\sin(\frac{\theta}{2}) \end{pmatrix},$$

and

$$\left|-\boldsymbol{n}\right\rangle = \hat{U}\left|-z\right\rangle = \begin{pmatrix} -e^{-i\frac{\phi}{2}}\sin(\frac{\theta}{2}) \\ e^{i\frac{\phi}{2}}\cos(\frac{\theta}{2}) \end{pmatrix}.$$

We note that

$$\hat{\sigma}_{\boldsymbol{n}}\hat{U}\left|+z\right\rangle = \hat{U}\left|+z\right\rangle \qquad \hat{U}^{+}\hat{\sigma}_{\boldsymbol{n}}\hat{U}\left|+z\right\rangle = \left|+z\right\rangle,$$

$$\hat{\sigma}_{\boldsymbol{n}}\left|+\boldsymbol{n}\right\rangle = -\left|+\boldsymbol{n}\right\rangle,$$

$$\hat{\sigma}_{\boldsymbol{n}}\hat{U}\left|-\boldsymbol{n}\right\rangle = \hat{U}\left|-\boldsymbol{n}\right\rangle \qquad \hat{U}^{+}\hat{\sigma}_{\boldsymbol{n}}\hat{U}\left|-z\right\rangle = -\left|-z\right\rangle,$$

$$\hat{U}^{+}\hat{\sigma}_{\boldsymbol{n}}\hat{U} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

(b) **Another method**
The above formula can be derived without Mathematica.

$$(\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{n})\left|\psi\right\rangle = \lambda\left|\psi\right\rangle.$$

Since $(\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{n})^2 = \hat{1}$,

$$(\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{n})^2\left|\psi\right\rangle = \lambda(\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{n})\left|\psi\right\rangle = \lambda^2\left|\psi\right\rangle, \text{ (eigenvalue problem)}$$

We get $\lambda^2 = 1$, or $\lambda = \pm 1$.

Thus

$$(\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{n})\left|+\boldsymbol{n}\right\rangle = \left|+\boldsymbol{n}\right\rangle,$$

$$(\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{n})\left|-\boldsymbol{n}\right\rangle = -\left|-\boldsymbol{n}\right\rangle,$$

$$\left|+\boldsymbol{n}\right\rangle = \hat{U}\left|+z\right\rangle = \begin{pmatrix} U_{11} & U_{12} \\ U_{21} & U_{22} \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} U_{11} \\ U_{21} \end{pmatrix},$$

$$\left|-\boldsymbol{n}\right\rangle = \hat{U}\left|-z\right\rangle = \begin{pmatrix} U_{11} & U_{12} \\ U_{21} & U_{22} \end{pmatrix}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} U_{12} \\ U_{22} \end{pmatrix},$$

where

$$\begin{pmatrix} U_{11}{}^* & U_{21}{}^* \\ U_{12}{}^* & U_{22}{}^* \end{pmatrix} \begin{pmatrix} U_{11} & U_{12} \\ U_{21} & U_{22} \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}.$$

(i) Derivation of the eigenket $\left|+\boldsymbol{n}\right\rangle$

$$\begin{pmatrix} \cos\theta & \sin\theta e^{-i\phi} \\ \sin\theta e^{i\phi} & -\cos\theta \end{pmatrix} \begin{pmatrix} U_{11} \\ U_{21} \end{pmatrix} = \begin{pmatrix} U_{11} \\ U_{21} \end{pmatrix},$$

or

$$\cos\theta U_{11} + \sin\theta e^{-i\phi} U_{21} = U_{11},$$

$$\sin\theta e^{i\phi} U_{11} - \cos\theta U_{21} = U_{21},$$

or

$$U_{21} = \frac{\sin\theta e^{i\phi}}{(1+\cos\theta)} U_{11} = \tan\frac{\theta}{2} e^{i\phi} U_{11}.$$

Since

$$\left|U_{11}\right|^2 + \left|U_{21}\right|^2 = 1, \qquad \text{(normalization)}$$

we get

$$\left|U_{11}\right|^2 = \cos^2\frac{\theta}{2}.$$

When we choose

$$U_{11} = e^{-i\frac{\phi}{2}} \cos\frac{\theta}{2},$$

we have

$$U_{21} = e^{i\frac{\phi}{2}} \sin\frac{\theta}{2}.$$

(ii) Derivation of the eigenket $\left|-\boldsymbol{n}\right\rangle$

$$\begin{pmatrix} \cos\theta & \sin\theta e^{-i\phi} \\ \sin\theta e^{i\phi} & -\cos\theta \end{pmatrix} \begin{pmatrix} U_{12} \\ U_{22} \end{pmatrix} = -\begin{pmatrix} U_{12} \\ U_{22} \end{pmatrix},$$

$$\cos\theta U_{12} + \sin\theta e^{-i\phi} U_{22} = -U_{12},$$

$$\sin\theta e^{i\phi} U_{12} - \cos\theta U_{22} = -U_{22},$$

$$U_{22} = -\frac{(1+\cos\theta)e^{i\phi}}{\sin\theta} U_{12} = -\cot(\frac{\theta}{2}) e^{i\phi} U_{12}.$$

Since

$$\left|U_{12}\right|^2 + \left|U_{22}\right|^2 = 1, \qquad \text{(normalization)},$$

we get

$$\left|U_{22}\right|^2 = \cos^2(\frac{\theta}{2}).$$

When we choose

$$U_{22} = e^{i\frac{\phi}{2}} \cos\frac{\theta}{2},$$

we have

$$U_{12} = -e^{-i\frac{\phi}{2}} \sin\frac{\theta}{2}.$$

(c) Special case for $\phi = 0$.

We consider the special case when $\phi = 0$.

$$\left|+\boldsymbol{n}\right\rangle = \begin{pmatrix} \cos(\frac{\theta}{2}) \\ \sin(\frac{\theta}{2}) \end{pmatrix},$$

and

$$|-\boldsymbol{n}\rangle = \begin{pmatrix} -\sin(\frac{\theta}{2}) \\ \cos(\frac{\theta}{2}) \end{pmatrix}.$$

When $\theta = 0$, we have

$$|+z\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |-z\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

When $\theta = \pi/2$,

$$|+x\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}, \qquad |-x\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} -1 \\ 1 \end{pmatrix} = -\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}.$$

This expression of $|-x\rangle$ is different from the conventional expression of $|-x\rangle$ only for the sign. So we may use the expression of $|-\boldsymbol{n}\rangle$ as

$$|-\boldsymbol{n}\rangle = \begin{pmatrix} \sin(\frac{\theta}{2}) \\ -\cos(\frac{\theta}{2}) \end{pmatrix}.$$

25. Derivation of the eigenkets in each SG configuration from the above formula

(i) SG$_x$ experiment:

$\theta = \pi/2$ and $\phi = 0$.

$$|+x\rangle = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix}, \qquad |-x\rangle = \begin{pmatrix} -\frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix}.$$

The eigenket of $|-x\rangle$ thus obtained is different from the conventional eigenket

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

except for the phase factor exp(iπ)=-1.

(ii) SG$_y$ experiment:

$\theta = \pi/2$ and $\phi = \pi/2$.

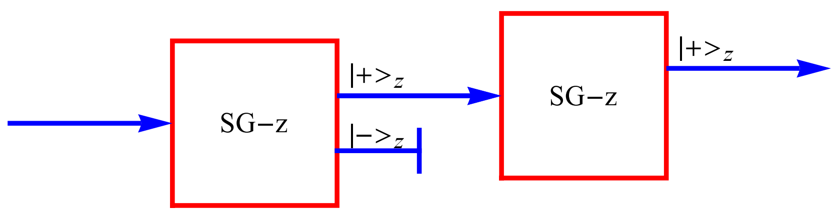
$$\left|+y\right\rangle = \begin{pmatrix} \frac{1}{\sqrt{2}} e^{-i\pi/4} \\ \frac{1}{\sqrt{2}} e^{i\pi/4} \end{pmatrix} = e^{-i\pi/4} \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{i}{\sqrt{2}} \end{pmatrix},$$

$$\left|-y\right\rangle = \begin{pmatrix} -\frac{1}{\sqrt{2}} e^{-i\pi/4} \\ \frac{1}{\sqrt{2}} e^{i\pi/4} \end{pmatrix} = -e^{-i\pi/4} \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{-i}{\sqrt{2}} \end{pmatrix}.$$

The eigenket of $\left|+y\right\rangle$ is different from the conventional $\left|+y\right\rangle$ except for the phase factor $e^{-i\pi/4}$. The eigenket of $\left|-y\right\rangle$ is different from the conventional $\left|-y\right\rangle$ except for the phase factor (-$e^{-i\pi/4}$).

26. SG Thinking experiment (gedanken experiment)

(1) Experiment



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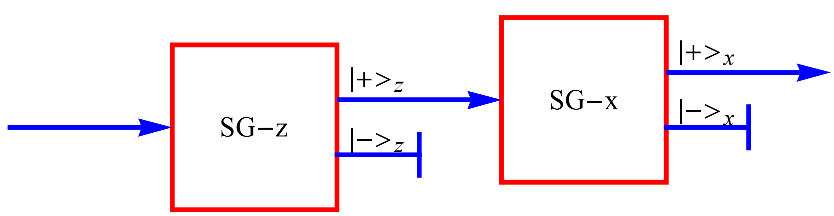
(2) Experiment



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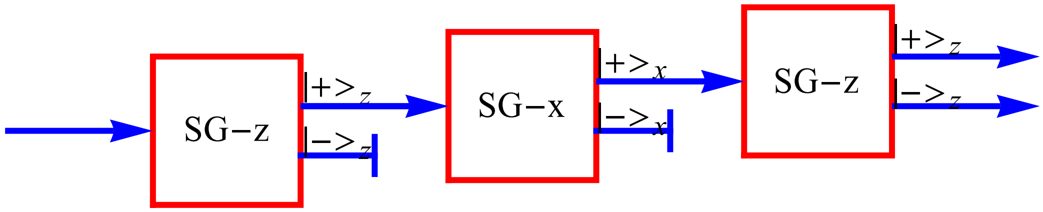
(3) Experiment



Analysis of experiment-3

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

The probability:

$$P_1 = \left|\left\langle +x \middle| +z \right\rangle\right|^2 = \left|\left\langle +z \middle| +x \right\rangle\right|^2 = \frac{1}{2},$$

$$P_2 = \left|\left\langle -x \middle| +z \right\rangle\right|^2 = \left|\left\langle +z \middle| -x \right\rangle\right|^2 = \frac{1}{2},$$

$$P_3 = \left|\left\langle +z \middle| +x \right\rangle\right|^2 = \frac{1}{2},$$

$$P_4 = \left|\left\langle -z \middle| +x \right\rangle\right|^2 = \frac{1}{2}.$$

The expectation value:

$$\left\langle S_z \right\rangle = \frac{\hbar}{2} \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix} = 0,$$

or

$$\left\langle S_z \right\rangle = \frac{\hbar}{2} P_3 + (-\frac{\hbar}{2}) P_4 = 0,$$

$$\left\langle S_z^{\ 2}\right\rangle = \frac{\hbar^2}{4}\begin{pmatrix}\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}}\end{pmatrix}\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}\begin{pmatrix}\frac{1}{\sqrt{2}}\\ \frac{1}{\sqrt{2}}\end{pmatrix} = \frac{\hbar^2}{4},$$

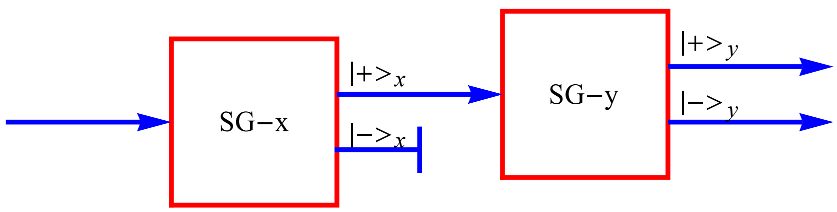
or

$$\left\langle S_z^{\ 2}\right\rangle = \frac{\hbar^2}{4}P_3 + \frac{\hbar^2}{4}P_4 = \frac{\hbar^2}{4},$$

$$\Delta S_z^{\ 2} = \left\langle S_z^{\ 2}\right\rangle - \left\langle S_z\right\rangle^2 = \frac{\hbar^2}{4}.$$

---

(4) Experiment



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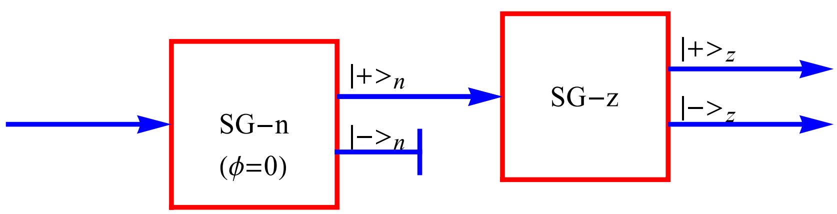
(5) Experiment



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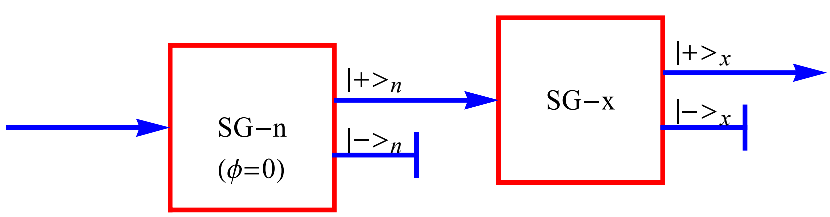
(6) Experiment



Analysis of experiment-6

$$|+\boldsymbol{n}\rangle = \begin{pmatrix} \cos\frac{\theta}{2} \\ \sin\frac{\theta}{2} \end{pmatrix}, \qquad |+x\rangle = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix}, \qquad |-x\rangle = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} \end{pmatrix},$$

$$\langle +x|+\boldsymbol{n}\rangle = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} \cos\frac{\theta}{2} \\ \sin\frac{\theta}{2} \end{pmatrix} = \frac{1}{\sqrt{2}}(\cos\frac{\theta}{2} + \sin\frac{\theta}{2}) = \frac{1}{\sqrt{2}}[\cos(\frac{\theta}{2} - \frac{\pi}{4})],$$

$$\langle -x|+\boldsymbol{n}\rangle = \begin{pmatrix} \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} \cos\frac{\theta}{2} \\ \sin\frac{\theta}{2} \end{pmatrix} = \frac{1}{\sqrt{2}}(\cos\frac{\theta}{2} - \sin\frac{\theta}{2}) = \frac{1}{\sqrt{2}}[\cos(\frac{\theta}{2} + \frac{\pi}{4})].$$

The probability;

$$P_{+x} = |\langle +x|+\boldsymbol{n}\rangle|^2 = \frac{1}{4}(\cos\frac{\theta}{2} + \sin\frac{\theta}{2})^2 = \frac{1}{4}(1+\sin\theta),$$

$$P_{-x} = |\langle -x|+\boldsymbol{n}\rangle|^2 = \frac{1}{4}(\cos\frac{\theta}{2} - \sin\frac{\theta}{2})^2 = \frac{1}{4}(1-\sin\theta).$$

The expectation value:

$$\langle S_x\rangle = \langle +\boldsymbol{n}|\hat{S}_x|+\boldsymbol{n}\rangle = \frac{\hbar}{2}\begin{pmatrix} \cos\frac{\theta}{2} & \sin\frac{\theta}{2} \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \cos\frac{\theta}{2} \\ \sin\frac{\theta}{2} \end{pmatrix}$$

$$= \hbar \sin\frac{\theta}{2}\cos\frac{\theta}{2} = \frac{\hbar}{2}\sin\theta$$

or

$$\langle S_x\rangle = \frac{\hbar}{2}P_{+x} + (-\frac{\hbar}{2})P_{-x} = \frac{\hbar}{2}\sin\theta,$$

$$\langle S_z \rangle = \langle +\boldsymbol{n}|\hat{S}_z|+\boldsymbol{n}\rangle = \frac{\hbar}{2}\begin{pmatrix} \cos\frac{\theta}{2} & \sin\frac{\theta}{2} \end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\begin{pmatrix} \cos\frac{\theta}{2} \\ \sin\frac{\theta}{2} \end{pmatrix}$$

$$= \frac{\hbar}{2}(\cos^2\frac{\theta}{2} - \sin^2\frac{\theta}{2}) = \frac{\hbar}{2}\cos\theta$$

27. Rotation operator and angular momentum

The relation between the rotation operator and angular momentum in detail will be discussed later in new topics. We assume that

$$\hat{U} = \hat{R}_z(d\phi) = \hat{1} - \frac{i}{\hbar}\hat{J}_z d\phi, \qquad \text{(infinitesimal rotation operator)}$$

where $\hat{J}_z$ is the angular momentum (in the unit of $\hbar$),

$$\hat{R}_z^{\ +}(d\phi) = \hat{1} + \frac{i}{\hbar}\hat{J}_z^{\ +} d\phi,$$

where

$$i^+ = -i^*,$$

$$(\hat{A}\hat{B})^+ = \hat{B}^+\hat{A}^+,$$

$$(i\hat{J}_z)^+ = \hat{J}_z^{\ +} i^+ = -i\hat{J}_z^{\ +}.$$

Here we note that

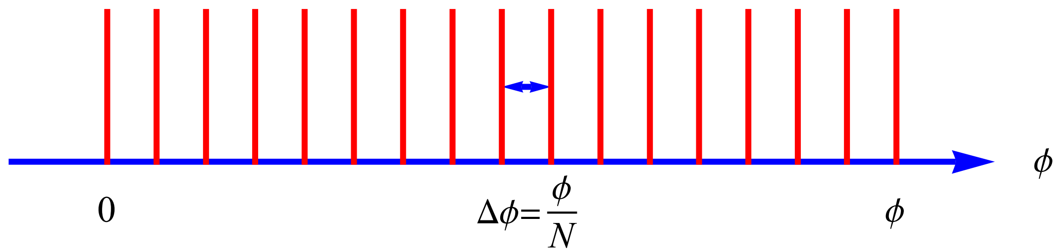
$$\hat{U}^+\hat{U} = \hat{R}_z^{\ +}(d\phi)\hat{R}_z d\phi) = (\hat{1} + \frac{i}{\hbar}\hat{J}_z^{\ +} d\phi)(\hat{1} - \frac{i}{\hbar}\hat{J}_z d\phi)$$

$$= \hat{1} + \frac{i}{\hbar}(\hat{J}_z^{\ +} - \hat{J}_z)d\phi) + O(d\phi)^2 = \hat{1}$$

leading to the relation

$$\hat{J}_z^{\ +} = \hat{J}_z. \qquad (\hat{J}_z \text{ is a Hermitian operator})$$

Suppose that $d\phi = \dfrac{\phi}{N}$ $\qquad (N \to \infty)$,



$$\hat{R}_z(\phi) = \lim_{N\to\infty}[\hat{R}_z(\frac{\phi}{N})\hat{R}_z(\frac{\phi}{N})\hat{R}_z(\frac{\phi}{N}).....\hat{R}_z(\frac{\phi}{N})]$$
$$= \lim_{N\to\infty}(\hat{1} - \frac{i}{\hbar}\hat{J}_z\frac{\phi}{N})^N = \exp(-i\frac{1}{\hbar}\hat{J}_z\phi)$$

((**Note**))

$$\lim_{N\to\infty}(1+\frac{1}{N})^N = e,$$ (from the definition of e).

$$\lim_{N\to\infty}(1+\frac{a}{N})^N = \lim_{N'\to\infty}[(1+\frac{1}{N'})^{N'}]^a = e^a,$$

where

$$N' = \frac{N}{a}.$$

28. Eigenstate and eigenvalues

We start with

$$\hat{R}_z(\phi)\left|+z\right\rangle = \exp(-\frac{i}{\hbar}\hat{J}_z\phi)\left|+z\right\rangle = e^{-i\frac{\phi}{2}}\left|+z\right\rangle,$$

where $e^{-i\frac{\phi}{2}}$ is the phase factor.

$$\hat{R}_z(d\phi)\left|+z\right\rangle = e^{-i\frac{d\phi}{2}}\left|+z\right\rangle.$$

Using the Taylor expansion, we get

$$(\hat{1} - \frac{i}{\hbar}\hat{J}_z d\phi)\left|+z\right\rangle = (1-\frac{i}{2}d\phi)\left|+z\right\rangle.$$

Then we have

$$\hat{J}_z|+z\rangle = \frac{\hbar}{2}|+z\rangle.$$ (Eigenvalue problem).

Similarly, we have

$$\hat{R}_z(\phi)|-z\rangle = e^{i\frac{\phi}{2}}|-z\rangle,$$

Using the Taylor expansion, we get

$$(\hat{1} - \frac{i}{\hbar}\hat{J}_z d\phi)|-z\rangle = (1 + \frac{i}{2}d\phi)|-z\rangle .$$

Then we have

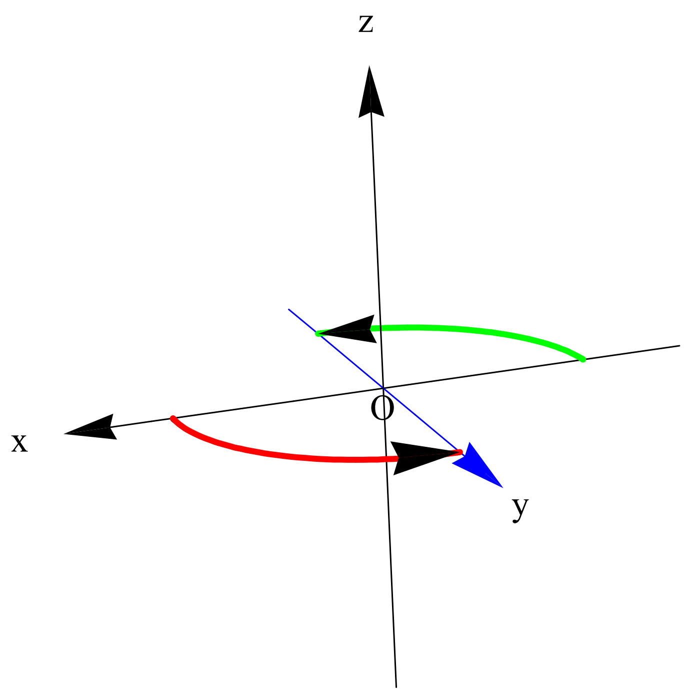
$$\hat{J}_z|-z\rangle = -\frac{\hbar}{2}|-z\rangle.$$ (Eigenvalue problem).

29. Calculation of $\hat{R}_z(\phi)|\pm\rangle_x$

$$\begin{aligned}
\hat{R}_z(\phi)|+x\rangle &= \hat{R}_z(\phi)\frac{1}{\sqrt{2}}(|+z\rangle + |-z\rangle) \\
&= \frac{1}{\sqrt{2}}[\hat{R}_z(\phi)|+z\rangle + \hat{R}_z(\phi)|-z\rangle] \\
&= \frac{1}{\sqrt{2}}[e^{-i\frac{\phi}{2}}|+z\rangle + e^{i\frac{\phi}{2}}|-z\rangle] \\
&= \frac{1}{\sqrt{2}}e^{-i\frac{\phi}{2}}[|+z\rangle + e^{i\phi}|-z\rangle]
\end{aligned}$$

$$\begin{aligned}
\hat{R}_z(\phi)|-x\rangle &= \hat{R}_z(\phi)\frac{1}{\sqrt{2}}(|+z\rangle - |-z\rangle) \\
&= \frac{1}{\sqrt{2}}[\hat{R}_z(\phi)|+z\rangle - \hat{R}_z(\phi)|-z\rangle] \\
&= \frac{1}{\sqrt{2}}[e^{-i\frac{\phi}{2}}|+z\rangle - e^{i\frac{\phi}{2}}|-z\rangle] \\
&= \frac{1}{\sqrt{2}}e^{-i\frac{\phi}{2}}[|+z\rangle - e^{i\phi}|-z\rangle]
\end{aligned}$$

When $\phi = \pi/2$,



$$\hat{R}_z(\frac{\pi}{2})\left|+x\right\rangle = \frac{1}{\sqrt{2}} e^{-i\frac{\pi}{4}} [\left|+z\right\rangle + e^{i\frac{\pi}{2}} \left|-z\right\rangle]$$

$$= \frac{1}{\sqrt{2}} e^{-i\frac{\pi}{4}} [\left|+z\right\rangle + i\left|-z\right\rangle] = e^{-i\frac{\pi}{4}} \left|+y\right\rangle$$

$$\hat{R}_z(\frac{\pi}{2})\left|-x\right\rangle_x = \frac{1}{\sqrt{2}} [e^{-i\frac{\phi}{2}} \left|+z\right\rangle - e^{i\frac{\phi}{2}} \left|-z\right\rangle]$$

$$= \frac{1}{\sqrt{2}} e^{-i\frac{\pi}{4}} [\left|+z\right\rangle - e^{i\frac{\pi}{2}} \left|-z\right\rangle]$$

$$= e^{-i\frac{\pi}{4}} \left|-y\right\rangle$$

When $\phi = 2\pi$,

$$\hat{R}_z(2\pi)\left|+x\right\rangle =$$

$$= \frac{1}{\sqrt{2}} e^{-i\pi} [\left|+z\right\rangle + e^{i(2\pi)} \left|-z\right\rangle]$$

$$= \frac{1}{\sqrt{2}} (-1) [\left|+z\right\rangle + \left|-z\right\rangle]$$

$$= -\left|+x\right\rangle$$

$$\hat{R}_z(2\pi)\left|-x\right\rangle =$$

$$= \frac{1}{\sqrt{2}} e^{-i\pi} [\left|+z\right\rangle - e^{i(2\pi)} \left|-z\right\rangle]$$

$$= \frac{1}{\sqrt{2}} (-1) [\left|+z\right\rangle - \left|-z\right\rangle]$$

$$= -\left|-x\right\rangle$$

For $\phi = \pi$,

$$\hat{R}_z(\pi)\left|+x\right\rangle =$$

$$= \frac{1}{\sqrt{2}} e^{-i\frac{\pi}{2}} [\left|+z\right\rangle + e^{i\pi} \left|-z\right\rangle]$$

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

$$= -i\left|-x\right\rangle$$

$$\hat{R}_z(\pi)\left|-x\right\rangle =$$

$$= \frac{1}{\sqrt{2}} e^{-i\frac{\pi}{2}} [\left|+z\right\rangle - e^{i\pi} \left|-z\right\rangle]$$

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

$$= -i\left|+x\right\rangle$$

30. Expression of the Pauli matrix $\hat{\sigma}_x$ under the basis of $\{\left|+z\right\rangle, \left|-z\right\rangle\}$

$$\hat{J}_x\left|+x\right\rangle = \frac{\hbar}{2}\left|+x\right\rangle, \qquad \hat{J}_x\left|-x\right\rangle = -\frac{\hbar}{2}\left|-x\right\rangle. \qquad (1)$$

where

$$|+x\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix}, \qquad |-x\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\-1\end{pmatrix}.$$

Note that

$$|+z\rangle = \frac{1}{\sqrt{2}}[|+x\rangle + |-x\rangle], \qquad |-z\rangle = \frac{1}{\sqrt{2}}[|+x\rangle - |-x\rangle].$$

Then we get

$$\hat{J}_x|+z\rangle = \frac{1}{\sqrt{2}}[\hat{J}_x|+x\rangle + \hat{J}_x|-x\rangle] = \frac{1}{\sqrt{2}}\frac{\hbar}{2}[|+x\rangle - |-x\rangle] = \frac{1}{\sqrt{2}}\frac{\hbar}{2}\sqrt{2}|-z\rangle = \frac{\hbar}{2}|-z\rangle,$$

$$\hat{J}_x|-z\rangle = \frac{1}{\sqrt{2}}[\hat{J}_x|+x\rangle - \hat{J}_x|-x\rangle] = \frac{1}{\sqrt{2}}\frac{\hbar}{2}[|+x\rangle + |-x\rangle] = \frac{1}{\sqrt{2}}\frac{\hbar}{2}\sqrt{2}|+z\rangle = \frac{\hbar}{2}|+z\rangle.$$

using Eq.(1). The matrix representation of $\hat{J}_x$ under the basis of $\{|+z\rangle, |-z\rangle\}$, is given by

$$\hat{J}_x = \frac{\hbar}{2}\sigma_x = \frac{\hbar}{2}\begin{pmatrix}0 & 1\\1 & 0\end{pmatrix}.$$

---

31. Expression of the Pauli matrix $\hat{\sigma}_y$ under the basis of $\{|+z\rangle, |-z\rangle\}$

$$\hat{J}_y|+y\rangle = \frac{\hbar}{2}|+y\rangle, \qquad ,\hat{J}_y|-y\rangle = -\frac{\hbar}{2}|-y\rangle \qquad (1)$$

where

$$|+y\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\i\end{pmatrix}, \qquad |-y\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\-i\end{pmatrix}.$$

Note that

$$|+z\rangle = \frac{1}{\sqrt{2}}[|+y\rangle + |-y\rangle], \qquad |-z\rangle = \frac{1}{i\sqrt{2}}[|+y\rangle - |-y\rangle].$$

Then we get

$$\hat{J}_y|+z\rangle = \frac{1}{\sqrt{2}}[\hat{J}_y|+y\rangle + \hat{J}_y|-y\rangle]$$
$$= \frac{1}{\sqrt{2}}\frac{\hbar}{2}[|+y\rangle - |-y\rangle]$$
$$= \frac{1}{\sqrt{2}}\frac{\hbar}{2}\sqrt{2}i|-z\rangle$$
$$= \frac{\hbar}{2}i|-z\rangle$$

$$\hat{J}_y|-z\rangle = \frac{1}{i\sqrt{2}}[\hat{J}_y|+y\rangle - \hat{J}_y|-y\rangle]$$
$$= \frac{1}{i\sqrt{2}}\frac{\hbar}{2}[|+y\rangle + |-y\rangle]$$
$$= \frac{1}{i\sqrt{2}}\frac{\hbar}{2}\sqrt{2}|+z\rangle$$
$$= -i\frac{\hbar}{2}|+z\rangle$$

using Eq.(1). The matrix representation of $\hat{J}_y$ under the basis of $\{|+z\rangle, |-z\rangle\}$, is given by

$$\hat{J}_y = \frac{\hbar}{2}\sigma_y = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}.$$

32. Commutation relation of the Pauli matrices

$$[\hat{J}_x, \hat{J}_y] = \left(\frac{\hbar}{2}\right)^2 [\hat{\sigma}_x, \hat{\sigma}_y] = \frac{\hbar^2}{4} 2i\hat{\sigma}_z = i\hbar\frac{\hbar}{2}\hat{\sigma}_z = i\hbar\hat{J}_z,$$

where

$$[\hat{\sigma}_x, \hat{\sigma}_y] = \hat{\sigma}_x\hat{\sigma}_y - \hat{\sigma}_y\hat{\sigma}_x$$
$$= \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} - \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$
$$= \begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix} - \begin{pmatrix} -i & 0 \\ 0 & i \end{pmatrix}$$
$$= 2i\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = 2i\hat{\sigma}_z$$

33. Formulation for the eigenvalue problem with 2 x 2 matrix

We consider the eigenvalue problem such that

$$\hat{A}|a_1\rangle = a_1|a_1\rangle, \qquad \hat{A}|a_2\rangle = a_2|a_2\rangle,$$

where $|a_1\rangle$ is the eigenket of $\hat{A}$ with the eigenvalue a_1, and $|a_2\rangle$ is the eigenket of $\hat{A}$ with the eigenvalue a_2. Note that

$$\langle a_i|\hat{A}|a_j\rangle = a_i\langle a_i|a_j\rangle = a_i\delta_{ij} \qquad \text{(diagonal)}$$

Suppose we have the matrix A under the basis of $\{|b_1\rangle$ and $|b_2\rangle\}$.

$$\hat{A} = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix},$$

where

$$\langle b_i|\hat{A}|b_j\rangle = A_{ij}.$$

In the eigenvalue problem, we need to find the unitary operator $\hat{U}$ such that

$$|a_1\rangle = \hat{U}|b_1\rangle = \begin{pmatrix} U_{11} & U_{12} \\ U_{21} & U_{22} \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} U_{11} \\ U_{21} \end{pmatrix},$$

$$|a_2\rangle = \hat{U}|b_2\rangle = \begin{pmatrix} U_{11} & U_{12} \\ U_{21} & U_{22} \end{pmatrix}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} U_{12} \\ U_{22} \end{pmatrix},$$

and

$$\begin{aligned} \hat{U} &= \hat{U}(|b_1\rangle\langle b_1| + |b_2\rangle\langle b_2|) \\ &= |a_1\rangle\langle b_1| + |a_2\rangle\langle b_2| \end{aligned}$$

where

$$\hat{U} = \begin{pmatrix} U_{11} & U_{12} \\ U_{21} & U_{22} \end{pmatrix},$$

$$\hat{U}^{+} = \begin{pmatrix} U_{11}^{*} & U_{21}^{*} \\ U_{12}^{*} & U_{22}^{*} \end{pmatrix}.$$

The condition for the unitary operator

$$\hat{U}^+\hat{U} = \begin{pmatrix} U_{11}^* & U_{21}^* \\ U_{12}^* & U_{22}^* \end{pmatrix}\begin{pmatrix} U_{11} & U_{12} \\ U_{21} & U_{22} \end{pmatrix}$$
$$= \begin{pmatrix} U_{11}^*U_{11} + U_{21}^*U_{21} & U_{11}^*U_{12} + U_{21}^*U_{22} \\ U_{12}^*U_{11} + U_{22}^*U_{21} & U_{12}^*U_{12} + U_{22}^*U_{22} \end{pmatrix}$$
$$= \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

The orthogonality of $|a_1\rangle$ and $|a_2\rangle$;

$$\langle a_2|a_1\rangle = (U_{12}^*U_{22}^*)\begin{pmatrix} U_{11} \\ U_{21} \end{pmatrix} = U_{12}^*U_{11} + U_{22}^*U_{21} = 0 .$$

The normalization of $|a_1\rangle$ and $|a_2\rangle$;

$$\langle a_1|a_1\rangle = (U_{11}^*U_{21}^*)\begin{pmatrix} U_{11} \\ U_{21} \end{pmatrix} = U_{11}^*U_{11} + U_{21}^*U_{21} = 1 ,$$

$$\langle a_2|a_2\rangle = (U_{12}^*U_{22}^*)\begin{pmatrix} U_{12} \\ U_{22} \end{pmatrix} = U_{12}^*U_{12} + U_{22}^*U_{22} = 1 .$$

Note that

$$\langle a_i|\hat{A}|a_j\rangle = \langle b_i|\hat{U}^+\hat{A}\hat{U}|b_j\rangle = a_i\delta_{ij} ,$$

or

$$\hat{U}^+\hat{A}\hat{U} = \begin{pmatrix} U_{11}^* & U_{12}^* \\ U_{12}^* & U_{22}^* \end{pmatrix}\begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{21} \end{pmatrix}\begin{pmatrix} U_{11} & U_{12} \\ U_{21} & U_{22} \end{pmatrix} = \begin{pmatrix} a_1 & 0 \\ 0 & a_2 \end{pmatrix} .$$

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34. Matrix representation of $\hat{S}_z$ under the basis of $\{|+x\rangle$ and $|-x\rangle\}$

Eigenvalue problem:

$$\hat{S}_x|+x\rangle = \frac{\hbar}{2}|+x\rangle , \qquad \hat{S}_x|-x\rangle = -\frac{\hbar}{2}|-x\rangle .$$

We define the unitary operator such that

$$\left|+x\right\rangle = \hat{U}\left|+z\right\rangle = \begin{pmatrix} U_{11} & U_{12} \\ U_{21} & U_{22} \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} U_{11} \\ U_{21} \end{pmatrix},$$

$$\left|-x\right\rangle = \hat{U}\left|-\right\rangle = \begin{pmatrix} U_{11} & U_{12} \\ U_{21} & U_{22} \end{pmatrix}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} U_{12} \\ U_{22} \end{pmatrix}.$$

The matrix representation of $\hat{S}_x$ is given by

$$\hat{S}_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},$$

under the basis of $\{\left|+z\right\rangle$ and $\left|-z\right\rangle\}$. Then the eigenvalue problem is as follows.

(a) $\lambda = 1$ (eigenvalue)

$$\frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} U_{11} \\ U_{21} \end{pmatrix} = \frac{\hbar}{2}\begin{pmatrix} U_{11} \\ U_{21} \end{pmatrix},$$

or

$$\begin{pmatrix} U_{11} \\ U_{21} \end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix},$$

(b) $\lambda = -1$ (eigenvalue)

$$\frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} U_{12} \\ U_{22} \end{pmatrix} = -\frac{\hbar}{2}\begin{pmatrix} U_{12} \\ U_{22} \end{pmatrix},$$

or

$$\begin{pmatrix} U_{11} \\ U_{21} \end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}.$$

Then we have the unitary operator (matrix form)

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

$$|+x\rangle = \hat{U}|+z\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}, \qquad |-x\rangle = \hat{U}|-z\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}.$$

Since

$$\langle +x| = \langle +z|\hat{U}^{+}, \qquad \text{and} \qquad \langle -x| = \langle -z|\hat{U}^{+},$$

we get

$$\langle +x|\hat{S}_z|+x\rangle = \langle +z|\hat{U}^{+}\hat{S}_z\hat{U}|+z\rangle .$$

The matrix representation of $\hat{S}_z$ under the basis of $\{|+x\rangle$ and $|-x\rangle\}$ is given by

$$\begin{aligned}
\hat{U}^{+}\hat{S}_z\hat{U} &= \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}\frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \\
&= \frac{\hbar}{4}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}\begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix} \\
&= \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}
\end{aligned}$$

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35. **Matrix presentation of $\hat{S}_y$ and $\hat{S}_z$ under the** basis of $\{|+y\rangle$ and $|-y\rangle\}$

Eigenvalue problem:

$$\hat{S}_y|+y\rangle = \frac{\hbar}{2}|+y\rangle, \qquad \hat{S}_y|-y\rangle = -\frac{\hbar}{2}|-y\rangle .$$

We define the unitary operator such that

$$|+y\rangle = \hat{U}|+z\rangle = \begin{pmatrix} U_{11} & U_{12} \\ U_{21} & U_{22} \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} U_{11} \\ U_{21} \end{pmatrix},$$

$$|-y\rangle = \hat{U}|-z\rangle = \begin{pmatrix} U_{11} & U_{12} \\ U_{21} & U_{22} \end{pmatrix}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} U_{12} \\ U_{22} \end{pmatrix}.$$

The matrix representation of $\hat{S}_y$ is given by

$$\hat{S}_y = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix},$$

under the basis of {$|+z\rangle$ and $|-z\rangle$}. Then the eigenvalue problem is as follows.

(a) λ = 1 (eigenvalue)

$$\frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}\begin{pmatrix} U_{11} \\ U_{21} \end{pmatrix} = \frac{\hbar}{2}\begin{pmatrix} U_{11} \\ U_{21} \end{pmatrix},$$

or

$$\begin{pmatrix} U_{11} \\ U_{21} \end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ i \end{pmatrix}.$$

(b) λ = -1 (eigenvalue)

$$\frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} U_{12} \\ U_{22} \end{pmatrix} = -\frac{\hbar}{2}\begin{pmatrix} U_{12} \\ U_{22} \end{pmatrix},$$

or

$$\begin{pmatrix} U_{12} \\ U_{22} \end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -i \end{pmatrix}.$$

Then we have the unitary operator (matrix form) as

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

$$|+y\rangle = \hat{U}|+\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ i \end{pmatrix}, \qquad |-y\rangle = \hat{U}|-\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -i \end{pmatrix},$$

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

The matrix $\hat{S}_y$ under the basis of {$|+y\rangle$ and $|-y\rangle$} is given by

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

$$= \frac{\hbar}{4}\begin{pmatrix} 1 & -i \\ 1 & i \end{pmatrix}\begin{pmatrix} 1 & -1 \\ i & i \end{pmatrix}$$

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

The matrix $\hat{S}_x$ under the basis of $\{\left|+y\right\rangle$ and $\left|-y\right\rangle\}$ is given by

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

$$= \frac{\hbar}{4}\begin{pmatrix} 1 & -i \\ 1 & i \end{pmatrix}\begin{pmatrix} 1 & 1 \\ -i & i \end{pmatrix}$$

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

36. The Vector operator under the rotation

Consider a rotation by a finite angle ϕ about the z axis.

$$\left|\psi'\right\rangle = \hat{R}_z(\phi)\left|\psi\right\rangle.$$

Let us calculate the expectation value of the spin operators $\hat{S}_x$, $\hat{S}_y$, and $\hat{S}_z$

$$\left\langle\psi'\right|\hat{S}_i\left|\psi'\right\rangle = \left\langle\psi\right|\hat{R}_z^{\,+}(\phi)\hat{S}_i\hat{R}_z(\phi)\left|\psi\right\rangle,$$

$$\hat{R}_z^{\,+}(\phi)\hat{S}_x\hat{R}_z(\phi) = \frac{\hbar}{2}\exp(\frac{i\phi\hat{\sigma}_z}{2})\hat{\sigma}_x\exp(-\frac{i\phi\sigma_z}{2}) = \frac{\hbar}{2}(\hat{\sigma}_x\cos\phi - \hat{\sigma}_y\sin\phi),$$

$$\hat{R}_z^{\,+}(\phi)\hat{S}_y\hat{R}_z(\phi) = \frac{\hbar}{2}\exp(\frac{i\phi\hat{\sigma}_z}{2})\hat{\sigma}_y\exp(-\frac{i\phi\hat{\sigma}_z}{2}) = \frac{\hbar}{2}(\hat{\sigma}_x\sin\phi + \hat{\sigma}_y\cos\phi),$$

$$\hat{R}_z^{\,+}(\phi)\hat{S}_z\hat{R}_z(\phi) = \frac{\hbar}{2}\exp(\frac{i\phi\hat{\sigma}_z}{2})\hat{\sigma}_z\exp(-\frac{i\phi\hat{\sigma}_z}{2}) = \frac{\hbar}{2}\hat{\sigma}_z.$$

Here we use the following theorem.

The operator

$$f(x) = \exp(\hat{A}x)\hat{B}\exp(-\hat{A}x)$$

can be expanded as

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

$$x = \frac{i\phi}{2}, \qquad \hat{A} = \hat{\sigma}_z, \qquad \hat{A} = \hat{\sigma}_y .$$

Thus we have

$$\langle\psi'|\hat{S}_x|\psi'\rangle = \langle\psi|\hat{S}_x\cos\phi - \hat{S}_y\sin\phi|\psi\rangle = \cos\phi\langle\psi|\hat{S}_x|\psi\rangle - \sin\phi\langle\psi|\hat{S}_y|\psi\rangle,$$

Similarly

$$\langle\psi'|\hat{S}_y|\psi'\rangle = \sin\phi\langle\psi|\hat{S}_x|\psi\rangle + \cos\phi\langle\psi|\hat{S}_y|\psi\rangle,$$

$$\langle\psi'|\hat{S}_z|\psi'\rangle = \langle\psi|\hat{S}_z|\psi\rangle .$$

Note that

$$\Re_z(\phi) = \begin{pmatrix} \cos\phi & -\sin\phi & 0 \\ \sin\phi & \cos\phi & 0 \\ 0 & 0 & 1 \end{pmatrix},$$

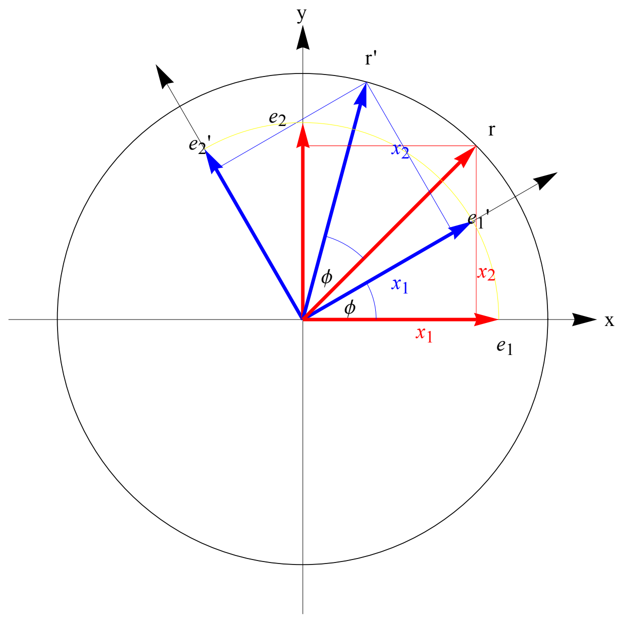
$$\langle\psi'|\hat{S}_i|\psi'\rangle = \sum_j \Re_{ij}\langle\psi|\hat{S}_j|\psi\rangle = \sum_j \langle\psi|\Re_{ij}\hat{S}_j|\psi\rangle .$$

In general for any vector operators, we have

$$\langle\psi'|\hat{A}_i|\psi'\rangle = \sum_j \langle\psi|\Re_{ij}\hat{A}_j|\psi\rangle .$$

APPENDIX 2D rotation matrix

Suppose that the vector ***r*** is rotated through θ (counter-clock wise) around the z axis. The position vector ***r*** is changed into ***r***' in the same orthogonal basis $\{\boldsymbol{e}_1, \boldsymbol{e}_2\}$.



In this Fig, we have

$$\mathbf{e}_1 \cdot \mathbf{e}_1' = \cos\phi \qquad \mathbf{e}_2 \cdot \mathbf{e}_1' = \sin\phi$$
$$\mathbf{e}_1 \cdot \mathbf{e}_2' = -\sin\phi, \qquad \mathbf{e}_2 \cdot \mathbf{e}_2' = \cos\phi.$$

We define ***r*** and ***r'*** as

$$\mathbf{r}' = x_1'\mathbf{e}_1 + x_2'\mathbf{e}_2 = x_1\mathbf{e}_1' + x_2\mathbf{e}_2',$$

and

$$\mathbf{r} = x_1\mathbf{e}_1 + x_2\mathbf{e}_2.$$

Using the relation

$$\mathbf{e}_1 \cdot \mathbf{r}' = \mathbf{e}_1 \cdot (x_1'\mathbf{e}_1 + x_2'\mathbf{e}_2) = \mathbf{e}_1 \cdot (x_1\mathbf{e}_1' + x_2\mathbf{e}_2')$$
$$\mathbf{e}_2 \cdot \mathbf{r}' = \mathbf{e}_2 \cdot (x_1'\mathbf{e}_1 + x_2'\mathbf{e}_2) = \mathbf{e}_2 \cdot (x_1\mathbf{e}_1' + x_2\mathbf{e}_2')$$

we have

$$x_1' = \mathbf{e}_1 \cdot (x_1\mathbf{e}_1' + x_2\mathbf{e}_2') = x_1\cos\phi - x_2\sin\phi$$
$$x_2' = \mathbf{e}_2 \cdot (x_1\mathbf{e}_1' + x_2\mathbf{e}_2') = x_1\sin\phi + x_2\cos\phi$$

or

$$\begin{pmatrix} x_1' \\ x_2' \end{pmatrix} = \Re(\phi)\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} \cos\phi & -\sin\phi \\ \sin\phi & \cos\phi \end{pmatrix}\begin{pmatrix} x_1 \\ x_2 \end{pmatrix}.$$

APPENDIX II Rotation operator for spin 1/2 (this will be discussed later chapter)

(a) Calculate the rotation operator $\hat{R}_z(\gamma) = \exp(-\frac{i\hat{S}_z}{\hbar}\gamma) = \exp(-\frac{i}{2}\hat{\sigma}_z\gamma)$, which rotates the ket counterclockwise by angle γ around the z axis.

(b) Calculate the rotation operator $\hat{R}_x(\alpha) = \exp(-\frac{i\hat{S}_x}{\hbar}\alpha) = \exp(-\frac{i}{2}\hat{\sigma}_x\alpha)$, which rotates the ket counterclockwise by angle α around the x axis.

(c) Calculate the rotation operator $\hat{R}_y(\beta) = \exp(-\frac{i\hat{S}_y}{\hbar}\beta) = \exp(-\frac{i}{2}\hat{\sigma}_y\beta)$, which rotates the ket counterclockwise by angle β around the y axis.

(d) Calculate the rotation operator defined by

$$\hat{R}_z(\phi)\hat{R}_y(\theta).$$

(e) Find the expressions for the state vectors $|+\boldsymbol{n}\rangle = \hat{R}_z(\phi)\hat{R}_y(\theta)|+z\rangle$ and $|-\boldsymbol{n}\rangle = \hat{R}_z(\phi)\hat{R}_y(\theta)|-z\rangle$, where the unit vector $\boldsymbol{n}$ is given by

$$\boldsymbol{n} = \sin\theta\cos\phi\boldsymbol{e}_x + \sin\theta\sin\phi\boldsymbol{e}_y + \cos\theta\boldsymbol{e}_z.$$

((**Solution**))

(a)

$$\hat{R}_z(\gamma) = \exp(-\frac{i}{\hbar}\hat{J}_z\gamma) = \exp(-\frac{i}{2}\hat{\sigma}_z\gamma),$$

$$\hat{R}_z(\gamma)|+z\rangle = \exp(-\frac{i}{2}\hat{\sigma}_z\gamma)|+z\rangle = e^{-\frac{i}{2}\gamma}|+z\rangle,$$

$$\hat{R}_z(\gamma)|-z\rangle = \exp(-\frac{i}{2}\hat{\sigma}_z\gamma)|-z\rangle = e^{\frac{i}{2}\gamma}|-z\rangle,$$

or

$$\hat{R}_z(\gamma) = \begin{pmatrix} e^{-\frac{i}{2}\gamma} & 0 \\ 0 & e^{\frac{i}{2}\gamma} \end{pmatrix}.$$

(b)

$$\hat{R}_x(\alpha) = \exp(-\frac{i}{\hbar}\hat{J}_x\alpha) = \exp(-\frac{i}{2}\hat{\sigma}_x\alpha).$$

Here we note that

$$|+x\rangle = \frac{1}{\sqrt{2}}(|+z\rangle + |-z\rangle) \qquad |-x\rangle = \frac{1}{\sqrt{2}}(|+z\rangle - |-z\rangle).$$

Then

$$|+z\rangle = \frac{1}{\sqrt{2}}(|+x\rangle + |-x\rangle), \qquad |-z\rangle = \frac{1}{\sqrt{2}}(|+x\rangle - |-x\rangle),$$

$$\begin{aligned}
\hat{R}_x(\alpha)|+z\rangle &= \exp(-\frac{i}{2}\hat{\sigma}_x\alpha)|+z\rangle \\
&= \frac{1}{\sqrt{2}}\exp(-\frac{i}{2}\hat{\sigma}_x\alpha)(|+x\rangle + |-x\rangle) \\
&= \frac{1}{\sqrt{2}}[e^{-\frac{i}{2}\alpha}|+x\rangle + e^{\frac{i}{2}\alpha}|-x\rangle] \\
&= \frac{1}{2}[e^{-\frac{i}{2}\alpha}(|+z\rangle + |-z\rangle) + e^{\frac{i}{2}\alpha}(|+z\rangle - |-z\rangle)] \\
&= \cos\frac{\alpha}{2}|+z\rangle - i\sin\frac{\alpha}{2}|-z\rangle
\end{aligned}$$

$$\begin{aligned}
\hat{R}_x(\alpha)|-z\rangle &= \exp(-\frac{i}{2}\hat{\sigma}_x\alpha)|-z\rangle \\
&= \frac{1}{\sqrt{2}}\exp(-\frac{i}{2}\hat{\sigma}_x\alpha)(|+x\rangle - |-x\rangle) \\
&= \frac{1}{\sqrt{2}}[e^{-\frac{i}{2}\alpha}|+x\rangle - e^{\frac{i}{2}\alpha}|-x\rangle] \\
&= \frac{1}{2}[e^{-\frac{i}{2}\alpha}(|+z\rangle + |-z\rangle) - e^{\frac{i}{2}\alpha}(|+z\rangle - |-z\rangle)] \\
&= -i\sin\frac{\alpha}{2}|+z\rangle + \cos\frac{\alpha}{2}|-z\rangle
\end{aligned}$$

or

$$\hat{R}_x(\alpha) = \begin{pmatrix} \cos\frac{\alpha}{2} & -i\sin\frac{\alpha}{2} \\ -i\sin\frac{\alpha}{2} & \cos\frac{\alpha}{2} \end{pmatrix}.$$

(c)

$$\hat{R}_y(\beta) = \exp(-\frac{i}{\hbar}\hat{J}_y\beta) = \exp(-\frac{i}{2}\hat{\sigma}_y\beta).$$

Here we note that

$$\left|+y\right\rangle = \frac{1}{\sqrt{2}}(\left|+z\right\rangle + i\left|-z\right\rangle), \qquad \left|-y\right\rangle = \frac{1}{\sqrt{2}}(\left|+z\right\rangle - i\left|-z\right\rangle).$$

Then

$$\left|+z\right\rangle = \frac{1}{\sqrt{2}}(\left|+y\right\rangle + \left|-y\right\rangle), \qquad \left|-z\right\rangle = \frac{1}{i\sqrt{2}}(\left|+y\right\rangle - \left|-y\right\rangle),$$

$$\begin{aligned}
\hat{R}_y(\beta)\left|+z\right\rangle &= \exp(-\frac{i}{2}\hat{\sigma}_y\beta)\left|+z\right\rangle \\
&= \frac{1}{\sqrt{2}}\exp(-\frac{i}{2}\hat{\sigma}_y\beta)(\left|+y\right\rangle + \left|-y\right\rangle) \\
&= \frac{1}{\sqrt{2}}[e^{-\frac{i}{2}\beta}\left|+y\right\rangle + e^{\frac{i}{2}\beta}\left|-y\right\rangle] \\
&= \frac{1}{2}[e^{-\frac{i}{2}\beta}(\left|+z\right\rangle + i\left|-z\right\rangle) + e^{\frac{i}{2}\beta}(\left|+z\right\rangle - i\left|-z\right\rangle)] \\
&= \cos\frac{\beta}{2}\left|+z\right\rangle + \sin\frac{\beta}{2}\left|-z\right\rangle
\end{aligned}$$

$$\begin{aligned}
\hat{R}_y(\beta)\left|-z\right\rangle &= \exp(-\frac{i}{2}\hat{\sigma}_y\beta)\left|-z\right\rangle \\
&= \frac{1}{\sqrt{2}i}\exp(-\frac{i}{2}\hat{\sigma}_y\beta)(\left|+y\right\rangle - \left|-y\right\rangle) \\
&= \frac{1}{\sqrt{2}i}[e^{-\frac{i}{2}\beta}\left|+y\right\rangle - e^{\frac{i}{2}\beta}\left|-y\right\rangle] \\
&= \frac{1}{2i}[e^{-\frac{i}{2}\beta}(\left|+z\right\rangle + i\left|-z\right\rangle) - e^{\frac{i}{2}\beta}(\left|+z\right\rangle - i\left|-z\right\rangle)] \\
&= -\sin\frac{\beta}{2}\left|+z\right\rangle + \cos\frac{\phi}{2}\left|-z\right\rangle
\end{aligned}$$

or

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

(d)

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

(e)

$$\hat{R}_z(\phi)\hat{R}_y(\theta)\left|+z\right\rangle = \begin{pmatrix} e^{-\frac{i}{2}\phi}\cos\frac{\theta}{2} \\ e^{\frac{i}{2}\phi}\sin\frac{\theta}{2} \end{pmatrix},$$

$$\hat{R}_z(\phi)\hat{R}_y(\theta)\left|+z\right\rangle = \begin{pmatrix} -e^{-\frac{i}{2}\phi}\sin\frac{\theta}{2} \\ e^{\frac{i}{2}\phi}\cos\frac{\theta}{2} \end{pmatrix}.$$

((Method II)) The use of formula for the rotation operator

We use the formula for the rotation operator given by

$$\hat{R}_u(\phi) = \exp[-\frac{i\phi}{2}(\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{u})] = \cos\frac{\phi}{2}\hat{1} - i(\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{u})\cos\frac{\phi}{2}.$$

(a)

$$\hat{R}_x(\alpha) = \exp[-\frac{i\alpha}{2}\hat{\sigma}_x] = \cos\frac{\alpha}{2}\hat{1} - i\hat{\sigma}_x\sin\frac{\alpha}{2}$$
$$= \begin{pmatrix} \cos\frac{\alpha}{2} & -i\sin\frac{\alpha}{2} \\ i\sin\frac{\alpha}{2} & \cos\frac{\alpha}{2} \end{pmatrix}$$

(b)

$$\hat{R}_y(\beta) = \exp[-\frac{i\beta}{2}\hat{\sigma}_y]$$

$$= \cos\frac{\beta}{2}\hat{1} - i\hat{\sigma}_y \sin\frac{\beta}{2}$$

$$= \begin{pmatrix} \cos\frac{\beta}{2} & -\sin\frac{\beta}{2} \\ \sin\frac{\beta}{2} & \cos\frac{\beta}{2} \end{pmatrix}$$

(c)

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

$$= \cos(\frac{\gamma}{2})\hat{1} - i\hat{\sigma}_z \sin(\frac{\gamma}{2})$$

$$= \begin{pmatrix} \cos\frac{\gamma}{2} - i\sin\frac{\gamma}{2} & 0 \\ 0 & \cos\frac{\gamma}{2} + i\sin\frac{\gamma}{2} \end{pmatrix}$$

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

((Method-III)) **The use of unitary operator**

Since

$$\langle +z|\hat{R}_x(\alpha)|+z\rangle = \langle +x|\hat{U}_x\hat{R}_x(\alpha)\hat{U}_x^{\ +}|+x\rangle,$$

we have

$$\hat{U}_x\hat{R}_x(\alpha)\hat{U}_x^{\ +} = \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}\begin{pmatrix} e^{\frac{-i}{2}\alpha} & 0 \\ 0 & e^{\frac{i}{2}\alpha} \end{pmatrix}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} = \begin{pmatrix} \cos\frac{\alpha}{2} & -\sin\frac{\alpha}{2} \\ \sin\frac{\alpha}{2} & \cos\frac{\alpha}{2} \end{pmatrix}.$$

Since

$$\langle +z|\hat{R}_y(\beta)|+z\rangle = \langle +y|\hat{U}_y\hat{R}_y(\beta)\hat{U}_y^{\ +}|+y\rangle,$$

we have

$$\hat{U}_y \hat{R}_y(\beta) \hat{U}_y^{\ +} = \frac{1}{2}\begin{pmatrix} 1 & 1 \\ i & -i \end{pmatrix}\begin{pmatrix} e^{\frac{-i}{2}\alpha} & 0 \\ 0 & e^{\frac{i}{2}\alpha} \end{pmatrix}\begin{pmatrix} 1 & -i \\ 1 & 1 \end{pmatrix} = \begin{pmatrix} \cos\frac{\alpha}{2} & -i\sin\frac{\alpha}{2} \\ -i\sin\frac{\alpha}{2} & \cos\frac{\alpha}{2} \end{pmatrix}.$$