Density operator

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(Date: November 08, 2014)

1. Introduction

The quantum-mechanical description based on an incomplete set of data concerning the system is effected by means of what is called a density operator. Such a density operator was introduced by von Neumann in 1927 to describe statistical concepts in quantum mechanics. Most physical systems consist of so many particles, or posses so many degrees of freedom. that it is impossible to specify completely the state of these systems. Nevertheless, physicists are forced to make predictions about the behavior of the systems they study from a knowledge of a very small number of parameters. To this end, one can use statistical methods and introduce representative ensembles which are collections of identical systems.

The density operator is an alternate representation of the state of a quantum system for which we have previously used the wavefunction. Although describing a quantum system with the density matrix is equivalent to using the wavefunction, one gains significant practical advantages using the density matrix for many physics problem. For a quantum mechanical system there are, in general, two reasons for statistical treatment: lack of detailed knowledge and the probabilistic nature of quantum mechanics. The statistical treatment is carried out by means of the density matrix which takes the place of the ensemble density in classical statistical mechanics. This operator – as all physical quantities in quantum mechanics, the density matrix is an operator – can be used to evaluate averages.

2. Definition of density operator

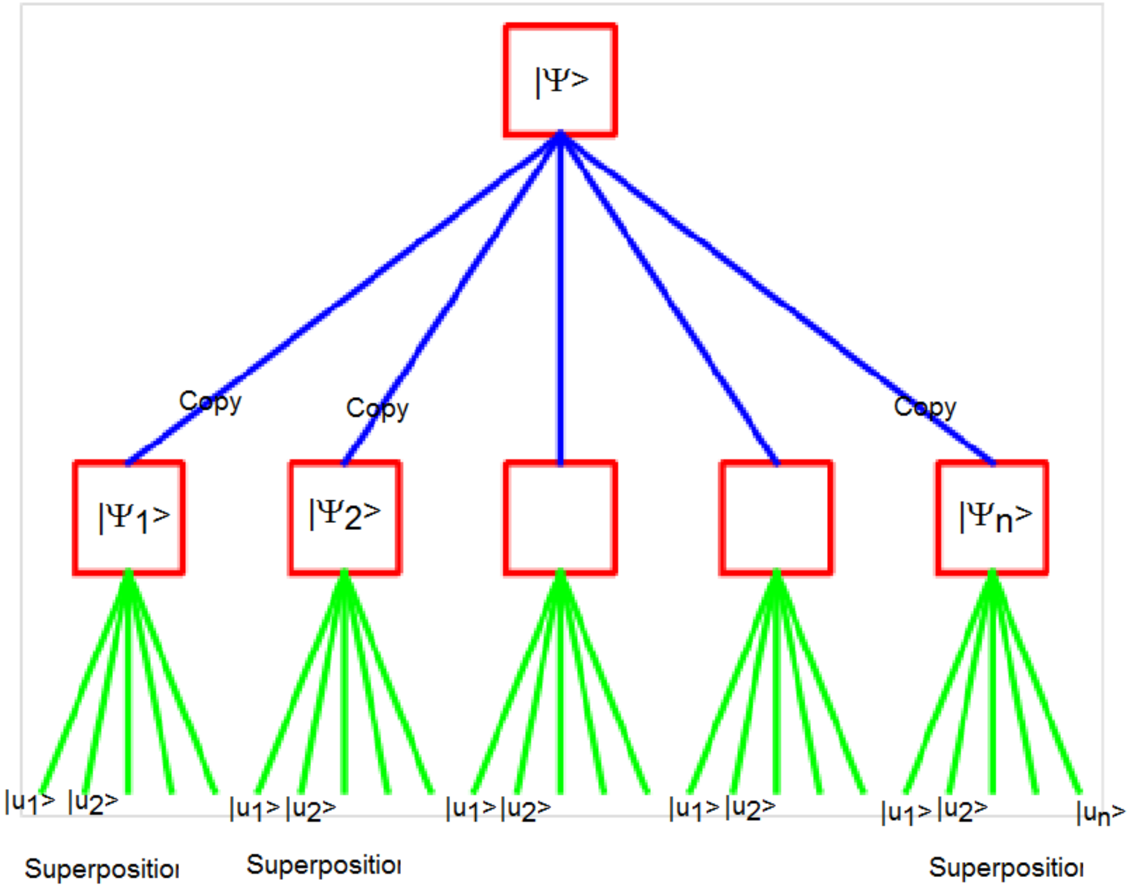

Fig. Ensemble average. Definition of the density operator

We suppose that the state ket vector of a system is represented by

$$|\psi\rangle = \sum_n c_n |u_n\rangle ,$$

for each ensemble, where

$$\langle u_n | u_m \rangle = \delta_{n,m} .$$

We define

$$\hat{\rho} = \overline{|\psi\rangle\langle\psi|} = \overline{\sum_{n,m} c_n |u_n\rangle c_m{}^* \langle u_m|} = \sum_{n,m} \overline{c_n c_m{}^*} |u_n\rangle\langle u_m| = \sum_{n,m} \rho_{nm} |u_n\rangle\langle u_m| ,$$

with the matrix element

$$\rho_{nm} = \langle u_n|\hat{\rho}|u_m\rangle = \overline{c_n c_m^*},$$

where the bar denotes ensemble average; that is, average over all the systems in the ensemble. Then the density operator $\hat{\rho}$ has the following properties.

(a) $\hat{\rho}^+ = \hat{\rho}$. (Hermitian operator)

(b) $Tr[\hat{\rho}] = 1$.

((**Proof**))

$$\overline{\langle\psi|\psi\rangle} = \overline{\sum_n c_n^* c_n} = \sum_n \overline{c_n^* c_n} = \sum_n \rho_{nn} = Tr[\hat{\rho}] = 1.$$

(c) The ensemble average of the expectation of an observable $\hat{A}$ is given by

$$\langle A\rangle = Tr[\hat{A}\hat{\rho}].$$

((**Proof**))

$$\begin{aligned}
\overline{\langle\psi|\hat{A}|\psi\rangle} &= \sum_{n,m} \overline{c_m^* c_n} \langle u_m|\hat{A}|u_n\rangle \\
&= \sum_{n,m} \rho_{nm} \langle u_m|\hat{A}|u_n\rangle \\
&= \sum_{n,m} \langle u_n|\hat{\rho}|u_m\rangle\langle u_m|\hat{A}|u_n\rangle \\
&= \sum_{n} \langle u_n|\hat{\rho}\hat{A}|u_n\rangle = Tr[\hat{\rho}\hat{A}]
\end{aligned}$$

(d)

We define a new density operator as

$$\hat{\rho}' = \overline{|\psi'\rangle\langle\psi'|} = \overline{\hat{U}|\psi\rangle\langle\psi|\hat{U}^+} = \hat{U}\overline{|\psi\rangle\langle\psi|}\hat{U}^+ = \hat{U}\hat{\rho}\hat{U}^+,$$

where

$$|\psi'\rangle = \hat{U}|\psi\rangle,$$

and $\hat{U}$ is the unitary operator.

(e) Equation of motion

The time dependence of $\hat{\rho}$ is given by

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

This equation is analogous to the Liouville theorem in classical theory.

$$\begin{aligned}
\frac{d}{dt}\hat{\rho} &= \overline{\frac{d}{dt}|\psi\rangle\langle\psi|} \\
&= \overline{\left(\frac{\partial}{\partial t}|\psi\rangle\right)\langle\psi| + |\psi\rangle\left(\frac{\partial}{\partial t}\langle\psi|\right)} \\
&= \frac{1}{i\hbar}\overline{\hat{H}|\psi\rangle\langle\psi| - |\psi\rangle\langle\psi|\hat{H}} \\
&= \frac{1}{i\hbar}\hat{H}\overline{|\psi\rangle\langle\psi|} - \overline{|\psi\rangle\langle\psi|}\hat{H} \\
&= \frac{1}{i\hbar}\hat{H}\hat{\rho} - \hat{\rho}\hat{H} = -\frac{1}{i\hbar}[\hat{\rho}, \hat{H}]
\end{aligned}$$

Note that this equation of motion is a little different (in sign) from the equation of motion of the Heisenberg operator $\hat{A}_H$.

$$\frac{d}{dt}\hat{A}_H = \frac{1}{i\hbar}[\hat{A}_H, \hat{H}].$$

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3. Pure state

$$\hat{\rho} = |\psi\rangle\langle\psi|,$$

$$\hat{\rho}^2 = |\psi\rangle\langle\psi|\psi\rangle\langle\psi| = \hat{\rho}.$$

Then we have

$$Tr[\hat{\rho}^2] = Tr[\hat{\rho}] = 1.$$

This is the definition of the density operator for the pure state.

$$\hat{\rho}^{+} = |\psi\rangle\langle\psi| = \hat{\rho} ,$$

$$\hat{\rho}|\psi\rangle = |\psi\rangle\langle\psi|\psi\rangle = |\psi\rangle .$$

Then $|\psi\rangle$ is the eigenket of $\hat{\rho}$ with the eigenvalue 1.

$$\rho_{nm} = c_n c_m^{*} .$$

4. Mixed state

We consider the eigenvalue problem of $\hat{\rho}$.

$$\hat{\rho}|\phi_n\rangle = p_n|\phi_n\rangle ,$$

where p_n is the eigenvalue and $|\phi_n\rangle$ is the eigenket of $\hat{\rho}$ with the eigenvalue p_n.

We define the unitary operator as

$$|\phi_n\rangle = \hat{U}|u_n\rangle ,$$

$$\hat{\rho}\hat{U}|u_n\rangle = p_n\hat{U}|u_n\rangle ,$$

or

$$\hat{U}^{+}\hat{\rho}\hat{U}|u_n\rangle = w_n|u_n\rangle .$$

Then we have

$$\hat{U}^{+}\hat{\rho}\hat{U} = \begin{pmatrix} p_1 & 0 & 0 & 0 & 0 \\ 0 & p_2 & 0 & 0 & 0 \\ 0 & 0 & p_3 & 0 & 0 \\ 0 & 0 & 0 & p_4 & 0 \\ 0 & 0 & 0 & 0 & p_5 \end{pmatrix}, \qquad \text{(diagonal matrix)}$$

under the basis of $\{|u_n\rangle\}$. So we define a new density operator as

$$\hat{\rho} = \hat{\rho}\sum_n |\phi_n\rangle\langle\phi_n| = \sum_n \hat{\rho}|\phi_n\rangle\langle\phi_n| = \sum_n p_n|\phi_n\rangle\langle\phi_n|,$$

where

$$p_n = \langle\phi_n|\hat{\rho}|\phi_n\rangle.$$

We note that

$$Tr[\hat{\rho}] = \sum_n p_n = 1,$$

$$\begin{aligned}
Tr[\hat{\rho}] &= \sum_n \langle u_n|\hat{\rho}|u_n\rangle \\
&= \sum_{n,k} \langle u_n|\hat{\rho}|\phi_k\rangle\langle\phi_k|u_n\rangle \\
&= \sum_{n,k} p_k\langle u_n|\phi_k\rangle\langle\phi_k|u_n\rangle \\
&= \sum_{n,k} p_k\langle\phi_k|u_n\rangle\langle u_n|\phi_k\rangle \\
&= \sum_k p_k\langle\phi_k|\phi_k\rangle = \sum_k p_k = 1
\end{aligned}$$

$$Tr[\hat{\rho}^2] = \sum_n p_n{}^2 \leq \sum_n p_n = 1,$$

since

$$p_k{}^2 \leq p_k.$$

The expectation value is given by

$$\langle A\rangle = \sum_n p_n\langle\phi_n|\hat{A}|\phi_n\rangle = Tr[\hat{A}\hat{\rho}],$$

since

$$
\begin{aligned}
Tr[\hat{A}\hat{\rho}] &= \sum_n \langle \phi_n | A\rho | \phi_n \rangle \\
&= \sum_{n,m} \langle \phi_n | A | \phi_m \rangle \langle \phi_m | \rho | \phi_n \rangle \\
&= \sum_{n,m} p_n \langle \phi_n | A | \phi_m \rangle \langle \phi_m | \phi_n \rangle \\
&= \sum_{n,m} p_n \langle \phi_n | A | \phi_m \rangle \delta_{m,n} \\
&= \sum_n p_n \langle \phi_n | A | \phi_n \rangle
\end{aligned}
$$

For the projection operator, we have

$$\hat{P}_{\phi_m} = |\phi_m\rangle\langle\phi_m|,$$

and

$$Tr[\hat{P}_{\phi_m}\hat{\rho}] = p_m,$$

since

$$Tr[\hat{P}_{\phi_m}\hat{\rho}] = \sum_n p_n \langle \phi_n | \hat{P}_{\phi_m} | \phi_n \rangle = \sum_n p_n \delta_{n,m} = p_m.$$

5. Example: density operator for the un-polarized light

(a) The pure state

We now consider the density operator of the linearly polarized photon,

$$\hat{\rho} = |\psi\rangle\langle\psi|, \qquad \text{(the pure state)}$$

where $|\psi\rangle = \cos\theta|x\rangle + \sin\theta|y\rangle$. The corresponding density matrix under the basis of $\{|x\rangle$ and $|y\rangle\}$ can be given by

$$\hat{\rho} = \begin{pmatrix} \cos\theta \\ \sin\theta \end{pmatrix} \begin{pmatrix} \cos\theta & \sin\theta \end{pmatrix}$$

$$= \begin{pmatrix} \cos^2\theta & \sin\theta\cos\theta \\ \sin\theta\cos\theta & \sin^2\theta \end{pmatrix} .$$

$$= \frac{1}{2} \begin{pmatrix} 1+\cos(2\theta) & \sin(2\theta) \\ \sin(2\theta) & 1-\cos(2\theta) \end{pmatrix}$$

$\hat{\rho}^2$ can be also calculated as

$$\hat{\rho}^2 = \begin{pmatrix} \cos^2\theta & \sin\theta\cos\theta \\ \sin\theta\cos\theta & \sin^2\theta \end{pmatrix} \begin{pmatrix} \cos^2\theta & \sin\theta\cos\theta \\ \sin\theta\cos\theta & \sin^2\theta \end{pmatrix}$$

$$= \begin{pmatrix} \cos^2\theta & \sin\theta\cos\theta \\ \sin\theta\cos\theta & \sin^2\theta \end{pmatrix} = \hat{\rho}$$

satisfying the condition for the pure state.

$$Tr[\hat{\rho}|x\rangle\langle x|] = Tr[\begin{pmatrix} \cos^2\theta & \sin\theta\cos\theta \\ \sin\theta\cos\theta & \sin^2\theta \end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}] = \cos^2\theta = |\langle x|\psi\rangle|^2 ,$$

$$Tr[\hat{\rho}|y\rangle\langle y|] = Tr[\begin{pmatrix} \cos^2\theta & \sin\theta\cos\theta \\ \sin\theta\cos\theta & \sin^2\theta \end{pmatrix}\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}] = \sin^2\theta = |\langle y|\psi\rangle|^2 ,$$

where

$$\langle x|\psi\rangle = \cos\theta\langle x|x\rangle + \sin\theta\langle x|y\rangle = \cos\theta ,$$

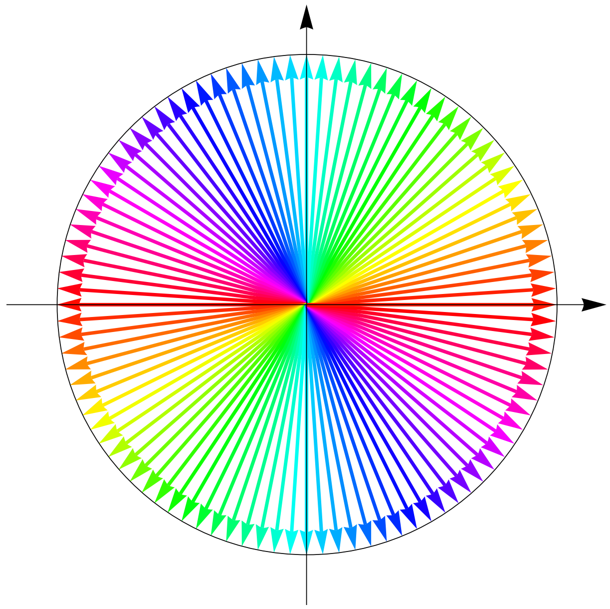
$$\langle y|\psi\rangle = \cos\theta\langle y|x\rangle + \sin\theta\langle y|y\rangle = \sin\theta .$$

(b) The mixed state

What is the density operator for the un-polarized light? To obtain it, we take the average of each matrix element of the density operator in the pure state over θ between 0 and 2π;

$$\hat{\rho}_{un} = \begin{pmatrix} \frac{1}{2\pi}\int_0^{2\pi}\cos^2\theta d\theta & \frac{1}{2\pi}\int_0^{2\pi}\sin\theta\cos\theta d\theta \\ \frac{1}{2\pi}\int_0^{2\pi}\sin\theta\cos\theta d\theta & \frac{1}{2\pi}\int_0^{2\pi}\sin^2\theta d\theta \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}.$$

which is the density matrix for the un-polarized light.



Since

$$\hat{\rho}_{un}{}^2 = \frac{1}{4}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \neq \hat{\rho}_{un},$$

the density operator for the un-polarized light $\hat{\rho}_{un}$ is for the mixed state. The transition from a pure state into a mixed state is connected with the loss of no-diagonal elements in the density matrix. The interference terms appear as non-diagonal elements in the density matrix.

We note that

$$Tr[\hat{\rho}_{un}|x\rangle\langle x|] = Tr[\begin{pmatrix} 1/2 & 0 \\ 0 & 1/2 \end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}] = Tr[\begin{pmatrix} 1/2 & 0 \\ 0 & 0 \end{pmatrix} = \frac{1}{2},$$

$$Tr[\hat{\rho}_{un}|y\rangle\langle y|] = Tr[\begin{pmatrix} 1/2 & 0 \\ 0 & 1/2 \end{pmatrix}\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}] = Tr[\begin{pmatrix} 0 & 0 \\ 0 & 1/2 \end{pmatrix} = \frac{1}{2}.$$

6. Example: the difference between the pure state and mixed state

We consider the state given by

$$|\psi\rangle = \begin{pmatrix} \cos\theta \\ e^{i\phi}\sin\theta \end{pmatrix}.$$

Does the density operator

$$\hat{\rho} = |\psi\rangle\langle\psi|,$$

define a density matrix?

((**Solution**))

$$\hat{\rho} = \begin{pmatrix} \cos^2\theta & e^{-i\phi}\sin\theta\cos\theta \\ e^{i\phi}\sin\theta\cos\theta & \sin^2\theta \end{pmatrix},$$

$$Tr[\hat{\rho}] = 1, \qquad Tr[\hat{\rho}^2] = 1,$$

$$\hat{\rho}^+ = \hat{\rho}.$$

For any $|\chi\rangle$, we have

$$\langle\chi|\hat{\rho}|\chi\rangle = |\langle\chi|\psi\rangle|^2 \geq 0$$

So $\hat{\rho}$ is the density operator for the pure state.

((**Mathematica**)

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

ψ1 = ( Cos[θ]
       Exp[ⅈ ϕ] Sin[θ] );
ψ11 = Transpose[ψ1][[1]];

ρ = Outer[Times, ψ11, ψ11*] // Simplify
```

$$\{\{\cos[\theta]^2,\ e^{-i\phi}\cos[\theta]\sin[\theta]\},\ \{e^{i\phi}\cos[\theta]\sin[\theta],\ \sin[\theta]^2\}\}$$

```
ρ // MatrixForm
```

$$\begin{pmatrix} \cos[\theta]^2 & e^{-i\phi}\cos[\theta]\sin[\theta] \\ e^{i\phi}\cos[\theta]\sin[\theta] & \sin[\theta]^2 \end{pmatrix}$$

```
ρ.ρ // Simplify
```

$$\{\{\cos[\theta]^2,\ e^{-i\phi}\cos[\theta]\sin[\theta]\},\ \{e^{i\phi}\cos[\theta]\sin[\theta],\ \sin[\theta]^2\}\}$$

```
Tr[ρ] // Simplify
```

1

```
Tr[ρ.ρ] // Simplify
```

1

7. Density matrix of a perfectly polarized spin (pure state) ((Cohen-Tannoudji et al.))

We start with the case of spin $S = 1/2$

$$|\psi\rangle = |+\boldsymbol{n}\rangle = \begin{pmatrix} e^{-i\frac{\phi}{2}}\cos\frac{\theta}{2} \\ e^{i\frac{\phi}{2}}\sin\frac{\theta}{2} \end{pmatrix},$$

where

$$\langle\psi|\hat{S}_x|\psi\rangle = \frac{\hbar}{2}\sin\theta\cos\phi,$$

$$\langle\psi|\hat{S}_y|\psi\rangle = \frac{\hbar}{2}\sin\theta\sin\phi,$$

$$\langle\psi|\hat{S}_z|\psi\rangle = \frac{\hbar}{2}\cos\theta,$$

or

$$\langle\psi|\hat{\boldsymbol{S}}|\psi\rangle = \frac{\hbar}{2}\boldsymbol{n},$$

and

$$\left|\langle\psi|\hat{\boldsymbol{S}}_\perp|\psi\rangle\right| = \frac{\hbar}{2}\sin\theta,$$

where

$\left|\langle\psi|\hat{\boldsymbol{S}}_\perp|\psi\rangle\right|$ is the projection of $\left|\langle\psi|\hat{\boldsymbol{S}}|\psi\rangle\right|$ onto the *x*-*y* plane.

The density operator (matrix) $\hat{\rho}(\theta,\phi)$, corresponding to the state $|+\boldsymbol{n}\rangle$.

$$\begin{aligned}
\hat{\rho}(\theta,\phi) &= |\psi\rangle\langle\psi| = |+\boldsymbol{n}\rangle\langle+\boldsymbol{n}| \\
&= \begin{pmatrix} e^{-i\frac{\phi}{2}}\cos\frac{\theta}{2} \\ e^{i\frac{\phi}{2}}\sin\frac{\theta}{2} \end{pmatrix} \begin{pmatrix} e^{i\frac{\phi}{2}}\cos\frac{\theta}{2} & e^{-i\frac{\phi}{2}}\sin\frac{\theta}{2} \end{pmatrix} \\
&= \begin{pmatrix} \cos^2\frac{\theta}{2} & e^{-i\phi}\sin\frac{\theta}{2}\cos\frac{\theta}{2} \\ e^{i\phi}\sin\frac{\theta}{2}\cos\frac{\theta}{2} & \sin^2\frac{\theta}{2} \end{pmatrix} \\
&= \begin{pmatrix} \rho_{++} & \rho_{+-} \\ \rho_{-+} & \rho_{--} \end{pmatrix}
\end{aligned}$$

The matrix is generally non-diagonal.

$$\rho_{++} = \cos^2\frac{\theta}{2}, \qquad \rho_{--} = \sin^2\frac{\theta}{2},$$

$$\rho_{+-} = e^{-i\phi}\sin\frac{\theta}{2}\cos\frac{\theta}{2}, \qquad \rho_{-+} = e^{i\phi}\sin\frac{\theta}{2}\cos\frac{\theta}{2}.$$

The "populations" ρ_{++} and ρ_{--} have a very simple physical significance,

$$\rho_{++} - \rho_{--} = \cos^2\frac{\theta}{2} - \sin^2\frac{\theta}{2} = \cos\theta = \frac{2}{\hbar}\langle \hat{S}_y \rangle,$$

$$\rho_{++} + \rho_{--} = \cos^2\frac{\theta}{2} + \sin^2\frac{\theta}{2} = 1.$$

The populations are therefore related to the longitudinal polarization.
The "coherence" ρ_{+-}, ρ_{-+}:

$$|\rho_{+-}| = |\rho_{-+}| = \sin\frac{\theta}{2}\cos\frac{\theta}{2} = \frac{1}{2}\sin\theta = \frac{1}{\hbar}\left|\langle \psi | \hat{\boldsymbol{S}}_\perp | \psi \rangle\right|,$$

where

$$\left|\langle \psi | \hat{\boldsymbol{S}}_\perp | \psi \rangle\right| = \frac{\hbar}{2}\sin\theta.$$

The argument of ρ_{+-}, ρ_{-+} is ϕ, that is, the angle between $\left|\langle \psi | \hat{\boldsymbol{S}}_\perp | \psi \rangle\right|$ and the x axis. Note that

$$\hat{\rho}^2(\theta,\phi) = |+\boldsymbol{n}\rangle\langle +\boldsymbol{n}|+\boldsymbol{n}\rangle\langle +\boldsymbol{n}| = |+\boldsymbol{n}\rangle\langle +\boldsymbol{n}| = \hat{\rho}(\theta,\phi),$$

is a relation characteristic of a pure state.

8. A statistical mixture; un-polarized spin

The only information we possess about the spin is the following. It can point in any direction of space and all directions are equally probable. The situation corresponds to a statistical mixture of the state $|+\boldsymbol{n}\rangle$ with equal weights.

$$\hat{\rho} = \frac{1}{4\pi}\int d\Omega \hat{\rho}(\theta,\phi) = \frac{1}{4\pi}\int_0^{2\pi} d\phi \int_0^{\pi} \sin\theta d\theta \hat{\rho}(\theta,\phi) = \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{pmatrix} = \frac{1}{2}\hat{1},$$

$$\begin{aligned}
\frac{1}{4\pi}\int_0^{2\pi} d\phi \int_0^{\pi} \sin\theta d\theta \hat{\rho}_{11}(\theta,\phi) &= \frac{1}{4\pi}\int_0^{2\pi} d\phi \int_0^{\pi} \sin\theta \cos^2\frac{\theta}{2} d\theta \\
&= \frac{1}{4\pi} 2\pi \frac{1}{2}\int_0^{\pi} \sin\theta(1+\cos\theta) d\theta \\
&= \frac{1}{4}\int_0^{\pi} (\sin\theta + \frac{1}{2}\sin 2\theta) d\theta \\
&= \frac{1}{2}
\end{aligned}$$

$$\begin{aligned}
\frac{1}{4\pi}\int_0^{2\pi} d\phi \int_0^{\pi} \sin\theta d\theta \hat{\rho}_{22}(\theta,\phi) &= \frac{1}{4\pi}\int_0^{2\pi} d\phi \int_0^{\pi} \sin\theta \sin s^2\frac{\theta}{2} d\theta \\
&= \frac{1}{4\pi} 2\pi \frac{1}{2}\int_0^{\pi} \sin\theta(1-\cos\theta) d\theta \\
&= \frac{1}{4}\int_0^{\pi} (\sin\theta - \frac{1}{2}\sin 2\theta) d\theta \\
&= \frac{1}{2}
\end{aligned}$$

$$\begin{aligned}
\frac{1}{4\pi}\int_0^{2\pi} d\phi \int_0^{\pi} \sin\theta d\theta \hat{\rho}_{12}(\theta,\phi) &= \frac{1}{4\pi}\int_0^{2\pi} e^{-i\phi} d\phi \int_0^{\pi} \sin\theta \sin\frac{\theta}{2}\cos\frac{\theta}{2} d\theta \\
&= 0
\end{aligned}$$

So we have

$$\hat{\rho}^2 = \frac{1}{2}\hat{\rho},$$

So $\hat{\rho}$ is the density operator for which a statistical mixture of states. Note that

$$\langle \hat{S}_i \rangle = Tr[\hat{\rho}\hat{S}_i] = Tr[\frac{1}{2}\hat{1}\hat{S}_i] = \frac{1}{2}Tr[\hat{S}_i] = 0 .$$

We again find that the spin is unpolarized: since all the directions are equivalent, the mean value of the spin is zero,

$$\langle \hat{S}_x \rangle = \langle \hat{S}_y \rangle = \langle \hat{S}_z \rangle = 0 .$$

((**Comment**))

(i) The coherence " ρ_{+-} and ρ_{-+} are related to the transverse polarization $\langle \hat{\boldsymbol{S}}_\perp \rangle$ of the spin. Upon summing the vector $\langle \hat{\boldsymbol{S}}_\perp \rangle$ corresponding to all (equiprobable) directions of the *x*-*y* plane, we obviously find a null result.

(ii) *It is impossible to describe a statistical mixture by an average state vector.*

We assume that we are trying to choose α and β so that the vector is given

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

with

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

represent an unpolarized spin, for which

$$\langle \hat{S}_x \rangle = \langle \hat{S}_y \rangle = \langle \hat{S}_z \rangle = 0 .$$

We note that

$$\langle \hat{S}_x \rangle = \frac{\hbar}{2}\begin{pmatrix}\alpha^* & \beta^*\end{pmatrix}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\begin{pmatrix}\alpha\\ \beta\end{pmatrix} = \frac{\hbar}{2}(\alpha^*\beta + \alpha\beta^*) = 0 ,$$

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

and

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

Then we get

$$\alpha^* \beta = 0, \qquad |\alpha|^2 = |\beta|^2 = \frac{1}{2}.$$

Thus we cannot find α and β so that $\langle \hat{S}_x \rangle = \langle \hat{S}_y \rangle = \langle \hat{S}_z \rangle = 0$.

9. Mixed state: another example of a statistical mixture

We could imagine other statistical mixture which would lead to the same density matrix.

(i) A statistical mixture of equal proportions of $|+z\rangle$ and $|-z\rangle$

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

(ii) A statistical mixture of equal proportions of $|+\boldsymbol{n}\rangle$ and $|-\boldsymbol{n}\rangle$

$$\begin{aligned} \hat{\rho} &= \frac{1}{2}(|+\boldsymbol{n}\rangle\langle +\boldsymbol{n}| + |-\boldsymbol{n}\rangle\langle -\boldsymbol{n}|) \\ &= \frac{1}{2}\hat{1} = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \end{aligned}$$

Since all the physical predictions depend only on the density matrix, it is impossible to distinguish physically between the various types of statistical mixtures which lead to the same density matrix.

We note that

$$\hat{\rho}_z^{\,2} = \hat{\rho}_x^{\,2} = \hat{\rho}_y^{\,2} = \begin{pmatrix} \frac{1}{4} & 0 \\ 0 & \frac{1}{4} \end{pmatrix},$$

$$Tr[\hat{\rho}_z^{\,2}] = Tr[\hat{\rho}_x^{\,2}] = Tr[\hat{\rho}_y^{\,2}] = \frac{1}{2}. \qquad \text{(mixed state)}$$

10. Mixed state: Spin 1/2 in the thermodynamic equilibrium in a static magnetic bfield

The spin of the electron has a magnetic moment (spin magnetic moment) as

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

where $\hat{\boldsymbol{S}}$ is the spin angular momentum. The spin Hamiltonian in the presence of a magnetic along the z axis is

$$\hat{H} = -\hat{\boldsymbol{\mu}}_s \cdot \boldsymbol{B} = \omega_0 \hat{S}_z = \frac{\hbar\omega_0}{2}\hat{\sigma}_z ,$$

where

$$\omega_0 = \frac{eB}{mc} . \qquad \text{(Larmor angular frequency)}$$

The eigenvalue problem:

$$\hat{H}\left|+z\right\rangle = \frac{\hbar\omega_0}{2}\hat{\sigma}_z\left|+z\right\rangle = \frac{\hbar\omega_0}{2}\left|+z\right\rangle ,$$

$$\hat{H}\left|-z\right\rangle = \frac{\hbar\omega_0}{2}\hat{\sigma}_z\left|-z\right\rangle = -\frac{\hbar\omega_0}{2}\left|-z\right\rangle .$$

The system is in the thermodynamic equilibrium at T. We can assert that it has a probability

$\frac{1}{Z}\exp(-\frac{\hbar\omega_0}{2k_B T})$, of being in the state $\left|+z\right\rangle$, and

$\frac{1}{Z}\exp(\frac{\hbar\omega_0}{2k_B T})$, of being in the state $\left|-z\right\rangle$,

where k_B is the Boltzmann constant and Z is the partition function is defined by

$$Z = \exp(-\frac{\hbar\omega_0}{2k_B T}) + \exp(\frac{\hbar\omega_0}{2k_B T}) .$$

We have another example of a statistical mixtures, described by the density matrix

$$\hat{\rho} = \frac{1}{Z}\begin{pmatrix} \exp(-\frac{\hbar\omega_0}{2k_B T}) & 0 \\ 0 & \exp(\frac{\hbar\omega_0}{2k_B T}) \end{pmatrix}$$

with

$$\hat{\rho}^2 \neq \hat{\rho}.$$

The non-diagonal elements are zero. We note that

$$\langle \hat{S}_x \rangle = Tr[\hat{\rho}\hat{S}_x] = 0,$$

$$\langle \hat{S}_y \rangle = Tr[\hat{\rho}\hat{S}_y] = 0,$$

$$\langle \hat{S}_z \rangle = Tr[\hat{\rho}\hat{S}_z] = \frac{\hbar}{2Z}[\exp(-\frac{\hbar\omega_0}{2k_B T}) - \exp(+\frac{\hbar\omega_0}{2k_B T})] = -\frac{\hbar}{2}\tanh(\frac{\hbar\omega}{2k_B T}).$$

Since $\left|\tanh(\frac{\hbar\omega}{2k_B T})\right| < 1$, this polarization is less than the value $\frac{\hbar}{2}$ which corresponds to a spin which is perfectly polarized along the *z* axis. "*Partially polarized along the z axis*.

---

11. Example: Cohen-Tannoudji Quantum Mechanics Chapter 4 exercise (4-4)

A beam of atom of spin 1/2 passes through one apparatus, which serves as a "polarizer" in a direction which makes an angle θ with Oz in the xOz plane, and then through another apparatus, the "analyzer," which measures the S_z component of the spin. We assume that between the polarizer and the analyzer, over a length L of the atomic beam, a magnetic field $\boldsymbol{B}_0$ is applied which is uniform and parallel to Ox. We call v the speed of the atoms and $T = L/v$ the time during which they are submitted to the field $\boldsymbol{B}_0$. We set $\omega_0 = -\gamma B_0$.

a. What is the state vector $|\psi_1\rangle$ of a spin at the moment it enters the analyzer?

b. Show that when the measurement is performed in the analyzer, there is a probability equal to $\frac{1}{2}[1+\cos\theta\cos(\omega_0 T)]$ of finding $+\frac{\hbar}{2}$ and $\frac{1}{2}[1-\cos\theta\cos(\omega_0 T)]$ of finding $-\frac{\hbar}{2}$. Give a physical interpretation.

c. Show that the density matrix $\hat{\rho}_1$ of a particle which enters the analyzer is written, in the $\{|+z\rangle, |-z\rangle\}$ basis:

$$\hat{\rho}_1 = \frac{1}{2}\begin{pmatrix} 1+\cos\theta\cos(\omega_0 T) & \sin\theta + i\cos\theta\sin(\omega_0 T) \\ \sin\theta - i\cos\theta\sin(\omega_0 T) & 1-\cos\theta\cos(\omega_0 T) \end{pmatrix}.$$

Calculate $Tr[\hat{\rho}_1\hat{S}_x]$, $Tr[\hat{\rho}_1\hat{S}_y]$, and $Tr[\hat{\rho}_1\hat{S}_z]$. Give an interpretation. Does the density operator $\hat{\rho}_1$ describes a pure state?

d. Now assume that the speed of an atom is a random variable, and hence the time T is known only to within a certain uncertainty ΔT. In addition, the field B_0 is assumed to be sufficiently strong that $\omega_0\Delta T >> 1$. The possible values of the product $\omega_0 T$ are then (modulus 2π) all values included between 0 and 2π, all of which are equally probable.

In this case, what is the density operator $\hat{\rho}_2$ of an atom at the moment it enters the analyzer? Does $\hat{\rho}_2$ correspond to a pure case? Calculate the quantities $Tr[\hat{\rho}_2\hat{S}_x]$, $Tr[\hat{\rho}_2\hat{S}_y]$, and $Tr[\hat{\rho}_2\hat{S}_z]$. What is your interpretation? In which case does the density operator describe a completely polarized spin? A completely unpolarized spin?

Describe quantitatively the phenomena observed at the analyzer exit when ω_0 varies from zero to a value where the condition $\omega_0\Delta T >> 1$ is satisfied.

((**Solution**))

(a)

$$|+\boldsymbol{n}\rangle = \begin{pmatrix} \cos\frac{\theta}{2} \\ \sin\frac{\theta}{2} \end{pmatrix} = \cos\frac{\theta}{2}|+z\rangle + \sin\frac{\theta}{2}|-z\rangle \text{ at } t = 0.$$

The Hamiltonian is given by

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

Time evolution operator:

$$\begin{aligned}
\left|\psi(t=T)\right\rangle &= \exp(-\frac{i}{\hbar}\hat{H}T)\left|+\boldsymbol{n}\right\rangle \\
&= \exp(-\frac{i}{2}\omega_0\hat{\sigma}_x T)\left|+\boldsymbol{n}\right\rangle \\
&= \begin{pmatrix} \cos\frac{\omega_0 T}{2} & -i\sin\frac{\omega_0 T}{2} \\ -i\sin\frac{\omega_0 T}{2} & \cos\frac{\omega_0 T}{2} \end{pmatrix} \begin{pmatrix} \cos\frac{\theta}{2} \\ \sin\frac{\theta}{2} \end{pmatrix} \\
&= \begin{pmatrix} \cos\frac{\theta}{2}\cos\frac{\omega_0 T}{2} - i\sin\frac{\theta}{2}\sin\frac{\omega_0 T}{2} \\ -i\cos\frac{\theta}{2}\sin\frac{\omega_0 T}{2} + \sin\frac{\theta}{2}\cos\frac{\omega_0 T}{2} \end{pmatrix}
\end{aligned}$$

Note that

$$\begin{aligned}
\exp(-\frac{i}{2}\omega_0\hat{\sigma}_x t) &= \exp(-\frac{i}{2}\omega_0\hat{\sigma}_x t)[\left|+x\right\rangle\left\langle +x\right| + \left|-x\right\rangle\left\langle -x\right|) \\
&= e^{-\frac{i}{2}\omega_0 t}\left|+x\right\rangle\left\langle +x\right| + e^{\frac{i}{2}\omega_0 t}\left|-x\right\rangle\left\langle -x\right|) \\
&= \hat{U}(e^{-\frac{i}{2}\omega_0 t}\left|+z\right\rangle\left\langle +z\right| + e^{\frac{i}{2}\omega_0 t}\left|-z\right\rangle\left\langle -z\right|)\hat{U}^+ \\
&= \hat{U}\begin{pmatrix} e^{-\frac{i}{2}\omega_0 t} & 0 \\ 0 & e^{\frac{i}{2}\omega_0 t} \end{pmatrix}\hat{U}^+ \\
&= \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}\begin{pmatrix} e^{-\frac{i}{2}\omega_0 t} & 0 \\ 0 & e^{\frac{i}{2}\omega_0 t} \end{pmatrix}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \\
&= \begin{pmatrix} \cos\frac{\omega_0 t}{2} & -i\sin\frac{\omega_0 t}{2} \\ -i\sin\frac{\omega_0 t}{2} & \cos\frac{\omega_0 t}{2} \end{pmatrix}
\end{aligned}$$

where

$$\left|+x\right\rangle = \hat{U}\left|+z\right\rangle, \qquad \left|-x\right\rangle = \hat{U}\left|-z\right\rangle,$$

with

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

Then we have

(b) Density matrix for the pure state

$$\left|\psi(t=T)\right\rangle = \begin{pmatrix} \alpha \\ \beta \end{pmatrix},$$

where

$$\alpha = \cos\frac{\theta}{2}\cos\frac{\omega_0 T}{2} - i\sin\frac{\theta}{2}\sin\frac{\omega_0 T}{2},$$

$$\beta = -i\cos\frac{\theta}{2}\sin\frac{\omega_0 T}{2} + \sin\frac{\theta}{2}\cos\frac{\omega_0 T}{2}.$$

We define the density matrix for the pure state as

$$\hat{\rho}_1 = \left|\psi(t=T)\right\rangle\left\langle\psi(t=T)\right| = \begin{pmatrix} \alpha \\ \beta \end{pmatrix}\begin{pmatrix} \alpha^* & \beta^* \end{pmatrix} = \begin{pmatrix} \alpha a^* & \alpha\beta^* \\ \alpha^*\beta & \beta\beta^* \end{pmatrix},$$

where

$$\begin{aligned} \rho_{++} &= \alpha a^* \\ &= \cos^2\frac{\theta}{2}\cos^2\frac{\omega_0 T}{2} + \sin^2\frac{\theta}{2}\sin^2\frac{\omega_0 T}{2} \\ &= \frac{1}{2}[1 + \cos\theta\cos(\omega_0 T)] \end{aligned}$$

$$
\begin{aligned}
\rho_{+-} &= \alpha\beta^* \\
&= \sin\frac{\theta}{2}\cos\frac{\theta}{2} + i\cos\theta\sin\frac{\omega_0 T}{2}\cos\frac{\omega_0 T}{2} \\
&= \frac{1}{2}[\sin\theta + i\cos\theta\sin(\omega_0 T)]
\end{aligned}
$$

$$
\begin{aligned}
\rho_{-+} &= \beta\alpha^* \\
&= \sin\frac{\theta}{2}\cos\frac{\theta}{2} - i\cos\theta\sin\frac{\omega_0 T}{2}\cos\frac{\omega_0 T}{2} \\
&= \frac{1}{2}[\sin\theta - i\cos\theta\sin(\omega_0 T)]
\end{aligned}
$$

$$
\begin{aligned}
\rho_{--} &= \beta\beta^* \\
&= \cos^2\frac{\theta}{2}\sin^2\frac{\omega_0 T}{2} + \sin^2\frac{\theta}{2}\cos^2\frac{\omega_0 T}{2} \\
&= \frac{1}{2}[1 - \cos\theta\cos(\omega_0 T)]
\end{aligned}
$$

Of course, we have

$$\hat{\rho}_1{}^2 = \hat{\rho}_1,$$

from the definition of

$$\hat{\rho}_1 = |\psi(t=T)\rangle\langle\psi(t=T)|, \qquad \text{for the pure state.}$$

$$
\begin{aligned}
\langle\hat{S}_x\rangle &= Tr[\hat{\rho}_1\hat{S}_x] \\
&= \frac{\hbar}{2}Tr[\begin{pmatrix}\alpha a^* & \alpha\beta^* \\ \alpha^*\beta & \beta\beta^*\end{pmatrix}\begin{pmatrix}0 & 1 \\ 1 & 0\end{pmatrix}] \\
&= \frac{\hbar}{2}Tr[\begin{pmatrix}\alpha\beta^* & \alpha\alpha^* \\ \beta^*\beta & \alpha^*\beta\end{pmatrix}] \\
&= \frac{\hbar}{2}(\alpha\beta^* + \alpha^*\beta) = \frac{\hbar}{2}\sin\theta
\end{aligned}
$$

$$\left\langle \hat{S}_y \right\rangle = Tr[\hat{\rho}_1 \hat{S}_y]$$

$$= \frac{\hbar}{2} Tr[\begin{pmatrix} \alpha a^* & \alpha\beta^* \\ \alpha^*\beta & \beta\beta^* \end{pmatrix}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}]$$

$$= \frac{\hbar}{2} Tr[\begin{pmatrix} i\alpha\beta^* & -i\alpha\alpha^* \\ i\beta^*\beta & -i\alpha^*\beta \end{pmatrix}]$$

$$= i\frac{\hbar}{2}(\alpha\beta^* - \alpha^*\beta) = -\frac{\hbar}{2}\cos\theta\sin(\omega_0 T)$$

$$\left\langle \hat{S}_z \right\rangle = Tr[\hat{\rho}_1 \hat{S}_z]$$

$$= \frac{\hbar}{2} Tr[\begin{pmatrix} \alpha a^* & \alpha\beta^* \\ \alpha^*\beta & \beta\beta^* \end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}]$$

$$= \frac{\hbar}{2} Tr[\begin{pmatrix} \alpha\alpha^* & -\alpha\beta^* \\ \alpha^*\beta & -\beta\beta^* \end{pmatrix}]$$

$$= \frac{\hbar}{2}(\alpha\alpha^* - \beta\beta^*) = \frac{\hbar}{2}\cos\theta\cos(\omega_0 T)$$

(d) The possible value of the product $\tau = \omega_0 T$ are all values included between 0 and 2π, all of which are equally probable.

$$\hat{\rho}_2 = \frac{1}{2\pi}\int_0^{2\pi} d\tau \hat{\rho}_1 = \frac{1}{2}\begin{pmatrix} 1 & \sin\theta \\ \sin\theta & 1 \end{pmatrix},$$

with

$$\tau = \omega_0 T \ .$$

Note that

$$\int_0^{2\pi} d\tau \sin(\tau) = 0\,, \qquad \int_0^{2\pi} d\tau \cos(\tau) = 0\,.$$

Then we find that

$$\hat{\rho}_2{}^2 = \frac{1}{4}\begin{pmatrix} 1 & \sin\theta \\ \sin\theta & 1 \end{pmatrix}\begin{pmatrix} 1 & \sin\theta \\ \sin\theta & 1 \end{pmatrix}$$
$$= \frac{1}{4}\begin{pmatrix} 1+\sin^2\theta & 2\sin\theta \\ 2\sin\theta & 1+\sin^2\theta \end{pmatrix} \neq \hat{\rho}_0$$

Therefore $\hat{\rho}_2$ correspond to the mixed state case.

$$\langle \hat{S}_x \rangle = Tr[\hat{\rho}_2 \hat{S}_x]$$
$$= \frac{\hbar}{4} Tr[\begin{pmatrix} 1 & \sin\theta \\ \sin\theta & 1 \end{pmatrix}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}]$$
$$= \frac{\hbar}{4} Tr[\begin{pmatrix} \sin\theta & 1 \\ 1 & \sin\theta \end{pmatrix}]$$
$$= \frac{\hbar}{2}\sin\theta$$

$$\langle \hat{S}_y \rangle = Tr[\hat{\rho}_2 \hat{S}_y]$$
$$= \frac{\hbar}{4} Tr[\begin{pmatrix} 1 & \sin\theta \\ \sin\theta & 1 \end{pmatrix}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}]$$
$$= \frac{\hbar}{4} Tr[\begin{pmatrix} i\sin\theta & -i \\ i & -i\sin\theta \end{pmatrix}]$$
$$= 0$$

$$\langle \hat{S}_z \rangle = Tr[\hat{\rho}_2 \hat{S}_z]$$
$$= \frac{\hbar}{4} Tr[\begin{pmatrix} 1 & \sin\theta \\ \sin\theta & 1 \end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}]$$
$$= \frac{\hbar}{4} Tr[\begin{pmatrix} 1 & -\sin\theta \\ \sin\theta & -1 \end{pmatrix}]$$
$$= 0$$

---

12. Eigenvalue problem (formulation)

Suppose that the density operator can be described by

$$\hat{\rho} = \sum_i p_i |a_i\rangle\langle a_i|,$$

under the basis of $\{|a_i\rangle\}$. $|a_i\rangle$ is the eigenket of $\hat{\rho}$ with the eigenvalue p_i.

$$\hat{\rho}|a_i\rangle = \sum_j p_j |a_j\rangle\langle a_j|a_i\rangle = \sum_j p_j |a_j\rangle\delta_{ij} = p_i|a_i\rangle .$$

Here we choose the basis $\{|b_i\rangle\}$, where

$$|a_i\rangle = \hat{U}|b_i\rangle, \quad |a_i\rangle = \hat{U}|b_k\rangle,$$

where

$$\hat{U} = \hat{U}\sum_i |b_i\rangle\langle b_i| = \sum_i \hat{U}|b_i\rangle\langle b_i| = \sum_i |a_i\rangle\langle b_i|,$$

$$\langle b_k|a_l\rangle = \langle b_k|\hat{U}|b_l\rangle = U_{kl} .$$

The matrix element under this basis is

$$\langle b_k|\hat{\rho}|b_l\rangle = \sum_i p_i \langle b_k|a_i\rangle\langle a_i|b_l\rangle .$$

The eigenvalue problem:

$$\hat{\rho}|a_i\rangle = p_i|a_i\rangle,$$

$$\sum_l \langle b_k|\hat{\rho}|b_l\rangle\langle b_l|a_i\rangle = p_i\langle b_k|a_i\rangle .$$

Since

$$\langle b_l|a_i\rangle = U_{li},$$

$$\sum_l \langle b_k|\hat{\rho}|b_l\rangle U_{li} = p_i U_{ki}, \qquad \text{(eigenvalue problem)}$$

$$\begin{pmatrix} \rho_{11} & \rho_{12} & . & . & . & . & . & \rho_{1n} \\ \rho_{21} & \rho_{22} & . & . & . & . & . & \rho_{2n} \\ . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . \\ \rho_{n1} & \rho_{n2} & . & . & . & . & . & \rho_{nn} \end{pmatrix} \begin{pmatrix} U_{1i} \\ U_{2i} \\ . \\ . \\ . \\ . \\ . \\ U_{ni} \end{pmatrix} = p_i \begin{pmatrix} U_{1i} \\ U_{2i} \\ . \\ . \\ . \\ . \\ . \\ U_{ni} \end{pmatrix},$$

$$\hat{\rho} = \sum_i p_i | a_i \rangle\langle a_i | = \sum_i p_i \hat{U} | b_i \rangle\langle b_i | \hat{U}^+ = \hat{U} (\sum_i p_i | b_i \rangle\langle b_i |) \hat{U}^+ .$$

13. The use of Mathematica for the calculation of the density operator

We use the following Mathematica program for the calculation of density operator.

(i)

$$Tr[\hat{A}].$$

(ii)

$$|\psi_1\rangle\langle\psi_2| .$$

(a)

$\psi_1.Transpose[\psi_2^*]$

when

$$|\psi_1\rangle = \begin{pmatrix} a_1 \\ a_2 \\ . \\ . \\ . \\ a_n \end{pmatrix}, \qquad |\psi_2\rangle = \begin{pmatrix} b_1 \\ b_2 \\ . \\ . \\ . \\ b_n \end{pmatrix}.$$

(b)

Outer[Times, ψ_1, ψ_2^*] $\rightarrow$ $|\psi_1\rangle\langle\psi_2|$

when $|\psi_1\rangle$ and $|\psi_2\rangle$ are given by

$$|\psi_1\rangle = (a_1 \quad a_2 \quad \cdot \quad \cdot \quad \cdot \quad \cdot \quad a_n), \qquad |\psi_2\rangle = (b_1 \quad b_2 \quad \cdot \quad \cdot \quad \cdot \quad \cdot \quad b_n)$$

(iii)

KroneckerProduct[ψ_1, ψ_2] $|\psi_1\rangle \otimes |\psi_2\rangle$

(iii) Eigenvalue problems
Eigensystem
Orthogonalize
Normalize

Suppose that the matrix of $\hat{\rho}$ is given in the form of n x n matrix. We solve the eigenvalue problem of the matrix of $\hat{\rho}$ using the Program "Eigensystem".

Eigensystem[$\hat{\rho}$]

Suppose that there are n eigenvalues and the corresponding normalized kets.

w_i $|\psi_i\rangle$ (i = 1, 2, .., n).

where

$$\langle\psi_i|\psi_j\rangle = \delta_{ij}.$$

Then we have the diagonal form of the density operator as

$$\hat{\rho} = \hat{\rho}\sum_i |\psi_i\rangle\langle\psi_i| = \sum_i \hat{\rho}|\psi_i\rangle\langle\psi_i| = \sum_i w_i|\psi_i\rangle\langle\psi_i|,$$

using the closure relation (completeness).

14. Example: eigenvalue problem

The density matrix (2 x 2 matrix) is not diagonal.

$$\hat{\rho} = \frac{1}{2}\begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} = \frac{1}{2}[|+z\rangle\langle+z| + |-z\rangle\langle-z| - |+z\rangle\langle-z| - |-z\rangle\langle+z|].$$

Note that

$$\hat{\rho}^2 = \hat{\rho},$$

$$Tr[\hat{\rho}^2] = Tr[\hat{\rho}] = 1,$$

satisfying the condition for the pure state.

Eigensystem[$\hat{\rho}$];

Eigenvalue	Eigenket
$w_1 = 1$	$\lvert\psi_1\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix} = \lvert -x\rangle$,
$w_2 = 0$	$\lvert\psi_2\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix} = \lvert +x\rangle$.

Then we have

$$\begin{aligned} \hat{\rho} &= \hat{\rho}(|\psi_1\rangle\langle\psi_1| + |\psi_2\rangle\langle\psi_2|) \\ &= w_1|\psi_1\rangle\langle\psi_1| + w_2|\psi_2\rangle\langle\psi_2| \\ &= w_1|\psi_1\rangle\langle\psi_1| \\ &= |-x\rangle\langle -x| \end{aligned}$$

15. Density operator for the spin 1/2 system

((L.I. Schiff))

In general the density operator for the spin 1/2 system can be described by

$$\hat{\rho} = \begin{pmatrix} \rho_{11} & \rho_{12} \\ \rho_{21} & \rho_{22} \end{pmatrix} = \frac{a\hat{1} + \alpha\hat{\sigma}_x + \beta\hat{\sigma}_y + \gamma\hat{\sigma}_y}{2} = \frac{1}{2}\begin{pmatrix} a+\gamma & \alpha - i\beta \\ \alpha + i\beta & a-\gamma \end{pmatrix},$$

where a, α, β, and γ are real numbers. Since $Tr[\hat{\rho}] = 1$, we get

$$\frac{a+\gamma+a-\gamma}{2}=1,$$

or

$$a=1.$$

Then the density operator can be rewritten as

$$\hat{\rho}=\hat{\rho}_{\boldsymbol{n}}=\frac{1}{2}\hat{1}+\frac{1}{2}\sqrt{\alpha^2+\beta^2+\gamma^2}(\frac{\alpha}{\sqrt{\alpha^2+\beta^2+\gamma^2}}\hat{\sigma}_x+\frac{\beta}{\sqrt{\alpha^2+\beta^2+\gamma^2}}\hat{\sigma}_y+\frac{\gamma}{\sqrt{\alpha^2+\beta^2+\gamma^2}}\hat{\sigma}_y)$$
$$=\frac{1}{2}[\hat{1}+\sqrt{\alpha^2+\beta^2+\gamma^2}(\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{n})]$$

with

$$|\boldsymbol{n}|=1, \qquad (\boldsymbol{n}\text{: unit vector})$$

and

$$\boldsymbol{n}=(\frac{\alpha}{\sqrt{\alpha^2+\beta^2+\gamma^2}},\frac{\beta}{\sqrt{\alpha^2+\beta^2+\gamma^2}},\frac{\gamma}{\sqrt{\alpha^2+\beta^2+\gamma^2}}).$$

Note that

$$\hat{\rho}^2=\frac{1}{4}\begin{pmatrix}\alpha^2+\beta^2+\gamma^2+1+2\gamma & 2(\alpha-i\beta)\\ 2(\alpha+i\beta) & \alpha^2+\beta^2+\gamma^2+1-2\gamma\end{pmatrix}.$$

For the pure state, we have

$$\hat{\rho}^2=\hat{\rho}, \qquad \text{or} \qquad Tr[\hat{\rho}^2]=Tr[\hat{\rho}]=1,$$

leading to the relation

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

Then the density operator for the pure state is

$$\hat{\rho}_{\boldsymbol{n}} = \frac{1}{2}(\hat{1} + \hat{\boldsymbol{\sigma}} \cdot \boldsymbol{n}) .$$

16. Comment on the density operator for the pure state

The density operator for the pure state can be described by

$$\hat{\rho}_{pure} = |\psi\rangle\langle\psi| = \begin{pmatrix} |\xi|^2 & \xi\eta^* \\ \xi^*\eta & |\eta|^2 \end{pmatrix},$$

where

$$|\psi\rangle = \xi|+z\rangle + \eta|-z\rangle = \begin{pmatrix} \xi \\ \eta \end{pmatrix}.$$

with

$$|\xi|^2 + |\eta|^2 = 1 .$$

We note that

$$\hat{\rho}_{pure} = \begin{pmatrix} |\xi|^2 & \xi\eta^* \\ \xi^*\eta & |\eta|^2 \end{pmatrix} = \frac{1}{2}(\hat{1} + \hat{\boldsymbol{\sigma}} \cdot \boldsymbol{n}) = \frac{1}{2}\begin{pmatrix} 1+n_z & n_x - in_y \\ n_x + in_y & 1-n_z \end{pmatrix},$$

or

$$n_x = \xi^*\eta + \xi\eta^* , \qquad n_y = -i(\xi^*\eta - \xi\eta^*) ,$$

$$n_z = 2|\xi|^2 - 1 = 1 - 2|\eta|^2 .$$

The expectation values of spin components are given by

$$\langle\psi|\hat{\sigma}_x|\psi\rangle = Tr(\hat{\sigma}_x\hat{\rho}_{\boldsymbol{n}}) = \frac{1}{2}Tr[\hat{\sigma}_x(\hat{1} + \hat{\boldsymbol{\sigma}} \cdot \boldsymbol{n})] = \frac{1}{2}Tr[\hat{\sigma}_x(\hat{\boldsymbol{\sigma}} \cdot \boldsymbol{n})] = n_x ,$$

$$\langle\psi|\hat{\sigma}_y|\psi\rangle = Tr(\hat{\sigma}_y\hat{\rho}_{\boldsymbol{n}}) = \frac{1}{2}Tr[\hat{\sigma}_y(\hat{1} + \hat{\boldsymbol{\sigma}} \cdot \boldsymbol{n})] = \frac{1}{2}Tr[\hat{\sigma}_y(\hat{\boldsymbol{\sigma}} \cdot \boldsymbol{n})] = n_y ,$$

$$\langle\psi|\hat{\sigma}_z|\psi\rangle = Tr(\hat{\sigma}_z\hat{\rho}_{\boldsymbol{n}}) = \frac{1}{2}Tr[\hat{\sigma}_z(\hat{1}+\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{n})] = \frac{1}{2}Tr[\hat{\sigma}_z(\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{n})] = n_z,$$

where

$$Tr[\hat{\sigma}_x\hat{\sigma}_y] = Tr[\hat{\sigma}_y\hat{\sigma}_x] = 0, \qquad Tr[\hat{\sigma}_y\hat{\sigma}_z] = Tr[\hat{\sigma}_z\hat{\sigma}_y] = 0,$$

$$Tr[\hat{\sigma}_z\hat{\sigma}_x] = Tr[\hat{\sigma}_x\hat{\sigma}_z] = 0,$$

$$Tr[\hat{\sigma}_x{}^2] = Tr[\hat{\sigma}_y{}^2] = Tr[\hat{\sigma}_z{}^2] = 2.$$

Then we have

$$\langle\psi|\hat{\sigma}_x|\psi\rangle = \begin{pmatrix}\xi^* & \eta^*\end{pmatrix}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\begin{pmatrix}\xi\\ \eta\end{pmatrix} = \xi^*\eta + \xi\eta^* = n_x,$$

$$\langle\psi|\hat{\sigma}_y|\psi\rangle = \begin{pmatrix}\xi^* & \eta^*\end{pmatrix}\begin{pmatrix}0 & -i\\ i & 0\end{pmatrix}\begin{pmatrix}\xi\\ \eta\end{pmatrix} = -i(\xi^*\eta - \xi\eta^*) = n_y,$$

$$\langle\psi|\hat{\sigma}_z|\psi\rangle = \begin{pmatrix}\xi^* & \eta^*\end{pmatrix}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}\begin{pmatrix}\xi\\ \eta\end{pmatrix} = |\xi|^2 - |\eta|^2 = 2|\xi|^2 - 1 = 1 - 2|\eta|^2 = n_z.$$

---

17. Density operator: the Bloch-sphere for mixed states

We discuss the general case (both the pure state and mixed state). For convenience we use

$$\alpha = r_x, \qquad \beta = r_y, \qquad \gamma = r_z.$$

An arbitrary single qubit density operator can be written as

$$\hat{\rho} = \frac{1}{2}(\hat{1} + r_x\hat{\sigma}_x + r_y\hat{\sigma}_y + r_z\hat{\sigma}_z) = \begin{pmatrix}\dfrac{1+r_z}{2} & \dfrac{r_x - ir_y}{2}\\ \dfrac{r_x + ir_y}{2} & \dfrac{1-r_z}{2}\end{pmatrix},$$

where $\boldsymbol{r} = (r_x, r_y, r_z)$ is an arbitrary real vector of length $|\boldsymbol{r}| \le 1$. We see that

$$Tr[\hat{\rho}] = 1.$$

We calculate

$$Tr[\hat{\rho}^2] = \frac{1}{2}(1 + \boldsymbol{r} \cdot \boldsymbol{r}),$$

When $|\boldsymbol{r}| < 1$, $\hat{\rho}$ is the density operator of a mixed state. When $|\boldsymbol{r}| = 1$ (i.e., the points are on the surface of the Bloch sphere), $\hat{\rho}$ is the density operator of a pure state;

$$Tr[\hat{\rho}^2] = 1.$$

$$Tr[\hat{\rho}] = 1,$$

$$\langle \sigma_x \rangle = Tr[\hat{\rho}\hat{\sigma}_x] = r_x, \qquad \langle \sigma_y \rangle = Tr[\hat{\rho}\hat{\sigma}_y] = r_y, \qquad \langle \sigma_z \rangle = Tr[\hat{\rho}\hat{\sigma}_z] = r_z$$

$$Tr[(|+x\rangle\langle +x|)\hat{\rho}] = \frac{1+r_x}{2}, \qquad Tr[(|-x\rangle\langle -x|)\hat{\rho}] = \frac{1-r_x}{2},$$

$$Tr[(|+y\rangle\langle +y|)\hat{\rho}] = \frac{1+r_y}{2}, \qquad Tr[(|-y\rangle\langle -y|)\hat{\rho}] = \frac{1-r_y}{2},$$

$$Tr[(|+z\rangle\langle +z|)\hat{\rho}] = \frac{1+r_z}{2}, \qquad Tr[(|-z\rangle\langle -z|)\hat{\rho}] = \frac{1-r_z}{2},$$

((**Mathematica**))

```
Clear["Global`*"];
expr_* :=
 expr /. Complex[a_, b_] :> Complex[a, -b];
```

$$\sigma x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix};\ \sigma y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix};\ \sigma z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix};$$

$$E1 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix};$$

$$\rho = \frac{E1 + rx\,\sigma x + ry\,\sigma y + rz\,\sigma z}{2} \text{ // Simplify}$$

$$\left\{\left\{\frac{1+rz}{2}, \frac{1}{2}(rx - i\,ry)\right\}, \left\{\frac{1}{2}(rx + i\,ry), \frac{1-rz}{2}\right\}\right\}$$

$$\psi xp = \frac{1}{\sqrt{2}}\{1, 1\};\ \psi xn = \frac{1}{\sqrt{2}}\{1, -1\};$$

$$\psi yp = \frac{1}{\sqrt{2}}\{1, i\};\ \psi yn = \frac{1}{\sqrt{2}}\{1, -i\};\ \psi zp = \{1, 0\};$$

$$\psi zn = \{0, 1\};\ \sigma x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix};\ \sigma y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix};$$

$$\sigma z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix};$$

```
Axp = Outer[Times, ψxp, ψxp*] // Simplify;
Axn = Outer[Times, ψxn, ψxn*] // Simplify;
Ayp = Outer[Times, ψyp, ψyp*] // Simplify;
Ayn = Outer[Times, ψyn, ψyn*] // Simplify;
Azp = Outer[Times, ψzp, ψzp*] // Simplify;
Azn = Outer[Times, ψzn, ψzn*] // Simplify;
```

```
Tr[σx.ρ] // Simplify
```

rx

```
Tr[σy.ρ] // Simplify
```

ry

```
Tr[σz.ρ] // Simplify
```

rz

```
Tr[Axp.ρ] // Simplify
```

$$\frac{1 + rx}{2}$$

```
Tr[Axn.ρ] // Simplify
```

$$\frac{1 - rx}{2}$$

```
Tr[Ayp.ρ] // Simplify
```

$$\frac{1+\mathrm{ry}}{2}$$

```
Tr[Ayn.ρ] // Simplify
```

$$\frac{1-\mathrm{ry}}{2}$$

```
Tr[Azp.ρ] // Simplify
```

$$\frac{1+\mathrm{rz}}{2}$$

```
Tr[Azn.ρ] // Simplify
```

$$\frac{1-\mathrm{rz}}{2}$$

18. Interpretation of the density matrix elements

What is the probability to find the qubit in the state $|+z\rangle$ when it is described by a density matrix ρ?

$$\hat{\rho}=\frac{1}{2}(\hat{1}+r_x\hat{\sigma}_x+r_y\hat{\sigma}_y+r_z\hat{\sigma}_z)=\begin{pmatrix}\frac{1+r_z}{2} & \frac{r_x-ir_y}{2}\\ \frac{r_x+ir_y}{2} & \frac{1-r_z}{2}\end{pmatrix}=\begin{pmatrix}\rho_{11} & \rho_{12}\\ \rho_{21} & \rho_{22}\end{pmatrix}.$$

The projection operator:

$$\hat{P}_+=|+z\rangle\langle+z|=\begin{pmatrix}1 & 0\\ 0 & 0\end{pmatrix}, \qquad \hat{P}_-=|-z\rangle\langle-z|=\begin{pmatrix}0 & 0\\ 0 & 1\end{pmatrix}.$$

The probability to find the qubit in the state $|+z\rangle$ is

$$P_+=Tr[\hat{P}_+\hat{\rho}]=\frac{1+r_x}{2}=\rho_{11}.$$

The probability to find the qubit in the state $|-z\rangle$ is

$$P_- = Tr[\hat{P}_-\hat{\rho}] = \frac{1-r_x}{2} = \rho_{22},$$

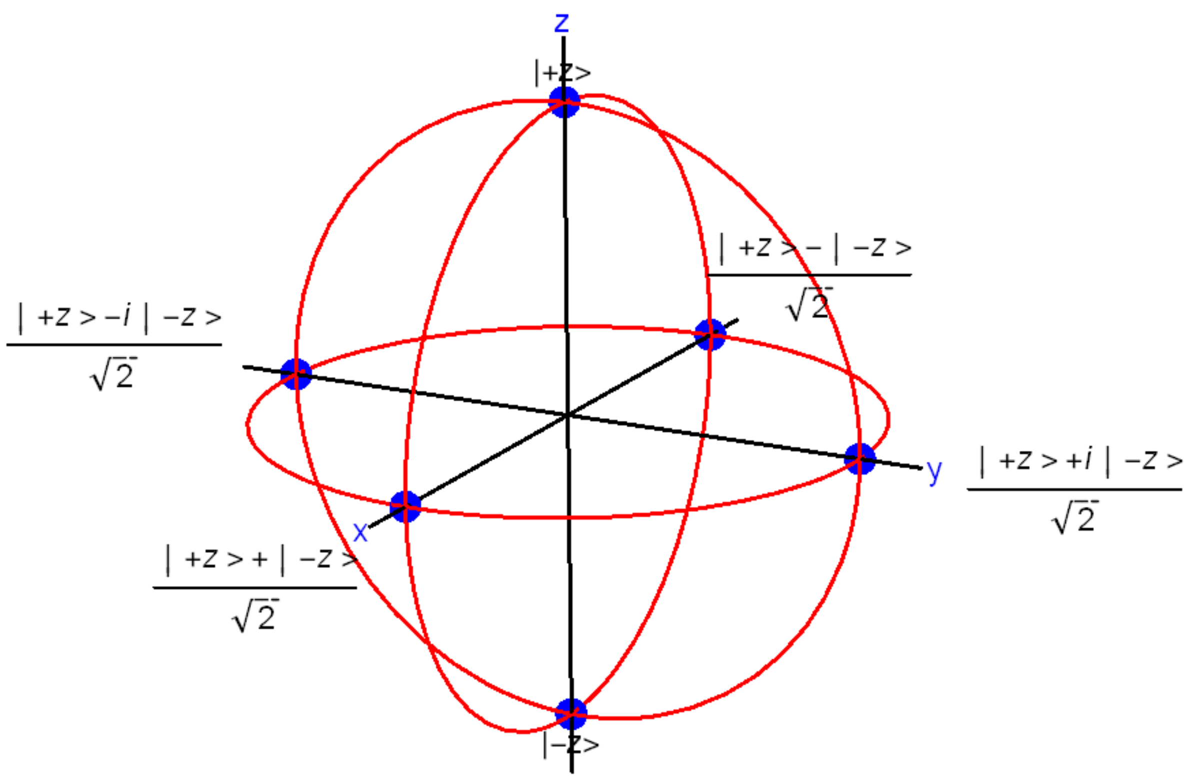
with

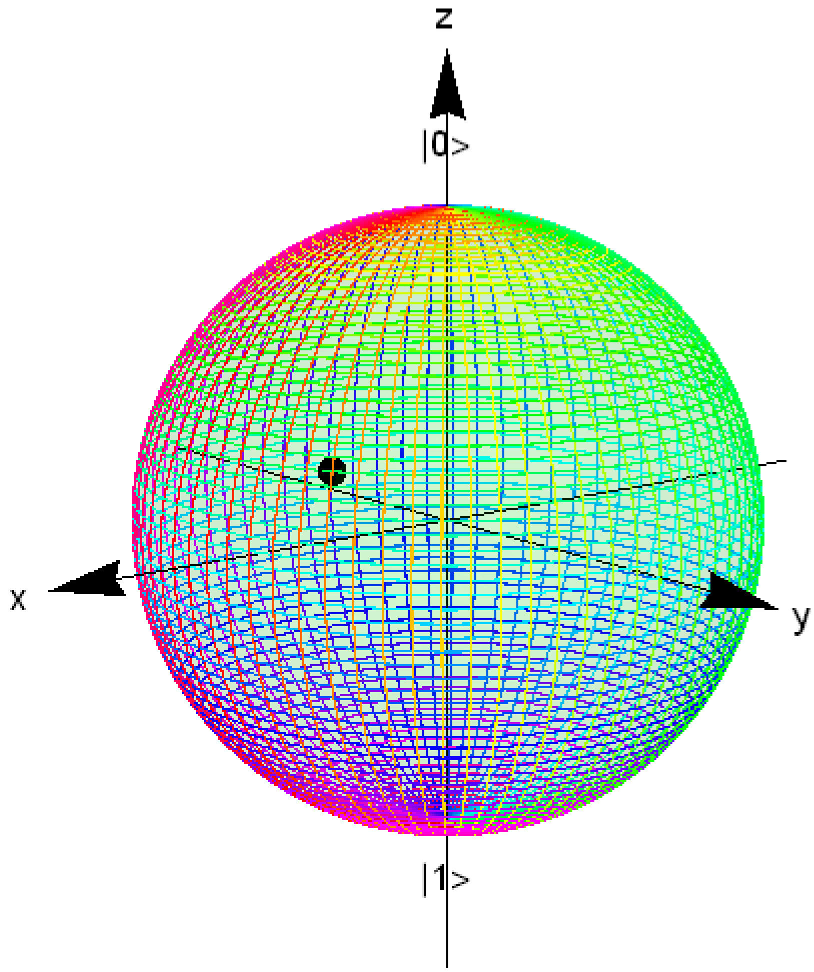
$$P_+ + P_- = \rho_{11} + \rho_{22} = 1.$$

So the probability to find the qubit in a certain state is given by the diagonal elements.

19. Bloch sphere picture

The Bloch sphere is a geometrical representation of the pure state space of a two-level quantum mechanical system (qubit). The north and south poles of the Bloch sphere are typically chosen to correspond to the ketvectors and $|+z\rangle$ and $|-z\rangle$, respectively, which correspond. to the spin-up and spin-down states of an electron. The points on the surface of the sphere correspond to the pure states of the system, whereas the interior points correspond to the mixed states.





Bloch sphere, $|\boldsymbol{r}|=1$ and the vector $\boldsymbol{r}$ pointing from the origin to a point on the sphere.

$$|\psi\rangle = |+\boldsymbol{r}\rangle = \cos\frac{\theta}{2}|+z\rangle + e^{i\phi}\sin\frac{\theta}{2}|-z\rangle = \begin{pmatrix} \cos\frac{\theta}{2} \\ e^{i\phi}\sin\frac{\theta}{2} \end{pmatrix},$$

$\boldsymbol{r} = (r_x, r_y, r_z)$, (called the Bloch vector).

$$r_x = Tr[\hat{\rho}\hat{\sigma}_x] = \langle\psi|\hat{\sigma}_x|\psi\rangle = \sin\theta\cos\phi,$$

$$r_y = Tr[\hat{\rho}\hat{\sigma}_y] = \langle\psi|\hat{\sigma}_y|\psi\rangle = \sin\theta\sin\phi,$$

$$r_z = Tr[\hat{\rho}\hat{\sigma}_z] = \langle\psi|\hat{\sigma}_z|\psi\rangle = \cos\theta .$$

The density operator (pure state) is defined as

$$\hat{\rho} = |\psi\rangle\langle\psi| = \begin{pmatrix} \cos^2(\frac{\theta}{2}) & \frac{1}{2}e^{-i\phi}\sin\theta \\ \frac{1}{2}e^{i\phi}\sin\theta & \sin^2(\frac{\theta}{2}) \end{pmatrix},$$

where

$$Tr[\hat{\rho}] = 1,$$

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

Pauli spin matrix representation of the density matrix is given by

$$\hat{\rho} = \frac{1}{2}(\hat{1} + \boldsymbol{r}\cdot\hat{\boldsymbol{\sigma}}).$$

((**Example-1**)) Plot the density matrix state $\hat{\rho} = \frac{1}{2}[|+z\rangle\langle+z| + |-z\rangle\langle-z|]$ in the Bloch sphere.

((**Solution**))

$$\hat{\rho} = \frac{1}{2}[|+z\rangle\langle+z| + |-z\rangle\langle-z|] = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix},$$

$$Tr(\hat{\rho}\hat{\sigma}_x) = 0,$$

$$Tr(\hat{\rho}\hat{\sigma}_y) = 0,$$

$$Tr(\hat{\rho}\hat{\sigma}_z) = 0.$$

The corresponding point of the Bloch sphere is the origin (0, 0, 0).

((**Example-2**)) Plot the density obtained by averaging

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

over ϕ with a uniform probability distribution in the interval $[0, 2\pi]$.

((**Solution**))

$$\hat{\rho} = \begin{pmatrix} \cos^2\left(\frac{\theta}{2}\right) & 0 \\ 0 & \sin^2\left(\frac{\theta}{2}\right) \end{pmatrix},$$

$$Tr(\hat{\rho}\hat{\sigma}_x) = 0,$$

$$Tr(\hat{\rho}\hat{\sigma}_y) = 0,$$

$$Tr(\hat{\rho}\hat{\sigma}_z) = \cos\theta.$$

Then the corresponding point of the Bloch sphere is the origin (0, 0, cosθ).

((**Example-3**)) The average $\langle \hat{\boldsymbol{\sigma}} \cdot \boldsymbol{n} \rangle$

We evaluate the average $\langle \hat{\boldsymbol{\sigma}} \cdot \boldsymbol{n} \rangle$ using the density operator,

$$\langle \hat{\boldsymbol{\sigma}} \cdot \boldsymbol{n} \rangle = Tr[\hat{\rho}(\hat{\boldsymbol{\sigma}} \cdot \boldsymbol{n})] = Tr[\frac{1}{2}(\hat{1} + \boldsymbol{r} \cdot \hat{\boldsymbol{\sigma}})(\hat{\boldsymbol{\sigma}} \cdot \boldsymbol{n})].$$

Noting that

$$(\boldsymbol{r} \cdot \hat{\boldsymbol{\sigma}})(\boldsymbol{n} \cdot \hat{\boldsymbol{\sigma}}) = (\boldsymbol{r} \cdot \boldsymbol{n})\hat{1} + i\hat{\boldsymbol{\sigma}} \cdot (\boldsymbol{r} \times \boldsymbol{n}), \qquad \text{(formula)}$$

we get

$$\langle \hat{\boldsymbol{\sigma}} \cdot \boldsymbol{n} \rangle = \frac{1}{2} Tr[\hat{\boldsymbol{\sigma}} \cdot \boldsymbol{n} + (\boldsymbol{r} \cdot \boldsymbol{n})\hat{1} + i\hat{\boldsymbol{\sigma}} \cdot (\boldsymbol{r} \times \cdot \boldsymbol{n})].$$

Since

$$Tr[\hat{\boldsymbol{\sigma}} \cdot \boldsymbol{n}] = Tr(\hat{\boldsymbol{\sigma}}) \cdot \boldsymbol{n} = 0, \qquad Tr[\hat{\boldsymbol{\sigma}} \cdot (\boldsymbol{r} \times \cdot \boldsymbol{n})] = Tr(\hat{\boldsymbol{\sigma}}) \cdot (\boldsymbol{r} \times \cdot \boldsymbol{n}) = 0,$$

we have

$$\langle \hat{\boldsymbol{\sigma}} \cdot \boldsymbol{n} \rangle = \frac{1}{2}(\boldsymbol{r} \cdot \boldsymbol{n}) Tr[\hat{1}] = (\boldsymbol{r} \cdot \boldsymbol{n}).$$

((**Example-4**)) Pure state $\hat{\rho} = \frac{1}{2}(\hat{I} + \boldsymbol{r} \cdot \hat{\boldsymbol{\sigma}})$

$$\begin{aligned}
\hat{\rho}^2 &= \frac{1}{2}(\hat{1} + \boldsymbol{r} \cdot \hat{\boldsymbol{\sigma}}) \frac{1}{2}(\hat{1} + \boldsymbol{r} \cdot \hat{\boldsymbol{\sigma}}) \\
&= \frac{1}{4}[\hat{1} + \boldsymbol{r} \cdot \hat{\boldsymbol{\sigma}} + \boldsymbol{r} \cdot \hat{\boldsymbol{\sigma}} + (\boldsymbol{r} \cdot \hat{\boldsymbol{\sigma}})(\boldsymbol{r} \cdot \hat{\boldsymbol{\sigma}})] \\
&= \frac{1}{4}[\hat{1}(1 + \boldsymbol{r} \cdot \boldsymbol{r}) + 2(\boldsymbol{r} \cdot \hat{\boldsymbol{\sigma}}) + i\hat{\boldsymbol{\sigma}} \cdot (\boldsymbol{r} \times \boldsymbol{r})] \\
&= \frac{1}{4}[\hat{1}(1 + \boldsymbol{r} \cdot \boldsymbol{r}) + 2(\boldsymbol{r} \cdot \hat{\boldsymbol{\sigma}})]
\end{aligned}$$

$$\begin{aligned}
Tr[\hat{\rho}^2] &= \frac{1}{4} Tr[\hat{1}(1 + \boldsymbol{r} \cdot \boldsymbol{r}) + 2(\boldsymbol{r} \cdot \hat{\boldsymbol{\sigma}})] \\
&= \frac{1}{2}(1 + r^2)
\end{aligned}$$

When $r = 1$ $\quad Tr[\hat{\rho}^2] = 1;$ $\quad$ (pure stae).
When $r<1$ $\quad Tr[\hat{\rho}^2] < 1:$ $\quad$ (mixed state)

20. Poincare sphere picture

Adopting a basis set $\{|R\rangle, |L\rangle\}$, representing right- and left-circularly polarized photons, a photon of any polarization can be represented, within an overall phase by the superposition

$$|\psi\rangle = \cos\frac{\theta}{2}|R\rangle + e^{i\phi}\sin\frac{\theta}{2}|L\rangle,$$

where the angles θ and ϕ define the point on the surface of the unit sphere (the Poincaré sphere) whose south and north poles represent the states $|L\rangle$ and $|R\rangle$, in analogy with $|-z\rangle$ and $|+z\rangle$ in the Bloch sphere, respectively.

$$|R\rangle = \frac{1}{\sqrt{2}}(|x\rangle + i|y\rangle), \qquad |L\rangle = \frac{1}{\sqrt{2}}(|x\rangle - i|y\rangle).$$

The orthogonal horizontal and vertical linear polarizations are given by

$$|H\rangle = \frac{1}{\sqrt{2}}(|R\rangle - |L\rangle), \text{ and } \qquad |V\rangle = \frac{1}{\sqrt{2}}(|R\rangle + |L\rangle),$$

respectively. They appear at diametrically opposite points on the equator. An incoherent polarization state is represented by a point within the Poincare sphere. For a pure photon state, the density operator can be expressed by

$$\hat{\rho} = \frac{1}{2}(1 + \boldsymbol{s} \cdot \boldsymbol{\sigma}),$$

where s_x, s_y and s_z are called Stokes parameters.

$$s_x = Tr[\hat{\rho}\sigma_x], \qquad s_y = Tr[\hat{\rho}\sigma_y], \qquad s_z = Tr[\hat{\rho}\sigma_z].$$

---

21. Example-I: eigenvalue problem

We consider the density matrix given by

$$\hat{\rho} = \begin{pmatrix} 3/4 & 1/4 \\ 1/4 & 1/4 \end{pmatrix} = \frac{3}{4}|+z\rangle\langle +z| + \frac{1}{4}|+z\rangle\langle -z| + \frac{1}{4}|-z\rangle\langle +z| + \frac{1}{4}|+z\rangle\langle +z|,$$

under the basis of $\{|+z\rangle, |-z\rangle\}$. This matrix is not diagonal. We now try to find the new basis under which the new density of matrix is diagonal. In order to do that, we need to solve the eigenvalue problem using the Mathematica.

The eigenvalue problem.

$$|\psi_1\rangle = \hat{U}|\phi_1\rangle, \qquad |\psi_2\rangle = \hat{U}|\phi_2\rangle,$$

$$\lambda_1 = \frac{2+\sqrt{2}}{4} = 0.85355, \qquad |\psi_1\rangle = \begin{pmatrix} 0.92388 \\ 0.382683 \end{pmatrix},$$

$$\lambda_2 = \frac{2-\sqrt{2}}{4} = 0.146447, \qquad |\psi_2\rangle = \begin{pmatrix} -0.382683 \\ 0.92388 \end{pmatrix},$$

$$\hat{U} = \begin{pmatrix} 0.92388 & 0.382683 \\ -0.382683 & 0.92388 \end{pmatrix},$$

$$\hat{\rho}_{new} = \hat{U}^{+}\hat{\rho}_{old}\hat{U}$$
$$= \begin{pmatrix} 0.853553 & 0 \\ 0 & 0.146447 \end{pmatrix}$$
$$= 0.853553|\psi_1\rangle\langle\psi_1| + +0.146447|\psi_2\rangle\langle\psi_2|$$

---

22. Example-II: eigenvalue problem

We consider the density matrix given by

$$\hat{\rho} = \begin{pmatrix} 1/2 & 1/2 \\ 1/2 & 1/2 \end{pmatrix} = \frac{1}{2}|+z\rangle\langle+z| + \frac{1}{2}|+z\rangle\langle-z| + \frac{1}{2}|-z\rangle\langle+z| + \frac{1}{2}|-z\rangle\langle-z|,$$

under the basis of $\{|+z\rangle, |-z\rangle\}$. This matrix is not diagonal.

$$\hat{\rho}^2 = \hat{\rho}. \qquad \text{(pure state)}$$

We now try to find the new basis under which the new density of matrix is diagonal. In order to do that, we need to solve the eigenvalue problem using the Mathematica.

The eigenvalue problem.

$$|\psi_1\rangle = \hat{U}|+z\rangle, \qquad |\psi_2\rangle = \hat{U}|-z\rangle,$$

$$\lambda_1 = 1, \qquad |\psi_1\rangle = |+x\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix},$$

$$\lambda_2 = 0 , \qquad |\psi_2\rangle = |-x\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix},$$

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

$$\hat{\rho}|\psi_i\rangle = \lambda_i|\psi_i\rangle,$$

or

$$\hat{\rho} = \hat{\rho}(|\psi_1\rangle\langle\psi_1| + |\psi_2\rangle\langle\psi_2|) = \lambda_1|\psi_1\rangle\langle\psi_1| = |\psi_1\rangle\langle\psi_1| = |+x\rangle\langle+x|,$$

which is the density matrix for the pure state.

23. Example-III: $|x\rangle$ representation

The probability of finding the system in the quantum state represented by the state vector $|\chi\rangle$ (of norm unity) is

$$P(\chi) = Tr[\hat{\rho}|\chi\rangle\langle\chi|].$$

Pure state in the $|x\rangle$ representation.

$$\hat{\rho} = |\psi\rangle\langle\psi|.$$

The probability of the system at the position *x*:

$$P(x) = Tr[\hat{\rho}(|x\rangle\langle x|)] = \int dx'\langle x'|\hat{\rho}|x\rangle\langle x|x'\rangle = \langle x|\hat{\rho}|x\rangle = |\langle x|\psi\rangle|^2.$$

We consider a system which is in either a coherent, or incoherent (mixture) superposition of two momenta $|k\rangle$ and $|-k\rangle$

(a) Coherent superposition

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

$$\begin{aligned}\hat{\rho} &= |\psi\rangle\langle\psi| \\ &= \frac{1}{2}[(|k\rangle + |-k\rangle)(\langle k| + \langle -k|)] \\ &= \frac{1}{2}[(|k\rangle\langle k| + |k\rangle\langle -k| + |-k\rangle\langle k| + |-k\rangle\langle -k|\end{aligned}$$

and

$$P(x) = Tr[\hat{\rho}|x\rangle\langle x|]$$
$$= \frac{1}{2}[\langle x|k\rangle\langle k|x\rangle + \langle x|k\rangle\langle -k|x\rangle + \langle x|-k\rangle\langle k|x\rangle + \langle x|-k\rangle\langle k|-x\rangle]$$

Using the transformation function,

$$\langle x|k\rangle = \frac{1}{\sqrt{2\pi}}e^{ikx},$$

we have

$$P(x) = \frac{1}{4\pi}(2 + e^{i2kx} + e^{-i2kx}) = \frac{1}{2\pi}[1 + \cos(kx)].$$

(b) Incoherent mixture

$$\hat{\rho} = \frac{1}{2}[(|k\rangle\langle k| + |-k\rangle\langle -k|)$$

$$P(x) = Tr[\hat{\rho}|x\rangle\langle x|]$$
$$= \frac{1}{2}[\langle x|k\rangle\langle k|x\rangle + \langle x|-k\rangle\langle k|-x\rangle]$$
$$= \frac{1}{2\pi}$$

24. Kronecker product

A classical bit of information is represented by a system that can be in either of two states, 0, 1. At the quantum mechanical level, the most natural candidate for replacing a classical bit is the state of a two-level system, whose basic components may be written as

$$|\psi_1\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} = |0\rangle, \qquad |\psi_2\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} = |1\rangle.$$

This is the so-called quantum bit of information, or, in short, a qubit. Here we define the combined state of two qubits as

$$|\psi_1\rangle \otimes |\psi_2\rangle = \text{KroneckerProduct}[\psi_1,\ \psi_2]$$

Then we have

$$|0\rangle \otimes |0\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \qquad |0\rangle \otimes |1\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}, \qquad |1\rangle \otimes |0\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix},$$

$$|1\rangle \otimes |1\rangle = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}.$$

$$|0\rangle \otimes |0\rangle)(\langle 0| \otimes \langle 0| = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad |0\rangle \otimes |1\rangle)(\langle 0| \otimes \langle 1| = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix},$$

$$|1\rangle \otimes |0\rangle)(\langle 1| \otimes \langle 0| = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad |1\rangle \otimes |1\rangle)(\langle 1| \otimes \langle 1| = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

25. Calculation of density operator by Mathematica

A classical bit of information is represented by a system that can be in either of two states, 0, 1. At the quantum mechanical level, the most natural candidate for replacing a classical bit is the state of a two-level system, whose basic components may be written as

$$|\psi_1\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} = |0\rangle, \qquad |\psi_2\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} = |1\rangle.$$

This is the so-called quantum bit of information, or, in short, a qubit.
The Kronecker product:

$$|\psi_1\rangle \otimes |\psi_2\rangle = \text{KroneckerProduct}[\psi_1,\ \psi_2]$$

Then we have

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

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

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

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

$$|0\rangle \otimes |0\rangle)(\langle 0| \otimes \langle 0| = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix},$$

$$|0\rangle \otimes |1\rangle)(\langle 0| \otimes \langle 1| = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix},$$

$$|1\rangle \otimes |0\rangle)(\langle 1| \otimes \langle 0| = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix},$$

$$|1\rangle \otimes |1\rangle)(\langle 1| \otimes \langle 1| = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

((**Example-1**))

$$|1\rangle = |+z\rangle_1 |+z\rangle_2, \qquad |2\rangle = |+z\rangle_1 |-z\rangle_2,$$

$$|3\rangle = |-z\rangle_1 |+z\rangle_2, \qquad |4\rangle = |-z\rangle_1 |-z\rangle_2,$$

where the index 1, 2 denote the particle number.

(a) For the state defined by

$$|\psi_a\rangle = \frac{1}{\sqrt{2}}(|2\rangle - |3\rangle) = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ 1 \\ -1 \\ 0 \end{pmatrix},$$

the density operator (the pure state) is given by

$$\hat{\rho}_a = |\psi_a\rangle\langle\psi_a| = \frac{1}{2}\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & -1 & 0 \\ 0 & -1 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}.$$

(b) For the state defined by

$$|\psi_s\rangle = \frac{1}{\sqrt{2}}(|2\rangle + |3\rangle) = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ 1 \\ 1 \\ 0 \end{pmatrix},$$

the density operator (the pure state) is given by

$$\hat{\rho}_s = |\psi_s\rangle\langle\psi_s| = \frac{1}{2}\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}.$$

---

26. Example

We consider the density operator (4x4 matrix) in the Hilbert space.

$$\hat{\rho} = \frac{1}{4}(1-\varepsilon)\hat{I}_4 + \varepsilon(|0\rangle \otimes |0\rangle)(\langle 0| \otimes \langle 0|),$$

where ε is a real parameter ($0<\varepsilon<1$). We examine the property of the density operator.

$$\hat{\rho} = \begin{pmatrix} \varepsilon + \frac{1-\varepsilon}{4} & 0 & 0 & 0 \\ 0 & \frac{1-\varepsilon}{4} & 0 & 0 \\ 0 & 0 & \frac{1-\varepsilon}{4} & 0 \\ 0 & 0 & 0 & \frac{1-\varepsilon}{4} \end{pmatrix}.$$

Thus

$$\hat{\rho}^+ = \hat{\rho},$$

$$Tr[\hat{\rho}^2] = \frac{1+3\varepsilon^2}{4}, \qquad Tr[\hat{\rho}] = 1.$$

For $0 < \varepsilon < 1$, we have

$$0 < Tr[\hat{\rho}^2] < 1,$$

which means that the system is mixed.

27. Problems and solutions (related to the density operator)

A. Example-1

A spin-1/2 particle is in the pure state $\left|\psi\right\rangle = a\left|+z\right\rangle + b\left|-z\right\rangle$

(a) Construct the density matrix in the S_z basis for this state.

(b) Starting with your result in (a), determine the density matrix in the S_x basis where

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

(c) Use your result for the density matrix in (b) to determine the probability that a measurement of S_x yields $\hbar/2$ for the state $\left|\psi\right\rangle$.

((**Solution**))

$$\left|\psi\right\rangle = \begin{pmatrix} a \\ b \end{pmatrix}, \qquad \text{under the basis of } \{\left|+z\right\rangle, \left|-z\right\rangle\}$$

We define the unitary operator as

$$\left|+x\right\rangle = \hat{U}\left|+z\right\rangle, \qquad \left|-x\right\rangle = \hat{U}\left|-z\right\rangle,$$

with

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

(a)

$$\hat{\rho}_z = \left|\psi\right\rangle\left\langle\psi\right| = \begin{pmatrix} a \\ b \end{pmatrix}\begin{pmatrix} a^* & b^* \end{pmatrix} = \begin{pmatrix} aa^* & ab^* \\ a^*b & bb^* \end{pmatrix},$$

under the basis of $\{\left|+x\right\rangle, \left|-x\right\rangle\}$

(b)

$$\begin{aligned}\hat{\rho}_x &= \hat{U}^+ \hat{\rho}_z \hat{U} \\ &= \frac{1}{\sqrt{2}}\begin{pmatrix}1 & 1\\ 1 & -1\end{pmatrix}\begin{pmatrix}aa^* & ab^*\\ a^*b & bb^*\end{pmatrix}\frac{1}{\sqrt{2}}\begin{pmatrix}1 & 1\\ 1 & -1\end{pmatrix} \\ &= \frac{1}{2}\begin{pmatrix}1 & 1\\ 1 & -1\end{pmatrix}\begin{pmatrix}a(a^*+b^*) & a(a^*-b^*)\\ b(a^*+b^*) & b(a^*-b^*)\end{pmatrix} \\ &= \frac{1}{2}\begin{pmatrix}(a+b)(a^*+b^*) & (a+b)(a^*-b^*)\\ (a-b)(a^*+b^*) & (a-b)(a^*+b^*)\end{pmatrix}\end{aligned}$$

The projection operator

$$\hat{P}_x = |+x\rangle\langle +x| = \begin{pmatrix}1\\ 0\end{pmatrix}\begin{pmatrix}1 & 0\end{pmatrix} = \begin{pmatrix}1 & 0\\ 0 & 0\end{pmatrix}$$

under the basis of $\{|+x\rangle, |-x\rangle\}$. Then we have

$$\begin{aligned}\hat{P}_x\hat{\rho}_x &= \begin{pmatrix}1 & 0\\ 0 & 0\end{pmatrix}\frac{1}{2}\begin{pmatrix}(a+b)(a^*+b^*) & (a+b)(a^*-b^*)\\ (a-b)(a^*+b^*) & (a-b)(a^*+b^*)\end{pmatrix} \\ &= \frac{1}{2}\begin{pmatrix}(a+b)(a^*+b^*) & (a+b)(a^*-b^*)\\ 0 & 0\end{pmatrix}\end{aligned}$$

and

$$Tr[\hat{P}_x\hat{\rho}_x] = \frac{1}{2}(a+b)(a^*+b^*)$$

((**Mathematica**))

```
Clear["Global`*"]; σx = (0 1
                        1 0); ψz = {a, b};
ψzc = {a*, b*}; ρz = Outer[Times, ψz, ψzc];
ρz // MatrixForm
```

$$\begin{pmatrix} a\, a^* & a\, b^* \\ b\, a^* & b\, b^* \end{pmatrix}$$

```
U = 1/√2 (1  1
          1 -1); UH = Transpose[U];
```

```
ρx = UH.ρz.U // Simplify; ρx // MatrixForm
```

$$\begin{pmatrix} \frac{1}{2}(a+b)(a^*+b^*) & \frac{1}{2}(a+b)(a^*-b^*) \\ \frac{1}{2}(a-b)(a^*+b^*) & \frac{1}{2}(a-b)(a^*-b^*) \end{pmatrix}$$

```
Px = Outer[Times, {1, 0}, {1, 0}];
```

```
Tr[Px.ρx]
```

$$\frac{1}{2}(a+b)\left(a^*+b^*\right)$$

B. Example-2

Given the density operator

$$\hat{\rho} = \frac{1}{2}[|+z\rangle\langle+z| + |-z\rangle\langle-z| - |-z\rangle\langle+z| - |+z\rangle\langle-z|] = \frac{1}{2}\begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix},$$

construct the density matrix. Use the density operator formalism to calculate $\langle S_x \rangle$ for this state. Is this the density operator for a pure state? Justify your answer in two different ways.

((**Solution**))

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

$$Tr[\hat{\rho}^2] = Tr[\hat{\rho}] = 1, \qquad \text{(pure state)}$$

$$Tr[\hat{\rho}\hat{S}_x] = -\frac{\hbar}{2}.$$

((**Mathematica**))

```
Clear["Global`*"]; Sx = ℏ/2 (0 1
                             1 0);

ρ =
 1/2 (Outer[Times, {1, 0}, {1, 0}] +
    Outer[Times, {0, 1}, {0, 1}] -
    Outer[Times, {0, 1}, {1, 0}] -
    Outer[Times, {1, 0}, {0, 1}])
```

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

```
Tr[Sx.ρ]
```

$-\frac{\hbar}{2}$

```
ρ.ρ - ρ // Simplify
```

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

C. Example-3

Given the density operator

$$\hat{\rho} = \frac{3}{4}|+z\rangle\langle +z| + \frac{1}{4}|-z\rangle\langle -z|,$$

construct the density matrix. Show that this is the density operator for a mixed state. Determine $\langle S_x \rangle$, $\langle S_y \rangle$, and $\langle S_z \rangle$ for this state.

((**Solution**))

$$\hat{\rho} = \frac{1}{4}\begin{pmatrix} 3 & 0 \\ 0 & 1 \end{pmatrix}.$$

$$Tr[\hat{\rho}^2] = \frac{5}{8} < 1, \qquad \text{(mixed state)}$$

$$\hat{S}_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \hat{S}_y = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \hat{S}_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},$$

$$\langle S_x \rangle = Tr[\hat{S}_x \hat{\rho}] = 0, \qquad \langle S_y \rangle = Tr[\hat{S}_y \hat{\rho}] = 0,$$

$$\langle S_z \rangle = Tr[\hat{S}_z \hat{\rho}] = \frac{\hbar}{4}.$$

((**Mathematica**))

```
Clear["Global`*"]; Sx = ℏ/2 (0 1
                              1 0); Sy = ℏ/2 (0 -i
                                               i  0);
Sz = ℏ/2 (1  0
          0 -1);
ρ = 3/4 Outer[Times, {1, 0}, {1, 0}] +
  1/4 Outer[Times, {0, 1}, {0, 1}]
```

$\{\{\frac{3}{4}, 0\}, \{0, \frac{1}{4}\}\}$

```
Tr[ρ.ρ] // Simplify
```

$\frac{5}{8}$

```
Tr[Sx.ρ]
```

0

```
Tr[Sy.ρ]
```

0

```
Tr[Sz.ρ]
```

$\frac{\hbar}{4}$

D. Example-4

Show that

$$\hat{\rho} = \frac{1}{2}[|+\boldsymbol{n}\rangle\langle+\boldsymbol{n}|+|-\boldsymbol{n}\rangle\langle-\boldsymbol{n}|] = \frac{1}{2}[|+z\rangle\langle+z|+|-z\rangle\langle-z|],$$

where

$$|+\boldsymbol{n}\rangle = \begin{pmatrix} \cos\frac{\theta}{2} \\ e^{i\phi}\sin\frac{\theta}{2} \end{pmatrix}, \qquad |-\boldsymbol{n}\rangle = \begin{pmatrix} \sin\frac{\theta}{2} \\ -e^{i\phi}\cos\frac{\theta}{2} \end{pmatrix}.$$

((**Solution**))

$$\hat{\rho}_z = \frac{1}{2}[|+z\rangle\langle +z| + |-z\rangle\langle -z|] = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix},$$

$$\hat{\rho}_{\boldsymbol{n}} = \frac{1}{2}[|+\boldsymbol{n}\rangle\langle +\boldsymbol{n}| + |-\boldsymbol{n}\rangle\langle -\boldsymbol{n}|] = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}.$$

Then we have

$$\hat{\rho}_{\boldsymbol{n}} = \hat{\rho}_z,$$

$$Tr[\hat{\rho}^2] = \frac{1}{2}. \qquad \text{(for mixed state)}$$

((**Mathematica**))

```
Clear["Global`*"];
expr_* := expr /. Complex[a_, b_] :→ Complex[a, -b];
ψpn = {Cos[θ/2], Exp[i ϕ] Sin[θ/2]};
ψmn = {Sin[θ/2], -Exp[i ϕ] Cos[θ/2]};
ρ =
 1/2 Outer[Times, ψpn, ψpn*] +
  1/2 Outer[Times, ψmn, ψmn*] // Simplify

{{1/2, 0}, {0, 1/2}}

Tr[ρ.ρ]

1/2
```

E. Example-5

Find states $|\psi_1\rangle$ and $|\psi_1\rangle$ for which the density operator

$$\hat{\rho} = \frac{3}{4}|+z\rangle\langle +z| + \frac{1}{4}|-z\rangle\langle -z|,$$

can be expressed in the form

$$\hat{\rho} = \frac{1}{2}|\psi_1\rangle\langle\psi_1| + \frac{1}{2}|\psi_2\rangle\langle\psi_2|.$$

((**Solution**))

Assume that

$$|\psi_1\rangle = \frac{\sqrt{3}}{2}|+z\rangle + \frac{1}{2}|-z\rangle = \begin{pmatrix} \frac{\sqrt{3}}{2} \\ \frac{1}{2} \end{pmatrix},$$

$$|\psi_2\rangle = \frac{\sqrt{3}}{2}|+z\rangle - \frac{1}{2}|-z\rangle = \begin{pmatrix} \frac{\sqrt{3}}{2} \\ -\frac{1}{2} \end{pmatrix}.$$

Then we have

$$\hat{\rho} = \frac{1}{2}|\psi_1\rangle\langle\psi_1| + \frac{1}{2}|\psi_2\rangle\langle\psi_2| = \frac{3}{4}|+z\rangle\langle +z| + \frac{1}{4}|-z\rangle\langle -z| = \begin{pmatrix} \frac{3}{4} & 0 \\ 0 & \frac{1}{4} \end{pmatrix}.$$

with

$$Tr[\hat{\rho}^2] = \frac{5}{8}.$$

((**Mathematica**))

```
Clear["Global`*"];
expr_* := expr /. Complex[a_, b_] :> Complex[a, -b];
ψ1 = {√3/2, 1/2}; ψ2 = {√3/2, -1/2};
ρ =
 1/2 Outer[Times, ψ1, ψ1*] + 1/2 Outer[Times, ψ2, ψ2*] //
  Simplify
```

$\{\{\frac{3}{4}, 0\}, \{0, \frac{1}{4}\}\}$

```
Tr[ρ.ρ]
```

$\frac{5}{8}$

F. Example-6

The density matrix for an ensemble of spin-1/2 particles in the S_z basis is

$$\hat{\rho} = \begin{pmatrix} \frac{1}{4} & n \\ n^* & p \end{pmatrix}.$$

(a) What value must p have? Why?

(b) What value(s) must n have for the density matrix to represent a pure state?

(c) What pure state is represented when n takes its maximum possible real value? Express your answer in terms of the state $|+\boldsymbol{n}\rangle$ given by

$$|+\boldsymbol{n}\rangle = \begin{pmatrix} \cos\frac{\theta}{2} \\ e^{i\phi}\sin\frac{\theta}{2} \end{pmatrix}.$$

((**Solution**)) Here we assume that n is the complex number,

(a)

$$n = a + \mathrm{i}\, b,$$

$$\hat{\rho} = \begin{pmatrix} \frac{1}{4} & a+ib \\ a-ib & p \end{pmatrix},$$

$$Tr[\hat{\rho}] = p + \frac{1}{4} = 1, \qquad p = \frac{3}{4},$$

(b)

$$Tr[\hat{\rho}^2] = \frac{5}{8} + 2(a^2+b^2) = 1. \qquad \text{for the pure state}$$

$$|n| = \sqrt{a^2+b^2} = \frac{\sqrt{3}}{4}.$$

(c)

$$|+\boldsymbol{n}\rangle = \begin{pmatrix} \cos\frac{\theta}{2} \\ e^{i\phi}\sin\frac{\theta}{2} \end{pmatrix},$$

$$\hat{\rho} = |+\boldsymbol{n}\rangle\langle+\boldsymbol{n}| = \begin{pmatrix} \cos^2\frac{\theta}{2} & \frac{1}{2}e^{-\phi}\sin\theta \\ \frac{1}{2}e^{\phi}\sin\theta & \sin^2\frac{\theta}{2} \end{pmatrix}.$$

So we have

$$a+ib = \frac{1}{2}e^{-\phi}\sin\theta.$$

When $b = 0$, $\phi = 0$. n is a real number.

$$a = \frac{1}{2}\sin\theta = \frac{\sqrt{3}}{4},$$

$$\sin\theta = \frac{\sqrt{3}}{2} \qquad \text{leading to the value of } \theta \text{ as } \theta = \frac{\pi}{3} \qquad \text{or} \qquad \theta = \frac{2\pi}{3}.$$

Here we note that

$$\cos^2\frac{\theta}{2} = \frac{1}{4}, \qquad \text{or} \qquad \cos\theta = -\frac{1}{2}.$$

So we get

$$\boxed{\theta = \frac{2\pi}{3}}.$$

((**Mathematica**))

```
Clear["Global`*"];
expr_* := expr /. Complex[a_, b_] :→ Complex[a, -b];
ρ = ( 1/4      a + ⅈ b
      a - ⅈ b  p       )
{{1/4, a + ⅈ b}, {a - ⅈ b, p}}

eq1 = Solve[Tr[ρ] == 1, p]
{{p → 3/4}}

ρ.ρ /. eq1[[1]] // Simplify
{{1/16 + a^2 + b^2, a + ⅈ b}, {a - ⅈ b, 9/16 + a^2 + b^2}}

eq2 = Tr[ρ.ρ] /. eq1[[1]] // Simplify
5/8 + 2 a^2 + 2 b^2
```

```
eq21 = eq2 /. {a^2 → x - b^2} // Simplify
```

$\frac{5}{8} + 2\,x$

```
Solve[eq21 == 1, x]
```

$\{\{x \to \frac{3}{16}\}\}$

```
ψpn = {Cos[θ/2], Exp[ⅈ ϕ] Sin[θ/2]};
```

```
ρn = Outer[Times, ψpn, ψpn*] // Simplify
```

$\{\{\mathrm{Cos}[\frac{\theta}{2}]^2, \frac{1}{2} e^{-i\phi}\,\mathrm{Sin}[\theta]\}, \{\frac{1}{2} e^{i\phi}\,\mathrm{Sin}[\theta], \mathrm{Sin}[\frac{\theta}{2}]^2\}\}$

G. Example-7

Show that the Curie constant for an ensemble of N spin-1 particles of mass m and charge q = -e immersed in a uniform magnetic field $\boldsymbol{B} = B\boldsymbol{k}$ is given by

$$C = \frac{2N\mu^2}{3k_B},$$

where $\mu = \frac{ge\hbar}{2mc}$. Compare this value of C with that for an ensemble of spin-1/2 particles,

((**Solution**))

The magnetic moment is defined as

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

The magnetic moment is antiparallel to the spin angular momentum. The Hamiltonian $\hat{H}$ is given by

$$\hat{H} = -\hat{\boldsymbol{\mu}}\cdot\boldsymbol{B} = -\hat{\mu}_z B_0 = \frac{g\mu_B B_0}{\hbar}\hat{S}_z,$$

$$\hat{H}|1,m\rangle = \frac{g\mu_B B_0}{\hbar}\hat{S}_z|1,m\rangle = \frac{g\mu_B B_0}{\hbar}\hbar m|1,m\rangle = g\mu_B B_0 m|1,m\rangle = E_0 m|1,m\rangle .$$

The energy eigenstate	energy eigenvalue	
$|1,m=1\rangle$,	E_0	(the magnetic moment is antiparallel to ***B***).
$|1,m=0\rangle$,	0	
$|1,m=-1\rangle$,	$-E_0$	(the magnetic moment is parallel to ***B***)

((**Solution**))

```
Clear["Global`*"];
expr_* := expr /. Complex[a_, b_] :> Complex[a, -b];
ψp1 = {1, 0, 0}; ψ0 = {0, 1, 0}; ψm1 = {0, 0, 1};
Sz = ℏ (1  0  0
        0  0  0
        0  0 -1);

rule1 = {Z1 → Exp[β E1] + 1 + Exp[-β E1], E1 → g μB B0};

ρ =
 1/Z1 (Exp[-β E1] Outer[Times, ψp1 , ψp1 ] +
     Outer[Times, ψ0 , ψ0 ] +
     Exp[β E1] Outer[Times, ψm1 , ψm1 ]) //
  FullSimplify
```

$$\left\{\left\{\frac{e^{-E1\,\beta}}{Z1}, 0, 0\right\}, \left\{0, \frac{1}{Z1}, 0\right\}, \left\{0, 0, \frac{e^{E1\,\beta}}{Z1}\right\}\right\}$$

```
M = -(g μB/ℏ) N1 Tr[Sz ρ] // Simplify
```

$$\frac{e^{-E1\,\beta}\left(-1 + e^{2\,E1\,\beta}\right) g\, N1\, \mu B}{Z1}$$

```
M1 = M //. rule1 // Simplify
```

$$\frac{\left(-1+e^{2\,\text{B0 g}\,\beta\,\mu\text{B}}\right)\text{g N1}\,\mu\text{B}}{1+e^{\text{B0 g}\,\beta\,\mu\text{B}}+e^{2\,\text{B0 g}\,\beta\,\mu\text{B}}}$$

```
M2 = M1 /. {B0 → x/(g μB β)}
```

$$\frac{\left(-1+e^{2\,x}\right)\text{g N1}\,\mu\text{B}}{1+e^{x}+e^{2\,x}}$$

```
M3 = Series[M2, {x, 0, 2}] // Normal
```

$$\frac{2}{3}\,\text{g N1 x}\,\mu\text{B}$$

```
M4 = M3 /. {x → g μB β B0} // Simplify
```

$$\frac{2}{3}\,\text{B0 g}^2\,\text{N1}\,\beta\,\mu\text{B}^2$$

H. Exmple-8

An attempt to perform a Bell-state measurement on two photons produces a mixed state, one in which the two photons are in the entangled state

$$\frac{1}{\sqrt{2}}[|x,x\rangle+|y,y\rangle],$$

with probability p and with probability $(1-p)/2$ in each of the states $|x,x\rangle$ and $|y,y\rangle$. Determine the density matrix for this ensemble using the linear polarization states of the photons as basis states.

((**Solution**))

$$|\psi_1\rangle = \frac{1}{\sqrt{2}}[|x,x\rangle + |y,y\rangle] = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\0\\0\\1\end{pmatrix},$$

$$|\psi_2\rangle = |x,x\rangle = \begin{pmatrix}1\\0\\0\\0\end{pmatrix}, \qquad |\psi_3\rangle = |y,y\rangle = \begin{pmatrix}0\\0\\0\\1\end{pmatrix}.$$

The density operator:

$$\begin{aligned}\hat{\rho} &= p|\psi_1\rangle\langle\psi_1| + \frac{1-p}{2}|\psi_2\rangle\langle\psi_2| + \frac{1-p}{2}|\psi_3\rangle\langle\psi_3| \\ &= \frac{1}{2}\begin{pmatrix}1 & 0 & 0 & p\\ 0 & 0 & 0 & 0\\ 0 & 0 & 0 & 0\\ p & 0 & 0 & 1\end{pmatrix}\end{aligned}$$

where

$$Tr[\hat{\rho}] = 1,$$

$$Tr[\hat{\rho}^2] = \frac{1+p^2}{2}.$$

((**Mathematica**))

```
Clear["Global`*"];
expr_* := expr /. Complex[a_, b_] :> Complex[a, -b];
ψ1 = 1/Sqrt[2] {1, 0, 0, 1}; ψ2 = {1, 0, 0, 0};
ψ3 = {0, 0, 0, 1};

ρ =
 p Outer[Times, ψ1, ψ1] + (1 - p)/2 Outer[Times, ψ2, ψ2] +
   (1 - p)/2 Outer[Times, ψ3, ψ3] // Simplify
```

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

```
ρ // MatrixForm
```

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

I. Example-9

Show for the density operator for a mixed state

$$\hat{\rho} = \sum_k p_k \left|\psi^{(k)}\right\rangle\left\langle\psi^{(k)}\right|,$$

that the probability of obtaining the state $|\phi\rangle$ as a result of a measurement is given by $Tr[P_{|\phi\rangle}\hat{\rho}]$, where

$$\hat{P}_{|\phi\rangle} = |\phi\rangle\langle\phi|.$$

((**Solution**))

$$
\begin{aligned}
Tr[P_{|\phi\rangle}\hat{\rho}] &= \sum_{m,k} p_k \langle\phi_m|\phi\rangle\langle\phi|\phi_k\rangle\langle\phi_k|\phi_m\rangle \\
&= \sum_{m,k} p_k \langle\phi_m|\phi\rangle\langle\phi|\phi_k\rangle\delta_{k,m} \\
&= \sum_{k} p_k \langle\phi_k|\phi\rangle\langle\phi|\phi_k\rangle \\
&= \sum_{k} p_k \left|\langle\phi_k|\phi\rangle\right|^2
\end{aligned}
$$

J. Example-10

Use the density operator formalism to show the probability that a measurement finds two spin-1/2 particles in the state $|+x,+x\rangle$ differs for the pure Bell state,

$$
|\Phi^{(+)}\rangle = \frac{1}{\sqrt{2}}[|+z,+z\rangle + |-z,-z\rangle],
$$

for which,

$$
\hat{\rho}_1 = |\Phi^{(+)}\rangle\langle\Phi^{(+)}|,
$$

and for the mixed state

$$
\hat{\rho}_2 = \frac{1}{2}|+z,+z\rangle\langle+z,+z| + \frac{1}{2}|-z,-z\rangle\langle-z,-z|.
$$

Thus, the disagreement between the predictions of quantum mechanics for the entangled state and those consistent with the views of a local realist are apparent without having to resort to Bell inequalities.

((**Solution**))

The Bell state $|\Phi^{(+)}\rangle$ is given by

$$\left|\Phi^{(+)}\right\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\0\\0\\1\end{pmatrix},$$

and, the first density operator is

$$\hat{\rho}_1 = \left|\Phi^{(+)}\right\rangle\left\langle\Phi^{(+)}\right| = \frac{1}{2}\begin{pmatrix}1 & 0 & 0 & 1\\0 & 0 & 0 & 0\\0 & 0 & 0 & 0\\1 & 0 & 0 & 1\end{pmatrix},$$

for the Bell state.

$$Tr(\hat{\rho}_1^{\,2}) = 1$$

which means that $\hat{\rho}_1$ is the density operator for the pure state.

When

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

the projection operator is given by

$$\hat{P}_{|+x,+x\rangle} = \left|+x,+x\right\rangle\left\langle+x,+x\right| = \frac{1}{4}\begin{pmatrix}1 & 1 & 1 & 1\\1 & 1 & 1 & 1\\1 & 1 & 1 & 1\\1 & 1 & 1 & 1\end{pmatrix}.$$

Then we have

$$Tr[\hat{P}_{|+x,+x\rangle}\hat{\rho}_1] = \frac{1}{2}.$$

The probability of finding the system in the state $\left|+x,+x\right\rangle$ is 1/2.

We now consider the second density operator given by

$$\hat{\rho}_2 = \frac{1}{2}\left|+z,+z\right\rangle\left\langle +z,+z\right| + \frac{1}{2}\left|-z,-z\right\rangle\left\langle -z,-z\right|$$
$$= \frac{1}{2}\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

Since

$$Tr(\hat{\rho}_2{}^2) = \frac{1}{2} \text{ (<1)}.$$

$\hat{\rho}_2$ is the density operator for the mixed state. We have

$$Tr[\hat{P}_{\left|+x,+x\right\rangle}\hat{\rho}_2] = \frac{1}{4}.$$

The probability of finding this system in the state $\left|+x,+x\right\rangle$ is 1/4.

((**Mathematica**))

```
Clear["Global`*"]; expr_* := expr /. Complex[a_, b_] :> Complex[a, -b];
```

$\psi xpT = \frac{1}{\sqrt{2}}\{1, 1\}$; $\phi xp = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix}$; $\phi zp = \begin{pmatrix}1\\0\end{pmatrix}$; $\phi zn = \begin{pmatrix}0\\1\end{pmatrix}$;

$\psi 11 = \frac{1}{\sqrt{2}}$ (KroneckerProduct[ϕzp, ϕzp] + KroneckerProduct[ϕzn, ϕzn]);

```
ψ1 = Transpose[ψ11][[1]]; ψ21 = KroneckerProduct[ϕxp, ϕxp]; ψ2 = Transpose[ψ21][[1]];
ψ3p1 = KroneckerProduct[ϕzp, ϕzp]; ψ3p = Transpose[ψ3p1][[1]];
ψ3n1 = KroneckerProduct[ϕzn, ϕzn];
ψ3n = Transpose[ψ3n1][[1]];
```

```
ψ11 // MatrixForm
```

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

```
ψ21 // MatrixForm
```

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

```
ρ1 =  Outer[Times, ψ1, ψ1] // Simplify; ρ1 // MatrixForm
```

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

```
Tr[ρ1.ρ1]
```

1

```
PX =  Outer[Times, ψ2, ψ2] // Simplify;
```

```
PX // MatrixForm
```

$$\begin{pmatrix} \frac{1}{4} & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} \\ \frac{1}{4} & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} \\ \frac{1}{4} & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} \\ \frac{1}{4} & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} \end{pmatrix}$$

```
Tr[PX.ρ1]
```

$\frac{1}{2}$

$$\rho 2 = \frac{1}{2}\,\text{Outer[Times, }\psi\text{3p, }\psi\text{3p]} + \frac{1}{2}\,\text{Outer[Times, }\psi\text{3n, }\psi\text{3n]};$$

```
ρ2 // MatrixForm
```

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

```
Tr[ρ2.ρ2]
```

$\frac{1}{2}$

```
Tr[PX.ρ2]
```

$\frac{1}{4}$

K. Example-11

Show that the equation governing time evolution of the density operator for a mixed state is given by

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

((**Solution**))

$$\begin{aligned}
\frac{d}{dt}\hat{\rho} &= \overline{\frac{d}{dt}|\psi\rangle\langle\psi|} \\
&= \overline{\left(\frac{\partial}{\partial t}|\psi\rangle\right)\langle\psi| + |\psi\rangle\left(\frac{\partial}{\partial t}\langle\psi|\right)} \\
&= \frac{1}{i\hbar}\overline{\hat{H}|\psi\rangle\langle\psi| - |\psi\rangle\langle\psi|\hat{H}} \\
&= \frac{1}{i\hbar}\hat{H}\overline{|\psi\rangle\langle\psi|} - \overline{|\psi\rangle\langle\psi|}\hat{H} \\
&= \frac{1}{i\hbar}\hat{H}\hat{\rho} - \hat{\rho}\hat{H} = -\frac{1}{i\hbar}[\hat{\rho}, \hat{H}]
\end{aligned}$$

or

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

L. Example-12

(a) Show that the time evolution of the density operator is given by

$$\hat{\rho}(t) = \hat{U}(t)\hat{\rho}(0)\hat{U}^{+}(t),$$

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

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

(b) Suppose that an ensemble of particles is in a pure state at t = 0. Show the ensemble cannot evolve into a mixed state as long as time evolution is governed by the Schrodinger equation.

((**Solution**))
(a)

$$\hat{\rho}(t) = \overline{|\psi(t)\rangle\langle\psi(t)|},$$

where

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

Then we get

$$\begin{aligned}\hat{\rho}(t) &= \overline{\hat{U}|\psi(t=0)\rangle\langle\psi(t=0)|\hat{U}^{+}} \\ &= \hat{U}\overline{|\psi(t=0)\rangle\langle\psi(t=0)|}\hat{U}^{+} \\ &= \hat{U}\hat{\rho}(t=0)\hat{U}^{+}\end{aligned}$$

(b)
Suppose that $\hat{\rho}(t=0)$ is the density operator for the pure state.

$$\begin{aligned}Tr[\hat{\rho}(t)\hat{\rho}(t)] &= Tr[\hat{U}\hat{\rho}(t=0)\hat{U}^{+}\hat{U}\hat{\rho}(t=0)\hat{U}^{+}] \\ &= Tr[\hat{U}\hat{\rho}(t=0)\hat{\rho}(t=0)\hat{U}^{+}] \\ &= Tr[\hat{U}^{+}\hat{U}\hat{\rho}(t=0)\hat{\rho}(t=0)] \\ &= Tr[\hat{\rho}(t=0)\hat{\rho}(t=0)] = 1\end{aligned}$$

Thus $\hat{\rho}(t)$ is still the density operator for the pure state.

26. Canonical ensemble in statistical mechanics

The time dependence of $\hat{\rho}$ is given by

$$i\hbar\frac{\partial}{\partial t}\hat{\rho} = -[\hat{\rho}, \hat{H}].$$

Note that the sign is opposite to that of the usual Heisenberg operator equation.We see that, if $\hat{\rho}(\hat{H})$ is a function only of $\hat{H}$, then

$$[\hat{\rho}, \hat{H}] = 0, \qquad \frac{\partial}{\partial t}\hat{\rho} = 0.$$

For a canonical ensemble we may write

$$\hat{\rho} = \exp(\frac{F - \hat{H}}{k_B T}) = \frac{1}{Z}\exp(-\frac{\hat{H}}{k_B T}),$$

where $\hat{H}$ is the Hamiltonian and Z is the partition function. Since

$$Tr[\hat{\rho}] = 1.$$

Z is given by

$$Z = \exp(-\frac{F}{k_B T}) = Tr[\exp(-\frac{\hat{H}}{k_B T})].$$

The Helmholtz free energy F is given by

$$F = -k_B T \ln Z .$$

Because of the invariance of the trace under unitary operators, we may calculate Z by taking the trace of $\exp(-\frac{\hat{H}}{k_B T})$ in any representation.

$$\begin{aligned}
\hat{\rho} &= \frac{1}{Z}\exp(-\frac{\hat{H}}{k_B T})\sum_n |E_n\rangle\langle E_n| \\
&= \frac{1}{Z}\sum_n \exp(-\frac{\hat{H}}{k_B T})|E_n\rangle\langle E_n| \\
&= \frac{1}{Z}\sum_n \exp(-\frac{E_n}{k_B T})|E_n\rangle\langle E_n|
\end{aligned}$$

where

$$\hat{H}\left|E_n\right\rangle = E_n\left|E_n\right\rangle,$$

and

$$Z = \sum_n \exp(-\frac{E_n}{k_B T}).$$

27. Multiparticle systems

27.1 The density operator of two-particles

The density operator for two spins is given by

$$\hat{\rho} = \begin{pmatrix} \rho_{11} & \rho_{12} & \rho_{13} & \rho_{14} \\ \rho_{21} & \rho_{22} & \rho_{23} & \rho_{24} \\ \rho_{31} & \rho_{32} & \rho_{33} & \rho_{34} \\ \rho_{41} & \rho_{42} & \rho_{43} & \rho_{44} \end{pmatrix}$$
$$= \begin{pmatrix} \left\langle ++\right|\hat{\rho}\left|++\right\rangle & \left\langle ++\right|\hat{\rho}\left|+-\right\rangle & \left\langle ++\right|\hat{\rho}\left|-+\right\rangle & \left\langle ++\right|\hat{\rho}\left|--\right\rangle \\ \left\langle +-\right|\hat{\rho}\left|++\right\rangle & \left\langle +-\right|\hat{\rho}\left|+-\right\rangle & \left\langle +-\right|\hat{\rho}\left|-+\right\rangle & \left\langle +-\right|\hat{\rho}\left|--\right\rangle \\ \left\langle -+\right|\hat{\rho}\left|++\right\rangle & \left\langle -+\right|\hat{\rho}\left|+-\right\rangle & \left\langle -+\right|\hat{\rho}\left|-+\right\rangle & \left\langle -+\right|\hat{\rho}\left|--\right\rangle \\ \left\langle --\right|\hat{\rho}\left|++\right\rangle & \left\langle --\right|\hat{\rho}\left|+-\right\rangle & \left\langle --\right|\hat{\rho}\left|-+\right\rangle & \left\langle --\right|\hat{\rho}\left|--\right\rangle \end{pmatrix}$$

The reduced density operator $\hat{\rho}_2$ is obtained from the full density operator by tracing over the diagonal matrix elements of particle 1

$$\hat{\rho}_2 = Tr_1[\hat{\rho}] = \begin{pmatrix} \rho_{11} & \rho_{12} \\ \rho_{21} & \rho_{22} \end{pmatrix} + \begin{pmatrix} \rho_{33} & \rho_{34} \\ \rho_{43} & \rho_{44} \end{pmatrix} = \begin{pmatrix} \rho_{11} + \rho_{33} & \rho_{12} + \rho_{34} \\ \rho_{21} + \rho_{43} & \rho_{22} + \rho_{44} \end{pmatrix}.$$

The reduced density operator $\hat{\rho}_1$ is obtained from the full density operator by tracing over the diagonal matrix elements of particle 2.

$$\hat{\rho}_1 = Tr_2[\hat{\rho}] = \begin{pmatrix} \rho_{11} & \rho_{13} \\ \rho_{31} & \rho_{33} \end{pmatrix} + \begin{pmatrix} \rho_{22} & \rho_{24} \\ \rho_{42} & \rho_{44} \end{pmatrix} = \begin{pmatrix} \rho_{11} + \rho_{22} & \rho_{13} + \rho_{24} \\ \rho_{31} + \rho_{42} & \rho_{33} + \rho_{44} \end{pmatrix}.$$

Note that the reduced density operator $\hat{\rho}_1$ describes completely all the properties/outcomes of measurements of the system 1, given that system 2 is left unobserved ("tracing out" system 2).

This represent the maximum information which is available about the particle 1 alone, irrespective of the state of particle 2.

The reduced density operator $\hat{\rho}_2$ describes completely all the properties/outcomes of measurements of the system 2, given that system 1 is left unobserved ("tracing out" system 1). This represent the maximum information which is available about the particle 2 alone, irrespective of the state of particle 1.

((**Example-1**)) Reduced density operator: Two spins (independent subsystems)
We consider the state of the composite system 1-2 consisting of independent subsystems

$$\left|\psi_{12}\right\rangle = \frac{1}{\sqrt{2}}(\left|+z,1\right\rangle + \left|-z,1\right\rangle) \otimes \left|+z,2\right\rangle = \left|+x,1\right\rangle \otimes \left|+z,2\right\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 0 \\ 1 \\ 0 \end{pmatrix}.$$

The density operator is obtained as

$$\begin{aligned}
\hat{\rho}_{12} &= \left|\psi_{12}\right\rangle\left\langle\psi_{12}\right| \\
&= (\left|+x,1\right\rangle \otimes \left|+z,2\right\rangle)(\left\langle +x,1\right| \otimes \left\langle +z,2\right|) \\
&= (\left|+x,1\right\rangle\left\langle +x,1\right|) \otimes (\left|+z,2\right\rangle\left\langle +z,2\right|) \\
&= \hat{\rho}_A \otimes \hat{\rho}_B
\end{aligned}$$

where A and B denote the particle-1 and particle-2, respectively.
The matrix form of $\hat{\rho}_{12}$ is given by

$$\hat{\rho}_{12} = \frac{1}{2}\begin{pmatrix} 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}.$$

The reduce density operators $\hat{\rho}_1$ and $\hat{\rho}_2$ are obtained as

$$\hat{\rho}_2 = Tr_1[\hat{\rho}_{12}] = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} + \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} = \hat{\rho}_B,$$

$$\hat{\rho}_{r1} = Tr_2[\hat{\rho}_{12}] = \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} + \frac{1}{2}\begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} = \hat{\rho}_A .$$

Note that

$$\hat{\rho}_2 = Tr_1[\hat{\rho}_{12}] = Tr_A[\hat{\rho}_A \otimes \hat{\rho}_B] = \hat{\rho}_B Tr_A[\hat{\rho}_A] = \hat{\rho}_B ,$$

$$\hat{\rho}_1 = Tr_2[\hat{\rho}_{12}] = Tr_B[\hat{\rho}_A \otimes \hat{\rho}_B] = \hat{\rho}_A Tr_B[\hat{\rho}_B] = \hat{\rho}_A .$$

((**Example-2**)) Two spins: independent subsystems

We start with the two-particle pure state $|\psi_{12}\rangle = |+z,1\rangle|+z,2\rangle$. The density operator is

$$\hat{\rho} = |+z,1\rangle|+z,2\rangle\langle+z;1|\langle+z,2| = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}.$$

The reduced density

$$\hat{\rho}_1 = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix},$$

$$\hat{\rho}_2 = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix},$$

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

((**Example-3**)) Bell's two-particle entangled state

$$|\Psi_{12}{}^{(-)}\rangle = \frac{1}{\sqrt{2}}[|+z;1\rangle|-z;2\rangle - |-z;1\rangle|+z;2\rangle] .$$

The density operator is given by

$$\hat{\rho} = \left|\Psi_{12}{}^{(-)}\right\rangle\left\langle\Psi_{12}{}^{(-)}\right| = \frac{1}{2}\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & -1 & 0 \\ 0 & -1 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}.$$

((**Mathematica**))

```
ψ1 = (1
      0); ψ2 = (0
                1);
ψ12 =
  1/√2 (KroneckerProduct[ψ1, ψ2] -
      KroneckerProduct[ψ2, ψ1]) // Simplify
```

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

```
ρ0 = ψ12.Transpose[ψ12] // Simplify;
ρ0 // MatrixForm
```

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

The reduced density operator

$$\hat{\rho}_1 = \frac{1}{2}\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} + \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix},$$

$$\hat{\rho}_2 = \frac{1}{2}\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} + \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix},$$

under the basis of $\{\left|+\right\rangle, \left|-\right\rangle\}$. Thus for measurements of particle 1 (or 2) the Bell's state behaves like the mixed states of completely un-polarized ensemble.

((**Note**))

M.A Nielsen and I.L. Chuang, Quantum computation and quantum information, 10th Anniversary Edition (Cambridge, 2010).

Notice that this state $\hat{\rho}_1$ (or $\hat{\rho}_2$) is a mixed state. This is a quite remarkable result. The state of the joint system of two qubits is a pure state, that is, it is known exactly, however, the first qubit is in a mixed state, that is a state about which we apparently do not have maximal knowledge. This strange property, that the joint state of a system can be completely known, yet a subsystem be in the mixed state, is another hallmark of quantum entanglement.

27.2 Density operator for three spins

$$\hat{\rho} = \begin{pmatrix} \rho_{11} & \rho_{12} & \rho_{13} & \rho_{14} & \rho_{15} & \rho_{16} & \rho_{17} & \rho_{18} \\ \rho_{21} & \rho_{22} & \rho_{23} & \rho_{24} & \rho_{25} & \rho_{26} & \rho_{27} & \rho_{18} \\ \rho_{31} & \rho_{32} & \rho_{33} & \rho_{34} & \rho_{35} & \rho_{36} & \rho_{37} & \rho_{18} \\ \rho_{41} & \rho_{42} & \rho_{43} & \rho_{44} & \rho_{45} & \rho_{46} & \rho_{47} & \rho_{18} \\ \rho_{51} & \rho_{52} & \rho_{53} & \rho_{54} & \rho_{55} & \rho_{56} & \rho_{57} & \rho_{18} \\ \rho_{61} & \rho_{62} & \rho_{63} & \rho_{64} & \rho_{65} & \rho_{66} & \rho_{67} & \rho_{18} \\ \rho_{71} & \rho_{72} & \rho_{73} & \rho_{74} & \rho_{75} & \rho_{76} & \rho_{77} & \rho_{78} \\ \rho_{81} & \rho_{82} & \rho_{83} & \rho_{84} & \rho_{85} & \rho_{86} & \rho_{87} & \rho_{88} \end{pmatrix}$$

where

$$\rho_{11} = \langle +++|\hat{\rho}|+++\rangle, \qquad \rho_{12} = \langle +++|\hat{\rho}|++-\rangle,$$

$$\rho_{13} = \langle +++|\hat{\rho}|+-+\rangle, \qquad \rho_{14} = \langle +++|\hat{\rho}|+--\rangle.$$

and so on. The reduced density operator $\hat{\rho}_{23}$ is obtained from the full density operator by tracing over the diagonal matrix elements of particle 1, leading to

$$\begin{aligned} \hat{\rho}_{23} &= Tr_1\hat{\rho} \\ &= \begin{pmatrix} \rho_{11} & \rho_{12} & \rho_{13} & \rho_{14} \\ \rho_{21} & \rho_{22} & \rho_{23} & \rho_{24} \\ \rho_{31} & \rho_{32} & \rho_{33} & \rho_{34} \\ \rho_{41} & \rho_{42} & \rho_{43} & \rho_{44} \end{pmatrix} + \begin{pmatrix} \rho_{51} & \rho_{52} & \rho_{53} & \rho_{54} \\ \rho_{61} & \rho_{62} & \rho_{63} & \rho_{64} \\ \rho_{71} & \rho_{72} & \rho_{73} & \rho_{74} \\ \rho_{81} & \rho_{82} & \rho_{83} & \rho_{84} \end{pmatrix} \\ &= \begin{pmatrix} \chi_{11} & \chi_{12} & \chi_{13} & \chi_{14} \\ \chi_{21} & \chi_{22} & \chi_{23} & \chi_{24} \\ \chi_{31} & \chi_{32} & \chi_{33} & \chi_{34} \\ \chi_{41} & \chi_{42} & \chi_{43} & \chi_{44} \end{pmatrix} \end{aligned}$$

The reduced density operator $\hat{\rho}_3$ is obtained from the full density operator by tracing over the diagonal matrix elements of particles 1 and 2, leading to

$$\hat{\rho}_3 = Tr_2\hat{\rho}_{23} = Tr_{1,2}\hat{\rho}$$
$$= \begin{pmatrix} \chi_{11} & \chi_{12} \\ \chi_{21} & \chi_{22} \end{pmatrix} + \begin{pmatrix} \chi_{33} & \chi_{34} \\ \chi_{43} & \chi_{44} \end{pmatrix}.$$

((**Example-1**)) Entangled GHS state

$$\left|\psi_{GHZ}{}^{(+)}\right\rangle = \frac{1}{\sqrt{2}}[\left|+++\right\rangle + \left|---\right\rangle].$$

The density operator is defined by

$$\hat{\rho} = \left|\psi_{GHZ}{}^{(+)}\right\rangle\left\langle\psi_{GHZ}{}^{(+)}\right|$$
$$=$$

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

The reduced density operators are obtained as

$$\hat{\rho}_{23} = \frac{1}{2}\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix},$$

and

$$\hat{\rho}_3 = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix},$$

which is equivalent to a completely un-polarized state,

((**Example-2**)) Another entangled GHZ state

$$\left|\psi_{GHZ}{}^{(-)}\right\rangle = \frac{1}{\sqrt{2}}[\left|+++\right\rangle - \left|---\right\rangle].$$

The density operator is defined by

$$\hat{\rho} = \left|\psi_{GHZ}{}^{(-)}\right\rangle\left\langle\psi_{GHZ}{}^{(-)}\right|$$
$$=$$

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

The reduced density operators are obtained as

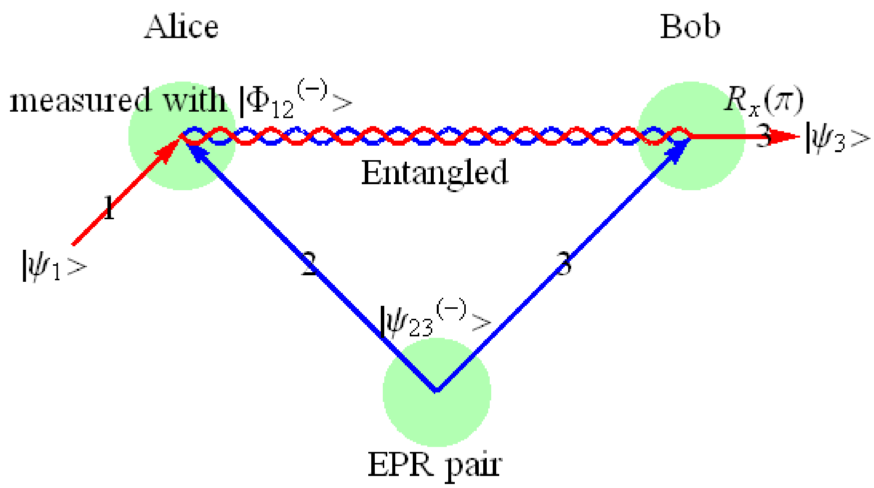
$$\hat{\rho}_{23} = \frac{1}{2}\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix},$$

and

$$\hat{\rho}_3 = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix},$$

which is equivalent to a completely un-polarized state,

28. Quantum teleportation



We consider the pure particle state $|\psi_{123}\rangle$ which is related to the quantum teleportation. The density operator for this pure state is given by

$$\hat{\rho} = |\psi_{123}\rangle\langle\psi_{123}|,$$

where

$$|\psi_{123}\rangle = \frac{1}{2}|\psi_{12}^{(-)}\rangle[-a|+z\rangle_3 - b|-z\rangle_3] + \frac{1}{2}|\psi_{12}^{(+)}\rangle[-a|+z\rangle_3 + b|-z\rangle_3]$$
$$+\frac{1}{2}|\Phi_{12}^{(-)}\rangle[a|-z\rangle_3 + b|+z\rangle_3] + \frac{1}{2}|\Phi_{12}^{(+)}\rangle[a(|-z\rangle_3 - b|+z\rangle_3)$$

with

$$|\psi_{12}^{(\pm)}\rangle = \frac{1}{\sqrt{2}}[|+z\rangle_1|-z\rangle_2 \pm |-z\rangle_1|+z\rangle_2] = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ 1 \\ \pm 1 \\ 0 \end{pmatrix},$$

$$\left|\Phi_{12}^{(\pm)}\right\rangle = \frac{1}{\sqrt{2}}[\left|+z\right\rangle_1\left|+z\right\rangle_2 \pm \left|-z\right\rangle_1\left|-z\right\rangle_2] = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 0 \\ 0 \\ \pm 1 \end{pmatrix}.$$

Note that

$$|a|^2 + |b|^2 = 1.$$

The density operator $\hat{\rho}$ can be obtained as

$$\hat{\rho} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & |a|^2/2 & -|a|^2/2 & 0 & 0 & (ab^*)/2 & -(ab^*)/2 & 0 \\ 0 & -|a|^2/2 & |a|^2/2 & 0 & 0 & -(ab^*)/2 & (ab^*)/2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & (a^*b)/2 & -(a^*b)/2 & 0 & 0 & |b|^2/2 & -|b|^2/2 & 0 \\ 0 & -(a^*b)/2 & (a^*b)/2 & 0 & 0 & -|b|^2/2 & |b|^2/2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

Tracing out particle 1, the reduced density operators are obtained as

$$\begin{aligned} \hat{\rho}_{23} &= \frac{1}{2}\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & |a|^2 & -|a|^2 & 0 \\ 0 & -|a|^2 & |a|^2 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} + \frac{1}{2}\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & |b|^2 & -|b|^2 & 0 \\ 0 & -|b|^2 & |b|^2 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \\ &= \frac{1}{2}\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & |a|^2+|b|^2 & -|a|^2-|b|^2 & 0 \\ 0 & -|a|^2-|b|^2 & |a|^2+|b|^2 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \\ &= \frac{1}{2}\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & -1 & 0 \\ 0 & -1 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \end{aligned}$$

Tracing over particle 2 furthermore, we have

$$\hat{\rho}_3 = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} + = \frac{1}{2}\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix},$$

which is equivalent to a completely un-polarized state. So Bob (particle 3) has no information about the state of the particle Alice is attempting to teleport. On the other hand, if Bob waits until he receives the result of Alice's Bell state measurement, Bob can then maneuver his particle into the state $|\psi\rangle$ that Alice's particle was in initially.

((**Mathematica**))

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

$$\psi 1 = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \\ -1 \\ 0 \end{pmatrix};\ \psi 2 = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \\ 1 \\ 0 \end{pmatrix};$$

$$\phi 1 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ 0 \\ -1 \end{pmatrix};$$

$$\phi 2 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ 0 \\ 1 \end{pmatrix};$$

$$\chi 1 = \begin{pmatrix} -a \\ -b \end{pmatrix};\ \chi 2 = \begin{pmatrix} -a \\ b \end{pmatrix};\ \chi 3 = \begin{pmatrix} b \\ a \end{pmatrix};\ \chi 4 = \begin{pmatrix} -b \\ a \end{pmatrix};$$

$$\psi 123 = \frac{1}{2} \text{KroneckerProduct}[\psi 1, \chi 1] + \frac{1}{2} \text{KroneckerProduct}[\psi 2, \chi 2] + \frac{1}{2} \text{KroneckerProduct}[\phi 1, \chi 3] + \frac{1}{2} \text{KroneckerProduct}[\phi 2, \chi 4] \,//\, \text{Simplify};$$

```
K1 = Transpose[ψ123][[1]];

K2 = Transpose[ψ123] //. {a → a1, b → b1};

ρ = Outer[Times, K1, K2[[1]]] // FullSimplify;
ρ // MatrixForm
```

$$\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{a\,a1}{2} & -\frac{a\,a1}{2} & 0 & 0 & \frac{a\,b1}{2} & -\frac{a\,b1}{2} & 0 \\ 0 & -\frac{a\,a1}{2} & \frac{a\,a1}{2} & 0 & 0 & -\frac{a\,b1}{2} & \frac{a\,b1}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{a1\,b}{2} & -\frac{a1\,b}{2} & 0 & 0 & \frac{b\,b1}{2} & -\frac{b\,b1}{2} & 0 \\ 0 & -\frac{a1\,b}{2} & \frac{a1\,b}{2} & 0 & 0 & -\frac{b\,b1}{2} & \frac{b\,b1}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

29. Average $\langle \hat{X}_1 \rangle$

We consider the average value of an operator $\hat{X}_1$ that acts only on the system 1 in a global density operator $\hat{\rho}$ for the particles 1 and 2;

$$\langle \hat{X}_1 \rangle = Tr[(\hat{X}_1 \otimes \hat{I}_2)\hat{\rho}] = Tr_1[\hat{X}_1 Tr_2 \hat{\rho}] = Tr_1[\hat{X}_1 \hat{\rho}_1],$$

where

$$\hat{\rho}_1 = Tr_2 \hat{\rho}.$$

If $\hat{\rho} = \hat{\alpha}_1 \otimes \hat{\alpha}_2$, we have

$$\begin{aligned}
\langle \hat{X}_1 \rangle &= Tr[(\hat{X}_1 \otimes \hat{I}_2)\hat{\rho}] \\
&= Tr[(\hat{X}_1 \otimes \hat{I}_2)(\hat{\alpha}_1 \otimes \hat{\alpha}_2)] \\
&= Tr[(\hat{X}_1 \hat{\alpha}_1 \otimes \hat{I}_2 \hat{\alpha}_2)] \\
&= Tr_1[\hat{X}_1 \hat{\alpha}_1] Tr[\hat{I}_2 \hat{\alpha}_2] \\
&= Tr_1[\hat{X}_1 \hat{\alpha}_1]
\end{aligned}$$

and

$$\hat{\rho}_1 = Tr_2[\hat{\alpha}_1 \otimes \hat{\alpha}_2] = \hat{\alpha}_1 Tr_2[\hat{\alpha}_2] = \hat{\alpha}_1.$$

30. Probability

Suppose that $\hat{P}$ is the projection operator,

$$\hat{P} = |\alpha\rangle\langle\alpha|,$$

then we have

$$Tr[\hat{P}\hat{\rho}] = Tr[|\alpha\rangle\langle\alpha|\hat{\rho}] = \sum_\beta \langle\beta|\alpha\rangle\langle\alpha|\hat{\rho}|\beta\rangle = \langle\alpha|\hat{\rho}|\alpha\rangle$$

So the probability of finding the state $|\alpha\rangle$ in the system is given by the diagonal element.

31. Examples

31.1 Problem and solution -1

Prove that the state of the form

$$|\psi\rangle_{12} = C_{xy}|x\rangle_1 \otimes |y\rangle_2 + C_{yx}|y\rangle_1 \otimes |x\rangle_2 = \begin{pmatrix} 0 \\ C_{xy} \\ C_{yx} \\ 0 \end{pmatrix},$$

where

$$|C_{xy}|^2 + |C_{yx}|^2 = 1,$$

and both coefficients are non-zero, cannot be written as a Kronecker product state

$$|\psi'\rangle_{12} = |\psi\rangle_1 \otimes |\phi\rangle_2,$$

with

$$|\psi\rangle_1 = \alpha_x|x\rangle_1 + \alpha_y|y\rangle_1,$$

$$|\phi\rangle_2 = \beta_x|x\rangle_2 + \beta_y|y\rangle_2.$$

((**Solution**))

$$|\psi'\rangle_{12} = |\psi\rangle_1 \otimes |\phi\rangle_2 = \begin{pmatrix} \alpha_x\beta_x \\ \alpha_x\beta_y \\ \alpha_y\beta_x \\ \alpha_y\beta_y \end{pmatrix}.$$

Suppose that $|\psi'\rangle_{12} = |\psi\rangle_{12}$. Then we have

$$\alpha_x\beta_x = 0, \qquad \alpha_y\beta_y = 0, \qquad C_{xy} = \alpha_x\beta_y, \qquad C_{yx} = \alpha_y\beta_x.$$

Then we get

$$C_{xy}C_{yx} = \alpha_x\beta_y\alpha_y\beta_x = \alpha_x\beta_x\alpha_y\beta_y = 0.$$

This is not consistent with the assumption that both C_{xy} and C_{yxy} are non-zero.

31.2 Problem and solution-2

Consider the state vector

$$|\psi\rangle_{12} = \frac{1}{2}[|x\rangle_1 \otimes |x\rangle_2 + |x\rangle_1 \otimes |y\rangle_2 + |y\rangle_1 \otimes |x\rangle_2 + |y\rangle_1 \otimes |y\rangle_2],$$

describing the polarization of two photons. Show that the reduced density operators

$$\hat{\rho}_1 = Tr_2[\hat{\rho}_{12}], \qquad \hat{\rho}_2 = Tr_1[\hat{\rho}_{12}],$$

describe pure states, where

$$\hat{\rho}_{12} = |\psi\rangle_{12\,12}\langle\psi|.$$

((**Solution**))

The density operator:

$$\hat{\rho}_{12} = \frac{1}{4}\begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \end{pmatrix}.$$

The reduced density operators:

$$\hat{\rho}_1 = Tr_2[\hat{\rho}_{12}] = \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}, \qquad \hat{\rho}_2 = Tr_1[\hat{\rho}_{12}] = \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}.$$

Since

$$\hat{\rho}_1^{\,2} = \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} = \hat{\rho}_1, \quad \hat{\rho}_2^{\,2} = \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} = \hat{\rho}_2,$$

the reduced density operators $\hat{\rho}_1$ and $\hat{\rho}_2$ describe pure state.

33. Schmidt decomposition

((**Theorem**))

Suppose that $|\psi\rangle$ is a pure state of a biparticle composite system, *AB*. Then there exist orthonormal states $|i_A\rangle$ for system *A*, and $|i_B\rangle$ for system, *B* such that

$$|\psi\rangle = \sum_i \sqrt{p_i}|i_A\rangle|i_B\rangle,$$

where $\lambda_i = \sqrt{p_i}$ is known as Schmidt coefficient and is non-negative real number satisfying

$$\sum_i \lambda_i^{\ 2} = 1, \qquad \text{or} \qquad \sum_i p_i = 1.$$

The states $|i_A\rangle$ and $|i_B\rangle$ are any fixed orthonormal bases for *A* and *B* (the relevant state spaces are here of the same dimension).

The density operator is defined by

$$\hat{\rho} = |\psi\rangle\langle\psi|.$$

Note that

$$Tr[\hat{\rho}^2] = \sum_i \lambda_i^{\ 2}.$$

If $Tr[\hat{\rho}^2] = 1$ (pure state), $\lambda_i = 1$ for one and only one *i* and zero for all others

---

We consider the simple case.

$$|\psi\rangle = C_{11}|a_1\rangle|b_1\rangle + C_{12}|a_1\rangle|b_2\rangle + C_{21}|a_2\rangle|b_1\rangle + C_{22}|a_2\rangle|b_1\rangle,$$

$$|\psi\rangle = \sqrt{p_{1}}{}_1|v_1\rangle|w_1\rangle + \sqrt{p_2}|v_2\rangle|w_2\rangle.$$

The unitary transformation:

$$|v_1\rangle = \hat{U}|a_1\rangle = U_{11}|a_1\rangle + U_{21}|a_2\rangle,$$

$$|v_2\rangle = \hat{U}|a_2\rangle = U_{12}|a_1\rangle + U_{22}|a_2\rangle,$$

where

$$\hat{U} = \begin{pmatrix} U_{11} & U_{12} \\ U_{21} & U_{22} \end{pmatrix}, \qquad \hat{U}^{+}\hat{U} = \hat{1}.$$

We also have

$$\left| w_1 \right\rangle = \hat{U}\left| b_1 \right\rangle = V_{11}\left| b_1 \right\rangle + V_{21}\left| b_2 \right\rangle,$$

$$\left| w_2 \right\rangle = \hat{U}\left| b_2 \right\rangle = V_{12}\left| b_1 \right\rangle + V_{22}\left| b_2 \right\rangle,$$

where

$$\hat{V} = \begin{pmatrix} V_{11} & V_{12} \\ V_{21} & V_{22} \end{pmatrix}, \qquad \hat{V}^{+}\hat{V} = \hat{1}.$$

Then

$$\begin{aligned}
\left| \psi \right\rangle &= \sqrt{p_1}\left| v_1 \right\rangle\left| w_1 \right\rangle + \sqrt{p_2}\left| v_2 \right\rangle\left| w_2 \right\rangle \\
&= \sqrt{p_1}(U_{11}\left| a_1 \right\rangle + U_{21}\left| a_2 \right\rangle\left| w_1 \right\rangle(V_{11}\left| b_1 \right\rangle + V_{21}\left| b_2 \right\rangle) \\
&\quad + \sqrt{p_2}(U_{12}\left| a_1 \right\rangle + U_{22}\left| a_2 \right\rangle(V_{12}\left| b_1 \right\rangle + V_{22}\left| b_2 \right\rangle) \\
&= (\sqrt{p_1}U_{11}V_{11} + \sqrt{p_2}U_{12}V_{12})\left| a_1 \right\rangle\left| b_1 \right\rangle + (\sqrt{p_1}U_{11}V_{21} + \sqrt{p_2}U_{12}V_{22})\left| a_1 \right\rangle\left| b_2 \right\rangle \\
&\quad + (\sqrt{p_1}U_{21}V_{11} + \sqrt{p_2}U_{22}V_{12})\left| a_2 \right\rangle\left| b_1 \right\rangle + (\sqrt{p_1}U_{21}V_{21} + \sqrt{p_2}U_{22}V_{22})\left| a_2 \right\rangle\left| b_2 \right\rangle
\end{aligned}$$

Then we have

$$C_{11} = U_{11}\sqrt{p_1}V_{11} + U_{12}\sqrt{p_2}V_{12}, \qquad C_{12} = U_{11}\sqrt{p_1}V_{21} + U_{12}\sqrt{p_2}V_{22},$$

$$C_{21} = U_{21}\sqrt{p_1}V_{11} + U_{22}\sqrt{p_2}V_{12} \qquad C_{22} = U_{21}\sqrt{p_1}V_{21} + U_{22}\sqrt{p_2}V_{22}.$$

Using the matrix form, we get

$$\hat{C} = \begin{pmatrix} U_{11} & U_{12} \\ U_{21} & U_{22} \end{pmatrix} \begin{pmatrix} \sqrt{p_1} & 0 \\ 0 & \sqrt{p_2} \end{pmatrix} \begin{pmatrix} V_{11} & V_{21} \\ V_{12} & V_{22} \end{pmatrix}$$
$$= \begin{pmatrix} U_{11} & U_{12} \\ U_{21} & U_{22} \end{pmatrix} \begin{pmatrix} \sqrt{p_1} & 0 \\ 0 & \sqrt{p_2} \end{pmatrix} \begin{pmatrix} V_{11} & V_{12} \\ V_{21} & V_{22} \end{pmatrix}^T$$
$$= \hat{U}\hat{d}\hat{V}^T$$

where $\hat{d}$ is a non-negative diagonal matrix, and $\hat{V}^T$ is the transpose matrix of $\hat{V}$.

$$\hat{d} = \begin{pmatrix} p_1 & 0 \\ 0 & p_2 \end{pmatrix}.$$

Thus we have

$$\hat{C}\hat{C}^+ = (\hat{U}\hat{d}\hat{V}^T)(\hat{U}\hat{d}\hat{V}^T)^+$$
$$= (\hat{U}\hat{d}\hat{V}^T)(\hat{V}^{+T}\hat{d}^+\hat{U}^+)$$
$$= (\hat{U}^+\hat{U}^+)$$
$$= \hat{d}\hat{d}^+$$

In order to determine the values of p_1 and p_2, we need to solve the eigenvalue problem of $\hat{C}\hat{C}^+$, if $\hat{C}\hat{C}^+$ is not a diagonal matrix.

Thus we can calculate the Schmidt numbers

((**Example-1**)) Pure state

$$|\psi\rangle = \frac{1}{\sqrt{2}}[|00\rangle + |01\rangle].$$

We construct $\hat{C}$ and $\hat{C}^+\hat{C}$.

$$\hat{C} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 0 & 0 \end{pmatrix}, \qquad \hat{C}^+\hat{C} = \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}.$$

The eigenvlaue problem of $\hat{C}^+\hat{C}$;

eigenvalue; $p_1 = 1$, eigenket: $\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}$,

eigenvalue; $p_2 = 0$, eigenket: $\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}$.

So there is only one nonzero Schmidt coefficient and thus $|\psi\rangle$ is a product state.

((**Example-2**)) Entangled state

$$|\psi\rangle = \frac{1}{\sqrt{2}}[|00\rangle + |11\rangle].$$

We construct $\hat{C}$ and $\hat{C}^{+}\hat{C}$.

$$\hat{C} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \qquad \hat{C}^{+}\hat{C} = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}.$$

The eigenvlaue problem of $\hat{C}^{+}\hat{C}$;

eigenvalue; $p_1 = \frac{1}{2}$, eigenket: $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$,

eigenvalue; $p_2 = \frac{1}{2}$, eigenket: $\begin{pmatrix} 0 \\ 1 \end{pmatrix}$.

So there are two nonzero Schmidt coefficients and thus $|\psi\rangle$ is an entangled state.

((**Example-3**)) Entangled state

$$|\psi\rangle = \frac{1}{\sqrt{2}}[|01\rangle + |10\rangle].$$

We construct $\hat{C}$ and $\hat{C}^{+}\hat{C}$.

$$\hat{C} = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \hat{C}^{+}\hat{C} = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}.$$

The eigenvlaue problem of $\hat{C}^{+}\hat{C}$;

eigenvalue; $p_1 = \frac{1}{2}$, eigenket: $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$.

eigenvalue; $p_2 = \frac{1}{2}$, eigenket: $\begin{pmatrix} 0 \\ 1 \end{pmatrix}$.

So there are two nonzero Schmidt coefficients and thus $|\psi\rangle$ is an entangled state

((**Example-4**))

$$|\psi\rangle = \frac{1}{\sqrt{3}}[|00\rangle + |01\rangle + |11\rangle].$$

We construct $\hat{C}$ and $\hat{C}^{+}\hat{C}$.

$$\hat{C} = \frac{1}{\sqrt{3}}\begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix}, \qquad \hat{C}^{+}\hat{C} = \frac{1}{3}\begin{pmatrix} 1 & 1 \\ 1 & 2 \end{pmatrix}.$$

The eigenvlaue problem of $\hat{C}^{+}\hat{C}$;

eigenvalue; $p_1 = 0.873$, eigenket: $\begin{pmatrix} 0.53 \\ 0.85 \end{pmatrix}$,

eigenvalue; $p_2 = 0.127$, eigenket: $\begin{pmatrix} 0.85 \\ -0.53 \end{pmatrix}$.

So there are two nonzero Schmidt coefficients and thus $|\psi\rangle$ is an entangled state.

((**Example-5**))

$$|\psi\rangle = \frac{1}{2}[|00\rangle - |01\rangle - |10\rangle + |11\rangle] = 1[\frac{1}{\sqrt{2}}|0\rangle - \frac{1}{\sqrt{2}}|1\rangle][\frac{1}{\sqrt{2}}|0\rangle - \frac{1}{\sqrt{2}}|1\rangle].$$

We construct $\hat{C}$ and $\hat{C}^{+}\hat{C}$.

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

The eigenvlaue problem of $\hat{C}^{+}\hat{C}$;

eigenvalue; $p_1 = 1$, eigenket: $\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}$.

eigenvalue; $p_2 = 0$, eigenket: $\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}$.

So there are one nonzero Schmidt coefficients and thus $|\psi\rangle$ is a product state.

((**Example-6**))

$$|\psi\rangle = \frac{1}{2\sqrt{6}}[(1+\sqrt{6})|00\rangle + (1-\sqrt{6})|01\rangle + (\sqrt{2}-\sqrt{3})|10\rangle + (\sqrt{2}+\sqrt{3})|11\rangle].$$

We construct $\hat{C}$ and $\hat{C}^{+}\hat{C}$.

$$\hat{C} = \frac{1}{2\sqrt{6}}\begin{pmatrix} 1+\sqrt{6} & 1-\sqrt{6} \\ \sqrt{2}-\sqrt{3} & \sqrt{2}+\sqrt{3} \end{pmatrix}, \qquad \hat{C}^{+}\hat{C} = \frac{1}{4}\begin{pmatrix} 2 & -1 \\ -1 & 2 \end{pmatrix}.$$

The eigenvlaue problem of $\hat{C}^{+}\hat{C}$;

eigenvalue; $p_1 = \frac{1}{4}$, eigenket: $\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}$.

eigenvalue; $p_2 = \frac{3}{4}$, eigenket: $\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}$.

So there are one nonzero Schmidt coefficients and thus $|\psi\rangle$ is an entangled state.

34. Schmidt decomposition application

It is very easy to compute the reduced density operator given the Schmidt decomposition

$$|\psi\rangle = \sum_i \sqrt{p_i}\,|i_A\rangle|i_B\rangle .$$

The density operator is

$$\hat{\rho} = \sum_{i,j} \sqrt{p_i p_j}\,|i_A\rangle|i_B\rangle\langle j_A|\langle j_B| .$$

The reduced density operator is given by

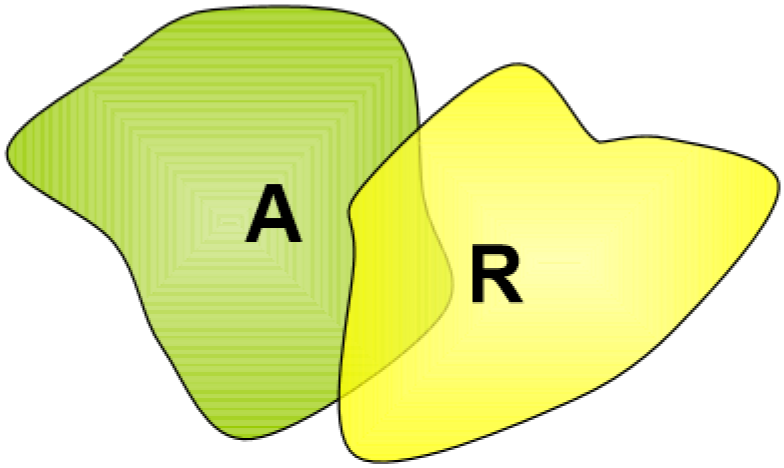
$$\begin{aligned} Tr_B(\hat{\rho}) &= \sum_{i,j,k} \sqrt{p_i p_j}\,\langle k_B|i_B\rangle\langle j_B|k_B\rangle|i_A\rangle\langle j_A| \\ &= \sum_i p_i |i_A\rangle\langle i_A| \end{aligned}$$

$$\begin{aligned} Tr_A(\hat{\rho}) &= \sum_{i,j,k} \sqrt{p_i p_j}\,\langle k_A|i_A\rangle\langle j_A|k_A\rangle|i_B\rangle\langle j_B| \\ &= \sum_i p_i |i_B\rangle\langle i_B| \end{aligned}$$

We note that the spectrum (i.e., set of eigenvalues) of both reduced density operators are the same.

35. Purification

Suppose we are given a state $\hat{\rho}_A$ of a quantum system *A*. It is possible to introduce an additional system, which we denote *R* (*R* has the same dimension as *A*) and define a pure state $|AR\rangle$ for the joint system *AR*



such that

$$\hat{\rho}_A = Tr_R |AR\rangle\langle AR|.$$

That is, the pure state $|AR\rangle$ reduces to $\hat{\rho}_A$ when we look at system *A* alone. This is a purely mathematical procedure, known as *purification*, which allows us to associate pure states with mixed states. For this reason we call system *R* a reference system: it is a fictitious system, without a direct physical significance.

((**Proof**))

To prove that purification can be done for *any* state, we explain how to construct a system *R* and purification $|AR\rangle$ for $\hat{\rho}_A$. Suppose $\hat{\rho}_A$ has orthonormal decomposition

$$\hat{\rho}_A = \sum_i p_i |i_A\rangle\langle i_A|. \qquad \text{(mixed state)}$$

To purify $\hat{\rho}_A$, we introduce an additional system *R* which has the same dimension as system *A*, with orthonormal basis states $|i_R\rangle$, and define a pure state for the combined system

$$|AR\rangle = \sum_i \sqrt{p_i}|i_A\rangle|i_R\rangle. \qquad \text{(pure state)}$$

We now calculate the reduced density operator for the system *A* corresponding to the state $|AR\rangle$

$$\begin{aligned}
Tr_R(|AR\rangle\langle AR|) &= \sum_{i,j}\sqrt{p_i}\sqrt{p_j}\,Tr(|i_A\rangle|i_R\rangle\langle j_A|\langle j_R|) \\
&= \sum_{i,j}\sqrt{p_i}\sqrt{p_j}\,|i_A\rangle\langle j_A|Tr(|i_R\rangle\langle j_R|) \\
&= \sum_{i,j}\sqrt{p_i}\sqrt{p_j}\,|i_A\rangle\langle j_A|\delta_{ij} \\
&= \sum_{i,j} p_i|i_A\rangle\langle i_A| \\
&= \hat{\rho}_A
\end{aligned}$$

Thus $|AR\rangle$ is a purification of $\hat{\rho}_A$.

Notice the close relationship of the Schmidt decomposition to purification: the procedure used to purify a mixed state of system *A* is to define a pure state whose Schmidt basis for system *A* is just the basis in which the mixed state is diagonal, with the Schmidt coefficients being the square root of the eigenvalues of the density operator being purified.

RFEFERENCES

L.D. Landau and E.M. Lifshitz, *Quantum Mechanics* (Pergamon Press, Oxford, 1977).

D. Ter Haar, *Fluctuation, Relaxation, and Resonance in Magnetic Systems, Scottisch Universities' Summer School* (Oliver and Boyd, Edinburgh and London, 1961).

L.I. Schiff, *Quantum Mechanics*, third edition (McGraw-Hill Book Company, New York, 1968).

J.J. Sakurai and J. Napolitano, *Modern Quantum Mechanics*, second edition (Addison-Wesley, New York, 2011). ISBN 978-0-8053-8291-4

J S. Townsend , *A Modern Approach to Quantum Mechanics*, second edition (University Science Books, 2012).

K. Blum, *Density matrix theory and applications, second edition* (Prenum Press, NY, 1996).

G. Aueletta, M. Fortunato, and G. Parisi, *Quantum Mechanics* (Cambridhe, 2009).

M.A Nielsen and I.L. Chuang, *Quantum computation and quantum information, 10th Anniversary Edition* (Cambridge, 2010).

APPENDIX

Density operator (problem)

A spin=1/2 particle is in the pure state,

$$|\psi\rangle = a|+z\rangle + b|-z\rangle .$$

(a) Construct the density matrix in the S_z basis for this state.

(b) Starting with your result in (a), determine the density matrix in the S_x basis, where

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

(c) Use your result for the density matrix in (b) to determine the probability that a measurement of S_x yields $-\hbar/2$ for the state.

(d) Starting with your result in (a), determine the density matrix in the S_y basis, where

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

(e) Use your result for the density matrix in (b) to determine the probability that a measurement of S_y yields $+\hbar/2$ for the state for the state.

((**Solution)**)

(a) The density matrix in the S_z basis:

$$\hat{\rho} = \begin{pmatrix} a \\ b \end{pmatrix}\begin{pmatrix} a^* & b^* \end{pmatrix} = \begin{pmatrix} aa^* & ab^* \\ a^*b & bb^* \end{pmatrix} = \begin{pmatrix} |a|^2 & ab^* \\ a^*b & |b|^2 \end{pmatrix}.$$

(b)

$$\begin{aligned}
\left\langle +x\right|\hat{\rho}\left|+x\right\rangle &= \sum_{b',b''} \left\langle +x | b'\right\rangle \left\langle b'\right|\hat{\rho}\left|b''\right\rangle \left\langle b'' | +x\right\rangle \\
&= \sum_{b',b''} \left\langle +z\right|\hat{U}_x^{+}\left|b'\right\rangle \left\langle b'\right|\hat{\rho}\left|b''\right\rangle \left\langle b''\right|\hat{U}_x\left|+z\right\rangle \\
&= \left\langle +z\right|\hat{U}_x^{+}\hat{\rho}\hat{U}_x\left|+z\right\rangle
\end{aligned}$$

Then the matrix density $\hat{\rho}_x$ under the basis of $\{\left|+x\right\rangle, \left|-x\right\rangle\}$ is obtained as

$$\hat{\rho}_x = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}\begin{pmatrix} |a|^2 & ab^* \\ a^*b & |b|^2 \end{pmatrix}\frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$
$$= \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}\begin{pmatrix} |a|^2 + ab^* & |a|^2 - ab^* \\ a^*b + |b|^2 & a^*b - |b|^2 \end{pmatrix}$$
$$= \frac{1}{2}\begin{pmatrix} |a|^2 + ab^* + a^*b + |b|^2 & |a|^2 - ab^* + a^*b - |b|^2 \\ |a|^2 + ab^* - a^*b - |b|^2 & |a|^2 - ab^* - a^*b + |b|^2 \end{pmatrix}$$

where $|b'\rangle = |\pm z\rangle$, $|b''\rangle = |\pm z\rangle$, $|a'\rangle = |\pm x\rangle$, $|a''\rangle = |\pm x\rangle$,

$$|+x\rangle = \hat{U}_x|+z\rangle, \qquad |-x\rangle = \hat{U}_x|-z\rangle,$$

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

(c)

$$Tr[(|-x\rangle\langle -x|)\hat{\rho}_x] = Tr[\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}\frac{1}{2}\begin{pmatrix} |a|^2 + ab^* + a^*b + |b|^2 & |a|^2 - ab^* + a^*b - |b|^2 \\ |a|^2 + ab^* - a^*b - |b|^2 & |a|^2 - ab^* - a^*b + |b|^2 \end{pmatrix}]$$
$$= \frac{1}{2}Tr[\begin{pmatrix} 0 & 0 \\ |a|^2 + ab^* - a^*b - |b|^2 & |a|^2 - ab^* - a^*b + |b|^2 \end{pmatrix}$$
$$= \frac{1}{2}[|a|^2 - ab^* - a^*b + |b|^2]$$
$$= \frac{1}{2}(a-b)(a^* - b^*)$$
$$= \frac{1}{2}|a-b|^2$$

((**Note**))
Since $\hat{\rho}$ is the density operator for the pure state, the probability that a measurement of S_x yields $-\hbar/2$ for the state for the state can be also calculated as

$$P(-x) = |\langle -x|\psi\rangle|^2 = \frac{1}{2}\left|\begin{pmatrix} 1 & -1 \end{pmatrix}\begin{pmatrix} a \\ b \end{pmatrix}\right|^2 = \frac{1}{2}|a-b|^2.$$

without using the density operator.

This method is not useful when $\hat{\rho}$ is the density operator for the mixed state.

(d)

$$\begin{aligned}
\langle +y|\hat{\rho}|+y\rangle &= \sum_{b',b''}\langle +y|b'\rangle\langle b'|\hat{\rho}|b''\rangle\langle b''|+y\rangle \\
&= \sum_{b',b''}\langle +z|\hat{U}_y{}^{+}|b'\rangle\langle b'|\hat{\rho}|b''\rangle\langle b''|\hat{U}_y|+z\rangle \\
&= \langle +z|\hat{U}_y{}^{+}\hat{\rho}\hat{U}_y|+z\rangle
\end{aligned}$$

Then the matrix density $\hat{\rho}_y$ under the basis of $\{|+y\rangle, |-y\rangle\}$ is obtained as

$$\begin{aligned}
\hat{\rho}_y &= \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & -i \\ 1 & i \end{pmatrix}\begin{pmatrix} |a|^2 & ab^* \\ a^*b & |b|^2 \end{pmatrix}\frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ i & -i \end{pmatrix} \\
&= \frac{1}{2}\begin{pmatrix} 1 & -i \\ 1 & i \end{pmatrix}\begin{pmatrix} |a|^2 + iab^* & |a|^2 - iab^* \\ a^*b + i|b|^2 & a^*b - i|b|^2 \end{pmatrix} \\
&= \frac{1}{2}\begin{pmatrix} |a|^2 + iab^* - ia^*b + |b|^2 & |a|^2 - iab^* - ia^*b - |b|^2 \\ |a|^2 + iab^* + ia^*b - |b|^2 & |a|^2 - iab^* + ia^*b + |b|^2 \end{pmatrix}
\end{aligned}$$

where $|b'\rangle = |\pm z\rangle$, $|b''\rangle = |\pm z\rangle$, $\quad |a'\rangle = |\pm y\rangle$, $|a''\rangle = |\pm y\rangle$,

$$|+y\rangle = \hat{U}_y|+z\rangle, \qquad |-y\rangle = \hat{U}_y|-z\rangle,$$

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

(e)

$$
\begin{aligned}
Tr[|+y\rangle\langle+y|\hat{\rho}_y] &= Tr[\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \frac{1}{2} \begin{pmatrix} |a|^2 + iab^* - ia^*b + |b|^2 & |a|^2 - iab^* - ia^*b - |b|^2 \\ |a|^2 + iab^* + ia^*b - |b|^2 & |a|^2 - iab^* + ia^*b + |b|^2 \end{pmatrix}] \\
&= \frac{1}{2} Tr[\begin{pmatrix} |a|^2 + iab^* - ia^*b + |b|^2 & |a|^2 - iab^* - ia^*b - |b|^2 \\ 0 & 0 \end{pmatrix} \\
&= \frac{1}{2}[|a|^2 + iab^* - ia^*b + |b|^2] \\
&= \frac{1}{2}(a - ib)(a^* + ib^*) \\
&= \frac{1}{2}|a - ib|^2
\end{aligned}
$$

((**Note**))

Since $\hat{\rho}$ is the density operator for the pure state, the probability that a measurement of S_y yields $+\hbar/2$ for the state for the state can be also calculated as

$$
P(+y) = |\langle +y|\psi\rangle|^2 = \frac{1}{2}\left| \begin{pmatrix} 1 & -i \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} \right|^2 = \frac{1}{2}|a - ib|^2 ,
$$

without using the density operator.