Density operator

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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 possess 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

We need to consider systems for which we do not possess the maximum knowledge allowed by quantum mechanics. In other words, we do not know the state vector of the system, but rather the classical probabilities for having various possible state vectors. Such situations are described by the density operator $\hat{\rho}$ which is a sum of projection operator $|u_k\rangle\langle u_k|$, each weighted by a classical probability w_i. (P. Meystre and M. Sargent III, Elements of Quantum Optics, 3rd edition (Springer 1998).

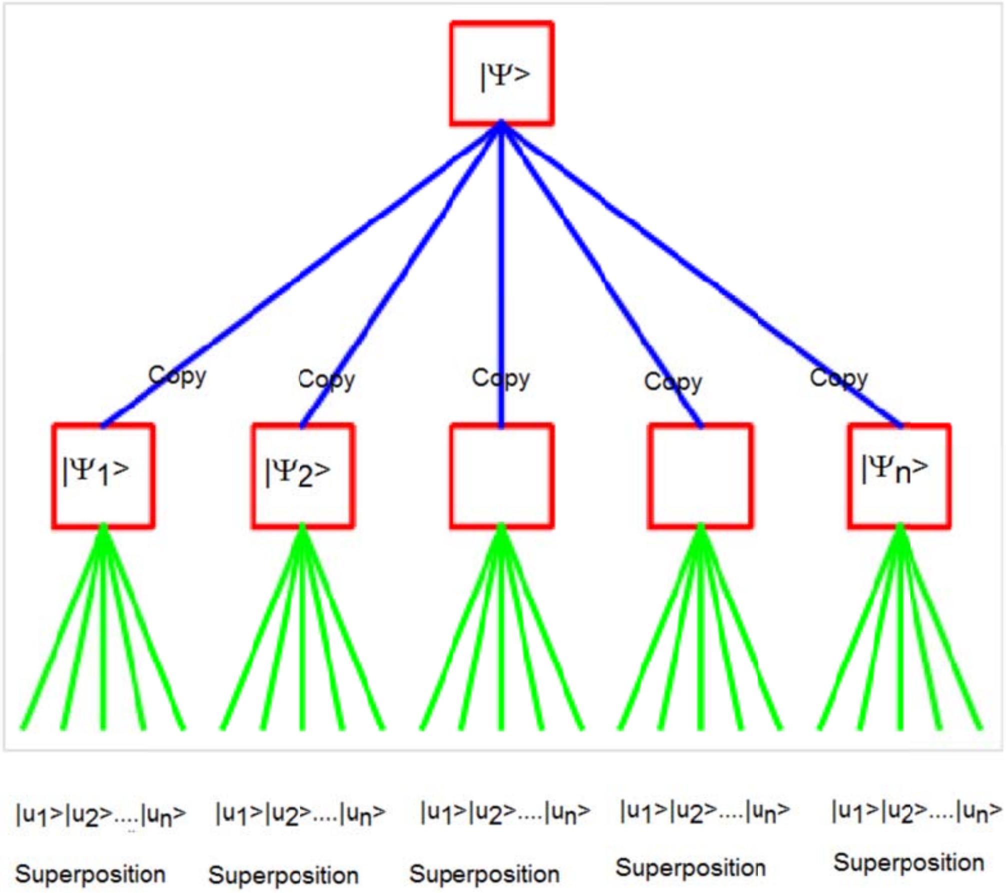


Fig. Ensemble average. Definition of the density operator

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)

((**Proof**))

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

leading to the relation $\hat{\rho}^+ = \hat{\rho}$.

(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**))

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

(d) Diagonalization of the density matrix

Suppose that the density operator is given by

$$\hat{\rho} = \sum_{i,j} \rho_{ij} \left| b_i \right\rangle \left\langle b_j \right| = \begin{pmatrix} \rho_{11} & \rho_{12} & \cdot & \cdot & \rho_{1n} \\ \rho_{21} & \rho_{22} & \cdot & \cdot & \rho_{2n} \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \rho_{n1} & \rho_{n2} & \cdot & \cdot & \rho_{nn} \end{pmatrix}$$

or

$$\begin{aligned} \hat{\rho} &= \sum_j \hat{\rho} \left| b_j \right\rangle \left\langle b_j \right| \\ &= \sum_{i,j} \left| b_i \right\rangle \left\langle b_i \right| \hat{\rho} \left| b_j \right\rangle \left\langle b_j \right| \\ &= \sum_{i,j} \left| b_i \right\rangle \left\langle b_i \right| \hat{\rho} \left| b_j \right\rangle \left\langle b_j \right| \\ &= \sum_{i,j} \rho_{ij} \left| b_i \right\rangle \left\langle b_j \right| \end{aligned}$$

We solve the eigenvalue problem for the density matrix ρ under the basis $\{\left| b_i \right\rangle\}$,

$$\hat{\rho} \left| a_i \right\rangle = w_i \left| a_i \right\rangle$$

$\left| a_i \right\rangle$ is the eigenket of $\hat{\rho}$ with the eigenvalue w_i. Using the basis $\{\left| a_i \right\rangle\}$, the density operator can be expressed by

$$\hat{\rho} = \sum_i \hat{\rho} \left| a_i \right\rangle \left\langle a_i \right| = \sum_i w_i \left| a_i \right\rangle \left\langle a_i \right| = \begin{pmatrix} w_1 & 0 & \cdot & \cdot & 0 \\ 0 & w_2 & \cdot & \cdot & 0 \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & \cdot & \cdot & w_n \end{pmatrix}$$

We note that

$$\left| a_i \right\rangle = \hat{U} \left| b_i \right\rangle \qquad \left\langle a_i \right| = \left\langle b_i \right| \hat{U}^+$$

where $\hat{U}$ is the unitary operator. The unitary operator can be determined by solving the eigenvalue problem. We start with

$$\hat{\rho}|a_k\rangle = w_k|a_k\rangle .$$

$$\sum_j \langle b_i|\hat{\rho}|b_j\rangle\langle b_j|a_k\rangle = w_k\langle b_1|a_k\rangle$$

where

$$\langle b_j|a_k\rangle = \langle b_j|\hat{U}|b_k\rangle = U_{jk}$$

The eigenvalue problem is

$$\begin{pmatrix} \rho_{11} & \rho_{12} & \cdot & \cdot & \rho_{1n} \\ \rho_{21} & \rho_{22} & \cdot & \cdot & \rho_{2n} \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \rho_{n1} & \rho_{n2} & \cdot & \cdot & \rho_{nn} \end{pmatrix} \begin{pmatrix} U_{1k} \\ U_{2k} \\ \cdot \\ \cdot \\ U_{nk} \end{pmatrix} = w_k \begin{pmatrix} U_{1k} \\ U_{2k} \\ \cdot \\ \cdot \\ U_{nk} \end{pmatrix}$$

where

$$\hat{U} = \begin{pmatrix} U_{11} & U_{12} & \cdot & \cdot & U_{1n} \\ U_{21} & U_{22} & \cdot & \cdot & U_{2n} \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ U_{n1} & U_{n2} & \cdot & \cdot & U_{nn} \end{pmatrix}$$

(e) Equation of motion for the density operator

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.

$$\frac{d}{dt}\hat{\rho} = \overline{\frac{d}{dt}|\psi\rangle\langle\psi|}$$

$$= \overline{\left(\frac{\partial}{\partial t}|\psi\rangle\right)\langle\psi| + |\psi\rangle\left(\frac{\partial}{\partial t}\langle\psi|\right)}$$

$$= \frac{1}{i\hbar}\overline{\hat{H}|\psi\rangle\langle\psi| - |\psi\rangle\langle\psi|\hat{H}}$$

$$= \frac{1}{i\hbar}\hat{H}\overline{|\psi\rangle\langle\psi|} - \overline{|\psi\rangle\langle\psi|}\hat{H}$$

$$= \frac{1}{i\hbar}\hat{H}\hat{\rho} - \hat{\rho}\hat{H} = -\frac{1}{i\hbar}[\hat{\rho},\hat{H}]$$

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

$$i\hbar\frac{d}{dt}\hat{A}_H = [\hat{A}_H,\hat{H}].$$ (Heisenberg's equation of motion)

3. Definition of the pure state

We consider the density operator for the pure state

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

We note that

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

since $\langle\psi|\psi\rangle = 1$. Then we have

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

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

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

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

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

4. Definition of the mixed state

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

$$\hat{\rho}|u_n\rangle = w_n|u_n\rangle$$

where $|u_n\rangle$ is the eigenket of $\hat{\rho}$ with the eigenvalue w_n. Then the density operator is expressed by

$$\hat{\rho} = \hat{\rho}\sum_n |u_n\rangle\langle u_n| = \sum_n \hat{\rho}|u_n\rangle\langle u_n| = \sum_n w_n|u_n\rangle\langle u_n|$$

where

$$w_n = \langle u_n|\hat{\rho}|u_n\rangle, \qquad \text{or} \qquad \begin{pmatrix} w_1 & 0 & 0 & 0 & 0 & 0 \\ 0 & w_2 & 0 & 0 & 0 & 0 \\ 0 & 0 & w_3 & 0 & 0 & 0 \\ 0 & 0 & 0 & . & 0 & 0 \\ 0 & 0 & 0 & 0 & . & 0 \\ 0 & 0 & 0 & 0 & & w_n \end{pmatrix}$$

We note that

$$\begin{aligned} Tr[\hat{\rho}] &= \sum_k \langle u_k|\hat{\rho}|u_k\rangle \\ &= \sum_k w_k\langle u_k|u_k\rangle \\ &= \sum_k w_k = 1 \end{aligned}$$

$$Tr[\hat{\rho}^2] = \sum_k w_k{}^2 \le \sum_k w_k = 1$$

or

$$Tr[\hat{\rho}^2] < Tr[\hat{\rho}] = 1 \qquad \text{(the condition of the mixed state)}$$

since

$$w_k{}^2 \le w_k .$$

with

$$w_k \le 1$$

5. Expectation value and probability

The expectation value is given by

$$\langle O \rangle = \sum_k w_k \langle u_k | \hat{O} | u_k \rangle = Tr[\hat{O}\hat{\rho}]$$

since

$$\begin{aligned} Tr[\hat{O}\hat{\rho}] &= \sum_k \langle u_k | \hat{O}\hat{\rho} | u_k \rangle \\ &= \sum_{k,l} \langle u_k | \hat{O} | u_l \rangle \langle u_l | \hat{\rho} | u_k \rangle \\ &= \sum_{k,l} w_k \langle u_k | \hat{O} | u_l \rangle \langle u_l | u_k \rangle \\ &= \sum_{k,l} w_k \langle u_k | \hat{O} | u_l \rangle \delta_{k,l} \\ &= \sum_k w_k \langle u_k | \hat{O} | u_k \rangle \end{aligned}$$

For the projection operator, we have

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

and

$$Tr[\hat{P}_{u_m}\hat{\rho}] = Tr[|u_m\rangle\langle u_m|\hat{\rho}] = w_m$$

which is the probability, since

$$Tr[\hat{P}_{u_m}\hat{\rho}] = \sum_n w_n \langle u_n|\hat{P}_{u_m}|u_n\rangle = \sum_n w_n \delta_{n,m} = w_m$$

((**Note**)) The notation used by Sakurai and Napolitano

Here we use the average of the operator $\langle O\rangle$. In their book, Sakurai and Napolitano used the notation $[O]$.

6. Change of the basis for the density operator

We now consider the change of basis for the density operator. Suppose that the density operator is described by the basis {$|b_i\rangle$ } with given matrix element $\langle b_j|\hat{\rho}|b_k\rangle$. Suppose that the basis is changed from {$|b_i\rangle$ } to {$|a_i\rangle$ }.by

$$|a_i\rangle = \hat{U}|b_i\rangle, \quad \langle a_i| = \langle b_i|\hat{U}^+$$

where $|a_i\rangle$ is not always the eigenket of $\hat{\rho}$. Then we have

$$\begin{aligned}\langle a_i|\hat{\rho}|a_j\rangle &= \sum_{j,k}\langle a_i|b_j\rangle\langle b_j|\hat{\rho}|b_k\rangle\langle b_k|a_j\rangle \\ &= \sum_{j,k}\langle b_i|\hat{U}^+|b_j\rangle\langle b_j|\hat{\rho}|b_k\rangle\langle b_k|\hat{U}|b_j\rangle \\ &= \langle b_i|\hat{U}^+\hat{\rho}\hat{U}|b_j\rangle\end{aligned}$$

In other words, the matrix of $\hat{\rho}$ under the basis {$|a_i\rangle$ is the same of the element $\hat{U}^+\hat{\rho}\hat{U}$ $\hat{\rho}$ under the basis {$|b_i\rangle$. Then we get

$$\hat{\rho} = \sum_{i,j}|a_i\rangle\langle a_i|\hat{\rho}|a_j\rangle\langle a_j| = \sum_{i,j}|a_i\rangle\langle b_i|\hat{U}^+\hat{\rho}\hat{U}|b_j\rangle\langle a_j|.$$

7. Density operator for the un-polarized spin state

The density operator for the un-polarized spin state

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

What is the expression of $\hat{\rho}$ under the basis of $\{|+\boldsymbol{n}\rangle, |-\boldsymbol{n}\rangle\}$ with

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

where $\boldsymbol{n}$ is the unit vector in the 3D real space; $\boldsymbol{n} = (\sin\theta\cos\phi, \sin\theta\cos\phi, \cos\theta)$.

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

We note that

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

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

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

since

$$\hat{\rho} = \sum_{i,j}|a_i\rangle\langle a_i|\hat{\rho}|a_j\rangle\langle a_j|, \qquad \text{and} \qquad \langle a_i|\hat{\rho}|a_j\rangle = \langle b_i|\hat{U}^{+}\hat{\rho}\hat{U}|b_j\rangle.$$

((**Note**)) This result is obvious since

$$|+z\rangle\langle+z| + |-z\rangle\langle-z| = \hat{1}, \qquad |+\boldsymbol{n}\rangle\langle+\boldsymbol{n}| + |-\boldsymbol{n}\rangle\langle-\boldsymbol{n}| = \hat{1}.$$

8. Density operator for the un-polarized light

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

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

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

$$
\begin{aligned}
\hat{\rho} &= |x'\rangle\langle x'| \\
&= \begin{pmatrix} \cos\theta \\ \sin\theta \end{pmatrix} \begin{pmatrix} \cos\theta & \sin\theta \end{pmatrix} \\
&= \begin{pmatrix} \cos^2\theta & \sin\theta\cos\theta \\ \sin\theta\cos\theta & \sin^2\theta \end{pmatrix} \\
&= \frac{1}{2}\begin{pmatrix} 1+\cos(2\theta) & \sin(2\theta) \\ \sin(2\theta) & 1-\cos(2\theta) \end{pmatrix}
\end{aligned}
.
$$

where

$$
|x'\rangle = \cos\theta|x\rangle + \sin\theta|y\rangle = \begin{pmatrix} \cos\theta \\ \sin\theta \end{pmatrix}, \quad \langle x'| = \begin{pmatrix} \cos\theta & \sin\theta \end{pmatrix}
$$

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

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

satisfying the condition for the pure state.

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

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

where

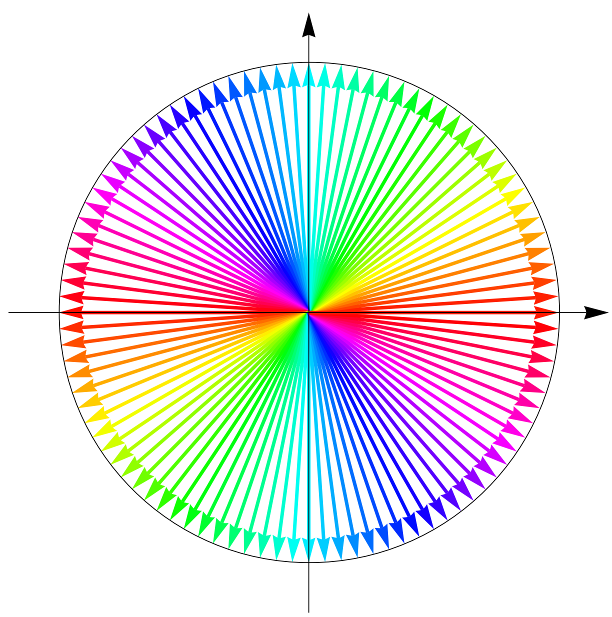
$$
\langle x|x'\rangle = \cos\theta\langle x|x\rangle + \sin\theta\langle x|y\rangle = \cos\theta,
$$

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

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. Note that we use the region of θ as $0 \le \theta \le 2\pi$ for the photon polarization.



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

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

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

((**Note**)) **Density operator for the un-polarized light using the $|R\rangle$ and $|L\rangle$.**

We consider the states $|R\rangle$ for the right-hand circularly polarized state and $|L\rangle$ for the left-hand circularly polarized state.

$$|R\rangle = \hat{U}|x\rangle, \qquad |L\rangle = \hat{U}|y\rangle$$

where

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

and

$$\hat{U}^{+}\hat{U} = \hat{1}.$$

We can show that

$$\hat{\rho}_{un} = \frac{1}{2}(|x\rangle\langle x| + |y\rangle\langle y|) = \frac{1}{2}|R\rangle\langle R| + \frac{1}{2}|L\rangle\langle L|$$

since

$$\langle R|\hat{\rho}_{un}|R\rangle = \langle x|\hat{U}^{+}\hat{\rho}_{un}\hat{U}|x\rangle$$

and

$$\hat{U}^{+}\hat{\rho}_{un}\hat{U} = \frac{1}{4}\begin{pmatrix} 1 & -i \\ 1 & i \end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}\begin{pmatrix} 1 & 1 \\ i & -i \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

under the basis $\{|x\rangle, |y\rangle\}$.

We also note that

$$Tr[\hat{\rho}_{un}(|x\rangle\langle x|)] = \frac{1}{2},$$

for the probability of the system in the $|x\rangle$ state after the X filter, and

$$Tr[\hat{\rho}_{un}(|y\rangle\langle y|)] = \frac{1}{2}$$

for the probability of the system in the $|y\rangle$ state after the Y filter.

9. Spin 1/2 system: 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 $0 \le \theta \le \pi$ and $0 \le \phi \le 2\pi$,

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

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

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

or

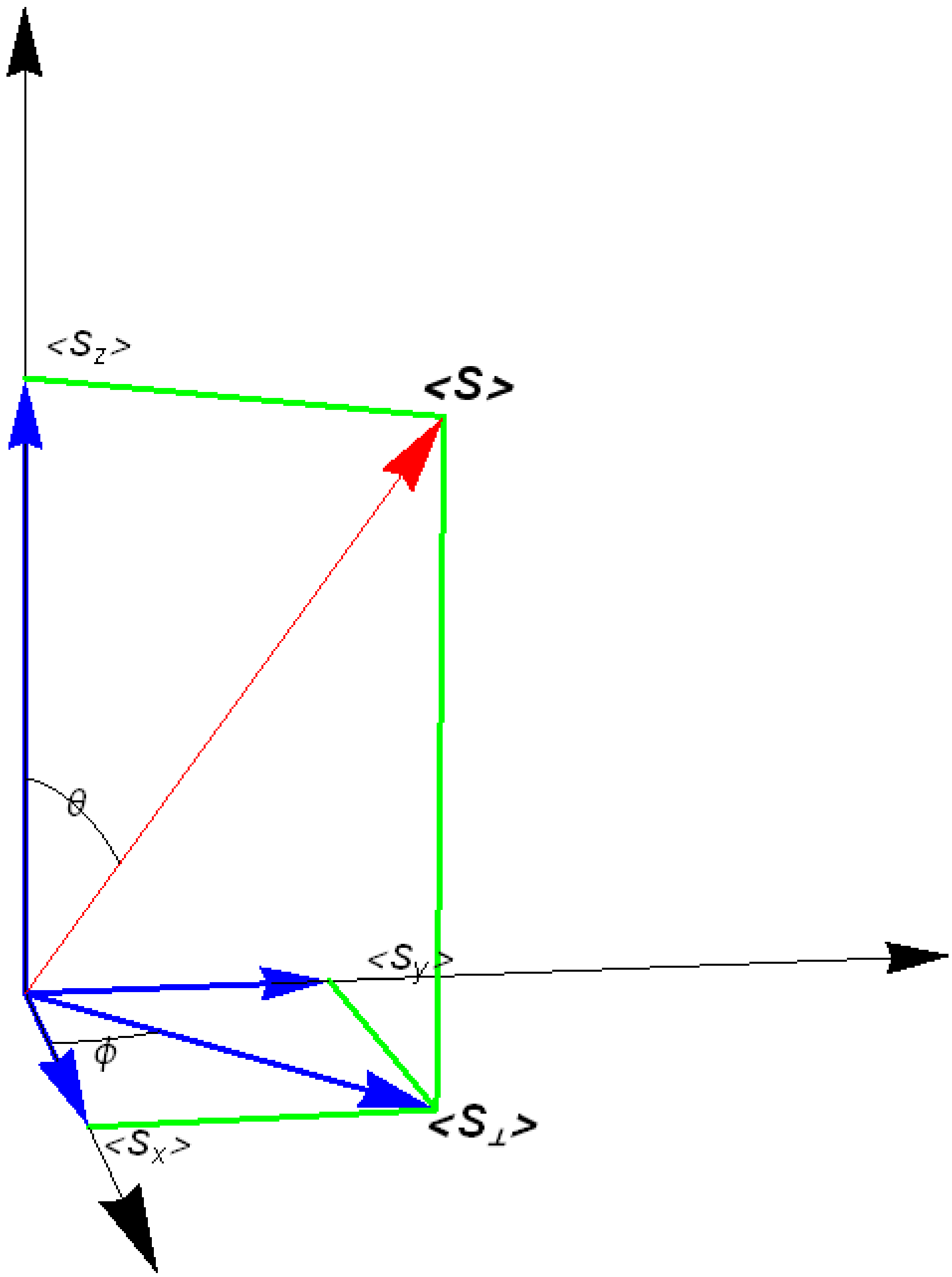
$$\langle \boldsymbol{S}\rangle = \langle\psi|\hat{\boldsymbol{S}}|\psi\rangle = \frac{\hbar}{2}\boldsymbol{n}$$

and

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

where

$\left|\langle \boldsymbol{S}_{\perp} \rangle\right|$ is the projection of $\langle \boldsymbol{S} \rangle$ onto the *x*-*y* plane. The density operator (matrix) $\hat{\rho}(\theta,\phi)$, corresponding to the state $|+\boldsymbol{n}\rangle$.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$$
\begin{aligned}
\hat{\rho}(\theta,\phi) &= |+\boldsymbol{n}\rangle\langle+\boldsymbol{n}| \\
&= \begin{pmatrix} e^{-i\frac{\phi}{2}}\cos\frac{\theta}{2} \\ e^{i\frac{\phi}{2}}\sin\frac{\theta}{2} \end{pmatrix} \begin{pmatrix} e^{i\frac{\phi}{2}}\cos\frac{\theta}{2} & e^{-i\frac{\phi}{2}}\sin\frac{\theta}{2} \end{pmatrix} \\
&= \begin{pmatrix} \cos^2\frac{\theta}{2} & e^{-i\phi}\sin\frac{\theta}{2}\cos\frac{\theta}{2} \\ e^{i\phi}\sin\frac{\theta}{2}\cos\frac{\theta}{2} & \sin^2\frac{\theta}{2} \end{pmatrix} \\
&= \begin{pmatrix} \rho_{++} & \rho_{+-} \\ \rho_{-+} & \rho_{--} \end{pmatrix}
\end{aligned}
$$

The matrix is generally non-diagonal. The matrix elements are obtained as

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

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

(a) Populations (diagonal): ρ_{++} and ρ_{--}

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

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

and

$$\rho_{++} + \rho_{--} = \cos^2\frac{\theta}{2} + \sin^2\frac{\theta}{2} = 1 \qquad (Tr(\hat{\rho}) = 1$$

The populations ($\rho_{++} - \rho_{--}$) are therefore related to the longitudinal polarization.

(b) Coherence (non-diagonal)

The "coherence" ρ_{+-}, ρ_{-+} is

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

where

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

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

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

is a relation characteristic of a pure state.

10. A statistical mixture; un-polarized spin state

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 $\left|+\boldsymbol{n}\right\rangle$ with equal weights.

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

since

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

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

$$= \frac{1}{4\pi} 2\pi \frac{1}{2}\int_0^{\pi} \sin\theta (1-\cos\theta) d\theta$$

$$= \frac{1}{4}\int_0^{\pi} (\sin\theta - \frac{1}{2}\sin 2\theta) d\theta$$

$$= \frac{1}{2}$$

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

$$= 0$$

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

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

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

$$\langle S_x \rangle = \langle S_y \rangle = \langle S_z \rangle = 0$$

((**Comment**))

(i) The coherence " ρ_{+-} and ρ_{-+} are related to the transverse polarization $\langle \boldsymbol{S}_\perp \rangle$ of the spin. Upon summing the vector $\langle \boldsymbol{S}_\perp \rangle$ corresponding to all (equi-probable) 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.*

((**Note**)) **Difference between the wave function and density operator**

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 un-polarized spin, for which

$$\langle S_x\rangle = \langle S_y\rangle = \langle S_z\rangle = 0.$$

We note that

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

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

and

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

Then we get

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

So we cannot find α and β, so that $\langle \hat{S}_x\rangle = \langle \hat{S}_y\rangle = \langle \hat{S}_z\rangle = 0$. There is no way to express the wave function satisfying the unpolarized spin state. So we need to introduce the concept of the density operator for such a case.

11. 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 $|-\boldsymbol{n}\rangle$

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

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

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

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

12. Probability

(a) The mixed state

The density operator for the un-polarized state is given by

$$\hat{\rho}_{un} = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \frac{1}{2}\hat{1} \qquad \text{(mixed state)}$$

Suppose that the electrons with un-polarized spin state is measured by using the Stern-Gerlach experiment, where the in-homogenous magnetic field ***B*** is applied along the direction of the unit vector (***n***).

$$|+\boldsymbol{n}\rangle\langle+\boldsymbol{n}| = \begin{pmatrix} \cos\frac{\theta}{2} \\ \sin\frac{\theta}{2} \end{pmatrix} \begin{pmatrix} \cos\frac{\theta}{2} & \sin\frac{\theta}{2} \end{pmatrix} = \begin{pmatrix} \cos^2\frac{\theta}{2} & \sin\frac{\theta}{2}\cos\frac{\theta}{2} \\ \sin\frac{\theta}{2}\cos\frac{\theta}{2} & \sin^2\frac{\theta}{2} \end{pmatrix}$$

$$|-\boldsymbol{n}\rangle\langle-\boldsymbol{n}| = \begin{pmatrix} \sin\frac{\theta}{2} \\ -\cos\frac{\theta}{2} \end{pmatrix} \begin{pmatrix} \sin\frac{\theta}{2} & -\cos\frac{\theta}{2} \end{pmatrix} = \begin{pmatrix} \sin^2\frac{\theta}{2} & -\sin\frac{\theta}{2}\cos\frac{\theta}{2} \\ -\sin\frac{\theta}{2}\cos\frac{\theta}{2} & \cos^2\frac{\theta}{2} \end{pmatrix}$$

Then we have

$$Tr[\hat{\rho}_{un}|+\boldsymbol{n}\rangle\langle+\boldsymbol{n}|] = \frac{1}{2}Tr[\hat{1}|+\boldsymbol{n}\rangle\langle+\boldsymbol{n}|] = \frac{1}{2}$$

$$Tr[\hat{\rho}_{un}|-\boldsymbol{n}\rangle\langle-\boldsymbol{n}|] = \frac{1}{2}Tr[\hat{1}|-\boldsymbol{n}\rangle\langle-\boldsymbol{n}|] = \frac{1}{2}$$

The probability of finding a particle in the state $|+\boldsymbol{n}\rangle$ is 1/2 and in the state $|-\boldsymbol{n}\rangle$ is 1/2. This result is independent of the angle θ, where θ is the angle between the z axis and the unit vector $\boldsymbol{n}$.

(b) The pure state

The state vector is given by

$$\hat{\rho}_p = |\psi\rangle\langle\psi| = \begin{pmatrix} c_+ \\ c_- \end{pmatrix} \begin{pmatrix} c_+^* & c_-^* \end{pmatrix} = \begin{pmatrix} |c_+|^2 & c_+c_-^* \\ c_-c_+^* & |c_-|^2 \end{pmatrix} \qquad \text{(pure state)}$$

where

$$|\psi\rangle = c_+|+z\rangle + c_-|-z\rangle .$$

Then we get

$$Tr[\hat{\rho}_p|+\boldsymbol{n}\rangle\langle+\boldsymbol{n}|] = Tr[\begin{pmatrix} |c_+|^2 & c_+c_-^* \\ c_-c_+^* & |c_-|^2 \end{pmatrix} \begin{pmatrix} \cos^2\frac{\theta}{2} & \sin\frac{\theta}{2}\cos\frac{\theta}{2} \\ \sin\frac{\theta}{2}\cos\frac{\theta}{2} & \sin^2\frac{\theta}{2} \end{pmatrix}]$$
$$= |c_+|^2\cos^2\frac{\theta}{2} + |c_-|^2\sin^2\frac{\theta}{2}$$

$$Tr[\hat{\rho}_p|-\boldsymbol{n}\rangle\langle-\boldsymbol{n}|] = Tr[\begin{pmatrix} |c_+|^2 & c_+c_-^* \\ c_-c_+^* & |c_-|^2 \end{pmatrix}\begin{pmatrix} \sin^2\frac{\theta}{2} & -\sin\frac{\theta}{2}\cos\frac{\theta}{2} \\ -\sin\frac{\theta}{2}\cos\frac{\theta}{2} & \cos^2\frac{\theta}{2} \end{pmatrix}]$$

$$= |c_+|^2\sin^2\frac{\theta}{2} + |c_-|^2\cos^2\frac{\theta}{2}$$

The probability of finding a particle in the state $|+\boldsymbol{n}\rangle$ and in the state $|-\boldsymbol{n}\rangle$ strongly depend on the angle θ, where θ is the angle between the z axis and the unit vector $\boldsymbol{n}$.

13. Entropy S (I)

In quantum statistical mechanics, the **von Neumann entropy**, named after John von Neumann, is the extension of classical Gibbs entropy concepts to the field of quantum mechanics. For a quantum-mechanical system described by a density operator $\hat{\rho}$, the von Neumann entropy S is defined by

$$S = -k_B Tr[\hat{\rho}\ln\hat{\rho}]$$

where k_B denotes the Boltzmann constant. The entropy vanishes for pure states only, exceeds zero for mixed states, and, most importantly, is an extensive quantity for non-entangled subsystems $\hat{\rho}_1 \otimes \hat{\rho}_2$ because in this case

$$S = S_1 + S_2$$

$$\begin{aligned} S &= -k_B Tr_{1,2}[(\hat{\rho}_1\hat{\rho}_2)\ln(\hat{\rho}_1\hat{\rho}_2)] \\ &= -k_B Tr_{1,2}[(\hat{\rho}_1\hat{\rho}_2)\{\ln(\hat{\rho}_1)+\ln(\hat{\rho}_2)\}] \\ &= -k_B Tr_{1,2}[(\hat{\rho}_1\hat{\rho}_2)\ln(\hat{\rho}_1)] - k_B Tr_{1,2}[(\hat{\rho}_1\hat{\rho}_2)\ln(\hat{\rho}_2)] \\ &= -k_B Tr_1[\hat{\rho}_1\ln(\hat{\rho}_1)] - k_B Tr_2[\hat{\rho}_2\ln(\hat{\rho}_2)] \\ &= S_1 + S_2 \end{aligned}$$

The von Neumann entropy is regarded as the fundamental measure of preparation impurity for quantum states. However, the entropy might be difficult to calculate. Another computationally more convenient option is the purity $tr[\hat{\rho}^2]$ or the purity parameter

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

Using the eigen-basis of the density operator, we see that

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

14. Entropy *S* (II)

As shown above, the entropy *S* is defined by

$$S = -k_B Tr[\hat{\rho} \ln \hat{\rho}]$$

where k_B is the Boltzmann constant. When

$$\hat{\rho}|u_k\rangle = w_k |u_k\rangle$$

the entropy *S* can be rewritten as

$$S = -k_B \sum_k \langle u_k | \hat{\rho} \ln \hat{\rho} | u_k \rangle = -k_B \sum_k w_k \ln w_k$$

For the two spin states $\{|+z\rangle, |+z\rangle\}$, we assume that the density operator is described by

$$\hat{\rho} = w|+z\rangle\langle +z| + (1-w)|-z\rangle\langle -z|$$

Then we get

$$\frac{S}{k_B} = -w \ln w - (1-w)\ln(1-w) .$$

We make a plot of S/k_B as s function of the probability *w*.

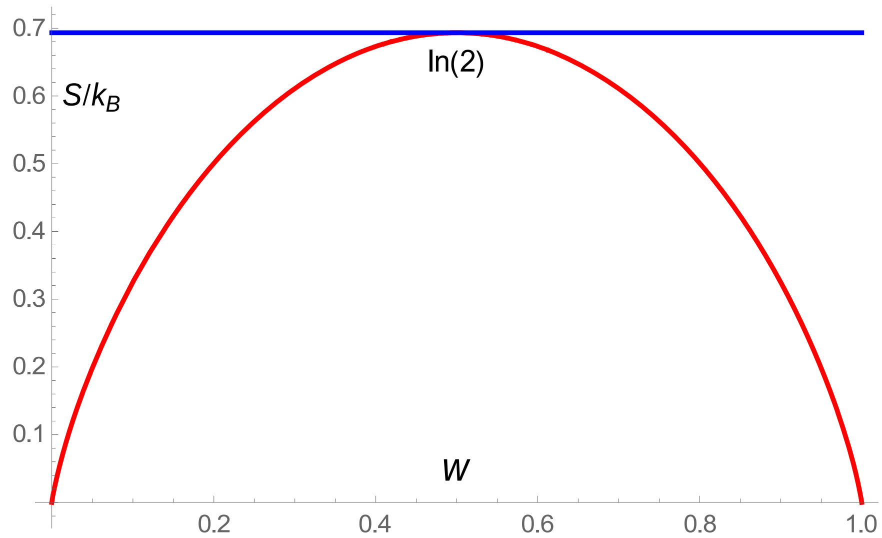


Fig. The reduced entropy (S/k_B) vs w. It exhibits a peak (= ln2 = 0.693147) at w = 1/2.

Using the Mathematica, one can evaluate the entropy even if the density matrix $\hat{\rho}$ is not diagonal;

$S/k_B = \sigma$ = -Tr[ρ MatrixLog[ρ]]

((**Example**))

The density operator (in the pure state) for the photon polarization $|x'\rangle$ is given by

$$\hat{\rho} = |x'\rangle\langle x'| = \frac{1}{2}\begin{pmatrix} 1+\cos(2\theta) & \sin(2\theta) \\ \sin(2\theta) & 1-\cos(2\theta) \end{pmatrix}$$

We calculate the entropy $\sigma = -k_B Tr[\hat{\rho}\ln\hat{\rho}]$ as a function of θ for $0 \le \theta \le \frac{\pi}{4}$, using the Mathematica. The result is as follows.

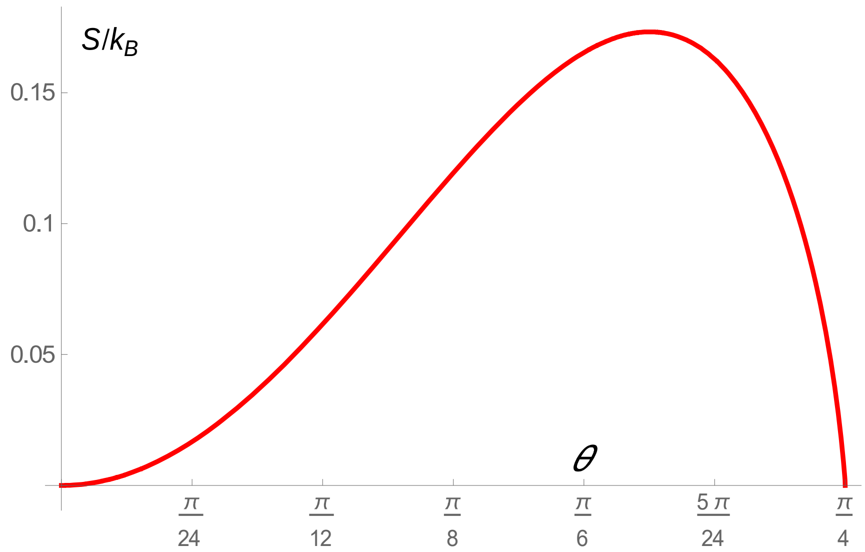


Fig. The entropy s for the photon polarization $|x'\rangle$ as a function of *θ*. $\hat{\rho} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$ for and $\hat{\rho} = \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$ for $\theta = \pi/4$.

How about the entropy for the density operator

$$\hat{\rho} = \frac{1}{2}\begin{pmatrix} 1 & a \\ a & 1 \end{pmatrix}.$$

where *a* is the parameter (0≤a≤1). Using the Mathematica, the entropy can be evaluated as

$$\sigma = \frac{S}{k_B} = \frac{1}{2}[a\ln(1-a) - a\ln(1+a) + \ln\frac{4}{1-a^2}$$

When $a = 1$, $\sigma = 0$. When $a = 0$, $\sigma = \ln 2$.

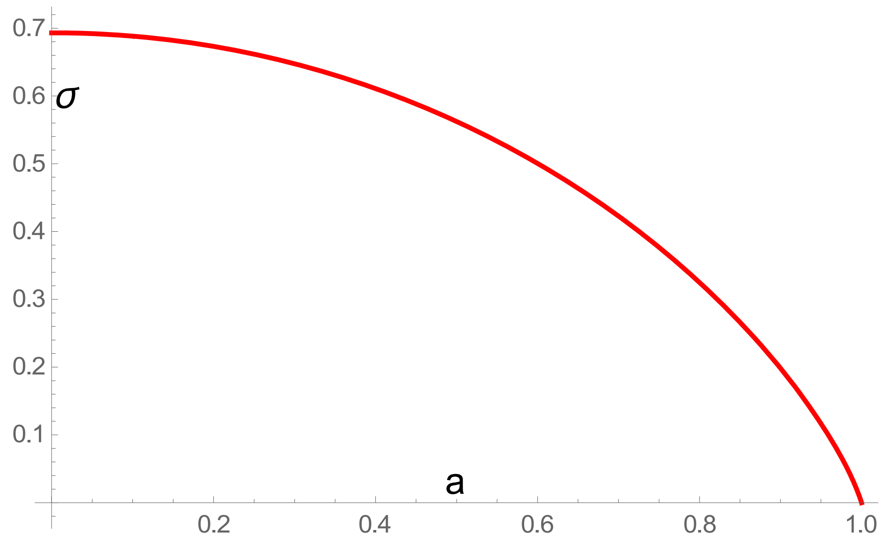


Fig. Entropy $\sigma = \dfrac{S}{k_B}$ a.s a function of the parameter a. $\sigma = \ln 2 = 0.69315$ at a = 0. $\sigma = 0$ at $a = 1$

15. Calculation of entropy with the use of Mathematica

Suppose that

$$\hat{\rho} = \frac{1}{8}\begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

Using the Mathematica, we can calculate the entropy

$$S = k_B \ln N$$

16. 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

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

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

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

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

17. 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)

$\psi_1.ComplexTranspose[\psi_2]$

when

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

(iii)

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

(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 $\quad |\psi_i\rangle \quad$ (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).

18. 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

$w_1 = 1$ $\quad\quad$ $|\psi_1\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix} = |-x\rangle$

$w_2 = 0$ $\quad\quad$ $|\psi_2\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix} = |+x\rangle$

Then we have

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

19. 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

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

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

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

20. 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

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

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

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

---

21. 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

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

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];
σx = (0 1
      1 0); σy = (0 -ⅈ
                  ⅈ 0); σz = (1 0
                              0 -1);
E1 = (1 0
      0 1);
ρ = (E1 + rx σx + ry σy + rz σz)/2 // Simplify
```

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

```
ψxp = 1/Sqrt[2] {1, 1}; ψxn = 1/Sqrt[2] {1, -1};
ψyp = 1/Sqrt[2] {1, ⅈ}; ψyn = 1/Sqrt[2] {1, -ⅈ}; ψzp = {1, 0};
ψzn = {0, 1}; σx = (0 1
                    1 0); σy = (0 -ⅈ
                                ⅈ 0);
σz = (1 0
      0 -1);
```

```
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
```

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

```
Tr[Ayn.ρ] // Simplify
```

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

```
Tr[Azp.ρ] // Simplify
```

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

```
Tr[Azn.ρ] // Simplify
```

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

22. Interpretation of the density matrix elements

What is the probability to find the qubit in the state $\left|+z\right\rangle$ 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:

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

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

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

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

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

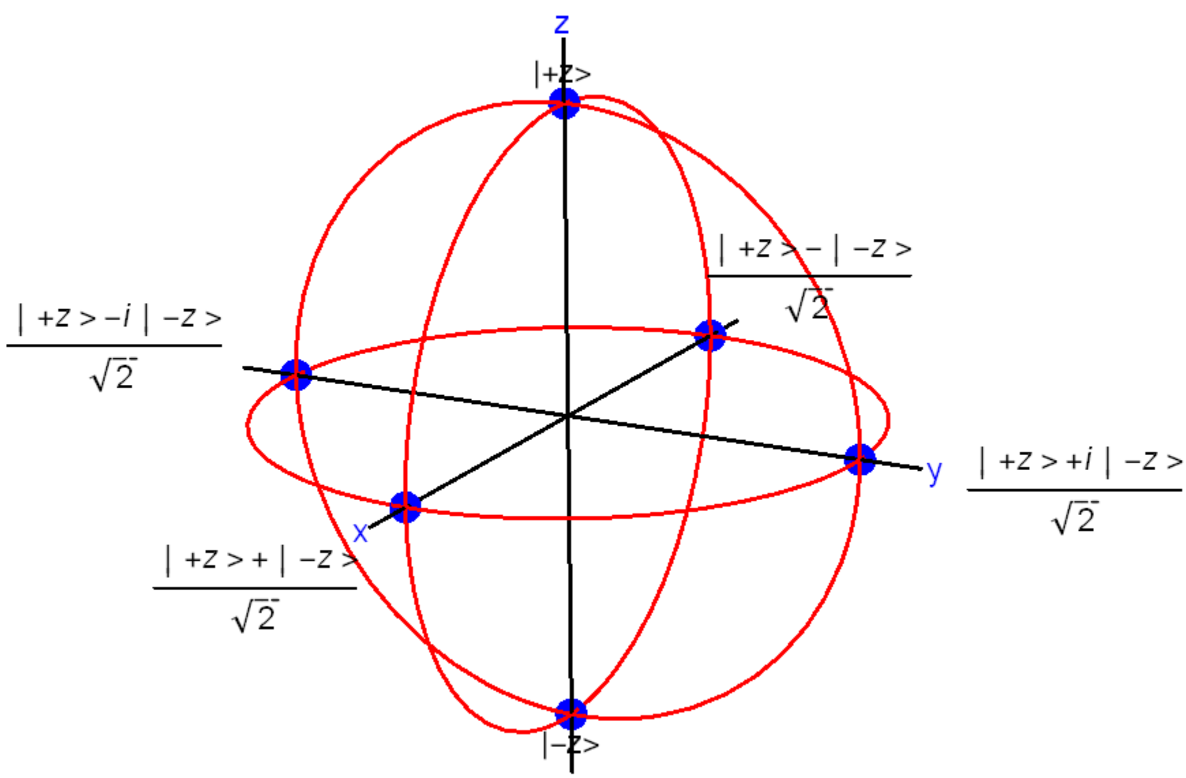
with

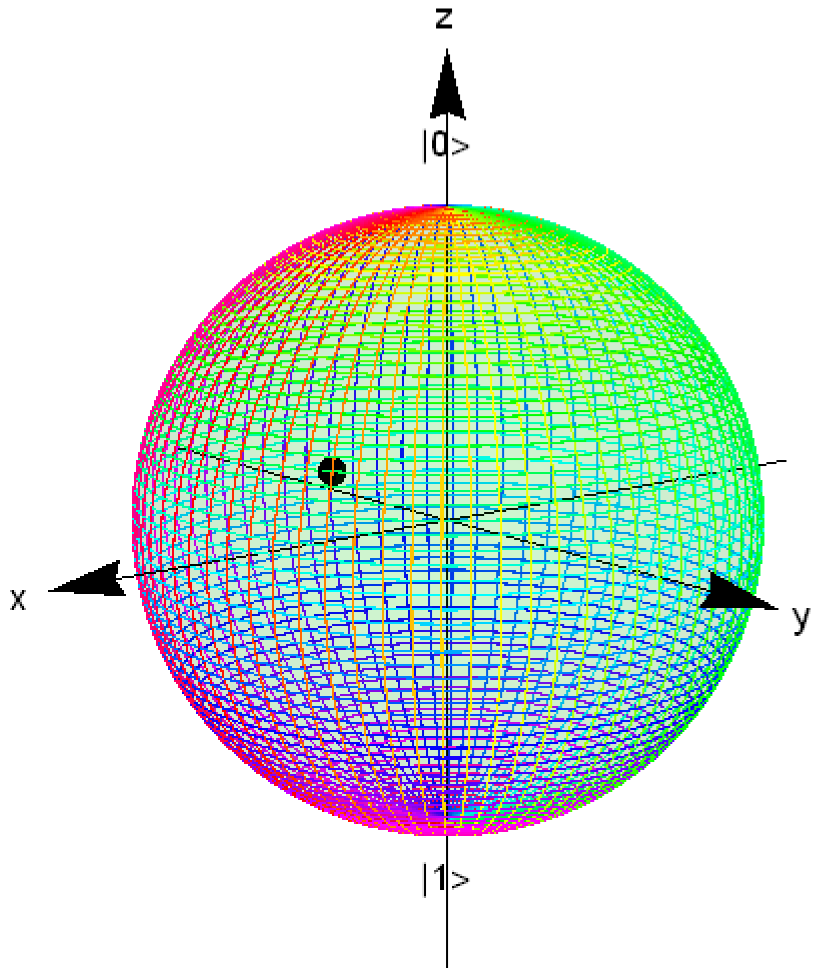
$$P_+ + P_- = \rho_{11} + \rho_{22} = 1 .$$

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

23. 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

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

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

((**Solution**))

$$\hat{\rho} = \begin{pmatrix} \cos^2\frac{\theta}{2} & 0 \\ 0 & \sin^2\frac{\theta}{2} \end{pmatrix}$$

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

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

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

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

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

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

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

24. 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

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

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.

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

---

25. 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.

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

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

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

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

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

26. 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.

27. 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

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

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

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

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

---

28 Application to the statistical mechanics; Spin in the presence of magnetic field

(a) Two-spin states

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

$$\omega_0 = \frac{eB}{mc} \qquad \text{(Larmor angular frequency, } e>0\text{)}$$

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

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

$\frac{1}{Z}\exp(\frac{\hbar\omega_0}{2k_BT})$, 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

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

The density operator is given by

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

with

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

The non-diagonal elements are zero. We note that

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

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

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

Since $\left|\tanh(\frac{\hbar\omega}{2k_BT})\right| < 1$, 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*.

(b) 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

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

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

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

Z is given by

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

The Helmholtz free energy F is given by

$$F = -k_BT\ln Z$$

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

$$\hat{H}|E_n\rangle = E_n|E_n\rangle$$

and

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

(c) Lagrange multiplier method: Derivation of canonical distribution

We define the entropy *S* as

$$S = -k_B Tr[\hat{\rho}\ln\hat{\rho}],$$

where k_B is the Boltzmann constant. The quantity $\sigma = S/k_B$ is expressed by

$$\frac{S}{k_B} = \sigma = -\sum_k \rho_{kk}\ln\rho_{kk}$$

when it is assumed that $\hat{\rho}$ is diagonal,

$$\hat{\rho} = \sum_k \rho_{kk}|E_k\rangle\langle E_k|$$

with

$$Tr[\hat{\rho}] = \sum_k \rho_{kk} = 1$$

The internal energy U is given by

$$U = \langle H \rangle = Tr[\hat{\rho}\hat{H}] = \sum_k E_k \rho_{kk}$$

Let us maximize σ by requiring that

$$\delta\sigma = -\sum_k (\ln \rho_{kk} + 1)\delta\rho_{kk} \qquad (1)$$

with two constraints

$$\delta\langle H \rangle = \sum_k E_k \delta\rho_{kk} \qquad (2)$$

$$\delta Tr[\hat{\rho}] = \sum_k \delta\rho_{kk} = 0 \qquad (3)$$

Using the Lagrange multiplier, we get:

$$\sum_k \delta\rho_{kk}[\ln \rho_{kk} + 1 + \beta E_k + \gamma] = 0$$

where β and γ are constants.

$$\ln \rho_{kk} + 1 + \beta E_k + \gamma = 0$$

Then we have

$$\rho_{kk} = \exp[-(1 + \beta E_k + \gamma)] = A\exp(-\beta E_k)$$

From the relation

$$\sum_k \rho_{kk} = A\sum_k \exp(-\beta E_k) = 1$$

where *A* is constant. The constant *A* can be determined as

$$A = \frac{1}{\sum_k \exp(-\beta E_k)} = \frac{1}{Z}$$

where Z is called the partition function

$$Z = \sum_k \exp(-\beta E_k) = Tr[e^{-\beta\hat{H}}]$$

Then we have

$$\rho_{kk} = \frac{1}{Z}\exp(-\beta E_k)$$

or

$$\begin{aligned}\hat{\rho} &= \sum_k \rho_{kk}|E_k\rangle\langle E_k| \\ &= \sum_k \frac{1}{Z}\exp(-\beta E_k)|E_k\rangle\langle E_k| \\ &= \frac{1}{Z}\exp(-\beta\hat{H})\end{aligned}$$

This system is called the canonical ensemble.

29. Spin with two energy levels

We now consider the system with two spin states with $|+z\rangle$ and $|-z\rangle$. Suppose that the magnetic field ***B*** is applied along the *z* axis. The spin Hamiltonian is given by

$$\hat{H} = -\left(\frac{-2\mu_B\hat{\boldsymbol{S}}}{\hbar}\cdot\boldsymbol{B}\right) = \mu_B B\hat{\sigma}_z$$

$$\hat{H}|+z\rangle = E_1|+z\rangle = \mu_B B|+z\rangle, \qquad \hat{H}|-z\rangle = E_2|-z\rangle = -\mu_B B|-z\rangle$$

where $E_1 = \mu_B B$ and $E_2 = -\mu_B B$.

$$\hat{H} = \begin{pmatrix} E_1 & 0 \\ 0 & E_2 \end{pmatrix}$$

$$Z = \exp(-\beta E_1) + \exp(-\beta E_2)$$

$$\hat{\rho} = \frac{1}{Z}\begin{pmatrix} \exp(-\beta E_1) & 0 \\ 0 & \exp(-\beta E_2) \end{pmatrix}$$

The internal energy U:

$$\begin{aligned} U &= \langle H \rangle = Tr(\hat{\rho}\hat{H}) \\ &= \frac{1}{Z}[E_1 \exp(-\beta E_1) + E_2 \exp(-\beta E_2)] \\ &= \frac{1}{\beta}\frac{1}{\frac{1}{x}+\frac{1}{y}}(\frac{\ln x}{x} + \frac{\ln y}{y}) \\ &= \frac{1}{\beta}\left(\frac{y\ln x + x\ln y}{x+y}\right) \end{aligned}$$

The entropy S:

$$\begin{aligned} S &= -k_B Tr[\hat{\rho}\ln(\hat{\rho})] \\ &= k_B[\frac{-x\ln x - y\ln y + (x+y)\ln(x+y)}{x+y}] \\ &= k_B[\frac{-(x\ln x + y\ln y)}{x+y} + \ln(x+y)] \end{aligned}$$

with

$$x = \exp(\beta E_1)\,, \qquad y = \exp(\beta E_2)$$

The Helmholtz free energy F:

$$\begin{aligned} F &= -k_B T\ln Z \\ &= -k_B T\ln[\exp(-\beta E_1) + \exp(-\beta E_2)] \\ &= -\frac{1}{\beta}[\ln(x+y) - \ln x - \ln y] \end{aligned}$$

Note that

$$F = E - ST \ .$$

The magnetization per unit mole is given by

$$M = N_A \mu_B \langle -\sigma_z \rangle = -N_A \mu_B Tr[\hat{\sigma}_z \hat{\rho}] = N_A \mu_B \tanh[\beta \mu_B B]$$

where N_A is the Avogadro number.

((**Mathematica**))

```
Clear["Global`*"]; H1 = ( E1  0 ;  0  E2 );
rule1 = {E1 → (1/β) Log[x], E2 → (1/β) Log[y]};
P1 = MatrixExp[-β H1]; σz = PauliMatrix[3];
Z1 = Tr[P1]
```

$$e^{-E1\,\beta} + e^{-E2\,\beta}$$

```
ρ1 = P1 / Z1
```

$$\left\{\left\{\frac{e^{-E1\,\beta}}{e^{-E1\,\beta} + e^{-E2\,\beta}},\ 0\right\},\ \left\{0,\ \frac{e^{-E2\,\beta}}{e^{-E1\,\beta} + e^{-E2\,\beta}}\right\}\right\}$$

```
Z1 /. rule1 // Simplify[#, {x > 0, y > 0, β > 0}] &
```

$$\frac{1}{x} + \frac{1}{y}$$

```
S1 = -kB Tr[ρ1 MatrixLog[ρ1]] /. rule1 //
  Simplify[#, {x > 0, y > 0, β > 0}] &
```

$$-\frac{kB\left(x\,\mathrm{Log}\left[\frac{x}{x+y}\right] + y\,\mathrm{Log}\left[\frac{y}{x+y}\right]\right)}{x + y}$$

```
F1 = -Log[Z1]/β /. rule1 //
  Simplify[#, {x > 0, y > 0, β > 0}] &
```

$$-\frac{\text{Log}\left[\frac{1}{x}+\frac{1}{y}\right]}{\beta}$$

```
U1 = Tr[H1.ρ1] /. rule1 //
  Simplify[#, {x > 0, y > 0, β > 0}] &
```

$$\frac{y\,\text{Log}[x]+x\,\text{Log}[y]}{x\,\beta+y\,\beta}$$

```
S11 = kB β (U1 - F1) /. rule1 //
  Simplify[#, {x > 0, y > 0, β > 0}] &
```

$$\frac{kB\left(y\,\text{Log}[x]+(x+y)\,\text{Log}\left[\frac{1}{x}+\frac{1}{y}\right]+x\,\text{Log}[y]\right)}{x+y}$$

```
(S1 - S11) // Simplify[#, {x > 0, y > 0, β > 0}] &
```

0

```
Aveσz = Tr[σz.ρ1] // ExpToTrig // Simplify;

M1 = -NA μB Aveσz /. {E1 → μB B, E2 → -μB B}
```

NA μB Tanh[B β μB]

30. Examples

(a) Example-1 Sakurai and Napolitano

As an example of a partially polarized beam, let us consider a 75-25 mixture of two pure ensembles, one with $|+z\rangle$ and the other with $|+x\rangle$. The corresponding ρ can be represented by

$$\hat{\rho} = \frac{3}{4}|+z\rangle\langle +z| + \frac{1}{4}|+x\rangle\langle +x| = \frac{3}{4}\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} + \frac{1}{8}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} = \frac{1}{8}\begin{pmatrix} 7 & 1 \\ 1 & 1 \end{pmatrix}$$

where

$$Tr[\hat{\rho}] = 1, \qquad S = -k_B Tr[\hat{\rho}\ln(\hat{\rho})] = 0.335322 k_B$$

$$Tr[\hat{S}_x\hat{\rho}] = \frac{\hbar}{8}, \qquad Tr[\hat{S}_y\hat{\rho}] = 0, \qquad Tr[\hat{S}_z\hat{\rho}] = \frac{3\hbar}{8}$$

Solving the eigenvalue problem, we have the diagonal form of $\hat{\rho}$,

$$\hat{\rho} = 0.8953|\phi_1\rangle\langle\phi_1| + 0.1047|\phi_2\rangle\langle\phi_2| = \begin{pmatrix} 0.8953 & 0 \\ 0 & 0.1047 \end{pmatrix}$$

with

$$|\phi_1\rangle = 0.9871|+z\rangle + 0.1672|-z\rangle$$

$$|\phi_2\rangle = -0.1672|+z\rangle + 0.9871|-z\rangle$$

(b) Example-2

We consider a 75-25 mixture of two pure ensembles, one with $|+z\rangle$ and the other with $|-x\rangle$. The corresponding p can be represented by

$$\hat{\rho} = \frac{3}{4}|+z\rangle\langle +z| + \frac{1}{4}|-x\rangle\langle -x| = \frac{3}{4}\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} + \frac{1}{8}\begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} = \frac{1}{8}\begin{pmatrix} 7 & -1 \\ -1 & 1 \end{pmatrix}$$

where

$$Tr[\hat{\rho}] = 1 \qquad S = -k_B Tr[\hat{\rho}\ln(\hat{\rho})] = 0.335322 k_B$$

$$Tr[\hat{S}_x\hat{\rho}] = -\frac{\hbar}{8}, \qquad Tr[\hat{S}_y\hat{\rho}] = 0, \qquad Tr[\hat{S}_z\hat{\rho}] = \frac{3\hbar}{8}$$

(c) Example-3

We consider a 75-25 mixture of two pure ensembles, one with $|+x\rangle$ and the other with $|-x\rangle$. The corresponding p can be represented by

$$\hat{\rho} = \frac{3}{4}|+x\rangle\langle +x| + \frac{1}{4}|-x\rangle\langle -x| = \frac{3}{8}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} + \frac{1}{8}\begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} = \begin{pmatrix} \frac{1}{2} & \frac{1}{4} \\ \frac{1}{4} & \frac{1}{2} \end{pmatrix}$$

where

$$Tr[\hat{\rho}] = 1 \qquad S = -k_B Tr[\hat{\rho}\ln(\hat{\rho})] = 0.562335 k_B$$

$$Tr[\hat{S}_x\hat{\rho}] = \frac{\hbar}{4}, \qquad Tr[\hat{S}_y\hat{\rho}] = 0, \qquad Tr[\hat{S}_z\hat{\rho}] = 0$$

(d) Example-4: 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[θ]^2, ⅇ^(-ⅈ ϕ) Cos[θ] Sin[θ]},
 {ⅇ^(ⅈ ϕ) Cos[θ] Sin[θ], Sin[θ]^2}}

ρ // MatrixForm

(       Cos[θ]^2          ⅇ^(-ⅈ ϕ) Cos[θ] Sin[θ] )
( ⅇ^(ⅈ ϕ) Cos[θ] Sin[θ]        Sin[θ]^2          )
ρ.ρ // Simplify

{{Cos[θ]^2, ⅇ^(-ⅈ ϕ) Cos[θ] Sin[θ]},
 {ⅇ^(ⅈ ϕ) Cos[θ] Sin[θ], Sin[θ]^2}}

Tr[ρ] // Simplify

1

Tr[ρ.ρ] // Simplify

1
```

31 Problems and solutions (collection)

31.1. 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)

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

The Hamiltonian is given by

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

Time evolution operator:

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

Note that

$$\exp(-\frac{i}{2}\omega_0\hat{\sigma}_x t) = \exp(-\frac{i}{2}\omega_0\hat{\sigma}_x t)[|+x\rangle\langle +x| + |-x\rangle\langle -x|)$$

$$= e^{-\frac{i}{2}\omega_0 t}|+x\rangle\langle +x| + e^{\frac{i}{2}\omega_0 t}|-x\rangle\langle -x|)$$

$$= \hat{U}(e^{-\frac{i}{2}\omega_0 t}|+z\rangle\langle +z| + e^{\frac{i}{2}\omega_0 t}|-z\rangle\langle -z|)\hat{U}^+$$

$$= \hat{U}\begin{pmatrix} e^{-\frac{i}{2}\omega_0 t} & 0 \\ 0 & e^{\frac{i}{2}\omega_0 t} \end{pmatrix}\hat{U}^+$$

$$= \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}\begin{pmatrix} e^{-\frac{i}{2}\omega_0 t} & 0 \\ 0 & e^{\frac{i}{2}\omega_0 t} \end{pmatrix}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

$$= \begin{pmatrix} \cos\frac{\omega_0 t}{2} & -i\sin\frac{\omega_0 t}{2} \\ -i\sin\frac{\omega_0 t}{2} & \cos\frac{\omega_0 t}{2} \end{pmatrix}$$

where

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

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

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

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

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

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

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

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

$$\begin{aligned}\langle \hat{S}_y \rangle &= Tr[\hat{\rho}_1 \hat{S}_y] \\ &= \frac{\hbar}{2} Tr[\begin{pmatrix} \alpha a^* & \alpha\beta^* \\ \alpha^*\beta & \beta\beta^* \end{pmatrix}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}] \\ &= \frac{\hbar}{2} Tr[\begin{pmatrix} i\alpha\beta^* & -i\alpha\alpha^* \\ i\beta^*\beta & -i\alpha^*\beta \end{pmatrix}] \\ &= i\frac{\hbar}{2}(\alpha\beta^* - \alpha^*\beta) = -\frac{\hbar}{2}\cos\theta\sin(\omega_0 T)\end{aligned}$$

$$\begin{aligned}\langle \hat{S}_z \rangle &= Tr[\hat{\rho}_1 \hat{S}_z] \\ &= \frac{\hbar}{2} Tr[\begin{pmatrix} \alpha a^* & \alpha\beta^* \\ \alpha^*\beta & \beta\beta^* \end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}] \\ &= \frac{\hbar}{2} Tr[\begin{pmatrix} \alpha\alpha^* & -\alpha\beta^* \\ \alpha^*\beta & -\beta\beta^* \end{pmatrix}] \\ &= \frac{\hbar}{2}(\alpha\alpha^* - \beta\beta^*) = \frac{\hbar}{2}\cos\theta\cos(\omega_0 T)\end{aligned}$$

(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

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

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

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

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

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

31.2 Problem and solution

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

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

(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 $|\psi\rangle$.

((**Solution**))

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

We define the unitary operator as

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

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)

$$\hat{\rho}_z = |\psi\rangle\langle\psi| = \begin{pmatrix} a \\ b \end{pmatrix}\begin{pmatrix} a^* & b^* \end{pmatrix} = \begin{pmatrix} aa^* & ab^* \\ a^*b & bb^* \end{pmatrix}$$ under the basis of $\{|+x\rangle, |-x\rangle\}$

(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]
```

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

31.3. Problem and solution

Given the density operator

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

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]
```

$\frac{\hbar}{4}$

31.4 Problem and solution

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
```

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

```
Tr[ρ.ρ]
```

$$\frac{1}{2}$$

31.5 Problem and solution

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
{{3/4, 0}, {0, 1/4}}

Tr[ρ.ρ]
5/8
```

31.6 Problem and solution

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.

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

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

Here we note that

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

So we get

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

((**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
```

5/8 + 2 x

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

{{x → 3/16}}

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

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

{{Cos[θ/2]^2, 1/2 ⅇ^(-ⅈ ϕ) Sin[θ]}, {1/2 ⅇ^(ⅈ ϕ) Sin[θ], Sin[θ/2]^2}}

31.7 Problem and solution

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 $\mu = \dfrac{ge\hbar}{2mc}$. 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};
```

$$Sz = \hbar \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix};$$

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

$$\rho = \frac{1}{Z1} (\text{Exp}[-\beta\, E1]\ \text{Outer}[\text{Times}, \psi p1, \psi p1] + \text{Outer}[\text{Times}, \psi 0, \psi 0] + \text{Exp}[\beta\, E1]\ \text{Outer}[\text{Times}, \psi m1, \psi m1]) \text{ // FullSimplify}$$

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

$$M = -\frac{g\,\mu B}{\hbar}\ N1\ \text{Tr}[Sz\,\rho] \text{ // Simplify}$$

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

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

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

```
M2 = M1 /. {B0 → x/(g μB β)}
```

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

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

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

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

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

31.8 Problem and solution

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**))

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

31.9 Problem and solution

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**))

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

or

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

31.10 Problem and solution

(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.

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