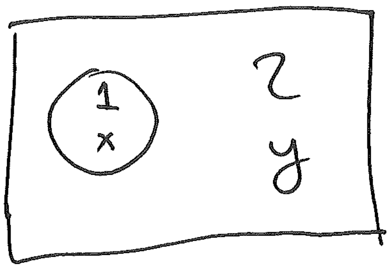
Physics 528 Lecture 12

Quantum Statistics III

1) Reduced density matrix



Suppose a system can be divided into two parts 1 and 2, described by variables x and y, respectively. A pure state of the system is described by a wavefunction

$$\psi(x,y) = \langle x|\langle y|\psi\rangle .$$

Let $\{|\psi_n\rangle\}$ be a complete set of states in region 1, and $\{|\phi_k\rangle\}$ a complete set in region 2.

$$|\psi\rangle = \sum_{n,k} C_{nk}\,|\psi_n\rangle|\phi_k\rangle$$

Let $\hat{A}$ be an operator defined in region 1 :

$$\hat{A} = \sum_{n,n'} |\psi_n\rangle A_{nn'} \langle\psi_{n'}| \otimes \underbrace{\mathbb{1}_2}_{\sum_k |\phi_k\rangle\langle\phi_k|}$$

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

$$\sum_{n',k'} \sum_{n,k} C^*_{nk} C_{n'k'} A_{nn'} \delta_{kk'}$$

$$= \sum_{\substack{n,n' \\ k}} C_{n'k} C^*_{nk} A_{nn'}$$

$$= \mathrm{Tr}\{\hat{\rho}_1 \hat{A}\},$$ where

$$(\rho_1)_{n'n} = \sum_k C_{n'k} C^*_{nk} .$$

$\hat{\rho}_1$ is called the <u>reduced density matrix</u> for sub-system 1.

Clearly $\hat{\rho}_1$ is Hermitian.

$$\mathrm{Tr}\{\hat{\rho}_1\} = \sum_{n,k} |C_{nk}|^2 = 1$$

due to normalization of $|\psi\rangle$.

Since $\hat{\rho}_1$ is Hermitian, it has an orthonormal set of eigenstates $|i\rangle$ with

$$\hat{\rho}_1 = \sum_i w_i |i\rangle\langle i| .$$

Let $\hat{A} = |j\rangle\langle j|$, where $|j\rangle$ is one of the eigenstates of $\hat{\rho}_1$.

$$w_j = \mathrm{Tr}\{\hat{\rho}_1 \hat{A}\} = \langle\psi|\hat{A}|\psi\rangle = |\langle j|\psi\rangle|^2 \geq 0.$$

Thus the eigenvalues of $\hat{\rho}_1$ satisfy

1) $w_i \geq 0$

2) $\sum_i w_i = 1$

Notice that

$$\langle \hat{Q} \rangle = Tr\{\hat{\rho}_1 \hat{Q}\} = \sum_i \langle i | \hat{\rho}_1 \hat{Q} | i \rangle$$

$$= \sum_i w_i \langle i | \hat{Q} | i \rangle,$$

where $\hat{Q}$ is any operator acting only on region 1.

Thus $\hat{\rho}_1$ has all of the properties required for a density matrix.

In terms of the coordinates x of system 1,

$$\langle \hat{A} \rangle = Tr\{\hat{\rho}_1 \hat{A}\} = \int dx \langle x | \hat{\rho}_1 \hat{A} | x \rangle$$

$$\langle \hat{A} \rangle = \int dx \int dx' \langle x | \hat{\rho}_1 | x' \rangle \langle x' | \hat{A} | x \rangle$$

$$= \int dx \int dx' \; \rho_1(x, x') \, A(x', x)$$

Moreover, in terms of $|\Psi\rangle$,

$$\langle \hat{A} \rangle = \langle \Psi | \hat{A} | \Psi \rangle = \int dx \int dx' \int dy \, \Psi^*(x', y) \, A(x', x) \, \Psi(x, y)$$

Thus

$$\rho_1(x, x') = \int dy \, \Psi(x, y) \, \Psi^*(x', y) .$$

$$= Tr_2 \{ \rho(x, y; x', y') \}$$

Notice that the reduced density matrix does not have the form required for a <u>pure state</u>. Pure states are thus not general enough to describe the state of a subsystem of a larger quantum system. The only known system that is not a part of a larger system is the universe as a whole.

It is unknown whether the universe as a whole is in a pure state.

<u>Example</u> Entangled (singlet) state of two spin-1/2 particles.

$$|\psi\rangle = \frac{|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle}{\sqrt{2}}$$ (a pure state)

$$\hat{\rho} = |\psi\rangle\langle\psi| = \frac{1}{2}|\uparrow\downarrow\rangle\langle\uparrow\downarrow| + \frac{1}{2}|\downarrow\uparrow\rangle\langle\downarrow\uparrow| - \frac{1}{2}|\uparrow\downarrow\rangle\langle\downarrow\uparrow| - \frac{1}{2}|\downarrow\uparrow\rangle\langle\uparrow\downarrow|$$

$$\hat{\rho}_1 = \mathrm{Tr}_2\{\hat{\rho}\} = \langle 2\uparrow|\hat{\rho}|2\uparrow\rangle + \langle 2\downarrow|\hat{\rho}|2\downarrow\rangle$$

$$= \frac{1}{2}|\downarrow\rangle\langle\downarrow| + \frac{1}{2}|\uparrow\rangle\langle\uparrow|$$ (a mixed state!)

$$S_1 = -k_B\,\mathrm{Tr}\{\hat{\rho}_1 \ln \hat{\rho}_1\} = k_B \ln 2$$

but $S = -k_B\,\mathrm{Tr}\{\hat{\rho}\ln\hat{\rho}\} = 0$

S_1 is sometimes refered to as <u>entanglement entropy</u>.

Discussion question

Is it possible that the universe as a whole is in a pure quantum state, whose initial wave function describes the big bang, but that the microscopic degrees of freedom of the observable universe are now entangled with degrees of freedom outside our light cone, so that the entropy of the observable universe is nothing but entanglement entropy?