Intermediate Quantum Mechanics
Lecture 26 Notes (4/29/15)

Density Matrices II

Density matrix for one particle of a two particle composite system

- Consider a two particle composite system and label the basis states as $|ab\rangle$ where a and b range over the dimension of the individual particles. For example, in the case of spin states of two electrons, the dimension of each particle would be two and a and b would each range over $|\uparrow\rangle$ and $|\downarrow\rangle$.

- The general state of the two particle system can be written as:

$$|\psi\rangle = \sum_{ab} \psi_{ab} \, |ab\rangle$$

- Now consider an operator $\hat{A}$ that only operates on particle a and therefore doesn't depend on b. The expectation value of the observable corresponding to $\hat{A}$ is given by:

$$\overline{A} = \sum_{aa'} \sum_{bb'} \psi^*_{a'b'} \langle a'b'|\hat{A}\,|ab\rangle \psi_{ab} = \sum_{aa'} \sum_{b} \psi^*_{a'b} \langle a'b|\hat{A}\,|ab\rangle \psi_{ab}$$

$$= \sum_{aa'} \sum_{b} \psi^*_{a'b} \langle a'|\hat{A}\,|a\rangle \psi_{ab} = \sum_{aa'} \sum_{b} A_{a'a} \psi_{ab} \psi^*_{a'b} = \sum_{aa'} A_{a'a} \rho_{aa'}$$

where $\rho_{aa'} = \sum_{b} \psi_{ab} \psi^*_{a'b}$ are the matrix elements of the density matrix of particle a.

- We then have: $$\overline{A} = \mathrm{Tr}\left(\hat{A}\hat{\rho}\right)$$

Density matrix for one particle of a two particle product state

- If two particle are in a product state then ψ_{ab} factorizes into $\phi_a \chi_b$. The general state of the two particle product system can then be written as:

$$|\psi\rangle = \sum_{ab} \psi_{ab} \, |ab\rangle = \sum_{ab} \phi_a \chi_b \, |ab\rangle$$

- The density matrix elements then become:

$$\rho_{aa'} = \sum_{b} \psi_{ab} \psi^*_{a'b} = \sum_{b} \phi_a \phi^*_{a'} \chi_b \chi^*_{b'} = \phi_a \phi^*_{a'}$$

$$\Rightarrow \quad \hat{\rho} = |\phi\rangle\langle\phi| \qquad \text{The individual particle is in a pure state.}$$

- The expectation value of $\hat{A}$ is then:

$$\overline{A} = \mathrm{Tr}\left(\hat{A}\hat{\rho}\right) = \sum_{aa'} A_{a'a} \rho_{aa'} = \sum_{aa'} A_{a'a} \phi_a \phi^*_{a'}$$

$$= \sum_{aa'} \langle \phi \,|\, a' \rangle \langle a'|\hat{A}\,|a\rangle \langle a \,|\, \phi \rangle = \langle \phi|\hat{A}\,|\phi\rangle$$

Density matrix elements for one electron in a two electron composite system

- For a two electron composite system, the density matrix elements of electron a are given by summing over the spin of electron b:

$$\rho_{aa'} \;=\; \sum_b \psi_{ab}\psi^*_{a'b}$$

- This gives the following useful table:

$$\rho_{\uparrow\uparrow} \;=\; \psi_{\uparrow\uparrow}\psi^*_{\uparrow\uparrow} + \psi_{\uparrow\downarrow}\psi^*_{\uparrow\downarrow} \qquad\qquad \rho_{\uparrow\downarrow} \;=\; \psi_{\uparrow\uparrow}\psi^*_{\downarrow\uparrow} + \psi_{\uparrow\downarrow}\psi^*_{\downarrow\downarrow}$$

$$\rho_{\downarrow\uparrow} \;=\; \psi_{\downarrow\uparrow}\psi^*_{\uparrow\uparrow} + \psi_{\downarrow\downarrow}\psi^*_{\uparrow\downarrow} \qquad\qquad \rho_{\downarrow\downarrow} \;=\; \psi_{\downarrow\uparrow}\psi^*_{\downarrow\uparrow} + \psi_{\downarrow\downarrow}\psi^*_{\downarrow\downarrow}$$

Example 1: the singlet state

$$|\psi\rangle \;=\; \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle \;-\; |\downarrow\uparrow\rangle\right)$$

$$\psi_{\uparrow\uparrow} \;=\; 0 \qquad \psi_{\uparrow\downarrow} \;=\; \frac{1}{\sqrt{2}} \qquad \psi_{\downarrow\uparrow} \;=\; -\frac{1}{\sqrt{2}} \qquad \psi_{\downarrow\downarrow} \;=\; 0$$

$$\rho_{\uparrow\uparrow} \;=\; \frac{1}{2} \qquad \rho_{\uparrow\downarrow} \;=\; 0 \qquad \rho_{\downarrow\uparrow} \;=\; 0 \qquad \rho_{\downarrow\downarrow} \;=\; \frac{1}{2}$$

$$\hat{\rho} \;\longrightarrow\; \begin{pmatrix} 1/2 & 0 \\ 0 & 1/2 \end{pmatrix}$$

- For each individual electron the entropy is: $S \;=\; \log 2$ and the electrons are maximally entangled.

- We can now easily calculate the expectation value of the spin of electron a in any direction:

$$\overline{\sigma}_n \;=\; \mathrm{Tr}\left(\hat{\rho}\hat{\sigma}_n\right) \;=\; \frac{1}{2}\,\mathrm{Tr}\left(\hat{I}\hat{\sigma}_n\right) \;=\; \frac{1}{2}\,\mathrm{Tr}\left(\hat{\sigma}_n\right) \;=\; 0$$

Example 2: the state $|\rightarrow\rightarrow\rangle$

$$|\psi\rangle \;=\; |\rightarrow\rangle \otimes |\rightarrow\rangle \;=\; \frac{1}{\sqrt{2}}\left(|\uparrow\rangle + |\downarrow\rangle\right) \otimes \frac{1}{\sqrt{2}}\left(|\uparrow\rangle + |\downarrow\rangle\right)$$

$$= \; \frac{1}{2}\Big(|\uparrow\uparrow\rangle \;+\; |\uparrow\downarrow\rangle \;+\; |\downarrow\uparrow\rangle \;+\; |\downarrow\downarrow\rangle\Big)$$

$$\psi_{\uparrow\uparrow} \;=\; \frac{1}{2} \qquad \psi_{\uparrow\downarrow} \;=\; \frac{1}{2} \qquad \psi_{\downarrow\uparrow} \;=\; \frac{1}{2} \qquad \psi_{\downarrow\downarrow} \;=\; \frac{1}{2}$$

$$\rho_{\uparrow\uparrow} \;=\; \frac{1}{2} \qquad \rho_{\uparrow\downarrow} \;=\; \frac{1}{2} \qquad \rho_{\downarrow\uparrow} \;=\; \frac{1}{2} \qquad \rho_{\downarrow\downarrow} \;=\; \frac{1}{2}$$

$$\hat{\rho} \;\longrightarrow\; \begin{pmatrix} 1/2 & 1/2 \\ 1/2 & 1/2 \end{pmatrix}$$

- This is the density matrix of a pure state. We scan check this in the following way using two matrix algebra identities. If we let λ_i be the N eigenvalues of an N-dimensional Hermitian matrix then:

$$\mathrm{Tr}\, M \;=\; \sum_i \lambda_i \qquad\qquad \det M \;=\; \prod_i \lambda_i$$

- In the present case of the two dimensional matrix ρ we have:

$$\mathrm{Tr}\,\rho \;=\; 1 \quad \text{and} \quad \det\rho \;=\; 0 \qquad \Rightarrow \qquad \lambda_1 + \lambda_2 \;=\; 1 \quad \text{and} \quad \lambda_1\lambda_2 \;=\; 0$$

  This can only be solved by one of the λ's equal to one and the other zero. This means that in the basis in which ρ is diagonalized we have:

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

  A two-dimensional system, is in a pure state if $\mathrm{Tr}\,\rho \;=\; 0$.

- This only works for a 2-dimensional system. For example, for a 3-dimensional system: $\quad \det\rho \;=\; 0 \quad \Rightarrow \quad \lambda_1\lambda_2\lambda_3 \;=\; 0$

  That means that ρ is either $\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$ or $\begin{pmatrix} p_1 & 0 & 0 \\ 0 & p_2 & 0 \\ 0 & 0 & 0 \end{pmatrix}$

  The state might be pure but it might also be partially mixed.

- Using the the density matrix that we found above $\rho \;=\; \begin{pmatrix} 1/2 & 1/2 \\ 1/2 & 1/2 \end{pmatrix}$ we can easily calculate the expectation values of $\hat{\sigma}_z$ and $\hat{\sigma}_z$:

$$\overline{\sigma}_z \;=\; \mathrm{Tr}\,(\hat{\rho}\hat{\sigma}_z) \;=\; \frac{1}{2}\,\mathrm{Tr}\left[\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\right] \;=\; \frac{1}{2}\,\mathrm{Tr}\begin{pmatrix} 1 & -1 \\ 1 & -1 \end{pmatrix} \;=\; 0$$

$$\overline{\sigma}_x \;=\; \mathrm{Tr}\,(\hat{\rho}\hat{\sigma}_z) \;=\; \frac{1}{2}\,\mathrm{Tr}\left[\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\right] \;=\; \frac{1}{2}\,\mathrm{Tr}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \;=\; 1$$

Summary for a two-dimensional system

Pure State: $\quad \rho = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$

Maximally mixed State: $\quad \rho = \begin{pmatrix} 1/2 & 0 \\ 0 & 1/2 \end{pmatrix}$

Partially mixed State: $\quad \rho = \begin{pmatrix} p_1 & 0 \\ 0 & p_2 \end{pmatrix} \quad$ with $p_1 \neq 0$ or 1 and $p_1 \neq 0$ or 1.

Summary of entropy for the singlet state

- The following table summarizer the entropy for the singlet state:

$$|\psi\rangle \;=\; \frac{1}{\sqrt{2}}\big(|\uparrow\downarrow\rangle \;-\; |\downarrow\uparrow\rangle\big)$$

  S_{sys} is the entropy for the composite system, S_{A} is the entropy for Alice and S_{B} is the entropy for Bob.

	S_{sys}	S_{A}	S_{B}
Initially:	0	$\log 2$	$\log 2$
After Alice, but not Bob, measures her electron:	0	0	$\log 2$
After Bob, but not Alice, measures his electron:	0	$\log 2$	0
After both Alice and Bob measure their electrons:	0	0	0