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PHY1520H Graduate Quantum Mechanics. Lecture 3: Density matrix (cont.). Taught by Prof. Arun Paramekanti

Disclaimer Peeter's lecture notes from class. These may be incoherent and rough.

These are notes for the UofT course PHY1520, Graduate Quantum Mechanics, taught by Prof. Paramekanti, covering ch. 1 [1] content.

Density matrix (cont.) An example of a partitioned system with four total states (two spin 1/2 particles) is sketched in fig. 1.1.

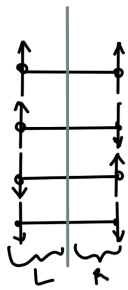

Figure 1.1: Two spins

An example of a partitioned system with eight total states (three spin 1/2 particles) is sketched in fig. 1.2.

The density matrix

$$\hat{\rho} = |\Psi\rangle \langle\Psi| \tag{1.1}$$

is clearly an operator as can be seen by applying it to a state

$$\hat{\rho} |\phi\rangle = |\Psi\rangle \left(\langle\Psi|\phi\rangle \right). \tag{1.2}$$

The quanitity in braces is just a complex number.

After expanding the pure state $|\Psi\rangle$ in terms of basis states for each of the two partitions

$$|\Psi\rangle = \sum_{m,n} C_{m,n} |m\rangle_{\mathrm{L}} |n\rangle_{\mathrm{R}}, \tag{1.3}$$

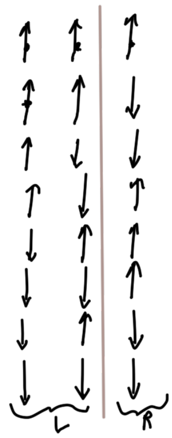

Figure 1.2: Three spins

With L and R implied for $|m\rangle, |n\rangle$ indexed states respectively, this can be written

$$|\Psi\rangle = \sum_{m,n} C_{m,n} |m\rangle |n\rangle . \tag{1.4}$$

The density operator is

$$\hat{\rho} = \sum_{m,n} C_{m,n} C^*_{m',n'} |m\rangle |n\rangle \sum_{m',n'} \langle m'| \langle n'| . \tag{1.5}$$

Suppose we trace over the right partition of the state space, defining such a trace as the reduced density operator $\hat{\rho}_{\text{red}}$

$$\begin{aligned}
\hat{\rho}_{\text{red}} &\equiv \text{Tr}_{\text{R}}(\hat{\rho}) \\
&= \sum_{\tilde{n}} \langle \tilde{n}| \hat{\rho} |\tilde{n}\rangle \\
&= \sum_{\tilde{n}} \langle \tilde{n}| \left(\sum_{m,n} C_{m,n} |m\rangle |n\rangle \right) \left(\sum_{m',n'} C^*_{m',n'} \langle m'| \langle n'| \right) |\tilde{n}\rangle \\
&= \sum_{\tilde{n}} \sum_{m,n} \sum_{m',n'} C_{m,n} C^*_{m',n'} |m\rangle \delta_{\tilde{n}n} \langle m'| \delta_{\tilde{n}n'} \\
&= \sum_{\tilde{n},m,m'} C_{m,\tilde{n}} C^*_{m',\tilde{n}} |m\rangle \langle m'|
\end{aligned} \tag{1.6}$$

Computing the matrix element of $\hat{\rho}_{\text{red}}$, we have

$$\begin{aligned}
\langle \tilde{m}| \hat{\rho}_{\text{red}} |\tilde{m}\rangle &= \sum_{m,m',\tilde{n}} C_{m,\tilde{n}} C^*_{m',\tilde{n}} \langle \tilde{m}|m\rangle \langle m'|\tilde{m}\rangle \\
&= \sum_{\tilde{n}} |C_{\tilde{m},\tilde{n}}|^2 .
\end{aligned} \tag{1.7}$$

This is the probability that the left partition is in state $\tilde{m}$.

Average of an observable Suppose we have two spin half particles. For such a system the total magnetization is

$$S_{\text{Total}} = S_1^z + S_1^z, \tag{1.8}$$

as sketched in fig. 1.3.

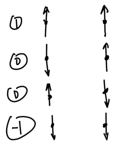

Figure 1.3: Magnetic moments from two spins.

The average of some observable is

$$\left\langle \hat{A} \right\rangle = \sum_{m,n,m',n'} C^*_{m,n} C_{m',n'} \left\langle m \right| \left\langle n \right| \hat{A} \left| n' \right\rangle \left| m' \right\rangle . \tag{1.9}$$

Consider the trace of the density operator observable product

$$\operatorname{Tr}(\hat{\rho}\hat{A}) = \sum_{m,n} \left\langle mn | \Psi \right\rangle \left\langle \Psi \right| \hat{A} \left| m, n \right\rangle . \tag{1.10}$$

Let

$$\left| \Psi \right\rangle = \sum_{m,n} C_{mn} \left| m, n \right\rangle , \tag{1.11}$$

so that

$$\begin{aligned} \operatorname{Tr}(\hat{\rho}\hat{A}) &= \sum_{m,n,m',n',m'',n''} C_{m',n'} C^*_{m'',n''} \left\langle mn | m', n' \right\rangle \left\langle m'', n'' \right| \hat{A} \left| m, n \right\rangle . \\ &= \sum_{m,n,m'',n''} C_{m,n} C^*_{m'',n''} \left\langle m'', n'' \right| \hat{A} \left| m, n \right\rangle . \end{aligned} \tag{1.12}$$

This is just

$$\boxed{\left\langle \Psi \right| \hat{A} \left| \Psi \right\rangle = \operatorname{Tr}(\hat{\rho}\hat{A}).} \tag{1.13}$$

Left observables Consider

$$\begin{aligned} \left\langle \Psi \right| \hat{A}_{\text{L}} \left| \Psi \right\rangle &= \operatorname{Tr}(\hat{\rho}\hat{A}_{\text{L}}) \\ &= \operatorname{Tr}_{\text{L}} \operatorname{Tr}_{\text{R}}(\hat{\rho}\hat{A}_{\text{L}}) \\ &= \operatorname{Tr}_{\text{L}} \left(\left(\operatorname{Tr}_{\text{R}} \hat{\rho} \right) \hat{A}_{\text{L}} \right) \\ &= \operatorname{Tr}_{\text{L}} \left(\hat{\rho}_{\text{red}} \hat{A}_{\text{L}} \right) . \end{aligned} \tag{1.14}$$

We see

$$\langle\Psi|\,\hat{A}_{\mathrm{L}}\,|\Psi\rangle = \mathrm{Tr}_{\mathrm{L}}\left(\hat{\rho}_{\mathrm{red,L}}\hat{A}_{\mathrm{L}}\right). \tag{1.15}$$

We find that we don't need to know the state of the complete system to answer questions about portions of the system, but instead just need $\hat{\rho}$, a "probability operator" that provides all the required information about the partitioning of the system.

Pure states vs. mixed states For pure states we can assign a state vector and talk about reduced scenerios. For mixed states we must work with reduced density matrices.

Example 1.1: Two particle spin half pure states

Consider

$$|\psi_1\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right) \tag{1.16}$$

$$|\psi_2\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle + |\uparrow\uparrow\rangle\right). \tag{1.17}$$

For the first pure state the density operator is

$$\hat{\rho} = \frac{1}{2}\left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right)\left(\langle\uparrow\downarrow| - \langle\downarrow\uparrow|\right) \tag{1.18}$$

What are the reduced density matrices?

$$\begin{aligned}\hat{\rho}_{\mathrm{L}} &= \mathrm{Tr}_{\mathrm{R}}\left(\hat{\rho}\right)\\ &= \frac{1}{2}(-1)(-1)\,|\downarrow\rangle\,\langle\downarrow| + \frac{1}{2}(+1)(+1)\,|\uparrow\rangle\,\langle\uparrow|\,,\end{aligned} \tag{1.19}$$

so the matrix representation of this reduced density operator is

$$\hat{\rho}_{\mathrm{L}} = \frac{1}{2}\begin{bmatrix}1 & 0\\ 0 & 1\end{bmatrix}. \tag{1.20}$$

For the second pure state the density operator is

$$\hat{\rho} = \frac{1}{2}\left(|\uparrow\downarrow\rangle + |\uparrow\uparrow\rangle\right)\left(\langle\uparrow\downarrow| + \langle\uparrow\uparrow|\right). \tag{1.21}$$

This has a reduced density matrice

$$\begin{aligned}\hat{\rho}_{\mathrm{L}} &= \mathrm{Tr}_{\mathrm{R}}\left(\hat{\rho}\right) \\ &= \frac{1}{2}\left|\uparrow\right\rangle\left\langle\uparrow\right| + \frac{1}{2}\left|\uparrow\right\rangle\left\langle\uparrow\right|, \\ &= \left|\uparrow\right\rangle\left\langle\uparrow\right|.\end{aligned} \tag{1.22}$$

This has a matrix representation

$$\hat{\rho}_{\mathrm{L}} = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}. \tag{1.23}$$

In this second example, we have more information about the left partition. That will be seen as a zero enganglement entropy in the problem set. In contrast we have less information about the first state, and will find a non-zero positive entanglement entropy in that case.

Bibliography

[1] Jun John Sakurai and Jim J Napolitano. *Modern quantum mechanics*. Pearson Higher Ed, 2014. 1