Physics 501-22

Density Matrix

Quantum Mechnics is a probabilistic theory. It is a theory which does not tell what the future is, given the past. Instead it gives probabilities for varios futures given the past. For a given state $|\psi\rangle$ (given by having knowledge of some feature of the system in the past, in the usual formulation, and a given attribute of a system $\mathcal{A}$, the possible future values for that attribute are given by the eigenvalues of the operator A associated with the attribute $\mathcal{A}$ The probability of finding that the system has some value for that attribute, one of the eigenvalues, is given by

$$\mathcal{P}(a) = |\langle a||\psi\rangle|^2 \tag{1}$$

where $|a\rangle$ is the normalised eigenvector associated with the eigenvalue a and $\mathcal{P}(a)$ is the probability. (If there are many eigenvectors with the same eigenvalue A you need to sum over the a complete orthonormal set of those eigenvectors for a).

One can imagine that one set up one's system so that, in addition to the probabilities that arise from Quantum mechanics, one also adds in classical probabilities. Lets say that one, instead of choosing one initial state $|\psi\rangle$ one instead chooses a set of them $|\psi_n\rangle$. One now correlates the state with some outside classically random event, such that the the nth value of the random generator has probability p_n. One now correlates that output with the nth state $|\psi_n\rangle$. If one wants to calculate the average value of some operator A, one would calculate the average for the nth state$|\psi_n\rangle$, and then average over the probabilities

$$\langle A\rangle = \sum_n p_n \langle\psi_n|A|\psi_n\rangle \tag{2}$$

Note that this is not a state.

Given an operators, B, one can define a operation on that operators called the trace. Consider a complete orthonormal set of states $|\phi_n\rangle$ define the trace as

$$\text{Tr}B = \sum_n \langle\psi_n|B|\psi_n\rangle \tag{3}$$

The trace has a number of features. In particular

$$\text{Tr}BC = \text{Tr}(CB) \tag{4}$$

If U is a unitary matrix, then

$$\text{Tr}(U^\dagger BU) = \text{Tr}(BUU^\dagger) = Tr(B) \tag{5}$$

Since the operator

$$U = \sum_n |\phi_n\rangle\langle\tilde{\phi_n}| \tag{6}$$

for two abitrary complete orthonormal sets,is a unitary matrix

$$UU^\dagger = \sum_{nm} |\phi_n\rangle(\langle\tilde{\phi_n}||\tilde{\phi_m}\rangle)\langle\tilde{\phi_m}| \tag{7}$$

$$= \sum_{nm} |\phi_n\rangle\delta_{nm}\langle\tilde{\phi_s}| = \sum_n |\phi_n\rangle\langle\tilde{\phi_n}| = I \tag{8}$$

. Thus $\mathrm{Tr}(UBU^\dagger) = \mathrm{Tr}(BU^\dagger U) = tr(B)$ Since $UBU^\dagger$ in the $|\tilde{\phi_n}\rangle$ basis, the trace is basis independent.

Furthrmore

$$\mathrm{Tr}(|\mu\rangle\langle\nu|) = \sum_n \langle\phi_n||\mu\rangle\langle\chi||\phi_n\rangle = \sum_n \langle\chi||\phi_n\rangle\langle\phi_n||\mu\rangle = \langle\chi|I|\mu\rangle = \langle\chi||\mu\rangle \tag{9}$$

(as can be seen by expanding $|\mu\rangle$ and $|\chi\rangle$ in the orthnormal basis of $|\phi_n\rangle$

We can write ρ as a density matrix

$$\rho = \sum_n p_n|\psi_n\rangle\langle\psi_n| \tag{10}$$

Note that $|\psi_n\rangle$ need not be a complete set, nor need it be an orthogonal set. But $|\psi_n\rangle$ are normalised. Then $\mathrm{Tr}\rho = \sum_n p_n = 1$

Now consider a two part system, and consider $|\psi\rangle$ as a state in that total system. If we have $|\phi_n\rangle$ to be a basis in the first of those two parts, and $||\phi\rangle_m\rangle$ to be an orthonormal basis in the second, we can write the state $|\psi\rangle$ in terms of the orthonoral basis $|\tilde{\phi_n}\rangle|\hat{\phi_m}\rangle$

$$|\psi\rangle = (\langle\tilde{\phi_n}|\langle\hat{\phi_m}||\psi\rangle)|\tilde{\phi_n}\rangle|\hat{\phi_m}\rangle \tag{11}$$

and the density matrix

$$\rho_T = |\psi\rangle\langle\psi| = \sum_{mnrs} (\langle\tilde{\phi_n}|\langle\hat{\phi_m}||\psi\rangle)|\tilde{\phi_n}\rangle|\hat{\phi_m}\rangle(\langle\tilde{\phi_r}|\langle\hat{\phi_s}||\psi\rangle) * \langle\tilde{\phi_r}|\langle\hat{\phi_s}| \tag{12}$$

The partial trace of ρ is to take the inner product of the state ψ with a vector which lives only in the first (second) space If the state can be written as $|\psi\rangle = |\phi\rangle\tilde{|}\phi\rangle$, then one one can define the partial product

$$\langle\tilde{\zeta}||\psi\rangle = (\langle\tilde{\zeta}||\tilde{\phi}\rangle)|\phi\rangle \tag{13}$$

Ie, as a map from the Hilbert space for the full system to the Hilbert space of the first subsystem. Since any state can be written as a sum of products, by defining this partial inner product to be linear, one can define the partial inner product for an arbitrary state of the system. One can use this to define the partial trace

$$\mathrm{Tr}_2\rho = \sum_n \langle\tilde{\phi_n}|\rho|\tilde{\phi_n}\rangle \tag{14}$$

where again $|\tilde{\phi_n}\rangle$ is a complete orthonormal set.

Now, The partial trace of a Hermitian density matrix is Hermitian. It thus has a complete orthonormal set of eigenvectors. Et us assume that $|\phi\rangle_n$ has been chosen to be those eigenvectors.Then

$$\mathrm{Tr}_2\rho|\phi\rangle_n = \lambda_n|\phi_n\rangle \tag{15}$$

and thus $\mathrm{Tr}_2\rho = \sum_n \lambda_n|\phi_n\rangle\langle\phi_n|$. But,

$$|\psi\rangle = \sum_n \mu_n|\psi\rangle_n|\tilde{\chi_n}\rangle \tag{16}$$

and

$$\sum_n |\psi\rangle\langle\psi| = \sum_{nm} \mu_n^*\nu_m\langle\tilde{\chi_n}||\tilde{\chi_m}\rangle|\phi_n\rangle\langle\phi_m| \tag{17}$$

But since the $|\phi_n\rangle$ are eigenstates of the reduced density matrix, the $\tilde{\chi}_n$ must be orthonormal as well. Thus $\mathrm{Tr}_1|\psi\rangle\langle\psi|$ must have the χ_n as eigenvectors.

$$\mathrm{Tr}_1|\psi\rangle\langle\psi| = |\mu_n|^2|\chi\rangle_n\langle\chi|_n \tag{18}$$

Ie, the reduced density matrices for system 1 and 2 must have the same set of eigenvalues. The number of such non-zero eigenvalues is called the rank of the operator.

Note that this is only true of the density matrix of the whole system is a pure state– ie, is a single state $|\psi\rangle$. If the density matrix of the whole system is a mixed state (has a density matrix or rank greater than 1), then the above Schmidt decomposition does not imply that the eigenvalues of the reduced density matrices have the same eigenvalues. A trivial example is

$$\rho = 1/2(|\tilde{\chi}\rangle|\psi\rangle_1\langle\psi|_1\langle\tilde{\chi}| + |\tilde{\chi}\rangle|\psi\rangle_2\langle\psi|_2\langle\tilde{\chi}|) \tag{19}$$

Then the reduced density matrix under the partial trace over 2 is

$$\rho_1 = 1/2(|\psi\rangle_1\langle\psi|_1 + |\psi\rangle_2\langle\psi|_2) \tag{20}$$

with two eigenvalues $\frac{1}{2}$ while the reduced density matrix under partial trace over the first system is

$$\rho_2 = |\tilde{\chi}\rangle\langle\tilde{\chi}| \tag{21}$$

with one eigenvalue of 1, and one eigenvector with non-zero eigenvalue $|\chi\rangle$.

Decoherence

Given a system with two parts, if one starts with a system which has a pure state, ψ as the intial (Schroedinger) state, then, on making a measurement on system 1, one can get interference. For example, if one starts with the state

$$|\psi\rangle = \tilde{0}(\frac{1}{\sqrt{2}}(|-1\rangle + |1\rangle) \tag{22}$$

then a measurement of the operator

$$|1\rangle\langle 1| \tag{23}$$

will give a 50% chance of getting a 1, and 50% chance of getting 0. However, if you measure the operator

$$(\frac{1}{\sqrt{2}}(|-1\rangle + |1\rangle)(\frac{1}{\sqrt{2}}(\langle -1| + \langle 1|) \tag{24}$$

one will always get a value of 1.

One the other hand, if one has the state

$$|\psi\rangle = \frac{1}{\sqrt{2}}(|\tilde{-}\rangle 1_2 |-1\rangle_1 + |\tilde{1}\rangle_2 |1\rangle_1) \tag{25}$$

One will always get 50% no matter which of the operators one measures. The interference has disappeared.

One could make this entangled state by interacting the two systems. If σ_i are the sigma matrices for the first system and Σ_i are those for the second. We could start in the state $|\psi_0\rangle = |-1\rangle_2 |-1\rangle_1$. Now we interact with this with the Unitary operator on the first system which is equal to

$$U_S = I_2 \frac{1}{\sqrt{2}}(\sigma_3 + \sigma_1) \tag{26}$$

to get

$$|\psi\rangle = U|\psi_0\rangle \tag{27}$$

We now make a measurement with the second system acting as the measuring apparatus.

$$U_M = \frac{1}{2}(\frac{1}{\sqrt{2}}(\Sigma_3 + \Sigma_1)(1 + \sigma_3) + I_2(1 - sigma_3) \tag{28}$$

with

$$U_M U_S |\psi_0\rangle = \frac{1}{\sqrt{2}}(|-1\rangle|-1\rangle + |1\rangle|1\rangle) \tag{29}$$

The reduced density matrix for the first system is just thei$\frac{1}{2}$ the Identity Matrix and the expectation value off all of the σ_1 are 0. There is no interference.

This state is an entangeled state, and entanglement destroys coherence for any subsystem.

One of the prototypical systems to which this is applied is the two slit interference experiment, or the interferometer.

If one sends a photon through an equal arm interferometer, then the photon will (depending on the exact design of the half silvered mirror one uses) will come back out of the same port it was sent into. One the other hand, if one places a non-destructive photon detector into one of the paths of the interferometer, which measures for certain which arm of the interferometer the particle went down, then the interference is destroyed, and the photon will exit out of either port with equal probability.

Now, let us set up this experiment with a slight twist. We put the photon detector into one of the paths of the interferometer. We measure which port the photon came out of and write it down in a book together with the experiment number. However we now place into storage the photon detector and do not determine which state it is in. We also make sure that this detector does not interact with anything. 20 years after the experiment was finished, the results recorded in the book, we now haul the detectors for each of the experiments out of storage. If we measure whether or not the detector is in the "detected" state, we will find that there is no correlation between that and the port out of which the photon exited the detector.

However, we now carry out a different experiment. We instead measure the state

$$\frac{1}{2}(|\tilde{1}\rangle + |\tilde{0}\rangle)(\langle\tilde{1}| + \langle\tilde{0}|) \tag{30}$$

This is an operator with the two eigenvectors $\frac{1}{\sqrt{2}}(|\tilde{1}\rangle+|\tilde{0}\rangle))$ and $\frac{1}{\sqrt{2}}(|\tilde{1}\rangle-|\tilde{0}\rangle)$ with eigenvalues of 1 and 0 We now find that the outcomes of this measurement are prefectly correlated with the outcomes of the experiment done 20 years earlier. If the measurement now has outcome 1, then the original photon came out of same port it went into, while if the outcome is 0, the original photon came out of the the other port of the interferometer. (Or vice versa, with the port being perfectly correlated with the meaurement). What seemed to be decoherence, has still retained at least some vestage of the correlation that was in the original state after the "measurement" type interaction with the photon.

The interference pattern is hidden, but is correlated with the value of the (till 20 years later) unmeasured measuring apparatus.

Determining the value of that measuring apparatus reveals the interference pattern.

Altrnatively, in the light of the next part, the time conditions, if one places on the 20-year determination of the vlaue of Σ_2 the condition that one demands that the value is 1, then one sees an interference pattern in the data collected 20 years earlier.