

§1. ENTANGLEMENT & DENSITY MATRICES

In basic Q.M. you are taught that an isolated system can be described using a wave-function, i.e., a state-vector in Hilbert space:

$$|\psi\rangle = \sum_j a_j |\psi_j\rangle. \quad \text{Pure STATE} \quad (1.1)$$

where the $\{|\psi_j\rangle\}$ span the Hilbert space of the system - unless specified otherwise we will assume the $\{|\psi_j\rangle\}$ are an orthonormal set. For the moment we ignore time-dependence.

However this description is inadequate in general. For various reasons which we will come to, it may be that the system cannot be described as a pure state, but has to be described as a "mixture" of different states, with different probabilities associated with each - this is analogous to classical probability distributions over classical states.

The crucial point is that no superposition or interference between different states in a mixture is possible. It is sometimes said that the "mixture" exists because of our inadequate "knowledge of" the system state, but this can be very misleading, particularly in any discussion of the "meaning" or physical significance of the state vector/wave function.

Suppose we have a system in a mixture of states $\langle\psi_j|$ with probabilities p_j . Then the density matrix is

$$\hat{\rho} = |\psi_j\rangle p_j \langle\psi_j| \quad (1.2)$$

It is diagonal in this representation, and has matrix elements

$$\rho_{ij} = \langle i | \hat{\rho} | j \rangle = p_j \delta_{ij} \quad (1.3)$$

i.e.,

$$\rho_{ij} = \begin{pmatrix} p_1 & & 0 \\ & p_2 & \\ 0 & & \ddots \end{pmatrix} \quad (1.4)$$

Clearly the density matrix can be defined in some other representation as well. Thus more generally we have, in some representation of states $\{|k\rangle\}$, etc., that

$$\hat{\rho} = |k\rangle \rho_{kk'} \langle k'| \quad (1.5)$$

$$\begin{aligned} \rho_{kk'} &= \langle k | \hat{\rho} | k' \rangle = \langle k | \sum_j |\psi_j\rangle p_j \langle\psi_j| \rangle \\ &= U_{jk}^\dagger p_j U_{jk'} \end{aligned} \quad (1.6)$$

From (1.2) it is obvious that in the diagonal basis we can write for any operator \hat{A} acting in the Hilbert space that

$$\langle A \rangle = \text{Tr}[\hat{\rho}\hat{A}] = \text{Tr}[\hat{A}\hat{\rho}] \quad (1.6)$$

and since the trace is invariant under Hilbert space rotations, this is true in other bases.

For a pure state, we see that the density matrix becomes

$$\rho = |\psi\rangle\langle\psi| = \sum_j |\psi_j\rangle \rho_{ij} \langle\psi_j| \quad \left. \vphantom{\rho} \right\} \text{(PURE)} \quad (1.7)$$

$$\rho_{ij} = a_i a_j^*$$

Simple example: A spin- $\frac{1}{2}$ system in a state $|\rightarrow\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle + |\downarrow\rangle)$ is compared with a mixture of states in which $\frac{1}{2}$ of the spins in an ensemble are $|\uparrow\rangle$ and half are down (or: that the probability to be in $|\uparrow\rangle/|\downarrow\rangle$ for a single spin is $\frac{1}{2}$ each). Then we have

$$\rho_{ij}^{\text{PURE}} = \frac{1}{2} \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \quad (1.8)$$

$$\rho_{ij}^{\text{MIXED}} = \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad (1.9)$$

As an exercise you should try spins in different directions / or rotate the basis. Note that we cannot distinguish the two by mmts of, eg., $\langle S_z \rangle$.

§1(a) 2 COUPLED SYSTEMS

Consider now 2 coupled Q. systems, whose state is now described in the product space $\mathcal{H}(1,2) = \mathcal{H}_1 \otimes \mathcal{H}_2$ of the individual Hilbert spaces of each. A pure state can then be written:

$$|\Psi\rangle = \sum_{i\alpha} C_{i\alpha} |\psi_i\rangle |\phi_\alpha\rangle = \sum_{i\alpha} C_{i\alpha} |i\alpha\rangle \quad (1.10)$$

where $\{|\psi_i(1)\rangle\}$ span \mathcal{H}_1 and $\{|\phi_\alpha(2)\rangle\}$ span \mathcal{H}_2 . In exactly the same way as above we have

$$\hat{\rho}(1,2) = |\Psi\rangle\langle\Psi| \quad (1.11)$$

Now the crucial point here is that the dynamics of the 2 systems becomes entangled by any interaction between them. Thus, if the 2 systems are completely separable (which would happen if the Hamiltonian had no

interaction in it), then the solution to Schrödinger's eqn clearly gives an unentangled PRODUCT state:

$$\begin{aligned} |\Psi\rangle &\rightarrow |\psi\rangle|\phi\rangle \\ &= \sum_{i,\alpha} a_i b_\alpha |i\rangle|\alpha\rangle \end{aligned} \quad \left. \vphantom{\begin{aligned} |\Psi\rangle &\rightarrow |\psi\rangle|\phi\rangle \\ &= \sum_{i,\alpha} a_i b_\alpha |i\rangle|\alpha\rangle \end{aligned}} \right\} \text{UNENTANGLED} \quad (1.12)$$

if $\hat{H}(1,2) = \hat{H}(1) + \hat{H}(2)$

Notice that in another basis the state might look entangled - we come below to criteria for distinguishing pure & mixed, entangled & unentangled states.

Now, suppose we have at our disposal operators that only operate on one of the 2 systems (eg., system 1). In this case it is clear that, for some such operator $\hat{A}(1)$

$$\begin{aligned} \langle \hat{A}(1) \rangle &= \text{Tr}_{1,2} [\rho(1,2) \hat{A}(1)] && \text{(MIXTURE)} \\ &\rightarrow \langle \bar{\Psi}(1,2) | \hat{A}(1) | \bar{\Psi}(1,2) \rangle && \text{(PURE)} \end{aligned} \quad \left. \vphantom{\begin{aligned} \langle \hat{A}(1) \rangle &= \text{Tr}_{1,2} [\rho(1,2) \hat{A}(1)] \\ &\rightarrow \langle \bar{\Psi}(1,2) | \hat{A}(1) | \bar{\Psi}(1,2) \rangle \end{aligned}} \right\} (1.13)$$

which we now write as

$$\langle \hat{A}(1) \rangle = \text{Tr}_1 [\bar{\rho}(1) \hat{A}(1)] \quad (1.14)$$

where $\bar{\rho}(1)$ is the REDUCED DENSITY MATRIX, given by

$$\bar{\rho}(1) = \text{Tr}_2 [\rho(1,2)] \quad (1.15)$$

or, written explicitly in the basis of states of system 1, we have

$$\begin{aligned} \bar{\rho}(1) &= \sum_{\alpha} \langle \alpha | \left(\sum_{i,j} \sum_{\beta} |i\rangle\langle j| c_{i\alpha} c_{j\beta}^* \langle j|\beta| \right) | \alpha \rangle \\ &= \sum_{\alpha} \sum_{i,j} |i\rangle\langle j| c_{i\alpha} c_{j\alpha}^* \end{aligned} \quad (1.16)$$

ie., $\bar{\rho}_{ij} = \langle i | \bar{\rho} | j \rangle = \sum_{\alpha} c_{i\alpha} c_{j\alpha}^* \quad (1.17)$

From this you see that it looks like we've averaged over all possible states in \mathcal{H}_2 , giving them all equal weight. Obviously one can think of more general averages, and we will later come to these.

Simple Example: Consider 2 spin- $\frac{1}{2}$ systems (2 qubits), described by Pauli matrices $\hat{\sigma}_i$ and $\hat{\tau}_i$. We will assume nothing for the moment about their Hamiltonians. The 2-spin density matrix is a 4×4 matrix, which we will define in the state-space representation of states $|TT\rangle$, $|Tb\rangle$, $|bT\rangle$, and $|bb\rangle$. Consider now 2 different states

of this system (the states are ordered as $|\uparrow\uparrow\rangle, |\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle, |\downarrow\downarrow\rangle$):

$$(i) |\Psi(1,2)\rangle = \frac{1}{\sqrt{2}} (|\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle e^{i\theta}) \quad (1.18)$$

$$\text{Then } \rho_{\alpha,\beta} = \frac{1}{2} \begin{pmatrix} 1 & 0 & 0 & e^{-i\theta} \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ e^{i\theta} & 0 & 0 & 1 \end{pmatrix} \quad (1.19)$$

$$\text{and } \bar{\rho}_{ij} = \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad (1.20)$$

ie., the reduced density matrix describes a simple mixture of $|\uparrow\rangle$ and $|\downarrow\rangle$ states for system 1; entanglement between \mathcal{H}_1 and \mathcal{H}_2 is gone.

$$(ii) |\Psi(1,2)\rangle = \frac{1}{\sqrt{2}} (|\uparrow\uparrow\rangle + |\downarrow\uparrow\rangle e^{i\phi}) \quad (1.21)$$

$$\text{So that } \rho_{\alpha,\beta} = \frac{1}{2} \begin{pmatrix} 1 & 0 & e^{-i\phi} & 0 \\ 0 & 0 & 0 & 0 \\ e^{i\phi} & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \quad (1.22)$$

$$\text{and } \bar{\rho}_{ij} = \frac{1}{2} \begin{pmatrix} 1 & e^{-i\phi} \\ e^{i\phi} & 1 \end{pmatrix} \quad (1.23)$$

and we now have a density matrix which contains off-diagonal interference terms - however, a little thought and you see that these terms have nothing to do with entanglement - they describe interference inside \mathcal{H}_1 alone.

Exercise: Consider more general states like $|\Psi\rangle = \sum_{\alpha} c_{\alpha} |\alpha\rangle = [a_1 |\uparrow\uparrow\rangle e^{i\phi_1} + a_2 |\uparrow\downarrow\rangle e^{i\phi_2} + a_3 |\downarrow\uparrow\rangle e^{i\phi_3} + a_4 |\downarrow\downarrow\rangle e^{i\phi_4}]$; try and understand the form of $\rho_j(i)$.

From these examples we already see some interesting things, as follows:

(a) Roughly speaking, we can say that correlations or interference terms between parts of the wave-function of system (ie., in \mathcal{H}_1) are not destroyed by averaging over system 2. However, entanglement between the 2 systems is destroyed. The point is that since $\bar{\rho}(i)$ has the matrix elements $\bar{\rho}_{\alpha\alpha}$ (summed over α), any correlation between $|i\rangle$

and $|\alpha\rangle$ implies the same correlation with $|j\rangle$ and $|\alpha\rangle$, i.e., it forces $\bar{p}_{j\alpha} \rightarrow \bar{p}_{\alpha\alpha}$, i.e. to a diagonal form. This is most clearly seen with the perfectly entangled wave function

$$|\Psi\rangle \rightarrow \sum_j c_j |\psi_j \phi_j\rangle = |\Psi_{ent}\rangle \quad (1.24)$$

in which all terms ψ_j in \mathcal{H}_1 are uniquely entangled with the terms ϕ_j in \mathcal{H}_2 (the notation here implies that the dimension of the 2 Hilbert spaces is the same, so that there is a 1-1 relationship between the ϕ_α and the ψ_j . We will see later how to generalize this). If we look at (1.12) it is clear that

$$\left. \begin{aligned} \rho_{\alpha\beta}^{(1,2)} &= c_i c_j^* \delta_{i\alpha} \delta_{j\beta} \\ \bar{p}_{ij}^{(1)} &= |c_j|^2 \delta_{ij} \equiv p_j \delta_{ij} \end{aligned} \right\} \quad (1.25)$$

As we shall discuss in more detail later, this result is nothing but the basis of the Born result for the probability of obtaining a given result for a measurement of an operator. Thus, imagine that system 2 is some quantum system which interacts with a measuring apparatus (system 1), and establishes the correlation embodied in (1.24). After this the systems can separate, but if we only have access to system 1, then it behaves as though in a mixture of states with probability p_j . More on this later.

(b) If we want to see entanglement in the combined state of the pair of systems. Then not any old operator will show this to us - some may not distinguish an entangled state from a simple mixture. This is easily seen formally by considering various operators acting on the pair of systems. If $\hat{O}^{(1,2)}$ is an operator acting on the 2 systems, we have

$$\begin{aligned} \langle \hat{O}^{(1,2)} \rangle &= \text{Tr}_{1,2} [\hat{\rho}^{(1,2)} \hat{O}^{(1,2)}] \\ &= \sum_{\alpha} c_{\alpha} c_{\alpha}^* \langle \alpha | O^{(1,2)} | \alpha \rangle \end{aligned} \quad (1.26)$$

which is indistinguishable from

$$\begin{aligned} \langle \hat{O}^{(1,2)} \rangle_{\text{MIXTURE}} &= \sum_{\alpha} c_{\alpha} c_{\alpha}^* O_{\alpha,\alpha} \\ &= \sum_{\alpha} p_{\alpha} O_{\alpha,\alpha} \quad (\text{if } \hat{O} \text{ is diagonal}) \end{aligned} \quad (1.27)$$

unless there are NON-DIAGONAL matrix elements in $O_{\alpha,\beta}$. For the completely entangled state (1.24), this gives

$$\langle \Psi_{ent} | \hat{O} | \Psi_{ent} \rangle = \sum_{ji} c_i c_j^* \langle \psi_i \phi_i | O^{(1,2)} | \psi_j \phi_j \rangle \quad (1.28)$$

and so we see that this state cannot be distinguished from a simple mixture of the different states $|\psi_i \phi_i\rangle$ (probability $|c_i|^2$) unless the operator has OFF-DIAGONAL matrix elements between the pair of states.

This should not surprise you - the same would be true of measurements on a single system. The superposition $\sum_j a_j \psi_j$ cannot be distinguished from the mixture of different ψ_j , having probabilities $|a_j|^2$, except by operators that are sensitive to the interference between the different components, i.e., having off-diagonal matrix elements A_{ij} .

Example: Consider 2 spins \hat{S}_1 and \hat{S}_2 (both spin $-\frac{1}{2}$), in some correlated state (choose, eg., the state

$$|\Psi\rangle = a_1 | \uparrow \uparrow \rangle e^{i\phi_1} + a_2 | \downarrow \downarrow \rangle e^{i\phi_2} \quad (1.29)$$

which is an example of (1.24)). Now, consider the effect of the following operators:

- (i) $\hat{S}_1^z \hat{S}_2^z$
- (ii) $\hat{S}_1^z \hat{S}_2^x$
- (iii) $\hat{S}_1^x \hat{S}_2^x$

It will easily be seen that only the 3rd operator, which has off-diagonal matrix elements between the 2 states in (1.29), will distinguish the superposition from a mixture. This is a special case of (1.28), with O taking the form $\hat{A}(1)\hat{B}(2)$, where $\hat{A}(1)$ is a spin operator acting on system 1 and $\hat{B}(2)$ another acting on system 2.

(c) The simplest way to distinguish a mixture from a pure state, if one has the density matrix, is to note the inequality

$$\left. \begin{aligned} \text{Tr}[\hat{\rho}^2] &< \text{Tr}[\hat{\rho}] && \text{(MIXTURE)} \\ \text{Tr}[\hat{\rho}^2] &= \text{Tr}[\hat{\rho}] && \text{(PURE STATE)} \end{aligned} \right\} (1.30)$$

These results are obvious in the representation where $\hat{\rho}$ is diagonal, and true in any representation because $\text{Tr}[\hat{\rho}^n]$ is invariant under rotations in Hilbert space.

§1(b) DENSITY MATRICES IN PICTURES

We can plot the form of the density matrix, provided it is not too complicated - this is a useful exercise for developing intuition. So we begin by considering some

examples, and then make a few observations about these.

(a) PARTICLE in 1-d MOTION

In this case it is most convenient to plot \hat{p} in a position representation, i.e., $\rho(Q, Q') = \langle Q | \hat{\rho} | Q' \rangle$. Let us consider a few interesting examples.

First consider a system with a pure state wave-function

$$\psi(Q) = \langle Q | \psi \rangle$$

$$= \frac{1}{2} [g(Q-Q_1) e^{ik_1 Q} + g(Q-Q_2) e^{ik_2 Q}] \quad (1.31)$$

i.e., a superposition of 2 wave-packets, each having the Gaussian normalised form

$$g(Q) = \frac{1}{\pi^{1/2} L_0} e^{-(Q/L_0)^2}$$

If these wave-packets are well separated (i.e. if $|Q_1 - Q_2| \geq 2L_0$) then the interference terms are small - note we can write the probability of finding a particle at Q as

$$|\psi(Q)|^2 \equiv \rho(Q, Q)$$

$$= \frac{1}{4} [g^2(Q-Q_1) + g^2(Q-Q_2) + 2g(Q-Q_1)g(Q-Q_2) \cos 2\kappa Q] \quad (1.32)$$

where we write

$$\left. \begin{aligned} K_0 &= \frac{1}{2}(k_1 + k_2) && \text{c.o.m. momentum} \\ \kappa &= \frac{1}{2}(k_1 - k_2) && \text{relative momentum} \end{aligned} \right\} \quad (1.33)$$

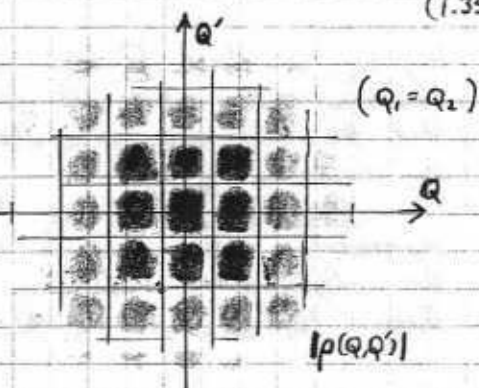
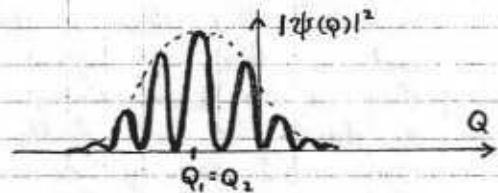
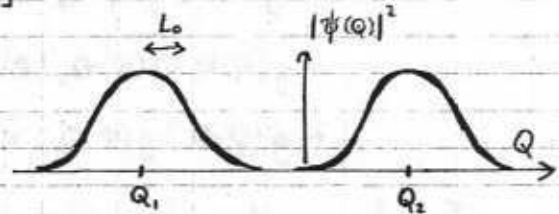
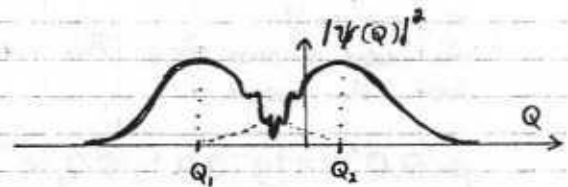
What now of the density matrix? Let's look at this first for the case where $Q_1 = Q_2$ (3rd figure above), in which case we have (assuming without loss of generality that $Q_1 = Q_2 = 0$)

$$\rho(Q, Q') \rightarrow g(Q)g(Q') e^{ik_0(Q-Q')} \cos \kappa Q \cos \kappa Q' \quad (1.34)$$

$$|\psi(Q)|^2 \rightarrow g^2(Q) \cos \kappa Q \quad (1.35)$$

The wave term $e^{ik_0(Q-Q')}$ is of less interest than the $\cos \kappa Q \cos \kappa Q'$ term, which is telling us about the relative interference between the 2 wave-packets - indeed, going to the c.o.m. frame removes this term ($K_0 \rightarrow 0$).

We see very clearly the contrasted between the 2 states $|k_1\rangle, |k_2\rangle$, with a characteristic length-scale $\sim \pi/\kappa$.

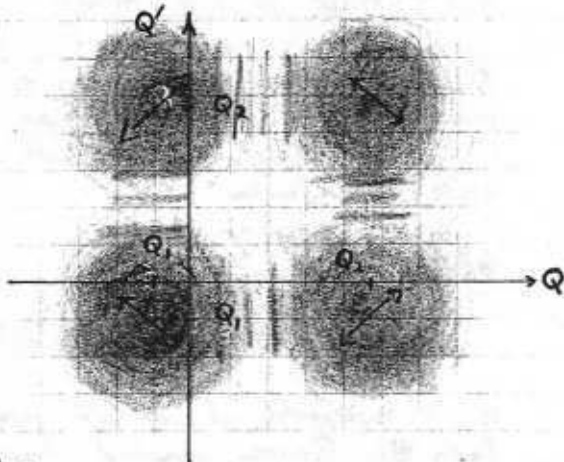


Now we go to the case where the interference involves not just that between different momentum states, but also the overlap (or not) between the 2 wave-packets. To make things simple let's assume that

$$K_0 = 0$$

ie., we go to the centre of mass frame. Then we have the result

$$\begin{aligned} \rho(Q, Q') = & [g(Q-Q_1)g(Q'-Q_1)e^{ik(Q-Q')} \\ & + g(Q-Q_2)g(Q'-Q_2)e^{-ik(Q-Q')} \\ & + g(Q-Q_1)g(Q'-Q_2)e^{ik(Q+Q')} \\ & + g(Q-Q_2)g(Q'-Q_1)e^{-ik(Q+Q')}] / 4 \end{aligned} \quad (1.36)$$



The diagram shows how this works when the 2 wave-packets are sufficiently separated that there is little interference between them. Nevertheless inside each of the 4 regions in the $Q-Q'$ plane where $\rho(Q, Q')$ is large, there is a wave having a certain direction or sense in the plane, which is shown by the double-headed arrows. Any overlap between these regions will show up as real interference (in $|\rho(Q, Q')|$), again on a length scale $\sim \pi/k$.

Now it is obvious that we could also plot these results in the momentum representation - since we are superposing 2 momentum states, this is more natural. In this representation we have

$$\begin{aligned} \psi_p & \equiv \langle p | \psi \rangle = \langle p | Q \rangle \langle Q | \psi \rangle \\ & = \int dQ \bar{e}^{ipQ} \frac{1}{2} [g(Q-Q_1)e^{ik_1Q} + g(Q-Q_2)e^{ik_2Q}] \\ & = \frac{1}{2} [\bar{g}(p-k_1)e^{-i(p-k_1)Q_1} + \bar{g}(p-k_2)e^{-i(p-k_2)Q_2}] \end{aligned} \quad (1.37)$$

where

$$\bar{g}(p) = \frac{L_0}{\pi^{1/2}} e^{-p^2 L_0^2} \quad (1.38)$$

ie., we now have Gaussian wave-packets centred round k_1 and k_2 in momentum space - but with width $1/L_0$ (instead of the width L_0 that the real space wave-packets have). If $L_0 \rightarrow 0$ these become δ -fns in momentum space.

Exercise: Work out the density matrix for this system in the momentum representation, and understand the role of the various phase factors, and the interference in momentum space as a function of both L_0 and the factors $|k_1 - k_2|$, and $|Q_1 - Q_2|$.

(b) TWO-LEVEL SYSTEM

There is no need here to draw the pictures - the physics is so simple that you can just imagine things from the matrices themselves. Thus the density matrix for the state

$$|\psi\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle + |\downarrow\rangle) \equiv |\mathcal{X}\rangle$$

which was given in (1.8), is shown here in the

$\hat{\tau}_z$ representation (i.e., the representation of eigenstates of $\hat{\tau}_z$). The interference terms are as big as the diagonal terms - on the other hand, if we went to the $\hat{\tau}_x$ representation, only one element of the density matrix will be occupied (i.e., the state is $|\mathcal{X}\rangle$ with probability 1).

Now, consider the mixture in (1.9). This has only diagonal elements. However, you will easily see that a rotation doesn't help this - we still have no interference terms.

Another way of saying this is to say that all coherence/interference between the states (either $|\uparrow\rangle$ and $|\downarrow\rangle$, or $|\rightarrow\rangle$ and $|\leftarrow\rangle$, etc) has been lost in the mixture - we have complete DECOHERENCE).

Thus, although off-diagonal terms can be changed by changing the representation (at best to give a single diagonal element if we have a pure state), they will be zero in any representation, if we have a completely decohered mixture.

In this context "entanglement" is just interference between 2 different systems, and disentanglement or suppression of this entanglement is a process of decoherence.

