

## Mixtures and the Density Matrix: Impure States

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Even in classical physics it is possible that the state of a system be unknown, or only partly known, simply because of our ignorance. Thus, in classical thermodynamics, knowledge of the temperature, pressure and density of a gas does not determine the specific state of all the constituent molecules. In classical physics this information would be regarded as knowable in principle, but just not known in practice. For a molecule chosen at random, there will be a certain probability that it possess a kinetic energy in the range, say,  $E$  to  $E + dE$ . Thus, the gas is a mixture of molecules of various energies, moving in various directions, and these quantities can be assigned probability densities. It is possible for this type of “deterministic” mixture to occur also in quantum mechanics. In which case the “deterministic” probabilities must be codified in the formalism as well as the quantum mechanical probabilities which arise from the Born Rule. How is this done?

It cannot be done simply by adding two quantum states together. This can be demonstrated with a simple example. Consider two spin  $\frac{1}{2}$  particles. One is prepared in the “spin up” state wrt the z-axis, and the other in the “spin up” state wrt the x-axis. Let us prepare a great many ( $N$ ) of these two-particle mixtures, and let us measure the spin of just one of the pair of particles chosen at random from each of the  $N$  mixtures. Suppose we choose to measure the spin in the z-direction. It is clear what the distribution of our measurements will be. About half the particles chosen will be in the z-spin-up state, and these will all give the result  $+1$  (measuring in units of  $\hbar/2$ ). The other half will be in the x-spin-up state. These particles will give a z-spin-up value of  $+1$  half the time, and  $-1$  the other half. So, overall, we must observe a z-spin of  $+1$  on 75% of the occasions and hence a z-spin of  $-1$  on 25% of the occasions.

But see what happens if we naïvely assumed that the two particle mixture could be described by adding their wavefunctions. If  $|\uparrow\rangle$  and  $|\downarrow\rangle$  represent spin up & down wrt the z axis, then the x-spin-up state is  $(|\uparrow\rangle + |\downarrow\rangle)/\sqrt{2}$ . Simply adding the states with the same weighting would give,

$$|\psi\rangle = A \left[ |\uparrow\rangle + \frac{|\uparrow\rangle + |\downarrow\rangle}{\sqrt{2}} \right] \quad (1.4.1)$$

where  $A$  is required to normalise, and hence takes the value  $A = \frac{1}{\sqrt{2 + \sqrt{2}}}$ . Hence (1.4.1)

becomes,  $|\psi\rangle = 0.92388|\uparrow\rangle + 0.38268|\downarrow\rangle$ . This state would produce measurements with z-spin-up 85.36% of the time, and z-spin-down 14.64% of the time. This is the wrong result, and hence the mixture of the two particles cannot be represented by simply adding the Hilbert space states as in (1.4.1).

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A more fundamental physical objection to (1.4.1) is that it represents a pure quantum state. But a pure quantum state cannot be made by throwing two particles together willy-nilly. Equ.(1.4.1) is a coherent quantum superposition, whereas in a classical mixture the two particles are incoherent. This is the crucial distinction.

So how can a mixture be codified correctly in quantum mechanics? The answer is in terms of the density matrix. Recall that a pure quantum state,  $|\psi\rangle$ , has a density matrix  $|\psi\rangle\langle\psi|$  (see Part 1 of these QM notes, QM1). So, for a pure state, specifying the density matrix is equivalent to specifying the state,  $|\psi\rangle$ . However, if we now have a classical (i.e. an incoherent) mixture in which state  $|\psi_1\rangle$  occurs with probability  $p_1$ , state  $|\psi_2\rangle$  occurs with probability  $p_2$ , etc., the density matrix of the mixture is defined by,

$$\hat{\rho} = \sum_{i=1}^n p_i |\psi_i\rangle\langle\psi_i| \quad (1.4.2)$$

where  $p_i$  are probabilities, and hence are real numbers in the range  $[0, 1]$  such that

$$\sum_{i=1}^n p_i = 1, \text{ where } n \text{ is the (arbitrary) number of terms in the mixture, (1.4.2).}$$

Thus, the density matrix is still an operator in Hilbert space, and hence is a well defined quantity in our formalism.

The reason why the density matrix is the correct vehicle for formulating a quantum mixture is that it represents probabilities, as contrasted with the state vector which represents probability amplitudes.

Note that there is no requirement for the states entering the sum in (1.4.2) to be orthogonal. In our example above the first state is a z-spin state whereas the second is an x-spin state, and these are not orthogonal. The density matrix for this example is thus,

$$\begin{aligned} \hat{\rho} &= 0.5|\uparrow\rangle\langle\uparrow| + 0.5 \times \frac{1}{\sqrt{2}} [|\uparrow\rangle + |\downarrow\rangle] \frac{1}{\sqrt{2}} [|\uparrow\rangle + \langle\downarrow|] \\ &= 0.75|\uparrow\rangle\langle\uparrow| + 0.25|\downarrow\rangle\langle\downarrow| + 0.25|\uparrow\rangle\langle\downarrow| + 0.25|\downarrow\rangle\langle\uparrow| \\ &= \begin{pmatrix} 0.75 & 0.25 \\ 0.25 & 0.25 \end{pmatrix} \end{aligned} \quad (1.4.3)$$

where the final matrix expression is in the obvious (z) representation.

When the components of the density matrix are expressed wrt an orthonormal basis, its diagonal elements are the probabilities of the corresponding measurement outcomes. So the 75% / 25% up/down result is reproduced correctly in this formalism.

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The expectation value is the sum of the product of these probabilities with the measurement eigenvalues. This can be written in exactly the same way as we saw for a pure state in QM1, i.e. as a trace over the product of the density matrix and the operator representing the observable,

$$\langle Q \rangle = \text{Tr}(\hat{\rho}\hat{Q}) \quad (1.4.4)$$

In this case we have,  $\langle z \text{ spin} \rangle = \langle \sigma_z \rangle = \text{Tr} \left[ \begin{pmatrix} 0.75 & 0.25 \\ 0.25 & 0.25 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \right] = \text{Tr} \begin{pmatrix} 0.75 & -.25 \\ 0.25 & -.25 \end{pmatrix} = 0.5$

An important property of the density matrix is that  $\text{Tr}(\hat{\rho}) = \sum_i p_i = 1$ . This follows directly from (1.4.2). Consider an orthonormal basis  $\{|\phi_j\rangle\}$ . Then

$$\begin{aligned} \text{Tr}(\hat{\rho}) &= \sum_{j=1}^{N_s} \sum_{i=1}^n p_i \langle \phi_j | \psi_i \rangle \langle \psi_i | \phi_j \rangle = \sum_{j=1}^{N_s} \sum_{i=1}^n p_i \langle \psi_i | \phi_j \rangle \langle \phi_j | \psi_i \rangle \\ &= \sum_{i=1}^n p_i \langle \psi_i | \psi_i \rangle = \sum_i p_i = 1 \end{aligned} \quad (1.4.5)$$

where  $N_s$  is the number of states and  $n$  is the (arbitrary) number of terms in the sum defining the density matrix in (1.4.1). We have used the fact that  $\sum_{j=1}^{N_s} |\phi_j\rangle \langle \phi_j| \equiv I$ , and the states  $|\psi_i\rangle$  must be normalised, though not necessarily orthogonal.

If  $\hat{\rho}$  is simply the pure state  $|\psi\rangle \langle \psi|$  then it is clear that  $\hat{\rho}^2 = \hat{\rho}$  and hence  $\text{Tr}(\hat{\rho}^2) = 1$ . In fact this is *only* true if  $\hat{\rho}$  is a pure state. Otherwise we have  $\text{Tr}(\hat{\rho}^2) < 1$ . This follows in a similar manner to (1.4.5), i.e.,

$$\begin{aligned} \text{Tr}(\hat{\rho}^2) &= \sum_{j=1}^{N_s} \sum_{i,k=1}^n p_i p_k \langle \phi_j | \psi_i \rangle \langle \psi_i | \psi_k \rangle \langle \psi_k | \phi_j \rangle = \sum_{j=1}^{N_s} \sum_{i,l=1}^n p_i p_k \langle \psi_k | \phi_j \rangle \langle \phi_j | \psi_i \rangle \langle \psi_i | \psi_k \rangle \\ &= \sum_{i,k=1}^n p_i p_k \langle \psi_k | \psi_i \rangle \langle \psi_i | \psi_k \rangle = \sum_{i,k=1}^n p_i p_k |\langle \psi_i | \psi_k \rangle|^2 < 1 \end{aligned} \quad (1.4.6)$$

where the strict inequality holds provided that  $\hat{\rho}$  is not a pure state. The last step follows because each of the  $|\langle \psi_i | \psi_k \rangle|^2$  is in the range  $[0, 1]$ , and hence  $\sum_{k=1}^n p_k |\langle \psi_i | \psi_k \rangle|^2 < 1$  and

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therefore  $\sum_{i,k=1}^n p_i p_k |\langle \psi_i | \psi_k \rangle|^2 < \sum_{i=1}^n p_i = 1$ . Note again that this holds even though the states  $|\psi_i\rangle$  may not be orthogonal (though they must be normalised).

In the particular case that the  $|\psi_i\rangle$  are orthogonal, then (1.4.6) gives  $\text{Tr}(\hat{\rho}^2) = \sum_{i=1}^n p_i^2 < 1$ , but this is not true in general.

The fact that  $\text{Tr}(\hat{\rho}^2) = 1$  only for a pure state provides a convenient test of a pure state. It will generally be simpler than diagonalising the density matrix to show explicitly that it has just one non-zero term.

It follows from (1.4.2) that the density matrix is Hermetian,  $\hat{\rho}^+ = \hat{\rho}$ , and hence that its real eigenvalues are orthogonal eigenvectors. The latter provide a unitary transformation which diagonalise the density matrix. That is, if we change to the basis  $\{|\phi_j\rangle\}$  which consists of the eigenvectors of  $\hat{\rho}$  then it becomes,

$$\hat{\rho} = \sum_{i=1}^{N_s} \lambda_i |\phi_i\rangle\langle\phi_i| \quad (1.4.7)$$

A key distinction between (1.4.2) and (1.4.7) is that the latter involves a sum over the number of possible states,  $N_s$ , i.e. the dimension of the Hilbert space, as opposed to (1.4.2) which is a sum over an arbitrary number of terms in the mixture. The diagonal components,  $\lambda_i$ , are, of course, the eigenvalues of the density matrix. Because we know that  $\text{Tr}(\hat{\rho}) = 1$  it follows that the eigenvalues sum to unity.

The density matrix is only diagonal in this specific representation. Transforming to an alternative orthonormal basis it will become a full matrix, i.e., putting  $|\phi_i\rangle = U_{ij} |\phi'_j\rangle$  gives,

$$\hat{\rho} = \sum_{i,j,k=1}^{N_s} \lambda_i U_{ij} U_{ik}^* |\phi'_j\rangle\langle\phi'_k| = \sum_{j,k=1}^{N_s} C_{jk} |\phi'_j\rangle\langle\phi'_k| \quad (1.4.8)$$

Thus, for example, even if we were dealing with a pure state, the density matrix would appear to be a full matrix when expressed in a general basis. The test  $\text{Tr}(\hat{\rho}^2) = 1$  is then the most efficient means of determining whether the state is actually pure. If not, the diagonal form can only be obtained from the general form by solving the eigenvalue problem.

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