Chapter 15

Density Matrices

15.1 Introduction

Density matrices are employed in quantum mechanics to give a *partial description* of a quantum system, one from which certain details have been omitted. For example, in the case of a composite quantum system consisting of two or more subsystems, one may find it useful to construct a quantum description of just one of these subsystems, either at a single time or as a function of time, while ignoring the other subsystem(s). Or it may be the case that the exact initial state of a quantum system is not known, and one wants to use a probability distribution or pre-probability as an initial state.

Probability distributions are used in classical statistical mechanics in order to construct partial descriptions, and density matrices play a somewhat similar role in quantum statistical mechanics, a subject which lies outside the scope of this book. In this chapter we shall mention a few of the ways in which density matrices are used in quantum theory, and discuss their physical significance.

Positive operators and density matrices were defined in Sec. 3.9. To recapitulate, a positive operator is a Hermitian operator whose eigenvalues are non-negative, and a density matrix ρ is a positive operator whose trace (the sum of its eigenvalues) is 1. If R is a positive operator but not the zero operator, its trace is greater than zero, and one can define a corresponding density matrix by means of the formula

$$\rho = R/\mathrm{Tr}(R). \tag{15.1}$$

The eigenvalues of a density matrix ρ must lie between 0 and 1. If one of the eigenvalues is 1, the rest must be 0, and $\rho = \rho^2$ is a projector onto a one-dimensional subspace of the Hilbert space. Such a density matrix is called a *pure state*. Otherwise there must be at least two non-zero eigenvalues, and the density matrix is called a *mixed state*.

Density matrices very often function as pre-probabilities which can be used to generate probability distributions in different bases, and averages of different observables. This is discussed in Sec. 15.2. Density matrices arise rather naturally when one is trying to describe a subsystem $\mathcal{A}$ of a larger system $\mathcal{A} \otimes \mathcal{B}$, and Secs. 15.3 to 15.5 are devoted to this topic. The use of a density matrix to describe an isolated system is considered in Sec. 15.6. Section 15.7 on conditional density matrices discusses a more advanced topic related to correlations between subsystems.

15.2 Density Matrix as a Pre-Probability

Recall that in some circumstances a quantum wave function or ket $|\psi\rangle$ need not denote an actual physical property $[\psi]$ of the quantum system; instead it can serve as a *pre-probability*, a mathematical device which allows one to calculate various probabilities. See the discussion in Sec. 9.4, and various examples in Sec. 12.1 and Ch. 13. In most cases (see the latter part of Sec. 15.6 below for one of the exceptions) a density matrix is best thought of as a pre-probability. Thus while it provides useful information about a quantum system, one should not think of it as corresponding to an actual physical property; it does not represent "quantum reality". For this reason, referring to a density matrix as the "state" of a quantum system can be misleading. However, in classical statistical mechanics it is customary to refer to probability distributions as "states", even though a probability distribution is obviously not a physical property, and hence it is not unreasonable to use the same term for a density matrix functioning as a quantum pre-probability.

A density matrix which is a pre-probability can be used to generate a probability distribution in the following way. Given a sample space corresponding to a decomposition of the identity

$$I = \sum_j P^j \tag{15.2}$$

into orthogonal projectors, the probability of the property P^j is

$$p_j = \mathrm{Tr}(P^j \rho P^j) = \mathrm{Tr}(\rho P^j), \tag{15.3}$$

where the traces are equal because of cyclic permutation, Sec. 3.8. The operator $P^j \rho P^j$ is positive—use the criterion (3.86)—and therefore its trace, the sum of its eigenvalues, cannot be negative. Thus (15.3) defines a set of probabilities: non-negative real numbers whose sum, in view of (15.2), is equal to 1, the trace of ρ. In particular, if for each j the projector $P^j = [j]$ is onto a state belonging to an orthonormal basis $\{|j\rangle\}$, then

$$p_j = \mathrm{Tr}\big(\rho|j\rangle\langle j|\big) = \langle j|\rho|j\rangle \tag{15.4}$$

is the j'th diagonal element of ρ in this basis. Hence the diagonal elements of ρ in an orthonormal basis form a probability distribution when this basis is used as the quantum sample space. As a special case, the probabilities given by the Born rule, Secs. 9.3 and 9.4, are of the form (15.4) when $\rho = |\psi_1\rangle\langle\psi_1|$ and $|j\rangle = |\phi_1^j\rangle$ in the notation used in (9.35).

From (15.3) it is evident that the average $\langle V\rangle$, see (5.42), of an observable

$$V = V^\dagger = \sum_j v_j P^j \tag{15.5}$$

can be written in a very compact form using the density matrix:

$$\langle V\rangle = \sum_j p_j v_j = \mathrm{Tr}(\rho V). \tag{15.6}$$

If ρ is a pure state $|\psi_1\rangle\langle\psi_1|$, then $\langle V\rangle$ is $\langle\psi_1|V|\psi_1\rangle$, as in (9.38). It is worth emphasizing that while the trace in (15.6) can be carried out using any basis, interpreting $\langle V\rangle$ as the average of a physical variable requires at least an implicit reference to a basis (or decomposition of the identity) in which V is diagonal. Thus if two observables V and W do not commute with each other, the two averages $\langle V\rangle$ and $\langle W\rangle$ cannot be thought of as pertaining to a single (stochastic) description of a quantum system, for they necessarily involve incompatible quantum sample spaces, and thus different probability distributions. The comments made about averages in Ch. 9 while discussing the Born rule, towards the end of Sec. 9.3 and in connection with (9.38), also apply to averages calculated using density matrices.

15.3 Reduced Density Matrix for Subsystem

Suppose we are interested in a composite system (Ch. 6) with a Hilbert space $\mathcal{A}\otimes\mathcal{B}$. For example, $\mathcal{A}$ might be the Hilbert space of a particle, and $\mathcal{B}$ that of some system (possibly another particle) with which it interacts. At t_0 let $|\Psi_0\rangle$ be a normalized state of the combined system which evolves, by Schrödinger's equation, to a state $|\Psi_1\rangle$ at time t_1. Assume that we are interested in histories for two times, t_0 and t_1, of the form $\Psi_0 \odot (A^j\otimes I)$, where Ψ_0 stands for the projector $[\Psi_0] = |\Psi_0\rangle\langle\Psi_0|$, and the A^j form a decomposition of the identity of the subsystem $\mathcal{A}$:

$$I_{\mathcal{A}} = \sum_j A^j. \tag{15.7}$$

The probability that system $\mathcal{A}$ will have the property A^j at t_1 can be calculated using the generalization of the Born rule found in (10.34):

$$\Pr(A^j) = \langle\Psi_1|A^j\otimes I|\Psi_1\rangle = \mathrm{Tr}\big[\Psi_1(A^j\otimes I)\big]. \tag{15.8}$$

The trace on the right side of (15.8) can be carried out in two steps, see Sec. 6.5: first a partial trace over $\mathcal{B}$ to yield an operator on $\mathcal{A}$, followed by a trace over $\mathcal{A}$. In the first step the operator A^j, since it acts on $\mathcal{A}$ rather than $\mathcal{B}$, can be taken out of the trace, so that

$$\mathrm{Tr}_{\mathcal{B}}\big[\Psi_1(A^j\otimes I)\big] = \rho A^j, \tag{15.9}$$

where

$$\rho = \mathrm{Tr}_{\mathcal{B}}(\Psi_1) \tag{15.10}$$

is called the *reduced density matrix*, because it is used to describe the subsystem $\mathcal{A}$ rather than the whole system $\mathcal{A}\otimes\mathcal{B}$. Since ρ is the partial trace of a positive operator, it is itself a positive operator: apply the test in (3.86). In addition, the trace of ρ is

$$\mathrm{Tr}_{\mathcal{A}}(\rho) = \mathrm{Tr}(\Psi_1) = \langle\Psi_1|\Psi_1\rangle = 1, \tag{15.11}$$

so ρ is a density matrix. Upon taking the trace of both sides of (15.9) over $\mathcal{A}$, one obtains, see (15.8), the expression

$$\Pr(A^j) = \mathrm{Tr}_{\mathcal{A}}\left(\rho A^j\right) \tag{15.12}$$

for the probability of the property A^j, in agreement with (15.3). Note that $|\Psi_1\rangle$, the counterpart of $|\psi_1\rangle$ in the discussion of the Born rule in Sec. 9.4, functions as a pre-probability, not as a physical property, and its partial trace ρ also functions as a pre-probability, which can be used to calculate probabilities for any sample space of the form (15.7). In the same way one can define the reduced density matrix

$$\rho' = \mathrm{Tr}_{\mathcal{A}}(\Psi_1) \tag{15.13}$$

for system $\mathcal{B}$ and use it to calculate probabilities of various properties of system $\mathcal{B}$.

Let us consider a simple example. Let $\mathcal{A}$ and $\mathcal{B}$ be the spin spaces for two spin-half particles a and b, and let

$$|\Psi_1\rangle = \alpha|z_a^+\rangle \otimes |z_b^-\rangle + \beta|z_a^-\rangle \otimes |z_b^+\rangle, \tag{15.14}$$

where the subscripts identify the particles, and the coefficients satisfy

$$|\alpha|^2 + |\beta|^2 = 1, \tag{15.15}$$

so that $|\Psi_1\rangle$ is normalized. The corresponding projector is

$$\begin{aligned}\Psi_1 = |\Psi_1\rangle\langle\Psi_1| = |\alpha|^2 |z_a^+\rangle\langle z_a^+| \otimes |z_b^-\rangle\langle z_b^-| + |\beta|^2 |z_a^-\rangle\langle z_a^-| \otimes |z_b^+\rangle\langle z_b^+| \\ + \alpha\beta^* |z_a^+\rangle\langle z_a^-| \otimes |z_b^-\rangle\langle z_b^+| + \alpha^*\beta |z_a^-\rangle\langle z_a^+| \otimes |z_b^+\rangle\langle z_b^-|.\end{aligned} \tag{15.16}$$

The partial trace in (15.10) is easily evaluated by noting that

$$\mathrm{Tr}_{\mathcal{B}}\left(|z_b^-\rangle\langle z_b^+|\right) = \langle z_b^+|z_b^-\rangle = 0, \tag{15.17}$$

etc.; thus

$$\rho = |\alpha|^2 [z_a^+] + |\beta|^2 [z_a^-]. \tag{15.18}$$

This is a positive operator, since its eigenvalues are $|\alpha|^2$ and $|\beta|^2$, and its trace is equal to 1, (15.15). If both α and β are nonzero, ρ is a mixed state.

Employing either (15.8) or (15.12), one can show that if the decomposition $[z_a^+]$, $[z_a^-]$, the S_{az} framework, is used as a sample space, the corresponding probabilities are $|\alpha|^2$ and $|\beta|^2$, whereas if one uses $[x_a^+]$, $[x_a^-]$, the S_{ax} framework, the probability of each is 1/2. Of course it makes no sense to suppose that these two sets of probabilities refer simultaneously to the same particle, as the two sample spaces are incompatible. Using either the S_{ax} or the S_{az} framework precludes treating Ψ_1 at t_1 as a physical property when α and β are both nonzero, since as a projector it does not commute with $[w_a^+]$ for any direction w. Thus Ψ_1 and its partial trace ρ should be thought of as pre-probabilities.

Except when $|\alpha|^2 = |\beta|^2$ there is a unique basis, $|z_a^+\rangle$, $|z_a^-\rangle$, in which ρ is diagonal. However, ρ can be used to assign a probability distribution for any basis, and thus there is nothing special about the basis in which it is diagonal. In this respect ρ differs from operators that represent physical variables, such as the Hamiltonian, for which the eigenfunctions do have a particular physical significance.

The expression on the right side of (15.14) is an example of the Schmidt form

$$|\Psi_1\rangle = \sum_j \lambda_j |\hat{a}_j\rangle \otimes |\hat{b}_j\rangle \tag{15.19}$$

introduced in (6.18), where $\{|\hat{a}_j\rangle\}$ and $\{|\hat{b}_k\rangle\}$ are special choices of orthonormal bases for $\mathcal{A}$ and $\mathcal{B}$. The reduced density matrices ρ and ρ' for $\mathcal{A}$ and $\mathcal{B}$ are easily calculated from the Schmidt form using (15.10) and (15.13), and one finds:

$$\rho = \sum_j |\lambda_j|^2 [\hat{a}_j], \quad \rho' = \sum_j |\lambda_j|^2 [\hat{b}_j]. \tag{15.20}$$

One can check that ρ in (15.18) is, indeed, given by this expression.

Relative to the physical state of the subsystem $\mathcal{A}$ at time t_1, ρ contains the same amount of information as Ψ_1. However, relative to the total system $\mathcal{A}\otimes\mathcal{B}$, ρ is much less informative. Suppose that

$$I_{\mathcal{B}} = \sum_k B^k \tag{15.21}$$

is some decomposition of the identity for subsystem $\mathcal{B}$, and we are interested in histories of the form $\Psi_0 \odot (A^j \otimes B^k)$. Then the joint probability distribution

$$\Pr(A^j \wedge B^k) = \mathrm{Tr}\left(\Psi_1 (A^j \otimes B^k)\right) \tag{15.22}$$

can be calculated using Ψ_1, whereas from ρ we can obtain only the marginal distribution

$$\Pr(A^j) = \sum_k \Pr(A^j \wedge B^k). \tag{15.23}$$

The other marginal distribution, $\Pr(B^k)$, can be obtained using the reduced density matrix ρ' for subsystem $\mathcal{B}$. However, from a knowledge of both ρ and ρ', one still cannot calculate the correlations between the two subsystems. For instance, in the two-spin example of (15.14), if we use a framework in which S_{az} and S_{bz} are both defined at t_1, Ψ_1 implies that $S_{az} = -S_{bz}$, a result which is not contained in ρ or ρ'. This illustrates the fact pointed out in the introduction, that density matrices typically provide partial descriptions of a quantum systems, descriptions from which certain features are omitted.

Rather than a projector on a one-dimensional subspace, Ψ_1 could itself be a density matrix on $\mathcal{A}\otimes\mathcal{B}$. For example, if the total quantum system with Hilbert space $\mathcal{A}\otimes\mathcal{B}\otimes\mathcal{C}$ consists of three subsystems $\mathcal{A}$, $\mathcal{B}$, and $\mathcal{C}$, and unitary time evolution beginning with a normalized initial state $|\Phi_0\rangle$ at t_0 results in a state $|\Phi_1\rangle$ with projector Φ_1 at t_1, then

$$\Psi_1 = \mathrm{Tr}_{\mathcal{C}}(\Phi_1) \tag{15.24}$$

is a density matrix. The partial traces of Ψ_1, (15.10) and (15.13) again define density matrices ρ and ρ' appropriate for calculating probabilities of properties of $\mathcal{A}$ or $\mathcal{B}$, since, for example,

$$\rho = \mathrm{Tr}_{\mathcal{B}}(\Psi_1) = \mathrm{Tr}_{\mathcal{BC}}(\Phi_1) \tag{15.25}$$

can be obtained from Ψ_1 or directly from Φ_1. Even when $\mathcal{A}\otimes\mathcal{B}$ is not part of a larger system it can be described by means of a density matrix as discussed in Sec. 15.6.

15.4 Time Dependence of Reduced Density Matrix

There is, of course, nothing very special about the time t_1 used in the discussion in Sec. 15.3. If $|\Psi_t\rangle$ is a solution to the Schrödinger equation as a function of time t for the composite system $\mathcal{A}\otimes\mathcal{B}$, and Ψ_t the corresponding projector, then one can define a density matrix

$$\rho_t = \mathrm{Tr}_{\mathcal{B}}(\Psi_t) \tag{15.26}$$

for subsystem $\mathcal{A}$ at any time t, and use it to calculate the probability of a history of the form $\Psi_0 \odot A^j$ based on the two times 0 and t, where A^j is a projector on $\mathcal{A}$. One should not think of ρ_t as some sort of physical property which develops in time. Instead, it is somewhat analogous to the classical single-time probability distribution $\rho_t(s)$ at time t for a particle undergoing a random walk, or $\rho_t(\boldsymbol{r})$ for a Brownian particle, discussed in Sec. 9.2. In particular, ρ_t provides no information about correlations of quantum properties at successive times. To discuss such correlations requires the use of quantum histories, see Sec. 15.5 below.

In general, ρ_t as a function of time does not satisfy a simple differential equation. An exception is the case in which $\mathcal{A}$ is itself an isolated subsystem, so that the time development operator for $\mathcal{A}\otimes\mathcal{B}$ factors,

$$T(t',t) = T_{\mathcal{A}}(t',t)\otimes T_{\mathcal{B}}(t',t), \tag{15.27}$$

or, equivalently, the Hamiltonian is of the form

$$H = H_{\mathcal{A}}\otimes I + I\otimes H_{\mathcal{B}} \tag{15.28}$$

during the times which are of interest. This would, for example, be the case if $\mathcal{A}$ and $\mathcal{B}$ were particles (or larger systems) flying away from each other after a collision. Using the fact that

$$\Psi_t = |\Psi_t\rangle\langle\Psi_t| = T(t,0)\Psi_0 T(0,t), \tag{15.29}$$

one can show (e.g., by writing Ψ_0 as a sum of product operators of the form $P\otimes Q$) that when $T(t,0)$ factors, (15.27),

$$\rho_t = T_{\mathcal{A}}(t,0)\rho_0 T_{\mathcal{A}}(0,t). \tag{15.30}$$

Upon differentiating this equation one obtains

$$i\hbar\frac{d\rho_t}{dt} = [H_{\mathcal{A}},\rho_t], \tag{15.31}$$

since for an isolated system $T_{\mathcal{A}}(t,0)$ satisfies (7.45) and (7.46) with $H_{\mathcal{A}}$ in place of H. Note that (15.31) is also valid when $H_{\mathcal{A}}$ depends on time. If $H_{\mathcal{A}}$ is independent of time and diagonal in the orthonormal basis $\{|e_n\rangle\}$,

$$H_{\mathcal{A}} = \sum_n E_n |e_n\rangle\langle e_n|, \tag{15.32}$$

one can use (7.48) to rewrite (15.30) in the form

$$\rho_t = e^{-itH_{\mathcal{A}}/\hbar}\rho_0 e^{itH_{\mathcal{A}}/\hbar}, \tag{15.33}$$

or the equivalent in terms of matrix elements:

$$\langle e_m|\rho_t|e_n\rangle = \langle e_m|\rho_0|e_n\rangle \exp\left(-i(E_m - E_n)t/\hbar\right). \tag{15.34}$$

There are situations in which (15.28) is only true in a first approximation, and there is an additional weak interaction between $\mathcal{A}$ and $\mathcal{B}$, so that $\mathcal{A}$ is not truly isolated. Under such circumstances it may still be possible, given a suitable system $\mathcal{B}$, to write an approximate differential equation for ρ_t in which additional terms appear on the right side. A discussion of open systems of this type lies outside the scope of this book.

15.5 Reduced Density Matrix as Initial Condition

Let Ψ_0 be a projector representing an initial pure state at time t_0 for the composite system $\mathcal{A}\otimes\mathcal{B}$, and assume that for $t > t_0$ the subsystem $\mathcal{A}$ is isolated from $\mathcal{B}$, so that the time time-development operator factors, (15.27). We shall be interested in histories of the form

$$Z^\alpha = \Psi_0 \odot Y^\alpha, \tag{15.35}$$

where

$$Y^\alpha = A_1^{\alpha_1} \odot A_2^{\alpha_2} \odot \cdots A_f^{\alpha_f} \tag{15.36}$$

is a history of $\mathcal{A}$ at the times $t_1 < t_2 < \cdots t_f$, with $t_1 > t_0$, and each of the projectors $A_j^{\alpha_j}$ at time t_j comes from a decomposition of the identity

$$I_\mathcal{A} = \sum_{\alpha_j} A_j^{\alpha_j} \tag{15.37}$$

of subsystem $\mathcal{A}$. A history of the form Z^α says nothing at all about what is going on in $\mathcal{B}$ after the initial time t_0, even though there might be non-trivial correlations between $\mathcal{A}$ and $\mathcal{B}$.

The Heisenberg chain operator for Z^α, Sec. 11.4, using a reference time $t_r = t_0$, can be written in the form

$$\hat{K}(Z^\alpha) = \big(\hat{K}_\mathcal{A}(Y^\alpha) \otimes I\big)\Psi_0, \tag{15.38}$$

where

$$\hat{K}_\mathcal{A}(Y^\alpha) = \hat{A}_f^{\alpha_f} \cdots \hat{A}_2^{\alpha_2} \hat{A}_1^{\alpha_1} \tag{15.39}$$

is the Heisenberg chain operator for Y^α, considered as a history of $\mathcal{A}$, with

$$\hat{A}_j^{\alpha_j} = T_\mathcal{A}(t_0, t_j) A_j^{\alpha_j} T_\mathcal{A}(t_j, t_0) \tag{15.40}$$

the Heisenberg counterpart of the Schrödinger operator $A_j^{\alpha_j}$, see (11.7).

By first taking a partial trace over $\mathcal{B}$, one can write the operator inner products needed to check consistency and calculate weights for the histories in (15.35) in the form

$$\begin{aligned} \langle \hat{K}(Z^\alpha), \hat{K}(Z^{\bar\alpha})\rangle &= \mathrm{Tr}\left(\Psi_0 \hat{K}_\mathcal{A}^\dagger(Y^\alpha)\hat{K}_\mathcal{A}(Y^{\bar\alpha})\right) \\ &= \mathrm{Tr}_\mathcal{A}\left(\rho \hat{K}_\mathcal{A}^\dagger(Y^\alpha)\hat{K}_\mathcal{A}(Y^{\bar\alpha})\right) = \langle \hat{K}_\mathcal{A}(Y^\alpha), \hat{K}_\mathcal{A}(Y^{\bar\alpha})\rangle_\rho, \end{aligned} \tag{15.41}$$

where the operator inner product $\langle , \rangle_\rho$ is defined for any pair of operators A and $\bar{A}$ on $\mathcal{A}$ by

$$\langle A, \bar{A}\rangle_\rho := \mathrm{Tr}_{\mathcal{A}}(\rho A^\dagger \bar{A}), \tag{15.42}$$

using the reduced density matrix

$$\rho = \mathrm{Tr}_{\mathcal{B}}(\Psi_0). \tag{15.43}$$

The definition (15.42) yields an inner product with all of the usual properties, including $\langle A, A\rangle_\rho \geq 0$, except that it might be possible (depending on ρ) for $\langle A, A\rangle_\rho$ to vanish when A is not zero.

The consistency conditions for the histories in (15.35) take the form

$$\langle \hat{K}_{\mathcal{A}}(Y^\alpha), \hat{K}_{\mathcal{A}}(Y^{\bar{\alpha}})\rangle_\rho = 0 \text{ for } \alpha \neq \bar{\alpha}, \tag{15.44}$$

and the probability of occurrence of Z^α or, equivalently, Y^α is given by

$$\Pr(Z^\alpha) = \Pr(Y^\alpha) = \langle \hat{K}_{\mathcal{A}}(Y^\alpha), \hat{K}_{\mathcal{A}}(Y^\alpha)\rangle_\rho. \tag{15.45}$$

Thus as long as we are only interested in histories of the form (15.35) that make no reference at all to $\mathcal{B}$ (aside from the initial state Ψ_0), the consistency conditions and weights can be evaluated with formulas which only involve $\mathcal{A}$ and make no reference to $\mathcal{B}$. They are of the same form employed in Ch. 10, except for replacing the operator inner product $\langle , \rangle$ defined in (10.12) by $\langle , \rangle_\rho$ defined in (15.42). It is also possible to write (15.44) and (15.45) using the Schrödinger chain operators $K(Y^\alpha)$ in place of the Heisenberg operators $\hat{K}(Y^\alpha)$, and this alternative form is employed in (15.48) and (15.50) in the next section.

If $\mathcal{A}$ is a small system and $\mathcal{B}$ is large, the second trace in (15.41) will be much easier to evaluate than the first. Thus using a density matrix can simplify what might otherwise be a rather complicated problem. To be sure, calculating ρ from Ψ_0 using (15.43) may be a nontrivial task. However, it is often the case that Ψ_0 is not known, so what one does is to assume that ρ has some form involving adjustable parameters, which might, for example, be chosen on the basis of experiment. Thus even if one does not know its precise form, the very fact that ρ exists can assist in analyzing a problem.

In the special case $f = 1$ in which the histories Y^α involve only a single time t, and the consistency conditions (15.44) are automatically satisfied, the probability (15.45) can be written in the form (15.3),

$$\Pr(A^j, t) = \mathrm{Tr}_{\mathcal{A}}(\rho_t A^j), \tag{15.46}$$

where ρ_t is a solution of (15.31), or given by (15.33) in the case in which $H_{\mathcal{A}}$ is independent of time. In this equation ρ_t is functioning as a time-dependent pre-probability; see the comments at the beginning of Sec. 15.4.

15.6 Density Matrix for Isolated System

It is also possible to use a density matrix ρ, thought of as a pre-probability, as the initial state of an isolated system which is not regarded as part of a larger, composite system. In such a case ρ embodies whatever information is available about the system, and this information does not have to be in the form of a particular property represented by a projector, or a probability distribution associated with some decomposition of the identity. As an example, the canonical density matrix

$$\rho = e^{-H/k\theta}/\mathrm{Tr}(e^{-H/k\theta}), \tag{15.47}$$

where k is Boltzmann's constant and H the time-independent Hamiltonian, is used in quantum statistical mechanics to describe a system in thermal equilibrium at an absolute temperature θ. While one often pictures such a system as being in contact with a thermal reservoir, and thus part of a larger, composite system, the density matrix (15.47) makes perfectly good sense for an isolated system, and a system of macroscopic size can constitute its own thermal reservoir.

The formulas employed in Sec. 15.5 can be used, with some obvious modifications, to check consistency and assign probabilities to histories of an isolated system for which ρ is the initial pre-probability at the time t_0. Thus for a family of histories of the form (15.36) at the times $t_1 < t_2 < \cdots t_f$, with $t_1 \geq t_0$, the consistency condition takes the form

$$\langle K(Y^\alpha), K(Y^{\bar\alpha})\rangle_\rho = \mathrm{Tr}\big[\rho K^\dagger(Y^\alpha)K(Y^{\bar\alpha})\big] = 0 \text{ for } \alpha \neq \bar\alpha, \tag{15.48}$$

where the (Schrödinger) chain operator is defined by

$$K(Y^\alpha) = A_f^{\alpha_f} T(t_f, t_{f-1}) \cdots A_2^{\alpha_2} T(t_2, t_1) A_1^{\alpha_1} T(t_1, t_0), \tag{15.49}$$

and the inner product $\langle , \rangle_\rho$ is the same as in (15.42), except for omitting the subscript on Tr. If the consistency conditions are satisfied, the probability of occurrence of a history Y^α is equal to its weight:

$$W(Y^\alpha) = \langle K(Y^\alpha), K(Y^\alpha)\rangle_\rho = \mathrm{Tr}\big[\rho K^\dagger(Y^\alpha)K(Y^\alpha)\big]. \tag{15.50}$$

One could equally well use Heisenberg chain operators $\hat K$ in (15.48) and (15.50), as in the analogous formulas (15.44) and (15.45) in Sec. 15.5. Note that (15.48) and (15.50) are essentially the same as the corresponding formulas (10.20) and (10.11) in Ch. 10, aside from the presence of the density matrix ρ inside the trace defining the operator inner product $\langle , \rangle_\rho$.

In the special case of histories involving only a *single* time $t > t_0$ and a decomposition of the identity $I = \sum A^j$ at this time, consistency is automatic, and the corresponding probabilities take the form

$$\Pr(A^j, t) = \mathrm{Tr}(\rho_t A^j), \tag{15.51}$$

or $\langle j|\rho_t|j\rangle$ when $A^j = |j\rangle\langle j|$ is a projector on a pure state, where ρ_t is a solution to the Schrödinger equation (15.31) with the subscript $\mathcal{A}$ omitted from H, or of the form (15.33) when the Hamiltonian H is independent of time. One should, however, not make the mistake of thinking that ρ_t as a function of time represents anything like a complete description of the time development of a quantum system; see the remarks at the beginning of Sec. 15.4. In order to discuss correlations it is necessary to employ histories with two or more times following t_0. For these the consistency conditions (15.48) are not automatic, and probabilities must be worked out using (15.50). Both of these formulas require more information about time development than is contained in ρ_t.

There are also situations in which information about the initial state of an isolated system is given in the form of a probability distribution on a set of initial states, and an initial density matrix is generated from this probability distribution. The basic idea can be understood by considering a family of histories

$$[\psi_0^j] \odot [\phi_1^k] \tag{15.52}$$

involving two times t_0 and t_1, where $\{|\psi_0^j\rangle\}$ and $\{|\phi_1^k\rangle\}$ are orthonormal bases, and the initial condition is that $[\psi_0^j]$ occurs with probability p_j. The probability that $[\phi_1^k]$ occurs at time t_1 is given by

$$\Pr(\phi_1^k) = \sum_j \Pr(\phi_1^k \,|\, \psi_0^j)\, p_j, \tag{15.53}$$

where the conditional probabilities come from the Born formula

$$\Pr(\phi_1^k \,|\, \psi_0^j) = |\langle \phi_1^k | T(t_1, t_0) | \psi_0^j \rangle|^2. \tag{15.54}$$

An alternative method for calculating $\Pr(\phi_1^k)$ is to define a density matrix

$$\rho_0 = \sum_j p_j [\psi_0^j] \tag{15.55}$$

at t_0 using the initial probability distribution. Since each summand is a positive operator, the sum is positive, Sec.3.9, and the trace of ρ_0 is $\sum_j p_j = 1$. Unlike the situations discussed previously, the eigenvalues of ρ_0 are of direct physical significance, since they are the probabilities of the initial distribution, and the eigenvectors are the physical properties of the system at t_0 for this family of histories. Next, let

$$\rho_1 = T(t_1, t_0) \rho_0 T(t_0, t_1) \tag{15.56}$$

be the result of integrating Schrödinger's equation, (15.31) with H in place of $H_{\mathcal{A}}$, from t_0 to t_1. Then the probabilities (15.53) can be written as

$$\Pr(\phi_1^k) = \mathrm{Tr}\big(\rho_1 [\phi_1^k]\big). \tag{15.57}$$

In this expression the density matrix ρ_1, in contrast to ρ_0, functions as a pre-probability, and its eigenvalues and eigenvectors have no particular physical significance.

The expression (15.57) is more compact than (15.53), as it does not involve the collection of conditional probabilities in (15.54). On the other hand, the description of the quantum system provided by ρ_1 is also less detailed. For example, one cannot use it to calculate correlations between the various initial and final states, or conditional probabilities such as

$$\Pr(\psi_0^j \,|\, \phi_1^k). \tag{15.58}$$

To be sure, a less detailed description is often more useful than one that is more detailed, especially when one is not interested in the details. The point is that a density matrix provides a partial description, and it is in principle possible to construct a more detailed description if one is interested in doing so.

15.7 Conditional Density Matrices

Suppose that at time t_0 a particle $\mathcal{A}$ has interacted with a device $\mathcal{B}$ and is moving away from it, so that the two no longer interact, and assume that the projectors $\{B^k\}$ in the decomposition of the identity (15.21) for $\mathcal{B}$ represent some states of physical significance. Given that $\mathcal{B}$ is in the state B^k at time t_0, what can one say about the future behavior of $\mathcal{A}$? For example, $\mathcal{B}$ might be a device which emits a spin-half particle with a spin polarization $S_v = +1/2$, where the direction v depends on some setting of the device indicated by the index k of B^k.

The question of interest to us can be addressed using a family of histories of the form

$$Z^{k\alpha} = B^k \odot Y^{k\alpha}, \tag{15.59}$$

defined for the times $t_0 < t_1 < \cdots$, where the $Y^{k\alpha}$ are histories of $\mathcal{A}$ of the sort defined in (15.36), except that they are labeled with k as well as with α to allow for the possibility that the decomposition of the identity in (15.7) could depend upon k. (One could also employ a set of times $t_1 < t_2 < \cdots$ that depend on k.)

Assume that the combined system $\mathcal{A} \otimes \mathcal{B}$ is described at time t_0 by an initial density matrix Ψ_0, which functions as a pre-probability. For example, Ψ_0 could result from unitary time evolution of an initial state defined at a still earlier time. Let

$$p_k = \mathrm{Tr}(\Psi_0 B^k) \tag{15.60}$$

be the probability of the event B^k. If p_k is greater than zero, the k'th *conditional density matrix* is an operator on $\mathcal{A}$ defined by the partial trace

$$\rho^k = (1/p_k)\mathrm{Tr}_{\mathcal{B}}(\Psi_0 B^k). \tag{15.61}$$

Each conditional density matrix gives rise to an inner product

$$\langle A, \bar{A}\rangle_k := \mathrm{Tr}_{\mathcal{A}}(\rho^k A^\dagger \bar{A}) \tag{15.62}$$

of the form (15.42).

Using the same sort of analysis as in Sec. 15.5, one can show that the family of histories (15.59) is consistent provided

$$\langle \hat{K}(Y^{k\alpha}), \hat{K}(Y^{k\bar{\alpha}})\rangle_k = 0 \text{ for } \alpha \neq \bar{\alpha} \tag{15.63}$$

is satisfied for every k with $p_k > 0$, where the Heisenberg chain operators $\hat{K}(Y^{k\alpha})$ are defined as in (15.39), but with the addition of a superscript k for each projector on the right side. Schrödinger chain operators could also be used, as in Sec. 15.6. Note that one does not have to check "cross terms" involving chain operators of histories with different values of k. If the consistency conditions are satisfied, the behavior of $\mathcal{A}$ given that $\mathcal{B}$ is in the state B^k at t_0 is described by the conditional probabilities

$$\Pr(Y^{k\alpha} \mid B^k) = \langle \hat{K}(Y^{k\alpha}), \hat{K}(Y^{k\alpha})\rangle_k. \tag{15.64}$$

The physical interpretation of the conditional density matrix is essentially the same as that of the simple density matrix ρ discussed in Sec. 15.5. Indeed, the latter can be thought of as a special case in which the decomposition of the identity of $\mathcal{B}$ in (15.21) consists of nothing but the identity itself. Note in particular that the eigenvalues and eigenvectors of ρ^k play no (direct) role in its physical interpretation, since ρ^k functions as a pre-probability.

Time-dependent conditional density matrices can be defined in the obvious way,

$$\rho_t^k = T_{\mathcal{A}}(t, t_0)\rho^k T_{\mathcal{A}}(t_0, t), \tag{15.65}$$

as solutions of the Schrödinger equation (15.31). One can use ρ_t^k to calculate the probability of an event A in $\mathcal{A}$ at time t conditional upon B_k, but not correlations between events in $\mathcal{A}$ at several different times. The comments about ρ_t at the beginning of Sec. 15.4 also apply to ρ_t^k.

The simple or "unconditional" density matrix of $\mathcal{A}$ at time t_0,

$$\rho = \mathrm{Tr}_{\mathcal{B}}(\Psi_0), \tag{15.66}$$

is an average of the conditional density matrices:

$$\rho = \sum_k p_k \rho^k. \tag{15.67}$$

While ρ can be used to check consistency and calculate probabilities of histories in $\mathcal{A}$ which make no reference to $\mathcal{B}$, for these purposes there is no need to introduce the refined family (15.59) in place of the coarser (15.35). To put it somewhat differently, the context in which the average (15.67) might be of interest is one in which ρ is not the appropriate mathematical tool for addressing the questions one is likely to be interested in.

Let us consider the particular case in which $\Psi_0 = |\Psi_0\rangle\langle\Psi_0|$ and the projectors

$$B^k = |b^k\rangle\langle b^k| \tag{15.68}$$

are pure states. Then one can expand $|\Psi_0\rangle$ in terms of the $|b^k\rangle$ in the form

$$|\Psi_0\rangle = \sum_k \sqrt{p_k}|\alpha^k\rangle \otimes |b^k\rangle, \tag{15.69}$$

where p_k was defined in (15.60). Inserting the coefficient $\sqrt{p_k}$ in (15.69) means that the $\{|\alpha^k\rangle\}$ are normalized, $\langle\alpha^k|\alpha^k\rangle = 1$, but there is no reason to expect $|\alpha^k\rangle$ and $|\alpha^l\rangle$ to be orthogonal for $k \neq l$. The conditional density matrices are now pure states represented by the dyads

$$\rho^k = |\alpha^k\rangle\langle\alpha^k|, \tag{15.70}$$

and (15.67) takes the form

$$\rho = \sum_k p_k |\alpha^k\rangle\langle\alpha^k| = \sum_k p_k[\alpha^k]. \tag{15.71}$$

The expression (15.71) is sometimes interpreted to mean that the system $\mathcal{A}$ is in the state $|\alpha^k\rangle$ with probability p_k at time t_0. However, this is a bit misleading, because in general the $|\alpha^k\rangle$ are not mutually orthogonal, and if two quantum states are not orthogonal to each other, it does not make sense to ask whether a system is in one or the other, as they do not represent mutually exclusive possibilities; see Sec. 4.6. Instead, one should assign a probability p_k at time t_0 to the state $|\alpha^k\rangle \otimes |b^k\rangle$ of the combined system $\mathcal{A} \otimes \mathcal{B}$. Such states are mutually orthogonal because the

$|b^k\rangle$ are mutually orthogonal. In general, $|\alpha^k\rangle$ is an event *dependent on* $|b^k\rangle$ in the sense discussed in Ch. 14, so it does not make sense to speak of $[\alpha^k]$ as a property of $\mathcal{A}$ by itself without making at least implicit reference to the state $|b^k\rangle$ of $\mathcal{B}$. If one wants to ascribe a probability to $|\alpha^k\rangle \otimes |b^k\rangle$, this ket or the corresponding projector must be an element of an appropriate sample space. The projector does not appear in (15.59), but one can insert it by replacing $B^k = [b^k]$ with $[\alpha^k] \otimes [b^k]$. The resulting collection of histories then forms the support of what is, at least technically, a different consistent family or histories. However, the consistency conditions and the probabilities in the new family are the same as those in the original family (15.59), so the distinction is of no great importance.