Chapter 14
Interpretations of Measurements. Decoherence. Density Matrix

The problem of getting the interpretation proved to be rather more difficult than just working out the equations [95].

Problems associated with the interpretation of the measurement processes are revisited in the present chapter. A brief survey of the orthodox line of thought is outlined in Sect. 14.1. Huge amounts of ink and paper have been devoted to the presentation of improved interpretations, without any of them having generated a general consensus.[1] However, a novel explanation of the coexistence between quantum and classical descriptions, based on the notion of *decoherence*, has been developed since the 1980s. The emergence of classicality from the quantum substrate interacting with the environment, outlined in Sect. 14.2†, appears to be a consistent approach. Its application to the measurement process is described in Sect. 14.3†.

In the present chapter, use is made of the density matrix, another formulation of quantum mechanics. It is appropriate for treating two entangled systems of which we have access to only one of them. The associated formalism is presented in Sect. 14.4.

14.1 Orthodox Interpretations

So far, predictions of quantum mechanics for isolated microsystems have never failed. However, the macroworld cannot be altogether forgotten even in the extreme Copenhagen interpretation, since it plays at least an essential role in the measurement process connecting quantum and classical systems.

If the quantum state of a system is denoted by $\Psi(t_0)$ at $t = t_0$, the system evolves swiftly and deterministically to the state $\Psi(t_1)$ at $t = t_1$, in accordance with the time-dependent Schrödinger equation. However, if a measurement takes place, it changes suddenly and impredictably.

[1] A critical discussion on alternative interpretations can be found, for instance, in [97].

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None of the difficulties with the collapse principle has been so caricatured as the one due to Schrödinger [96]. He imagined an unstable nucleus inside a box. Its decay product, an α-particle, may free some poison that would also kill a cat staying inside the box.[2] Let $\mathcal{S}_0$, $\mathcal{S}_1$ represent the two states of the system (not-decayed-atom and decayed-atom) and $\mathcal{C}_0$, $\mathcal{C}_1$ those of the cat (alive and dead). The quantum evolution implies

$$\mathcal{S}_0\,\mathcal{C} \to \mathcal{S}_0\,\mathcal{C}_0,$$
$$\mathcal{S}_1\,\mathcal{C} \to \mathcal{S}_1\,\mathcal{C}_1, \tag{14.1}$$

where $\mathcal{C}$ is an initial, ready state for the cat. If the atom is in a quantum superposition, the linear evolution requires[3]

$$(c_0\mathcal{S}_0 + c_1\mathcal{S}_1)\,\mathcal{C} \to c_0\mathcal{S}_0\mathcal{C}_0 + c_1\mathcal{S}_1\mathcal{C}_1. \tag{14.2}$$

The collapse principle that we have been applying so far tells us that the cat will be either dead or alive after the measurement. Note that the composite system + cat is in an entangled state at the beginning of the measurement. Thus neither the atom nor the cat are in a definite state. But a superposition of an alive and a dead cat has never been seen![4]

Two orthodox interpretations are outlined in the following sections:

14.1.1 The Standard Interpretation

The standard interpretation is not much more than an enunciation of the basic Principle 3. Therefore, its main contents are:

- Every measurement performed on a quantum system induces a breakdown of the continuous evolution associated with the Schrödinger evolution, as a consequence of the collapse of the state Ψ into an eigenstate φ_n of the measured observable Q.
- The probability of a particular outcome q_n is given by $|\langle\Psi|\varphi_n\rangle|^2$.
- It is the observer who chooses the observable to be measured.

According to Zeilinger, "If we accept that the quantum state is no more than a representation of the information we have, then the spontaneous change of the state upon observation, the so-called collapse or reduction of the wave packet, is just a

[2] The link between the nuclear microsystem and the meter (the animal cat) goes through a chain of amplifying stages with intermediate systems (detector, poison, etc.) also getting correlated. In the text, we use the word "cat" to represent all of these items plus the animal.

[3] A similar operation may be accomplished by the controlled-NOT gate (13.21).

[4] Entangled states representing N spins pointing together in opposite directions $\Psi = \frac{1}{\sqrt{2}}[\varphi_0(1)\varphi_0(2)...\varphi_0(N) + \varphi_1(1)\varphi_1(2)...\varphi_1(N)]$ are called Schrödinger cat states or GHZ states.

very natural consequence of the fact that, upon observation, our information changes and therefore we have to change our representation of the information, that is, the quantum state." [78].

14.1.2 The Copenhagen Interpretation

Although the standard interpretation has often been confused with the Copenhagen interpretation, this last one includes the classical world in the process of measurement.

Intermediate classical apparatuses are necessary to convey to our classical minds the results of measurements on the quantum level. When particles are detected, the atoms of the detector become ionized, producing first a few electrons, and then a cascade of electrons. The state vector should take these macroscopic effects into account. Because of the linearity of the Schrödinger evolution, there is no mechanism to stop the evolution and yield a single result for the measurement.

Ultimately the evolution may involve the observer's brain, since the disappearance of macroscopic superpositions is attributed to the existence of the observer. Some extreme advocates of this interpretation have even argued that this mechanism may be linked to the property of consciousness in the human brain. Thus, it has been argued that quantum mechanics has an anthropocentric foundation, a concept which had disappeared from science after the Middle Ages.

However, the frontier between the quantum and the classical domains remained an ill-defined concept. This division was never accepted by Bell and other thinkers. In fact, there exist mesoscopic and even macroscopic quantum systems that are described with a global quantum wave function [Bose–Einstein condensates (Sect. 7.5†), superconductors (Sect. 10.1), neutron stars, etc.].

14.2† The Emergence of Classicality from the Quantum Substrate. Decoherence

In this section we present a derivation of Newtonian mechanics as a limiting case of quantum mechanics.[5] Zurek was the first to emphasize the relevance of the interaction of systems with the environment [99], which in this case is represented by the initial state ε and the two states ε_0 and ε_1 that are obtained through the linear evolution

$$\begin{aligned} \varphi_0\, \varepsilon &\rightarrow \varphi_0\, \varepsilon_0, \\ \varphi_1\, \varepsilon &\rightarrow \varphi_1\, \varepsilon_1. \end{aligned} \tag{14.3}$$

[5]We mostly follow Chap. 2 of [98] throughout this section.

The system–environment interaction frequently manifests through a scattering process of surrounding particles interacting with the system (photons, air molecules, etc.).

If the initial state is a quantum superposition $\varphi_\pm = \frac{1}{\sqrt{2}}(\varphi_0 \pm \varphi_1)$, the evolution yields entangled states

$$\varphi_\pm\,\varepsilon \rightarrow \frac{1}{\sqrt{2}}\left(\varphi_0\,\varepsilon_0 \;\pm\; \varphi_1\varepsilon_1\right). \tag{14.4}$$

The reduced density matrix[6] operator for the system may be written[7]

$$\begin{aligned}\hat{\rho}_{\mathcal{S}} &= \frac{1}{2}\left(|\varphi_0\rangle\langle\varphi_0| \;+\; |\varphi_1\rangle\langle\varphi_1| \;\pm\; |\varphi_0\rangle\langle\varphi_1|\langle\varepsilon_1|\varepsilon_0\rangle \;\pm\; |\varphi_1\rangle\langle\varphi_0|\langle\varepsilon_0|\varepsilon_1\rangle\right)\\ &\approx \frac{1}{2}\left(|\varphi_0\rangle\langle\varphi_0| \;+\; |\varphi_1\rangle\langle\varphi_1|\right).\end{aligned} \tag{14.5}$$

In deriving the last line we have assumed that the environment states are almost orthogonal to each other. This assumption is based on the complexity of the environment: if, for instance, we consider a beam of light quanta impinging over the system, the overlap between states before and after the collision may not be very much smaller than one for each individual photon, but the overlap of N photons may be close to vanishing in the limit of large N. If this is the case, the density matrix becomes similar to the one associated with an uncorrelated admixture of two separate states and thus, it is not able to display interference phenomena. Moreover, the larger the system, the more likely that the environment states become mutually orthogonal.

Therefore, classical macroscopic systems emerge as a consequence of being monitored by the rest of the universe. The environment acts as a device yielding information about which path in the two slit experiment (Fig. 2.5), which destroys the interference pattern.

Equation (14.5) does not imply that the system is in a mixture of states φ_0 and φ_1. Since these two states are simultaneously present in (14.4), the composite system + environment displays superposition and associated interferences. However, (14.5) says that such quantum manifestations will not appear as long as experiments are performed only on the system $\mathcal{S}$. Thus, there has been a leakage of coherence from the system to the composite entity. Since we are not able to control this entity, the decoherence has been completed to all practical purposes.

For many system–environment models the overlaps

$$\langle\varepsilon_i(t)|\varepsilon_j(t)\rangle \propto \exp(-t/\tau_d) \tag{14.6}$$

[6]The density matrix formalism is outlined in Sect. 14.4.

[7]An expansion of the environmental states in terms of an orthonormal set, $\varepsilon_i = \sum_l c_l^i \phi_l$, yields: $\mathrm{trace}(|\varepsilon_i\rangle\langle\varepsilon_j|) = \sum_l c_l^i c_l^{j*} = \langle\varepsilon_j|\varepsilon_i\rangle$.

display an extremely fast exponential decay for $i \neq j$. Calculations for simplified cases yield decay times between $\mathcal{O}\left(10^{-14}\right)$ s and much less. In particular, the estimated decoherence times for neural superpositions (10^{-19}–10^{-20}) s is much smaller than typical times for cognitive processes (10^{-2}–1) s [98].

In contrast with the states $\varphi_{\pm}$ of the system, the states φ_0 and φ_1 do not become entangled with the environment, according to (14.3). We thus conclude that there are states less prone to decoherence than others. They are called *pointer* states and make up the pointer subspace of the Hilbert space of the system. They play two essential roles:

- Sets of pointer states are made up from states most immune to decoherence. The composite pointer state + environment remains in a product state at all subsequent times. The selection of these states is determined through the structure of the system–environment Hamiltonian using methods developed in [99].
- Pointer states are also the states for which information is redundantly stored in a large number of fragments of the environment, in such a way that multiple observers can retrieve this information without disturbing the state of the system (as, for instance, through visual registration of photons that have been scattered from the system).

Since these are characteristic features of classical systems, classical reality has emerged from the quantum substrate.

Decoherence therefore explains why we do not see quantum superpositions in our everyday world: macroscopic objects are more difficult to keep isolated than microscopic objects. It also explains why spin up and down states are more easily preserved than their linear combinations through their interaction with the environment. This promising result is presently the subject of many studies.

14.2.1† A Mathematical Model of Decoherence

Consider a qubit (the system) coupled to other $N - 1$ qubits representing the environment.[8] Let the Hamiltonian be

$$\hat{H} = -\frac{4}{\hbar}\,\hat{S}_z^{(1)} \sum_{k=2}^{k=N} j_k\,\hat{S}_z^{(k)}, \tag{14.7}$$

where any interaction between the qubits of the environment is disregarded. Assume an initial state of the form

$$\Phi(0) = \Psi(0) \prod_{k=2}^{k=N} \Psi^{(k)}(0)$$

[8] See [100], Sect. 2.5.

$$\Psi(0) = c_0\varphi_0 + c_1\varphi_1, \qquad \Psi^{(k)}(0) = c_0^{(k)}\varphi_0^{(k)} + c_1^{(k)}\varphi_1^{(k)}. \tag{14.8}$$

The evolution of the system yields

$$\begin{aligned}
\Phi(t) &= \exp\left(-\mathrm{i}\hat{H}t/\hbar\right)\,\Phi(0) \\
&= c_0\varphi_0 \prod_{k=2}^{k=N}\left[c_0^{(k)}\exp\left(\mathrm{i}j_k t\right)\varphi_0^{(k)} + c_1^{(k)}\exp\left(-\mathrm{i}j_k t\right)\varphi_1^{(k)}\right] \\
&\quad + c_1\varphi_1 \prod_{k=2}^{k=N}\left[c_0^{(k)}\exp\left(-\mathrm{i}j_k t\right)\varphi_0^{(k)} + c_1^{(k)}\exp\left(\mathrm{i}j_k t\right)\varphi_1^{(k)}\right].
\end{aligned} \tag{14.9}$$

The density operator is

$$\hat{\rho}(t) = |\Phi(t)\rangle\,\langle\Phi(t)|. \tag{14.10}$$

Since we are interested in the system consisting of the first qubit, we trace out the remaining ones

$$\begin{aligned}
\hat{\rho}^{(1)} &= |c_0|^2\,|0\rangle\langle 0| + |c_1|^2\,|1\rangle\langle 1| + z(t)\,c_0c_1^*|0\rangle\langle 1| + z^*(t)\,c_0^*c_1|1\rangle\langle 0|, \\
z(t) &= \prod_{k=2}^{k=N}\left[|c_0^{(k)}|^2\exp\left(\mathrm{i}j_k t\right) + |c_1^{(k)}|^2\exp\left(-\mathrm{i}j_k t\right)\right].
\end{aligned} \tag{14.11}$$

The time-dependence $z(t)$ included in the non-diagonal terms encompasses the relevant information concerning the coherence of the system. If $|z(t)| \to 0$, we are in the presence of a non-unitary process with an irreversible loss of information. This simple model is not quite up to this task, since there is a recurrence time τ_r for the function z to reassume the value 1. Nevertheless, there is an effective loss of coherence, since

$$\begin{aligned}
\langle z(t)\rangle &= \lim_{T\to\infty}\frac{1}{T}\int_0^T \mathrm{d}t'z(t') = 0, \\
\langle|z(t)|^2\rangle &= \frac{1}{2^{N-1}}\prod_{k=2}^{k=N}\left[1 + \left(\left|c_0^{(k)}\right|^2 - \left|c_1^{(k)}\right|^2\right)^2\right],
\end{aligned} \tag{14.12}$$

which tell us that the fluctuations of $z(t)$ around the mean value 0 are inversely proportional to a function which increases exponentially with of the dimensions of the Hilbert space. Therefore, for a sufficiently large interval, and if the spins of the environment are initially oriented on the xy plane, the loss of information becomes irreversible.[9] The φ_0 and φ_1 are the pointer states of the simplified model and there is decoherence.

14.2.2† An Experiment with Decoherence

Since 1996, many experiments have demonstrated the dynamics of decoherence, by showing how superposition states become unobservable due to decoherence. In the following, we present one of such experiments.

As mentioned in Sect. 2.5.2, two-slit experiments were carried out even with relatively large objects such as fullerenes. The "matter" category of these objects appears evident from the fact that a molecule C_{70} has more than 10^3 particle components (electrons and nucleons). It is also possible to assign to them a temperature, and thermal radiation has also been observed.

A variation of the two-slit experiment consists of an application of the Talbot–Lau effect: if a wave impinges perpendicularly on a grating composed of parallel slits, as a consequence of interference the pattern of the grating will be reproduced at multiples of the distance $L_\lambda = d^2/\lambda$. Here d is the spacing between adjacent slits and λ, the wavelength.

Experiments clearly display the oscillatory fluctuations in the density of the C_{70} molecule along an axis perpendicular both to the incident direction and to the grating, at the distance L_λ. The confirmation of the existence of interference effects due to the Talbot–Lau effect was obtained by varying the velocity of the particles and thus the wavelength according to the de Broglie prescription.

Decoherence is produced by collisions between C_{70} molecules and molecules in the background gas. The amount of decoherence can be tuned by changing the density of the gas. Let us define the visibility factor as the ratio

$$V = \frac{I_{\max} - I_{\min}}{I_{\max} + I_{\min}}, \tag{14.13}$$

where $I_{\max}$ and $I_{\min}$ are the maximum and minimum amplitudes in the interference pattern, respectively. The visibility decays exponentially with the increase in the density, as shown in Fig. 14.1.

"Thus these experiments provide impressive direct evidence for how the interaction with the environment gradually delocalizes the quantum coherence required for the interference effects to be observed... So we can smoothly navigate and explore the quantum-classical boundary, and we find our observations to be in excellent agreement with theoretical predictions." (M. Schlosshauer [98], p. 265).

Decoherence is currently the subject of a great deal of research. Many questions have been clarified to a large extent in recent years. These include the rate of

[9]This is due to the fact that (14.11) is a sum of periodic terms. However, for macroscopic environments of realistic size, Zurek has pointed out that τ_r can exceed the life of the universe.

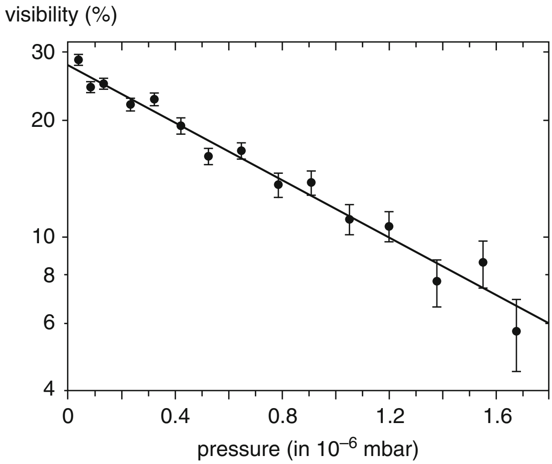

Fig. 14.1 Dependence of the visibility (14.13) of the interference pattern on the pressure of the background gas [102] (reproduced with permission from the authors and from Springer Science and Business Media)

decoherence, the dynamical selection of the pointer states, the dissipation of energy into the environment, and many others.

14.3† Quantum Measurements

A quantum measurement is an experiment coupling a microscopic system to a macroscopic meter. This last piece of the experiment is coupled to the environment. Decoherence ensures the classical description of the meter.

The von Neumann scheme for measurements assumes that all states are quantum mechanical, including the much smaller set of classical states. This is a different starting point than the one upon which the Copenhagen interpretation is based. Even though the possible superpositions in Hilbert space are potentially expanded with the Schrödinger equation, we have seen in Sect. 14.2† that the process of decoherence, i.e. the interaction between systems and environment, leads to the elimination of quantum superposition effects within the observed system, and to the selection of a small subset of classical, pointer states [100].

In the following, we sketch how this may be applied for the measurement of a two-state system (Fig. 14.2). Consider, for instance Schrödinger's thought experiment. At the quantum end (left side of the figure) the microsystem is represented by the two nuclear states, with an α-particle inside or outside the nucleus

$$\Psi^{\mathcal{S}}(0) = c_0\varphi_0 + c_1\varphi_1. \tag{14.14}$$

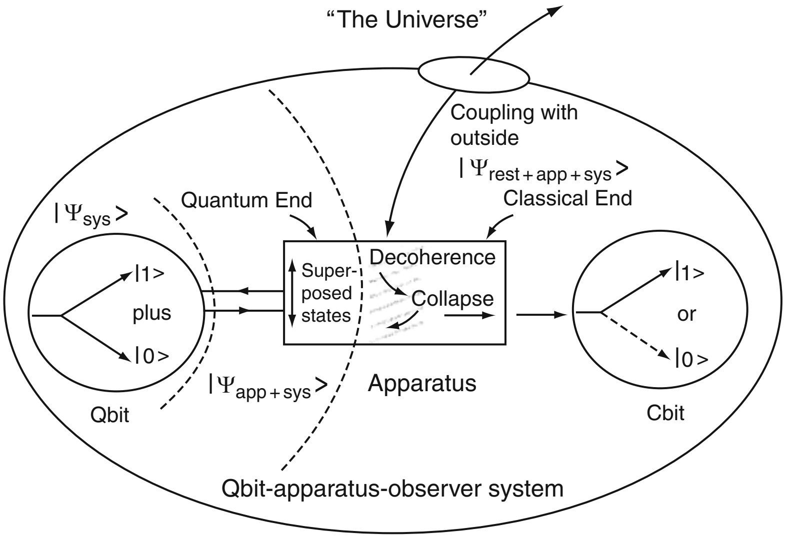

Fig. 14.2 Sketch of the measurement of a qubit. "Rest" is called "environment" in the text. Initially, there is a superposition of the two nuclear states. One of the two alternatives for the Schrödinger cat occurs at the classical end. (Reproduced from J. Roederer [20], with permission from Springer-Verlag)

We consider a quantum apparatus $\mathcal{Z}$ (cat et al.) with a Hilbert space spanned by the two states χ_1, χ_0. One can assume that the initial state of the binary microsystem-apparatus is

$$\Psi^{\mathcal{S},\mathcal{Z}}(0) = (c_0\varphi_0 + c_1\varphi_1)\,\chi_1. \tag{14.15}$$

The entanglement of the composite system may be produced by means of the interaction represented by a controlled-NOT gate [see (13.22)]. It is represented by the two arrows linking the qubit with the apparatus. Thus,

$$\Psi_t^{\mathcal{S},\mathcal{Z}} = c_0\varphi_0\chi_1 + c_1\varphi_1\chi_0. \tag{14.16}$$

If the detector is in the state χ_1, the microsystem is guaranteed to be found in the state φ_0, and vice versa. However, there is an ambiguity in a correlated state of the form (14.16), since we may rotate both the system and the apparatus without changing $\Psi_t^{\mathcal{S},\mathcal{Z}}$ (see p. 221). The ambiguity may be superseded by introducing another system, the environment $\mathcal{E}$, which is also represented by two quantum states $\varepsilon_1, \varepsilon_0$. From now on we apply the decoherence process to the composite system + apparatus

$$\Psi^{\mathcal{S},\mathcal{Z},\mathcal{E}}(0) = \Psi_t^{\mathcal{S},\mathcal{Z}}\varepsilon_1 \longrightarrow \Psi_t^{\mathcal{S},\mathcal{Z},\mathcal{E}} = c_0\varphi_0\chi_1\varepsilon_1 + c_1\varphi_1\chi_0\varepsilon_0. \tag{14.17}$$

Since we cannot control the environment, we are limited to evaluate expectation values of observables belonging to the $(\mathcal{S}, \mathcal{Z})$ subsystems. In the state (14.17), any such expectation value is

$$\langle Q\rangle = |c_0|^2\langle\varphi_0\chi_1|Q|\varphi_0\chi_1\rangle + |c_1|^2\langle\varphi_1\chi_0|Q|\varphi_1\chi_0\rangle \\ +2\mathrm{Re}\left(c_0c_1^*\langle\varphi_1\chi_0|Q|\varphi_0\chi_1\rangle\ \langle\varepsilon_0|\varepsilon_1\rangle\right). \qquad (14.18)$$

The third term in this equation is responsible for introducing interference. Interaction with the environment has the effect of modulating this interference term, whose magnitude is reduced by a factor determined by the absolute value of the overlap $\langle\varepsilon_0|\varepsilon_1\rangle$. When this overlap is sufficiently small, quantum interference effects become dynamically suppressed. The two (curved) arrows inside the box represent the correlation between the state of the system and the cat after decoherence has taken place.

The classical end appears at the extreme right of the figure, the word "Cbit" labels the cat, *either* dead *or* alive (and the observer looking at it).

As pointed out by M. Schlosshauer [98], p. 50, there are three issues in the measurement problem:

1. The problem of non-observability of interference. Through the interaction with the environment, decoherence explains why patterns of interference between macroscopic objects dissapear and only one of the possible outcomes is observed. An observer would only see the Schrödinger cat *either* dead *or* alive, because the duration of the weird state (14.2) will be incredibly short in a system with so many components. "Decoherence produces an effect that looks and smells like a collapse." [125].
2. The problem of the preferred basis. The preferred states of the system–apparatus are those that become least entangled with the environment in the course of the evolution and are thus most immune to decoherence. If the interaction between the (microscopic) system and the environment is neglected, the different pointer positions of the apparatus are the robust preferred states "superallowed" by the environment.
3. The question about why a particular outcome appears to the observer, rather than another possible one, is outside the domain of decoherence. It belongs to the philosophical aspects of the relation between quantum mechanics and reality.

14.4 The Density Matrix

The density matrix operator corresponding to a state Ψ is defined as the projector

$$\hat{\rho} = |\Psi\rangle\langle\Psi|. \qquad (14.19)$$

In particular, $\hat{\rho}_i = |i\rangle\langle i|$ is used in (2.57). The expectation value of an operator $\hat{Q}$ in the state φ_i is given by

$$\text{trace}(\rho_i\, Q) = \sum_{i'} \langle i'|i\rangle\langle i|Q|i'\rangle = \langle i|Q|i\rangle. \tag{14.20}$$

If our system is in a state Ψ, the descriptions in terms of Ψ and in terms of the density matrix (14.19) are completely equivalent.

14.4.1 Mixed Density Matrix

In a mixed state we do not know in which state φ_i the system is. Therefore, only probabilities π_i can be ascribed to each state

$$0 \le \pi_i \le 1, \qquad \sum_i \pi_i = 1, \tag{14.21}$$

which can be interpreted as a classical probability distribution of quantum states. The projection operator can be generalized in terms of the density matrix

$$\hat{\rho} = \sum_i \pi_i\, |i\rangle\langle i|\,. \tag{14.22}$$

Thus, the present formalism is especially useful when we have less than complete information on the system. For instance, the silver atoms leaving the furnace in a Stern–Gerlach experiment are randomly oriented in space (as in Fig. 2.4). In this case, $\pi_+ = \pi_- = 1/2$, the probabilities of the spin being up or down being the same. We say that the system is in a *mixed state* and the density matrix is given by

$$\hat{\rho} = \frac{1}{2}\,(|0\rangle\langle 0| + |1\rangle\langle 1|)\,. \tag{14.23}$$

If $\pi_{i'} = \delta_{i'i}$, we say that the system is in a *pure state*, like all those that we have studied so far in the present text. In this case the density matrix reduces to the projection $|i\rangle\langle i|$.

Some consequences of the definition (14.22) are:

- The expectation value of an operator $\hat{Q}$ acting within the complete set of states φ_i, is given by

$$\begin{aligned} \langle|Q|\rangle = \text{trace}(\rho\, Q) &= \sum_{i'i} \pi_i\, \langle i'|i\rangle\langle i|Q|i'\rangle \\ &= \sum_i \pi_i\, \langle i|Q|i\rangle, \end{aligned} \tag{14.24}$$

where the expectation values $\langle i|Q|i\rangle$ are weighted for each of the possible states φ_i by their respective classical probability.

- The matrix elements of the density matrix are given by

$$\langle i|\rho|j\rangle = \sum_k \pi_k \langle i|k\rangle\langle k|j\rangle \tag{14.25}$$

and therefore,

$$\text{trace}(\rho) = \prod_{ik} \pi_k\, |\langle i|k\rangle|^2 = \sum_k \pi_k = 1, \tag{14.26}$$

where trace$(\rho^2) < 1$, unless we are dealing with a pure state.
The matrix elements $\langle i|\rho|i\rangle$ represent the probability of finding the system in the state φ_i. The non-diagonal matrix elements $\langle i|\rho|j\rangle$ may vanish, even if none of their terms do.

- Let us rotate the spin axis by means of the transformation (5.26). In such a case (14.23) is transformed to

$$\hat{\rho} = \frac{1}{2}\left(|0^{(\beta,\phi)}\rangle\langle 0^{(\beta,\phi)}| + |1^{(\beta,\phi)}\rangle\langle 1^{(\beta,\phi)}|\right). \tag{14.27}$$

Thus, the mixed density matrix does not provide information about the particular axis in which the state has been prepared.

- A mixed state *is not* a superposition of pure states $\Psi = \sum_i \sqrt{\pi_i}\,\varphi_i$, which correspond to a density matrix with off diagonal terms

$$\hat{\rho} = \sum_i \pi_i |i\rangle\langle i| + \sum_{i\neq j} \sqrt{\pi_i \pi_j}\, |i\rangle\langle j|. \tag{14.28}$$

- The (useless) overall phase multiplying the state vector disappears from the formalism.
- As time changes,

$$\hat{\rho}(t) = \sum_i \pi_i\, |i(t)\rangle\langle i(t)|,$$

$$\langle i|\rho(t)|j\rangle = \sum_k \pi_k \langle i|k(t)\rangle\langle k(t)|j\rangle. \tag{14.29}$$

Therefore, according to the time principle (9.4),

$$\dot{\hat{\rho}} = -\mathrm{i}[\hat{H}, \hat{\rho}]. \tag{14.30}$$

14.4.2 Reduced Density Matrix

The reduced density matrix is the appropriate tool for the treatment of two (or more) entangled systems A, B, if we have access only to system A.

$$\hat{\rho}^{(A)} = \text{trace}_B \left(\hat{\rho}^{(AB)}\right), \tag{14.31}$$

where the operator $\hat{\rho}^{(A)}$ is obtained by performing a partial trace over the subsystem B. If we denote by $\Psi^{(AB)}$ a pure eigenstate of the whole system

$$\Psi^{(AB)} = \sum_{i,\nu} c_{i\nu}\, \varphi_i^{(A)}\, \chi_\nu^{(B)} \tag{14.32}$$

and $\hat{Q}$ is an operator acting only within the (complete) subspace $\varphi_i^{(A)}$, its expectation value can be written

$$\langle \Psi^{(AB)}|Q|\Psi^{(AB)}\rangle = \sum_{i,j,\nu} \langle i^{(A)}|Q|j^{(A)}\rangle = \text{trace}(\hat{\rho}^{(A)}Q). \tag{14.33}$$

The reduced density matrix can be written as

$$\hat{\rho}^{(A)} = \sum_{i,j,\nu} c_{i\nu}^{*} c_{j\nu}\, |i^{(A)}\rangle\langle j^{(A)}|,$$

$$\text{trace}(\rho^{(A)}) = 1 \qquad \langle k^{(A)}|\hat{\rho}^{(A)}|k^{(A)}\rangle \geq 0, \tag{14.34}$$

which are conditions equivalent to (14.21). Therefore, $\hat{\rho}^{(A)}$ satisfies the definition of a density matrix, upon the diagonalization within the subspace A.

As an example, consider the case of two qubits, A and B, in the Bell state Ψ_{B_0} (Sect. 12.2). The density matrix operator is written

$$\hat{\rho}_{B_0}^{(AB)} = \frac{1}{2}\left(|0^{(A)}0^{(B)}\rangle + |1^{(A)}1^{(B)}\rangle\right)\left(\langle 0^{(A)}0^{(B)}| + |\langle 1^{(A)}1^{(B)}|\right). \tag{14.35}$$

Since this is a pure state, $\text{trace}(\rho^2) = 1$. Let us assume that we do not have access to qubit B. We obtain the reduced density matrix for qubit A by tracing out qubit B

$$\hat{\rho}^{(A)} = \frac{1}{2}\left(|0^{A}\rangle\langle 0^{(A)}| \,+\, |1^{(A)}\rangle\langle 1^{(A)}|\right) = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \tag{14.36}$$

which behaves as a mixed state, since $\text{trace}\left[(\rho^{(A)})^2\right] = 1/2$. In a Bell state we have incomplete information on the properties of each qubit. Moreover, the information encoded in (14.36) is the same for any of the Bell states.

The expectation value of the spin of qubit A along the x-direction vanishes

$$\langle|S_x|\rangle = \frac{\hbar}{2}\,\text{trace}\left(\sigma_x \rho^{(A)}\right) = 0. \tag{14.37}$$

The reduced density matrix is used in Sect. 14.2† to formalize the concept of decoherence. In such case, the universe is divided into two parts: A, the system upon which we are interested, and B, the rest of the universe.

Problems

Problem 1. A C_{70} molecule moves with a velocity of about 100 m/s. Calculate the Talbot–Law distance if the separation between two consecutive slits is 1 μm.

Problem 2. Show that the mean value of the density matrix is always positive.

Problem 3. Show that the density operator is Hermitian.

Problem 4. Consider the pure spin state $\varphi_{\uparrow}^{\beta\phi}$ (5.25).

1. Construct the density operator.
2. Obtain the averages $\langle S_x\rangle, \langle S_y\rangle, \langle S_z\rangle$.

Problem 5. Consider the unpolarized mixed spin state ($\pi_{\beta\phi} \to \mathrm{d}\Omega/4\pi$).

1. Construct the density operator and compare the result with (14.36).
2. Obtain the averages $\langle S_x\rangle, \langle S_y\rangle, \langle S_z\rangle$.
3. Interpret the difference between these averages and those obtained in Problem 4.

Problem 6. Calculate the value of Δx for a particle moving in a harmonic oscillator potential at temperature T. Assume a Maxwell–Boltzmann distribution [$\pi_n = \exp(-\hbar\omega\, n/k_B T)$] and use $\int_0^\infty \exp(-x)\, x^n \mathrm{d}x = \Gamma(n)$.