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Quantum mechanics for quantum engineers

> Shall I refuse my dinner because I do not fully understand the process of digestion? No, not if I am satisfied with the result.
>
> O. Heaviside, *Electromagnetic Theory*, vol. 2, 1899

1.1 Basic notions of quantum mechanics

1.1.1 Quantum axioms

Let us start with a brief recapitulation of quantum mechanics on the "how to" level. According to the standard lore, the instantaneous state of any quantum system (that is, *everything* that can be known about it at a given moment of time) is given by its wave function (state vector)[1] – a complex-valued vector in some abstract Hilbert space; the nature of this space is determined by the system. All the *observables* (i.e., physical quantities defined for the system and determined by its state – e.g., the position or momentum of a free particle, the energy of an oscillator) are described by Hermitian operators defined in the same Hilbert space. All three elements – the Hilbert space, the state vector, and the set of observables – are necessary to describe the outcome of any experiment one could perform with the system. Since humans cannot directly observe the behaviour of quantum objects, these outcomes are also called *measurements*, being the result of using some classical apparatus in order to translate the state of a quantum system into the state of the apparatus, which can then be read out by the experimentalist. The classical (i.e., non-quantum) nature of the apparatus is essential, as we shall see in a moment.

In addition, we need to know how the state of the system changes in time, and how it determines the measured values of the observables. All of the above can be presented as four textbook "axioms of quantum theory":

1) The state of a quantum system at time t is described by a normalized[2] vector $|\psi(t)\rangle$ belonging to the Hilbert space $\mathcal{H}$, which is specific for the system in question.

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[1] A very important generalization of the wave function, the density matrix (statistical operator), will be discussed in Section 1.2.

[2] This is not strictly necessary, but makes the explanations shorter without much loss of generality.

2) [Schrödinger equation] The state evolves with time according to $\imath\hbar|\dot{\psi}(t)\rangle = H|\psi(t)\rangle$, where H, the Hamiltonian, is a Hermitian operator associated with the energy of the system.

3) [Collapse of the wave function] The measured value of an observable is always one of the eigenvalues of its operator A, a_j; whatever the state of the system was *before* the measurement, immediately *after* it the state vector of the system is the corresponding normalized eigenvector of A, $|a_j\rangle$ ($A|a_j\rangle \equiv a_j|a_j\rangle$).

4) [Born's rule] The probability of measuring a particular eigenvalue, a_j, of the observable A (collapsing the wave function $|\psi(t)\rangle$ into a given eigenvector $|a_j\rangle$) is given by the square modulus of the former's projection on the latter, $p_j(t) = \left|\langle a_j|\psi(t)\rangle\right|^2$.

The most striking features of these axioms are the special roles played by time and energy (Hamiltonian) of all the other physical quantities associated with the quantum system, and the jarring difference between the linear, reversible, unitary quantum evolution determined by the Schrödinger equation, and the nonlinear, irreversible, non-unitary measurement process. Indeed, the equation

$$\imath\hbar|\dot{\psi}(t)\rangle = H|\psi(t)\rangle \tag{1.1}$$

has the solution (in the sufficiently general case of a time-independent Hamiltonian)

$$|\psi(t)\rangle = U(t)|\psi(0)\rangle; \ \ U(t) = \mathrm{e}^{-\frac{1}{\hbar}Ht}, \tag{1.2}$$

and for Hermitian H the *evolution operator* is unitary, $U(t)^\dagger U(t) = U(t)U(t)^\dagger = I$ (where I is the identity operator in the Hilbert space of the system). The latter property ensures that the normalization of the state vector is preserved. On the other hand, after the measurement at moment t we find the system in a state $|a_j\rangle$, which is not related to the state $|\psi(t)\rangle$ before the measurement by any reversible transformation ($\psi(t)\rangle$ instantaneously collapses to $|a_j\rangle$). The after-collapse state $|a_j\rangle$ could be obtained from *any* state $|\psi(t)\rangle$ as long as $|a_j\rangle$ and $|\psi(t)\rangle$ are not mutually orthogonal. Taken together, axioms (3) and (4) are often called the *projection postulate*: the measurement of the observable A *projects* the state vector $|\psi(t)\rangle$ on the eigenvectors of A; the square modulus of the projection gives the probability with which the system is likely to be found in the corresponding eigenstate of A. The eigenvectors of a Hermitian operator A can be chosen to form a complete orthonormal basis of the Hilbert space; therefore the sum of squared projections of the state vector $|\psi\rangle$ on the vectors of this basis is, by Parseval's equality, the square of the norm of $|\psi\rangle$,

$$||\psi(t)\rangle||^2 = \langle\psi(t)|\psi(t)\rangle = \sum_j |\langle a_j|\psi(t)\rangle|^2 = \sum_j p_j. \tag{1.3}$$

Once we have chosen the state vector such that it is normalized to unity, Eq. (1.3) ensures that the probabilities of finding different outcomes of the measurement of the observable *A* sum to one, as they should. The unitarity of the evolution given by Eq. (1.2) ensures that the probabilities "don't leak".

1.1.2 Quantum–classical boundary: the Schrödinger's cat paradox

This picture does lead to serious questions. First of all, time is *very* different from spatial coordinates: it is not an observable, but a parameter, which governs the evolution of the state vector between the instantaneous "collapses". Fortunately, we do not have to deal with it, since our problems are strictly non relativistic. More pertinent is the question of the nature of "measurement" and "collapse" and their presumed instantaneity.

Measurement is understood as an interaction of the quantum system with a macroscopic object ("apparatus") such that the final state of the latter is determined by the value of the observable a_j, and different states of the apparatus are distinguishable and immutable (i.e., can be observed without perturbation). The terminology originates from the early days of quantum mechanics. Of course, there is no need for somebody to actually set up the apparatus; any appropriate macroscopic system will do, and now the tradition forces us to talk about, e.g., the liquid "measuring" or "observing" the quantum state of a particle travelling through it.

The classical states of the apparatus correlated to the different outcomes of the measurement are called "pointer states". (The corresponding eigenstates of the observable that is being measured we will also call pointer states, where it does not lead to confusion.) In the Copenhagen interpretation, it is the apparatus that predetermines what observables can be measured (so called "complementarity with respect to the means of observation"). In principle, for any classical variable we should be able to design an apparatus which would measure its quantum counterpart, an observable.

One problem here is that there exists no well-defined boundary between the "measured", or "observed" microscopic system, and the macroscopic "apparatus" or "observer". The Copenhagen interpretation of quantum mechanics simply posits the quantum behaviour for the one, and classical for the other, which is somewhat circular. What is worse, it does not allow a description of the system and the apparatus within a single formalism, denying us any quantitative description of the *process* of measurement. This was not too troubling when dealing with (quantum) electrons going through double slits in a (classical) screen, since it was obvious which was which, and the time of the electron's interaction with the detector can be neglected compared to all other relevant timescales. It becomes of crucial importance when the quantum systems we deal with contain huge numbers of elementary particles,

almost comparable with the number of particles in our "apparatus", or are being "measured" continually. How do we describe such a situation in a consistent way?

A natural thing to do is to directly extend the quantum description (as the more fundamental one) to macroscopic systems. A difficulty of this approach lies in the fact that only very special states can be measured by a macroscopic apparatus, while at the quantum level they seem to be no different from all the rest of them. The situation is highlighted by the famous "Schrödinger's cat" paradox. Let us put together a deadly contraption: a tank of poisonous gas with an electrically controlled valve, connected to a Geiger counter. Put it in a sealed container with a live cat and a radioactive atom (e.g., ^{210}Po, which decays into the stable lead-206, ^{206}Pb, with the half-life $T \approx 138$ days), and wait (Fig. 1.1).

If we had to deal just with the radioactive atom, the description would be simple. Its wave function can be written as[3]

$$|\psi(t)\rangle = 2^{-t/2T}\left|^{210}\text{Po}\right\rangle + \sqrt{1 - 2^{-t/T}}\left|^{206}\text{Pb} + \alpha \text{ particle}\right\rangle. \qquad (1.4)$$

If at any given time we measure (observe) this atom, with the probability $1 - 2^{-t/T}$ we'll find lead-206. But putting the atom in the box with a cat makes things look bizarre, once we try to describe the cat (and the rest of the contraption) by a wave
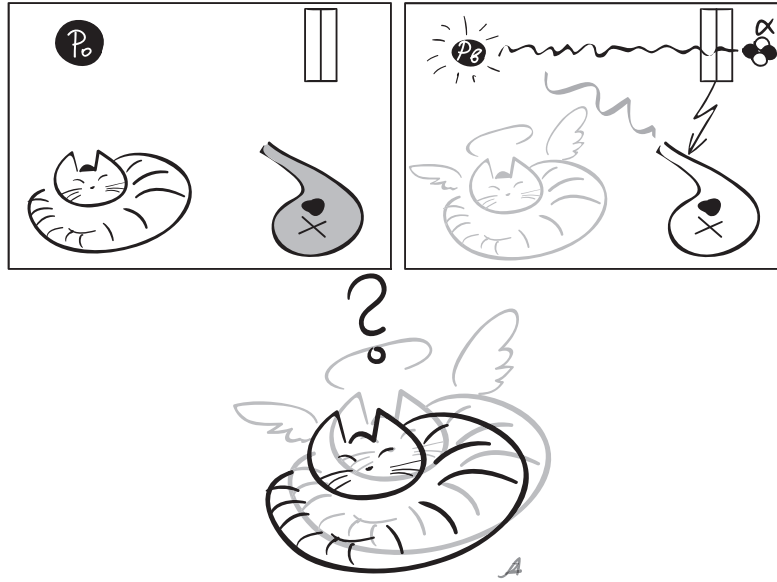

Fig. 1.1. Schrödinger's cat paradox: Should we describe macroscopic systems by wave functions, and if not, why not?

[3] This expression is only valid for not too short and not too long times; see § 5.5.6.

function. Now the state of the system before the observation will be

$$|\psi(t)\rangle = 2^{-t/2T}\left|^{210}\text{Po} + \text{live cat}\right\rangle + \sqrt{1 - 2^{-t/T}}\left|^{206}\text{Pb} + \alpha\text{ particle} + \text{dead cat}\right\rangle.$$
(1.5)

We don't doubt that after opening the box one will find either a live or a dead cat, with the probabilities $2^{-t/T}$ and $1 - 2^{-t/T}$ respectively. This intuitively clear outcome is in no way trivial. On the quantum side, we can always introduce an observable, which is a linear combination of other observables with real coefficients – there is nothing in the formalism to prohibit it. For example, we can build an observable, which will have as one of its eigenstates the superposition given by Eq. (1.5). Nevertheless, we evidently cannot build a classical apparatus, which would measure such a "zombie" state of the poor animal. The set of admissible classical states thus must impose some preferred set of bases on the Hilbert state of our quantum system.

Is the description (1.5) of a hybrid micro/macro system justified at all? And, what does precipitate the transition from the "live–dead" superposition to the "either–or" classical picture? The proposed answers run the full philosophical gamut from the many-worlds interpretation to the key role of the observer's conscience in the collapse. Instead of plunging into these fascinating ontological and epistemological depths, we will take a pragmatic approach and see how far it will take us.

We will not make any special difference between the "measurement" or "observation" and the interaction of our quantum system with its macroscopic surroundings.
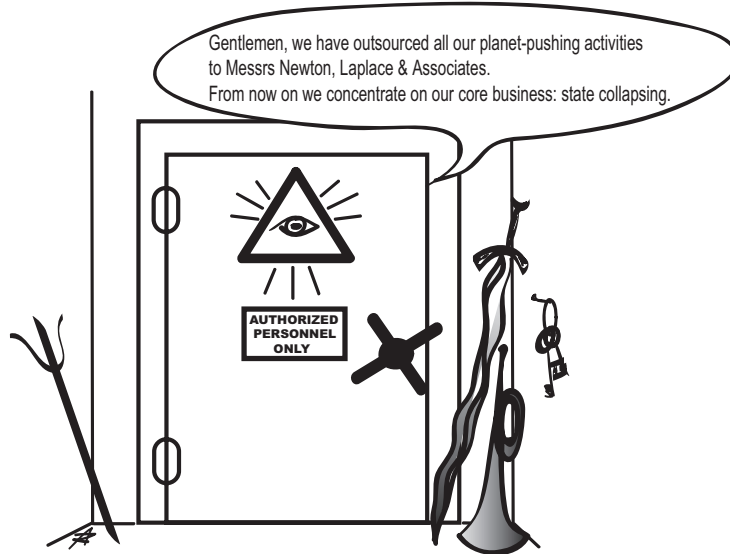

Fig. 1.2. The canonical view of the quantum–classical transition.

Indeed, explaining the "collapse" through the action of conscience would be exorcizing Asmodeus with Beelzebub's help, since we currently understand the latter, if anything, less than the former.

We will assume that on the fundamental level every system is governed (and described) by the laws of quantum mechanics, of which classical mechanics is a limiting case – in full agreement with Bohr's *correspondence principle*. The difference between "quantum" and "classical" systems must naturally emerge from the formalism.[4]

1.2 Density matrix formalism

1.2.1 Justification and properties

The notion of the state vector is inadequate for our purposes, but it can be generalized to the *density matrix*, or *statistical operator*, first introduced independently by Landau and von Neumann in 1927. To make the motivation clear, let us start from a quantum system, which consists of two subsystems, A and B, which we can measure independently. Suppose, for example, that we have two particles with spin $\hbar/2$, and have an apparatus, which can measure the z-component of spin of either particle. Let the system be in state

$$|\Psi\rangle_{AB} = \sum_{j,k=\uparrow,\downarrow} C_{jk}|j_A k_B\rangle, \tag{1.6}$$

which is obviously the most general form of such two-particle wave functions. Now measure the spin of particle B. The corresponding observable is the operator $(\hbar/2)\sigma_z$, such that $(\hbar/2)\sigma_z|\uparrow\rangle = \hbar/2|\uparrow\rangle$, and $(\hbar/2)\sigma_z|\downarrow\rangle = -\hbar/2|\downarrow\rangle$. The result of the measurement can then be written as

$$|\Psi\rangle_{AB} \rightarrow \begin{cases} \text{spin B} = \hbar/2, |\uparrow_A\rangle, \text{probability}|C_{\uparrow\uparrow}|^2; \\ \text{spin B} = \hbar/2, |\downarrow_A\rangle, \text{probability}|C_{\downarrow\uparrow}|^2; \\ \text{spin B} = -\hbar/2, |\uparrow_A\rangle, \text{probability}|C_{\uparrow\downarrow}|^2; \\ \text{spin B} = -\hbar/2, |\downarrow_A\rangle, \text{probability}|C_{\downarrow\downarrow}|^2. \end{cases} \tag{1.7}$$

If now we measure the spin of particle A, its average value will be

$$\left\langle \frac{\hbar}{2}\sigma_z \right\rangle = \frac{\hbar}{2}\left(|C_{\uparrow\uparrow}|^2 + |C_{\uparrow\downarrow}|^2 - |C_{\downarrow\uparrow}|^2 - |C_{\downarrow\downarrow}|^2 \right). \tag{1.8}$$

The normalization of the initial state vector, $|||\Psi\rangle_{AB}||^2 = \sum_{ij}|C_{ij}|^2 = 1$, ensures that the probabilities of the outcomes of (1.7) add up to unity, so everything is fine,

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[4] We are encouraged by the emergence of time-irreversible Boltzmann equations from time-reversible Newtonian dynamics of point-like particles.

except that Eq. (1.7) is a very awkward way of dealing with even such a small system. Just imagine we had three particles!

The situation improves once the state vector is replaced with the density matrix. Let us choose a set of normalized, but not necessarily mutually orthogonal states in the Hilbert space, $\{|\Psi_j\rangle\}$, and write an operator

$$\rho = \sum_j p_j |\Psi_j\rangle\langle\Psi_j|, \tag{1.9}$$

where $p_j \geq 0$, and $\sum_j p_j = 1$. This obviously Hermitian operator can be interpreted as describing a *statistical ensemble* of quantum systems, which can be in a state $|\Psi_j\rangle$ with probability p_j. This is exactly the situation described by Eq. (1.7).

The convenience of using this operator becomes clear when calculating average values of the observables. According to rule (3) of quantum mechanics, the measured value of an observable A is always one of the eigenvalues of A, and according to rule (4), the probability of measuring a particular a_k in state $|\Psi_j\rangle$ is $|\langle a_k|\Psi_j\rangle|^2$. Therefore

$$\langle A \rangle_{\Psi_j} = \sum_k |\langle a_k|\Psi_j\rangle|^2 a_k = \sum_k \langle\Psi_j|a_k\rangle a_k \langle a_k|\Psi_j\rangle$$

$$= \sum_k \langle\Psi_j|a_k|a_k\rangle\langle a_k|\Psi_j\rangle = \langle\Psi_j|A\left(\sum_k |a_k\rangle\langle a_k|\right)|\Psi_j\rangle = \langle\Psi_j|A|\Psi_j\rangle, \tag{1.10}$$

a standard formula. Since now the system is in state $|\Psi_j\rangle$ only with some probability p_j, we must average over these too, with the result

$$\langle A \rangle = \sum_j p_j \langle A \rangle_{\Psi_j} = \sum_j p_j \langle\Psi_j|A|\Psi_j\rangle \equiv \mathrm{tr}(\rho A). \tag{1.11}$$

The system, described by a density matrix, is said to be in a *mixed state*, instead of a *pure state* (when a single state vector suffices). One can write a density matrix for a pure state: it will include only one component, $\rho_{\mathrm{pure}} = |\Psi\rangle\langle\Psi|$.

As a Hermitian operator, the density matrix has an orthonormal set of eigenstates, $|\rho_j\rangle$, with corresponding eigenvalues, ρ_j. It can be, therefore, written in the *spectral representation*,

$$\rho = \sum_j \rho_j |\rho_j\rangle\langle\rho_j|. \tag{1.12}$$

Since ρ_j can be interpreted as the probability of finding the system in state $|\rho_j\rangle$, all $\rho_j \geq 0$; in other words, the density matrix is *positive semidefinite*.

The density matrix can be written in any basis in the Hilbert space, and will usually have neither the explicit form (1.9) nor (1.12). We will therefore list here its invariant properties.

1) $\text{tr}\,\rho = 1$ (follows directly from the definition (1.9)).
2) $\rho^2 = \rho$ if and only if the state is pure. Indeed, if $\rho = |\Psi\rangle\langle\Psi|$, then $\rho^2 = |\Psi\rangle\langle\Psi||\Psi\rangle\langle\Psi| = |\Psi\rangle\langle\Psi| = \rho$. Conversely, if $\rho^2 = \rho$, then (from (1.12)) $\rho_j^2 = \rho_j$, and the eigenvalues of the density matrix are either zeros, or ones. Since its trace is one, then only one eigenvalue can be equal to one, i.e., there is only one term in the spectral decomposition, and the state is indeed pure.
3) $\text{tr}(\rho^2) \leq 1$, and there is equality if and only if the state is pure (therefore the quantity $\varsigma = \text{tr}(\rho^2)$ is sometimes called *purity*). Starting from (1.9) and recalling that $|\langle\Psi_j|\Psi_k\rangle| \leq 1$,

$$\text{tr}(\rho^2) = \text{tr}\left(\sum_{jk} p_j p_k |\Psi_j\rangle\langle\Psi_j|\Psi_k\rangle\langle\Psi_k|\right)$$

$$= \sum_j p_j \sum_k p_k \left|\langle\Psi_j|\Psi_k\rangle\right|^2 \leq \sum_j p_j = 1.$$

On the other hand, if $\text{tr}(\rho^2) = 1$, then $\sum_j p_j \left(\sum_k p_k \left|\langle\Psi_j|\Psi_k\rangle\right|^2\right) = 1$. Since the non negative p_j's add up to one, there is equality only if $p_j = \delta_{jq}$ for some q, that is, if the state is pure.

These properties provide us with a reliable way to check any approximate calculations of a density matrix, as well as a criterion of whether a given system is in a pure or a mixed state.

1.2.2 Averages, probabilities and coherences

Consider now, as before, a quantum-mechanical system in the pure state (1.6). Its density matrix is

$$\rho_{AB} = |\Psi\rangle_{AB}\langle\Psi|_{AB} = \sum_{j,k,l,m=\uparrow,\downarrow} C_{jk}C_{lm}^*|j_A k_B\rangle\langle l_A m_B|.$$

Let's take a partial trace of this operator over the states of particle B:

$$\rho_A \equiv \text{tr}_B\rho_{AB} = \sum_{q=\uparrow,\downarrow} \langle q_B|\Psi\rangle_{AB}\left(\langle\Psi|_{AB}\right)|q_B\rangle$$

$$= \sum_{q,j,k,l,m=\uparrow,\downarrow} C_{jk}C_{lm}^*\delta_{qk}|j_A\rangle\langle l_A|\delta_{qm} = \sum_{q,j,l=\uparrow,\downarrow} C_{jq}C_{lq}^*|j_A\rangle\langle l_A|. \quad (1.13)$$

To find the observed value of the *z*-component of spin of particle A, we now take the trace of the spin operator with *reduced density matrix* ρ_A:

$$\left\langle \frac{\hbar}{2}\sigma_z^A \right\rangle = \frac{\hbar}{2}\text{tr}\left(\rho_A\sigma_z^A\right) = \frac{\hbar}{2}\text{tr}\sum_{q,j,l=\uparrow,\downarrow} C_{jq}C_{lq}^*\sigma_z|j_A\rangle\langle l_A|$$

$$= \frac{\hbar}{2}\text{tr}\sum_{q,j=\uparrow,\downarrow}|C_{jq}|^2\langle j_A|\sigma_z|j_A\rangle. \tag{1.14}$$

This equation automatically yields the same result as Equations (1.7) and (1.8), and in a compact form. We see that as long as we are interested only in the results of measurement on one subsystem, we can use the reduced density matrix by taking the trace of the full density matrix over all the irrelevant degrees of freedom. This is an important procedure, which is crucial for describing open quantum systems, i.e., systems for which one can neither neglect their interaction with the environment nor take the latter into account explicitly.

Let us look at Eq. (1.13) in more detail. This expression contains more information than just the average value of the operator σ_z. The diagonal terms provide the probabilities of finding the system with spin up/down. What about the off-diagonal ones?

Let us write a density matrix in an orthonormal basis of eigenstates of some observable *A*, and we chose *A* such that its eigenstates are macroscopically observable pointer states – e.g., charges, positions or momenta: $\rho = \sum_{ij}\rho_{ij}|a_i\rangle\langle a_j|$. Its diagonal elements give the probabilities of finding the system in appropriate eigenstates, and if we are only performing the measurements of *A* this is all we care about or can extract from the experiment. The off-diagonal terms could have never been there. Nevertheless, they are crucially important.

We have seen that a diagonal density matrix describes a pure state if and only if its only element is unity (invariant property number 2). If this is the case, we will always measure the same eigenvalue a_j of the operator *A* and leave the system in the same state $|a_j\rangle$.[5] (This is called *quantum non demolition (QND) measurement*, and we will discuss the implications of such experiments in § 5.5.2.) If not, the density matrix must describe a mixed state, so the absence of the off-diagonal matrix elements is a tell-tale sign. These elements describe *quantum coherence*. If they are zero, mathematically there is no basis in which the density matrix contains a single diagonal element; physically, the system is in a mixed state; from the point of view of the observation, there is no observable of which the system is in an eigenstate, and its measurement will yield some eigenstate at random, with a given

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[5] We need not bother here with the cases of degenerate eigenstates or the continuous spectrum of the operator *A*.

probability. This is why the evolution of the off-diagonal elements of the density matrix *("coherences")* is of special interest: their disappearance – "decoherence", due to whatever processes that cause it – means the reduction of the state of the system to a mixture, with the loss of specifically quantum correlations. The rate of this reduction can, therefore, be taken as the *decoherence rate*, and its inverse as the *decoherence time*.

1.2.3 Entanglement

We have already seen that when several distinct systems (e.g., a cat and a ^{210}Po atom) are described by a single quantum state, this can lead to quite counterintuitive conclusions. Suppose that two quantum systems (e.g., spin-1/2 particles A and B) are in a pure quantum state $|\Psi\rangle_{AB}$. Then, generally speaking, separately, neither of them can be in a definite quantum state. Consider, for example, the expectation value of σ_z for particle A, Eq. (1.14):

$$\left\langle \frac{\hbar}{2}\sigma_z^A \right\rangle = \frac{\hbar}{2}\text{tr}\left(\rho_A\sigma_z^A\right).$$

The reduced density matrix $\rho_A = \text{tr}_B\left[|\Psi\rangle_{AB}\langle\Psi|_{AB}\right]$ can only have the form $|\psi\rangle_A\langle\psi|_A$, corresponding to particle A being in a pure quantum state $|\psi\rangle_A$, if the quantum state of the whole system is factorized:

$$|\Psi\rangle_{AB} = |\psi\rangle_A \otimes |\psi\rangle_B. \tag{1.15}$$

Otherwise, particle A by itself is in a mixed state, even though the whole system consisting of A and B is in a pure state, and there is no interaction between A and B. The non factorized states of multipartite systems are called *entangled*, which expresses this specifically quantum correlation between its components. Essentially, it means that the properties of a quantum system in general can never be reduced to the sum of the properties of its constituents.

For a pure state $|\Psi\rangle_{ABC...}$ of a system, comprising any number of subsystems, the test for entanglement is straightforward: if all reduced density matrices correspond to pure states, the state $|\Psi\rangle_{ABC...}$ can be written as $|\psi\rangle_A \otimes |\psi\rangle_B \otimes |\psi\rangle_C ...$, and there is no entanglement. But entanglement is not limited to pure states: certain quantum correlation can exist even if the system itself is described by a density matrix. For a given density matrix one can find different numerical measures of entanglement (all of which are zero for a factorized state; see, e.g., Horodecki et al., 2009).

1.2.4 Liouville–von Neumann equation

As a generalization of the state vector, the density matrix contains all the information about the system that can possibly be obtained. It is a counterpart of the classical density function in the phase space, $f(X_a, P_a, t)$, which describes an arbitrary classical system (e.g., a non-ideal gas). The equation of motion for $f(X_a, P_a, t)$ follows from the Hamiltonian dynamics and is called the Liouville equation:

$$\frac{\partial f(X_a, P_a, t)}{\partial t} = -[\mathcal{H}, f]_P \equiv -\sum_a \left(\frac{\partial \mathcal{H}}{\partial P_a} \frac{\partial f}{\partial X_a} - \frac{\partial f}{\partial P_a} \frac{\partial \mathcal{H}}{\partial X_a} \right), \qquad (1.16)$$

where $\mathcal{H}$ is the classical Hamilton function of the system, and $[.,.]_P$ is the Poisson bracket.

Similarly, the equation of motion for the density matrix (the *Liouville–von Neumann equation*) follows directly from the Schrödinger equation:

$$\frac{d\rho}{dt} = \sum_j \frac{d}{dt}\left(p_j|\Psi_j\rangle\langle\Psi_j|\right) = \sum_j p_j \frac{1}{\imath\hbar}\left(H|\Psi_j\rangle\langle\Psi_j| - |\Psi_j\rangle\langle\Psi_j|H\right) = \frac{1}{\imath\hbar}[H, \rho].$$
$$(1.17)$$

Not surprisingly, it has the same structure as the classical Eq. (1.16), with the Poisson bracket replaced by a commutator. It can be rewritten as

$$\frac{d\rho}{dt} = \mathcal{L}[\rho(t)], \qquad (1.18)$$

where the action of the *Liouvillian* on any operator A is given by $\mathcal{L}[A] \equiv \frac{1}{\imath\hbar}[H, A]$.

First of all, the evolution described by Eq. (1.17) is unitary. The solution can be written as (cf. (1.2))

$$\rho(t) = U(t)\rho(0)U(t)^\dagger \equiv \mathcal{U}(t, 0)[\rho(0)]; \quad U(t) = e^{-\frac{1}{\hbar}Ht}, \qquad (1.19)$$

with an obviously unitary evolution operator $U(t)$. Unitarity means, in particular, that the evolution is time-reversible, since $U^{-1} = U^\dagger$ always exists. Therefore for any $\mathcal{U}(t, 0)$ there exists the unique inverse operator: $(\mathcal{U}(t, 0))^{-1}[A(t)] = \mathcal{U}(-t, 0)[A(t)] = U(t)^\dagger A(t)U(t) = A(0)$.

There is an interesting difference between the Liouville–von Neumann equation and the Schrödinger equation from the point of view of symmetry. In the Schrödinger picture the time dependence of the energy eigenstates, $H|e_j\rangle = E_j|e_j\rangle$, is given by $\exp[-\imath E_j t/\hbar]$, and therefore a special role is played by the degenerate energy eigenstates (with $E_j = E_k$). For the Liouville–von Neumann equation,

the corresponding phase factors, obviously, contain the energy *differences*, $\exp[-\mathrm{i}(E_j - E_k)t/\hbar]$. This yields a new (so-called Liouvillian) symmetry between the *pairs* of eigenstates with the same energy differences, which can be used, as any symmetry, to simplify the analysis (Maassen van den Brink and Zagoskin, 2002).

The purity is conserved:

$$\varsigma(t) \equiv \mathrm{tr}(\rho(t)^2) = \mathrm{tr}[U(t)\rho(0)U(t)^\dagger U(t)\rho(0)U(t)^\dagger] = \mathrm{tr}(\rho(0)^2) = \varsigma(0).$$
(1.20)

This means that the evolution of a pure state into a mixed state, including the process of measurement, cannot be described by (1.17) and is an essentially non-unitary process.

1.2.5 Wigner function

The relation between the classical density function and the quantum density matrix becomes more clear if we use for the latter a representation that was first proposed by Wigner (1932) for the wave function. Consider for simplicity the case of a single particle in one dimension. In the position representation its density matrix is (omitting the explicit time dependence)

$$\rho(x, x') \equiv \langle x|\rho|x'\rangle,$$
(1.21)

where $\hat{X}|x\rangle = x|x\rangle$. If we denote the average position and the deviation from it by $X = (x + x')/2$, $\xi = x - x'$, respectively, and take the Fourier transform over the latter, we obtain a function, which depends on *both* position and momentum:

$$W(X, P) = \frac{1}{2\pi\hbar} \int d\xi \left\langle X + \frac{\xi}{2} \middle| \rho \middle| X - \frac{\xi}{2} \right\rangle e^{-\mathrm{i}P\xi/\hbar}.$$
(1.22)

This *Wigner function* looks similar to the classical distribution function $f(X, P)$. They indeed have common properties. For example, integrating $f(X, P)$ with respect to one variable leaves a positively defined probability distribution for the other. The same holds for $W(X, P)$:

$$\int dP\, W(X, P) = \int d\xi \left\langle X + \frac{\xi}{2} \middle| \rho \middle| X - \frac{\xi}{2} \right\rangle \frac{1}{2\pi\hbar} \int dP\, e^{-\mathrm{i}P\xi/\hbar}$$
$$= \int d\xi \left\langle X + \frac{\xi}{2} \middle| \rho \middle| X - \frac{\xi}{2} \right\rangle \delta(\xi) = \langle X|\rho|X\rangle \geq 0;$$
(1.23)

$$\int dX\, W(X, P) = \frac{1}{2\pi\hbar} \int d\xi \int dX \left\langle X + \frac{\xi}{2} \middle| \rho \middle| X - \frac{\xi}{2} \right\rangle e^{-\imath P\xi/\hbar}$$

$$= \int dx\, dx'\, \langle x|\rho|x'\rangle \left[\frac{1}{2\pi\hbar} e^{-\imath P(x-x')/\hbar} \right]$$

$$= \int dx\, dx'\, \langle x|\rho|x'\rangle \langle x'|P\rangle \langle P|x\rangle = \langle P|\rho|P\rangle \geq 0. \qquad (1.24)$$

We took into account that the eigenfunctions of momentum in the position representation are simply plane waves, $\langle x|P\rangle = e^{\imath Px/\hbar}/\sqrt{2\pi\hbar}$, and that they comprise a basis of the Hilbert space (see, e.g., Messiah, 2003; Landau and Lifshitz, 2003). We also used the fact that the density matrix is positive semidefinite, Eq. (1.12).

From (1.23) and (1.24) immediately follows that the Wigner function is normalized to unity,

$$\int dX\, dP\, W(X, P) = 1. \qquad (1.25)$$

In addition to the relations

$$\langle \hat{X}^m \rangle = \int dX\, dP\, W(X, P) X^m; \quad \langle \hat{P}^n \rangle = \int dX\, dP\, W(X, P) P^n, \qquad (1.26)$$

which follow from Eqs. (1.23) and (1.24), it can be shown that, in general,

$$\int dX\, dP\, W(X, P) X^m P^n = \langle \{\hat{X}^m \hat{P}^n\}_{\text{sym}} \rangle, \qquad (1.27)$$

where $\{\hat{X}^m \hat{P}^n\}_{\text{sym}}$ is a *symmetrized* product of noncommuting operators $\hat{X}$, $\hat{P}$. For example, $\{\hat{X}\hat{P}\}_{\text{sym}} = \frac{1}{2}(\hat{X}\hat{P} + \hat{P}\hat{X})$, $\{\hat{X}^2\hat{P}^2\}_{\text{sym}} = \frac{1}{6}(\hat{X}^2\hat{P}^2 + \hat{P}^2\hat{X}^2 + \hat{X}\hat{P}^2\hat{X} + \hat{P}\hat{X}^2\hat{P} + \hat{X}\hat{P}\hat{X}\hat{P} + \hat{P}\hat{X}\hat{P}\hat{X})$, etc. The Wigner function, therefore, reduces the task of finding average values of a product of the observables to calculating an ordinary integral (1.27) (where X's and P's are, of course, just numbers), but imposes a specific (*Wigner*) ordering of the operators to be averaged.

Where the drastic difference between $W(X, P)$ and $f(X, P)$ does arise, it is that Eqs. (1.23) and (1.24) notwithstanding, $W(X, P)$ is not non-negative. Therefore, it is not a probability, but a *quasiprobability* distribution function, and here lies its essential quantumness. One can show, on the other hand, that the Wigner function averaged on the scale of $2\pi\hbar$ becomes non-negative and reduces to the classical distribution function $f(X, P)$ (Röpke, 1987, §2.2.2; Zubarev et al., 1996). This is another way of looking at the quantum–classical transition.[6]

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[6] Of course, one has eventually to discuss reasons and specific mechanisms for such averaging.

The generalization to more degrees of freedom or different observables is straightforward. The similarity between the Wigner function and the classical probability density makes use of $W(X, P)$ very convenient in, e.g., quantum statistical physics and quantum kinetics (Balescu, 1975; Pitaevskii and Lifshitz, 1981).

The Wigner function for the states of a harmonic oscillator – i.e., quantized field modes – is particularly useful for our purposes and will be introduced in Section 4.4.[7]

1.2.6 Perturbation theory for density matrix. Linear response theory

Any system in the Universe is isolated only to a degree. Therefore, a reasonable theory must allow for a consistent treatment of *open systems*, i.e., systems coupled to their environment (which is weakly influenced by the system and can only be described by average macroscopic parameters, like temperature and pressure).

If the system is in equilibrium, its density matrix has the Gibbs form:

$$\rho_{CE} = e^{(F-H)/k_B T}; \quad F = -k_B T \ln \mathrm{tr}\, e^{-H/k_B T} \tag{1.28}$$

or

$$\rho_{GCE} = e^{(\Omega - H')/k_B T}; \quad \Omega = -k_B T \ln \mathrm{tr}\, e^{-H'/k_B T}. \tag{1.29}$$

The first of these equations describes the *canonical ensemble*, where the system can exchange only energy with the environment. The second corresponds to the *grand canonical ensemble*, where particles can also be exchanged. (Therefore, instead of the Hamiltonian H one uses the operator $H' = H - \mu N$, where μ is the chemical potential and N is the particle number operator; N obviously commutes with H.) These expressions are routinely derived in quantum statistical mechanics (e.g., Landau and Lifshitz, 1980, Chapter III). They are very similar to their classical analogues, and the normalization factors F and Ω are the quantum counterparts of the (Helmholtz) free energy and of the grand potential, respectively. Here we should observe that as long as the number of particles in the system is large, the two ensembles are equivalent, but in small systems, where a single particle may make a difference, one must take care to use the physically appropriate ensemble. This is precisely the case of, e.g., charge qubits.

Looking at Equations (1.28) and (1.29), we see that in equilibrium the system is in a mixed state. Nevertheless, the systems we are interested in are far from equilibrium, and the Liouville–von Neumann equations should be solved with appropriate initial conditions, which is usually impossible. The general approach to the problem

---

[7] On a more general plane, the Wigner function is a version of a non-equilibrium Green's function, which finds broad applications all across physics (see, e.g., Pitaevskii and Lifshitz, 1981, Chapter X; Zagoskin, 1998, Chapter 3).

is based on perturbation theory. Assuming that the coupling between the system and the environment is weak and the initial state of both is known, one can, e.g., iterate the equations, obtaining the answer as a series of powers of the coupling.

To demonstrate this approach and introduce (or remind the reader of) some useful ideas, we start by deriving the equations of *linear response theory*. We assume that the system is weakly perturbed by an external force and are interested in what will be the change in the average value of some observable A due to the perturbation, in the first order, in the perturbation strength.

The Hamiltonian of the problem is then

$$H(t) = H_0 + H_I(t), \tag{1.30}$$

where the unperturbed Hamiltonian H_0 is time-independent, and the perturbation $H_I(t)$ is small compared to H_0. It is convenient to use the *interaction representation*, in which every operator is put between the "brackets":

$$A \rightarrow A_{\text{int}}(t) = U_0(t)^\dagger A U_0(t), \ \ U_0(t) = \mathrm{e}^{-\imath H_0 t / \hbar}. \tag{1.31}$$

Performing this operation on the density matrix, we see that

$$\begin{aligned} \frac{\mathrm{d}\rho_{\text{int}}}{\mathrm{d}t} &= -\frac{1}{\imath\hbar}[H_0, \rho_{\text{int}}(t)] + U_0(t)^\dagger \frac{\mathrm{d}\rho}{\mathrm{d}t} U_0(t) \\ &= -\frac{1}{\imath\hbar}[H_0, \rho_{\text{int}}(t)] + U_0(t)^\dagger \frac{1}{\imath\hbar}[H_0 + H_I(t), \rho(t)] U_0(t) \\ &\equiv \frac{1}{\imath\hbar}[H_{I,\text{int}}(t), \rho_{\text{int}}(t)]. \end{aligned} \tag{1.32}$$

Integrating this from $t = -\infty$, we find

$$\rho_{\text{int}}(t) = \rho_{\text{int}}(-\infty) + \frac{1}{\imath\hbar} \int_{-\infty}^{t} \mathrm{d}t' [H_{I,\text{int}}(t'), \rho_{\text{int}}(t')]. \tag{1.33}$$

The system initially being in equilibrium, $\rho_{\text{int}}(-\infty) \equiv \rho_0$ is given either by (1.29) or by (1.30). (In the case of the grand canonical ensemble we should everywhere use instead of the Hamiltonian, H, the operator $H' = H - \mu N$.) Equation (1.33) can be formally iterated:

$$\rho_{\text{int}}(t) = \rho_0 + \rho_1(t) + \rho_2(t) + \dots;$$
$$\rho_1(t) = \frac{1}{\imath\hbar} \int_{-\infty}^{t} \mathrm{d}t' [H_{I,\text{int}}(t'), \rho_0]; \ \text{ad inf}. \tag{1.34}$$

This series usually converges only asymptotically; moreover, its higher-order terms contain unpleasant nested commutators, but the linear response of the system to the perturbation – the first term in the series – can be readily obtained.

Due to the cyclic invariance of the trace, the average $\langle A \rangle$ is the same in the interaction representation, $\langle A \rangle = \mathrm{tr}\ A\rho(t) = \mathrm{tr}\ A_{\mathrm{int}}(t)\rho_{\mathrm{int}}(t)$. The shift due to the perturbation (the linear response of the measured observable) is then

$$\Delta A(t) = \mathrm{tr}\ \rho_1(t)A_{\mathrm{int}}(t) = \frac{1}{\mathrm{i}\hbar}\int_{-\infty}^{t}\mathrm{d}t'\,\mathrm{tr}\left([H_{I,\mathrm{int}}(t'),\rho_0]A_{\mathrm{int}}(t)\right)$$

$$= \frac{1}{\mathrm{i}\hbar}\int_{-\infty}^{t}\mathrm{d}t'\,\big\langle[A_{\mathrm{int}}(t),H_{I,\mathrm{int}}(t')]\big\rangle_0, \tag{1.35}$$

where $\langle\ldots\rangle_0 \equiv \mathrm{tr}(\rho_0\ldots)$ is the equilibrium average. This expression can be used as is, but it is both convenient and insightful to transform this *Kubo formula* to the form that allows us to link the linear response of a system to the equilibrium fluctuations in it.

There are different ways of writing Kubo formulas. We will do so by assuming, without restricting the generality, that the perturbation $H_I(t)$ has the form

$$H_I(t) = -f(t)B, \tag{1.36}$$

where B is an operator, and $f(t)$ is a conventional function called a *generalized force*. We will also introduce the *retarded Green's function* of the operators A and B,

$$\ll A(t)B(t') \gg^R \equiv \frac{1}{\mathrm{i}\hbar}\big\langle[A(t),B(t')]\big\rangle_0\,\theta(t-t'). \tag{1.37}$$

Here $\theta(t-t')$ is Heaviside's step function, and retarded means that (1.36) is zero unless $t \geq t'$. Using this definition, we can rewrite (1.35) as

$$\Delta A(t) = -\int_{-\infty}^{\infty}\mathrm{d}t'\,f(t') \ll A(t)B(t') \gg^R. \tag{1.38}$$

As would be expected, from causality, only the perturbations at times earlier than t can influence $\Delta A(t)$.

The Green's function is calculated at equilibrium; therefore, it depends only on the difference $t-t'$, and the expression (1.38) is a convolution. Taking its Fourier transform, we obtain simply

$$\Delta A(\omega) = -f(\omega) \ll AB \gg_{\omega}^R. \tag{1.39}$$

Defining the *generalized susceptibility* via

$$\chi(\omega) = \Delta A(\omega)/f(\omega), \tag{1.40}$$

we see that it is equal to $- \ll AB \gg_{\omega}^R$. Examples of generalized susceptibilities are electrical conductivity $\sigma_{\alpha\beta}(\omega)$ (where the current density $j_{\alpha}(\omega) = \sigma_{\alpha\beta}(\omega)E_{\beta}(\omega)$), magnetic susceptibility $\chi_{\alpha\beta}(\omega)$ (with the magnetic moment $m_{\alpha}(\omega) = \chi_{\alpha\beta}(\omega)H_{\beta}(\omega)$), etc.

1.2.7 Fluctuation-dissipation theorem

Now we will, as promised, relate the susceptibility to the equilibrium fluctuations in the system. The latter are described by the *autocorrelation function* of the given observable,

$$K_A(t) = \langle A(t)A(0)\rangle_0 \equiv K_{A,s}(t) + K_{A,a}(t);$$

$$K_{A,s(a)}(t) = \frac{K_A(t) \pm K_A(-t)}{2}. \tag{1.41}$$

Since A is an operator, $A(t)$ and $A(0)$ do not necessarily commute, and the anti-symmetric part $K_{A,a}(t)$ is generally nonzero, but we are here concerned with the symmetric part of the autocorrelator. Its Fourier transform $S_{A,s}(\omega)$ (*symmetric spectral density of fluctuations*) gives the intensity of fluctuations of the observable.[8]

Let us invoke a useful *Kubo–Martin–Schwinger identity* for an equilibrium average of any two operators,

$$\langle A(\tau)B(0)\rangle_0 \equiv \mathrm{tr}\left(e^{(F_0-H_0)/k_BT}e^{\imath H_0\tau/\hbar}A(0)e^{\imath H_0\tau/\hbar}B(0)\right)$$

$$= \langle B(0)A(\tau + \imath\hbar/k_BT)\rangle_0, \tag{1.42}$$

which immediately follows from the cyclic invariance of the trace. Then we can write for the Fourier transforms of a commutator and an anticommutator,

$$\langle [A, A]\rangle_{0,\omega} \equiv \int_{-\infty}^{\infty} dt\,e^{\imath\omega t}\langle [A(t), A(0)]\rangle_0 = \left(e^{\hbar\omega/k_BT} - 1\right)\int_{-\infty}^{\infty} dt\,e^{\imath\omega t}\langle A(0)A(t)\rangle_0;$$

$$\langle \{A, A\}\rangle_{0,\omega} \equiv \int_{-\infty}^{\infty} dt\,e^{\imath\omega t}\langle \{A(t), A(0)\}\rangle_0 = \left(e^{\hbar\omega/k_BT} + 1\right)\int_{-\infty}^{\infty} dt\,e^{\imath\omega t}\langle A(0)A(t)\rangle_0.$$

$$\tag{1.43}$$

This allows us to express the symmetric spectral density through the average commutator,

$$S_{A,s}(\omega) \equiv \langle \{A, A\}\rangle_{0,\omega}/2 = \langle [A, A]\rangle_{0,\omega} \coth(\hbar\omega/2k_BT)/2. \tag{1.44}$$

---

[8] To be more precise, in order to investigate fluctuations around the average value $\langle A\rangle_0$ one should consider the *autocovariance function*, $K'_A(t) = \langle (A(t) - \langle A\rangle_0)(A(0) - \langle A\rangle_0)\rangle_0 \equiv K_A(t) - \langle A\rangle_0^2$. In the following we assume $\langle A\rangle_0 = 0$, which makes only a trivial difference.

On the other hand, by splitting the integration interval and changing variables we get

$$
\begin{aligned}
\langle [A, A]\rangle_{0,\omega} &= \int_{\infty}^{0} \mathrm{d}(-t)\mathrm{e}^{\imath\omega(-t)} \langle [A(-t), A(0)]\rangle_0 + \int_{0}^{\infty} \mathrm{d}t\mathrm{e}^{\imath\omega t} \langle [A(t), A(0)]\rangle_0 \\
&= -\int_{0}^{\infty} \mathrm{d}t\mathrm{e}^{-\imath\omega t} \langle [A(t), A(0)]\rangle_0 + \int_{0}^{\infty} \mathrm{d}t\mathrm{e}^{\imath\omega t} \langle [A(t), A(0)]\rangle_0 \\
&= -2\hbar\mathtt{Im} \ll AA \gg_{\omega}^{R} \equiv 2\hbar\mathtt{Im}\chi(\omega).
\end{aligned}
\tag{1.45}
$$

We have, therefore, established the relation between the intensity of *equilibrium* fluctuations in a system and its linear response to an external perturbation, known as the *fluctuation–dissipation theorem*:

$$
S_{A,s}(\omega) = \hbar\mathtt{Im}\chi(\omega)\coth(\hbar\omega/2k_B T).
\tag{1.46}
$$

The relation between the equilibrium properties of the system and its nonequilibrium behaviour is not only physically insightful, but practically useful. Equilibrium Green's functions like (1.37) can be obtained perturbatively, using the well-developed and relatively simple *Matsubara formalism* (an extension of Feynman's diagrammatic approach).[9] One can also go on and calculate higher-order response functions (i.e., quadratic susceptibility, cubic susceptibility, etc.), which will again be expressed in terms of equilibrium properties of the system, but the expressions soon become unwieldy, and their practical usefulness diminishes.

1.3 Evolution of density matrix in open systems

1.3.1 Getting rid of the environment

Let us return to the Liouville–von Neumann equation (1.17) for a system and its environment described by the Hamiltonian

$$
H = H_S + H_E + H_I.
\tag{1.47}
$$

Our goal is to reconcile the unitary evolution given by Eq. (1.17) with the existence of non unitary processes, like measurement, and in general, transition from a pure to a mixed state. We will see that this can be done based on several plausible assumptions.

First, we plausibly assume that H_I is a small perturbation, and that the environment is so big that the influence of the system on it is also small. As in (1.31) we will use the interaction representation with respect to the Hamiltonian $H_0 \equiv H_S + H_E$,

---

[9] See, e.g., Zagoskin (1998), Chapter 3.

so that

$$\frac{\mathrm{d}\rho}{\mathrm{d}t} = \frac{1}{\imath\hbar}[H_I(t), \rho(t)]; \quad \rho(t) = \rho(-\infty) + \frac{1}{\imath\hbar}\int_{-\infty}^{t} \mathrm{d}t'[H_I(t'), \rho(t')] \qquad (1.48)$$

(we dropped the subscripts "int" to unclutter the formulas). By substituting in the right-hand side of the first equation (1.48) the expression for $\rho(t)$ from the second equation, we get

$$\frac{\mathrm{d}\rho}{\mathrm{d}t} = \frac{1}{\imath\hbar}[H_I(t), \rho(-\infty)] + \frac{1}{(\imath\hbar)^2}\int_{-\infty}^{t} \mathrm{d}t'[H_I(t), [H_I(t'), \rho(t')]]. \qquad (1.49)$$

Now we continue making plausible assumptions. First, assume that not only initially the system and the environment were statistically independent of each other, but they will remain so:

$$\rho(-\infty) = \rho_S(-\infty) \otimes \rho_E; \quad \rho(t) = \rho_S(t) \otimes \rho_E. \qquad (1.50)$$

This assumption rests on the bigness of the environment and the weakness of its interaction with the system, and is physically reasonable. (Of course, every part of the physical environment, which violates this assumption, must be included in the system.) Then we can trace out the environment and find for the reduced density matrix of the system, $\mathrm{tr}_E\rho(t) \equiv \rho_S(t)$ (compare to Eq. (1.14)),

$$\frac{\mathrm{d}\rho_S}{\mathrm{d}t} = \frac{1}{\imath\hbar}\mathrm{tr}_E([H_I(t), \rho_S(-\infty) \otimes \rho_E])$$

$$+ \frac{1}{(\imath\hbar)^2}\int_{-\infty}^{t} \mathrm{d}t'\mathrm{tr}_E([H_I(t), [H_I(t'), \rho_S(t') \otimes \rho_E]]). \qquad (1.51)$$

Second, realistically assume that the interaction Hamiltonian has the form (in the Schrödinger representation)

$$H_I = \sum_{ab} g_{ab} A_a B_b, \qquad (1.52)$$

where the operators A act on the system, and B on the environment, and $\langle B \rangle \equiv \mathrm{tr}_E[\rho_E B] = 0$. (If $\langle B \rangle \neq 0$, the corresponding term in (1.52), $\sum_{ab} g_{ab} A_a \langle B_b \rangle$, would only depend on the operators acting on the system and should have been included in H_S.) From here it follows that the first term in (1.51) vanishes. Finally, make a really important *Markov approximation*. Namely, assume that the density matrix in the system changes more slowly than the characteristic correlation times of the environment. Then we can neglect the difference between t and t' in the argument of ρ_S and reduce the integro-differential equation (1.51) to the differential

master equation

$$\frac{\mathrm{d}\rho_S}{\mathrm{d}t} = -\frac{1}{\hbar^2}\int_{-\infty}^{t}\mathrm{d}t'\,\mathrm{tr}_E([H_I(t),[H_I(t'),\rho_S(t)\otimes\rho_E]]), \qquad (1.53)$$

which contains *only the current value* of the reduced density matrix. (Independence of the previous history is precisely what Markovian means in the mathematical theory of random processes.) We could have an additional term in (1.53), of the form $(1/\mathrm{1}\hbar)[h(t),\rho_S(t)]$, with $h(t)$ describing some processes in the system we decided not to cancel by the transition to the interaction picture (e.g., the influence of an external field, as in Eq. (1.36)).

1.3.2 Master equation for the density matrix; Lindblad operators

Equation (1.53) does not look like a finished job yet. We should have substituted (1.52) for H_I, taken the trace over the environmental variables, and calculated the integral over t'. Nevertheless, it is more convenient to do this with a concrete Hamiltonian, to make use of the specific commutation relations of the operators A, B.

Let us consider, as an example, an environment that consists of a single bosonic mode with frequency ω_E. That is, our system is coupled to a linear oscillator, which is somehow maintained in a given stationary state ρ_E. It is usually, but not always, justified to assume that this state is an equilibrium state (1.28) with some temperature T.

The simplest form of a coupling term in the interaction representation is then (reminding us of Eq. (1.36))

$$H_I(t) = gB(t)(a^\dagger(t)+a(t)) = gB(t)\left(a^\dagger\mathrm{e}^{\mathrm{1}\omega_E t}+a\mathrm{e}^{-\mathrm{1}\omega_E t}\right). \qquad (1.54)$$

We took into account that in the interaction representation the Bose operators depend on time trivially, $a(t)=a\exp[-\mathrm{1}\omega_E t]$, $a^\dagger(t)=a^\dagger\exp[\mathrm{1}\omega_E t]$. The time dependence of the Hermitian operator B, acting on the system, is determined by H_S, whatever it is, and B generally does not commute with the density matrix ρ_S (neither $B(t)$ and $B(t')$ should commute, unless $t'=t$). Substituting (1.54) into (1.53), we will obtain several tedious expressions, which are all written down below:

$$\frac{\mathrm{d}\rho_S}{\mathrm{d}t} = -\frac{g^2}{\hbar^2}\{(a)-(b)-(c)+(d)\}; \qquad (1.55)$$

$$(a) = \left\langle\left(a^\dagger\right)^2\right\rangle B(t)\left[\int_{-\infty}^{t}\mathrm{d}t'B(t')\mathrm{e}^{\mathrm{1}\omega_E(t'+t)}\right]\rho_S(t)$$
$$+\langle aa^\dagger\rangle B(t)\left[\int_{-\infty}^{t}\mathrm{d}t'B(t')\mathrm{e}^{\mathrm{1}\omega_E(t'-t)}\right]\rho_S(t)$$

$$+ \langle a^\dagger a \rangle B(t) \left[\int_{-\infty}^{t} dt' B(t') e^{-\imath \omega_E (t'-t)} \right] \rho_S(t)$$

$$+ \langle (a)^2 \rangle B(t) \left[\int_{-\infty}^{t} dt' B(t') e^{-\imath \omega_E (t'+t)} \right] \rho_S(t);$$

$$(b) = \left\langle \left(a^\dagger \right)^2 \right\rangle B(t) \rho_S(t) \left[\int_{-\infty}^{t} dt' B(t') e^{\imath \omega_E (t'+t)} \right]$$

$$+ \langle a^\dagger a \rangle B(t) \rho_S(t) \left[\int_{-\infty}^{t} dt' B(t') e^{\imath \omega_E (t'-t)} \right]$$

$$+ \langle a a^\dagger \rangle B(t) \rho_S(t) \left[\int_{-\infty}^{t} dt' B(t') e^{-\imath \omega_E (t'-t)} \right]$$

$$+ \langle (a)^2 \rangle B(t) \rho_S(t) \left[\int_{-\infty}^{t} dt' B(t') e^{-\imath \omega_E (t'+t)} \right];$$

$$(c) = \left\langle \left(a^\dagger \right)^2 \right\rangle \left[\int_{-\infty}^{t} dt' B(t') e^{\imath \omega_E (t'+t)} \right] \rho_S(t) B(t)$$

$$+ \langle a^\dagger a \rangle \left[\int_{-\infty}^{t} dt' B(t') e^{-\imath \omega_E (t'-t)} \right] \rho_S(t) B(t)$$

$$+ \langle a a^\dagger \rangle \left[\int_{-\infty}^{t} dt' B(t') e^{\imath \omega_E (t'-t)} \right] \rho_S(t) B(t)$$

$$+ \langle (a)^2 \rangle \left[\int_{-\infty}^{t} dt' B(t') e^{-\imath \omega_E (t'+t)} \right] \rho_S(t) B(t);$$

$$(d) = \left\langle \left(a^\dagger \right)^2 \right\rangle \rho_S(t) \left[\int_{-\infty}^{t} dt' B(t') e^{\imath \omega_E (t'+t)} \right] B(t)$$

$$+ \langle a a^\dagger \rangle \rho_S(t) \left[\int_{-\infty}^{t} dt' B(t') e^{-\imath \omega_E (t'-t)} \right] B(t)$$

$$+ \langle a^\dagger a \rangle \rho_S(t) \left[\int_{-\infty}^{t} dt' B(t') e^{\imath \omega_E (t'-t)} \right] B(t)$$

$$+ \langle (a)^2 \rangle \rho_S(t) \left[\int_{-\infty}^{t} dt' B(t') e^{-\imath \omega_E (t'+t)} \right] B(t).$$

The averages are taken over the density matrix of the environment: $\langle a^\dagger a \rangle = \mathrm{tr}(\rho_E a^\dagger a) = \mathrm{tr}(a \rho_E a^\dagger)$, etc. Unless the bosonic mode is in a so-called *squeezed state* (see § 4.4.4), then the off-diagonal averages are zero: $\langle (a)^2 \rangle = \langle (a^\dagger)^2 \rangle = 0$. The rest are expressed through the average values of the *number operator*,

$N = a^\dagger a$; $\langle N \rangle = n$:

$$(a) = (n+1)B(t)\bar{B}(t)\rho_S(t) + nB(t)\bar{B}^\dagger(t)\rho_S(t);$$

$$(b) = nB(t)\rho_S(t)\bar{B}(t) + (n+1)B(t)\rho_S(t)\bar{B}^\dagger(t);$$

$$(c) = n\bar{B}^\dagger(t)\rho_S(t)B(t) + (n+1)\bar{B}(t)\rho_S(t)B(t);$$

$$(d) = (n+1)\rho_S(t)\bar{B}^\dagger(t)B(t) + n\rho_S(t)\bar{B}(t)B(t),$$

where

$$\bar{B}(t) = \int_{-\infty}^{t} dt'\, B(t') e^{\imath \omega_E (t'-t)}. \tag{1.56}$$

A further simplification can be achieved if we assume that

$$B(t) = B_- e^{-\imath \omega_B t} + B_+ e^{\imath \omega_B t}; \quad B_+ \equiv B_-^\dagger. \tag{1.57}$$

Then the integral in (1.56) is taken explicitly,

$$\bar{B}(t) = B_- e^{-\imath \omega_E t} \frac{e^{\imath(\omega_E - \omega_B)t}}{\imath(\omega_E - \omega_B) + \varepsilon} + B_+ e^{-\imath \omega_E t} \frac{e^{\imath(\omega_E + \omega_B)t}}{\imath(\omega_E + \omega_B) + \varepsilon}.$$

Here $\varepsilon \to 0$ is the infinitesimally small term added to ensure that the integrals will converge at the lower limit (this procedure is called *regularization*). Using the well-known Weierstrass formula[10]

$$\lim_{\varepsilon \to 0} \frac{1}{x - \imath \varepsilon} = \mathcal{P}\frac{1}{x} + \imath \pi \delta(x), \tag{1.58}$$

where $\mathcal{P}$ means that when the expression is integrated around the singular point (in our case, $x = 0$), the integral must be taken in the sense of the principal value, we obtain

$$\bar{B}(t) = B_- e^{-\imath \omega_B t} \left(\pi \delta(\omega_E - \omega_B) - \imath \mathcal{P}\frac{1}{\omega_E - \omega_B} \right)$$

$$+ B_+ e^{\imath \omega_B t} \left(\pi \delta(\omega_E + \omega_B) - \imath \mathcal{P}\frac{1}{\omega_E + \omega_B} \right)$$

$$\equiv \kappa_- B_- e^{-\imath \omega_B t} + \kappa_+ B_+ e^{\imath \omega_B t}. \tag{1.59}$$

In the general case, the spectra of both the system and the environment – especially the environment! – contain many frequencies, all of which will contribute to $\kappa'_\pm(\omega) \equiv \mathrm{Re}\ \kappa_\pm(\omega)$ and $\kappa''_\pm(\omega) \equiv \mathrm{Im}\ \kappa_\pm(\omega)$. (Note that since we consider the spectra at positive frequencies only, $\kappa'_+ = 0$.)

---

[10] See, e.g., Zagoskin (1998) Eq. (2.31) or Richtmyer (1978), Section 2.9.

Substituting expression (1.59) in Eq. (1.55), we obtain some terms that explicitly depend on time via $\exp[\pm 2\imath \omega_B t]$. They can be dropped (the so-called *rotating wave approximation (RWA)*) on the grounds that they oscillate so fast on the scale of changes of the density matrix $\rho_S(t)$, that they will average to zero. This is usually valid (unless there are resonances!). The remaining terms are

$$
\begin{aligned}
\frac{\mathrm{d}\rho_S}{\mathrm{d}t} = {} & \frac{1}{\imath\hbar}\frac{g^2}{\hbar}\Big[((n+1)\kappa''_+ - n\kappa''_-)B_-B_+ + ((n+1)\kappa''_- - n\kappa''_+)B_+B, \rho_S(t)\Big] \\
& + \frac{g^2}{\hbar^2}(n+1)\Big[\kappa'_-\,(2B_-\rho_S(t)B_+ - \{\rho_S(t), B_+B_-\}) \\
& \quad + \kappa'_+\,(2B_+\rho_S(t)B_- - \{\rho_S(t), B_-B_+\})\Big] \\
& + \frac{g^2}{\hbar^2}n\Big[\kappa'_-\,(2B_+\rho_S(t)B_- - \{\rho_S(t), B_-B_+\}) \\
& \quad + \kappa'_+\,(2B_-\rho_S(t)B_+ - \{\rho_S(t), B_+B_-\})\Big].
\end{aligned}
\tag{1.60}
$$

The first line represents the usual unitary Hamiltonian dynamics. We could have added the two terms in the commutator with the density matrix to the system's Hamiltonian as a small correction (of order $g^2/\hbar\omega_{E,B}$).

It is the rest that we are interested in. They have the so-called *Lindblad form*

$$
2L\rho_S L^\dagger - L^\dagger L\rho_S - \rho_S L^\dagger L.
\tag{1.61}
$$

It was indeed shown by Lindblad (1976) (see also Gardiner and Zoller, 2004) that the most general form of a linear differential equation for the density matrix, which would preserve its properties, has the form

$$
\frac{\mathrm{d}\rho}{\mathrm{d}t} = \frac{1}{\imath\hbar}[H, \rho] + \sum_a (2L_a\rho L_a^\dagger - L_a^\dagger L_a\rho - \rho L_a^\dagger L_a)
\tag{1.62}
$$

with a Hermitian H and arbitrary operators L_a (so-called *Lindblad operators*, or simply Lindblads). It is straightforward to check (using the cyclic invariance of the trace) that such an equation indeed preserves the trace of the density matrix.

The fact that the master equation (1.60) is of the Lindblad form is not a trivial matter. We made a number of assumptions and approximations when deriving first (1.53), and then (1.60), and there was no guarantee that they will not catch up with us and lead to an equation with unphysical solutions. Fortunately this did not happen.

What makes Eq. (1.62) so important is that it models the non-unitary evolution of the density matrix of the system – the very behaviour that could not be described by our initial equation (1.17) for the whole set: system + environment. We will show this on a simple, but relevant, example of a two-level quantum system (e.g., a spin-1/2 particle fixed in space, or, if you wish, a qubit).

1.3.3 An example: a non-unitary evolution of a two-level system. Dephasing and relaxation

The density matrix of a two-level system is a two-by-two Hermitian matrix, and all calculations can easily be done explicitly. We choose the energy representation, in which the Hamiltonian of the system is

$$H_S = \begin{pmatrix} E_0 & 0 \\ 0 & E_1 \end{pmatrix},$$

and consider three examples of Lindblad operators:

$$L_1 = L_1^\dagger = \sqrt{\gamma}\sigma_+\sigma_- \equiv \sqrt{\gamma}\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}; \tag{1.63}$$

$$L_2 = \sqrt{\Gamma/2}\sigma_- \equiv \sqrt{\Gamma/2}\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}; \; L_2^\dagger = \sqrt{\Gamma/2}\sigma_+ \equiv \sqrt{\Gamma/2}\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}; \tag{1.64}$$

$$L_3 = \sqrt{\Gamma/2}\sigma_+; \; L_3^\dagger = \sqrt{\Gamma/2}\sigma_-. \tag{1.65}$$

The master equation (1.62) in the first case becomes (assuming that the Hamiltonian term is removed in the interaction representation)

$$\begin{pmatrix} \dot{\rho}_{00} & \dot{\rho}_{01} \\ \dot{\rho}_{10} & \dot{\rho}_{11} \end{pmatrix} = \begin{pmatrix} 0 & -\gamma\rho_{01} \\ -\gamma\rho_{10} & 0 \end{pmatrix}, \tag{1.66}$$

with solution

$$\rho(t) = \begin{pmatrix} \rho_{00}(0) & \rho_{01}(0)e^{-\gamma t} \\ \rho_{10}(0)e^{-\gamma t} & \rho_{11}(0) \end{pmatrix}. \tag{1.67}$$

This is an obviously non-unitary evolution, with the density matrix being reduced to a diagonal form. The diagonal terms are not changed at all, so this choice of Lindblads realizes what is called *pure dephasing*. Equation (1.67) can be considered as a model of the measurement process, in which the upper/lower state of the system is being detected, with γ giving the rate of the state collapse. The purity, $\varsigma(t) = \text{tr}\,\rho^2(t)$, also decays exponentially,

$$\varsigma(t) = \rho_{00}(0)^2 + \rho_{11}(0)^2 + |\rho_{01}(0)|^2 e^{-2\gamma t}. \tag{1.68}$$

In the other two cases we get

$$\begin{pmatrix} \dot{\rho}_{00} & \dot{\rho}_{01} \\ \dot{\rho}_{10} & \dot{\rho}_{11} \end{pmatrix} = \begin{pmatrix} -\Gamma\rho_{00} & -(\Gamma/2)\rho_{01} \\ -(\Gamma/2)\rho_{10} & \Gamma\rho_{00} \end{pmatrix}, \tag{1.69}$$

with solution

$$\rho(t) = \begin{pmatrix} \rho_{00}(0)e^{-\Gamma t} & \rho_{01}(0)e^{-(\Gamma/2)t} \\ \rho_{10}(0)e^{-(\Gamma/2)t} & 1 - \rho_{00}(0)e^{-\Gamma t} \end{pmatrix}, \tag{1.70}$$

and similarly

$$\begin{pmatrix} \dot{\rho}_{00} & \dot{\rho}_{01} \\ \dot{\rho}_{10} & \dot{\rho}_{11} \end{pmatrix} = \begin{pmatrix} \Gamma\rho_{11} & -(\Gamma/2)\rho_{01} \\ -(\Gamma/2)\rho_{10} & -\Gamma\rho_{11} \end{pmatrix}, \tag{1.71}$$

$$\rho(t) = \begin{pmatrix} 1 - \rho_{11}(0)e^{-\Gamma t} & \rho_{01}(0)e^{-(\Gamma/2)t} \\ \rho_{10}(0)e^{-(\Gamma/2)t} & \rho_{11}(0)e^{-\Gamma t} \end{pmatrix}. \tag{1.72}$$

In addition to dephasing, these equations also show the *relaxation* of the diagonal elements (to the upper or lower level). Physically, this means that the Lindblads L_2, L_3 describe the competing processes of energy transmission between the system and the environment. Note that the evolution of Eqs. (1.70) and (1.72) leads eventually to a *pure* state – an eigenstate of the system's Hamiltonian. In order to make the system relax to a mixed state, the master equation must include both terms like (1.69) and (1.71), with appropriate weights.

Note also the relation between the relaxation and the dephasing rate in (1.72); this is a frequent occurrence, because Lindblads of the type (1.64) and (1.65) often appear in realistic models. The decoherence rate, which characterizes the sum total of all contributions to the loss of the off-diagonal elements of the density matrix, is, in this case, the sum of the pure dephasing rate plus half the relaxation rate.

If we include all the Lindblads (1.63, 1.64, 1.65), the solution to the master equation will have the form

$$\rho(t) = \begin{pmatrix} \overline{\rho_{00}} + (\rho_{00}(0) - \overline{\rho_{00}})e^{-\Gamma t} & \rho_{01}(0)e^{-(\Gamma/2+\gamma)t} \\ \rho_{10}(0)e^{-(\Gamma/2+\gamma)t} & \overline{\rho_{11}} + (\rho_{11}(0) - \overline{\rho_{11}})e^{-\Gamma t} \end{pmatrix}, \tag{1.73}$$

where the stationary values $\overline{\rho_{00}} + \overline{\rho_{11}} = 1$ are the eventual occupation probabilities of the levels. If the system relaxes towards the equilibrium at some temperature T^*, then $\overline{\rho_{11}}/\overline{\rho_{00}} = \exp[-(E_1 - E_0)/k_B T^*]$, from which one can restore the scaling factors for the Lindblad operators L_2, L_3. If, on the other hand, we know the properties of the environment, then the Lindblad terms, and therefore the stationary state of the system, can be calculated from there (see, e.g., Eq. (1.60)). If we formally ascribe to the environment a *negative* temperature, then the two-level system will undergo a *population inversion*, with a higher probability to be found on the upper, than on the lower level.[11]

The particular form of the Lindblad operators depends on the environment and on the details of its coupling to the system. Earlier in this section we found for the

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[11] This is a common and convenient way of modelling pumping in active media, e.g., lasers.

coupling of a two-level system to a Bose mode the following Lindblad operators:

$$L_1 = \frac{g}{\hbar}\sqrt{\mathrm{Re}(\kappa_-)(n+1)}\,B_-; \quad L_2 = \frac{g}{\hbar}\sqrt{\mathrm{Re}(\kappa_+)(n+1)}\,B_+;$$

$$L_3 = \frac{g}{\hbar}\sqrt{\mathrm{Re}(\kappa_-)n}\,B_+; \qquad L_4 = \frac{g}{\hbar}\sqrt{\mathrm{Re}(\kappa_+)n}\,B_-.$$

The last two disappear if the Bose mode is empty ($n = 0$). Obviously they correspond to the absorption of quanta by the system, while the first two describe the contribution of stimulated and spontaneous emission processes to the decoherence. In many cases it is impossible to provide a precise theoretical description of the environment. Then the Lindblad operators are chosen on a phenomenological basis. Very often it is sufficient to describe the situation with the simple Lindblads of Eqs. (1.63), (1.64) and (1.65) and two parameters of Eq. (1.73): the relaxation rate Γ and total dephasing (i.e., decoherence) rate $\Gamma/2 + \gamma$.

1.3.4 *Non-unitary vs. unitary evolution*

The non unitary master equation in its Lindblad form (1.62) can be written formally in the same way as the unitary Liouville–von Neumann equation (1.18), i.e.,

$$\frac{\mathrm{d}\rho}{\mathrm{d}t} = \mathcal{L}(t)[\rho(t)], \tag{1.74}$$

where now the Liouvillian includes the unitarity-violating Lindblad terms. Of course, there is no solution of the form (1.19), since the evolution is now irreversible: non-unitarity means that many initial states (density matrices) evolve into the same final state of the system. Let us write

$$\rho(t) = \mathcal{S}(t,0)[\rho(0)], \tag{1.75}$$

where $\mathcal{S}(t_f, t_i)[A]$ is the operator non-unitary evolution of an arbitrary operator A from the moment t_i to $T_f \geq t_i$. Obviously, $\mathcal{S}(t,t)[\cdot] = \hat{1}$, the unit operator, and

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{S}(t,t_0)[\cdot] = \mathcal{L}(t)[\mathcal{S}(t,t_0)[\cdot]]. \tag{1.76}$$

Since for any later time t' both $\rho(t') = \mathcal{S}(t',t)[\rho(t)]$ and $\rho(t') = \mathcal{S}(t',0)[\rho(0)]$ should hold, then

$$\mathcal{S}(t',0)[A] = \mathcal{S}(t',t)[\mathcal{S}(t,0)[A]], \ \ t' \geq t \geq 0 \tag{1.77}$$

(the composition property): two consecutive evolutions described by the master equation form some other such evolution. For a unitary transformation of (1.19) this property obviously holds: recall that the evolution is there given by

$\mathcal{U}(t,0)[A] \equiv U(t)AU^{\dagger}(t)$. The difference is that the unitary transformations can be inverted: it is clear from (1.19) that identically $\mathcal{U}(t,0)[\mathcal{U}(-t,0)[A]] = A$. Therefore, from the mathematical point of view, the unitary evolutions constitute a *group*, while the non-unitary evolutions of Eq. (1.75) are only a *semigroup*.[12]

1.4 Quantum dynamics of a two-level system

1.4.1 Bloch vector and Bloch sphere

We are often – and rightly – awed by the power and beauty of universal mathematical methods. Nevertheless, all of them started as one-off tricks for solving some specific problem, and were later generalized. The approaches that defied generalization are not to be neglected, since they are often as powerful in their area and allow significant simplification. One such special trick is the representation of the density matrix of a two-level quantum system through the *Bloch vector* in a 3D space. It employs our hard-wired abilities and lifelong experience of imagining and manipulating objects in space, and has helpful analogies with classical physics. It is fortunate that all these advantages can be used to describe such important two-level systems as qubits.[13]

The density matrix in question can be written as

$$\rho = \left(\begin{array}{cc} (1+\mathcal{R}_z)/2 & (\mathcal{R}_x - i\mathcal{R}_y)/2 \\ (\mathcal{R}_x + i\mathcal{R}_y)/2 & (1-\mathcal{R}_z)/2 \end{array} \right) = \frac{1}{2}\left(\hat{1} + \mathcal{R}_x \sigma_x + \mathcal{R}_y \sigma_y + \mathcal{R}_z \sigma_z \right),$$

(1.78)

where $\mathcal{R}_x$, $\mathcal{R}_y$, $\mathcal{R}_z$ are real numbers, $\hat{1}$ is the unit two-by-two matrix, and σ_x, σ_y, σ_z are the Pauli matrices:

$$\sigma_x = \left(\begin{array}{cc} 0 & 1 \\ 1 & 0 \end{array} \right); \ \sigma_y = \left(\begin{array}{cc} 0 & -i \\ i & 0 \end{array} \right); \ \sigma_z = \left(\begin{array}{cc} 1 & 0 \\ 0 & -1 \end{array} \right). \qquad (1.79)$$

(We can check that the combinations $\sigma_{\pm} = (\sigma_x \pm i\sigma_y)/2$ are the same matrices that we used in Eqs. (1.64) and (1.65).)

The expression (1.78) looks like an expansion of a 3D vector with components $\mathcal{R}_x$, $\mathcal{R}_y$, $\mathcal{R}_z$ over the unit vectors $\sigma_{x,y,z}$, which it actually is: the space of all

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[12] In common mathematical notation, the compositions of the elements of (semi)groups (i.e., evolutions $\mathcal{U}(t_2,t_1)[\cdots]$ or $\mathcal{S}(t_2,t_1)[\cdots]$) are written as, e.g., $g \circ h$, where the evolution g happens after h. The composition property, $g_2 \circ g_1 = g_3$ (i.e., two consecutive evolutions are also equivalent to an evolution), and the associativity, $(g_3 \circ g_2) \circ g_1 = g_3 \circ (g_2 \circ g_1)$, hold both for groups and semigroups. In addition, in groups for any g there exists an inverse g^{-1}: $g^{-1} \circ g = \hat{1}$.

[13] We will call an arbitrary two-level quantum system a "qubit", irrespective of whether it is an actual qubit, as long as this does not create confusion. The reason is that "qubit" is shorter than "two-level system", while the abbreviation "TLS" often refers to a special (and mostly troublesome) kind of two-state object (see Section 5.2).

Hermitian matrices with zero trace is three-dimensional, and the Pauli matrices can be chosen as its orthonormal basis. (There is, of course, also the term $\hat{1}$, but its role is only to ensure that the density matrix has the unit trace.) This 3D vector $\mathcal{R}$ is the *Bloch vector*, and

$$\rho = \frac{1}{2}\left(\hat{1} + \mathcal{R}_\alpha \sigma_\alpha\right). \tag{1.80}$$

Now recall that $\mathrm{tr}\left[\rho^2\right] \leq \mathrm{tr}\rho$, with equality if and only if the system is actually in a pure state. Since

$$\mathrm{tr}\left[\rho^2\right] = \mathrm{tr}\left[\frac{1}{4}\left(\begin{array}{cc}(1+\mathcal{R}_z)^2 + \mathcal{R}_x^2 + \mathcal{R}_y^2 & 2(\mathcal{R}_x - i\mathcal{R}_y) \\ 2(\mathcal{R}_x + i\mathcal{R}_y) & (1-\mathcal{R}_z)^2 + \mathcal{R}_x^2 + \mathcal{R}_y^2\end{array}\right)\right]$$

$$= \frac{1 + \mathcal{R}_x^2 + \mathcal{R}_y^2 + \mathcal{R}_z^2}{2} = \frac{|\mathcal{R}|^2 + 1}{2} \leq 1, \tag{1.81}$$

we see that the length of the Bloch vector cannot exceed unity. Therefore it is convenient to represent the density matrix using the unit *Bloch sphere*, Fig. 1.3. Any point on its surface corresponds to some pure state, and any point inside to some mixed state. The pure states on the opposite sides of the sphere's diameters are mutually orthogonal. Indeed, for two pure states with opposite Bloch vectors
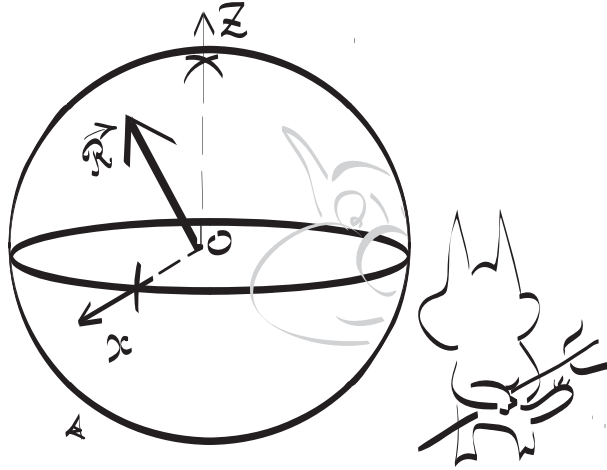

Fig. 1.3. Bloch sphere. Points on its surface correspond to the pure states of a qubit (quantum two-level system), points inside to mixed states.

the density matrices are

$$\rho_1 = |\Psi_1\rangle\langle\Psi_1| = \frac{\hat{1} + \mathcal{R}_\alpha\sigma_\alpha}{2}; \quad \rho_2 = |\Psi_2\rangle\langle\Psi_2| = \frac{\hat{1} - \mathcal{R}_\alpha\sigma_\alpha}{2}; \quad (1.82)$$

$$\mathrm{tr}\,(\rho_1\rho_2) = |\langle\Psi_1|\Psi_2\rangle|^2 = \mathrm{tr}\frac{1}{4}\left(\hat{1} - \mathcal{R}_\alpha\mathcal{R}_\beta\sigma_\alpha\sigma_\beta\right) = \frac{1}{2}\left(1 - |\mathcal{R}|^2\right) = 0.$$

For example, if we choose the eigenstates of the unperturbed Hamiltonian, $|0\rangle$ and $|1\rangle$, as the basis of the Hilbert space, then the north and south poles of the Bloch sphere would correspond to the pure states $|0\rangle$ and $|1\rangle$. At equilibrium at temperature T, the density matrix has the Gibbs form $a_0|0\rangle\langle0| + a_1|1\rangle\langle1|$, with the Boltzmann ratio $a_1/a_0 = \exp(-(E_1 - E_0)/k_BT)$. Therefore, all the equilibrium states lie on the positive vertical axis of the Bloch sphere, with the ground state ($\rho = |0\rangle\langle0|$) at its north pole, and the state at infinite temperature (when both qubit states are equipopulated) in the centre of the sphere. The "equilibrium states with negative temperatures", for which $a_1 > a_0$, fill the negative vertical axis; they terminate at the pure excited state $|1\rangle\langle1|$ at the south pole. The points away from the vertical axes represent mixed states with nonzero coherences.

The evolution of the qubit state is visually represented by the hodograph of the Bloch vector. In the presence of decoherence (dephasing and relaxation), it will approach the positive vertical axis and terminate at some point there, determined by the temperature of the bath with which the qubit eventually equilibrates.

Using the Bloch sphere we can give a clear geometrical meaning to the density matrix representation as a weighted sum of projectors on pure states, Eq. (1.9). Take a section of the Bloch sphere by a plane, containing the Bloch vector $\mathcal{R} \equiv \vec{OR}$ (Fig.1.4). (There is a continuum of such sections, of course.) Choose an *arbitrary* point A on the boundary and draw the chord AB through the point R. Then the Bloch vector $\vec{OR}$ can be written as[14]

$$\vec{OR} = \frac{|RB|}{|AB|}\vec{OA} + \frac{|RA|}{|AB|}\vec{OB} \equiv a\mathcal{A} + b\mathcal{B} \quad (1.83)$$

(obviously $a, b \geq 0$, $a + b = 1$), and the density matrix can be *unravelled* (e.g., Percival, 2008, 3.2) as

$$\rho = \frac{1}{2}\left[(a + b)\hat{1} + (a\mathcal{A}_\alpha + b\mathcal{B}_\alpha)\sigma_\alpha\right] = a|\Psi_A\rangle\langle\Psi_A| + b|\Psi_B\rangle\langle\Psi_B|. \quad (1.84)$$

There is a continuum of such unravellings of the density matrix into a sum of projectors: we are free to choose both a point on the great circle, and the great

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[14] This is easy to see if we write $\vec{OR} = a\vec{OA} + b\vec{OB}$ and notice that R lies on the line AB if and only if $\vec{AR}||\vec{AB}$ (or $\vec{RB}||\vec{AB}$), and that these conditions can be written as $\vec{AR} \times \vec{AB} = 0$ ($\vec{RB} \times \vec{AB} = 0$). Here $\times$ denotes the vector product – another very useful operation, which only works in the special case of 3D space!
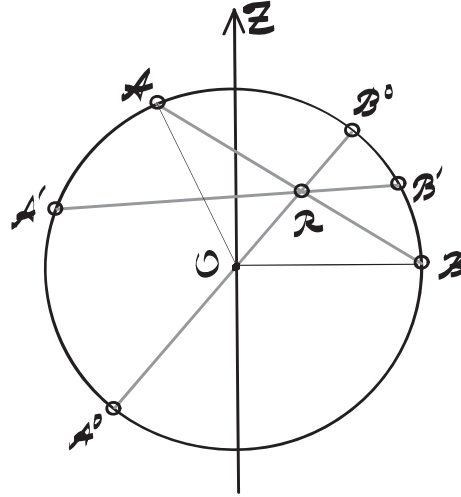
Fig. 1.4. Section of the Bloch sphere, which contains the Bloch vector $\mathcal{R} = \vec{OR}$. Different chords AB, $A'B'$, ... represent different unravellings of the density matrix, $\rho = W_A|\Psi_A\rangle\langle\Psi_A| + W_B|\Psi_B\rangle\langle\Psi_B|$. The chord passing through the centre of the sphere, A^0B^0, corresponds to the spectral representation of the density matrix. Only in this representation are the constituent states orthogonal, $\langle\Psi_{A^0}|\Psi_{B^0}\rangle = 0$.

circle itself. There exists, though, a special unravelling, represented by the chord A^0B^0, which passes through the centre of the Bloch sphere. According to Eq. (1.83), the states $|\Psi_{A^0}\rangle$ and $|\Psi_{B^0}\rangle$ are mutually orthogonal, being on the opposite ends of the diameter, and such an unravelling is obviously unique. This is the spectral representation (1.12) of the density matrix, and the state vectors $|\Psi_{A^0}\rangle$ and $|\Psi_{B^0}\rangle$ are the eigenvectors of ρ.

1.4.2 Bloch equations and quantum beats

Now consider a qubit in an external field, described in the so-called diabatic or "physical" basis by the Hamiltonian

$$H(t) = -\frac{1}{2}\left(\Delta\sigma_x + \epsilon(t)\sigma_z\right). \tag{1.85}$$

The basis is called "physical", since we assume that the two eigenstates of the operator σ_z, $|0\rangle$ and $|1\rangle$, correspond to the pointer states, which can eventually be read out. For example, if the qubit is a spin, then these states are "up" and "down"; if it is a superconducting loop with current, they are "clockwise" and "anticlockwise"; if it is a quantum dot, then they are "charge zero" and "charge one" etc. For clarity, we will call these states "left", $|L\rangle$, and "right", $|R\rangle$, whatever their actual physical meaning.

The σ_x-term describes quantum-mechanical tunnelling with amplitude Δ between $|L\rangle$ and $|R\rangle$, and the term $\epsilon(t) = (\epsilon_0 + \epsilon_1(t))\sigma_z$ is the time-dependent bias. (Without losing generality, we can assume that the average $\langle\epsilon_1(t)\rangle = 0$.)

To begin, let us write the Liouville–von Neumann equation,

$$\frac{d\rho}{dt} = \frac{1}{1\hbar}[H, \rho],$$

in terms of the Bloch vector as

$$\frac{d}{dt}\mathcal{R} = \mathbf{M}(t)\mathcal{R}, \tag{1.86}$$

where the antisymmetric matrix $\mathbf{M}$

$$\mathbf{M} = \begin{pmatrix} 0 & \Delta & 0 \\ -\Delta & 0 & \epsilon(t) \\ 0 & -\epsilon(t) & 0 \end{pmatrix} \tag{1.87}$$

describes the unitary evolution. This equation can be rewritten as

$$\frac{d\mathcal{R}}{dt} = \frac{2}{\hbar}\mathcal{H}(t) \times \mathcal{R}, \tag{1.88}$$

where the vector $\mathcal{H}(t) = (\Delta/2, 0, \epsilon(t)/2)^{\mathrm{T}}$. (In other words, $\mathcal{H}$ is the Hamiltonian (1.85) considered as another vector in the space of traceless two-by-two Hermitian matrices.) We can also check, for the sake of completeness, that Eq. (1.88) holds if the Hamiltonian (1.85) also contains the y-term, $-\Delta_y\sigma_y/2$ (that is, $\mathcal{H}(t) = (\Delta/2, \Delta_y/2, \epsilon(t)/2)^{\mathrm{T}}$).

If our qubit was actually a spin-1/2, and we had N such independent elementary magnets per unit volume, then the α-th component of the macroscopic magnetization of the system would be

$$M_\alpha = \frac{Ng\hbar}{2}\langle\sigma_\alpha\rangle, \quad \alpha = x, y, z, \tag{1.89}$$

where g is the gyromagnetic ratio. In the external magnetic field $\vec{H}(t) = \vec{H}_0 + \vec{H}_1(t)$ (assuming that the stationary field component is in the z-direction, and $\langle\vec{H}_1(t)\rangle = 0$) the magnetization vector would rotate around the direction of the field, while simultaneously relaxing to the stationary state with $M_x = M_y = 0$ (in the absence of a time-dependent field) and $M_z = \bar{M}_z$ (determined by the temperature and the energy splitting between the "up" and "down" states in the field), which is described

by the *Bloch equations*

$$\frac{\mathrm{d}M_x}{\mathrm{d}t} = g\left[\vec{M} \times \vec{H}(t)\right]_x - \frac{M_x}{T_2};$$

$$\frac{\mathrm{d}M_y}{\mathrm{d}t} = g\left[\vec{M} \times \vec{H}(t)\right]_y - \frac{M_y}{T_2}; \qquad (1.90)$$

$$\frac{\mathrm{d}M_z}{\mathrm{d}t} = g\left[\vec{M} \times \vec{H}(t)\right]_z - \frac{M_z - \bar{M}_z}{T_1}$$

of nuclear magnetic resonance (NMR) theory (see, e.g., Blum, 2010, Section 8.4). Here $T_{1,2}$ are the longitudinal and transverse relaxation times. These equations describe the Larmor precession of the average magnetic moment in the external magnetic field and its relaxation. On the other hand, mathematically they are – *mutatis mutandis* – the same as Eq. (1.88) for the components of the Bloch vector. Moreover, the simplest Lindblad operators (1.69) and (1.71) lead (in a basis of the energy eigenstates) to the relaxation terms exactly like in (1.90), with the relaxation rate Γ and the dephasing rate $\Gamma/2 + \gamma$ corresponding to the rates $1/T_1$ and $1/T_2$.

This is why Eq. (1.90) using the Bloch vector is also called the Bloch equations:

$$\frac{\mathrm{d}\mathcal{R}_x}{\mathrm{d}t} = \frac{2}{\hbar}[\mathcal{H}(t) \times \mathcal{R}]_x - \frac{\mathcal{R}_x}{T_2};$$

$$\frac{\mathrm{d}\mathcal{R}_y}{\mathrm{d}t} = \frac{2}{\hbar}[\mathcal{H}(t) \times \mathcal{R}]_y - \frac{\mathcal{R}_y}{T_2}; \qquad (1.91)$$

$$\frac{\mathrm{d}\mathcal{R}_z}{\mathrm{d}t} = \frac{2}{\hbar}[\mathcal{H}(t) \times \mathcal{R}]_z - \frac{\mathcal{R}_z - \bar{\mathcal{R}}_z}{T_1}.$$

Eqs. (1.88) and (1.91) describe a rotation of the vector $\mathcal{R}$ with the instantaneous angular velocity $2\mathcal{H}(t)/\hbar$. The absolute value of this velocity is $\Omega(t) = 2|\mathcal{H}(t)|/\hbar = \sqrt{\Delta^2 + \epsilon^2(t)}/\hbar$, that is, the transition frequency between the ground state and the excited state of the qubit, produced by the tunnelling Δ and bias ϵ between its two physical states.

For a time-independent bias, the rotation (1.88) represents *quantum beats* between the eigenstates of the system. If it was initially in the "left"/"right" state, it will rotate around $\mathcal{H}$ between the north/south pole and a point close to the opposite pole of the Bloch sphere (Fig. 1.5); in the limit of zero bias, the rotation is around the x-axis, and the hodograph is the great circle through both poles.

Quantum beats are a natural way of switching the qubit between its "left" and "right" states. If we start from any other point of the Bloch sphere, they will carry the system around the corresponding trajectory, as shown in Fig.1.5. To be precise,
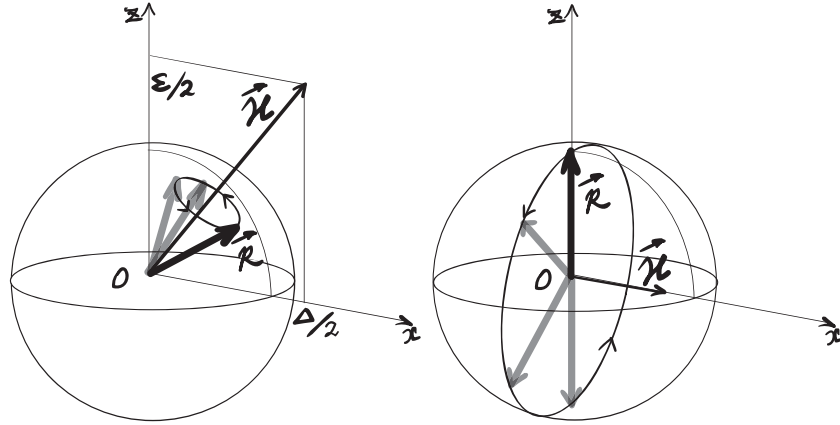
Fig. 1.5. Quantum beats: the Bloch vector $\mathcal{R}$ rotates around the "field vector" $\mathcal{H}$ with the angular velocity $\Omega = \sqrt{\Delta^2 + \epsilon^2}/\hbar$ (left). For zero bias the rotation axis coincides with Ox, and the trajectory of a pure state is a great circle (right).

the *probability* of finding the system in either state will be a periodic function of time.[15]

Nevertheless, if the system was initially in an equilibrium state, it will remain there, since then its Bloch vector is parallel to $\mathcal{H}$. Transitions between such states can be produced by applying a harmonic resonant field to the system. This effect is called *Rabi oscillations*.

1.4.3 Rabi oscillations

Let us act on the qubit with a harmonic perturbation, which in the diabatic ("physical") basis has the form $H_1(t) = \hbar\eta\cos\omega t\ \sigma_z$. In the absence of the static bias ($\epsilon_0 = 0$) the physical states $|L\rangle$, $|R\rangle$ have the same energy, so the qubit is at its *degeneracy point*. Then the unperturbed Hamiltonian is

$$H_0 = -\frac{1}{2}\Delta\sigma_x \equiv -\frac{\hbar\Omega}{2}\sigma_x, \tag{1.92}$$

and in the eigenbasis of H_0 (note that now the z- and x-directions change places)

$$H(t) = H_0 + H_1(t) = -\frac{\hbar\Omega}{2}\sigma_z + \hbar\eta\cos\omega t\ \sigma_x. \tag{1.93}$$

---

[15] A simpler way to come to the same conclusion for a pure state is to write the wave function as $|\Psi(t)\rangle = a_0|0\rangle\exp[-\imath E_0 t/\hbar] + a_1|1\rangle\exp[-\imath E_1 t/\hbar] = \exp[-\imath E_0 t/\hbar]\,(a_0|0\rangle + a_1|1\rangle\exp[-\imath\Omega t])$ and the density matrix as $\rho(t) = |\Psi(t)\rangle\langle\Psi(t)|$.

If we do not assume that the qubit is at the degeneracy point, the perturbation in (1.93) will also have a component proportional to σ_z. This does not actually make the solution any harder, but the formulas get messier (see, e.g., Scully and Zubairy, 1997, Chapter 5).

Without the perturbation, the unitary evolution of the qubit is given by

$$\rho(t) = \exp[-\imath H_0 t/\hbar]\rho(0)\exp[\imath H_0 t/\hbar]. \tag{1.94}$$

Expanding the exponents in series and using the properties of the Pauli matrices,

$$[\sigma_x, \sigma_y] = 2\sigma_z, \ [\sigma_y, \sigma_z] = 2\sigma_x, \ [\sigma_z, \sigma_x] = 2\sigma_y, \ (\sigma_x)^2 = (\sigma_y)^2 = (\sigma_z)^2 = \hat{1}, \tag{1.95}$$

it is easy to see that

$$\exp[\pm\imath H_0 t/\hbar] = \hat{1}\cos(\Omega t/2) \pm \imath\sigma_z \sin(\Omega t/2). \tag{1.96}$$

Here $\hat{1}$ is a unit two-by-two matrix. The corresponding rotation of the Bloch vector $\mathcal{R}$ with the angular velocity Ω around the axis Oz is given by

$$\mathcal{R}(t) = \mathbf{U}(t)^{\mathrm{T}}\mathcal{R}(0), \tag{1.97}$$

where

$$\mathbf{U}(t)^{\mathrm{T}} = \begin{pmatrix} \cos\Omega t & -\sin\Omega t & 0 \\ \sin\Omega t & \cos\Omega t & 0 \\ 0 & 0 & 1 \end{pmatrix}. \tag{1.98}$$

We chose to write it this way using the operation of matrix transposition; we also use the fact that the matrix $\mathbf{U}$ is real unitary (that is, orthogonal, as it should be, since it describes rotations in a 3D space):

$$\mathbf{U}\mathbf{U}^{\dagger} = \mathbf{U}\mathbf{U}^{\mathrm{T}} = \mathbf{1}. \tag{1.99}$$

Eq. (1.97) describes quantum beats, which in our 3D picture are nothing else but a Larmor precession of the fictitious "magnetic moment" $\mathcal{R}$ in the fictitious "magnetic field" $\mathcal{H}$. To cancel the effects of this evolution, which we after all have already discussed, it is convenient to switch to the rotating frame of reference, which is equivalent to using the standard quantum-mechanical interaction representation. To do so, we represent the Bloch vector as

$$\mathcal{R}(t) = \mathbf{U}(t)^{\mathrm{T}}\mathcal{R}_I(t), \tag{1.100}$$

with the time dependence of $\mathcal{R}_I(t)$ caused by everything else apart from the unperturbed Hamiltonian H_0. Using Eq. (1.99), we obtain

$$\frac{d\mathcal{R}_I(t)}{dt} = \frac{d[\mathbf{U}(t)\mathcal{R}(t)]}{dt} = \mathbf{M}_I(t)\mathcal{R}_I(t), \tag{1.101}$$

where

$$\mathbf{M}_I(t) = \mathbf{U}(t)\mathbf{M}(t)\mathbf{U}(t)^{\mathrm{T}} - \mathbf{U}(t)\frac{\mathrm{d}\mathbf{U}(t)^{\mathrm{T}}}{\mathrm{d}t} \qquad (1.102)$$

describes the evolution of the Bloch vector with respect to the rotating frame. It is only due to the harmonic perturbation. (We will deal with the non-unitary terms in a moment.) The matrix $\mathbf{M}$ (we have dropped the subscript I to unclutter the formulas) is now

$$\mathbf{M}(t) = \begin{pmatrix} 0 & 0 & \eta(\sin(2\Omega+\delta)t- \\ & & \sin\delta t) \\ 0 & 0 & -\eta(\cos(2\Omega+\delta)t- \\ & & \cos\delta t) \\ -\eta(\sin(2\Omega+\delta)t- & \eta(\cos(2\Omega+\delta)t- & 0 \\ \sin\delta t) & \cos\delta t) & \end{pmatrix}. \qquad (1.103)$$

Here we have introduced the *detuning*

$$\delta = \omega - \Omega \qquad (1.104)$$

between the driving frequency ω and the interlevel distance.

If we neglect the "fast" terms (with frequency $2\Omega+\delta \sim 2\omega$), which will average to almost zero, the matrix (1.103) becomes

$$\mathbf{M}(t) \approx \begin{pmatrix} 0 & 0 & -\eta\sin\delta t \\ 0 & 0 & \eta\cos\delta t \\ \eta\sin\delta t & -\eta\cos\delta t & 0 \end{pmatrix}. \qquad (1.105)$$

It describes the rotation of the Bloch vector with the angular velocity $\mathcal{Y}(t)$

$$\frac{\mathrm{d}\mathcal{R}}{\mathrm{d}t} = \mathbf{M}(t)\mathcal{R}(t) \approx \mathcal{Y}(t) \times \mathcal{R}(t); \ \ \mathcal{Y}(t) = -\eta\begin{pmatrix} \cos\delta t \\ \sin\delta t \\ 0 \end{pmatrix}, \qquad (1.106)$$

which itself slowly rotates around the axis Oz.

Dropping the fast terms is called the *rotating wave approximation* (RWA). The name can be better understood with the magnetic analogy and considering a magnetic moment in a constant magnetic field parallel to the axis Oz and a small harmonic field along the axis Ox. The harmonic field can always be represented as a sum of two fields with opposite circular polarizations: "rotating waves", one co-rotating and the other counter-rotating with the Larmor precession of the magnetic moment. When the perturbation frequency is close to the Larmor frequency,

we can neglect the counter-rotating wave, since in the frame of reference of the rotating magnetic moment it changes too fast to produce a significant effect.

Clearly, RWA is justified only as far as the evolution of the Bloch vector in the rotating frame is slow, that is, near the resonance, $\delta \ll \omega$, but this is exactly where we need it. More formally, we can average the equations over the period $\tau_\omega = 2\pi/\omega$ of fast drive oscillations: $\langle \cdots \rangle_{\tau_\omega} \equiv \tau_\omega^{-1} \int_t^{t+\tau_\omega} (\cdots) dt$. The slow terms vary little during this time and can be approximated by constants taken at any point inside the interval $[t, t+\tau_\omega]$ (for example, at the moment t). Then integration eliminates the fast terms.

Now let us return to Eq. (1.106). The rotation of the vector of angular velocity $\mathcal{Y}(t)$ can be compensated by the counter-rotation

$$
\mathbf{U}'(t) = \begin{pmatrix} \cos \delta t & -\sin \delta t & 0 \\ \sin \delta t & \cos \delta t & 0 \\ 0 & 0 & 1 \end{pmatrix}. \tag{1.107}
$$

In this new frame of reference the rotation matrix becomes (cf. Eq. (1.102)),

$$
\mathbf{M}(t) \rightarrow \mathbf{U}'(t)\mathbf{M}(t)\mathbf{U}'(t)^{\mathrm{T}} - \mathbf{U}'(t)\frac{d\mathbf{U}'(t)^{\mathrm{T}}}{dt}
$$

$$
= \begin{pmatrix} 0 & -\delta & \eta \sin 2\omega t \\ \delta & 0 & -2\eta \cos^2 \omega t \\ -\eta \sin 2\omega t & 2\eta \cos^2 \omega t & 0 \end{pmatrix}. \tag{1.108}
$$

The Bloch vector now satisfies the equation

$$
\frac{d\mathcal{R}}{dt} = \mathbf{M}(t)\mathcal{R}(t) \approx \mathcal{Y}' \times \mathcal{R}(t); \quad \mathcal{Y}' = \begin{pmatrix} \eta \\ 0 \\ \delta \end{pmatrix}. \tag{1.109}
$$

Here we again used RWA and dropped the fast terms. We see already that in the new frame of reference the Bloch vector rotates with the angular velocity

$$
\omega_R = \sqrt{\delta^2 + \eta^2}; \tag{1.110}
$$

ω_R is the *Rabi frequency*. If the harmonic field is exactly in resonance with the qubit, this frequency is directly proportional to the amplitude of the applied field, $\hbar \eta$.

To tidy things up, we align the x-axis of the rotating frame with the vector $\mathcal{Y}'$:

$$\mathbf{U}'' = \begin{pmatrix} \dfrac{\eta}{\omega_R} & 0 & \dfrac{\delta}{\omega_R} \\ 0 & 1 & 0 \\ -\dfrac{\delta}{\omega_R} & 0 & \dfrac{\eta}{\omega_R} \end{pmatrix} ; \ \mathbf{U}''\mathcal{Y}' = \begin{pmatrix} \omega_R \\ 0 \\ 0 \end{pmatrix}. \tag{1.111}$$

The Bloch equations become

$$\frac{\mathrm{d}\mathcal{R}}{\mathrm{d}t} \approx \omega_R \hat{\mathbf{x}} \times \mathcal{R}(t). \tag{1.112}$$

This is what we were looking for: we found the frame of reference in which the evolution of the Bloch vector is a simple precession with a known angular velocity, and a solution with any initial conditions is obvious, for example,

$$\mathcal{R}(t) = \begin{pmatrix} R_\parallel \\ R_\perp \cos \omega_R t \\ R_\perp \sin \omega_R t \end{pmatrix}. \tag{1.113}$$

All that remains is to transform it back to the laboratory frame of reference (i.e., the energy basis). Since the Bloch vector in the rotating frame was obtained by the consecutive application of three rotations,

$$\mathcal{R}(t) \rightarrow \mathbf{U}''\mathbf{U}'(t)\mathbf{U}(t)\mathcal{R}(t), \tag{1.114}$$

we now need to invert the matrix

$$\mathbf{W}(t) \equiv \mathbf{U}''\mathbf{U}'(t)\mathbf{U}(t), \tag{1.115}$$

which transforms the Bloch vector from the laboratory to the rotating frame of reference, that is,

$$\mathbf{W}(t) = \begin{pmatrix} (\eta/\omega_R)\cos\omega t & -(\eta/\omega_R)\sin\omega t & \delta/\omega_R \\ \sin\omega t & \cos\omega t & 0 \\ -(\delta/\omega_R)\cos\omega t & (\delta/\omega_R)\sin\omega t & \eta/\omega_R \end{pmatrix}. \tag{1.116}$$

Note that we did *not* make any approximations in our frame-to-frame transformations $\mathbf{U}$, $\mathbf{U}'$, $\mathbf{U}''$. Nevertheless in the final matrix $\mathbf{W}(t)$ all the complicated time dependences of separate rotations miraculously reduce to the single frequency ω. But it would not be easy to come up with this simple transformation, if we did not use our intuition for 3D rotations.

The matrix $\mathbf{W}(t)$ provides a direct transformation for the matrix $\mathbf{M}(t)$ between the laboratory and rotating frames. After making the "formal" RWA in the final result, we obtain

$$\left\langle \mathbf{W}(t)\mathbf{M}(t)\mathbf{W}^{\mathrm{T}}(t) - \mathbf{W}(t)\frac{\mathrm{d}\mathbf{W}(t)^{\mathrm{T}}}{\mathrm{d}t} \right\rangle_{\tau_\omega} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -\omega_R \\ 0 & \omega_R & 0 \end{pmatrix}, \quad (1.117)$$

so that the Bloch equations in the rotating frame are indeed Eq. (1.112). The transformation is unitary (even orthogonal), as it should be:

$$[\mathbf{W}(t)]^{-1} = \mathbf{W}(t)^{\dagger} = \mathbf{W}(t)^{\mathrm{T}}. \quad (1.118)$$

Applying $\mathbf{W}(t)^{\mathrm{T}}$ to the solution Eq. (1.113), we find

$$\mathcal{R}(t) = \begin{pmatrix} [(\eta/\omega_R)R_\parallel - (\delta/\omega_R)R_\perp \sin\omega_R t]\cos\omega t + R_\perp \cos\omega_R t \sin\omega t \\ -[(\eta/\omega_R)R_\parallel - (\delta/\omega_R)R_\perp \sin\omega_R t]\sin\omega t + R_\perp \cos\omega_R t \cos\omega t \\ (\delta/\omega_R)R_\parallel + (\eta/\omega_R)R_\perp \sin\omega_R t \end{pmatrix}.$$

$$(1.119)$$

Note the behaviour of the z-component of the Bloch vector in the laboratory frame, which describes the populations of the energy levels. While the other components are oscillating with the fast driving-field frequency (plus slow modulations at ω_R), the z-component oscillates at the Rabi frequency only.

The fact that the Rabi frequency, $\omega_R = \sqrt{\delta^2 + \eta^2}$, can be controlled by varying the field amplitude and detuning, and that it is small compared to the drive frequency, can be (and is) used for the coherent control of the quantum state of a qubit. Suppose, for example, that a qubit is initially in its ground state. After applying an external field at the resonance frequency $\omega = \Delta$ and with the amplitude $\hbar\eta$ and waiting for the interval $\tau = \pi/\eta$, we will find the qubit in its excited state with probability 1; generally this probability will behave as $P_{\mathrm{up}}(t) = \sin\eta t$. On the other hand, the telltale periodic oscillations of $P_{\mathrm{up}}(t)$ in the external field, with the frequency behaving like $\sqrt{\delta^2 + \eta^2}$, indicate that the system in question is indeed a quantum-mechanical two-level system. In the following chapters we will see a number of examples of how this works in real hardware.

1.4.4 *Rabi oscillations in the presence of dissipation

Now let us consider a more general case, when the density matrix evolution is non unitary due to the effects of dissipation. Using the simple Lindblad operators (1.69)

and (1.71), we find in the energy basis (which is, in our case of zero static bias, the same as the laboratory frame of reference for the Bloch vector) the Bloch equations

$$
\begin{aligned}
\frac{d\mathcal{R}_x}{dt} &= [\text{unitary evolution}] - \Gamma_2 \mathcal{R}_x; \\
\frac{d\mathcal{R}_y}{dt} &= [\text{unitary evolution}] - \Gamma_2 \mathcal{R}_y; \\
\frac{d\mathcal{R}_z}{dt} &= [\text{unitary evolution}] - \Gamma_1 (\mathcal{R}_z - Z_T).
\end{aligned}
\tag{1.120}
$$

Here $Z_T = \tanh(\Delta/2k_B T)$ is the equilibrium value of the z-component of the Bloch vector, and $\Gamma_{1,2}$ are the rates of the longitudinal and transverse relaxation (i.e., relaxation proper and dephasing), respectively.

It is convenient to write the non-unitary part of the evolution operator as

$$
\mathbf{L}[\mathcal{R}] = -\Gamma_2 \mathcal{R} - (\Gamma_1 - \Gamma_2) \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \mathcal{R} + \Gamma_1 Z_T \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}.
\tag{1.121}
$$

Then in the rotating frame we will have

$$
\mathbf{L}[\mathcal{R}] \to \mathbf{W}(t)\mathbf{L}[\mathcal{R}] = -\Gamma_2 \mathcal{R} - (\Gamma_1 - \Gamma_2)\mathbf{W}(t) \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \mathbf{W}(t)^{\mathrm{T}} \mathcal{R}
$$

$$
+ \Gamma_1 Z_T \mathbf{W}(t) \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix};
$$

$$
\mathcal{R} \to \mathbf{W}(t)\mathcal{R}.
\tag{1.122}
$$

Explicitly, in the rotating frame

$$
\mathbf{L}[\mathcal{R}] = -\Gamma_2 \mathcal{R} - (\Gamma_1 - \Gamma_2) \begin{pmatrix} (\delta/\omega_R)^2 & 0 & \delta\eta/\omega_R^2 \\ 0 & 0 & 0 \\ \delta\eta/\omega_R^2 & 0 & (\eta/\omega_R)^2 \end{pmatrix} \mathcal{R} + \Gamma_1 Z_T \begin{pmatrix} \delta/\omega_R \\ 0 \\ \eta/\omega_R \end{pmatrix}.
\tag{1.123}
$$

Therefore, the Bloch equations in the rotating frame and in the RWA are:

$$\frac{d\mathcal{R}_x}{dt} = -\Gamma_2\mathcal{R}_x - (\Gamma_1 - \Gamma_2)\left[\left(\frac{\delta}{\omega_R}\right)^2 \mathcal{R}_x + \frac{\eta\delta}{\omega_R^2}\mathcal{R}_z\right] + \Gamma_1 Z_T\left(\frac{\delta}{\omega_R}\right);$$

$$\frac{d\mathcal{R}_y}{dt} = -\Gamma_2\mathcal{R}_y - \omega_R\mathcal{R}_z; \tag{1.124}$$

$$\frac{d\mathcal{R}_z}{dt} = \omega_R\mathcal{R}_y - \Gamma_2\mathcal{R}_z - (\Gamma_1 - \Gamma_2)\left[\left(\frac{\eta}{\omega_R}\right)^2 \mathcal{R}_z + \frac{\eta\delta}{\omega_R^2}\mathcal{R}_x\right] + \Gamma_1 Z_T\left(\frac{\eta}{\omega_R}\right).$$

These equations are valid in the rotating wave approximation (i.e., when $|\delta|, \omega_R \ll \omega$) and under the assumption of weak non-unitarity ($\Gamma_1, \Gamma_2 \ll \omega_R, \omega$).

Let us consider for simplicity the special case $\Gamma_2 = \Gamma_1 = \Gamma$. Now in (1.124) the equations for $\mathcal{R}_x$ and for $\mathcal{R}_y, \mathcal{R}_z$ decouple:

$$\frac{d\mathcal{R}_x}{dt} = -\Gamma\mathcal{R}_x(t) + \Gamma Z_T \frac{\delta}{\omega_R};$$

$$\frac{d\mathcal{R}_y}{dt} = -\Gamma\mathcal{R}_y(t) - \omega_R\mathcal{R}_z(t); \tag{1.125}$$

$$\frac{d\mathcal{R}_z}{dt} = -\Gamma\mathcal{R}_z(t) + \omega_R\mathcal{R}_y(t) + \Gamma Z_T \frac{\eta}{\omega_R}.$$

The first equation describes the pure decay of $\mathcal{R}_x$, while the other two correspond to the rotation in the y-z-plane with decaying amplitude, so that a solution can be sought in the form:

$$\mathcal{R}_x(t) = a + b e^{-\Gamma t};$$

$$\mathcal{R}_y(t) = c + r e^{-\Gamma t}\cos(\omega_R t + \alpha); \tag{1.126}$$

$$\mathcal{R}_z(t) = d + r e^{-\Gamma t}\sin(\omega_R t + \alpha).$$

It is straightforward to check that the expressions (1.126) satisfy Eq. (1.125). The constants a, c and d are determined from the stationary limit of the Bloch equations (i.e., taking $d\mathcal{R}_{x,y,z}/dt = 0$ and $t \to \infty$):

$$a = Z_T\delta/\omega_R; \quad c = Z_T\eta\frac{\Gamma}{\Gamma^2 + \omega_R^2}; \quad d = Z_T\frac{\eta}{\omega_R}\frac{\Gamma^2}{\Gamma^2 + \omega_R^2}; \tag{1.127}$$

the rest must be chosen to satisfy the initial conditions.

Suppose we start from equilibrium. Then in the laboratory frame of reference the Bloch vector has only a z-component, $\mathcal{R}_z(0) = Z_T = \tanh(\Delta/2k_B T)$. After applying the transformation matrix $\mathbf{W}(0)$, we find in the rotating frame

$$\mathcal{R}(0) = Z_T \begin{pmatrix} \delta/\omega_R \\ 0 \\ \eta/\omega_R \end{pmatrix}. \tag{1.128}$$

Therefore, we must choose in Eq. (1.126)

$$b = 0; \quad r = Z_T \frac{\eta}{\sqrt{\omega_R^2 + \Gamma^2}}; \quad \alpha = \arctan\frac{\omega_R}{\Gamma}. \tag{1.129}$$

Transforming the solution back to the laboratory frame, we see that the Bloch vector participates in two distinct motions: forced oscillations of its x-, y-components with frequency ω (plus exponentially decaying transients at frequencies $\omega \pm \omega_R \approx \omega$), and exponentially decaying Rabi oscillations of its z-component:

$$\mathcal{R}(t) = \begin{pmatrix} \text{fast terms} \\ \text{fast terms} \\ Z_T \frac{\delta^2 + \Gamma^2}{\omega_R^2 + \Gamma^2} + r\exp(-\Gamma t)\sin(\omega_R t + \alpha) \end{pmatrix}. \tag{1.130}$$

The quantity

$$R(t) = r\exp(-\Gamma t) \tag{1.131}$$

is the instantaneous amplitude of decaying Rabi oscillations.

1.5 Slow evolution of a quantum system

1.5.1 Adiabatic theorem

After having investigated the evolution of a qubit under the influence of a fast resonant perturbation, we will now consider a different important limiting case. Let us return to the qubit Hamiltonian (1.85):

$$H(t) = -\frac{1}{2}(\Delta\sigma_x + \epsilon(t)\sigma_z) \tag{1.85}$$

and consider an arbitrary $\epsilon(t)$.

Suppose that initially, at $t = 0$, the qubit was in a pure state. Direct diagonalization of (1.85) yields the *instantaneous eigenstates* $|g(t)\rangle$, $|e(t)\rangle$:

$$H(t)|g(t)\rangle = -\frac{\hbar\Omega(t)}{2}|g(t)\rangle; \quad H(t)|e(t)\rangle = \frac{\hbar\Omega(t)}{2}|e(t)\rangle;$$

$$\hbar\Omega(t) = \sqrt{\Delta^2 + \epsilon(t)^2}; \tag{1.132}$$

$$|g(t)\rangle = \begin{pmatrix} \sqrt{\frac{1}{2}(1 + \epsilon(t)/\Omega(t))} \\ \sqrt{\frac{1}{2}(1 - \epsilon(t)/\Omega(t))} \end{pmatrix}; \quad |e(t)\rangle = \begin{pmatrix} \sqrt{\frac{1}{2}(1 - \epsilon(t)/\Omega(t))} \\ -\sqrt{\frac{1}{2}(1 + \epsilon(t)/\Omega(t))} \end{pmatrix}.$$

The states $|g(t)\rangle$, $|e(t)\rangle$ at any moment form an orthonormal basis – the so-called *adiabatic basis*[16] of the qubit's Hilbert space, i.e., the instantaneous eigenbasis of the time-dependent Hamiltonian. In the limit of infinitely strong bias, obviously,

$$\lim_{\epsilon\to\infty} |g\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \equiv |0\rangle; \quad \lim_{\epsilon\to\infty} |e\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \equiv |1\rangle, \tag{1.133}$$

and the adiabatic basis coincides with the diabatic ("physical") one. If we change the polarity ($\epsilon \to -\infty$), then the limits of $|g(t)\rangle$, $|e(t)\rangle$ change places (see Fig. 1.6).

The applicability of the simple Hamiltonian (1.85) is actually much wider than just qubit dynamics. In a quantum system with discrete energy levels and a Hamiltonian dependent on some external parameter λ, only two levels can get close together at any given value of λ (unless the system has a special symmetry). Moreover, in
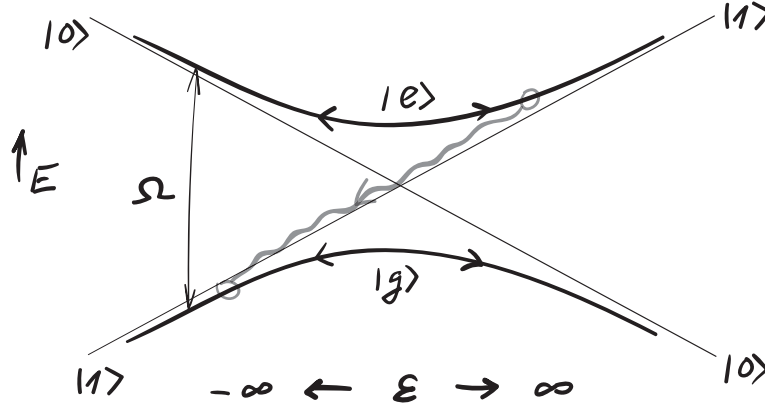

Fig. 1.6. Adiabatic evolution of a two-level system and the Landau–Zener-Stückelberg effect. Adiabatic transitions between the diabatic lines ("physical states") $|0\rangle$ and $|1\rangle$ and Landau–Zener tunnelling (wavy arrow) between the excited state $|e\rangle$ and the ground state $|g\rangle$ in the adiabatic basis are shown.

[16] Why it is called adiabatic will become clear directly.

the generic case the levels do not cross (see, e.g. Stöckmann, 1999, Chapter 3). The Hamiltonian (1.85), with λ replacing time, thus describes the one-parametric *level anticrossing* in a system with a discrete energy spectrum.[17]

The solution to the Schrödinger equation,

$$\imath\hbar\frac{\mathrm{d}}{\mathrm{d}t}|\psi(t)\rangle = H(t)|\psi(t)\rangle, \tag{1.134}$$

can still be written as in (1.2),

$$|\psi(t)\rangle = U(t)|\psi(0)\rangle,$$

only this time the unitary operator $U(t)$ is given by the standard *time-ordered* exponent (e.g. Zagoskin, 1998, § 1.3):

$$U(t) = \mathrm{Te}^{-\frac{1}{\hbar}\int_0^t H(t')\mathrm{d}t'}. \tag{1.135}$$

The time-ordering operator $\mathbb{T}$ arranges all the operators standing to the right of it in chronological order; for example, $\mathbb{T}A(t_1)B(t_2) = A(t_1)B(t_2)$ if $t_1 \geq t_2$, and $\mathbb{T}A(t_1)B(t_2) = B(t_2)A(t_1)$ otherwise. (The operator exponent is to be understood, as usual, as its Taylor expansion.) The nontriviality of the time ordering is due to the fact that $H(t_1)$ and $H(t_2)$ do not necessarily commute. Otherwise, the action of $U(t)$ would reduce to producing phase factors multiplying the instantaneous basis states: $U(t)|g(0)\rangle \rightarrow \exp[-\frac{1}{2}\int_0^t E_0(t')\,\mathrm{d}t']|g(t)\rangle$, $U(t)|e(0)\rangle \rightarrow \exp[-\frac{1}{2}\int_0^t E_1(t')\,\mathrm{d}t']|e(t)\rangle$, where $E_{0,1}(t) = \mp\hbar\Omega(t)/2$. These formulas are, of course, wrong, but they are almost right in an important special case when $H(t)$ changes *adiabatically*. (In this context "adiabatic" means, as in classical mechanics, "slow enough for our purposes".)

A pure state of the qubit can always be written as

$$|\psi(t)\rangle = C_0(t)|g(t)\rangle + C_1(t)|e(t)\rangle. \tag{1.136}$$

Taking the matrix elements of the Schrödinger equation:

$$\imath\hbar\left[\dot{C}_0(t)|g(t)\rangle + C_0(t)|\dot{g}(t)\rangle + \dot{C}_1(t)|e(t)\rangle + C_1(t)|\dot{e}(t)\rangle\right]$$
$$= E_0(t)C_0(t)|g(t)\rangle + E_1(t)C_1(t)|e(t)\rangle, \tag{1.137}$$

---

[17] To describe the general case, when the diabatic lines (i.e., the asymptotes of the anticrossing levels) are asymmetrically inclined, would require a more general Hamiltonian,

$$H = -\frac{1}{2}\left[\Delta\sigma_x + \epsilon(\lambda)(\alpha\sigma_z + \beta\hat{1})\right],$$

but it would lead to trivial changes only. Moreover, the Hamiltonian (1.85) accurately describes the behaviour of the systems we are actually interested in, i.e., qubits.

we find

$$\dot{C}_0(t) = -\frac{1}{\hbar}E_0(t)C_0(t) - C_1(t)\langle g(t)|\dot{e}(t)\rangle; \tag{1.138}$$

$$\dot{C}_1(t) = -\frac{1}{\hbar}E_1(t)C_1(t) - C_0(t)\langle e(t)|\dot{g}(t)\rangle.$$

If not for the scalar products $\langle g(t)|\dot{e}(t)\rangle$ and $\langle e(t)|\dot{g}(t)\rangle$, the solutions would have, indeed, been trivial. But if the Hamiltonian changes slowly, so do its instantaneous eigenstates, therefore, their time derivatives can be neglected, and indeed

$$C_0(t) \approx C_0(0)e^{-\frac{1}{\hbar}\int_0^t E_0(t')\,dt'}; \;\; C_1(t) \approx C_1(0)e^{-\frac{1}{\hbar}\int_0^t E_1(t')\,dt'}. \tag{1.139}$$

In the case of a mixed state we obtain the elements of the density matrix, $\rho(t) = \sum_{i,j} \rho_{ij}(t)|i(t)\rangle\langle j(t)|$, in the same way:

$$\dot{\rho}_{00} = -\rho_{10}(t)\langle g(t)|\dot{e}(t)\rangle - \rho_{01}(t)\langle \dot{e}(t)|g(t)\rangle;$$

$$\dot{\rho}_{11} = -\rho_{01}(t)\langle e(t)|\dot{g}(t)\rangle - \rho_{10}(t)\langle \dot{g}(t)|e(t)\rangle;$$

$$\dot{\rho}_{01} = -\rho_{11}(t)\langle g(t)|\dot{e}(t)\rangle - \rho_{00}(t)\langle \dot{g}(t)|e(t)\rangle + \frac{1}{\hbar}(E_1(t) - E_0(t))\rho_{01}(t);$$

$$\dot{\rho}_{10} = -\rho_{00}(t)\langle e(t)|\dot{g}(t)\rangle - \rho_{11}(t)\langle \dot{e}(t)|g(t)\rangle - \frac{1}{\hbar}(E_1(t) - E_0(t))\rho_{10}(t), \tag{1.140}$$

and the diagonal terms are approximately time-independent under the same conditions:

$$\dot{\rho}_{00} \approx 0; \;\; \dot{\rho}_{11} \approx 0. \tag{1.141}$$

It does not actually matter for our reasoning how many levels the system has, as long as they are discrete. Therefore, we have obtained the *adiabatic theorem* (see, e.g., Messiah, 2003, Chapter XVII, §§7–12):

In a system with a discrete energy spectrum under certain conditions an infinitely slow, or adiabatic, change of the Hamiltonian does not change the level populations.

The change of the *off*-diagonal elements of the density matrix under an adiabatic evolution – as well as the phase gain by a pure state – can be observed and has an important physical meaning, but this does not concern us now. What does concern us are the conditions of applicability of the "theorem".

For a qubit "slow change" should mean that $d\Omega/dt$ is small, i.e.,

$$\frac{\hbar}{\Omega^2(t)}\frac{d\Omega}{dt} \ll 1 \tag{1.142}$$

(this is the simplest dimensionless combination of relevant variables). Indeed, if we use the explicit solutions (1.133), calculate the values of $|\langle e|\dot{g}\rangle| (= |\langle g|\dot{e}\rangle|)$, and require that they can be neglected in Eqs. (1.138) and (1.140), we come to the above condition. For a general multilevel system the adiabatic condition is usually stated as

$$\left| \hbar \frac{\langle m(t)|\dot{n}(t)\rangle}{E_n(t) - E_m(t)} \right| \equiv \left| \hbar \frac{\langle m(t)|\dot{H}(t)|n(t)\rangle}{(E_n(t) - E_m(t))^2} \right| \ll 1. \tag{1.143}$$

Here we have used

$$\langle m(t)|\dot{n}(t)\rangle = \frac{\langle m(t)|\dot{H}(t)|n(t)\rangle}{E_n(t) - E_m(t)}, \quad m \neq n, \tag{1.144}$$

which directly follows from considering the expression $\frac{d}{dt}(H(t)|n(t)\rangle)$.

It is clear from (1.143) that for the adiabatic theorem to hold the *levels must not cross*: $E_m(t) \neq E_n(t)$, if $m \neq n$. But even if this is satisfied, there are problems with (1.143). Let us, e.g., take the qubit Hamiltonian (1.85) with $\epsilon(t) = \hbar\eta\cos(\omega t)$ with $\omega \approx \Delta$ and $\hbar\eta \ll \Delta$. Then

$$\frac{\hbar}{\Omega^2(t)} \frac{d\Omega}{dt} \approx \frac{1}{2}\left(\frac{\hbar\eta}{\Delta}\right)^2 \ll 1. \tag{1.145}$$

Nevertheless, we have seen that such a small harmonic perturbation produces Rabi oscillations. Even though their frequency η is small, the periodic changes of the density matrix elements is of order unity, and the theorem as stated above breaks down. This situation is not exclusive to quantum mechanics and is not surprising: small resonant perturbations *do* produce large cumulative effects. Therefore, another condition of validity of the criterion (1.143) is the absence of such terms.

It is actually possible to formulate the condition of adiabaticity in such a way as to include the case of resonant perturbations (Amin, 2009). We will do this here considering the evolution of a density matrix rather than of a pure state. For a multilevel system, Eqs. (1.140) easily generalize to

$$\dot{\rho}_{mn} = -\frac{1}{\hbar}\rho_{mn}(E_m(t) - E_n(t)) - \sum_j \left(\rho_{jn}\langle m|\dot{j}\rangle + \rho_{mj}\langle\dot{j}|n\rangle\right), \tag{1.146}$$

where $H(t)|j(t)\rangle = E_j(t)|j(t)\rangle$. By separating the adiabatic phase gain,

$$\rho_{mn}(t) = \widetilde{\rho}_{mn}(t)e^{-\frac{1}{\hbar}\int_0^t (E_m(t') - E_n(t'))\, dt'}, \tag{1.147}$$

where

$$\omega_{mn}(t) = \frac{E_m(t) - E_n(t)}{\hbar},$$

we obtain

$$\dot{\tilde{\rho}}_{mn} = -\sum_{j\neq m} \tilde{\rho}_{jn}\left(\langle m|\dot{j}\rangle e^{-1\int_0^t \omega_{jm}(t')\,dt'}\right) - \sum_{j\neq n} \tilde{\rho}_{mj}\left(\langle \dot{j}|n\rangle e^{-1\int_0^t \omega_{nj}(t')\,dt'}\right)$$

(1.148)

(obviously, $\langle m|\dot{m}\rangle = 0$, etc.).

Integrating (1.148) over the time interval $[0, \tau]$ we find the change of the diagonal density matrix element $\tilde{\rho}_{nn}$:

$$\Delta\rho_{nn}(\tau) = -2\mathrm{Re}\int_0^\tau \left[\sum_{j\neq n}\tilde{\rho}_{jn}\langle n|\dot{j}\rangle e^{-1\int_0^t \omega_{jn}(t')\,dt'}\right]dt \equiv -2\mathrm{Re}\sum_{j\neq n}\alpha_{jn}(\tau).$$

(1.149)

For the adiabatic theorem to hold, $|\Delta\rho_{nn}(\tau)|$ must be zero in the limit of infinitely slow evolution. Introducing the quantity

$$r_{jn}(t) = \frac{\tilde{\rho}_{jn}(t)\langle n(t)|\dot{j}(t)\rangle}{\omega_{jn}(t)} \equiv \frac{\tilde{\rho}_{jn}(t)\langle n(t)|\dot{H}(t)|j(t)\rangle}{\hbar\omega_{jn}(t)^2}$$

(1.150)

we can express the contribution from the transitions $j \leftrightarrow n$ as follows:

$$\alpha_{jn}(\tau) = 1\int_0^\tau dt\ r_{jn}(t)\left[-1\omega_{jn}(t)e^{-1\int_0^t \omega_{jn}(t')\,dt'}\right]$$

$$= 1\int_0^\tau dt\ r_{jn}(t)\frac{d}{dt}\left[e^{-1\int_0^t \omega_{jn}(t')\,dt'}\right].$$

(1.151)

Integrating this by parts, we find

$$\alpha_{jn}(\tau) = 1\left[r_{jn}(\tau)e^{-1\int_0^\tau \omega_{jn}(t')\,dt'} - r_{jn}(0)\right] - 1\int_0^\tau dt\ \left[\frac{dr_{jn}(t)}{dt}e^{-1\int_0^t \omega_{jn}(t')\,dt'}\right].$$

(1.152)

Looking at the definition of r_{jn}, Eq. (1.150), we see that the absolute value of the first term in (1.152) is infinitesimally small if the adiabaticity condition (1.143) is satisfied. Therefore, the violation of the adiabatic theorem can only come from the second term. Using the Fourier transform of $r_{jn}(t) = \int \frac{d\omega}{2\pi} R^*(\omega)\exp(1\omega t)$, we can write this term as

$$-1\int_0^\tau dt\ \left[\frac{dr_{jn}(t)}{dt}e^{-1\int_0^t \omega_{jn}(t')\,dt'}\right] = \tau\int \frac{d\omega}{2\pi}\omega R^*(\omega)\int_0^1 ds\ e^{-1\int_0^s (u(s')-v)\,ds'},$$

(1.153)

where $u = \omega_{jn}\tau$ and $v = \omega\tau$ are dimensionless frequencies.

If the Hamiltonian does not contain resonant terms for the transition $j \leftrightarrow n$, then this integral is small due to fast oscillations of the integrand. Indeed, integrating by parts:

$$\tau \int \frac{d\omega}{2\pi} \omega R^*(\omega) \int_0^1 ds \, e^{-\imath \int_0^s (u(s')-v) \, ds'}$$

$$= \tau \int \frac{d\omega}{2\pi} \omega R^*(\omega) \int_0^1 ds \left[\frac{d}{ds} \left(\frac{e^{-\imath \int_0^s (u(s')-v) \, ds'}}{-\imath(u(s)-v)} \right) - \frac{e^{-\imath \int_0^s (u(s')-v) \, ds'}}{\imath(u(s)-v)^2} \frac{du}{ds} \right]$$

$$= \int \frac{d\omega}{2\pi} \omega R^*(\omega) \left[\frac{e^{-\imath \int_0^\tau (\omega_{jn}(t')-\omega) \, dt'}}{-\imath(\omega_{jn}(\tau)-\omega)} - \frac{1}{-\imath(\omega_{jn}(0)-\omega)} \right] + \ldots$$

we see that the dominating term in the expansion is infinitesimally small if the condition (1.143) holds, independently of the length of the evolution interval τ.

On the other hand, if $R^*(\omega)$ is nonzero at frequencies close to $\omega_{jn}(t)$, the main contribution to the integral will be due to these resonant frequencies, and

$$-\imath \int_0^\tau dt \left[\frac{dr_{jn}(t)}{dt} e^{-\imath \int_0^t \omega_{jn}(t') \, dt'} \right] \approx \tau \int \frac{d\omega}{2\pi} \omega R^*(\omega) \approx -i\tau \left. \frac{d}{dt} r_{jn}(t) \right|_{t=t^*, \, 0 \leq t^* \leq \tau}.$$

The error is proportional to the duration of the evolution, and however small is r_{jn} or its derivative, for large enough τ the adiabatic theorem will break down.[18]

Therefore, for resonance there is an upper limit on the duration of the adiabatic evolution. It is easy to see that both cases are incorporated if instead of (1.143) we use (Amin, 2009)

$$\max_{0 \leq s \leq 1} \left| \hbar \frac{\langle m(s)|dH/ds|n(s)\rangle}{(E_n(s) - E_m(s))^2} \right| \ll \tau, \; s = t/\tau. \tag{1.154}$$

1.5.2 Landau–Zener–Stückelberg effect

The adiabatic theorem shows a different way of controlling the quantum state. Instead of relying on a free evolution of an initial superposition of eigenstates of a system (as in the case of quantum beats), or applying a harmonic resonant perturbation to induce the transition between them (as in the case of Rabi oscillations), a slow and smooth variation of the Hamiltonian changes the eigenstates themselves without changing their occupation numbers. As we have seen, this ideal situation can be achieved only in the unrealistic limit of infinitesimally slow change. For any finite speed of the variation of $H(t)$, even in the absence of resonant terms,

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[18] Another, extrinsic mechanism, which limits the duration of an adiabatic evolution of a system, is through its interaction with the environment (Sarandy and Lidar, 2005a).

the adiabatic theorem will be violated. The corresponding process is called the Landau–Zener–Stückelberg effect, or – more often – the Landau–Zener transition, or Landau–Zener tunnelling. In addition to being an important physical process, showing up in such different areas as molecular collisions, quantum control and, of course, quantum computing, this is a nice example of an exactly solvable problem with a nonanalytical dependence on the parameters.

Let us return to the qubit Hamiltonian:

$$H(t) = -\frac{1}{2}\left(\Delta\sigma_x + \epsilon(t)\sigma_z\right), \tag{1.85}$$

which, up to trivial changes, can be considered as representing two levels of any multilevel system near an anticrossing, if $\epsilon(t)$ changes monotonically between a large negative and a large positive value.

Despite what was done in the previous subsection, we expand the wave function over the diabatic basis,

$$|\psi(t)\rangle = C_0(t)e^{-\frac{1}{\hbar}\int_{-\infty}^{t} E_0(t')\,dt'}|0\rangle + C_1(t)e^{-\frac{1}{\hbar}\int_{-\infty}^{t} E_1(t')\,dt'}|1\rangle$$

(we have explicitly written the phase factors). Given that $E_1(t) - E_0(t) = \epsilon(t)$, we find from the Schrödinger equation:

$$\dot{C}_0 = \imath\frac{\Delta}{2\hbar}C_1 e^{-\frac{1}{\hbar}\int_{-\infty}^{t} \epsilon(t')\,dt'}, \quad \dot{C}_1 = \imath\frac{\Delta}{2\hbar}C_0 e^{\frac{1}{\hbar}\int_{-\infty}^{t} \epsilon(t')\,dt'}. \tag{1.155}$$

Differentiating these equations by time, making obvious substitutions and taking into account that $E_1(t) + E_0(t) = 0$, we decouple the system:

$$\ddot{C}_0 - \frac{1}{\hbar}\epsilon(t)\dot{C}_0 + \left(\frac{\Delta}{2\hbar}\right)^2 C_0 = 0; \tag{1.156}$$

$$\ddot{C}_1 + \frac{1}{\hbar}\epsilon(t)\dot{C}_1 + \left(\frac{\Delta}{2\hbar}\right)^2 C_1 = 0. \tag{1.157}$$

Notably, for a linear sweep,

$$\epsilon(t) = vt,$$

these equations allow an explicit solution. We will see that the effect is dominated by the time when the bias $|\epsilon(t)| \leq \Delta$, where such a linear approximation is very plausible.[19] Instead of following Zener (1932) in reducing (1.156) to a known in the mathematical physics Weber equation, solvable using special functions, we use the elegant result of Wittig (2005), where solving the equations is avoided altogether.

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[19] The case of nonlinear sweep is considered in detail, e.g., by Garanin and Schilling (2002).

To begin, let us find the answer in the limit of weak tunnelling, when Δ is small. Consider a system, which is at $t = -\infty$ in the excited state (that is, $C_1(-\infty) = 1$). In the absence of the tunnelling term in the Hamiltonian, at $t = \infty$ the system would remain in this state, which – of course – would be the ground state (see Fig. 1.6), i.e., $C_1(\infty) = 1$ as well. Therefore, we expect that in the presence of tunnelling ($\Delta \neq 0$) this coefficient will remain close to unity, and correspondingly $C_0 \ll 1$. Substituting $C_1 = 1$ in the first equation of (1.155), we find (up to a non-essential phase factor originating from the lower integration limit by t' in the exponent)

$$\dot{C}_0 \approx \mathrm{i}\frac{\Delta}{2\hbar}e^{-\frac{\mathrm{i}vt^2}{2\hbar}}; \ \ C_0(\infty) \approx \int_{-\infty}^{\infty} \mathrm{i}\frac{\Delta}{2\hbar}e^{-\frac{\mathrm{i}vt^2}{2\hbar}}\,\mathrm{d}t = \mathrm{i}\frac{\Delta}{2\hbar}\sqrt{\frac{2\pi\hbar}{\mathrm{i}v}}. \tag{1.158}$$

The probability of *not* switching from the state $|1\rangle$ to the state $|0\rangle$ at the end of the evolution is, therefore (now you see why the phase factor does not matter),

$$P_{LZ} = 1 - |C_0|^2 = 1 - \frac{\pi\Delta^2}{2\hbar v}, \tag{1.159}$$

which is essentially the result obtained by Landau (1932). Note that P_{LZ} is the probability of not switching between the *diabatic* states, $|0\rangle$ and $|1\rangle$, and, therefore, it is the probability of *switching* between the *a*diabatic states (the eigenstates of the qubit Hamiltonian (1.85)), $|g\rangle$ and $|e\rangle$.

The ratio $\Delta^2/\hbar v$ can be written as $(\Delta/\hbar) \cdot (\Delta/\dot{\epsilon})$, that is, as the product of the frequency of quantum beats[20] (see Fig. 1.5) and the anticrossing passage time during which the bias changes by Δ. Note that – up to a factor of order unity – we could derive from dimensional considerations only. What we can't do this way is to find the whole functional dependence, which we will now proceed to derive.

Dividing (1.157) by $tC_1(t)$ and integrating over time from minus to plus infinity, we find

$$\int_{-\infty}^{\infty} \frac{\ddot{C}_1}{tC_1}\,\mathrm{d}t + \frac{1}{\hbar}\int_{-\infty}^{\infty} v\frac{\dot{C}_1}{C_1}\,\mathrm{d}t + \left(\frac{\Delta}{2\hbar}\right)^2 \int_{-\infty}^{\infty} \frac{\mathrm{d}t}{t} = 0, \tag{1.160}$$

that is,

$$\ln\left(\frac{C_1(\infty)}{C_1(-\infty)}\right) = \frac{\mathrm{i}\hbar}{v}\left\{\left(\frac{\Delta}{2\hbar}\right)^2 \int_{-\infty}^{\infty} \frac{\mathrm{d}t}{t} + \int_{-\infty}^{\infty} \frac{\ddot{C}_1}{tC_1}\,\mathrm{d}t\right\}. \tag{1.161}$$

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[20] For some mysterious reason this frequency is often called the Rabi frequency. It *is not*. The Rabi frequency describes the effects of a resonant harmonic perturbation, and is nothing to do with quantum beats, which are free evolution of a superposition of eigenstates of a static Hamiltonian.
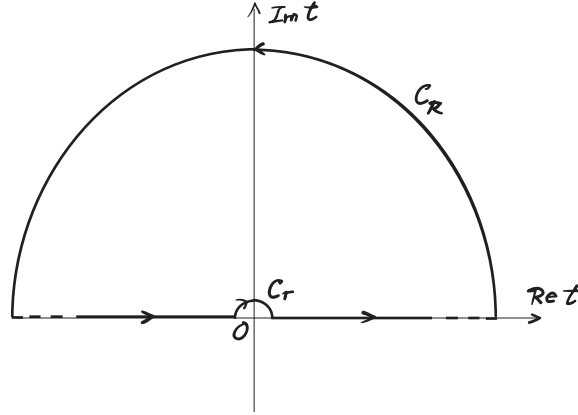
Fig. 1.7. Calculation of the integral (1.163). The closed contour $\mathcal{C}$ consists of the real positive and negative semiaxes plus an infinitesimal semicircle $\mathcal{C}_r$ around zero, and an infinitely large semicircle $\mathcal{C}_R$. The contour does not enclose the singularity at $t = 0$.

The integral of $1/t$ can be found using regularization (1.58):

$$\int_{-\infty}^{\infty} \frac{\mathrm{d}t}{t} \rightarrow \int_{-\infty}^{\infty} \frac{\mathrm{d}t}{t \pm \imath\varepsilon} \rightarrow \mathcal{P} \int_{-\infty}^{\infty} \frac{\mathrm{d}t}{t} \mp \imath\pi = \mp \imath\pi. \qquad (1.162)$$

We will fix the sign later.

The remaining integral,

$$J \equiv \int_{-\infty}^{\infty} \frac{\ddot{C}_1}{t C_1} \, \mathrm{d}t \qquad (1.163)$$

requires a little more attention. Let us consider $F(t) \equiv \ddot{C}_1(t)/(t C_1(t))$ as a function of a complex variable t (Fig. 1.7). In the general case, $F(t)$ should be an analytical function, except, possibly, at $t = 0$. Any exponential dependence on t in $C_1(t)$ – e.g., from the phase factors – which could cause trouble, will obviously cancel in the combination $\ddot{C}_1/C_1$. Therefore, the integral of $F(t)$ along the contour $\mathcal{C}$ in the complex plane is the sum of the residues in the singularities of $F(t)$, which are enclosed by this contour, in accordance with Cauchy's theorem.[21] We choose the contour as in Fig. 1.7, so that

$$J + J_R = 0, \qquad (1.164)$$

and we need only to calculate the integral along the infinite semicircle $\mathcal{C}_R$ to find J. This integral is easily found. Looking at (1.157) with $\epsilon(t) = vt$ we see that, since $|C_1(t)| \leq 1$, the last two terms must cancel when $t \rightarrow \pm\infty$, and the second

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[21] See any textbook on complex analysis (e.g. Gamelin, 2001, Chapter VI).

derivative should be negligible:

$$\frac{\dot{C}_1}{C_1} \sim -\frac{1}{vt}\frac{\hbar}{}\left(\frac{\Delta}{2\hbar}\right)^2; \quad C_1(t) \sim (t)^{-1\frac{\hbar}{v}\left(\frac{\Delta}{2\hbar}\right)^2}.$$

(1.165)

Then indeed $\ddot{C}_1/\dot{C}_1 \sim 1/t$, $\ddot{C}_1/C_1 \sim 1/t^2$, and our initial assumption (that the second derivative can be neglected) holds. Therefore, for large values of $|t| \, |F(t)| = |\ddot{C}_1/(t\dot{C}_1)| \sim 1/|t|^3$. Since the integral J_R

$$J_R = \int_{C_R} F(t)\,\mathrm{d}t \le \int_{C_R} |F(t)|\,\mathrm{d}t \sim \frac{\pi R}{R^3} \xrightarrow{R\to\infty} 0,$$

we see that $J = 0$ as well.

Returning to (1.161), we see that

$$\ln\left(\frac{C_1(\infty)}{C_1(-\infty)}\right) = \pm\frac{\pi\hbar}{v}\left(\frac{\Delta}{2\hbar}\right)^2.$$

(1.166)

Since $C_1(-\infty) = 1$ and the probability of staying in the same state is $|C_1(\infty)|^2$, we see that

$$P_{LZ} = \mathrm{e}^{-\frac{\pi\Delta^2}{2\hbar v}}.$$

(1.167)

The choice of the sign was obvious: the probability cannot exceed unity. Eq. (1.167) agrees with the perturbative result (1.159) in the limit $\Delta^2 \ll \hbar v$, as it should. Note that the speed of the sweep, v, plays a crucial role: the faster the sweep, the less the probability of switching diabatic states (or, equivalently, of staying in the same adiabatic state). Moreover, the dependence of P_{LZ} on v is essentially non-analytical.

Of course, we would obtain the same result if starting from the state $|0\rangle$ instead. That particular case is of special interest, since it is sometimes easier to cool a system down to its ground state and then manoeuvre the state into something we would like to have (like, e.g., in *adiabatic quantum computing*, Section 6.2). The Landau–Zener effect would then be one of the leading sources of failure of such a scheme.[22]

Concluding remarks

Before proceeding to practical applications, let us recapitulate what has been achieved so far. First, the introduction of the density matrix provides a unified description of the quantum system before, during and after the measurement, that is, the reduction of the density matrix to an appropriate diagonal form. Second, the non-unitary evolution of the density matrix has been shown to be explainable

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[22] This has been directly observed, e.g., in a superconducting flux qubit (Izmalkov et al., 2004a).

Fig. 1.8. Quantum–classical transition: two possibilities.

by averaging over – tracing out – the "environment", i.e., averaging over the huge number of degrees of freedom, which interact with our system but are affected by it only to a negligibly weak degree. This "restricted description" is commonly employed for the same reason in classical statistical mechanics. It is not our purpose here to establish under what strict conditions this kind of explanation works – it is good enough for our purposes. The key physical effect leading to this is the loss of correlation via its "removal" from the system – to the environment, or to infinity, as we will see when considering the effective impedance of a transmission line in Chapter 5. There appears to be no "fundamental size", exceeding which a system *must* drop all quantum behaviour in favour of classical physics, no matter what. Third, this still *does not* resolve the problem indicated after Eq. (1.5), namely, that the formalism of the density matrix still does not give us a clue as to which bases in the Hilbert state can describe macroscopic measurements, and which cannot. We can have a diagonal density matrix, but its elements may – for all we know – give the probabilities of finding the system in different Schrödinger-cat-type states.

   In other words, we still must answer the question as to why we can build the apparatus for measuring eigenstates of only certain observables and not others, and how to tell the difference *from the quantum mechanics itself*. This is a fascinating and still open question, and again it is beyond the scope of this book.[23] We will be, therefore, pragmatically minded and satisfy ourselves that these special observables and states can be found from macroscopic experience. With this restriction, and evading finer ontological points of the description based on a density matrix,[24] we have now laid a sufficient foundation for dealing with the more practical side of quantum engineering.

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[23] A very attractive possibility is the "quantum Darwinism" approach (Zurek, 2003), which argues that the "macroscopic" observables are the ones with the eigenstates that are the least disrupted by their interaction with different subsystems of the environment.

[24] A very good and accessible resume of the problem, together with an extensive bibliography, is given in Penrose, (2004), Chapter 29.