Spin $\frac{1}{2}$ Quantum Systems: Dynamics and Circuit Models

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OUTLINE

1. Quantum Binary Devices
2. Classical definition of the Cell
3. Classical Dynamics of the Cell
4. Quantum Definition of the Cell
5. Quantum Dynamics of the Closed Cell
6. Quantum Dynamics of the Open Cell
7. Passage to the Rotating Reference Frame
8. Quantum Dynamics in Bloch Space
9. Rabi's Problem
10. Power Dissipation
11. Linearisation
12. The Equivalent Circuit Synthesis

APPENDIX

A Refresher of Quantum Mechanics

A1. The Mathematics of Quantum Mechanics

A2. The Interpretative Postulates

A3. Main Theorems

A4. Pure States and Mixtures

A5. Dissipative Quantum Systems

A6. The Bloch Space

1. **Quantum Binary Devices**

Quantum binary devices are important in two respects:

(a) In quantum computers each number represented by n binary digits is stored in a set of n two–state devices (or *qubits*). Since the state of each qubit is a quantum–mechanical superposition of two states (representing digits 0 and 1), the entire set stores simultaneously 2^n numbers (parallel computing).

(b) In classical computers use of nanodevices interacting among themselves in a classical way (so that the state space dimensions increase as n instead of as 2^n) provides consistent reduction in size and dissipation.

In these lectures we examine the dynamics and the circuit modelling of potential nanodevices (or *cells*) – spin $\frac{1}{2}$ particles immersed in a magnetic field supporting both the bias and the signal.

Before entering the quantum treatment, we sketch the dynamics of such particles in a purely classical way.

2. **Classical Definition of the Cell**

The cell is assumed to be a particle endowed with an *angular momentum* $\mathbf{J}$ and a *magnetic moment*

$$\mathbf{M} = \gamma \mathbf{J} \tag{1}$$

where γ is the *gyromagnetic ratio*, whose expression is not of interest by now. We only assume, to comply with further developments, that $\gamma < 0$, i.e. that angular momentum and magnetic moment are *antiparallel*.

We assume a Cartesian reference frame with unit vectors $\mathbf{e}_x, \mathbf{e}_y, \mathbf{e}_z$.

The cell is immersed in a magnetic field

$$\mathbf{B} = B_0 \mathbf{e}_z + \mathbf{B}_1(t) \tag{2}$$

where B_0 is a constant bias and

$$\mathbf{B}_1(t) = B_1 \cos \omega t \, \mathbf{e}_x + B_1 \sin \omega t \, \mathbf{e}_y \tag{3}$$

is the magnetic harmonic component at angular frequency ω of a circularly polarized TEM wave signal impinging on the cell.

We assume that the electric field has negligible effect on the system.

3. **Classical Dynamics of the Cell**

The energy of the system cell+magnetic field is

$$W = -\mathbf{M} \cdot \mathbf{B} = -MB\cos\theta \tag{4}$$

where θ is the angle from $\mathbf{B}$ to $\mathbf{M}$.

a. *Motion in the static field* $\mathbf{B}_0$

The torque acting on the cell is

$$\Gamma = -\frac{\mathrm{d}W}{\mathrm{d}\theta} = -MB_0 \sin\theta \tag{5}$$

or vectorially

$$\mathbf{\Gamma} = \mathbf{M} \times \mathbf{B}_0 \tag{6}$$

The rate of increase of angular momentum

$$\frac{\mathrm{d}\mathbf{J}(t)}{\mathrm{d}t} = \mathbf{\Gamma}(t) \tag{7}$$

thus becomes from eqs. (1) and (6)

$$\frac{\mathrm{d}\mathbf{M}(t)}{\mathrm{d}t} = \gamma \mathbf{M}(t) \times \mathbf{B}_0 \tag{8}$$

From eq. (8)

$$\begin{aligned} \frac{\mathrm{d}M^2}{\mathrm{d}t} &= 2\mathbf{M}\cdot\frac{\mathrm{d}\mathbf{M}}{\mathrm{d}t} = 2\gamma\mathbf{M}\times\mathbf{B}_0\cdot\mathbf{M} = 0 \\ \frac{\mathrm{d}}{\mathrm{d}t}(\mathbf{M}\cdot\mathbf{B}_0) &= \frac{\mathrm{d}\mathbf{M}}{\mathrm{d}t}\cdot\mathbf{B}_0 = \gamma\mathbf{M}\times\mathbf{B}_0\cdot\mathbf{B}_0 = 0 \end{aligned} \tag{9}$$

Moreover, by projecting eq. (8) on the (x, y)–plane, we find the equations

$$\begin{cases} \dfrac{\mathrm{d}M_x}{\mathrm{d}t} = \gamma B_0 M_y \\ \dfrac{\mathrm{d}M_y}{\mathrm{d}t} = -\gamma B_0 M_x \end{cases} \tag{10}$$

Eqs. (9) show that the magnetic moment $\mathbf{M}$ has constant modulus and forms a constant angle with the magnetic field $\mathbf{B}_0 = B_0\mathbf{e}_z$; eqs. (10) that it rotates around $\mathbf{e}_z$ with angular speed

$$\omega_0 = -\gamma B_0 \tag{11}$$

(Larmor's precession).

A well known mechanical analogue is the *spinning top*.

b. *Influence of a rotating field* $\mathbf{B}_1(t)$

Eq. (8) is replaced by

$$\frac{\mathrm{d}\mathbf{M}(t)}{\mathrm{d}t} = \gamma \mathbf{M}(t) \times [\mathbf{B}_0 + \mathbf{B}_1(t)] \tag{12}$$

Define

$$\omega_0 = -\gamma B_0, \qquad \omega_1 = -\gamma B_1 \tag{13}$$

Thus, taking into account eqs. (13), eq. (12) becomes

$$\frac{\mathrm{d}\mathbf{M}(t)}{\mathrm{d}t} = \mathbf{M}(t) \times [-\omega_0 \mathbf{e}_z - \omega_1 \mathbf{e}_X(t)] \tag{14}$$

where $\mathbf{e}_X$ is the unit vector parallel to $\mathbf{B}_1(t)$.

We now introduce a rotating reference frame $(\mathbf{e}_X, \mathbf{e}_Y, \mathbf{e}_z)$ with $\mathbf{e}_Y$ perpendicular to $\mathbf{e}_X$ and $\mathbf{e}_z$. With respect to the latter the precession angular speed is $-\Delta\omega = \omega_0 - \omega$. Thus eq. (14) becomes

$$\left(\frac{\mathrm{d}\mathbf{M}(t)}{\mathrm{d}t}\right)_{\mathrm{rel}} = \mathbf{M}(t) \times [\Delta\omega \mathbf{e}_z - \omega_1 \mathbf{e}_X] \tag{15}$$

While eq. (14) is time–dependent because the vector $\mathbf{e}_X$ rotates, eq. (15) is time-independent because the same vector is now fixed. Thus the solution is greatly simplified.

Now precession takes place around a relative resultant field

$$\mathbf{B}_{\text{eff}} = \frac{1}{\gamma}(\varDelta\omega \mathbf{e}_z - \omega_1 \mathbf{e}_X) \tag{16}$$

If $\varDelta\omega = 0$ we have *magnetic* resonance. The magnetic moment spins around $\mathbf{e}_X$, that is a vector lying in the (x, y)-plane, and therefore it has positive and negative components along the z-axis for equal times.

If $\varDelta\omega \gg \omega_1$, $\mathbf{B}_{\text{eff}}$ as almost the same direction as $B_0\mathbf{e}_z$ and thus the precession occurs around the z-axis.

The motion, as seen from the fixed reference frame, is the resultant of the rotation of the magnetic moment $\mathbf{M}$ around the effective magnetic field $\mathbf{B}_{\text{eff}}$, with angular speed

$$\varOmega = \sqrt{\varDelta\omega^2 + \omega_1^2} \tag{17}$$

and of the rotation of vector $\mathbf{B}_{\text{eff}}$ around $\mathbf{e}_z$ with angular speed ω. While the last motion gives rise to *precession*, the former develops into *nutation*.

4. **Quantum Definition of the Cell**

The cell is assumed to be a particle endowed with a two–state *angular momentum* $\hat{\mathbf{J}}$ and a *magnetic moment*

$$\hat{\mathbf{M}} = \gamma \hat{\mathbf{J}} \tag{18}$$

where

$$\gamma = g \frac{q_{\mathrm{e}}}{2m} \tag{19}$$

is the *gyromagnetic ratio*, $q_{\mathrm{e}} < 0$ the electric charge of the electron, m the mass the particle, g the LANDÉ factor. $\hat{\mathbf{M}}$ and $\hat{\mathbf{J}}$ are operators in HILBERT space $\mathbb{H}$.

The LANDÉ factor has the value 1 for pure electron orbital moment, 2 for pure electron spin moment, $2{\cdot}2.79$ for proton spin, $2(-1.93)$ for neutron spin, other values of the order of 1 for nuclei and atoms.

In the following we usually will make reference to the case of the electron spin ($\gamma = q_{\mathrm{e}}/m$) for which

$$\hat{\mathbf{M}} = \gamma \hat{\mathbf{S}} = \frac{q_{\mathrm{e}}\hbar}{2m} \hat{\boldsymbol{\sigma}} \tag{20}$$

The cell is immersed in a magnetic field

$$\mathbf{B} = B_0\mathbf{e}_z + \mathbf{B}_1(t) \tag{21}$$

where B_0 is a constant bias and

$$\mathbf{B}_1(t) = B_1 \cos \omega t \, \mathbf{e}_x + B_1 \sin \omega t \, \mathbf{e}_y \tag{22}$$

is the magnetic harmonic component at angular frequency ω of a circularly polarized TEM wave signal impinging on the cell.

Again we assume that the electric field has negligible effect on the system.

The energy operator of the system cell+magnetic field (the Hamiltonian operator) is by analogy with the classical case

$$\hat{H} = -\hat{\mathbf{M}} \cdot \mathbf{B} = \frac{|q_\mathrm{e}|\hbar}{2m} \, \hat{\boldsymbol{\sigma}} \cdot \mathbf{B} \tag{23}$$

Note that the magnetic field is treated as an ordinary vector function, not as a vector operator: the description of the interaction is semiclassical.

The vector spin operator $\hat{\boldsymbol{\sigma}}$ is expanded along the axes x, y, z:

$$\hat{\boldsymbol{\sigma}} = \hat{\sigma}_x \mathbf{e}_x + \hat{\sigma}_y \mathbf{e}_y + \hat{\sigma}_z \mathbf{e}_z \tag{24}$$

Thus eq. (23) becomes

$$\hat{H} = \frac{|q_\mathrm{e}|\hbar}{2m}\, \hat{\boldsymbol{\sigma}} \cdot \mathbf{B} = \frac{|q_\mathrm{e}|\hbar}{2m}\, (\hat{\sigma}_x B_x + \hat{\sigma}_y B_y + \hat{\sigma}_z B_z) \tag{25}$$

We choose the up and down spin states along the z-axis as the basis: they are denoted as $|{+z}\rangle$ and $|{-z}\rangle$.

In such a basis the operators $\hat{\sigma}_x$, $\hat{\sigma}_y$ and $\hat{\sigma}_z$ have the representations

$$\begin{aligned} \hat{\sigma}_x &= |{-z}\rangle \langle{+z}| + |{+z}\rangle \langle{-z}| \\ \hat{\sigma}_y &= \mathrm{i}\, |{-z}\rangle \langle{+z}| - \mathrm{i}\, |{+z}\rangle \langle{-z}| \\ \hat{\sigma}_z &= -\, |{-z}\rangle \langle{-z}| + |{+z}\rangle \langle{+z}| \end{aligned} \tag{26}$$

Note: operators of the type $|m\rangle \langle n|$ form the basis for the space of matrices representing the operators: matrix representing the operator above has just a 1 at the crossing of row m and column n and 0 everywhere else.

The matrix representation associated to the previous basis in Hilbert space $\mathbb{H}$ is

$$(\sigma_x) = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad (\sigma_y) = \begin{pmatrix} 0 & \mathrm{i} \\ -\mathrm{i} & 0 \end{pmatrix}, \quad (\sigma_z) = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} \tag{27}$$

where ordering of rows and columns is $|{-z}\rangle\,, |{+z}\rangle$.

Using eqs. (27), we obtain the z-representation of the Hamiltonian $\hat{H}$ defined in eq. (25)

$$(H)_z = \frac{|q_\mathrm{e}|\hbar}{2m} \begin{pmatrix} -B_z & B_x + \mathrm{i}B_y \\ B_x - \mathrm{i}B_y & B_z \end{pmatrix} \tag{28}$$

or, taking into account eqs. (21), (22) and leaving out index z

$$(H) = \frac{|q_\mathrm{e}|\hbar}{2m} \begin{pmatrix} -B_0 & B_1\mathrm{e}^{\mathrm{i}\omega t} \\ B_1\mathrm{e}^{-\mathrm{i}\omega t} & B_0 \end{pmatrix} \tag{29}$$

Now define

$$\omega_0 = \frac{|q_\mathrm{e}|B_0}{m}, \qquad \omega_1 = \frac{|q_\mathrm{e}|B_1}{m} \tag{30}$$

Thus the final form of the Hamiltonian matrix is

$$(H) = \frac{\hbar}{2} \begin{pmatrix} -\omega_0 & \omega_1 e^{i\omega t} \\ \omega_1 e^{-i\omega t} & \omega_0 \end{pmatrix} \tag{31}$$

The Hamiltonian operator completely characterises the cell as a *closed* system.

Such a description is not sufficient for our purposes for two reasons:

(a) It is not completely realistic since the cell is in contact with environment not only through the electromagnetic excitation, but also through thermal exchanges.

(b) We need that the computer, at the end of processing, reach a steady state, instead of evolving quasi-periodically for ever.

Thus we assume that

The cell interacts with a thermal bath of infinite capacity at some fixed temperature T, that in our applications can be chosen ≈ 0.

5. **Quantum Dynamics of the Closed Cell**

We temporarily assume that the interaction between the cell and the bath is interrupted.

1. **Pure states**

A *pure state* is a system whose evolution between *preparation* and *measurement* is completely defined by a *state vector* $|\psi\rangle \in \mathbb{H}$.

Its dynamical evolution is ruled by SCHRÖDINGER equation

$$\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}|\psi(t)\rangle = \hat{H}(t)\,|\psi(t)\rangle \tag{32}$$

with the initial condition

$$|\psi(0)\rangle = \left|\psi_0\right\rangle \tag{33}$$

$\left|\psi_0\right\rangle$ being any ket of $\mathbb{H}$.

Eq. (33), when $\hat{H}$ does not depend on t, is solved as follows

$$|\psi(t)\rangle = \mathrm{e}^{-\mathrm{i}\hat{H}t/\hbar}\left|\psi_0\right\rangle = \sum_n \mathrm{e}^{-\mathrm{i}E_n t/\hbar}\,|E_n\rangle\,\langle E_n|\psi_0\rangle \tag{34}$$

with E_n and $|E_n\rangle$ the eigenvalues and eigenvectors of $\hat{H}$.

2. **Mixtures**

A *mixture* is a system composed of several pure states $|\psi_\nu\rangle$, each of which enters the mixture with some probability ρ_ν (with $\sum_\nu \rho_\nu = 1$).

The state of a mixture is described by the Hermitian *density operator*

$$\hat{\rho}(t) = \sum_\nu \rho_\nu \, |\psi_\nu(t)\rangle \, \langle\psi_\nu(t)| \tag{35}$$

Using eq. (32) for each of the pure states, we obtain that the dynamical evolution of the mixture is ruled by the LIOUVILLE–VON NEUMANN equation

$$\frac{\mathrm{d}\hat{\rho}(t)}{\mathrm{d}t} = -\frac{\mathrm{i}}{\hbar}\,[\hat{H}(t)\hat{\rho}(t) - \hat{\rho}(t)\hat{H}(t)] \tag{36}$$

For a two–state system eq. (36) reads

$$\left\{\begin{array}{rcl} \dfrac{\mathrm{d}\rho_{11}}{\mathrm{d}t} & = & +\mathrm{i}\frac{\omega_1}{2}\,(\mathrm{e}^{-\mathrm{i}\omega t}\rho_{12} - \mathrm{e}^{\mathrm{i}\omega t}\rho_{12}^*) \\ \dfrac{\mathrm{d}\rho_{22}}{\mathrm{d}t} & = & -\mathrm{i}\frac{\omega_1}{2}\,(\mathrm{e}^{-\mathrm{i}\omega t}\rho_{12} - \mathrm{e}^{\mathrm{i}\omega t}\rho_{12}^*) \\ \dfrac{\mathrm{d}\rho_{12}}{\mathrm{d}t} & = & \mathrm{i}\frac{\omega_1}{2}\,\mathrm{e}^{\mathrm{i}\omega t}(\rho_{11} - \rho_{22}) + \mathrm{i}\omega_0\rho_{12} \end{array}\right. \tag{37}$$

where index 1 refers to state $|{-z}\rangle$, index 2 to state $|{+z}\rangle$.

6. **Quantum Dynamics of the Open Cell**

The dynamical evolution of the two–state system in contact with the bath defined at the end of slide 13 is ruled by eqs. (37) supplemented by phenomenological terms taking into account thermal exchanges.

We assume that a particle in the state of higher energy (excited state) has a probability per unit time W_{12} of decaying to the state of lower energy (ground state) emitting a quantum of energy $\hbar\omega_0$ which is absorbed by the bath; and that conversely a particle in the ground state has a probability per unit time W_{21} of rising to the excited state absorbing a quantum of energy $\hbar\omega_0$ which is released by the bath.

We further assume that the two probabilities are related by Boltzmann's Law

$$\frac{W_{21}}{W_{12}} = \mathrm{e}^{-\hbar\omega_0/kT} \tag{38}$$

We assume that incoherent dynamics, due to the interaction of the system with the bath, be simply additive to the coherent dynamics described by equations (37), which thus become

$$\begin{cases} \frac{d\rho_{11}}{dt} &= +i\frac{\omega_1}{2}\left(e^{-i\omega t}\rho_{12} - e^{i\omega t}\rho_{12}^*\right) + W_{12}\rho_{22} - W_{21}\rho_{11} \\ \frac{d\rho_{22}}{dt} &= -i\frac{\omega_1}{2}\left(e^{-i\omega t}\rho_{12} - e^{i\omega t}\rho_{12}^*\right) - W_{12}\rho_{22} + W_{21}\rho_{11} \\ \frac{d\rho_{12}}{dt} &= i\frac{\omega_1}{2}e^{i\omega t}(\rho_{11} - \rho_{22}) + i\omega_0'\rho_{12} - \left[\frac{1}{2}(W_{12} + W_{21}) + W_{12}^{\mathrm{adi}}\right]\rho_{12} \end{cases} \tag{39}$$

The incoherent term in the last equation states that the logarithmic decrement of coherence depends additively on the *nonadiabatic* transition probabilities between the states W_{12} and W_{21} (each counted for one half), due to the mechanism of emission and absorption of energy quanta, and from an *adiabatic* decoherence probability within the states $W_{12}^{\mathrm{adi}} = W_{21}^{\mathrm{adi}}$ due to collisions between particles. The latter give rise also to a shift in frequency $\omega_0' = \omega_0 - \Delta\omega_0$.

Note: the last statement is an interpretation, not an assumption, which could hardly be justified. All incoherent terms in eqs. (39) can be derived in a theoretical way.

Note:

Open systems cannot be treated by SCHRÖDINGER equation, since a pure state immediately degenerates into a mixture, when in contact with the bath.

The density operator of a pure state has the form

$$\hat{\rho} = |\psi\rangle \langle\psi| \tag{40}$$

For a two–state system the state vector has the form $|\psi\rangle = \psi_1 |1\rangle + \psi_2 |2\rangle$ and the density operator has the representation

$$(\rho) = \begin{pmatrix} \psi_1\psi_1^* & \psi_1\psi_2^* \\ \psi_2\psi_1^* & \psi_2\psi_2^* \end{pmatrix} \tag{41}$$

The density matrix of a pure system has rank one.

In a decoherence process in absence of external actions ρ_{12} decreases and converges to zero while ρ_{11} and ρ_{22} remain both nonzero, since they must satisfy the conservation of probability and BOLTZMANN's Law. So the rank of the density matrix becomes 2.

7. **Passage to the Rotating Reference Frame**

If a system is rotated of angle ϕ around an axis, say $\mathbf{e}_z$, its state vector $|\psi\rangle$ transforms to $|\psi'\rangle$ according to the rule

$$|\psi'\rangle = \exp\left(-\frac{\mathrm{i}}{\hbar}\phi \hat{J}_z\right)|\psi\rangle \tag{42}$$

This is the same as to leave the system fixed and to rotate the axes (x, y) of an angle $-\phi$.

Thus the passage from fixed to rotating axes is equivalent to a system rotation

$$|\psi'\rangle = \exp\left(\frac{\mathrm{i}}{\hbar}\omega t \hat{J}_z\right)|\psi\rangle = \exp\left(\mathrm{i}\frac{\omega t}{2}\hat{\sigma}_z\right)|\psi\rangle \tag{43}$$

or, taking into account eq. (27),

$$\begin{cases} \psi_1' = \mathrm{e}^{-\mathrm{i}\omega t/2}\psi_1 \\ \psi_2' = \mathrm{e}^{\mathrm{i}\omega t/2}\psi_2 \end{cases} \tag{44}$$

The density matrix is a sum of rank one matrices of the type in eq. (41). For each of them, and hence for their sum, we can calculate the transformation from fixed to rotating axes using eqs. (44).

Thus

$$\begin{aligned}\rho'_{11} &= \mathrm{e}^{-\mathrm{i}\omega t/2}\rho_{11}\mathrm{e}^{\mathrm{i}\omega t/2} = \rho_{11}\\ \rho'_{22} &= \mathrm{e}^{\mathrm{i}\omega t/2}\rho_{22}\mathrm{e}^{-\mathrm{i}\omega t/2} = \rho_{22}\\ \rho'_{12} &= \mathrm{e}^{-\mathrm{i}\omega t/2}\rho_{11}\mathrm{e}^{-\mathrm{i}\omega t/2} = \mathrm{e}^{-\mathrm{i}\omega t}\rho_{12}\end{aligned} \tag{45}$$

By replacing in eqs. (39) variables ρ_{ij} with variables ρ'_{ij} according to eqs. (45), we obtain

$$\left\{\begin{aligned}\frac{\mathrm{d}\rho'_{11}}{\mathrm{d}t} &= +\mathrm{i}\tfrac{\omega_1}{2}\,(\rho'_{12}-\rho'^{*}_{12}) + W_{12}\rho'_{22} - W_{21}\rho'_{11}\\ \frac{\mathrm{d}\rho'_{22}}{\mathrm{d}t} &= -\mathrm{i}\tfrac{\omega_1}{2}\,(\rho'_{12}-\rho'^{*}_{12}) - W_{12}\rho'_{22} + W_{21}\rho'_{11}\\ \frac{\mathrm{d}\rho'_{12}}{\mathrm{d}t} &= \mathrm{i}\tfrac{\omega_1}{2}\,(\rho'_{11}-\rho'_{22}) - \mathrm{i}\Delta\omega_0\rho'_{12} - \left[\tfrac{1}{2}(W_{12}+W_{21}) + W^{\mathrm{adi}}_{12}\right]\rho'_{12}\end{aligned}\right. \tag{46}$$

Eqs. (46) are time–independent like eqs. (15) for the classical case.

Eqs. (46) can be rewritten compactly as

$$\frac{\mathrm{d}\hat{\rho}}{\mathrm{d}t} = \mathrm{i}\mathcal{L}\hat{\rho} + \mathcal{D}\hat{\rho} \tag{47}$$

where $\mathcal{L}$ and $\mathcal{D}$ are respectively the Hermitian LIOUVILLE and *dissipation* superoperators. This opens the way to the analysis in BLOCH space.

8. **Quantum Dynamics in Bloch Space**

Representation of the density operator in the canonic basis (rotating reference frame)

$$\hat{\rho} = \frac{1}{2}\hat{1}_2 + \frac{1}{2}\lambda_1'\hat{\sigma}_x + \frac{1}{2}\lambda_2'\hat{\sigma}_y + \frac{1}{2}\lambda_3'\hat{\sigma}_z \tag{48}$$

Representation of the density operator in the $|\pm z\rangle$ basis (rotating reference frame) (eq. (27))

$$(\rho) = \frac{1}{2}\begin{pmatrix} 1-\lambda_3' & \lambda_1' + \mathrm{i}\lambda_2' \\ \lambda_1' - \mathrm{i}\lambda_2' & 1+\lambda_3' \end{pmatrix} \tag{49}$$

Using the Bloch variables $(\lambda_1', \lambda_2', \lambda_3')$, eqs. (46) assume the form

$$\frac{\mathrm{d}}{\mathrm{d}t}\begin{pmatrix} \lambda_1' \\ \lambda_2' \\ \lambda_3' \end{pmatrix} = \begin{pmatrix} -\frac{1}{T_2} & \Delta\omega' & 0 \\ -\Delta\omega' & -\frac{1}{T_2} & -\omega_1 \\ 0 & \omega_1 & -\frac{1}{T_1} \end{pmatrix}\begin{pmatrix} \lambda_1' \\ \lambda_2' \\ \lambda_3' \end{pmatrix} + \begin{pmatrix} 0 \\ 0 \\ W_{12} - W_{21} \end{pmatrix} \tag{50}$$

where

$$\frac{1}{T_1} = W_{12} + W_{21}, \qquad \frac{1}{T_2} = \frac{1}{2}(W_{12} + W_{21}) + W_{12}^{\mathrm{adi}}$$
$$\Delta\omega' = \Delta\omega + \Delta\omega_0 \tag{51}$$

Note that the *relaxation times* are connected by the equation

$$\frac{2}{T_2} = \frac{1}{T_1} + \frac{1}{\tau^*} \tag{52}$$

where

$$\tau^* = \frac{1}{W_{12}^{\mathrm{adi}}} \tag{53}$$

Eq. (50) can be rewritten compactly as a vector equation in the three–dimensional Bloch space

$$\frac{\mathrm{d}\vec{\lambda}}{\mathrm{d}t} = \Omega\vec{\lambda} + D\lambda + \vec{f} \tag{54}$$

with evident meaning of the symbols.

From eq. (54)

$$\frac{\mathrm{d}\lambda^2}{\mathrm{d}t} = \vec{\lambda}\cdot D\vec{\lambda} + \vec{f}\cdot\vec{\lambda} \tag{55}$$

since Ω is skew–symmetric. For a closed system

$$|\vec{\lambda}| = \mathrm{const} \tag{56}$$

or the “state vector” $\vec{\lambda}$ moves on Bloch’s sphere.

The average value of the magnetic moment is

$$\langle \mathbf{m} \rangle = \mathrm{Tr}(\rho \hat{\boldsymbol{\sigma}}) = -\frac{|q_\mathrm{e}|\hbar}{2m}(\lambda_1' \mathbf{e}_X + \lambda_2' \mathbf{e}_Y + \lambda_3' \mathbf{e}_z) \tag{57}$$

Thus eqs. (50) are equivalent to the following

$$\frac{\mathrm{d}}{\mathrm{d}t}\begin{pmatrix} \langle m_X' \rangle \\ \langle m_Y' \rangle \\ \langle m_z' \rangle \end{pmatrix} = \begin{pmatrix} -\frac{1}{T_2} & \Delta\omega' & 0 \\ -\Delta\omega' & -\frac{1}{T_2} & -\omega_1 \\ 0 & \omega_1 & -\frac{1}{T_1} \end{pmatrix} \begin{pmatrix} \langle m_X' \rangle \\ \langle m_Y' \rangle \\ \langle m_z' \rangle \end{pmatrix} + \frac{|e|\hbar}{2m}\begin{pmatrix} 0 \\ 0 \\ W_{12} - W_{21} \end{pmatrix} \tag{58}$$

which describe the time evolution of the *classical* magnetic moment.

The dynamical system described by eqs. (58), started from any initial condition $\langle \mathbf{m}_0 \rangle$, after a transient whose duration depends on the relaxation times, will reach an equilibrium, that in the fixed reference frame corresponds to steady precession around $\mathbf{e}_z$.

The equilibrium is found by equating the time derivatives in eqs. (58) to zero and solving the obtained algebraic equations. We find

$$\begin{aligned}
\tilde{\lambda}'_1 &= \frac{(W_{12} - W_{21})\omega_1(\Delta\omega')}{\frac{1}{T_2^2 T_1} + \frac{1}{T_1}(\Delta\omega')^2 + \frac{1}{T_2}\omega_1^2} \\
\tilde{\lambda}'_2 &= \frac{(W_{12} - W_{21})\frac{1}{T_2}\omega_1}{\frac{1}{T_2^2 T_1} + \frac{1}{T_1}(\Delta\omega')^2 + \frac{1}{T_2}\omega_1^2} \\
\tilde{\lambda}'_3 &= -\frac{(W_{12} - W_{21})\left[\frac{1}{T_2^2} + (\Delta\omega')^2\right]}{\frac{1}{T_2^2 T_1} + \frac{1}{T_1}(\Delta\omega')^2 + \frac{1}{T_2}\omega_1^2}
\end{aligned} \tag{59}$$

where tilde means asymptotic value.

From eqs. (49) and (59) we obtain

$$\tilde{\rho}_{22} = \frac{1}{2}(1 + \lambda_3') = \frac{1}{2}\left\{1 - \frac{(W_{12} - W_{21})\left[\frac{1}{T_2^2} + (\Delta\omega')^2\right]}{\frac{1}{T_2^2 T_1} + \frac{1}{T_1}(\Delta\omega')^2 + \frac{1}{T_2}\omega_1^2}\right\}. \tag{60}$$

From eqs. (38) and (51) we get

$$W_{12} - W_{21} = \frac{1}{T_1}\tanh\frac{\hbar\omega_0}{2kT} \tag{61}$$

Finally $\tilde{\rho}_{22}$ can be written as

$$\tilde{\rho}_{22} = \frac{1}{2}\left\{1 - \frac{\left[\frac{1}{T_2^2} + (\Delta\omega')^2\right]}{\frac{1}{T_2^2} + (\Delta\omega')^2 + \frac{T_1}{T_2}\omega_1^2}\tanh\frac{\hbar\omega_0}{2kT}\right\} \tag{62}$$

At any temperature, however large be the field B_1, $\tilde{\rho}_{22}$ cannot be larger than $\frac{1}{2}$.

At $T = 0\,\mathrm{K}$ eq. (62) simplifies to

$$\tilde{\rho}_{22} = \frac{1}{2}\frac{\frac{T_1}{T_2}\omega_1^2}{\frac{1}{T_2^2} + (\Delta\omega')^2 + \frac{T_1}{T_2}\omega_1^2} \tag{63}$$

Assume that in eq. (52) τ^* tend to $+\infty$ as T_1. Then

$$\lim_{T_1 \to +\infty} \frac{T_1}{T_2} = 1 \tag{64}$$

Then eq. (63) becomes

$$\tilde{\rho}_{22} = \frac{1}{2}\frac{\omega_1^2}{(\Delta\omega)^2 + \omega_1^2} \tag{65}$$

In the case of a closed system, $\rho_{22}(t)$ is a periodic function of angular frequency $\Omega = \sqrt{\Delta\omega^2 + \omega_1^2}$. The above quantity $\tilde{\rho}_{22}$ is its time average value!

Although the derivation is mathematically questionable, it gives the right answer, as it will be proved rigorously in the following.

For the sake of completeness, we present the stationary components of the magnetic moment from eqs. (57) and (59)

$$\langle \tilde{m}'_X \rangle = -\frac{(W_{12} - W_{21})\omega_1(\varDelta\omega')}{\frac{1}{T_2^2 T_1} + \frac{1}{T_1}(\varDelta\omega')^2 + \frac{1}{T_2}\omega_1^2}$$

$$\langle \tilde{m}'_Y \rangle = -\frac{(W_{12} - W_{21})\dfrac{1}{T_2}\omega_1}{\frac{1}{T_2^2 T_1} + \frac{1}{T_1}(\varDelta\omega')^2 + \frac{1}{T_2}\omega_1^2} \tag{66}$$

$$\langle \tilde{m}'_z \rangle = \frac{(W_{12} - W_{21})\left[\dfrac{1}{T_2^2} + (\varDelta\omega')^2\right]}{\frac{1}{T_2^2 T_1} + \frac{1}{T_1}(\varDelta\omega')^2 + \frac{1}{T_2}\omega_1^2}$$

9. Rabi's Problem

Assume a closed two–state system with $\rho_{22}(0) = 1$. Then find the time evolution of ρ_{22}.

We must solve eqs. (50) with $1/T_1 = 1/T_2 = W_{12} = W_{21} = 0,\ \varDelta\omega' = \varDelta\omega$.

$$\frac{\mathrm{d}}{\mathrm{d}t}\begin{pmatrix} \lambda_1' \\ \lambda_2' \\ \lambda_3' \end{pmatrix} = \begin{pmatrix} 0 & \varDelta\omega & 0 \\ -\varDelta\omega & 0 & -\omega_1 \\ 0 & \omega_1 & 0 \end{pmatrix}\begin{pmatrix} \lambda_1' \\ \lambda_2' \\ \lambda_3' \end{pmatrix} \tag{67}$$

The eigenvalues are

$$\lambda_{1,2}' = \pm\varOmega = \pm\sqrt{\varDelta\omega^2 + \omega_1^2}, \qquad \lambda_3 = 0 \tag{68}$$

Then

$$\lambda_3' = A\sin\varOmega t + B\cos\varOmega t + C \tag{69}$$

where A, B, and C are constants to be determined by the initial conditions.

From the third of eqs. (67)

$$\lambda_2' = \frac{1}{\omega_1}\frac{\mathrm{d}\lambda_3'}{\mathrm{d}t} = \frac{\Omega}{\omega_1}(A\cos\Omega t - B\sin\Omega t) \tag{70}$$

From the second of eqs. (67)

$$\lambda_1' = -\frac{1}{\Delta\omega}\frac{\mathrm{d}\lambda_2'}{\mathrm{d}t} - \frac{\omega_1}{\Delta\omega}\frac{\mathrm{d}\lambda_3'}{\mathrm{d}t} \tag{71}$$

Condition $\rho_{22}(0) = 0$ gives (eq. (49)) $\lambda_3'(0) = -1$. Thus eq. (69) yields

$$A = 0, \qquad B + C = -1 \tag{72}$$

Hence

$$\begin{aligned} \lambda_1' &= \frac{1}{\Delta\omega}\frac{\Omega^2}{\omega_1}B\cos\Omega t - \frac{\omega_1}{\Delta\omega}(B\cos\Omega t + C) \\ \lambda_2' &= -\frac{\Omega}{\omega_1}B\sin\Omega t \\ \lambda_3' &= B\cos\Omega t + C \end{aligned} \tag{73}$$

Since the density matrix (ρ) is nonnegative definite,

$$\rho_{22}(0) = 0 \Rightarrow \rho_{12}(0) = 0$$

and therefore $\lambda_1'(0) = \lambda_2'(0) = 0$.

From the first of eqs. (73), the second of eqs. (72) we obtain

$$\frac{\Omega^2}{\omega_1 \Delta\omega} B + \frac{\omega_1}{\Delta\omega} = 0 \tag{74}$$

and finally

$$A = 0, \qquad B = -\frac{\omega_1^2}{\Omega^2}, \qquad C = -1 + \frac{\omega_1^2}{\Omega^2} \tag{75}$$

Thus from eqs. (49), (73) and (75) we find

$$\begin{aligned} \rho_{11}(t) &= 1 - \frac{\omega_1^2}{\Delta\omega^2 + \omega_1^2} \sin^2 \frac{\Omega t}{2} \\ \rho_{22}(t) &= \frac{\omega_1^2}{\Delta\omega^2 + \omega_1^2} \sin^2 \frac{\Omega t}{2} \\ \rho_{12}(t) &= \frac{1}{2} \frac{\omega_1}{\Omega} \left[\frac{\Delta\omega}{\Omega} (1 - \cos \Omega t) + \sin \Omega t \right] \end{aligned} \tag{76}$$

The second of eqs. (76) solves RABI's problem. It is immediately seen that the time average of $\rho_{22}(t)$ over the period is just given by eq. (65).

10. **Power Dissipation**

The energy that a particle exchanges with the bath in one transition is $\hbar\omega_0$. If N is the total number of particles, $W_{12}N\rho_{22}$ of them decay per unit time while $W_{21}N\rho_{11}$ rise up. Hence the total power released to the bath is

$$p_\mathrm{d}(t) = N\hbar\omega_0[W_{12}\rho_{22}(t) - W_{21}\rho_{11}t] \tag{77}$$

or, at zero bath temperature

$$p_\mathrm{d}(t) = N\hbar\omega_0 W_{12}\rho_{22}(t) \tag{78}$$

Such powers become asymptotically constant since $\rho_{11}(t)$ and $\rho_{22}(t)$ converge to $\tilde{\rho}_{11}$ and $\tilde{\rho}_{22}$ when $t \to +\infty$.

Hence the dissipated power has the steady state form

$$P_\mathrm{d} = N\hbar\omega_0 W_{12}\tilde{\rho}_{22} \tag{79}$$

$\tilde{\rho}_{22}$ is calculated from $\tilde{\lambda}_3$ (eq. (59)) by using eq. (49)

$$\tilde{\rho}_{22} = \frac{1}{2}\frac{\omega_1^2}{\dfrac{1}{T_1T_2} + \dfrac{T_2}{T_1}(\Delta\omega')^2 + \omega_1^2} \tag{80}$$

Now

$$\omega_1^2 = \gamma B_1^2 = \frac{q_\mathrm{e}^2}{m^2} B_1^2 \tag{81}$$

The incident power of the rotating TEM wave can be expressed in terms of B_1 as

$$P_\mathrm{i} = \frac{1}{2}\epsilon_0 c^3 B_1^2 \sigma \tag{82}$$

(ϵ_0 permittivity of vacuum, c speed of electromagnetic waves in vacuum, σ the area illuminated by the field)

Hence

$$\omega_1^2 = \frac{q_\mathrm{e}^2}{m^2} B_1^2 = \frac{2q_\mathrm{e}^2}{m^2 \epsilon_0 c^3 \sigma} P_\mathrm{i} \tag{83}$$

Finally

$$P_\mathrm{d} = \frac{N\hbar\omega_0 W_{12} q_\mathrm{e}^2}{m^2 \epsilon_0 c^3 \sigma} \frac{P_\mathrm{i}}{\dfrac{1}{T_1 T_2} + \dfrac{T_2}{T_1}(\Delta\omega')^2 + \dfrac{2q_\mathrm{e}^2}{m^2 \epsilon_0 c^3 \sigma} P_\mathrm{i}} \tag{84}$$

Eq. (84) expresses the dissipated power in terms of the incident one.

11. **Linearisation**

Eq. (84) can be linearised when

$$\frac{2T_1T_2q_e^2}{m^2\epsilon_0c^3\sigma}P_i \ll 1 \qquad (85)$$

and reduces to

$$P_d = \frac{N\hbar\omega_0W_{12}q_e^2}{m^2\epsilon_0c^3\sigma}\frac{1}{1+T_2^2(\Delta\omega')^2}P_i \qquad (86)$$

The cell illuminated by the TEM circularly polarized wave can be considered as a *linear time–invariant one–port*.

Electromagnetic power entering it is partly dissipated (released to the bath) and partly supplies the increase rate of stored electromagnetic energy.

In steady state only the first part is the *active power* constant in time, the second part is the *reactive power*, whose time average on a period is zero.

12. **The Equivalent Circuit Synthesis**

We represent the linear time–invariant one–port in DARLINGTON's form, i.e. as a lossless two–port terminated on a resistor.

The two–port is characterized by its *scattering matrix*

$$S = \begin{pmatrix} s_{11} & s_{12} \\ s_{21} & s_{22} \end{pmatrix} \tag{87}$$

In absence of nonreciprocal media, $s_{12} = s_{21}$ (condition of *reciprocity*).

Due to losslessness, matrix S is *unitary* on the imaginary axis.

The scattering matrix yields the *reflected* waves b_i in terms of the *incident* ones a_i at both ports.

Wave amplitudes are so normalized that $|a_i|^2$ represents the incident power, $|b_i|^2$ the reflected power at port i.

Since there is no incident power at port 2, the equation

$$|b_2|^2 = |s_{21}|^2 |a_1|^2 \tag{88}$$

relates the reflected power at port 2 (i.e. the power released to the resistor) to the incident power at port 1. Thus comparing with eq. (86), we obtain

$$|s_{21}|^2 = \frac{K}{1 + T_2^2(\omega - \omega_0')^2} \tag{89}$$

with

$$K = \frac{N\omega_0 T_2 q_e^2}{m^2 \epsilon_0 c^3 \sigma} \tag{90}$$

Analytic continuation of eq. (89) in the complex plane $p = \sigma + \mathrm{i}\omega$ gives

$$s_{21*}(p)s_{21}(p) = \frac{K}{1 - T_2^2(p - \mathrm{i}\omega_0')^2} \tag{91}$$

where the *paraconjugate* $s_{21*}(p)$ of $s_{21}(p)$ is defined as

$$s_{21*}(p) = s_{21}^*(-p^*) \tag{92}$$

(note that the paraconjugate reduces to the conjugate on the imaginary axis $\mathrm{i}\omega$.)

Eq. (91) admits of the Hurwitzian factorization

$$s_{21}(p) = \frac{\sqrt{K}}{1 + T_2(p - \mathrm{i}\omega_0')}, \quad s_{21*}(p) = \frac{\sqrt{K}}{1 - T_2(p - \mathrm{i}\omega_0')} \tag{93}$$

Analytic continuation of the unitary conditions leads to the paraunitary conditions. In particular

$$s_{11*}(p)s_{11}(p) = 1 - s_{21*}(p)s_{21}(p) \tag{94}$$

and therefore

$$s_{11*}(p)s_{11}(p) = \frac{1 - K - T_2^2(p - \mathrm{i}\omega_0')^2}{1 - T_2^2(p - \mathrm{i}\omega_0')^2} \tag{95}$$

Again we perform Hurwitz factorisation

$$\begin{aligned} s_{11}(p) &= \sqrt{1-K}\frac{1 + \dfrac{T_2}{\sqrt{1-K}}(p - \mathrm{i}\omega_0')}{1 + T_2(p - \mathrm{i}\omega_0')} \\ s_{11*}(p) &= \sqrt{1-K}\frac{1 - \dfrac{T_2}{\sqrt{1-K}}(p - \mathrm{i}\omega_0')}{1 - T_2(p - \mathrm{i}\omega_0')} \end{aligned} \tag{96}$$

Let Z_0 be the (real) characteristic impedance of the transmission line carrying the incident wave.

Then the impedance of the one–port is

$$Z(p) = Z_0 \frac{1 + s_{11}(p)}{1 - s_{11}(p)} \tag{97}$$

or, taking into account the first of eqs. (96),

$$Z(p) = Z_0 \frac{2T_2}{1 - \sqrt{1-K}} p - \mathrm{i} Z_0 \frac{\omega_0' T_2}{1 - \sqrt{1-K}} + Z_0 \frac{1 + \sqrt{1-K}}{1 - \sqrt{1-K}} \tag{98}$$

Thus the equivalent circuit is the series connection of an inductor, of an imaginary resistor and of a real resistor. The first two elements are lossless and form the DARLINGTON two–port.

APPENDIX

A Refresher of Quantum Mechanics

A1. The Mathematics of Quantum Mechanics

The *state space* of Quantum Mechanics is a HILBERT space $\mathbb{H}$, whose elements, *kets*, are denoted as $|\psi\rangle$, where ψ is a label to distinguish a particular ket.

The dual space of $\mathbb{H}$, $\mathbb{H}'$, can be identified with $\mathbb{H}$. Hence each of its elements, the *bras*, can be labelled as the ket which it can be identified with and represented as $\langle\psi|$.

The scalar product $\langle\phi|\psi\rangle$ is a mapping of the Cartesian product $\mathbb{H}'\times\mathbb{H}$ into the complex plane $\mathbb{C}$ with the properties

$$\begin{aligned}
&1. \quad \langle\phi|(c_1\,|\psi_1\rangle + c_2\,|\psi_2\rangle) = c_1\langle\phi|\psi_1\rangle + c_2\langle\phi|\psi_2\rangle \\
&\qquad c_1, c_2 \in \mathbb{C} \\
&2. \quad \langle\phi|\psi\rangle = \langle\psi|\phi\rangle^* \\
&3. \quad \langle\psi|\psi\rangle \geq 0 \quad (= 0 \quad \text{iff} \quad \psi = 0)
\end{aligned} \tag{A1}$$

Thus the scalar product is *linear* in the second factor and *antilinear* in the first.

A *linear operator* $\hat{A}$ from $\mathbb{H}$ to $\mathbb{H}$ is defined by the property

$$\hat{A}(c_1 |\psi_1\rangle + c_2 |\psi_2\rangle) = c_1\hat{A} |\psi_1\rangle + c_2\hat{A} |\psi_2\rangle \qquad \text{(A2)}$$

Let $|\chi\rangle$ be the mapping of $|\psi\rangle$ through $\hat{A}$. Then the mapping between the corresponding bras is defined by the *adjoint* of $\hat{A}$ denoted as $\hat{A}^+$:

$$\langle\chi| = \langle\psi|\hat{A}^+ \qquad \text{(A3)}$$

Thus

$$\langle\phi|\hat{A}|\psi\rangle = \langle\psi|\hat{A}^+|\phi\rangle^* \qquad \text{(A4)}$$

An operator such that

$$A = A^+ \qquad \text{(A5)}$$

is said to be *Hermitian*.

An Hermitian operator $\hat{A}$ has the following properties:

1. Its eigenvalues a_i are *real*.

2. Its eigenvectors $|a\rangle$ are *orthonormal* ($\langle a_i|a_j\rangle = \delta_{ij}$).

Any set of orthonormal kets $|\xi_i\rangle$ such that any $|\psi\rangle$ can be *uniquely* represented as

$$|\psi\rangle = \sum_i c_i\, |\xi_i\rangle \tag{A6}$$

is a *basis* for the Hilbert space $\mathbb{H}$. Since

$$c_i = \langle \xi_i | \psi \rangle \tag{A7}$$

eq. (A6) can be rewritten as

$$|\psi\rangle = \sum_i |\xi_i\rangle\, \langle \xi_i | \psi \rangle \tag{A8}$$

Accordingly the operator $\hat{A}$ can be represented as

$$\hat{A} = \sum_{i,j} a_{ij}\, |i\rangle\, \langle j| \tag{A9}$$

with

$$a_{ij} = \langle i|\hat{A}|j\rangle \tag{A10}$$

If the operator is Hermitian

$$a_{ij} = a^*_{ji} \tag{A11}$$

The non-Hermitian operator

$$|i\rangle\, \langle j| := \hat{P}_{ij} \tag{A12}$$

is the *projection operator* of state j on state i.

A2. **The Interpretative Postulates**

Postulate 1 *The state of a physical system is represented by a normalized ket* $|\psi\rangle$ *(or equivalently by the corresponding bra* $\langle\psi|$*.)*

Postulate 2 *An* observable *(a dynamical variable that can be measured) is represented by an Hermitian operator* $\hat{A}$ *whose eigenvectors form a basis for* $\mathbb{H}$*.*

Postulate 3 *The result of a measurement of an observable* $\hat{A}$ *can only be an eigenvalue* a_i *of* $\hat{A}$*. After the measurement the state vector* $|\psi\rangle$ collapses *into the eigenvector corresponding to that eigenvalue, i.e.* $|a_i\rangle$*.*

Postulate 4 *When the state* $|\psi\rangle$ *is expanded in eigenvectors of the operator* $\hat{A}$ *according to eqs. (A6) or (A8), the coefficients* $c_i = \langle a_i|\psi\rangle$ *represent the* probability amplitudes *that the system in state* $|\psi\rangle$ *be found after the measurement of* $\hat{A}$ *in state* $|a_i\rangle$*. The squared modulus of the probability amplitude is the* probability *of the same event:* $P(a_i|\,|\psi\rangle) = |\langle a_i|\psi\rangle|^2$*.*

Postulate 5 *The time evolution of the state vector* $|\psi\rangle$ *is determined by the* SCHRÖDINGER *equation*

$$i\hbar\frac{\mathrm{d}}{\mathrm{d}t}\,|\psi(t)\rangle = \hat{H}(t)\,|\psi(t)\rangle \tag{A13}$$

with the initial condition

$$|\psi(0)\rangle = \left|\psi_0\right\rangle, \qquad \left|\psi_0\right\rangle \in \mathbb{H} \tag{A14}$$

where $\hat{H}(t)$ *is the* energy *or* Hamiltonian *operator.*

Postulate 6 *The commutator of two Hermitian operators* $\hat{A}$ *and* $\hat{B}$ *having classical analogues is given by*

$$[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A} = i\hbar\{A, B\}\hat{1} \tag{A15}$$

where

$$\{A, B\} = \sum_n \left(\frac{\partial A}{\partial q_n}\frac{\partial B}{\partial p_n} - \frac{\partial A}{\partial p_n}\frac{\partial B}{\partial q_n}\right) \tag{A16}$$

is the POISSON *bracket of the classical quantities* A *and* B*;* q_n *and* p_n *are the classical coordinates and momenta.*

A3. **Main Theorems**

From Postulates 1 to 4 follows the

Theorem 1 *The expected value of a dynamical variable* $\hat{A}$ *for a system in state* $|\psi\rangle$ *is given by*

$$\langle A\rangle = \langle\psi|\hat{A}|\psi\rangle \tag{A17}$$

From Postulate 5 follows the

Theorem 2 *The solution of eq. (A13) with the initial condition (A14) has the form*

$$|\psi(t)\rangle = \hat{U}(t)\left|\psi_0\right\rangle \tag{A18}$$

where $\hat{U}(t)$ *is a unitary operator satisfying*

$$\hat{U}^+\hat{U} = \hat{1} \tag{A19}$$

The evolution operator $\hat{U}(t)$ *defines on* $(-\infty < t < +\infty)$ *a one–parameter group i.e.*

$$\hat{U}(t_1 + t_2) = \hat{U}(t_1)\hat{U}(t_2) \tag{A20}$$

If $\hat{H}$ *does not depend on time* (conservative *system), we have*

$$\hat{U}(t) = \mathrm{e}^{-\mathrm{i}\hat{H}t/\hbar} \tag{A21}$$

A4. **Pure States and Mixtures**

A *pure state* is characterised by a single state vector $|\psi\rangle$. A *mixture* is characterised by several state vectors $|\psi_i\rangle$, each of which is present in the mixture with (classical) probability ρ_i.

Definition 1 *The* density operator *of a mixture is defined as*

$$\hat{\rho} = \sum_i \rho_i |\psi_i\rangle \langle\psi_i| \tag{A22}$$

In particular for a pure state it reduces to

$$\hat{\rho} = |\psi\rangle \langle\psi| \tag{A23}$$

The density operator is Hermitian and nonnegative definite. Its rank is equal to the number of linearly independent $|\psi_i\rangle$; in particular it is 1 for pure states.

In a given base the diagonal elements ρ_{ii} are called *populations*, since they give the densities of systems in the various states, the nondiagonal ones ρ_{ij} are called *coherences*, since they take into account the phase differences between the various states.

Theorem 3 *The expected value of a dynamical variable* $\hat{A}$ *for a mixture characterised by a density operator* $\hat{\rho}$ *is*

$$\langle \hat{A} \rangle = \mathrm{Tr}\{\hat{\rho}\hat{A}\} = \sum_i \rho_i \langle \psi_i | \hat{A} | \psi_i \rangle \tag{A24}$$

Theorem 4 *The time evolution of the density operator* $\hat{\rho}$ *is determined by the* LIOUVILLE–VON NEUMANN *equation*

$$\frac{\partial \hat{\rho}}{\partial t} = -\frac{\mathrm{i}}{\hbar}[\hat{H}, \hat{\rho}] \tag{A25}$$

with the initial condition

$$\hat{\rho}(0) = \hat{\rho}_0, \qquad \hat{\rho}_0 \in \mathbb{H} \times \mathbb{H} \tag{A26}$$

Theorem 5 *The solution of eq. (A25) with the initial condition (A26) has the form*

$$\hat{\rho}(t) = \hat{U}(t)\hat{\rho}_0 U^+(t) \tag{A27}$$

If $\hat{H}$ *does not depend on time* (conservative *system), we have*

$$\hat{\rho}(t) = \mathrm{e}^{-\mathrm{i}\hat{H}t/\hbar}\hat{\rho}_0 \mathrm{e}^{\mathrm{i}\hat{H}t/\hbar} \tag{A28}$$

A5. **Dissipative Quantum Systems**

Dissipation is introduced by assuming that the system S is in contact with a thermal bath of infinite capacity at temperature T.

The treatment is limited to two–state systems.

We introduce the PAULI spin operators in the z-representation

$$\hat{\sigma}_x \doteq \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \hat{\sigma}_y \doteq \begin{pmatrix} 0 & \mathrm{i} \\ -\mathrm{i} & 0 \end{pmatrix} \quad \hat{\sigma}_z \doteq \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} \tag{A29}$$

and the *projection operators*

$$\begin{aligned} \hat{\sigma}^+ &= \tfrac{1}{2}(\hat{\sigma}_x + \mathrm{i}\hat{\sigma}_y) \doteq \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \\ \hat{\sigma}^- &= \tfrac{1}{2}(\hat{\sigma}_x - \mathrm{i}\hat{\sigma}_y) \doteq \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \end{aligned} \tag{A30}$$

that can also be represented as

$$\sigma^+ = \hat{P}_{21} = |2\rangle\langle 1| \qquad \sigma^- = \hat{P}_{12} = |1\rangle\langle 2| \tag{A31}$$

The effect of the interaction on the equations of the system can be represented according to the following

Theorem 6 *The master equation corresponding to irreversible dynamics which preserves the semigroup property for the non–unitary evolution operator $\hat{\Phi}(t)$, i.e.*

$$\hat{\Phi}(t_1 + t_2) = \hat{\Phi}(t_1)\hat{\Phi}(t_2) \qquad (t_1, t_2) \geq 0 \tag{A32}$$

must have the LINDBLAD *form*

$$\begin{aligned} \frac{\partial\hat{\rho}}{\partial t} &= -\frac{\mathrm{i}}{\hbar}[\hat{H}, \hat{\rho}] \\ &\quad + W^{\mathrm{adi}}[[\hat{\sigma}_z, \hat{\rho}], \hat{\sigma}_z] + \mathrm{i}\frac{\Delta\omega_0}{2}[\hat{\sigma}_z, \hat{\rho}] \\ &\quad + \frac{1}{2}W_{12}\left([\hat{\sigma}^-, \hat{\rho}\hat{\sigma}^+] + [\hat{\sigma}^-\hat{\rho}, \hat{\sigma}^+]\right) \\ &\quad + \frac{1}{2}W_{21}\left([\hat{\sigma}^+, \hat{\rho}\hat{\sigma}^-] + [\hat{\sigma}^+\hat{\rho}, \hat{\sigma}^-]\right) \end{aligned} \tag{A33}$$

where W^{adi} can be interpreted as the adiabatic *transition probability within the states (decoherence due to elastic collisions), $\Delta\omega_0$ as the connected frequency shift, W_{12} and W_{21} as the* nonadiabatic *transition probabilities from state 2 to state 1 and viceversa (with release or absorption of a quantum of energy to or from the bath).*

Eq. (A33) can be rewritten in a less compact but more convenient form as

$$
\begin{aligned}
\frac{\partial\hat{\rho}}{\partial t} &= -\frac{\mathrm{i}}{\hbar}[\hat{H},\hat{\rho}] \\
&+W^{\mathrm{adi}}[[\hat{\sigma}_z,\hat{\rho}],\hat{\sigma}_z] + \mathrm{i}\frac{\Delta\omega_0}{2}[\hat{\sigma}_z,\hat{\rho}] \\
&+\tfrac{1}{2}W_{12}\,(\hat{\sigma}^-\hat{\rho}\hat{\sigma}^+ - \hat{\sigma}^+\hat{\sigma}^-\hat{\rho} - \hat{\rho}\hat{\sigma}^+\hat{\sigma}^-) \\
&+\tfrac{1}{2}W_{21}\,(\hat{\sigma}^+\hat{\rho}\hat{\sigma}^- - \hat{\sigma}^-\hat{\sigma}^+\hat{\rho} - \hat{\rho}\hat{\sigma}^-\hat{\sigma}^+)
\end{aligned}
\qquad \text{(A34)}
$$

Finally, taking into account the definition of projection operators in eq. (A12) and eq. (A31), eq. (A34) can be written as

$$
\begin{aligned}
\frac{\partial\hat{\rho}}{\partial t} &= -\frac{\mathrm{i}}{\hbar}[\hat{H},\hat{\rho}] \\
&+W^{\mathrm{adi}}_{12}(\rho_{12}\,|1\rangle\,\langle 2| + \rho_{21}\,|2\rangle\,\langle 1|) \\
&+(W_{12}\rho_{22} - W_{21}\rho_{11})\,|1\rangle\,\langle 1| \\
&+(W_{21}\rho_{11} - W_{12}\rho_{22})\,|2\rangle\,\langle 2| \\
&-\frac{1}{2}(W_{12} + W_{21})(\rho_{12}\,|1\rangle\,\langle 2| + \rho_{21}\,|2\rangle\,\langle 1|)
\end{aligned}
\qquad \text{(A35)}
$$

Eq. (A35), written in scalar form, coincides with eqs. (39).

A6. **The Bloch Space**

The set of linear Hermitian operators from $\mathbb{H}$ to $\mathbb{H}$ is itself a vector space $\mathcal{L}(\mathbb{H}, \mathbb{H})$ on the real field, since

1. The sum of two Hermitian operators is an Hermitian operator.

2. The product of a *real* constant times an Hermitian operator is an Hermitian operator.

3. The above sum and product obey the usual rules of algebra.

The space of Hermitian operators can be given the structure of an Hilbert space by defining the *internal product* as

$$(\hat{A}, \hat{B}) = \mathrm{Tr}\{\hat{A}\hat{B}\} \tag{A36}$$

i.e. the internal product of two operators is the trace of their ordinary product.

In the Bloch space the natural basis is obtained from that of eq. (A9), $|i\rangle\langle j|$, by a nonsingular linear transformation yielding Hermitian elements.

For a two–dimensional Hilbert space, such a basis is provide by the unit operator and the three components of the spin operator

$$\hat{A} = \frac{1}{2}\mathcal{A}_0\hat{1} + \mathcal{A}_1\hat{\sigma}_x + \mathcal{A}_2\hat{\sigma}_y + \mathcal{A}_3\hat{\sigma}_z \tag{A37}$$

where

$$\begin{aligned} \mathcal{A}_0 &= a_{11} + a_{22} = \mathrm{Tr}\{\hat{A}\hat{1}\} \\ \mathcal{A}_1 &= a_{12} + a_{21} = \mathrm{Tr}\{\hat{A}\hat{\sigma}_x\} \\ \mathcal{A}_2 &= -\mathrm{i}(a_{12} - a_{21}) = \mathrm{Tr}\{\hat{A}\hat{\sigma}_y\} \\ \mathcal{A}_3 &= -a_{11} + a_{22} = \mathrm{Tr}\{\hat{A}\hat{\sigma}_z\} \end{aligned} \tag{A38}$$

Thus $\hat{A}$ can be represented in matrix form as

$$\hat{A} = \begin{pmatrix} \dfrac{\mathcal{A}_0 - \mathcal{A}_3}{2} & \dfrac{\mathcal{A}_1 + \mathrm{i}\mathcal{A}_2}{2} \\ \dfrac{\mathcal{A}_1 - \mathrm{i}\mathcal{A}_2}{2} & \dfrac{\mathcal{A}_0 + \mathcal{A}_3}{2} \end{pmatrix} \tag{A39}$$

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