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Spin relaxation and dissipative Schrödinger like evolution equations

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Abstract. A microscopic model of spin relaxation is proposed. In order to describe the energy exchange between the spins and the bath the idea is to add to the usual Schrödinger equation a non-linear term which acts as a damping term. This splitting in two competitive parts has the advantage of giving rise to relaxation and equilibrium magnetization without any approximation. Furthermore, it explains why the relaxation time T_1 which characterizes a dissipative phenomenon, is mainly given by a process described by the usual Schrödinger equation. The case of spin relaxation in zero magnetic field is also contained in this model.

In the case of a magnetic field with a rotating component our model predicts relaxation towards the effective magnetic field, i.e. recovers Redfield phenomenological theory, but without the usual constraint $\omega_1 \ll \omega_0$.

1. Introduction

Nuclear spin relaxation and Bloch's phenomenological equations [1] are by now largely known. Corresponding microscopic models have been proposed already in 1948 by Bloembergen, Purcell and Pound (BPP) [2], and in 1953 by Bloch himself and by Wangsness [3]. For an account of these and other models we refer to [4].

All these microscopic models have the common feature that the dissipative properties and the equilibrium states are inserted by procedures of limits and approximations applied to the Schrödinger equation (or to the Von Neumann equation). For example in the BPP model the procedure roughly goes as follows: using some perturbative approximations one computes transition probabilities. Then, adding terms which take the Boltzmann equilibrium state into account, one gets an evolution equation for the population [5, 6]. Another example is the master equation approach [3, 7], which has been shown to be rigorous [8, 9] only if one takes the thermodynamical and weak coupling limits one after the other and if one uses a rescaled time (Van Hove limit) [10, 11]). Abragam [12], among others, has emphasized that the problem of describing an irreversible dissipative behaviour starting from the conservative Schrödinger equation is far from being solved.

In the present paper we expose a quite different approach, which moreover allows to explain the good behaviour of the above mentioned models in the

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experimental situation. In order to present the ideas of our model we recall some elementary facts.

The evolution of the state vector ψ of a spin $\frac{1}{2}$ in an external magnetic field $\mathbf{B}$ is given by the Schrödinger equation:

$$\dot{\psi} = i\frac{\gamma}{2}\mathbf{B}\cdot\boldsymbol{\sigma}\psi$$

with obvious notations. Accordingly, the evolution of the macroscopic magnetic moment $\mathbf{M}$ is given by:

$$\dot{\mathbf{M}} = \gamma(\mathbf{M}\wedge\mathbf{B})$$

In order to take into account relaxation phenomena Bloch [1] proposed to add to this equation phenomenological terms:

$$\dot{M}_z = \frac{M^{\text{equ.}} - M_z}{T_1} \tag{1.a}$$

$$\dot{M}_x = \gamma M_y B - \frac{M_x}{T_2} \tag{1.b}$$

$$\dot{M}_y = -\gamma M_x B - \frac{M_y}{T_2} \tag{1.c}$$

where $M^{\text{equ.}}$ is the equilibrium magnetization and T_1, T_2 are the relaxation times. We have chosen, as usual, $\mathbf{B} = (0, 0, B)$. However in general no evolution equation corresponding to (1) exists for state vectors, nor for density matrices (Section 2).

We propose to add a phenomenological term directly to the Schrödinger equation and to use the structure of the state space and arguments of simplicity to deduce the form of this term (Section 3). The interpretation of our proposed term is analogous to the interpretation of Block's longitudinal relaxation term, i.e. it describes the energy exchange between the spins and the heat reservoir. In this way, as we shall see, no approximation is necessary for obtaining relaxation effects and equilibrium states. Furthermore adding terms to the Schrödinger equation – and not to the Von Neumann equation or to the population evolution equations – implies that the pure states ($\rho^2 = \rho$) remain pure during the evolution. Thus, in our model the use of statistical mixture is not fundamental but might, as in classical mechanics, be technically convenient. We believe that this point is important since a dissipative process may be predetermined as well in Quantum mechanics as in classical mechanics. This brings us back to our initial motivation which was to describe jointly spin relaxation and spin echo [20, 21]. Indeed, if one describes the relaxation by means of some stochastic Markovian process, then the spin echo phenomenon is out of the scope of the model [26]. On the other hand if the relaxation is predetermined, so that one can trace back the motion of each individual spin, then spin echo is easily explained [27].

In Section 4 we show that in our model the longitudinal relaxation phenomenon is due to two distinct and competitive processes: first a dissipative one, corresponding to a general tendency of spins to line up in a magnetic field, which is described by the additional term in the Schrödinger equation. Secondly a non dissipative process corresponding to a loss of coherence, i.e. a tendency towards the uniformization of the spin distribution, described by the usual Schrödinger equation (including the interactions between the spins). A process of this second kind occurs for example, in the spin relaxation in zero magnetic field: suppose a sample is set in a magnetic field until thermal equilibrium is reached. Then the field is suddenly turned off and one observes an exponential decay of the macroscopic magnetic moment with a time constant λ^{-1}. This phenomenon is not dissipative, in contrast to the longitudinal relaxation in a magnetic field and it thus indicates that in this case the evolution of the spins is described by the usual Schrödinger equation, the relaxation effect being due to the fact that one has prepared the system in a very special initial state [13].

Thus we are led to propose an evolution equation of the macroscopic magnetic moment M_z which is quite different from the corresponding Bloch equation. However, since in actual experiments the thermal energy is much larger than the magnetic energy, $K\theta \gg \hbar|\omega|$, the difference between the solutions is unobservable.

In Section 5 we apply our model to the case of a magnetic field with a rotating component.

2. Geometric picture of an ensemble of spins $\frac{1}{2}$

This section is devoted to a brief review of the correspondence between the (pure and mixed) density matrices on $\mathbb{C}^2$ and the points of the unit ball of $\mathbb{R}^3$. We show that the state and the evolution of a spin $\frac{1}{2}$ can be described as a classical magnetic moment, i.e. by a vector in $\mathbb{R}^3$ of fixed length.

The reader already familiar with this connection may proceed immediately to Section 3.

Let $\psi \in \mathbb{C}^2$ be a normalized state vector of one spin $\frac{1}{2}$. It is always possible to write ψ as follows:

$$\psi = e^{i\alpha/2} \begin{pmatrix} e^{-i\varphi/2}\sqrt{\dfrac{1+\eta}{2}} \\ e^{i\varphi/2}\sqrt{\dfrac{1-\eta}{2}} \end{pmatrix} \tag{2}$$

where α is a global phase factor and $\varphi \in [0, 2\pi[$, $\eta \in [-1, 1]$ are two parameters which we shall call the classical canonical variables (the motivation for this terminology will become clear from (7) and (9)). The parameters η, φ are in one-to-one correspondence with the directions of space given by the unit vector $\mathbf{m}_\psi$:

$$\mathbf{m}_\psi = (\sqrt{1-\eta^2}\cos\varphi; \sqrt{1-\eta^2}\sin\varphi; \eta) = \langle\psi|\boldsymbol{\sigma}|\psi\rangle \tag{3}$$

where $\boldsymbol{\sigma}$ are the Pauli matrices. The connection between ψ and $\mathbf{m}_\psi$ given by (2) is completed by the fact that a spin $\frac{1}{2}$ in the state ψ is actually in the direction $\mathbf{m}_\psi$, that is to say a measurement of the spin component in the direction $\mathbf{m}_\psi$ made on a spin in the state ψ always gives the result $+\hbar/2$, i.e.

$$\mathbf{m}_\psi \cdot \mathbf{S}\,|\psi\rangle = +\frac{\hbar}{2}|\psi\rangle$$

where $\mathbf{s} = (\hbar/2)\boldsymbol{\sigma}$ are the spin operators.

Some care has to be taken for the notion of orthogonality of two state vectors ψ and χ. One indeed has:

$$\langle\psi \mid \chi\rangle = 0 \quad \Leftrightarrow \quad \mathbf{m}_\psi = -\mathbf{m}_\chi \tag{4}$$

Let us now turn to the evolution of a spin $\frac{1}{2}$. The following results hold: if

$$\dot{\psi} = i\frac{\gamma}{2}\mathbf{B} \cdot \boldsymbol{\sigma}\psi \tag{5}$$

then

$$\dot{\eta} = \gamma\sqrt{1-\eta^2}(B_y \cos\varphi - B_x \sin\varphi) \tag{6}$$

$$= -\partial_\varphi h(\eta, \varphi) \tag{7}$$

$$\dot{\gamma} = \gamma(B_x \cos\varphi + B_y \sin\varphi)\frac{\eta}{\sqrt{1-\eta^2}} - \gamma B_z \tag{8}$$

$$= \partial_\eta h(\eta, \varphi) \tag{9}$$

$$\dot{\mathbf{m}}_\psi = \gamma(\mathbf{m}_\psi \wedge \mathbf{B}) \tag{10}$$

where

$$h(\eta, \varphi) = -\gamma\mathbf{B} \cdot \mathbf{m}_\psi \tag{11}$$

The equations (7) and (9) are canonical equations for the Hamiltonian $h(\eta, \varphi)$ given by (11). Notice that the symplectic 2-form $\Omega = d\eta \wedge d\varphi$ represents geometrically a small surface element of the unit sphere. The relation (10) shows that the vector $\mathbf{m}_\psi$ turns around the magnetic field $\mathbf{B}$ with the Larmor frequency $\omega = -\gamma|\mathbf{B}|$.

Let us now consider an ensemble of N spins: $\{\psi_i\}_{i=1\ldots N}$. The density operator of this ensemble is given by the following 2×2 matrix:

$$\rho = \frac{1}{N}\sum_{i=1}^{N} |\psi_i\rangle\langle\psi_i| \tag{12}$$

Analogously to relation (2) we associate to each density operator a vector $\mathbf{M} \in \mathbb{R}^3$:

$$\mathbf{M} = \mathrm{Tr}(\boldsymbol{\sigma}\rho) \tag{13}$$

The practical use of this operator ρ is that $\mathrm{Tr}\,(A\rho) = (1/N)\sum_{i=1}^{N}\langle A\rangle_{\psi_i}$ for all operators A, in particular:

$$\mathbf{M} = \frac{1}{N}\sum_{i=1}^{N} \mathbf{m}_{\psi_i} \tag{14}$$

i.e. the vector associated to ρ is the mean vector of the ones associated with the ψ_i.

The relation (13) between ρ and $\mathbf{M}$ can be inverted:

$$\rho = \frac{\mathbb{1} + \mathbf{M} \cdot \boldsymbol{\sigma}}{2} \tag{15}$$

However this last relation does not always define a density operator. Indeed a density operator must satisfy the three following conditions:

(i) $\rho = \rho^+$

(ii) $\mathrm{Tr}\,|\rho| = 1$

(iii) $\rho \geq 0$

All matrices of the form (15) satisfy (i) and (ii), but for (iii) one has the following condition:

$$\rho \geq 0 \quad \Leftrightarrow \quad |\mathbf{M}| \leq 1 \tag{16}$$

The proof of (16) is elementary if one chooses the z axis parallel to $\mathbf{M}$. Notice that if $\mathbf{M}$ is of the form (14), then necessarily $\mathbf{M} \leq 1$, the equality holding iff all the $\mathbf{m}_{\psi_i}$ are parallel.

Among all the density operators the ones corresponding to pure states have the characteristic property $\rho^2 = \rho$, which is equivalent to $|\mathbf{M}| = 1$.

This completes the geometric picture (see Fig. 1): the space of the density operators is identified with the unit ball of $\mathbb{R}^3$, the unit sphere being identified with the pure states.

This picture makes it easy to see that to one mixed density operator, represented by some vector $\mathbf{M} \in \mathbb{R}^3$ with $|\mathbf{M}| < 1$, correspond several ensembles of spins represented by $\{\mathbf{m}_{\psi_i}\}$ with

$$|\mathbf{m}_{\psi_i}| = 1 \quad \text{and} \quad \mathbf{M} = \frac{1}{N} \sum_{i=1}^{N} \mathbf{m}_{\psi_i}.$$

The evolution of $\mathbf{M}$ corresponding to the unitary evolution of ρ:

$$\dot{\rho} = i\frac{\gamma}{2}[\mathbf{B} \cdot \boldsymbol{\sigma}; \rho] \tag{17}$$

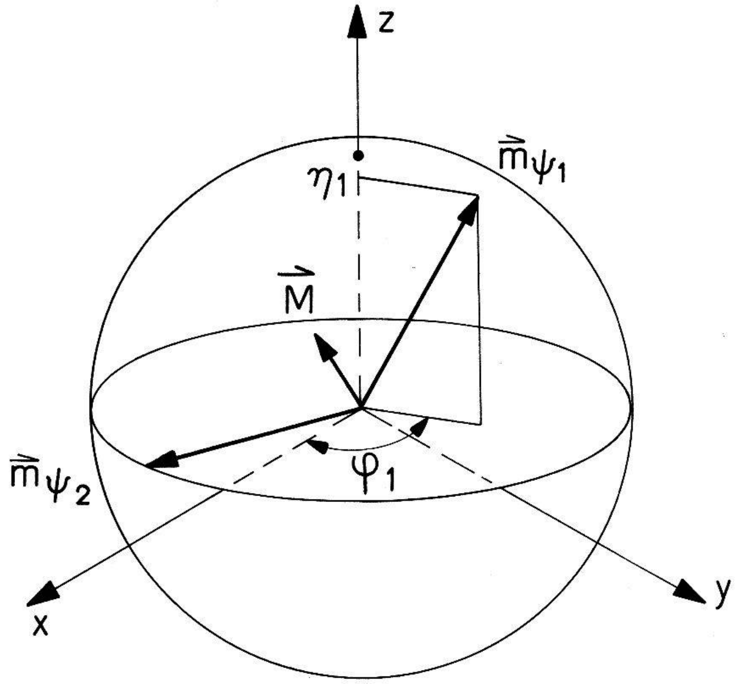

Figure 1

Correspondence between the pure and the mixed density matrices of spins $\frac{1}{2}$ and the unit ball of $\mathbb{R}^3$. To pure states ψ_i correspond unit vectors $\mathbf{m}_{\psi_i}$. To a mixed density matrice ρ corresponds a vector $\mathbf{M}$ with $|M| < 1$.

is

$$\dot{\mathbf{M}} = \gamma(\mathbf{M} \wedge \mathbf{B}) \tag{18}$$

We now apply the preceeding results, in particular relation (15), to deduce the evolution equation for ρ which corresponds to the Bloch equations (1):

$$\dot{\rho} = \frac{i\gamma B}{2}[\sigma_z; \rho] + \frac{M_0 - \mathrm{Tr}(\sigma_z \rho)}{2T_1} \cdot \sigma_z - \frac{\mathrm{Tr}(\sigma_x \rho)}{2T_2} \cdot \sigma_x - \frac{\mathrm{Tr}(\sigma_y \rho)}{2T_2} \cdot \sigma_y \tag{20}$$

Due to (16) the equation (20) can be interpreted as an evolution equation for density matrices only if the condition $|\mathbf{M}| \leq 1$ is preserved during the evolution. A simple computation shows however that this is generally not the case. This fact reduces the import of the Bloch equations. Similar results have also been obtained in the framework of quantum dynamical semi-groups which deals with general linear evolution equation for density operators [14].

3. Relaxation equations for one spin $\frac{1}{2}$

In the preceeding section the state space of one spin $\frac{1}{2}$ is identified with the unit sphere of $\mathbb{R}^3$. The evolution equation for the classical variables η, φ are deduced from the evolution equation of the state vector. In this section we shall go the other way round. We shall look for the evolution equations for ψ which correspond to definite equations for η and φ. More precisely we add to the Hamiltonian equation for $\dot{\eta}$ and $\dot{\varphi}$ some friction terms such that $\eta(t)$ tends to 1 for t going to infinity, i.e. such that the spin relaxes to the parallel state, and then deduce the corresponding evolution for ψ.

Leaving out long but straightforward computations, we present the results (see fig. 2):

a) if $\dot{\eta} = k(1-\eta)$ with $k > 0$
$\dot{\varphi} = \omega$

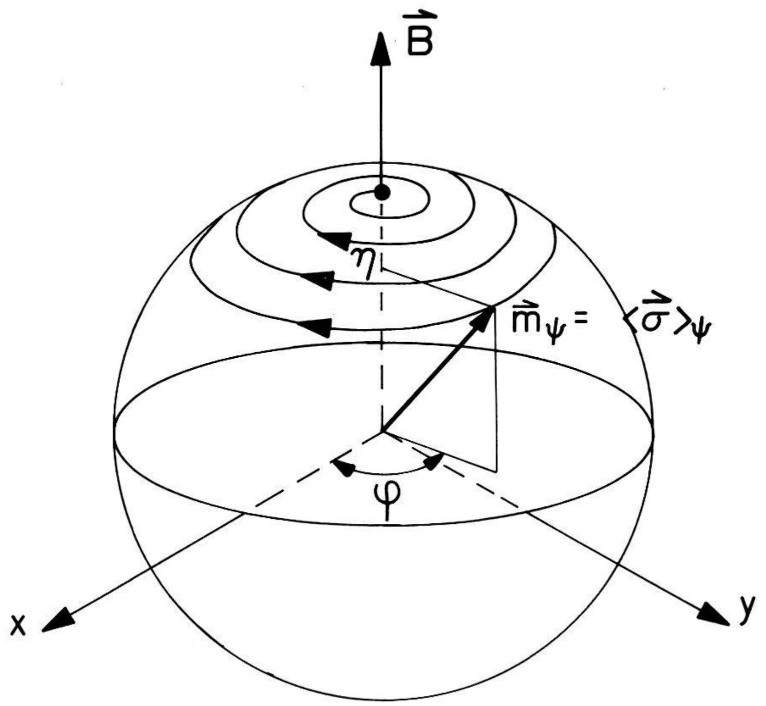

Figure 2
Solution of the equation (25) describing the spiroïdal motion of a spin turning around and simultaneously lining up on the magnetic field **B**.

(i.e. $\eta(t)=1-(1-\eta(0))\cdot e^{-kt} \xrightarrow{t\to\infty} 1$) then the corresponding evolution equation for ψ and $\mathbf{m}_\psi$ are:

$$\dot{\psi}=-i\frac{\omega}{2}\sigma_z\psi+k\frac{\sigma_z-\langle\sigma_z\rangle\psi}{2(1+\langle\sigma_z\rangle_\psi)}\cdot\psi \tag{22}$$

$$\begin{aligned}\dot{m}_x&=-\omega m_y-k\frac{m_z}{1+m_z}\cdot m_x\\ \dot{m}_y&=\omega m_x-k\frac{m_z}{1+m_z}\cdot m_y\\ \dot{m}_z&=k(1-m_z)\end{aligned} \tag{23}$$

where $\langle\sigma_z\rangle_\psi=\langle\psi\,|\sigma_z|\,\psi\rangle/\langle\psi\mid\psi\rangle$.

b) if $\dot{\eta}=2k(1-\eta^2)$ with $k>0$

$\dot{\rho}=\omega$

(i.e. $\eta(t)=\text{th}\,(2kt+\text{arth}\,\eta(0)) \xrightarrow{t\to\infty} 1$), then the corresponding evolution equation for ψ and $\mathbf{m}_\psi$ are:

$$\dot{\psi}=-i\frac{\omega}{2}\sigma_z\psi+k(\sigma_z-\langle\sigma_z\rangle_\psi)\cdot\psi \tag{25}$$

$$\begin{aligned}\dot{m}_x&=-\omega m_y-2km_z\cdot m_x\\ \dot{m}_y&=\omega m_x-2km_z\cdot m_y\\ \dot{m}_z&=2k(1-m_z^2)\end{aligned} \tag{26}$$

It is interesting that the solution of (25) has a simple form:

$$\psi_t=\frac{\exp[(-i(\omega/2)+k)\sigma_z t]\cdot\psi_0}{(\langle e^{2k\sigma_z t}\rangle_{\psi_0})^{1/2}}$$

The above results ask for several comments:

(1) First we would like to emphasize that non linear evolution equation for the state vector are compatible with the fundamental postulates of quantum mechanic [10].

(2) The equations (22) and (25) preserve the norm of ψ. This is clear from the construction, and one may also explicitily verify that $d/dt\langle\psi\mid\psi\rangle=0$. The vector $\mathbf{m}$ also remains normalized under the evolution equations (23) or (26). Thus its motion must be a sequence of instantaneous rotations. Similarily the evolution of ψ is a sequence of 'instantaneous Hamiltonians'. Indeed the equations (25) and (26) can be rewritten in the following equivalent form:

$$i\dot{\psi}=\frac{\omega}{2}\sigma_z\psi+ik[\sigma_z;|\psi\rangle\langle\psi|]\cdot\psi \tag{27}$$

$$\dot{\mathbf{m}}=-\omega(\mathbf{m}\wedge\mathbf{e}_z)-2k\mathbf{m}\wedge(\mathbf{m}\wedge\mathbf{e}_z) \tag{28}$$

where $(\omega/2)\sigma_z+ik[\sigma_z,|\psi\rangle\langle\psi|]$ is the 'instantaneous Hamiltonian', and $-\omega\mathbf{e}_z-2k\mathbf{m}\wedge\mathbf{e}_z$ is the vector parametrizing the instantaneous rotation. The equations (22) and (23) can be rewritten in a similar form. The second term on the right hand side of the equation (28) is called the Landau-Lifshitz friction term [16].

(3) So far we have supposed that the magnetic field **B** is parallel to the z axis. For the general case one has to replace everywhere σ_z by $\mathbf{B}\boldsymbol{\sigma}$. The generalization of (25) is linear in **B**, contrarily to the generalization of (22) which is non-linear in **B**. This fact is a strong argument in favour of the equation (25). Indeed the superposition of two magnetic fields $\mathbf{B}_1$ and $\mathbf{B}_2$ is given by their sum $\mathbf{B}_1+\mathbf{B}_2$. Furthermore (25) is the unique quasi linear (in ψ) Schrödinger equation which preserves the norm of ψ and is linear in **B**.

(4) The equation (22) predicts an exponential longitudinal relaxation for each individual spin, whereas the equation (25) predicts an hyperbolic tangent relaxation. Experimentally the relaxation is exponential. However, as explained in the next section, an hyperbolic tangent microscopic relaxation is not incompatible with an exponential macroscopic relaxation.

(5) The equation (25) has a very natural extension to arbitrary quantum system. Let H be any Hamiltonian acting on an Hilbert space $\mathcal{H}$, then the extended equation reads:

$$\dot{\psi}=-iH\psi+k(\langle H\rangle_\psi-H)\cdot\psi \tag{29}$$

From (29) one deduces:

$$\begin{aligned}\frac{d}{dt}\langle H\rangle_\psi&=-2k(\langle H^2\rangle_\psi-\langle H\rangle_\psi^2)\\&=-2k(\Delta H)^2\leq 0\end{aligned} \tag{30}$$

The interpretation of this last inequality is that the system dissipates energy iff the state vector is not an eigenstate of the Hamiltonian. The equation (29) has been studied in [17]. Two of its main properties are listed below:

(i) The eigenstates of H are stationary semi stable solutions of (29), except the ground state which is stable. In the case of a spin $\frac{1}{2}$ this fact appears as follows: the antiparallel state is a stationary solution of (29), but all other states, even arbitrarily close to it, evolve to the parallel state.

(ii) Applying equation (29) to the damped quantum harmonic oscillator it turns out that the solution corresponding to a coherent initial state is itself a coherent state at each time. Furthermore the point of the classical phase space which labels such a coherent state, follows the path of the classical damped harmonic oscillator.

(6) Finally we would like to make a short additional comment in relation with the equation (25) which is independent from the main subject of this paper.

Let ρ be the density matrix of a statistical mixture of N spins $\{\psi_i\}_{i=1\ldots N}$. Suppose that the Hamiltonian of each individual spin contains the usual term $\mathbf{B}\boldsymbol{\sigma}$ and a term proportional to the macroscopic magnetic moment $\mathrm{Tr}\,(\boldsymbol{\sigma}\rho)\boldsymbol{\sigma}$. Furthermore suppose that the individual spins react to this macroscopic magnetic moment with a small delay ε. Then, developing the evolution equation for the state vector of the kth spin up to order ε one finds:

$$\begin{aligned}\dot{\psi}_k(t)&=-i\frac{\omega}{2}\sigma_z\psi_k(t)-i\alpha\,\mathrm{Tr}\,(\boldsymbol{\sigma}\cdot\rho(t-\varepsilon))\cdot\boldsymbol{\sigma}\psi_k(t)\\&=-i\frac{\omega}{2}\sigma_z\psi_k(t)-i\alpha\{2\rho(t)-\mathbb{1}+\\&\quad+i\varepsilon\omega[\sigma_z,\rho(t)]+0(\varepsilon^2)\}\psi_k(t)\end{aligned}$$

and consequently

$$\dot{\rho} = \frac{1}{N}\sum_{i=1}^{N}\frac{d}{dt}(|\psi_i\rangle\langle\psi_i|)$$

$$\cong -i\frac{\omega}{2}[\sigma_z, \rho] + \alpha\omega\varepsilon[[\sigma_z, \rho], \rho] \tag{31}$$

If $N = 1$, equation (31) is equivalent to equation (25). So it seems that the assumption introduced above leads naturally to relaxation. Nevertheless a deeper study shows that only the self-interaction of a spin with its own magnetic moment is responsible for the relaxation effect.

4. Relaxation model at finite temperature

In this section we present one simple model of macroscopic spin relaxation based on the dissipative Schrödinger like equation (25).

The solution of equation (25) is such that $\mathbf{B} \cdot \mathbf{m}_\psi$ tends asymptotically to its maximum value. This corresponds to the thermal equilibrium value at zero temperature. For N spins at finite temperature θ one has:

$$M^{\text{equilibrium}} = \frac{N\gamma\hbar}{2} \cdot \text{th}\left(\frac{-\hbar\omega}{2K\theta}\right) \tag{34}$$

where $\omega = -\gamma B$ is the Larmor frequency and K is the Boltzmann constant.

Consequently, at finite temperature, in addition to the tendency of the spins to line up in a magnetic field, another process must occur to prevent an alignment of all the spins in the same direction. In particular if no magnetic field is present $M^{\text{equ.}} = 0$, and experimentally one finds that the macroscopic magnetic moment goes exponentially to zero. This process is not dissipative, thus we describe it by the usual Schrödinger equation, including the interactions between the different spins. The transition probabilities due to the interaction Hamiltonian $H_I(t)$ can be computed as in the BPP model [2, 4]. In this way one obtains symmetric transition probabilities, and thus predicts an exponential uniformization of the population of the different levels. Orginally BPP added ad hoc terms to the evolution equation of the population in order to take into account the Boltzmann equilibrium state. This is not necessary in our model. Let λ^{-1} denote the time characterizing this uniformization. Notice that λ depends, in particular, on the strength of the magnetic field and on the correlation time of the particles motion.

In the case of an external field $\mathbf{B} = (0, 0, -\omega/\gamma)$ we assume that the evolution equation of each spin reads:

$$\dot{\psi} = i\frac{\omega}{2}\sigma_z\psi + \frac{k\omega}{2}(\langle\sigma_z\rangle_\psi - \sigma_z)\psi - iH_I\psi_t \tag{35}$$

The corresponding evolution equation for the microscopic distribution function $\rho(\psi, t)$ (or $\rho(\eta, \varphi, t)$ with the notations of Section 2) can easily be deduced. However, since $H_I(t) = \mathbf{B}_1(t) \cdot \boldsymbol{\sigma}$, where $\mathbf{B}_1(t)$ is an extremely rapidly fluctuating field, equation (35) cannot be exactly solved. A useful tool to tackle this difficulty is a stochastic model. Such a model for a classical spin has been proposed for the narrowing limit case by R. Kubo and N. Hashitsame [18], see also [19]. Another method uses the above mentioned transition probability $\lambda/2$. We follow the latter. For our purpose only the (normalized) distribution function $\rho(\eta, t)$ of the spin projection along the magnetic field is needed. According to (35) we assume that its evolution equation is given by:

$$\partial_t \rho(\eta, t) = -\partial_\eta(-\omega k(1-\eta^2)\rho) + \lambda(\rho_0 - \rho) \tag{36}$$

where $\rho_0(\eta) \equiv \frac{1}{2}$ corresponds to the distribution of the spins uniform in all directions.

Notice that due to the non linearity of the equation (35) no corresponding evolution equation exist for density matrices. This particularity of the density matrices formalism also shows up in the spin echo phenomenon [20, 21]: if each spin has a different Larmor frequency no consistent evolution equation exist for the density matrix of the ensemble of spins.

Defining the mean value of η by

$$\langle \eta \rangle_\rho = \int_{-1}^{1} \eta \cdot \rho(\eta, t)\, d\eta$$

one has:

$$\partial_t \langle \eta \rangle_\rho = -\omega k(1 - \langle \eta^2 \rangle_\rho) - \lambda \langle \eta \rangle_\rho \tag{37}$$

The non linearity of the evolution equation of η (24) makes it impossible to deduce from (36) a consistent equation for $\langle \eta \rangle_\rho$. From here on we assume that $\hbar\,|\omega| \ll K\theta$. Accordingly

$$\langle \eta \rangle_{\text{equilibrium}} \cong -\frac{\hbar\omega}{2K\theta} \ll 1$$

and the distribution function $\rho(\eta, t)$ is always very close to the uniform distribution ρ_0. Thus we replace in equation (37) the mean square deviation $(\Delta\eta)^2_\rho = \langle \eta^2 \rangle_\rho - \langle \eta \rangle^2_\rho$ by $(\Delta\eta)^2_{\rho_0} = \frac{1}{3}$:

$$\begin{aligned} \partial_t \langle \eta \rangle_\rho &= -\omega k(1 - (\Delta\eta)^2_\rho - \langle \eta \rangle^2_\rho) - \lambda \langle \eta \rangle_\rho \\ &\cong -\omega k(\tfrac{2}{3} - \langle \eta \rangle^2_\rho) - \lambda \langle \eta \rangle_\rho \end{aligned} \tag{38}$$

Let $M_z = (N\gamma\hbar/2)\langle \eta \rangle_\rho$, then:

$$\dot{M}_z = -\frac{N\gamma\hbar\omega k}{2}\left(\frac{2}{3} - \frac{4}{N^2\gamma^2\hbar^2} \cdot M_z^2\right) - \lambda M_z \tag{39}$$

This last equation describes the evolution of the macroscopic magnetic moment component parallel to the magnetic field, and is to be compared with Bloch equation (1.c). Although the structures of (39) and (1.c) are very different, the solutions are very similar in the region $|M_z| \ll N\gamma h/2$ (i.e. $\langle \eta \rangle_\rho \ll 1$). Indeed the solution of (39) reads:

$$M_z(t) = \frac{N\gamma\hbar}{4T_1\omega k}\left\{\text{th}\left(\frac{t}{2T_1} + C_0\right) - 1\right\} + M_z(\infty) \tag{40}$$

with

$$T_1 = (\lambda^2 + \tfrac{8}{3}\omega^2 k^2)^{-1/2} \tag{41}$$

$$M_z(\infty) = \frac{N\gamma\hbar}{2} \cdot \frac{\lambda - T_1^{-1}}{2\omega k} \tag{42}$$

and where C_0 is the integration constant depending on the initial condition at $t_0 = 0$. Notice that according to the assumption $|\hbar\omega| \ll K\theta$, only the asymptotic part of $M_z(t)$ corresponds to the equation (37). The equation (39) thus predicts that as t goes to infinity, $M_z(t)$ tends exponentially to $M_z(\infty)$ with a time constant T_1:

$$M_z(t) \simeq M_z(\infty) - [M_z(\infty) - M_z(0)]e^{-t/T_1}$$

The relation (41) gives the longitudinal relaxation time in function of the Larmor frequency, the characteristic time of loss of coherence λ^{-1}, and the friction constant k. The latter can be eliminated using the condition:

$$M_z(\infty) = M_z^{\text{equilibrium}}$$

and can be further simplified using the inequality $\hbar|\omega| \ll K\theta$. One obtains:

$$T_1^{-1} \cong \lambda\left(1 + \frac{3}{4} \cdot \frac{\hbar^2\omega^2}{k^2\theta^2}\right) \tag{43}$$

$$\omega k \cong \lambda \cdot \frac{3}{4} \cdot \frac{\hbar\omega}{k\theta} \tag{44}$$

The dependence of k on the bath variables, like the temperature θ and the correlation times (via λ), is compatible with our interpretation of k as describing phenomenologically the interaction between the spins and the bath.

5. Rotating field

Let us apply our model to the case of a magnetic field with a rotating component:

$$\mathbf{B}(t) = -\frac{1}{\gamma}(\omega_1 \cdot \cos\omega t; \omega_1 \cdot \sin\omega t; \omega_0)$$

In this case equation (25) reads:

$$\dot{\psi}_t = i\frac{\gamma}{2}\mathbf{B}(t) \cdot \boldsymbol{\sigma}\psi_t - \frac{k\gamma}{2}(\langle \mathbf{B}(t) \cdot \boldsymbol{\sigma}\rangle_{\psi_t} - \mathbf{B}(t) \cdot \boldsymbol{\sigma})\psi_t \tag{45}$$

In the rotating frame, $\tilde{\psi}_t = \exp\{i(\omega/2)\sigma_z t\}\psi_t$, the equation (45) is time independent and can be explicitly solved:

$$\dot{\tilde{\psi}}_t = -\frac{i}{2}\mathbf{B}_{ef} \cdot \boldsymbol{\sigma}\tilde{\psi}_t + \frac{k}{2}(\langle \mathbf{B}_{fr} \cdot \boldsymbol{\sigma}\rangle_{\tilde{\psi}_t} - \mathbf{B}_{fr} \cdot \boldsymbol{\sigma})\tilde{\psi}_t \tag{46}$$

$$\tilde{\psi}_t = (\langle \exp(i\mathbf{B}_{ef} - k\mathbf{B}_{fr})\boldsymbol{\sigma}t/2 \cdot \exp(-i\mathbf{B}_{ef} - k\mathbf{B}_{fr})\boldsymbol{\sigma}t/2\rangle_{\tilde{\psi}_0})^{-1/2} \cdot \exp -[(i\mathbf{B}_{ef} + k\mathbf{B}_{fr})\boldsymbol{\sigma}t/2]\tilde{\psi}_0$$

with $\mathbf{B}_{ef} = (\omega_1; 0; \delta)$ the effective field, $\delta = \omega_0 - \omega$, and $\mathbf{B}_{fr} = (\omega_1; 0; \omega_0)$.

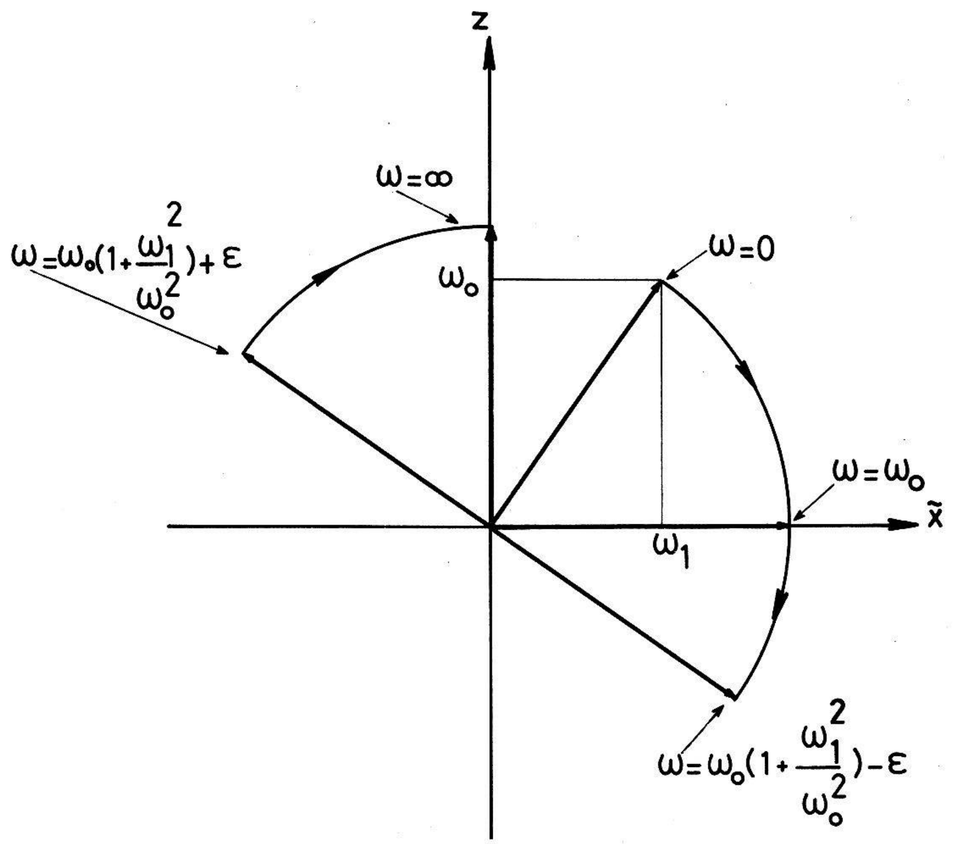

Figure 3
Quasi periodic state of a spin $\frac{1}{2}$ in the rotating frame (equation (47)) in function of the frequency ω of the rotating field.

For $\omega \neq \omega_0(1+\omega_1^2/\omega_0^2)$, i.e. $\mathbf{B}_{ef}$ and $\mathbf{B}_{fr}$ nor orthogonal, equation (46) has two stationary solutions. If $k \ll 1$, then the directions corresponding to these solutions are arbitrary close to $\mathbf{B}_{ef}$. Indeed, denoting these stationary solutions by $\tilde{\psi}^{\pm}$, one has:

$$\mathbf{m}^{\pm} \equiv \langle \boldsymbol{\sigma} \rangle_{\tilde{\psi}^{\pm}} = \left(\frac{\pm \omega_1}{\xi\sqrt{w_1^2+\delta^2}}; k \cdot \frac{\omega \cdot \omega_1}{\omega_1^2+\delta^2}; \frac{\pm \delta}{\xi\sqrt{\omega_1^2+\delta^2}} \right) + 0(k^2) \tag{47}$$

where $\xi = +1$ if $\omega < \omega_0(1+\omega_1^2/\omega_0^2)$ and $\xi = -1$ if not. $\mathbf{m}^-$ corresponds to the stable solution.

This last result is quite remarkable, since it proves that the way we introduced friction at a microscopic level unifies in a natural way Bloch ($\omega_1 = 0$) and Redfield ($\omega_1 \ll \omega_0$) [23] phenomenological theories. The Figure 3 shows the dependence of $\mathbf{m}^+$ on ω (in the rotation frame). To the author's knowledge the case of large ω_1 has so far not been tested experimentally. It is interesting to note that in the limit $k \to 0$ the asymptotic states (47) are adiabatic invariants of the linear time dependent Schrödinger equation [28]. For an approach to spin systems in a rotating field based on the (non dynamical) principle of adiabatic invariance, see [24].

6. Conclusion

The correspondence between the classical and the quantum spin $\frac{1}{2}$ explicitly given in Section 2 clearly indicates how to construct dissipative Schrödinger like evolution equations. In Section 3 we saw that in this way the quantum analogue of the Landau-Lifshitz friction term arises very naturally. According to this friction term the microscopic relaxation of a spin $\frac{1}{2}$ is not exponential, but follows a hyperbolic tangent. However the simple model of macroscopic relaxation proposed in Section 4 shows that, close to the uniform distribution (i.e. when the thermal energy $K\theta$ is much larger than the magnetic energy $|\hbar\omega|$), such a microscopic relaxation is completely compatible with the well known phenomenological Bloch equations [1]. Furthermore the relaxation time predicted by this model is equal, up to order $(\hbar\omega/K\theta)^2$, to the one predicted by the known models based on the Schrödinger equation. The higher order approximate solutions of the equation (36) exhibit non linear relaxation [22].

In Section 5 we showed that the case of a magnetic field with a rotating component is particularly simple to treat in our approach. The predictions recover Redfield's phenomenological theory, i.e. relaxation toward the effective magnetic field, and are not constrained by the usual inequality $\omega_1 \ll \omega_0$. New experiments should be made to investigate the area $\omega_1 \gtrsim \omega_0$.

As we wrote in introduction all the microscopic models of spin relaxation introduce dissipation via some limits on approximations. It should be noticed that the fundamental equation (25) of our approach can also be deduced from the linear Schrödinger equation using some approximations. Actually it happens that exactly the same type of projection techniques and approximations which are necessary to deduce the Pauli master equation can be used to derive equation (25) [25]. But, by doing so, we would inherit most of the problems of the usual approaches. And our purpose was to split clearly in the microscopic evolution equations the dissipative irreversible energy exchange process and the Hamiltonian evolution. Indeed the dichotomy between the time reversal invariant Schrödinger equation and the longitudinal relaxation time T_1 which characterizes a dissipative irreversible phenomenon is enlightened by the description of the longitudinal relaxation phenomenon as due to the competition of a dissipative process and a non dissipative one. In the experimental condition, $|\hbar\omega| \ll K\theta$, the value of T_1 is mainly determined by the non dissipative mechanism described by the Schrödinger equation.

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REFERENCES

[1] F. Bloch, Phys. Rev. *70*, 460 (1946).
[2] N. Bloembergen, E. M. Purcell and R. V. Pound, Phys. Rev. *73*, 679 (1948)
[3] F. Bloch and R. K. Wangness, Phys. Rev. *89*, 728 (1953).
[4] D. Wolf, *Spin-temperature and nuclear-spin relation in matter*, Clarendon Press, Oxford 1979.
[5] A. Abragam, *The principles of nuclear magnetism*, Clarendon Press, Oxford, Section VIII.C, 1973.
[6] C. P. Slicher, *Principles of magnetic resonance*, Springer-Verlag, Section I.3, 1978.
[7] A. G. Redfield, IBM J. Res. Develop. *1*, 19 (1957).

[8] E. B. DAVIES, *Master equations, survey of rigorous results* in Rend. Sem. Mat. Fis. Milano (1977).
[9] J. V. PULÈ, Comm. Math. Phys. *38*, 241 (1974).
[10] L. VAN HOVE, Physica *23*, 441 (1957).
[11] PH. A. MARTIN, *Modèles en mécanique statistique des processus irréversibles*, Lecture Notes in Physics *103*, Springer-Verlag, Section 3.2, 1979.
[12] A. ABRAGAM, Loc. cit. p. 274.
[13] L. VAN HOVE, Physica *21*, 517 (Section 10), (1955).
[14] A. KOSSAKOWSKI, Bull. Acad. Polon. Sci. Math. Astronom. Phys. *21*, 649 (1973).
[15] C. PIRON, *Foundation of Quantum Physics*, Benjamin, Reading, Mass., 1976.
[16] L. D. LANDAU and E. M. LIFSHITZ, Physik. Z. Sowjetunion *8*, 153 (1935), see also references 18 and 19.
[17] N. GISIN, J. Phys. *14A*, 2259 (1981).
[18] R. KUBO and N. HASHITSUME, Prog. Th. Phys. suppl. *46*, 210 (1970).
[19] A. KAWABATA, Prog. Th. Phys. *48*, 2237 (1972) and N. GISIN, Prog. Th. Phys. Lett. vol. 66, no. 6 (1981).
[20] E. L. HAHN, Phys. Rev. *77*, 746 (1950); *80*, 580 (1950).
[21] G. J. BÉNÉ, Pure and Applied chem. *32*, 67 (1972).
[22] F. SHIBATA, J. Phys. Soc. Japan, *49*, 15 (1980).
[23] A. G. REDFIELD, Phys. Rev. *98*, 1787 (1955).
[24] A. ALAOUI and G. LOCHAK, C. R. Acad. Sc., *280-B*, 589 (1975).
[25] N. GISIN, *Microscopic derivation of a class of non-linear Schrödinger like equations*, to appear in Physica A.
[26] G. LINBLAD, *A General H-Theorem for Quantum Stochastic Processes: Markovicity is equivalent to a monotone loss of information* Preprint KTH, S-10044, Stockholm (1979).
[27] G. J. BENE, *Base Phénéménologiques des échos de spins*, cours avancé de résonance magnétique, Université de Genève (1975).
[28] N. GISIN, *Dissipative Quantum Dynamics for Hamiltonians Periodic in Time*, UGVA-DPT 1981/11-324.