On the standard form of the Bloch equation

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Abstract

The requirement is often made in non-equilibrium statistical mechanics that a transport equation should be derived as that which governs the subdynamics relative to a (small) part of a (large) conservative dynamical system close to equilibrium. We show that such a requirement on the Markovian relaxation of a $\frac{1}{2}$-spin imposes that this process be described by a Bloch equation of a very specific form, which we call standard. We show that this reduced dynamics is quasi-free if, and only if, the relaxation time is maximally anisotropic.

The Bloch equation for a $\frac{1}{2}$-spin reads:

$$(d/dt)\,[\tau_i(t) - \varepsilon_j\,1] = \sum_{k=1}^{3} \lambda_{jk}\,[\tau_k(t) - \varepsilon_k\,1], \qquad j = 1, 2, 3, \tag{1}$$

with $\tau_j(0)$ being the usual Pauli matrices.

We say that this equation is **standard** if there exists a unitary transformation U on $\mathbb{C}^2$ such that $\sigma_j(t) = U\tau_j(t)U^{-1}$ satisfies

$$\begin{aligned} (d/dt)\,\sigma_1(t) &= -\lambda\,\sigma_1(t) - \omega\,\sigma_2(t), \\ (d/dt)\,\sigma_2(t) &= +\omega\,\sigma_1(t) - \lambda\,\sigma_2(t), \\ (d/dt)\,[\sigma_3(t) - \varepsilon\,1] &= -\mu\,[\sigma_3(t) - \varepsilon\,1], \end{aligned} \tag{2}$$

with $-1 < \varepsilon < 1$, ω real, and $0 \leqslant \mu \leqslant 2\lambda$.

Here ε is the equilibrium value $\langle\sigma_3\rangle$ of the component σ_3 of the spin, whereas $\langle\sigma_1\rangle = \langle\sigma_2\rangle = 0$; ω is the transverse frequency; there are only two relaxation times $T_\parallel = \mu^{-1}$ and $T_\perp = \lambda^{-1}$, which moreover satisfy the very remarkable relation $T_\parallel \geqslant T_\perp/2$.

Favre and Martin [6] seem to have been the first authors to argue that the Bloch equation would take this standard form whenever the $\frac{1}{2}$-spin system is 'weakly coupled' to a bath at 'high' temperature. More recently Gorini *et al* [7, 15] gave a *thermodynamical*, model-independent argument showing that if $T_j^{-1} = \lambda_j$ is the inverse relaxation time relative to the jth component of

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the spin, then $\lambda_j + \lambda_k \geqslant \lambda_l$ for all permutations (j, k, l) of the indices $(1, 2, 3)$. In particular, they pointed out that the standard Bloch equation (with $\lambda_1 = \lambda_2 = \lambda$ and $\lambda_3 = \mu$) fully describes the axially symmetric relaxation of a $\frac{1}{2}$-spin in a 'strong' magnetic field.

The purpose of the present note is to give an argument, which is both mathematically simple and physically general, to the effect that this standard form does in fact *always* occur in the non-equilibrium *statistical mechanics* of the approach to equilibrium; that it is valid for all finite temperatures, independently of the strength of the coupling with external forces, and independently of any specific Hamiltonian model. We impose only two restrictions. The first, also implicit in the works cited above, is that we are interested in a time-scale compatible with a *Markovian* regime, where the reduced evolution can be described by a linear differential equation of the first order in the time. The second is that the reduced description, as well as that of the conservative system, is at finite temperature.

Recent investigations [11, 13, 14] indicate that in the framework of (infinite) statistical mechanics, a *conservative dynamical system at finite temperature* is described, under quite general circumstances, by a triple $\{\mathfrak{N}, \psi, \alpha(\mathbb{R})\}$ where $\mathfrak{N}$ is a von Neumann algebra acting on a (separable) Hilbert space $\mathcal{H}$; ψ is a faithful normal state on $\mathfrak{N}$, given by $\langle \psi\,; N\rangle := (N\Psi, \Psi)$ for every $N \in \mathfrak{N}$, with Ψ a vector in $\mathcal{H}$, cyclic and separating with respect to $\mathfrak{N}$; α is a w^*-continuous group homomorphism from $\mathbb{R}$ to $\mathrm{Aut}(\mathfrak{N})$ with $\psi \circ \alpha(t) = \psi$ for all $t \in \mathbb{R}$. It should be noted (see, e.g., [2–4]) that in general $\alpha(\mathbb{R})$ is not necessarily to be assumed to coincide with the modular group $\Sigma(\mathbb{R})$ canonically associated to ψ by the KMS condition.

In this framework, the *reduced description* of a dynamical subsystem is defined from a triple $\{\mathfrak{M}, \mathcal{E}, i\}$ where $\mathfrak{M}$ is a von Neumann algebra; i is an injective $*$-representation of $\mathfrak{M}$ into $\mathfrak{N}$; and $\mathcal{E}$ is a faithful normal conditional expectation from $\mathfrak{N}$ onto $\mathfrak{M}$ such that $\mathcal{E} \circ i = \mathrm{id}$ and $\psi \circ i \circ \mathcal{E} = \psi$. The reduced description consists then of the triple $\{\mathfrak{M}, \phi, \gamma(\mathbb{R}^+)\}$ where $\phi := \psi \circ i$, and for each $t \in \mathbb{R}^+$: $\gamma(t) \equiv \mathcal{E} \circ \alpha(t) \circ i$.

Lemma. *Let $\{\mathfrak{M}, \phi, \gamma(\mathbb{R}^+)\}$ be the reduced description of a dynamical subsystem of the conservative dynamical system $\{\mathfrak{N}, \psi, \alpha(\mathbb{R})\}$. Then for every $t \in \mathbb{R}^+$, $\gamma(t)$ is a completely positive linear map from $\mathfrak{M}$ onto itself such that:*

(i) $\gamma(t)[1] = 1$;

(ii) $\phi \circ \gamma(t) = \phi$;

(iii) there exists a linear, completely positive map $\nu(t)$ of $\mathfrak{M}$ into itself such that for every pair A, B of elements of $\mathfrak{M}$, $\langle \phi\,; \gamma(t)[A]\, B\rangle = \langle \phi\,; A\, \nu(t)[B]\rangle$; and

(iv) with $\sigma(\mathbb{R})$ denoting the modular group canonically associated to ϕ by the KMS condition, $\sigma(s) \circ \gamma(t) = \gamma(t) \circ \sigma(s)$ for all $s \in \mathbb{R}$.

Proof. $\mathcal{E}$, $\alpha(t)$ and i are linear, completely positive and identity preserving; so are then $\gamma(t)$ and $\nu(t) := \mathcal{E} \circ \alpha(-t) \circ i$. Also

$$\phi \circ \gamma(t) = \psi \circ i \circ \mathcal{E} \circ \alpha(t) \circ i = \psi \circ \alpha(t) \circ i = \psi \circ i = \phi,$$

and

$$
\begin{aligned}
\langle\phi\,;\gamma(t)[A]\,B\rangle &= \langle\psi\circ i\circ\mathcal{E}\,;\alpha(t)\circ i[A]\,i[B]\rangle \\
&= \langle\psi\,;\alpha(t)\,[i[A]\,\alpha(-t)\circ i[B]]\rangle = \langle\psi\circ i\circ\mathcal{E}\,;i[A]\,\alpha(-t)\circ i[B]\rangle \\
&= \langle\phi\,;A\,\nu(t)[B]\rangle.
\end{aligned}
$$

Finally, (iv) follows as in [1, 8] by defining $S(t)$ [resp. $T(t)$] by $S(t)\,A\Phi := \gamma(t)[A]\,\Phi$ [resp. $T(t)\,A\Phi := \nu(t)[A]\,\Phi$]; checking that $S(t)* = T(t)$ follows from (iii); and by verifying that this latter result implies that $S(t)$ commutes with the modular operator Δ. □

We now say that the reduced description $\{\mathfrak{M},\phi,\gamma(\mathbb{R}^+)\}$ is **Markovian** if $\gamma\colon\mathbb{R}^+\to\mathrm{CP}(\mathfrak{M},\phi)$ is a semigroup homomorphism, i.e., $\gamma(s)\gamma(t)=\gamma(s+t)$ for all $s,t\in\mathbb{R}^+$.

Theorem. *If $\{\mathfrak{M},\phi,\gamma(\mathbb{R}^+)\}$ is a Markovian reduced description for a subsystem of a conservative dynamical system at finite temperature, if $\mathfrak{M}=\mathfrak{M}(2,\mathbb{C})$ and if ϕ is not a trace, then the time evolution $a\in\mathfrak{M}\mapsto A(t)\equiv\gamma(t)[A]\in\mathfrak{M}$ satisfies a standard Bloch equation.*

Proof. From ψ and i faithful follows that ϕ is faithful; there exists therefore an orthonormal basis in $\mathbb{C}^2$ such that ϕ is given by the density matrix $\rho := \exp(\beta B\sigma_3)/\mathrm{Tr}\exp(\beta B\sigma_3)$ with $0<\beta<\infty$, $B\neq 0$ real, and σ_3 the third Pauli matrix. Let L [resp. L_0] be the generator of $\gamma(\mathbb{R}^+)$ [resp. $\sigma(\mathbb{R})$] and let $a^* := (\sigma_1+i\sigma_2)/2$. One first checks easily that $L_0 = i[H_0,-]$ with $H_0=\omega_0\,a^*a$ and that L commutes with L_0. This implies that $L[a]=-\nu a$ and $L[a^*a]=-\mu(a^*a-\eta\,1)$ with μ, ν and η in $\mathbb{C}$. Upon making use of $\phi\circ\gamma(t)=\phi$ one gets $\eta=\langle\phi\,;a^*a\rangle$ and thus $0<\eta<1$. Since L is the generator of a continuous semigroup of completely positive maps on $\mathfrak{M}(2,\mathbb{C})$ it is 2-dissipative [10], i.e., for every $X\in\mathfrak{M}(2,\mathfrak{M}(2,\mathbb{C}))$: $D(L_2;X,X) := L_2[X^*X]-L_2[X^*]\,X-X^*\,L_2[X]$ must be positive. With

$$
X=\begin{pmatrix} a^*a & a^* \\ a & 0\end{pmatrix},
$$

it is now straightforward to check that L_2-dissipativity, together with the conditions we found earlier on L, implies $0\leqslant\mu\leqslant 2\lambda$ where $\lambda=\mathrm{Re}\,\nu$. Upon writing $\omega=\mathrm{Im}\,\nu$, and going back from the basis $\{1,a^*,a,a^*a\}$ in $\mathfrak{M}(2,\mathbb{C})$ to the basis $\{1,\sigma_1,\sigma_2,\sigma_3\}$ one obtains indeed the Bloch equation in standard form (2). □

Evans [5] introduced the notion of *quasi-free completely positive map*. In this connection, it is interesting to note that we know exactly when the standard Bloch equation corresponds to a quasifree evolution; the following result follows indeed immediately from the definition [5], and from the above theorem.

Corollary. *Let $\gamma(\mathbb{R}^+)$ be as in the Theorem. Its generator is then of the form $L=i[H,-]+L_1+L_2+L_3$ with $H=\omega\,a^*a$ and*

$$
L_j[A] = V_j^* A V_j - \tfrac{1}{2}\{V_j^*V_j, A\}\quad \textit{for all}\quad A\in\mathfrak{M}(2,\mathbb{C}),
$$

where $V_1=\nu_1 a$, $V_2=\nu_2 a^*$ and $V_3=\nu_3 a^*a$; and

$$
\mu=\nu_1^*\nu_1+\nu_2^*\nu_2,\qquad \nu=\tfrac{1}{2}(\nu_1^*\nu_1+\nu_2^*\nu_2+\nu_3^*\nu_3)+i\omega,\qquad \eta=\frac{\nu_1^*\nu_1}{\nu_1^*\nu_1+\nu_2^*\nu_2}\,.
$$

This evolution is quasi-free in the sense of [5] if and only if $\nu_3=0$, i.e., $\mu=2\lambda$.

Upon using an adaptation to the CAR of the technique developed in [4] for the CCR, one can construct explicitly a minimal quasi-free dilation $\{\mathfrak{N}, \psi, \alpha(\mathbb{R})\}$ for the maximally anisotropic case $\mu = 2\lambda$. In fact, a Hamiltonian model has been constructed [12] which, in the weak coupling limit, leads to such a quasi-free standard Bloch equation. It should nevertheless be emphasized that all the results obtained here are model-independent, and hence are of complete general validity within the algebraic framework for finite-temperature statistical mechanics outlined at the beginning of this note.

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