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Simple Derivation of the Bloch Equation

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It is shown how one can derive Bloch's induction equation from the equation of motion of the density matrix by coarse-graining in time. The relaxation of the magnetization is assumed to be due to a fluctuating magnetic field acting upon the spins. The derivation does not provide any new information but is sufficiently simple that it may be used as a lecture application of the density matrix.

I. INTRODUCTION

IN his discussion of nuclear magnetic resonance, Bloch[1] introduced the following equation of motion for the magnetization $\mathbf{M}$ of a substance

$$\frac{d\mathbf{M}}{dt}=\gamma[\mathbf{M}\times\mathbf{B}]-\frac{\mathbf{i}M_x+\mathbf{j}M_y}{T_2}-\frac{\mathbf{k}(M_z-M_0)}{T_1}. \quad (1)$$

It is assumed here that the applied magnetic field $\mathbf{B}$ consists of a steady field $\mathbf{B}_0$ along the z axis and an oscillating field $\mathbf{B}_1$ in the xy plane; $\mathbf{i}$, $\mathbf{j}$, and $\mathbf{k}$ are unit vectors along the x, y, and z directions; γ is the magnetogyric ratio ($\gamma=\mu/\hbar S$ for a spin-S particle with magnetic moment μ), M_0 is the equilibrium magnetization in the field B_0, and T_1 and T_2 are, respectively, the spin–lattice or longitudinal and the spin–spin or transverse relaxation times.

Andrew[2] has given a very simple, phenomenological explanation of the various terms of Eq. (1). To see this we assume now and in what follows that we are dealing with a system of N spin-$\frac{1}{2}$ particles interacting with their surroundings (the lattice or bath). If $\mathbf{S}_i$ is the spin vector of the spin i, the total magnetization will be given by the equation

$$\mathbf{M}=\sum_i \gamma\hbar\mathbf{S}_i=N\gamma\hbar\langle\mathbf{S}\rangle, \quad (2)$$

where $\langle\cdots\rangle$ denotes an average. If a field $\mathbf{B}$ is acting upon the spins, they will experience a torque and the classical equation of motion will be

$$d\hbar\mathbf{S}/dt=[\boldsymbol{\mu}\times\mathbf{B}] \quad (3)$$

or

$$\frac{d\mathbf{M}}{dt}=\gamma[\mathbf{M}\times\mathbf{B}], \quad (4)$$

leading to the first term on the right-hand side of (1). That the same relation also holds for a quantum-mechanical system follows then from Ehrenfest's theorem on the equation of motion of quantum-mechanical averages, provided we interpret the averages $\langle\cdots\rangle$ as proper quantum statistical averages.

If a spin-$\frac{1}{2}$ particle is placed in a steady magneticfield B_0, its spin energy will be $\mp\frac{1}{2}\hbar B_0$, depending on whether it is parallel or antiparallel to the field. At equilibrium the numbers of spins parallel (N_+) or antiparallel (N_-) to the field is given by the equation

$$N_\pm^{\text{eq}}=N\exp[\pm\tfrac{1}{2}\beta\gamma\hbar B_0]/2\cosh[\tfrac{1}{2}\beta\gamma\hbar B_0], \quad (5)$$

where β^{-1} is the absolute temperature multiplied by Boltzmann's constant. As for practically experimental situations $\frac{1}{2}\beta\gamma\hbar B_0\ll1$, we can replace (5) to a very good approximation by

$$N_\pm^{\text{eq}}=\tfrac{1}{2}N[1\pm\tfrac{1}{2}\beta\gamma\hbar B_0]. \quad (6)$$

As the magnetization of the system is given by the equation

$$M=\tfrac{1}{2}\gamma\hbar(N_+-N_-), \quad (7)$$

the equilibrium magnetization satisfies the equation

$$M_0=\tfrac{1}{4}\beta\gamma^2\hbar^2B_0. \quad (8)$$

Because of the interaction with the lattice, there are transitions from the parallel to the antiparallel position and vice versa. If $W_+(W_-)$ is the transition probability for the parallel (antiparallel) to change to the antiparallel

[1] F. Bloch, Phys. Rev. **70**, 460 (1946).
[2] E. R. Andrew, *Nuclear Magnetic Resonance* (University Press, Cambridge, England, 1955).

(parallel) position, we find

$$dN_{\pm}/dt = \pm W_-N_- \mp W_+N_+, \tag{9}$$

which leads to the following equation of motion for the magnetization:

$$dM/dt = \gamma\hbar(W_-N_- - W_+N_+). \tag{10}$$

At equilibrium, $dN_{\pm}/dt = 0$ so that we have from (9) and (6)

$$\frac{W_+}{W_-} = \frac{N_-^{\text{eq}}}{N_+^{\text{eq}}} = \frac{1-\frac{1}{2}\beta\gamma\hbar B_0}{1+\frac{1}{2}\beta\gamma\hbar B_0}, \tag{11}$$

or

$$W_{\pm} = W(1 \mp \tfrac{1}{2}\beta\gamma\hbar B_0). \tag{12}$$

The $W_{\pm}$ as transition probabilities are independent of $N_{\pm}$; the fact that W_- is larger than W_+ is because there are spontaneous transitions from a higher to a lower energy level in addition to the induced transitions which go either way with the same probability (compare the case of blackbody radiation). Substituting (12) into (10) and using (8) we find

$$dM/dt = -(M-M_0)/T_1, \quad T_1 = 1/2W, \tag{13}$$

which shows the nature of the last term on the right-hand side of (1).

To see the physical meaning of the remaining terms on the right-hand side of (1), we remind ourselves that the magnetic moment will precess around a magnetic field according to Eq. (3). As there is no steady field in the xy plane, there will be no nonvanishing magnetization in that plane but, due to fluctuations, at some moment there might occur a resultant moment in the xy plane. If all spins were precessing with the same frequency $\omega(=\gamma B)$ this nonvanishing moment would persist. However, apart from the field B_0 which is the same for all the spins, there will also be other fields B_{fl} acting upon the spins which are due to the magnetic moments of the other spins. The magnitude of those fields will be of the order of μ/r^3 (r: average distance apart of the spins) which is several orders of magnitude less than the applied field. These fields will fluctuate both in magnitude and in direction and we must thus expect that the fields acting upon the different spins will fluctuate by something of the order of B_{fl} and that therefore the precessional frequencies of the spins will vary by an amount $\Delta\omega \sim \gamma B_{\text{fl}}$. This would entail that after a period of the order $1/\Delta\omega$ the nonvanishing moment in the xy plane will have become zero. This is the origin of the terms with T_2.

Basing our derivation of the Bloch equation upon the idea that the relaxation is due to the presence of a fluctuating magnetic field, the origin of which we leave open, we assume as our basic spin-Hamiltonian the expression

$$\hat{H} = -\tfrac{1}{2}\gamma\hbar(\boldsymbol{\sigma}\cdot\mathbf{B}_0+\mathbf{B}_1+\mathbf{B}_{\text{fl}}), \tag{14}$$

where we have introduced the Pauli matrices,

$$\hat{\sigma}_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \hat{\sigma}_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \hat{\sigma}_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \tag{15}$$

to describe the spin vector of the spin-$\frac{1}{2}$ particle. The field $\mathbf{B}_0$ is a steady field which we assume to be much larger than the oscillating field $\mathbf{B}_1$ and the fluctuating field $\mathbf{B}_{\text{fl}}$. We assume that $\mathbf{B}_1$ contains the time as a factor $e^{i\omega t}$ and that $\omega \approx \omega_0 = \gamma\mathbf{B}_0$, that is, that we consider the resonance region. The fact that $\mathbf{B}_{\text{fl}}$ is a fluctuating field can be expressed by the equations

$$\lim_{T\to\infty} \frac{1}{T}\int_t^{t+T} B_{\text{fl}}(t')dt' = 0, \tag{16}$$

$$\lim_{T\to\infty} \frac{1}{T}\int_t^{t+T} dt'\int_t^{t'} dt'' B_{\text{fl}}^{\mu}(t')B_{\text{fl}}^{\nu}(t'') = \delta_{\mu\nu}k, \qquad \mu,\ \nu = x,\ y,\ z. \tag{17}$$

Equation (16) expresses the fact that the average value of the components of $\mathbf{B}_{\text{fl}}$ is zero, while the constant k measures for how long a period the field $\mathbf{B}_{\text{fl}}$ remembers what value it had earlier. If the correlation time—that is, the time over which the field retains its value—is τ_c, we expect k to be of the order of τ_c times the amplitude of the fluctuating field. The factor $\delta_{\mu\nu}$ in (17) expresses the independence of the various components of $\mathbf{B}_{\text{fl}}$.

II. DENSITY MATRIX[3]

In quantum statistical mechanics, the properties of a system are fully determined by the

[3] For a general discussion of density matrix theory see, for instance, D. ter Haar, Rept. Progr. Phys. **24**, 304 (1961) or D. ter Haar, *Elements of Thermostatistics* (Holt, Rinehart, and Winston, Inc., New York, 1966).

density matrix $\hat{\rho}$. Its equation of motion is

$$i\hbar(d\hat{\rho}/dt)=[\hat{H},\hat{\rho}]_-, \tag{18}$$

and the average value of a physical quantity, corresponding to an operator $\hat{G}$, is given by the equation

$$\langle G\rangle=\mathrm{Tr}\hat{\rho}\hat{G}. \tag{19}$$

From (18) and (19) it follows that the equation of motion of $\langle G\rangle$ is

$$i\hbar d\langle G\rangle/dt=\langle[\hat{G},\hat{H}]_-\rangle. \tag{20}$$

To illustrate the general theory we show how one can derive (4). The derivation we give here is for the spin-$\frac{1}{2}$ case, but it will be seen that it also holds for the general, spin-S case. If the spin is in a constant external field $\mathbf{B}$, the spin-Hamiltonian is

$$\hat{H}=-\tfrac{1}{2}\gamma\hbar(\boldsymbol{\sigma}\cdot\mathbf{B}), \tag{21}$$

and from (20) and (2) we get

$$\frac{d\mathbf{M}}{dt}=\tfrac{1}{2}N\gamma\hbar\frac{d\langle\boldsymbol{\sigma}\rangle}{dt}=\frac{N\gamma\hbar}{i\hbar}\langle[\boldsymbol{\sigma},\ -\tfrac{1}{2}\gamma\hbar(\boldsymbol{\sigma}\cdot\mathbf{B})]_-\rangle. \tag{22}$$

Using the commutation relations of the components of $\boldsymbol{\sigma}$, which in symbolic form can be written as follows,

$$[\boldsymbol{\sigma}\times\boldsymbol{\sigma}]=2i\boldsymbol{\sigma}, \tag{23}$$

we find from (22) that (4) holds.

III. COARSE GRAINING

Before deriving Eq. (1)—or at least an equation which resembles (1)—we must briefly discuss how it is possible to obtain an equation such as (1), which describes an irreversible approach to an equilibrium situation, starting from reversible equations of motion such as (18). This is one of the basic problems of statistical mechanics.[4] The irreversibility is obtained by an averaging or "course-graining" process. Many authors[5] have obtained (1) by using an ensemble average over both the variables. In the treatment discussed here[6] a coarse-graining in time is used instead. This means that we calculate $d\langle\boldsymbol{\sigma}\rangle/dt$ as follows:

$$\frac{d\langle\boldsymbol{\sigma}\rangle}{dt}=\frac{\langle\boldsymbol{\sigma}\rangle_{t+\Delta t}-\langle\boldsymbol{\sigma}\rangle_t}{\Delta t}=\frac{1}{\Delta t}\int_t^{t+\Delta t}\frac{d\langle\boldsymbol{\sigma}\rangle}{dt}dt'. \tag{24}$$

In (23), Δt is a time interval sufficiently short that the difference quotient is a good approximation to the differential quotient and sufficiently long that we can use Eqs. (16) and (17). This means that Δt must be much longer than τ_c. If the change in the system during Δt is to be small, Δt must satisfy the inequalities

$$\omega_0\Delta t\ll 1 \quad\text{and}\quad \omega\Delta t\ll 1, \tag{25}$$

which are the same in the resonance region. The two conditions on Δt can clearly only be satisfied, if

$$\omega_0\tau_c\ll 1, \tag{26}$$

a condition which corresponds to the extreme narrowing case[7] and which we assume to be satisfied.

For $d\langle\boldsymbol{\sigma}\rangle/dt$ in the last member of (24), we use (20). Let us now first of all consider the equation of motion for the density matrix. From (18) and (14) we have

$$i\hbar(d\hat{\rho}/dt)=-\tfrac{1}{2}\gamma\hbar[(\boldsymbol{\sigma}\cdot\mathbf{B}_0+\mathbf{B}_1+\mathbf{B}_{fl}),\hat{\rho}]_-, \tag{27}$$

which to a first approximation, neglecting the terms in $\mathbf{B}_1$ and $\mathbf{B}_{fl}$ is

$$d\hat{\rho}/dt=\tfrac{1}{2}i\gamma[(\boldsymbol{\sigma}\cdot\mathbf{B}_0),\hat{\rho}]_-, \tag{28}$$

which we can integrate as follows:

$$\hat{\rho}(t+\Delta t)=\exp[\tfrac{1}{2}i\gamma(\boldsymbol{\sigma}\cdot\mathbf{B}_0)\Delta t]\hat{\rho}(t)\times\exp[-\tfrac{1}{2}i\gamma(\boldsymbol{\sigma}\cdot\mathbf{B}_0)\Delta t], \tag{29}$$

and as $\omega_0=\gamma B_0$ we see that by virtue of (25) to a first approximation $\hat{\rho}$ does not change over the period Δt.

[4] See, for instance, D. ter Haar, Rev. Mod. Phys. **27**, 289 (1955), or R. Jancel, *Les Fondements de la Mécanique Statistique Classique et Quantique* (Gauthiers-Villars, Paris, 1962) (English translation to be published by Pergamon Press).

[5] R. K. Wangsness and F. Bloch, Phys. Rev. **89**, 728 (1953); F. Bloch, *ibid.* **102**, 104 (1956); **105**, 1206 (1957); A. G. Redfield, IBM J. Res. Develop. **1**, 19 (1957).

[6] The detailed calculations were made by S. Stenholm; see, S. Stenholm and D. ter Haar, Physica **32**, 136 (1966).

[7] A. Abragam, *Principles of Nuclear Magnetism* (Oxford University Press, London, 1961), p. 279.

Consider now the equation of motion for $\langle\boldsymbol{\sigma}\rangle$ and substitute it into (24). We then get, using (19), (20), and (14),

$$\frac{d\langle\boldsymbol{\sigma}\rangle}{dt}=\frac{1}{\Delta t}\frac{-i}{\hbar}\int_t^{t+\Delta t}\mathrm{Tr}\hat{\rho}\times[\boldsymbol{\sigma},\ -\tfrac{1}{2}\gamma\hbar(\boldsymbol{\sigma}\cdot\mathbf{B}_0+\mathbf{B}_1+\mathbf{B}_{\mathrm{fl}})]_-dt'. \quad (30)$$

As we have just seen, to a first approximation $\hat{\rho}$ is independent of t' so that the term involving $\mathbf{B}_0$ leads, just as in the evaluation of (22), to $\gamma[\langle\boldsymbol{\sigma}\rangle\times\mathbf{B}_0]$. As Δt satisfies (25), to the same approximation $\mathbf{B}_1$ is independent of t' and the term involving $\mathbf{B}_1$ thus leads to $\gamma[\langle\boldsymbol{\sigma}\rangle\times\mathbf{B}_1]$. These two terms combined thus give $\gamma[\langle\boldsymbol{\sigma}\rangle\times\mathbf{B}]$, that is, the first term on the right-hand side of (1). As far as the term with $\mathbf{B}_{\mathrm{fl}}$ is concerned, in the approximation where $\hat{\rho}$ is taken to be independent of t', it vanishes by virtue of (16), and we must go to the next approximation. In this approximation, we solve (27) as follows

$$\hat{\rho}(t')=\tfrac{1}{2}i\gamma\int_t^{t'}[(\boldsymbol{\sigma}\cdot\mathbf{B}_{\mathrm{fl}}(t'')),\hat{\rho}(t)]_-dt''+\hat{\rho}(t), \quad (31)$$

where we use the fact that the terms in $\mathbf{B}_0$ and $\mathbf{B}_1$ will not contribute [by virtue of (25)] and where we may in the second approximation neglect the time dependence of $\hat{\rho}$ in the integral. We get, therefore, from the term in $\mathbf{B}_{\mathrm{fl}}$ in (30), the following contribution to $d\langle\boldsymbol{\sigma}\rangle/dt$:

$$\begin{aligned}&\frac{i\gamma}{2\Delta t}\int_t^{t+\Delta t}dt'\ \mathrm{Tr}(\tfrac{1}{2}i\gamma)\\&\quad\times\int_t^{t'}[(\boldsymbol{\sigma}\cdot\mathbf{B}_{\mathrm{fl}}(t'')),\hat{\rho}(t)]_-[\boldsymbol{\sigma},(\boldsymbol{\sigma}\cdot\mathbf{B}_{\mathrm{fl}}(t'))]_-dt''\\&=\frac{-\gamma^2}{4\Delta t}\int_t^{t+\Delta t}dt'\int_t^{t'}dt''\ \mathrm{Tr}\hat{\rho}\\&\qquad\times[[\boldsymbol{\sigma},(\boldsymbol{\sigma}\cdot\mathbf{B}_{\mathrm{fl}}(t'))]_-,(\boldsymbol{\sigma}\cdot\mathbf{B}_{\mathrm{fl}}(t''))]_- \quad (32)\\&=-2\gamma^2k\langle\boldsymbol{\sigma}\rangle,\end{aligned}$$

where we have used (23) and (17).

Combining all results and using (2), we obtain thus the following equation of motion for $\mathbf{M}$

$$d\mathbf{M}/dt=\gamma[\mathbf{M}\times\mathbf{B}]-(\mathbf{M}/T), \quad (33)$$

with

$$T^{-1}=2\gamma^2k. \quad (34)$$

As k is of the order of $\tau_c|\mathbf{B}_{\mathrm{fl}}|^2$ which is smaller than $\tau_cB_0^2=(\omega_0\tau_c)^2/\gamma^2\tau_c$, we see that $T\gg\tau_c$, a condition which is, of course, necessary for the validity of our calculations.

IV. DISCUSSION

We see that we have derived a simplified form of the Bloch equation and the question arises whether we can improve our theory in such a way as to include two relaxation times as well as a nonvanishing equilibrium magnetization. It is easily seen that this is not possible in the simple-minded theory we have presented here. We only consider one cause for relaxation: the fluctuating magnetic field. We could artificially introduce in (17) three constants k_μ rather than one, and in that case, different relaxation times would occur. Also, different relaxation times appear when we extend the theory to higher powers of $\omega_0\Delta t$ (see the paper by Stenholm and ter Haar[6]).

A more serious shortcoming of the theory, however, is the absence of M_0. This should not surprise us, however, as we have described the influence of the surroundings by a classical field, while we are dealing with spin-$\frac{1}{2}$ particles. In other words, in describing the relaxation we have thus essentially considered the limit as $\hbar\to0$ and we see from (8) that this is equivalent to putting $M_0=0$. Moreover, we must bear in mind that the nonvanishing magnetization comes about because the spin system is kept at a constant temperature by the bath. In deriving Eq. (13) it was essential that there was a feedback from the spins to the lattice and as in our theory this feedback is of necessity absent, we cannot hope to recover M_0. The only way to remedy the absence of M_0 would thus be by introducing instead of the classical correlation functions of (17) quantum-mechanical correlation functions and at the same time either to take the spin–bath interaction into account in more detail or to impose the nonvanishing magnetization upon the system as a boundary condition in a way similar to what was done by Lamb and Scully for the case of lasers. This would, however, considerably complicate the theory and as the main object of the discussion given here was to present a relatively simple derivation of the Bloch equation, there does not seem to be much point in trying to improve this theory, if at the same time it becomes more complicated.

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Quantum-Mechanical Tunneling

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An elementary method is given for the exact determination of the quantum mechanical transmission and reflection coefficients for a rectangular one-dimensional potential barrier. The method also finds application in approximate solutions for multistep barriers.

THE method commonly used in calculating the transmission and reflection coefficients for a particle incident at a rectangular one-dimensional potential barrier, (see, e.g., Condon[1]) depends on solving the Schrödinger equation for the region within the barrier and on either side, and eliminating the two constants which were introduced in the solution for the region within the barrier. Solutions for barriers with several steps involve the elimination of two constants for each region of constant potential within the barrier. In all cases, the constants are eliminated by using the conditions for continuity of ψ and $d\psi/dx$ at the discontinuities in potential. The treatment to be found in modern books on the subject (e.g., Merzbacher,[2] and Dicke and Wittke[3]) is usually that for a symmetrical barrier and in some cases is only approximate.

The present method consists, firstly, in writing down the reflected and the transmitted components of an elementary wavefunction ψ incident at each discontinuity of potential to be found in the barrier. The resultant ψ wave in a region of interest is then calculated, following the principle of superposition, by summing in a geometric series the components resulting from multiple reflection and transmission. In this way, one arrives easily at the transmission and reflection coefficients for the barrier without the introduction of unnecessary constants and the necessity for their subsequent elimination. An approximate solution for the case of a multistep barrier is found by including only those terms of the series which are found to be of appreciable size.

The solution of the Schrödinger equation $H\psi=E\psi$ for a particle in a region of constant potential energy V may be written as

$$\psi=\exp(ikx), \tag{1}$$

where

$$k=[2m(E-V)]^{\frac{1}{2}}/h. \tag{2}$$

For $E>V$, k is real and the solution represents a complex harmonic wave traveling in the direction of increasing x; while if $E<V$, the physically meaningful solution for ψ is an exponentially decreasing real function of x. (For $E=V$, $\psi=1$, representing a stationary particle of undetermined position.) Thus, for the present purpose,

[1] E. U. Condon, Rev. Mod. Phys. **3**, 43–74 (1931).

[2] E. Merzbacher, *Quantum Mechanics* (John Wiley & Sons, Inc., New York, 1961), pp. 91–92.

[3] R. H. Dicke and J. P. Wittke, *Introduction to Quantum Mechanics* (Addison-Wesley Publ. Co., Inc., Reading, Mass., 1960), pp. 40–46.