The Bloch Equations

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Abstract. We consider a spinor interacting with a heat bath of harmonic oscillators in equilibrium and we prove that the phenomenological Bloch equations for time development are satisfied exactly if the spin is $\frac{1}{2}$ and to first order in the inverse temperature if the spin exceeds $\frac{1}{2}$.

§ 1. Introduction

In 1946 Bloch [1] proposed the differential equation

$$\frac{dM}{dt} = \gamma M \times H - \frac{M_1}{T_2} e_1 - \frac{M_2}{T_2} e_2 - \frac{(M_3 - M_0)}{T_1} e_3 \tag{1}$$

for the time dependence of the macroscopic nuclear polarization M(t)under the influence of an external magnetic field H. $\gamma = \mu/jh$ is the gyromagnetic ratio of the nuclei under consideration with magnetic moment μ and spin j. The constants T_1 and T_2 are the longitudinal and transverse relaxation times respectively. Later Bloch and Wangness [2] attempted to justify these phenomenological equations theoretically with the simplifying assumption that the nucleus under consideration reacts independently of the other nuclei. In this paper we consider a fully quantum mechanical model by replacing the electromagnetic field by an infinite heat bath of harmonic oscillators in equilibrium keeping the simplifying assumption in [2]. We show that if $j = \frac{1}{2}$, our model, described in § 2, satisfies an equation of the same form as (1) in the weak coupling limit if the time is rescaled; we find also that if j exceeds $\frac{1}{2}$, to first order in the inverse temperature the model satisfies an equation of the form of (1). In § 3 we obtain an equation for the time development of an observable while in § 4 we obtain the Bloch equations by taking the spin as the observable.

This work is very similar to [4] which considers a harmonic oscillator interacting with a heat bath of harmonic oscillators though in the latter, expressions are simpler due to the fact that the particle is of the same type as those of which the bath is composed. We have used the description of the infinite heat bath provided in [4].

§ 2. The Model

The description of an infinite heat bath of harmonic oscillators is well known [3, 4]. The Hamiltonian is given formally by

$$\tilde{H}_0 = \frac{1}{2} : \sum_{n=-\infty}^{\infty} p_n^2 + \sum_{n,m=-\infty}^{\infty} a_{m,n} q_m q_n :$$

where p_m , q_m are the canonical co-ordinates of the infinite heat bath. We suppose that $a_{mn} = a_{m-n}$ where a is a real symmetric positive definite sequence and that

$$\varrho(\theta) = \sum_{n=-\infty}^{\infty} a_n e^{in\theta} > 0 \quad \text{for} \quad \theta[0, 2\pi].$$

Then ϱ is a real analytic periodic function on $[0, 2\pi]$ with strictly positive minimum and maximum values and consequently the corresponding convolution operator C on \mathcal{H} , the space of square-summable complex sequences, is positive, bounded and invertible. We can find real numbers $C_1 \ldots C_N(C_r > 0)$ so that there is a unitary equivalence $V:\mathcal{H} \to \sum_{r=1}^N \oplus L^2(C_{r-1}, C_r)$ such that $C^{\frac{1}{2}}$ acts on $\sum_{r=1}^N \oplus L^2(C_{r-1}, C_r)$ as the usual multiplication operator

$$(C^{\frac{1}{2}}\psi)_{r}(x) = x \psi_{r}(x)$$
.

Let $\mathscr{F}(\mathscr{H})$ be the Bose Fock space over \mathscr{H} . Then we can realise \tilde{H}_0 , above, as the self-adjoint operator constructed on $\mathscr{F}(\mathscr{H})$ from $C^{\frac{1}{2}}$ on \mathscr{H} . For $h \in \mathscr{H}$ let $W_F(h)$ be the usual Weyl operators on Fock space satisfying

 $W_F(h_1) W_F(h_2) = \exp\{i/2 \, \mathcal{I}_m \langle h_1, h_2 \rangle \, W_F(h_1 + h_2)$ $e^{i\tilde{H}_0 t} W_F(h) e^{-i\tilde{H}_0 t} = W_F(e^{iC^{\frac{1}{2}}t} h) \, .$

The equilibrium state of the bath at the inverse temperature β is given by the generating functional

where $\mu(h) = \exp\left\{-\frac{1}{4} \|Th\|^2\right\}$ $T = \left(\coth\frac{\beta C^{\frac{1}{2}}}{2}\right)^{\frac{1}{2}}.$

and

It is more convenient in our case to change to another representation of the CCR in which $\mu(h)$ is given by the vacuum expectation of the Weyl operator W(h). This representation is given explicitly by Chaiken [5]. We shall denote this representation by $\{W_c, \Omega, \mathcal{H}_c\}$ where in fact $\mathcal{H}_c = \mathcal{F}(\mathcal{H}) \times \mathcal{F}(M)$, M being the closure of the range of $\left(\frac{T^2-1}{2}\right)^{\frac{1}{2}}$. Let R(h)

be the self-adjoint field operator corresponding to the Weyl operator $W_c(h)$ that is $W_c(h) = e^{iR(h)}$. Then it is straightforward to verify that

$$\langle \Omega, R(h_1) R(h_2) \Omega \rangle = \frac{1}{2} \left\{ \Re \left\{ \langle T^2 h_1, h_2 \rangle + i \operatorname{Im} \langle h_1, h_2 \rangle \right\} \right\}$$
 (2)

and that

$$\begin{split} &\langle \Omega, R(h_1) \dots R(h_{2m+1}) \Omega \rangle = 0 \; . \\ &\langle \Omega, R(h_1) \dots R(h_{2n}) \Omega \rangle \\ &= \frac{1}{2^n n!} \sum_{\sigma \in S_n} \prod_{i=1}^n \langle \Omega : R(h_{\sigma(2j-1)}) R(h_{\sigma(2j)}) : \Omega \rangle \end{split}$$

where :: means that the original order is preserved.

Define H_0 on \mathcal{H}_c by

$$H_0 = \tilde{H}_0 \otimes 1 - 1 \otimes \tilde{H}_0$$
.

Then as in the Fock representation for h in the domain of C,

$$e^{iH_0t}W_c(h)^{-iH_0t}=W_c(e^{iC^{\frac{1}{2}}t}h)$$
.

We shall take $\mathbb{C}^{2j+1} \otimes \mathcal{H}_c$ as the composite spinor-bath space with the Hamiltonian

$$\begin{split} H = \omega \, J_3 + H_0 + \lambda \{ J_- \, \psi^*(b) + J_+ \, \psi(b) \} + \lambda^2 \, \omega_0 \, J_3 &\equiv H_\lambda + \lambda \, H_1 \; , \\ H_\lambda = \omega \, J_3 + H_0 + \lambda^2 \, \omega_0 \, J_3 \\ H_1 = J_- \, \psi^*(b) + J_+ \, \psi(b) \; , \end{split}$$

where J is the spin operator acting on \mathbb{C}^{2j+1} and $J_{\pm} = J_1 \pm iJ_2, b \in \mathcal{H}$ gives the mode of the bath to which the spinor is coupled, $\psi^*(b)$ and $\psi(b)$ are the creation and annihilation operators corresponding to the Weyl operators, that is

$$\psi^*(h) = 2^{-\frac{1}{2}} \{ R(h) + iR(ih) \}$$

$$\psi(h) = 2^{-\frac{1}{2}} \{ R(h) - iR(ih) \}.$$

The operator H is a self-adjoint operator with the same domain as H_{λ} . Let $(Vb)_r = b_r$ r = 1, ... N. We shall require $\{b_r\}_{r=1}^N$ to be C^{∞} functions of compact support. We shall assume also that for some r

$$C_{r-1} < -\omega < C_r$$
 and $b_r(-\omega) \neq 0$.

This condition may be interpreted physically as in [4], that is that $-\omega$ should be one of the range of frequencies of the heat bath and that the interaction should couple the oscillator to that frequency.

The dynamics of the spinor is given in the Heisenberg picture by α_t ,

$$\langle y, \alpha_t(B) x \rangle = \langle y \otimes \Omega, e^{iHt} B \otimes 1 e^{-iHt} x \otimes \Omega \rangle$$

where B is a $2j + 1 \times 2j + 1$ self-adjoint complex matrix. This corresponds to taking the expectation with respect to the canonical equilibrium state of the bath of all expressions involving the bath. We want to follow the time evolution in the weak coupling limit. As λ approaches zero the diffusion becomes slower so that this must be done using re-scaled time. But in re-scaling the time that part of Hamiltonian which is independant of λ gives rise to oscillating terms so that we must work in the interaction picture. In this representation the dynamics of the spinor is given by

$$\tilde{\alpha}_t(B) = e^{-i\omega J_3 t} \alpha_t(B) e^{i\omega J_3 t}.$$

§ 3. Time Evolution in the Weak Coupling Limit

It is clear that we cannot obtain a closed expression for $\tilde{\alpha}_t(B)$. But we can expand $\tilde{\alpha}_t(B)$ in a perturbation series. Let

$$\beta_t(B) = e^{-i(\omega + \lambda^2 \omega_0)J_3t} \alpha_t(B) e^{i(\omega + \lambda^2 \omega_0)J_3t}$$

so that $\tilde{\alpha}_t(B) = e^{i\lambda^2 \omega_0 J_3 t} \beta_t(B) e^{-i\lambda^2 \omega_0 J_3 t}$.

Since Ω is invariant under H_0

$$\langle y, \beta_t(B) x \rangle = \langle y \Omega, e^{-iH_{\lambda}t} e^{iHt} B e^{-iHt} e^{+iH_{\lambda}t} \times \Omega \rangle$$

where we write $y\Omega$ for $y\otimes\Omega$ and B for $B\otimes 1$. With

$$U_{\lambda}(t) = e^{-iH_{\lambda}t}e^{iHt}, \langle y, \beta_t(B)x \rangle = \langle y\Omega, U_{\lambda}(t)BU_{\lambda}^*(t) \times \Omega \rangle.$$

For an operator C on $\mathbb{C}^n \otimes \mathcal{H}_c$ let D(t) $C = [H_1(t), C]$ where

$$\begin{split} H_1(t) &= e^{-iH_{\lambda}t} H_1 \, e^{iH_{\lambda}t} = J_- \, \psi^*(e^{it(\omega + \lambda^2 \omega_0 + C^{\frac{1}{2}})} b) \\ &+ J_+ \, \psi(e^{it(\omega + \lambda^2 \omega_0 + C^{\frac{1}{2}})} b) \, . \end{split}$$

Theorem 1.
$$\langle y, \beta_t(B) x \rangle = \sum_{k=0}^{\infty} (-i\lambda)^k \int_{t_1=0}^{t} \cdots \int_{t_k=0}^{t_{k-1}} dt_1 \dots dt_k$$

$$\cdot \langle y \Omega, D(t_1) \dots D(t_k) B \times \Omega \rangle, \qquad (3)$$

where the series on the right is uniformly convergent on $\{(\lambda, t) : t \lambda^2 = \tau\}$.

Proof. If θ is in the domain of H, then by [6]

$$U_{\lambda}(t)\theta = \theta - i\lambda \int_{s=0}^{t} H_{1}(s) U_{\lambda}(s)\theta ds.$$
 (4)

Now H has the same domain as H_{λ} . $e^{iH_{\lambda}t}\Omega$ is in the domain of H_{λ} and therefore in the domain of H, which means that $Be^{-iHt}e^{iH_{\lambda}t}\Omega$ or $BU^*(t)\Omega$ is in the domain of H.

Therefore by using (4)

$$\langle y, \beta_{t}(B) x \rangle = \langle y\Omega, BU_{\lambda}^{*}(t) x\Omega \rangle$$

$$-i\lambda \int_{s=0}^{t} \langle y\Omega, H_{1}(s) U_{\lambda}(s) BU_{\lambda}^{*}(t) x\Omega \rangle ds$$

$$= \langle y\Omega, Bx\Omega \rangle + i\lambda \int_{s=0}^{t} \langle y\Omega, BH_{1}(s) U_{\lambda}^{*}(s) x\Omega \rangle ds$$

$$-i\lambda \int_{s=0}^{t} \langle y\Omega, H_{1}(s) U_{\lambda}(s) BU_{\lambda}^{*}(t) x\Omega \rangle ds.$$

By repeating the process m times we obtain

$$\langle y, \beta_t(B)x \rangle = \sum_{k=0}^{m-1} (-i\lambda)^k \int_{t_1=0}^t \int_{t_2=0}^{t_1} \cdots \int_{t_k=0}^{t_{k-1}} dt_1 \dots dt_k$$

 $\langle y\Omega, D(t_1) \dots D(t_k)Bx\Omega \rangle + r_m$ where

$$r_m = (-1)^k (i\lambda)^m \sum_{k+l=m, k \le m-1} \int_{t_1=0}^t \int_{t_2=0}^{t_1} \cdots \int_{t_k=0}^{t_{k-1}} dt_1 \dots dt_k$$

$$ds_1 \dots ds_1 \langle y\Omega, H_1(t_1) \dots H_1(t_k) BH_1(s_1) \dots H_1(s_l) U_{\lambda}^*(s_l) x\Omega \rangle$$

$$+ (-i\lambda)^m \int_{t_1=0}^t \int_{t_2=0}^{t_1} \cdots \int_{t_m=0}^{t_{m-1}} \langle y\Omega, H_1(t_1) \dots H_1(t_m) U_{\lambda}(t_m) BU_{\lambda}^*(t) x\Omega \rangle$$

$$\cdot dt_1 \dots dt_m$$
.

We now prove that r_m vanishes as m tends to infinity which means that the series in (3) is equal to $\langle y, \beta_t(B)x \rangle$.

$$\begin{aligned} |\langle y\Omega, H_1(t_1) \dots H_1(t_k) B H_1(s_1) \dots H_1(s_l) U_{\lambda}^*(s_l) x \Omega \rangle| \\ &\leq ||x|| ||H_1(s_l) \dots H_1(s_1) B H_1(t_k) \dots H_1(t_1) y \Omega||. \end{aligned}$$

For $b \in \mathcal{H}$ let

$$G(b) = J_{-} \psi^{*}(b) + J_{+} \psi(b)$$

$$= 2\{J_{1} R(b) + J_{2} R(ib)\}$$

$$= 2 \sum_{i=1,2} J_{j} R(e^{i\pi/2(j-1)}b).$$

Therefore

$$\langle y\Omega, G(b_{1}) \dots G(b_{k}) BG(b_{k+1}) \dots G(b_{2m}) x\Omega \rangle$$

$$= 2^{m} \sum_{\substack{j_{1}=1,2\\j_{2m}=1,2\\j_{2m}=1,2\\}} \langle y, J_{j_{1}} \dots J_{j_{k}} BJ_{j_{k+1}} \dots J_{j_{1}} BJ_{j_{1+1}} \dots J_{j_{2m}} x \rangle$$

$$\langle \Omega, R(e^{i\pi/2'(j_{1}-1)}b_{1}) \dots R(e^{i\pi/2(j_{2m}-1)}b_{2m}) \cdot \Omega \rangle .$$
If $K = \max(\|J_{1}\|, \|J_{2}\|, \|B\|, \|x\|, \|y\|)$

$$|\langle y\Omega, G(b_{1})B \dots B \dots G(b_{2m}) x\Omega \rangle|$$

$$\leq 2^{m} K^{2m+6} \sum_{j_{1}=1,2} \langle \Omega, R(e^{i\pi/2(j_{1-1})}b_{1}) \dots R(e^{i\pi/2(j_{2m}-1)}b_{2m})\Omega \rangle .$$
 (5)

Now if α and β take the values 1 or i,

$$\begin{split} |\langle \Omega, R(\alpha e^{it(\omega + \lambda^2 \omega_0 + C^{\frac{1}{2}})}b) \, R(\beta e^{it'(\omega + \lambda^2 \omega_0 + C^{\frac{1}{2}})}b)\Omega \rangle| \\ & \leq \frac{1}{2} \, \|T^2 b\| \, \|b\| + \frac{1}{2} \, \|b\|^2 = M \ (\text{say}) \, . \end{split}$$

But
$$H_1(t) = G(e^{it(\omega + \lambda^2 \omega_0 + C^{\frac{1}{2}})}b)$$
 so that from (5)

$$|\langle y\Omega, H_1(t_1) \dots B \dots B \dots H_1(t_{2m}) x\Omega \rangle|$$

$$\leq K^{2(m+3)} 2^{2m} M^m \cdot \frac{(2m)!}{m!} = L^m \frac{(2m)!}{m!}$$

which gives

$$|r_m| \le t^m \lambda^m L^{m/2} 2^{m/2} \sum_{l+k=m} \frac{1}{(k! l!)^{\frac{1}{2}}}$$

which tends to zero as m tends to infinity. We still have to prove that the series in (3) is uniformly convergent in λ and t. From (5) and (2) we obtain

$$\begin{aligned} |\langle y\Omega, H_1(t_1) \dots H_1(t_j)BH_1(t_{j+1}) \dots H_1(t_{2n})x\Omega \rangle| \\ & \leq \frac{K^{2n+3} 2^n}{n!} \sum_{\sigma \in S_{2n}} \prod_{j=1}^n \theta(t_{\sigma(2j-1)} - t_{\sigma(2j)}) \end{aligned}$$

where
$$\theta(s) = \theta(-s) = \frac{1}{2} |z(s)| + |\zeta(s)|$$

 $z(s) = \langle b, e^{-isC^{\frac{1}{2}}} T^2 b \rangle e^{-is\omega}$ and $\zeta(s) = \langle b, e^{-isC^{\frac{1}{2}}} b \rangle e^{-is\omega}$.

Therefore

$$|\langle y\Omega, D(t_1) \dots D(t_{2n})Bx\Omega \rangle|$$

$$\leq 2^{3n} \frac{K^{2n+3}}{n!} \sum_{\sigma \in S_{2n}} \prod_{j=1}^{n} \theta(t_{\sigma(2j-1)} - t_{\sigma(2j)}).$$
(6)

Now

$$z(s) = e^{i\omega s} \sum_{r=1}^{N} \int_{-\infty}^{\infty} e^{ixs} \coth \beta \frac{x}{2} |b_r(x)|^2 dx$$

$$= \int_{-\infty}^{\infty} e^{ix} \coth \beta \frac{(x-\omega)}{2} \sum_{r=1}^{N} |b_r(x-\omega)|^2 dx.$$
(7)

Since b_r are C^{∞} functions of compact support and $C_r > 0$, z(s) lies in the Schwartz space \mathcal{S} . Similarly

$$\zeta(s) = \int_{-\infty}^{\infty} e^{ixs} \sum_{r=1}^{N} |b_r(x-\omega)|^2$$
 (8)

and lies in \mathcal{S} . Therefore $\int_{-\infty}^{\infty} \theta(s) ds < \infty$.

Combining (6) with Lemma 3 in the appendix we have

$$\lambda^{2n} \int_{t_{1}=0}^{t/\lambda^{2}} \cdots \int_{t_{2n}=0}^{t_{2n-1}} |\langle y\Omega, D(t_{1}) \dots D(t_{2n})Bx\Omega \rangle| dt_{1} \dots dt_{2n}$$

$$\leq 2^{3n} \frac{K^{2n+3}}{n!} \left(\int_{-\infty}^{\infty} \theta(s) ds \right)^{n} \cdot t^{n}$$

so that the series (3) is uniformly convergent.

Theorem 2. $\lim_{\lambda \to 0} \tilde{\alpha}_{\tau \lambda^{-2}}(B) = e^{-\tau \varrho} B$ where $\varrho B = \tilde{\varrho} B + i \omega_0 [J_3, B]$ and

$$\begin{split} \tilde{\varrho}B &= -\frac{1}{8\pi} \sum_{r=1}^{N} |b_r(-\omega)|^2 \left\{ ([J_1, [J_1, B]] + [J_2, [J_2, B]]) \coth \frac{\beta \omega}{2} \right. \\ &\left. - i(J_1[J_2, B] + [J_2; B]J_1 - J_2[J_1, B] - [J_1, B]J_2) \right\} \\ &\left. - \frac{1}{2} \int\limits_{0}^{\infty} ds \int\limits_{0}^{\infty} dx \sin xs \sum_{r=1}^{N} |b_r(x - \omega)|^2 \left\{ ([J_2, [J_1, B]] - [J_1, [J_2, B]]) \right. \\ &\left. \cdot \coth \beta \frac{(x - \omega)}{2} + i(J_1[J_1, B] + [J_1, B]J_1 + J_2[J_2, B] + [J_2, B]J_2) \right\}. \end{split}$$

Proof. Clearly as a consequence of (2) the odd terms on the series (3) do not contribute. Let us therefore look at the first even term of the series for $\beta_{\tau\lambda^{-2}}(B)$,

$$\lambda^2 \int_{t_1=0}^{\tau\lambda^{-2}} \int_{t_2=0}^{t_1} \langle y\Omega, D(t_1)D(t_2)Bx\Omega \rangle dt_2 dt_1.$$
 (9)

One can check that the integrand is equal to

$$\frac{1}{2} \left\{ \left\langle y, ([J_{1}, [J_{1}, B]] + [J_{2}, [J_{2}, B]]) x \right\rangle \mathcal{R}e(e^{i\lambda^{2}\omega_{0}(t_{1}-t_{2})}z(t_{1}-t_{2})) + \left\langle y, ([J_{2}, [J_{1}, B]] - [J_{1}, [J_{2}, B]]) x \right\rangle \mathcal{I}_{\mathcal{H}}(e^{i\lambda^{2}\omega_{0}(t_{1}-t_{2})}z(t_{1}-t_{2})) \right\} + \frac{i}{2} \left\{ \left\langle y, (J_{1}[J_{2}, B] + [J_{2}, B]J_{1} - J_{2}[J_{1}, B] - [J_{1}, B]J_{2}) x \right\rangle \right. \\
\left. \mathcal{R}e(e^{i\lambda^{2}\omega_{0}(t_{1}-t_{2})}\zeta(t_{1}-t_{2})) + \left\langle y, (J_{1}[J_{1}, B] + [J_{1}, B]J_{1} + J_{2}[J_{2}, B] + [J_{2}, B]J_{2}) x \right\rangle \\
\left. \mathcal{I}_{\mathcal{H}}(e^{i\lambda^{2}\omega_{0}(t_{1}-t_{2})}\zeta(t_{1}-t_{2})) \right\}.$$
(10)

Now

$$\lambda^{2} \int_{t_{1}=0}^{\tau\lambda^{-2}} \int_{t_{2}=0}^{t_{1}} e^{-i\lambda^{2}\omega_{0}(t_{1}-t_{2})} z(t_{1}-t_{2}) dt_{2} dt_{1}$$

$$= \lambda^{-2} \int_{t_{1}=0}^{\tau} \int_{t_{2}=0}^{t_{1}} e^{i\omega_{0}(t_{1}-t_{2})} z(\lambda^{-2}(t_{1}-t_{2})) dt_{2} dt_{1}$$

which according to Lemma 2 approaches $\tau \int_{0}^{\infty} z(s) ds$ as λ tends to zero. Similarly

$$\lambda^2 \int\limits_{t_1=0}^{\tau\lambda^{-2}} \int\limits_{t_2=0}^{t_1} e^{i\lambda^2 \omega_0(t_1-t_2)} \zeta(t_1-t_2) \, dt_2 \, dt_1 \to \tau \int\limits_0^\infty \zeta(s) \, ds \quad \text{as} \quad \lambda \to 0 \, .$$

Since $z \in \mathcal{S}$ and $z(-s) = \overline{z(s)}$, from (7)

$$\int_{0}^{\infty} \mathcal{R}e(z(s)) dx = \frac{1}{2} \int_{-\infty}^{\infty} z(s) ds$$

$$= \frac{-1}{4\pi} \coth \frac{\beta \omega}{2} \sum_{r=1}^{N} |b_{r}(-\omega)|^{2}.$$
(11)

Similarly

$$\mathcal{R}_e(\zeta(s)) ds = \frac{1}{4\pi} \sum_{r=1}^N |b_r(-\omega)|^2.$$
 (12)

Hence the expression (10) approaches $\tau \langle y, \tilde{\varrho} Bx \rangle$ as λ tends to zero. We now turn to terms of higher order and prove by induction on n that

$$\lambda^{2n} \int_{t_1=0}^{\tau\lambda^{-2}} \cdots \int_{t_{2n}=0}^{t_{2n}=1} \langle y\Omega, D(t_1) \dots D(t_{2n}) Bx\Omega \rangle dt_{2n} \dots dt_1$$
 (13)

tends to $\frac{\tau^n}{n!} \langle y, \tilde{\varrho}^n B x \rangle$ as λ tends to zero.

Since the integrand in (13) is of the form

$$\sum_{\sigma \in S_{2n}} \langle y, A_{\sigma} x \rangle f_1^{\sigma}(t_{\sigma(1)} - t_{\sigma(2)}) \dots f_n^{\sigma}(t_{\sigma(2n-1)} - t_{\sigma(2n)})$$
 (14)

where for each $\sigma \in S_n$ and each i, $1 \le i \le n$, $f_i^{\sigma} \in \mathcal{S}$, we deduce from Lemma 1 that only terms for which there is a k satisfying $\sigma(2k-1)=1$ and $\sigma(2k) = 2$ or satisfying $\sigma(2k-1) = 2$ and $\sigma(2k) = 1$, contribute to the limit of (13). That is, the only contribution comes from the term which couples t_1 and t_2 . Now

$$D(t_1) \dots D(t_{2n})B = H_1(t_1) H_1(t_2) X - H_1(t_1) X H(t_2)$$
$$- H_1(t_2) X H_1(t_2) + X H_1(t_2) H_1(t_1)$$

where $X(t_2 \dots t_{2n}) = D(t_3) \dots D(t_{2n})B$. Therefore this contribution to the limit of (13) must come from the term

$$\lambda^{2n} \int_{t_{1}=0}^{t\lambda^{-2}} \cdots \int_{t_{2n}=0}^{t_{2n}-1} dt_{2n} \dots dt_{1}$$

$$\frac{1}{2} \left\{ \left\langle y, ([J_{1}, [J_{1}, \overline{X}]] + [J_{2}, [J_{2}, \overline{X}]]) x \right\rangle \Re(e^{-i\lambda^{2}\omega_{0}(t_{1}-t_{2})} z(t_{1}-t_{2})) + \left\langle y, ([J_{2}, [J_{1}, \overline{X}]] - [J_{1}, [J_{2}, \overline{X}]]) x \right\rangle \Im(e^{-i\lambda^{2}\omega_{0}(t_{1}-t_{2})} z(t_{1}-t_{2})) \right\}$$

$$+ \frac{i}{2} \left\{ \left\langle y, (J_{1}[J_{2}, \overline{X}] + [J_{2}, \overline{X}] J_{1} - J_{2}[J_{1}, \overline{X}] - [J_{1}, \overline{X}] J_{1}) x \right\rangle \right.$$

$$\left. \Re(e^{i\lambda^{2}\omega_{0}(t_{1}-t_{2})} \zeta(t_{1}-t_{2})) + \left\langle y, (J_{1}[J_{1}, \overline{X}] + [J_{1}, \overline{X}] J_{1} + J_{2}, [J_{2}, \overline{X}] + [J_{2}, \overline{X}] J_{2}) x \right\rangle$$

$$\left. \Im(e^{i\lambda^{2}\omega_{0}(t_{1}-t_{2})} \zeta(t_{1}-t_{2})) \right\}$$
where

$$\langle y, \overline{X}(t_{3} \dots t_{2n}) x \rangle = \langle y\Omega, X(t_{3} \dots t_{2n}) x\Omega \rangle$$

$$= \lambda^{2n} \int_{t_{1}=0}^{\tau\lambda^{-2}} \dots \int_{t_{2n}=0}^{t_{2n-1}} dt_{2n} \dots dt_{1} F_{1}(t_{3} \dots t_{2n}) \mathcal{R}e(e^{-i\lambda^{2}\omega_{0}(t_{1}-t_{2})} z(t_{1}-t_{2}))$$

$$+ F_{2}(t_{3} \dots t_{2n}) \mathcal{I}_{m}(e^{-i\lambda^{2}\omega_{0}(t_{1}-t_{2})} z(t_{1}-t_{2})) + F_{3}(t_{3} \dots t_{2n})$$

$$\mathcal{R}e(\zeta(t_{1}-t_{2})e^{-i\lambda^{2}\omega_{0}(t_{1}-t_{2})})$$

$$+ F_{4}(t_{3} \dots t_{2n}) \mathcal{I}_{m}(e^{-i\lambda^{2}\omega_{0}(t_{1}-t_{2})} \zeta(t_{1}-t_{2})).$$

$$(16)$$

Now

$$\lambda^{2n} \int_{t_{1}=0}^{\tau\lambda^{-2}} \cdots \int_{t_{2n}=0}^{t_{2n-1}} dt_{2n} \dots dt_{1} F_{1}(t_{3} \dots t_{2n}) \mathcal{R}e(e^{-i\lambda^{2}\omega_{0}(t_{1}-t_{2})}z(t_{1}-t_{2}))$$

$$= \frac{1}{\lambda^{2}} \int_{t_{1}=0}^{\tau} \int_{t_{2}=0}^{t_{1}} dt_{1} dt_{2} \mathcal{R}e\left\{e^{-i\omega_{0}(t_{1}-t_{2})}z\left(\frac{t_{1}-t_{2}}{\lambda^{2}}\right)\lambda^{2(n-1)}\right\}$$

$$= \int_{t_{3}=0}^{t_{2}\lambda^{-2}} dt_{2n} \dots dt_{3} F_{1}(t_{3} \dots t_{2n}).$$
(17)

By the induction hypothesis

$$\lambda^{2(n-1)} \int_{t_1=0}^{\tau} \int_{t_2=0}^{t_1 \lambda^{-2}} dt_3 \dots dt_{2n} F_1(t_3 \dots t_{2n})$$

tends to

$$\frac{t_2^{n-1}}{(n-1)!} \stackrel{1}{=} \{ \langle y, ([J_1, [J_1, \tilde{\varrho}^{n-1}B]] + [J_2, [J_2, \tilde{\varrho}^{n-1}B]]) x \rangle \}$$

as λ tends to zero and from (14) and Lemma 3 one can see that (17) is bounded in modulus by a constant independent of λ so that from Lemma 2 it follows that the expression in (16) tends to

$$\int_{0}^{\infty} \Re(z(s)) ds \int_{t_{2}=0}^{\tau} \frac{t_{2}^{n-1}}{(n-1)!} \frac{1}{2} \{ \langle y, ([J_{1}, [J_{1}, \tilde{\varrho}^{n-1}B]]) + [J_{2}, [J_{2}, \tilde{\varrho}^{n-1}B]]) x \rangle \}$$

$$= \frac{\tau^{n}}{n!} \int_{0}^{\infty} \Re(z(s)) ds \frac{1}{2} \{ \langle y, ([J_{1}, [J_{1}, \tilde{\varrho}^{n-1}B]]) + [J_{2}, [J_{2}, \tilde{\varrho}^{n-1}B]]) x \rangle \}.$$

Treating the other three terms similarly and using the expressions (7), (8), (11), (12) we see that (13) tends to $\frac{\tau^n}{n!} \langle y, \varrho^n Bx \rangle$. Since the convergence of the series (3) is uniform on $\{(\lambda, t): t = \tau \lambda^{-2}\}$,

$$\lim_{\lambda \to 0} \beta_{\tau \lambda^{-2}}(B) = e^{-\tau \tilde{\varrho}} B.$$

 $\underset{e^{iJ_3\tau\omega_0}(e^{-\tau\tilde{\varrho}}B)e^{-iJ_3\tau\omega_0}}{\text{Now}} (\beta_{\tau\lambda^{-2}}(B)) \, e^{-iJ_3\tau\omega_0} \qquad \text{which} \qquad \text{tends} \qquad \text{to} \\ e^{iJ_3\tau\omega_0}(e^{-\tau\tilde{\varrho}}B)e^{-iJ_3\tau\omega_0} \text{ or } e^{-(\varrho-\tilde{\varrho})}(e^{-\tau\tilde{\varrho}}B).$

By direct verification or by noting that

$$\langle y\Omega, D(t_1)D(t_2) [J_3, B] x\Omega \rangle = \langle y\Omega, [J_3, D(t_1)D(t_2)B] x\Omega \rangle,$$

one can show that $[\varrho - \tilde{\varrho}, \tilde{\varrho}] = 0$ so that the limit of $\tilde{\alpha}_{\tau \lambda^{-2}}(B)$ is $e^{-\tau \varrho} B$.

§ 4. The Bloch Equations

Let $\gamma_t(B)$ denote $\lim_{\lambda \to 0} \tilde{\alpha}_{t\lambda^{-2}}(B)$, that is $\gamma_t(B) = e^{-t\varrho} B$. Then

$$\frac{d\gamma_t}{dt}(B) = -e^{-t\varrho}\varrho B = -\gamma_t(\varrho B). \tag{18}$$

We now turn to the case when $B = J = (J_1, J_2, J_3)$. One can verify that

$$\varrho J_{3} = \frac{1}{T_{1}} \left\{ J_{3} + (J^{2} - J_{3}^{2}) \tanh \frac{\beta \omega}{2} \right\}.$$

$$\varrho J_{1} = \frac{1}{2T_{1}} \left\{ J_{1} - (J_{1} J_{3} + J_{3} J_{1}) \tanh \frac{\beta \omega}{2} \right\}$$

$$- J_{2} H_{\text{eff}} + \frac{1}{T_{2}} (J_{2} J_{3} + J_{3} J_{2}),$$

$$\varrho J_{2} = \frac{1}{2T_{1}} \left\{ J_{2} - (J_{2} J_{3} + J_{3} J_{2}) \tanh \frac{\beta \omega}{2} \right\}$$

$$+ J_{1} H_{\text{eff}} + \frac{1}{T} (J_{1} J_{3} + J_{3} J_{1}),$$
(19)

where

$$\frac{1}{T_1} = \frac{-1}{4\pi} \sum_{r=1}^{N} |b_r(-\omega)|^2 \coth \frac{\beta \omega}{2}$$

$$H_{\text{eff}} = \omega_0 + \frac{1}{2} \int_0^\infty ds \int_{-\infty}^\infty ds \sin ds \sum_{r=1}^{N} |b_r(x-\omega)|^2 \coth \frac{1}{2} \beta(x-\omega)$$

and

$$\frac{1}{T} = -\frac{1}{2} \int_{0}^{\infty} ds \int_{-\infty}^{\infty} dx \sin xs \sum_{r=1}^{N} |b_r(x-\omega)|^2.$$

If $j = \frac{1}{2}$, that is for spin $\frac{1}{2}$ particles, $J^2 - J_3^2 = \frac{1}{2}$ and $J_1 J_3 + J_3 J_1 = J_2 J_3 + J_3 J_2 = 0$ so that the Eqs. (19) reduce to, (20)

$$\varrho J_{3} = \frac{1}{T_{1}} \{J_{3} + J_{0}\} \quad \text{where} \quad J_{0} = \frac{1}{2} \tanh \frac{\beta \omega}{2}$$

$$\varrho J_{1} = \frac{1}{2T_{1}} J_{1} - J_{2} H_{\text{eff}}$$

$$\varrho J_{2} = \frac{1}{2T_{1}} J_{2} + J_{1} H_{\text{eff}}$$
(21)

so that we can write Eq. (18) vectorially as

$$\frac{d\gamma_t}{dt}(\mathbf{J}) = \gamma_t \left(\mathbf{J} \times H_{\text{eff}} - \frac{1}{T_1} \left\{ J_3 + J_0 \right\} \mathbf{e}_3 - \frac{1}{2T_1} J_1 \mathbf{e}_1 - \frac{1}{2T_1} J_2 \mathbf{e}_2 \right)$$
(22)

which has the same form as (1). For $j \ge 1$ we cannot make use of the Eqs. (20) so that the Eqs. (19) do not lead directly to the Bloch equations.

It is only for large temperatures that (19) give approximately the Bloch equations. Because of the singularity in $\frac{1}{T_1(\omega,\beta)}$ as β approaches 0 we suppose that for each β the mode to which the spinor interacts, $b(\beta)$, is such that $\frac{1}{T_1(\omega,\beta)}$ approaches a finite limit as β tends to zero. Then

$$e^{-t\tilde{\varrho}}B = e^{-t\varrho_0}B + O(\beta)$$

where

$$\varrho_{0}B = \frac{1}{2T_{1}(\omega,\beta)} ([J_{1},[J_{1},B]] + [J_{2},[J_{2},B]]) - 2\pi \int_{0}^{\infty} ds \int_{0}^{\infty} dx \sin xs$$

$$\frac{1}{T_{1}(\omega-x,\beta)} ([J_{2},[J_{1},B]] - [J_{1},[J_{2},B]]).$$

Therefore $e^{-t\tilde{\varrho}}\tilde{\varrho}B = e^{-t\tilde{\varrho}}\varrho_0B + e^{-t\varrho_0}(\tilde{\varrho}-\varrho_0)B$.

We now suppose that the state of the system is the uniform state,

$$\sigma = \frac{1}{2i+1}$$

and let

$$\delta_{t}(B) = \lim_{\lambda \to 0} \quad \text{trace} \quad (\sigma \alpha_{t \lambda^{-2}}(B)) = \frac{1}{2j+1} \lim_{\lambda \to 0} \quad \text{trace} \quad (\beta_{t \lambda^{-2}}(B))$$
$$= \frac{1}{2j+1} \quad \text{trace} \quad (e^{-t\tilde{\varrho}}B).$$

Then

$$\frac{d\delta_{t}(B)}{dt} = \frac{-1}{2j+1} \quad trace \quad (e^{-t\tilde{\varrho}}\tilde{\varrho}B)$$

$$= \delta_{t}(-\varrho_{0}B) - \frac{1}{2j+1} \quad trace \quad (e^{-t\varrho_{0}}(\varrho - \varrho_{0})B) + O(\beta^{2}).$$

Now $\varrho_0 A$ has zero trace so that trace $(e^{-t\varrho_0}A)$ = trace A = trace $(e^{-t\varrho}(\text{trace }A)I)$.

Thus

$$\frac{d\delta_t(B)}{dt} = \delta_t(-\varrho_0 B) - \operatorname{trace}\left((\tilde{\varrho} - \varrho_0) B\right) + O(\beta^2)$$

which for $B = J = (J_1, J_2, J_3)$ reduces to

$$\begin{split} \frac{d\delta_{t}}{dt}(J_{3}) &= \delta_{t} \left(\frac{-1}{T_{1}} \left\{ J_{3} + \operatorname{trace}(J^{2} - J_{3}^{2}) \tanh \frac{\beta \omega}{2} \right\} \right) + O(\beta^{2}) \,, \\ \frac{d\delta_{t}}{dt}(J_{1}) &= \delta_{t} \left(\frac{-1}{2T_{1}} \left\{ J_{1} - \operatorname{trace}(J_{1}J_{3} + J_{3}J_{1}) \tanh \frac{\beta \omega}{2} \right\} \right) \\ &+ J_{2}H_{\text{eff}} + \frac{1}{T} \quad \operatorname{trace} \quad \left((J_{2}J_{3} + J_{3}J_{2}) \right) + O(\beta^{2}) \,, \end{split} \tag{23}$$

$$\frac{d\delta_{t}}{dt}(J_{2}) &= \delta_{t} \left(\frac{-1}{2T_{1}} \left\{ J_{2} - \operatorname{trace}(J_{2}J_{3} + J_{3}J_{2}) \tanh \frac{\beta \omega}{2} \right\} \right) \\ &+ J_{1}H_{\text{eff}} + \frac{1}{T} \quad \operatorname{trace} \quad (J_{1}J_{3} + J_{3}J_{1}) + O(\beta^{2}) \,. \end{split}$$

Since trace $(J^2 - J_3^2) = (2/3)(2j+1)(j+1)j$ and trace $(J_1 J_3 + J_3 J_1) = \text{trace} (J_2 J_3 + J_3 J_2) = 0$ we can write the Eqs. (23) as

$$\frac{d\delta_{t}}{dt}(\mathbf{J}) = \delta_{t} \left(\mathbf{J} \times \mathbf{H}_{eff} - \frac{1}{T_{1}} \left\{ J_{3} + J_{0} \right\} \mathbf{e}_{3} - \frac{1}{2T_{1}} J_{1} \mathbf{e}_{1} - \frac{1}{2T_{1}} J_{2} \mathbf{e}_{2} \right) + O(\beta^{2})$$

with $J_0 = (2/3)(2j+1)(j+1)j$. This again is of the form of (1).

§ 5. Appendix

Lemma 1. Let $f_1, f_2, ... f_n$ be in \mathcal{S} and let σ be a permutation on $\{1, 2, ... 2n\}$ such that $|\sigma^{-1}(1) - \sigma^{-1}(2)| > 1$, then

$$\frac{1}{\lambda^{2n}} \int_{t_1=0}^{\tau} \int_{t_2=0}^{t_1} \cdots \int_{t_{2n}=0}^{t_{2n-1}} f_1\left(\frac{t_{\sigma(1)}-t_{\sigma(2)}}{\lambda^2}\right) \cdots \\
\dots f_n\left(\frac{t_{\sigma(2n-1)}-t_{\sigma(2n)}}{\lambda^2}\right) dt_{2n} \dots dt_1$$
(24)

tends to zero as λ tends to zero.

Proof. Let $S_{\tau} = \{t \in \mathbb{R}^{2n} : \tau > t_1 > \dots > t_{2n} > 0\}$ and define $\sigma : \mathbb{R}^{2n} \to \mathbb{R}^{2n}$ by

$$\sigma t = (t_{\sigma(1)}, t_{\sigma(3)}, \dots, t_{\sigma(2n-1)}, t_{\sigma(2)} \dots t_{\sigma(2n)}).$$

With the substitution $(s + \lambda^2 x, s) = \sigma t, s, x \in \mathbb{R}^n$ (24) becomes

$$\int_{s_1=0}^{\infty} \cdots \int_{s_n=0}^{\infty} \int_{x_1=-s_1\lambda^{-2}}^{\infty} \cdots \int_{x_n=-s_n\lambda^{-2}}^{\infty} f_1(x_1) \dots f_n(x_n) \chi_{S_{\tau}}(\sigma^{-1}(s+\lambda^2 x,s)) dx_1 \dots dx_n ds_1 \dots ds_n.$$
(25)

The modulus of (25) is bounded by

$$\int_{s_1=0}^{\tau} \cdots \int_{s_n=0}^{\tau} \int_{x_1=-\infty}^{\infty} \cdots \int_{x_n=-\infty}^{\infty} |f_1(x_1)| \dots |f(x_n)| \chi_{S_{\tau}}(\sigma^{-1}(s+\lambda^2 x, s))$$

$$dx_1 \dots dx_n ds_1 \dots ds_n$$

so that it is enough to prove that $\chi_{S_{\tau}}(\sigma^{-1}(s+\lambda^2 x,s))$ converges to zero pointwise as λ tends to zero.

Suppose that $\sigma^{-1}(1) = 2k - 1$, and that $\sigma^{-1}(2) = 2p - 1$ where $k \neq p$ and let $\sigma(2k) = l > 2$. By noting that $(\sigma^{-1}t)_{(2j-1)} = t_j$ and $(\sigma^{-1}t)_{(2j)} = t_{n+j}$, j = 1, ..., n, we see that if $s_k = s_p$ then $\sigma^{-1}(s + \lambda^2 x, s) \in S_\tau$ and therefore $\chi_{S_\tau}(\sigma^{-1}(s + \lambda^2 x, s)) = 0$.

Suppose now that $|s_k - s_n| \neq 0$ and choose λ such that

$$\min(\lambda^2 |x_p|, \lambda^2 |x_p - x_k|) < |s_p - s_k|.$$

Since

$$(\sigma^{-1}(s+\lambda^2 x, s))_1 = (\sigma^{-1}(s+\lambda^2 x, s))_{\sigma(2k-1)} = s_k + \lambda^2 x_k, (\sigma^{-1}(s+\lambda^2 x, s))_2 = (\sigma^{-1}(s+\lambda^2 x, s))_{\sigma(2k-1)} = s_k + \lambda^2 x_k,$$

and

$$(\sigma^{-1}(s+\lambda^2 x, s))_l = (\sigma^{-1}(s+\lambda^2 x, s))_{\sigma(2k)} = s_k$$
,

 $\sigma^{-1}(s+\lambda^2 x, s) \in S_{\tau}$ implies that $\tau > s_k + \lambda^2 x_k > s_p + \lambda^2 x_p > s_k$ which means that if $s_k - s_p > 0$

$$\begin{split} |s_k-s_p| &= s_k-s_p < \lambda^2 \, x_p < \lambda^2 |x_p| \quad \text{and that if} \quad s_k-s_p > 0 \\ |s_k-s_p| &= s_p-s_k < \lambda^2 (x_k-x_p) < \lambda^2 |x_k-x_p| \end{split}$$

both of which contradict our choice of λ . Thus for sufficiently small λ , $\sigma^{-1}(s+\lambda^2 x,s) \notin S_{\tau}$, as required. The other three possibilities corresponding to whether $\sigma^{-1}(1)$ and $\sigma^{-1}(2)$ are even or odd can be dealt with similarly.

Lemma 2. If $g \in \mathcal{S}$ and $|f(t_2, \lambda^2)| \leq M$ for all λ and for $t_2 \in [0, t]$, and $f(t_2, \lambda^2)$ tends to $f(t_2)$ as λ tends to zero then

$$\frac{1}{\lambda^2} \int_{t_1=0}^{t} \cdots \int_{t_2=0}^{t_1} e^{i(t_1-t_2)} g\left(\frac{t_1-t_2}{\lambda^2}\right) f(t_2,\lambda^2) dt_1 dt_2$$
 (26)

converges to

$$\int_{0}^{\infty} g(x) \, dx \, \int_{0}^{t} f(t_2) \, dt_2 \,. \tag{27}$$

Proof. We can rewrite the integral as

$$\int_{t_{2}=0}^{t} \int_{x=0}^{(t-t_{2})\lambda^{-2}} e^{i\lambda^{2}x} g(x) f(t_{2}\lambda^{2}) dx dt_{2}$$

$$\int_{t_{2}=0}^{t} \int_{x=0}^{\infty} g(x) F(x, t_{2}, \lambda^{2}) dx dt_{2}$$

$$F(x, t_{2}, \lambda^{2}) = 0 \quad \text{if} \quad x \ge \frac{t - t_{2}}{\lambda^{2}}$$

$$= e^{i\lambda^{2}x} f(t_{2}, \lambda^{2}) \quad \text{if} \quad x < \frac{t - t_{2}}{\lambda^{2}}.$$

Therefore

or

where

$$|(26) - (27)| \le \int_{t_2=0}^{t} \int_{x=0}^{\infty} |g(x)| |f(t_2) - F(x, t_2, \lambda^2)| dx dt_2.$$

Now $|f(t_2) - F(x, t, \lambda^2)| \le 2M$ and $f(t_2) - F(x, t_2, \lambda^2)$ tends to zero as λ tends to zero which means that $\{(26) - (27)\}$ approaches zero as λ tends to zero.

Lemma 3. If
$$\theta_{j}(s) \geq 0$$
 and $\int_{-\infty}^{\infty} \theta_{j}(s) ds < \infty$ for $j = 1, ..., n$ then
$$\sum_{\sigma \in S_{2n}} \frac{1}{\lambda^{2n}} \int_{t_{1}=0}^{t} \cdots \int_{t_{2n}=0}^{t_{2n-1}} \prod_{j=1}^{n} \theta_{j} \left(\frac{t_{\sigma(2j-1)} - t_{\sigma(2j)}}{\lambda^{2}} \right) dt_{1} \dots dt_{2n}$$

$$\leq t^{n} \prod_{i=1}^{n} \left[\int_{-\infty}^{\infty} \theta_{j}(s) ds \right]. \tag{28}$$

Proof. With the notation of Lemma 1, (28) is equal to

$$\int_{s_1=0}^{\infty} \cdots \int_{s_n=0}^{\infty} \int_{x_1=-s_1\lambda^{-2}}^{\infty} \cdots \int_{x_n=-s_n\lambda^{-2}}^{\infty} \prod_{j=1}^{n} \theta_j(x_j) \sum_{\sigma \in s_{2n}} \chi_{S_t}(\sigma^{-1}(s+\lambda^2 x,s))$$

$$ds_1 \dots ds_n dx_1 \dots dx_n.$$

Now if $\sigma \neq \tilde{\sigma}$ and $\sigma^{-1}(s + \lambda^2 x, s) \in S_t$ then $\tilde{\sigma}^{-1}(s + \lambda^2 x, s) \notin S_t$ and $\sigma^{-1}(s + \lambda^2 x, s) \in S_t$ implies that $s_i < t$ for $i = 1 \dots n$.

Therefore $\sum_{\sigma \in s_{2n}} \chi_{S_t}(\sigma^{-1}(s+\lambda^2 x,s)) \leq \chi_{\{y:0 < y_i < t\}}$ which means that (28) is less than or equal to

$$\int_{s_1=0}^{t} \cdots \int_{s_n=0}^{t} \int_{x_1=-\infty}^{\infty} \cdots \int_{x_n=-\infty}^{\infty} \prod_{j=1}^{n} \theta_j(x_j) ds_1 \dots ds_n dx_1 \dots dx_n$$

$$= t^n \prod_{j=1}^{n} \left(\int_{y=-\infty}^{\infty} \theta_j(y) dy \right).$$

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