Derivation of a time dependent Schrödinger equation as the quantum mechanical Landau–Lifshitz–Bloch equation

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Abstract
The derivation of the time dependent Schrödinger equation with transversal and longitudinal relaxation, as the quantum mechanical analog of the classical Landau–Lifshitz–Bloch equation, has been described. Starting from the classical Landau–Lifshitz–Bloch equation the transition to quantum mechanics has been performed and the corresponding von-Neumann equation deduced. In a second step the time Schrödinger equation has been derived. Analytical proofs and computer simulations show the correctness and applicability of the derived Schrödinger equation.

Keywords: spin dynamics, Landau–Lifshitz–Bloch equation, time dependent Schrödinger equation

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(Some figures may appear in colour only in the online journal)

1. Introduction

The Landau–Lifshitz equation [1] respectively Landau–Lifshitz–Gilbert (LLG) equation [2] are the most prominent equations describing spin dynamics. These equations are intensively used to describe any kind of magnetization dynamics in ferromagnetic, antiferromagnetic or ferrimagnetic materials with diameters from a few Ångström (atomistic description) to a micrometer length scale (micromagnetism). The Landau–Lifshitz respectively LLG equation describes the motion of a magnetic moment under the influence of an effective field $H_{\text{eff}}$ which causes a precessional motion and an additional friction (transversal relaxation) which leads to a parallel alignment of the magnetic moment and the effective field. During the relaxation the length of the magnetic moment is conserved. However, there are situations, e.g. during ultrafast reversal processes [3] or the dynamics near the critical temperature $T_c$ [4], where the description using the Landau–Lifshitz or LLG equation fails because the magnetization is not necessarily constant. This has been already pointed out by Callen in 1957 [5]: the general equation of motion of a ferromagnetic material has to be obtained by expanding the change of the magnetization $M$ in the three orthogonal vectors $M, (M \times H_{\text{eff}})$, and $M \times (M \times H_{\text{eff}})$.

$$\frac{dM}{dt} = -\gamma M \times H_{\text{eff}} - \gamma \alpha_0 M \times (M \times H_{\text{eff}}) - \gamma \alpha_1 (M \cdot H_{\text{eff}})M.$$  

(1)

While $\gamma = g\mu_B/\hbar$ is the gyromagnetic ratio, $\alpha_0$ and $\alpha_1$ are scalar functions of $M$, and $H_{\text{eff}}$. This equation is called Landau–Lifshitz–Bloch equation and without the last term ($\alpha_1 = 0$) equal to the Landau–Lifshitz equation. In many cases this equation can be found for the corresponding magnetic moment $m = MV$, where $V$ is the volume of the sample, or the normalized magnetic moment $S = m/|m|$. Depending on the characteristics of the sample $\alpha_0, \alpha_1$ and $H_{\text{eff}}$ will be different. In general $H_{\text{eff}}$ is given by the negative gradient of the Hamiltonian $H$ with respect to the magnetization or magnetic
moment e.g. $H_{\text{eff}} = -\nabla_{\mathbf{m}} H$, eventually modified by an additional stochastic noise term $\xi$ describe the influence of temperature [6] and further modification to take into account that the magnetization and most of the material parameters itself like the anisotropy are temperature dependent [7].

As for the effective field we can find for $\alpha_{\tau}$ and $\alpha_{l}$ different descriptions. The first proposal has been given by Callen [5]. The assumption there is that the dissipative process is dominated by spin wave transitions from ($\mathbf{k} = 0$) to ($\mathbf{k} = \infty$) where $\mathbf{k}$ is the wave vector of the spin wave. Callen deduces for $\alpha_{\tau}$ and $\alpha_{l}$ (equation (36) in [5]):

$$\alpha_{\tau} = \frac{1}{\gamma[H_{\text{eff}}]} \left[ \frac{1}{n_{0}} \frac{dn_{0}}{dt} + \frac{2\gamma h}{M} \frac{dn'}{dt} \right], \alpha_{l} = \frac{h}{M} \frac{dn'}{dt},$$

with $n' = \sum_{k=0}^{\infty} n_{k}$ and $n_{k} = a_{k}^{\dagger} a_{k}$, where $a_{k}^{\dagger}$ and $a_{k}$ are the Bose creation and annihilation operators.

Gehk et al propose the following functions (see equation (3.4) in [8]):

$$\alpha_{\tau} = \alpha, \quad \alpha_{l} = \frac{2\alpha \gamma k_{B} T}{m},$$

with $\alpha$ the Gilbert damping constant, $k_{B}$ the Boltzmann constant, $T$ the temperature and $m = |\mathbf{m}|$. The assumption behind this proposal is the temperature dependence of the magnetization.

In 1990, the same idea following, Garanin et al [9, 10] and Plefka [11, 12] proposed independently the following functions for $\alpha_{\tau}$ and $\alpha_{l}$ which can be found with just slightly changes in nearly all recent publications [4, 13–16] dealing with the Landau–Lifshitz–Bloch equation. Here in the writing of Xu and Zhang [15, 16]:

$$\alpha_{\tau} = \frac{m_{\text{eq}}}{\gamma \tau_{T} m[H_{\text{eff}}]}, \alpha_{l} = \frac{1}{\gamma \tau_{T}} \left[ \frac{m}{m[H_{\text{eff}}]} - \frac{m_{\text{eq}}}{m[H_{\text{eff}}]} \right],$$

$m_{\text{eq}} = |\mathbf{m}_{\text{eq}}|$ is the equilibrium magnetization and $\tau_{T}$ the relaxation time, similar to $T_{1}$ and $T_{2}$ in the case of the Bloch equation [17]. In the most cases the temperature dependence of $m_{\text{eq}}$ is for simplicity reasons taken into account via a mean field theory.

In all these cases, even if the derivation starts with a quantum mechanical description, the authors end up with the (semi-) classical LLB equation (equation (1)) where $\mathbf{M}$ is either the magnetization $\mathbf{M}$, the magnetic moment $\mathbf{m}$ or $\mathbf{S}$ or at least the spin expectation value $\langle \mathbf{S} \rangle$ of the spin operator $\mathbf{S}$. There are two reasons: The first reason can be seen in the Ehrenfest theorem [18], which says that the quantum mechanical expectation values behave classical. However, in the mean time it is known that the Ehrenfest theorem fails if the potential $V(x)$ is not linear: $\langle x^{n} \rangle \neq \langle x \rangle^{n}$ if $a \geq 2$. In the case of the Heisenberg model this means a classical behavior of the spin expectation values can be expected only if the terms of the Hamiltonian are linear in $\mathbf{S}_{n}$, where $n$ is the spin index [19]. This excludes especially crystalline anisotropies which are proportional to $S_{n}^{2}$.

The second reason is the fact that with the classical description larger system sizes as with a quantum mechanical description can be addressed. This can be explained with the fact that in the classical description the spins are local: every spin can be addressed separately and is affected by a local effective field. This makes it possible to simulate up to $10^{6}$ spins [6]. In the quantum mechanical description we are dealing with wave functions describing all spins at the same time. The corresponding matrices are huge and actual it impossible to address more than 64 spins $S = 1/2$ in maximum using exact diagonalization [20]. The larger system sizes can be seen as an advantage. On the other hand with a classical description quantum effects get lost. The comparison between classical and quantum spin dynamics shows that a similar dynamics can be found only in some special cases:

1. in the classical limit ($S \to \infty$, $h \to 0$, and $hS \to 1$)
2. only linear terms in $\mathbf{S}_{n}$, where $n$ is the lattice site, in the Hamilton operator $H$ [19]
3. in the case of no entanglement [21], e.g. if the system is described by a product state [22]
4. $|\psi\rangle$ corresponds to a superposition of the basis states $|S, m_{S}\rangle = |S, \pm S\rangle$ only: $|\psi\rangle = \psi_{+}|S, +S\rangle + \psi_{-}|S, -S\rangle$.

The last scenario (point 4.) is the case for:

(a) ferromagnetic spin waves: in this case $|\psi\rangle$ is approximately given by $|\psi\rangle \approx |S, \pm S\rangle$ [23, 24]
(b) coherent states where $|\psi\rangle$ is given by $|\psi\rangle = U(\theta, \phi)|S, \pm S\rangle$, $U(\theta, \phi)$ is a unitary transformation describing a rotation with the rotation angles $\theta$ and $\phi$ [25]
(c) a single spin with $S = 1/2$: in this case the wave function is always given by: $|\psi\rangle = \psi_{+}|S, +\rangle + \psi_{-}|S, -\rangle$ (Bloch sphere) [26]
(d) a single spin with $S > 1/2$ if the only contribution to $H$ is a external field in direction of the quantization axis (in the most cases $\mathbf{B} = B\mathbf{z}$). Perpendicular fields lead to quantum tunneling which can lead to states $|\psi\rangle = |S, m_{S}\rangle$, with $m_{S} = \pm S$ [21, 27–29].

As said before, the mentioned examples in the introduction using the Landau–Lifshitz–Bloch equation describing a classical or semiclassical spin dynamics which means they exclude quantum effects like entanglement. The spin dynamics with or without entanglement is totally different. The spin expectation values $\langle \mathbf{S} \rangle$ follow the same trajectories as the classical spin $\mathbf{S}$ only if there is no entanglement [21]. This together with the possibility to find quantum tunneling in anisotropic spin systems [27–29] are the main differences between the quantum mechanical description which takes these effects into account and the classical or a semiclassical description which do not take into account these effects.

To take into account these quantum effects it is necessary to describe the system fully quantum mechanical and to calculate the spin expectation values at the end. The goal of this publication is to give a time dependent Schrödinger equation which enables us to address all quantum effects and at the same time to take into account transversal and longitudinal relaxation similar to the (semi-) classical description using the LLB equation (equation (1)).
The outline of the publication is the following: In section 2 first the von Neumann equation will be introduced and after that the corresponding time dependent Schrödinger equation will be derived. The reason for this is the facts that the von Neumann equation is easier to understand and closer to the (semi-) classical description than the time dependent Schrödinger equation. However, the time dependent Schrödinger equation has a reduced numerical effort with respect to the von Neumann equation. For a Hilbert space of dimension $N$ the number of components of the corresponding wave function $|\psi\rangle$ is $N$ while the number of matrix components of the density operator matrix $\hat{\rho} = |\psi\rangle\langle\psi|$ is equal to $N^2$ [30]. In section 3 the derived time dependent Schrödinger equation will be proved analytical. Here the Hamiltonian is chosen in such a way that the we can expect a classical behavior of the spin expectation value $\langle \hat{S} \rangle$. This gives us a direct proof of the correctness of our description. Section 4 demonstrates the possibility to solve the derived time dependent Schrödinger equation under some more complex condition and the stability of the numerical calculation. The publication ends with a summary (section 5).

2. Equation of motion

In a recently published manuscript [21] it has been shown that the following von Neumann equation:

$$\frac{d\hat{\rho}}{dt} = -\frac{i}{\hbar} [\hat{\rho}, \hat{H}] = -\frac{i}{\hbar} \left( \hat{\rho} \hat{H} - \hat{H} \hat{\rho} \right)$$

and the corresponding self-consistent nonlinear Schrödinger equation:

$$i\hbar \frac{d}{dt} |\psi\rangle = \hat{H}|\psi\rangle - i\alpha_{\mu} (\hat{H} - \langle\hat{H}\rangle)|\psi\rangle,$$  \hspace{1cm} (3)

with $\langle\hat{H}\rangle = \langle\psi|\hat{H}|\psi\rangle$, and $\hat{H}$ an arbitrary Hermitian Heisenberg Hamiltonian, can be used to describe the dynamics of quantum spin. In both equations the first term on the right hand side describes a precessional motion and the second term a transversal relaxation.

It has been further shown that in the case of a spin $\hat{S}_n$, where $n$ corresponds to the $n$th spin at lattice site $r_n$, in an effective field $\mathbf{B}_n$ the trajectories of the spin expectation value $\langle\hat{S}_n\rangle = \langle\psi|\hat{S}_n|\psi\rangle$, where the wave function $|\psi\rangle$ has been calculated with equation (3), are similar to the trajectories of the classical spin $\mathbf{S}$ with dynamics described by the Landau–Lifshitz equation:

$$\frac{d(\mathbf{S}_n)}{dt} = \gamma (\mathbf{S}_n) \times \mathbf{B}_n - \gamma \alpha_{\mu} (\mathbf{S}_n) \times \langle(\mathbf{S}_n) \times \mathbf{B}_n\rangle.$$  \hspace{1cm} (4)

The only difference between both descriptions is the reversed sense of rotation of the precessional motion (first term: $\gamma \rightarrow -\gamma$).

However, there are two restrictions: equation (4) holds only if the Hamiltonian is linear in $\hat{S}_n$ (point 2 in the list before). This means as long as we can write $\hat{H} = -\sum_n \mathbf{B}_n \cdot \hat{S}_n$. Thereby, the effective field $\mathbf{B}_n$ itself can be a function of the surrounding spins $\hat{S}_m$, $m \neq n$, interacting with $\hat{S}_n$. Higher order contributions as uniaxial anisotropies or the biquadratic exchange (both quadratic in $\hat{S}_n$), will lead to additional terms of the order $\hbar$, which disappear in the classical limit $\hbar \rightarrow 0$ [19].

The second restriction is related to the entanglement. While equation (4) looks similar to the classical Landau–Lifshitz equation the trajectories of spin expectation values $\langle\hat{S}_n\rangle$ and the corresponding classical spin $\mathbf{S}_n$ are not necessary equal. The trajectories differ if entanglement plays a role. While in the (semi-) classical description the length of the spin $|\langle\hat{S}_n\rangle|$ only changes if there is an additional longitudinal relaxation as in the Landau–Lifshitz–Bloch equation the value $|\langle\hat{S}_n\rangle|$ can also change if there is no longitudinal relaxation in the equation of motion as in equation (4). Indeed, $|\langle\hat{S}_n\rangle|$ is a direct indicator for entanglement: $|\langle\hat{S}_n\rangle| = \hbar |\mathbf{S}|$ can be expected only if the system shows no entanglement [21]. In all the other cases we have $|\langle\hat{S}_n\rangle| < \hbar |\mathbf{S}|$. In a case of maximal entanglement as in the case of singlet state $\text{singlet} = \langle 1| - \langle 1|$ we have $|\langle\hat{S}_n\rangle| = 0$ [22].

To take the entanglement into account it is mandatory necessary that we solve the time dependent Schrödinger equation (3) or the corresponding von Neumann equation (2) and in a second step calculate the spin expectation values $\langle\hat{S}_n\rangle$. Equation (4) does not take into account the change of $|\langle\hat{S}_n\rangle|$ and therefore entanglement. This means the description where we solve equation (4) to calculate the trajectories of $\langle\hat{S}_n\rangle$ has to be considered as semiclassical. The resulting trajectories in this case will be the same as for the classical Landau–Lifshitz equation but not necessarily the same as in the case of the quantum mechanical description. The same is true for the Landau–Lifshitz–Bloch equation and the corresponding Schrödinger equation which we will derive in the following.

The first step will be to derive the corresponding von Neumann equation. As going from the Landau–Lifshitz equation (equation (4)) to the Landau–Lifshitz–Bloch equation (equation (1)) we have to add to the von Neumann equation (equation (2)) an additional longitudinal relaxation term which can be derived from the longitudinal relaxation term of the classical Landau–Lifshitz–Bloch equation: $\gamma \alpha_{\nu} (\mathbf{S} \cdot \mathbf{B}) \mathbf{S}$ (we assume $\mathbf{H}_{\text{eff}} = \mathbf{B}$) in the following way: we replace the classical spin $\mathbf{S}$ by the expectation value $\langle \hat{S} \rangle$ and correct the dimension. $\mathbf{S}$ is assumed to be dimensionless, but $\langle \hat{S} \rangle$ has the dimension of $\hbar$. We correct the dimension by an additional $1/\hbar$ to keep $\gamma\nu$ dimensionless:

$$-\gamma \alpha_{\nu} (\mathbf{S} \cdot \mathbf{B}) \mathbf{S} \rightarrow -2 \gamma \alpha_{\nu} \left( \frac{\gamma \hbar}{h} \mathbf{B} \cdot \langle \hat{S} \rangle \right) \langle \hat{S} \rangle = 2 \alpha_{\nu} \left( \frac{\hbar}{h} \langle \hat{H} \rangle \langle \hat{S} \rangle \right).$$

The same dimension problem also appears for $\alpha_{\mu}$. We have to correct the dimension there too. The additional factor 2 is needed to guarantee later a symmetric decoupling during the derivation of the time-dependent Schrödinger equation. Furthermore, it can be shown that this factor is needed to get the correct spin length (see supplementary material (stacks.iop.org/JPhysCM/28/396003/mmedia)). The next step is to write $\langle \hat{H} \rangle \langle \hat{S} \rangle$ as:
\[ (\hat{H})(\hat{S}) = \text{Tr}(\hat{\rho} \hat{H}) \text{Tr}(\hat{\rho} \hat{S}) = \text{Tr}(\hat{\rho} \hat{H} \hat{\rho} \hat{S}) \]  \hfill (5)

[21]. The relaxation term in terms of the density operator \( \hat{\rho} \) appears if we skip \( \text{Tr} \) and \( \hat{S} \) in equation (5): \( \text{Tr}(\hat{\rho} \hat{H} \hat{\rho} \hat{S}) = \hat{\rho} \hat{H} \hat{\rho} \hat{S} \).

Adding the resulting expression to equation (2) leads to the von Neumann equation containing transversal and longitudinal relaxation:

\[ \frac{d\hat{\rho}}{dt} = \frac{i}{\hbar} [\hat{\rho}, \hat{H}] - \frac{\alpha_\parallel}{\hbar}[\hat{\rho}, [\hat{\rho}, \hat{H}]] + 2 \frac{\alpha_\perp}{\hbar}(\hat{\rho} \hat{H} \hat{\rho}) \hat{\rho}. \]  \hfill (6)

To derive the corresponding Schrödinger equation we use the definition of the density operator in the case of a pure state:

\[ \hat{\rho} = |\psi\rangle \langle \psi|. \]  \hfill (7)

Inserting \( \hat{\rho} \) in equation (6) we find after some algebra the following two differential equations:

\[ \frac{d|\psi\rangle}{dt} = \left[ -\frac{i}{\hbar} \hat{H} |\psi\rangle - \frac{\alpha_\parallel}{\hbar} [\hat{\rho}, \hat{H}] - \langle \hat{\rho} | \hat{H} | \psi \rangle \right] |\psi\rangle \]
\[ + \frac{\alpha_\perp}{\hbar} \langle \psi | (\hat{\rho} \hat{H}) | \psi \rangle, \]  \hfill (8)

\[ |\psi\rangle \frac{d|\psi\rangle}{dt} = |\psi\rangle \left[ \langle \psi | \hat{H} \frac{i}{\hbar} - \frac{\alpha_\parallel}{\hbar} [\hat{\rho}, \hat{H}] - \langle \hat{\rho} | \hat{H} | \psi \rangle \right] \]
\[ + \frac{\alpha_\perp}{\hbar} \langle \psi | (\hat{\rho} \hat{H}) | \psi \rangle. \]  \hfill (9)

After multiplying equation (8) with \( |\psi\rangle \) from the right and dividing both sides by \( \langle \psi | \psi \rangle \) we find the Schrödinger equation:

\[ i\hbar \frac{d}{dt} |\psi\rangle = (\hat{H} - i\alpha_\parallel [\hat{\rho}, \hat{H}] - \langle \hat{\rho} | \hat{H} | \psi \rangle) |\psi\rangle. \]  \hfill (10)

The three terms on the right hand side are the same as in the case of the classical Landau–Lifshitz–Bloch equation. The first term describes an undamped precession. The second term provides a transversal and the last term a longitudinal relaxation. In the case of the Landau–Lifshitz–Bloch equation the transversal and longitudinal relaxation act separate, which means independent. However, a careful analysis shows that this is not the case for the recently proposed Schrödinger equation. This equation has a problem if we assume a spin oriented parallel to an external field \( \hat{B} = B \hat{z} \). In this case only the longitudinal relaxation should contribute and lead to a change the length of the spin. A transversal relaxation should take place. However, it can be shown that in this simple scenario both relaxation terms influence the change of the spin length. The influence of the transversal relaxation term can be seen with \( \hat{H} = -g\mu_B B \hat{S}_z / \hbar = -b \hat{\sigma}_z \) and \( |\psi(t)\rangle = \psi_0(t) \uparrow \) is \( \psi_0(t) \) of (1, 0)\(^T\) by:

\[ -i\alpha_\parallel [\hat{\rho}, \hat{H}] |\psi\rangle = ib \alpha_\parallel \psi_0(1, 0)^T \left( \begin{array}{c} 1 \\ 0 \end{array} \right). \]

This equation only becomes zero if \( |\psi_0|^2 = \langle \psi | \psi \rangle = 1 \), which means in the case of a normalized wave function. This is surely the case for \( \alpha_\parallel = 0 \) (no longitudinal relaxation), where we deal with normalized wave functions [21]. However, in the cases \( \alpha_\parallel > 0 \) we have a decrease or increase of the norm of the wave function \( n = \langle \psi | \psi \rangle \) due to the longitudinal relaxation. In this case we have \( 0 < \langle \psi | \psi \rangle \leq 1 \) and therefore a contribution of the transversal relaxation. This means we need a modification to fix this problem:

\[ i\hbar \frac{d}{dt} |\psi\rangle = (\hat{H} - i\alpha_\parallel [\hat{\rho}, \hat{H}] - \langle \hat{\rho} | \hat{H} | \psi \rangle) |\psi\rangle. \]  \hfill (11)

The modification is to add \( \langle \psi | \psi \rangle \) into the transversal relaxation term which leads to \( -i\alpha_\parallel [\langle \psi | \psi \rangle \hat{H} - \langle \hat{\rho} | \hat{H} | \psi \rangle] = 0 \) in any case. With this modification the transversal relaxation does not contribute in this constellation and we can expect the correct results.

### 3. Analytical proof

It is easy to show that the conjugate transposed equation corresponding to equation (11) is given by:

\[ -i\hbar \frac{d}{dt} |\psi\rangle = (\hat{H} + i\alpha_\parallel [\hat{\rho}, \hat{H}] - \langle \hat{\rho} | \hat{H} | \psi \rangle) |\psi\rangle. \]  \hfill (12)

Next, we are looking for the time development of a single spin in an external field \( \hat{B} \) described by:

\[ \mathbf{m} = \frac{\langle \hat{S} \rangle}{\hbar \mathcal{S}}, \]  \hfill (13)

with \( \langle \hat{S} \rangle = \langle \psi | \hat{S} | \psi \rangle \). Furthermore, we assume \( \mathcal{S} = 1/2 \) which means \( \hat{S} = \frac{1}{2} \hat{\sigma} \) and

\[ \mathbf{m} = \langle \psi | \hat{\sigma} | \psi \rangle. \]  \hfill (14)

Therefore, the time derivative of \( \mathbf{m}(t) \) is given by:

\[ \frac{d\mathbf{m}}{dt} = \langle \psi | \hat{\sigma} | \psi \rangle + \langle \psi | \hat{\sigma} | \psi \rangle, \]  \hfill (15)

where \( |\psi \rangle = \frac{d}{dt} |\psi\rangle \) and \( \langle \psi | = \frac{d}{dt} \langle \psi | \) are represented by the time dependent Schrödinger equation (11) and the corresponding conjugate transposed equation (12).

It is more convenient to look for one component of \( \mathbf{m} \), e.g. \( z \)-component \( m_z \). The time development of \( m_z \) is given by:

\[ \frac{dm_z}{dt} = \langle \psi | \hat{\sigma}_z | \psi \rangle + \langle \psi | \hat{\sigma}_z | \psi \rangle. \]  \hfill (16)

Due to the assumption \( \mathcal{S} = 1/2 \) the Hamilton operator of a single spin in an external field is given by:

\[ \hat{H} = \frac{-g\mu_B}{\hbar} \mathbf{B} \cdot \hat{\mathbf{S}} = \frac{-g\mu_B}{\hbar} \mathbf{B} \cdot \hat{\sigma}, \]  \hfill (17)

and \( \langle \hat{\rho} \rangle \) as:

\[ \langle \hat{\rho} \rangle = \frac{-g\mu_B}{\hbar} \mathbf{B} \cdot \mathbf{m}. \]  \hfill (18)
Inserting the equations of motions equation (11) and (12), together with equation (17) and (18) in equation (16) we get after some algebra:

\[
\frac{dm_z}{dt} = -\frac{i\mu_B}{2\hbar}(B_z(\langle |\hat{\sigma}_z| \rangle |\psi\rangle + B_z(\langle |\hat{\sigma}_z| \rangle |\psi\rangle) \\
+ \frac{\mu_B}{2\hbar}(\langle |\psi\rangle |\psi\rangle B_z(\langle |\hat{\sigma}_z| \rangle |\psi\rangle) \\
+ \frac{\mu_B}{2\hbar}(\langle |\psi\rangle |\psi\rangle B_z(\langle |\hat{\sigma}_z| \rangle |\psi\rangle) \\
+ \frac{\mu_B}{\hbar}B_z(\langle |\psi\rangle |\psi\rangle)^2 - \frac{\mu_B(\alpha + \alpha_1)}{\hbar}(B \cdot m) m_z. (19)
\]

Here, we have used the definition of \( m_z = \langle |\hat{\sigma}_z| \rangle \) and \( \hat{\sigma}_z = \hat{1} \), where \( \hat{1} \) is the identity matrix. The same is true for the other Pauli matrices: \( \hat{\sigma}_x = \hat{\sigma}_y = \hat{\sigma}_z = \hat{1} \). In equation (19) the \( \{\hat{\sigma}_x, \hat{\sigma}_y\} = \{\hat{\sigma}_y, \hat{\sigma}_z\} = \{\hat{\sigma}_z, \hat{\sigma}_x\} \) are commutators while the \( \{\hat{\sigma}_x, \hat{\sigma}_y\} = \{\hat{\sigma}_y, \hat{\sigma}_z\} = \{\hat{\sigma}_z, \hat{\sigma}_x\} \) are anticommutators. Independent of \( S \) the commutators are given by \( \{\hat{\sigma}_x, \hat{\sigma}_y\} = 2i\epsilon_{x,y,z} \hat{\sigma}_z \), where \( \epsilon_{x,y,z} \) is the Levi-Civita tensor. With changing \( S \), only the Pauli matrices change. This is not the case for the anticommutators \( \{\hat{\sigma}_x, \hat{\sigma}_y\} \). They are changing with \( S \). In the case of \( S = 1/2 \) the anticommutators are given by: \( \{\hat{\sigma}_x, \hat{\sigma}_y\} = 2\delta_{\alpha,\beta} \hat{1} \). However, this is not the case for \( S > 1/2 \). The general anticommutator relations for the spin operator \( \hat{S}_i \) are given by: \( \{\hat{S}_x, \hat{S}_y\} = 4iN\hat{S}_z \hat{1} + 2g_{\alpha\beta} g_{\gamma} \hat{S}_\gamma \), where \( g_{\alpha\beta} \) is the completely symmetric tensor of the Lie algebra sl(2N), and \( N \) the number of quantum level [31]. For \( S = 1/2 \) we have \( N = 2 \), and \( g_{\alpha\beta} = 0 \).

After working out the commutators and anticommutators we find with \( \gamma = \frac{\mu_B}{\hbar} \):

\[
\frac{dm_z}{dt} = \gamma[m_x B_y - m_y B_x] - \alpha_0 \gamma(B \cdot m) m_z \\
- \alpha_0 \gamma[m_x B_y - m_y B_x] - \alpha_0 \gamma(B \cdot m) m_z. (20)
\]

Here, the definitions for \( m_z = \langle |\hat{\sigma}_z| \rangle |\psi\rangle \) and \( m_y = \langle |\hat{\sigma}_y| \rangle |\psi\rangle \) have been used and the assumption that \( \hat{m} = \langle |\psi\rangle |\psi\rangle \langle \psi |\psi\rangle \) is normalized: \( \langle \hat{m} \cdot \hat{m} \rangle = m_z \). The last equation can be written in a more compact form using the vector triple product identity and \( \hat{m} = \hat{m}(\langle |\psi\rangle |\psi\rangle) \):

\[
\frac{dm_z}{dt} = \gamma[m_x B_y - m_y B_x] - \alpha_0 \gamma[m_x \times (m \times B)]_z \\
- \alpha_0 \gamma(B \cdot m) m_z. (21)
\]

The equations for \( m_x \) and \( m_y \) can be derived in a similar way and therefore, we finally get:

\[
\frac{dm_z}{dt} = \gamma[m_x B_y - m_y B_x] - \alpha_0 \gamma[m_x \times (m \times B)]_z \\
- \alpha_0 \gamma(B \cdot m) m_z. (22)
\]

This equation is identical to the classical Landau–Lifshitz–Bloch equation, if we ignore the sign problem of the precessional motion \( (\gamma \rightarrow -\gamma) \).

4. Numerical examples

In the last section 3 the proposal has been proved analytically for the case of a single spin with \( S = 1/2 \). We have seen that in this case the Schrödinger equation (equation (11)) leads to an equation for the expectation values \( m = \langle |\psi\rangle |\hat{S}| \rangle |\psi\rangle \) which is similar to the classical Landau–Lifshitz–Bloch equation. To strengthen this statement we present in this section computer simulations to show the correctness and the possibilities of the given description.

For the computer simulations we have solved the time dependent Schrödinger equation (equation (10)) numerical for different scenarios. In the following we set \( \hbar = 1 \) which means that the time will be in natural units: \( t_{\text{sim}} = h_{\text{real}} \). Under the assumption that we have energies in units of electronvolts the time scales of the simulations are in the femtosecond regime.

In the first scenario we assume a starting configuration of one spin with spin quantum number \( S = 1/2 \) oriented in \(+ x\)-direction: \( |\psi\rangle_{\text{init}} = (|\uparrow\rangle + |\downarrow\rangle)/\sqrt{2} \) and a length \( |\langle \hat{S}\rangle|/hS = 1 \). Furthermore, an external field in \(+ z\)-direction: \( B = B_x \hat{z} \). The scenario has been chosen in such a way that, following the description (point 4c), we can expect a behavior of the spin expectation value \( \langle \hat{S}\rangle \) similar to the dynamics of a classical spin \( S \) (except the different sense of rotation). The Hamiltonian of this scenario is given by:

\[
\hat{H} = -\frac{\mu_B}{\hbar} B \cdot \hat{S}. (23)
\]

Due to the relaxation terms the spin will relax into the direction of the external field and shrink to the equilibrium length \( |\langle \hat{S}\rangle|/hS = 0.7 \). For \( \alpha_0 \) and \( \alpha_1 \) we use the definitions:

\[
\alpha_0 = \alpha_0^0 \quad \text{and} \quad \alpha_1 = \alpha_1^0 \cdot \frac{|\langle \hat{S}\rangle| - |\langle \hat{S}\rangle|_{\text{eq}}|}{hS} . (24)
\]

with \( \alpha_0^0 = 0.02 \) and \( \alpha_1^0 = 0.04 \).

Figure 1 presents the relaxation process of a quantum spin (\( S = 1/2 \)) compared with a classical spin (\( S = \infty \)). In the later case we have solved the Landau–Lifshitz equation. In both cases the spin has been normalized and in the case of the classical spin we have used the double field value: \( 2B_z \) instead of \( B_z \). The doubling of the field value is necessary to make the quantum mechanical and the classical trajectories comparable. The reason for that are the different Zeeman energies \( q_{\text{m}} \): \( \hat{H} = -\mu_B B \cdot \hat{S} (\text{see equation (17)}) \) and cl.: \( \hat{H} = -\mu_B B \cdot \hat{S} \). Figure 1 clearly shows that in this case we find a perfect agreement between the classical trajectories \( S \) and quantum mechanical expectation values \( \langle \hat{S}\rangle \). The only difference appears for \( \langle \hat{S}\rangle \). Here, we see a phase difference of \( 180^\circ \) coming from the different rotation senses of the precession in the classical and quantum spin dynamics (\( \gamma \rightarrow -\gamma \) problem). However, the amplitude and frequency are are same.

To show the reliability of the given description we have performed more complex simulations. The next scenario has an initial configuration with a single spin with \( S = 1/2 \) oriented in \(+ z\)-direction with \( |\langle \hat{S}\rangle|/hS = 1 \). As before we assume an external magnetic field in \(+ z\) direction plus an additional Gaussian field pulse:

\[
B_x(t) = B_0 e^{-\left(\frac{t-n_{\text{tr}}}{\tau_W}\right)^2} \hat{x} . (25)
\]
in $x$-direction to excite the spin. Therefore, the Hamilton operator of this scenario is:

$$\hat{H} = -\frac{g\mu_B}{\hbar}(B_z(t)\hat{S}_z + B_x\hat{S}_x),$$

with $B_z(t)$ given by equation (25).

For the damping parameters $\alpha_{tr}$ and $\alpha_1$ the definitions given by Xu and Zhang [15, 16] have been used. Within their publication Xu and Zhang have proposed the following von Neumann equation:

$$\frac{d\hat{\rho}}{dt} = \frac{i}{\hbar}[\hat{H}, \hat{\rho}] = \frac{\hat{\rho} - \hat{\rho}_{eq}}{\tau_5},$$

which becomes with $\hat{H} = -\frac{g\mu_B}{\hbar}\hat{S}$ in the classical limit:

$$\frac{d\mathbf{m}}{dt} = \gamma\mathbf{m} \times \mathbf{B} - \frac{\mathbf{m} - \mathbf{m}_{eq}}{\tau_5},$$

$m_{eq}$ is the equilibrium magnetization and $\tau_5$ is a constant describing the strength of the relaxation.

Xu and Zhang have shown that with the identity: $\mathbf{B} = m^{-2}[(\mathbf{m} \cdot \mathbf{B})\mathbf{m} - \mathbf{m} \times (\mathbf{m} \times \mathbf{B})]$ this equation becomes:

$$\frac{d\mathbf{m}}{dt} = \gamma\mathbf{m} \times \mathbf{B} - \gamma\alpha_{tr}\mathbf{m} \times (\mathbf{m} \times \mathbf{B}) - \gamma\alpha_1(\mathbf{m} \cdot \mathbf{B})\mathbf{m},$$

which is identical to the Landau–Lifshitz–Bloch equation (1).

The damping parameters are given by:

$$\alpha_{tr} = \frac{m_{eq}}{\gamma\tau_5\mu_B},$$

as well as

$$\alpha_1 = \frac{1}{\tau_6}\left[\frac{\mathbf{m} \cdot \mathbf{B}}{\mathbf{m} \cdot \mathbf{B}} - \frac{m_{eq}}{\mu_B}\right].$$

To make equation (29) more general we replace $\tau_5$ in equation (30) by $\tau_{tr}$ and in equation (31) by $\tau_6$. $\tau_{tr}$ and $\tau_6$ are similar to $\tau_5$ constants. Furthermore, we replace the classical

Figure 1. Relaxation of a single spin ($S = 1/2$) with initial orientation in $+x$-direction and length $|\langle S \rangle|/\hbar S = 1$ in an external field in $+z$-direction and a final spin length $|\langle S \rangle|/\hbar S = 0.7$. The solid lines correspond to the quantum mechanical expectation values $\langle \hat{S}_z \rangle$ and the circles the classical trajectories $S$. (Simulation parameter: $\hbar = 1$, $\gamma\tau_{tr} = 10$, $\alpha_6^0 = 0.02$, $\alpha_1^0 = 0.04$.)

Figure 2. Longitudinal relaxation and combined transversal + longitudinal relaxation after a Gaussian field pulse at $t = 20$ for a quantum spin with $S = 1/2$, initial and final spin length $|\langle S \rangle|/\hbar S = 0.5$, $|\langle S \rangle|/\hbar S = 0.5$. (Simulation parameter: $\hbar = 1$, $\gamma\tau_{tr} = 10$, $\gamma\tau_{eq} = 46.54$, $\gamma\tau_{eq}^{-1} = 0.1$, $(\gamma\tau_{tr})^{-1} = 0.2$, $\tau_{tr} = 20$, $T_w = 0.02$.)

$m$, $m_{eq}$ by their quantum mechanical counterparts $\langle \hat{S} \rangle$, $|\langle S \rangle|$, and $|\langle S \rangle|_{eq}$. The results are the following two damping parameters:

$$\alpha_{tr} = \frac{\hbar}{g\mu_B\tau_{tr}}|\langle \hat{S} \rangle|/B,$$

and

$$\alpha_1 = \frac{\hbar}{g\mu_B\tau_{eq}}\left[\frac{|\langle S \rangle|}{\langle S \rangle} - \frac{|\langle S \rangle|_{eq}}{|\langle S \rangle|} \right].$$

Figure 2 shows the $x$ and $z$ components of the spin expectation value $\langle \hat{S} \rangle$ as well as the length $|\langle S \rangle|$ of a single spin in an external field oriented in $+z$ direction as function of time. The initial spin is oriented parallel to the external field and has a length of $|\langle S \rangle| = 1$. The equilibrium length $|\langle S \rangle|_{eq}$ has been chosen as $|\langle S \rangle|_{eq} = 0.5$. Therefore, and due to the fact that there is only the external field in $+z$ direction only the longitudinal relaxation contributes to the dynamics. Figure 2 clearly shows that the $z$ component of $\langle \hat{S} \rangle$ decays exponentially with the time until it reaches the equilibrium length $|\langle S \rangle|_{eq} = 0.5$. After reaching the equilibrium a Gaussian field pulse has been applied bringing the $z$ component $\langle \hat{S}_z \rangle$ close to zero. After the field pulse the spin relaxes back to equilibrium, but this time all three terms: precession, transverse and longitudinal relaxation contribute to the dynamics.

The last example shall demonstrate that the given description is not restricted to a single spin. In the following we assume two spins $S = 1/2$ antiferromagnetically exchange coupled and where the first spin can be manipulated by an external field:

$$\hat{H} = J\hat{S}_1 \cdot \hat{S}_2 + \frac{g\mu_B}{\hbar} \frac{B_z(t)\hat{S}_1^z}{\hbar^2}$$

(34)
The first term describes the antiferromagnetic exchange coupling with $J > 0$. The second term describes the coupling between first spin and an external field which is time dependent. This external field can be seen as a rough description of an electric current of an spin-polarized scanning tunneling microscope [32] or as an approximate description of the coupling to a magnetic island as described in [33]. In both cases we assume that we can switch the field and therefore the influence on and off.

In the case of a magnetic island it means that we e.g. increase the temperature above the Curie temperature $T_C$ to switch the field off and let the island cool down to switch it on again. We further assume that we start with a zero external field which increases with the time:

$$B_0(t) = B_0 \tanh[\kappa(t - t_0)] + B_0^0,$$

where $B_0^0 = 3.0$ and $\kappa = 0.5$ are constants describing the maximum field strength and the inclination with the time and $t_0 = 10$.

As long as the field is switched off ($B_0(t) > 0$) the spins are in the ground state configuration which means in this case the singlet state:

$$|\psi\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle).$$

With $B_0(t) > 0$ the first spin becomes stabilized and we find as final state:

$$|\psi\rangle = \sqrt{\langle \hat{S}_{\text{eq}} \rangle} |\uparrow\downarrow\rangle.$$  

$\langle \hat{S}_{\text{eq}} \rangle$ has been determined at the beginning of the calculation as part of the definition of $\alpha_1$ (see equation (24) or (33)). During the simulation for the damping terms the definition equation (24) with $\alpha_0 = 0.2$ and $\alpha_0^0 = 1.0$ has been used. Figure 3 shows the normalized spin expectation values $\langle \hat{S}_{\alpha} \rangle/hS$, $n \in \{1, 2\}$ of the first and second spin, as well as the time dependent external field $B_0(t)$. The zero expectation values $\langle \hat{S}_1 \rangle/hS = \langle \hat{S}_2 \rangle/hS = 0$ correspond to the initial singlet state (equation (36)) and $B_0^0 = 0$. With $B_0 > 0$ the expectation values $\langle \hat{S}_\alpha \rangle/hS$ increase / decrease to their final values $\pm \langle \hat{S}_{\text{eq}} \rangle$ corresponding to $|\psi\rangle_{\text{final}}$ given by equation (37) (classical Néel state). The other expectation values $\langle \hat{S} \rangle/hS$ and $\langle \hat{S}_\alpha \rangle/hS$ are zero for all times.

5. Summary

Within this publication the way how to derive the time dependent Schrödinger equation which can be seen as the quantum mechanical analog to the classical Landau–Lifshitz–Bloch equation has been demonstrated. The starting point is the Landau–Lifshitz–Bloch equation itself. From this equation the corresponding von Neumann equation can be deduced. And the von Neumann equation is the starting point to derive the corresponding time dependent Schrödinger equation. Therefore, with von Neumann equation and the time dependent Schrödinger equation we have two equations which can be seen as quantum mechanical analogs to the classical Landau–Lifshitz–Bloch equation. This opens the opportunity to extend the spin dynamics with transversal and longitudinal relaxation to the quantum regime and to compare the classical with the quantum spin dynamics.

The correctness of the time dependent Schrödinger equation and therefore indirectly also of the von Neumann equation has been proved analytical and with computer simulations. It has been shown that derived Schrödinger equation can lead to the same dynamics as the classical Landau–Lifshitz–Bloch equation. However, in the most scenarios we have to expect a different dynamics due to quantum effects. With the given description we have a general description of the quantum spin dynamics with transversal and longitudinal relaxation which is simple to understand. However, the given description will not give an insight to the microscopic processes of the damping. The energy gain and loss is introduced by phenomenological damping functions. This is the same in the case of the classical description. This can be seen as a disadvantage. On the other hand the Landau–Lifshitz–Gilbert as well as the Bloch equation became successful due to their simplicities and the fact that it is not necessary to know the underlying damping mechanism. In the given description this is the same and can be seen as an advantage. Furthermore, due to the fact that the damping parameters are no longer constant, but functions the given description is quite general. E.g. using the description of coherent states for $|\psi\rangle$ [25, 34] together with the definition for $\alpha_0$ and $\alpha_0^0$ in [35] reproduces the Landau–Lifshitz–Bloch equation which has been successful used to describe ultrafast magnetization dynamics measurements.

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