Quantum spin dynamics

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The classical Landau-Lifshitz equation has been derived from quantum mechanics. Starting point is the assumption of a non-Hermitian Hamilton operator to take the energy dissipation into account. The corresponding quantum mechanical time dependent Schrödinger, Liouville and Heisenberg equation have been described and the similarities and differences between classical and quantum mechanical spin dynamics have been discussed. Furthermore, a time dependent Schrödinger equation corresponding to the classical Landau-Lifshitz-Gilbert equation and two ways to include temperature into the quantum mechanical spin dynamics have been proposed.

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I. INTRODUCTION

The increasing need of faster and more powerful computer technology provides more and more new fields in magnetism like the field of magnonics [1] or the field antiferromagnetic spintronics [2,3]. In all these new fields as well as in the established areas like the ferromagnetic spintronics [4,5] the interest is mostly focused in the dynamics. To describe the dynamics of magnetic structures it is need to have an equation of motion. In the most cases this equation is the Landau-Lifshitz-Gilbert (LLG) equation [10]. Together with the Maxwell equations [11] this equation is the main equation of Micromagnetism [12], the field which describes the dynamics of nearly all magnetic devices of our daily life. There are more equations describing the dynamics in magnetism like the Bloch equation [13], the Landau-Lifshitz-Bloch equation [14,16] or the Ishimori equation [17]. However, the most important equation is the LLG equation.

The LLG equation was originally introduced by T. L. Gilbert in 1955 [18] as a reaction of the fact that the Landau-Lifshitz (LL) equation which was proposed by L. D. Landau and E. M. Lifshitz in 1932 contains a purely phenomenological damping term [19]. Gilbert’s original equation, the Gilbert equation, is an implicit differential equation. The explicit form of the Gilbert equation is similar to the original LL equation, therefore this equation is called Landau-Lifshitz-Gilbert (LLG) equation. Both equations contain two terms describing the dynamics of a single spin. The first term describes a precessional motion within an effective field and the second term a relaxation of the spin into the direction of the effective field. During this relaxation the energy will be reduced. The difference between the LL and LLG equation is the fact that in the LLG equation both terms, the precessional as well as the relaxation term are damped. In the original LL equation the precession term does not contain a damping constant, which means that this motion is not affected by the damping.

In 1956 Kikuchi [20] has shown that the LLG equation describes the correct physics while the LL equation fails in the limit of a huge damping. The reason is the missing damping for the precession in the LL equation.

The goal of this publication is to show that the LLG equation can be derived from quantum mechanics which gives new insight in the underlying physics and makes it possible to study the quantum-classical transition. Text books [21,22] as well as previous publications [23,24] describe only the derivation of the precessional term. In all cases, the damping term has been added later phenomenological. However, complete derivations using a classical description are known [10,26].

Furthermore, the paper discusses the difference between the classical and quantum mechanical description of the spin dynamics and shall correct the mistakes made in the former publication [27].

The manuscript is organized as follows. After this introduction, in Sec. II the equation of motion for a single spin will be derived and extended to a multi-spin system (Sec. III). In Sec. IV the results of the previous sections will be proved by numerical calculations and the last Sec. V describes two ways how to include temperature and quantum fluctuations into the computer simulations. The publication ends with a summary (Sec. VI).

II. EQUATION OF MOTION

It is a well know fact that a non-Hermitian Hamiltonian $\hat{H} = \hat{H} - i\lambda \hat{F}$, with $\hat{H}$ and $\hat{F}$ Hermitian operators and $\lambda \in \mathbb{R}_0^+$ a constant, lead to energy dissipation [28,29]. On the other hand such a Hamiltonian does not conserve the norm of the wave function $|\psi(t)\rangle = \exp(-i\hat{H}t)|\psi_0\rangle$:

$$n = \langle \psi(t)|\psi(t)\rangle = \langle \psi_0| e^{-2\lambda \hat{F}t} |\psi_0\rangle = e^{-2\lambda \langle \hat{F} \rangle t}. \quad (1)$$

However, the norm can be conserved by replacing $\hat{F}$ by $\hat{F} - \langle \hat{F} \rangle$. In this case we the following wave function:

$$|\psi(t)\rangle = e^{-i\hat{H}t} e^{-\lambda \langle \hat{F} \rangle t} |\psi_0\rangle, \quad (2)$$
which is conserved: \( n = 1 \). The corresponding Schrödinger equation is given by:
\[
\frac{d}{dt} \psi(t) = (\hat{H} - i\lambda(\hat{\Gamma} - \langle \hat{\Gamma} \rangle))\psi(t) .
\] (3)

The energy dissipation itself depends on \( \lambda \) and \( \hat{\Gamma} \). In the following we assume that \( \hat{\Gamma} \) is equal \( \hat{H} \) and therefore, \( \hat{H} = \hat{H} - i\lambda(\hat{H} - \langle \hat{H} \rangle) \). With this assumption the Schrödinger equation becomes [31]:
\[
\frac{d}{dt} \psi(t) = (\hat{H} - i\lambda[\hat{H} - \langle \hat{H} \rangle])\psi(t) .
\] (4)

We will see that this Schrödinger equation can be seen as the quantum mechanical analog of the classical Landau-Lifshitz equation, where \( \lambda \) is the damping constant.

Now, it is quite easy to show that this equation corresponds to the following Liouville (von Neumann) equation [27]:
\[
\frac{d\rho}{dt} = i[\hat{\rho}, \hat{H}] - \lambda[\hat{\rho}, [\hat{\rho}, \hat{H}]] .
\] (5)

We assume that the system is in a pure state therefore the density operator is given by:
\[
\hat{\rho} = |\psi(t)\rangle\langle \psi(t)| .
\] (6)

Equation (5) has already the form of the Landau-Lifshitz equation because the commutator \([\ , \ ]\) in the case of spin systems lead to a vector product.

So far, we have derived the quantum mechanical Liouville equation. The next step is the Heisenberg equation. Therefore, we concentrate ourselves first on the time dependence of the expectation value \( \langle \hat{\mathbf{S}} \rangle \):
\[
\frac{d}{dt} \langle \hat{\mathbf{S}} \rangle = \text{Tr} \left( \frac{d}{dt} \hat{\rho} \hat{\mathbf{S}} \right) .
\] (7)

Including the Liouville equation (5) in Eq. (7), written in the alternative form:
\[
\frac{d\hat{\rho}}{dt} = i[\hat{\rho}, \hat{H}] - \lambda \left( [\hat{\rho}, \hat{H}] + 2\hat{\rho}\hat{H}\hat{\rho} \right) ,
\] (8)

and get immediately the following differential equation:
\[
\frac{d}{dt} \langle \hat{\mathbf{S}} \rangle = -i\langle [\hat{\mathbf{S}}, \hat{H}] \rangle - \lambda \left( \langle [\hat{\mathbf{S}}, \hat{H}] \rangle + 2\langle \hat{H} \rangle \langle \hat{\mathbf{S}} \rangle \right) .
\] (9)

Here, the \([\ , \ ]\) is the anticommutator and we have used the fact that the trace is invariant under cyclic permutations. Furthermore:
\[
\text{Tr} \left( \hat{\rho} \hat{H} \hat{\rho} \hat{\mathbf{S}} \right) = \sum_m \langle \psi | \hat{\mathbf{S}} | \psi \rangle \langle \psi | \psi \rangle \langle \psi | \hat{\mathbf{S}} | \psi \rangle = \sum_m \langle \psi | \hat{\mathbf{S}} | \psi \rangle \langle \psi | \psi \rangle \langle \psi | \psi \rangle = \langle \psi | \psi \rangle \langle \psi | \psi \rangle = \langle \psi | \psi \rangle = \text{Tr} \left( \hat{\rho} \hat{H} \right) \text{Tr} \left( \hat{\rho} \hat{\mathbf{S}} \right) .
\] (10)

Then, the Heisenberg equation appears after replacing the expectation values \( \langle \hat{\mathbf{S}} \rangle \) by \( \hat{\mathbf{S}} \):
\[
\frac{d}{dt} \hat{\mathbf{S}} = -i[\hat{\mathbf{S}}, \hat{H}] - \lambda \left( [\hat{\mathbf{S}}, \hat{H}] + 2\langle \hat{H} \rangle \hat{\mathbf{S}} \right) .
\] (11)

Now, the Heisenberg equation (11) as well as the Liouville equation (5) can be used to derive the Landau-Lifshitz equation. Therefore, we have to insert these equations in (7) and to determine the traces. However, we need to know the exact form of the density operator \( \hat{\rho} \).

In the case of a Heisenberg spin system with spin quantum number \( S \) the density operator is given by the following multivector expansion [32]:
\[
\hat{\rho} = \frac{1}{2S+1} \mathbf{1} + \frac{1}{n_S} \sum_m \langle \hat{S}_m \rangle \hat{S}_m + \frac{1}{n_{2S}} \sum_{ml} \langle \hat{S}_{ml} \rangle \hat{S}_{ml} + \ldots
\] (12)

The first term is the Identity matrix which behaves under rotation like a scalar. The next term is the sum over the three spin matrices \( \hat{S}_x, \hat{S}_y, \hat{S}_z \). These matrices behave under rotation like a vector. The next term is the sum over multivectors \( \hat{S}_{ml} = \frac{1}{2}[\hat{S}_m, \hat{S}_l] + \frac{1}{3}S(S+1)\delta_{ml} \), (13)

and the next term (not shown) is the sum over trivectors \( \hat{S}_{mlk} \) and so on. All higher order terms have the same scheme as the previous ones but with higher order tensors. The prefactors \( n_S \) and \( n_{2S} \) are given by traces \( n_S = \text{Tr}(\hat{S}_x \hat{S}_x) \) and \( n_{2S} = \text{Tr}(\hat{S}_{xy} \hat{S}_{xy}) \) (these values only depend on the spin quantum number \( S \) and are independent of the direction \( a, b \in \{x, y, z\} \)). The prefactors of the higher expansion terms are similar.

This expansion is highly related to the magnetic multipolar expansion [33], and the number of terms depend on the spin quantum number \( S \). In the case \( S = 1/2 \) the expansion ends with the vector term
\[
\hat{\rho} = \frac{1}{2} \left( \mathbf{1} + \sum_m \langle \hat{\mathbf{S}}_m \rangle \hat{\mathbf{S}}_m \right) .
\] (14)

Here, \( \hat{\mathbf{S}}_m \) are the Pauli matrices. In the case \( S = 1 \) the expansion ends with the bivector term
\[
\hat{\rho} = \frac{1}{3} \mathbf{1} + \frac{1}{2} \sum_m \langle \hat{\mathbf{S}}_m \rangle \hat{\mathbf{S}}_m + \frac{1}{2} \sum_{ml} \langle \hat{\mathbf{S}}_{ml} \rangle \hat{\mathbf{S}}_{ml} ,
\] (15)

and in the case \( S = 3/2 \) the expansion ends with the trivector term, and so on.

After this small digression let us come back to the derivation of the Landau-Lifshitz equation. We have already noticed that it is necessary to insert the Liouville equation (5) or the Heisenberg equation (11) in Eq. (7) to derive a complete solvable equation for the expectation value \( \langle \hat{\mathbf{S}} \rangle \). The result is the following equation for the components of \( \langle \hat{\mathbf{S}} \rangle \) (\( n \in \{x, y, z\} \)):
\[
\text{Tr} \left( \frac{d}{dt} \hat{\rho} \hat{\mathbf{S}}_n \right) = i\text{Tr} \left( [\hat{\rho}, \hat{H}] \hat{\mathbf{S}}_n \right) - \lambda \text{Tr} \left( [\hat{\rho}, [\hat{\rho}, \hat{H}]] \hat{\mathbf{S}}_n \right) .
\] (16)
Inserting $\hat{\rho}$ in (10) and calculating the traces lead to an equation for $\langle \hat{S} \rangle$ which is similar to the Landau-Lifshitz equation if the Heisenberg Hamilton operator can be written as external field $\hat{H} = -\hat{B}_{\text{eff}} \cdot \hat{S}$.

During the calculation we can ignore the first term of $\hat{\rho}$ because the identity matrix $\hat{1}$ commutes with any operator and therefore all the commutators with the identity matrix become zero. Furthermore, we can see that only the vector term $\sum_m \langle \hat{S}_m \rangle \hat{S}_m$ participate to the differential equation of $\langle \hat{S} \rangle$. All the higher order expansion terms (bivector, trivector, $\ldots$) are not contributing. The reason for that is the conservation of the rank $k$ of a tensor under rotation. Now, each term of the multivector expansion has its own rank $k$. The expansion starts with the Identity matrix with rank $k = 0$ (scalar). The vector term has rank $k = 1$, the bivector rank $k = 2$, the trivector rank $k = 3$, and so on. The rank of each additional term increases by a factor 1.

Now, we assume that the trajectories of $\langle \hat{S} \rangle$ shall behave classical. This means that the length of the spin is conserved, and the spin only fulfills precession and relaxation. However, any precession as well as relaxation can be described as a rotation of the coordinate system and we have already mentioned that the rank of a tensor is conserved under such a rotation. This also means that the motion of $\langle \hat{S}_n \rangle$ is only described by the tensors $\hat{S}_n$ which are responsible for $\langle \hat{S}_n \rangle$:

$$\langle \hat{S}_n \rangle = \text{Tr}(\hat{\rho} \hat{S}_n) = \frac{1}{2S+1} \text{Tr}(\hat{S}_n) + \frac{1}{n_S} \sum_m \langle \hat{S}_m \rangle \text{Tr}(\hat{S}_m \hat{S}_n)_{m,0} + \frac{1}{n_{2S}} \sum_{ml} \langle \hat{S}_{ml} \rangle \text{Tr}(\hat{S}_{ml} \hat{S}_n)_{m,0} + \ldots + 0.$$  \tag{17}

The higher order expansion terms disappear due to

$$\text{Tr}\left(\hat{S}_n \hat{S}_{k'}\right) = n_{S_k} \delta_{\alpha \beta} \delta_{kk'}.$$  \tag{18}

$k$ and $k'$ are the rank of the tensor and $\alpha$ and $\beta$ its components: e.g. $S_3^3 = S_z$, or $S_4^2 = S_{zx}$.

Inserting the vector term $\sum_m \langle \hat{S}_m \rangle \hat{S}_m$ of $\hat{\rho}$ in Eq. (10) we find after some algebra:

$$\frac{d}{dt} \langle \hat{S}_n \rangle = \left(\langle \hat{S} \rangle \times \hat{B}_{\text{eff}}\right)_n - \lambda \left(\langle \hat{S} \rangle \times \left(\langle \hat{S} \rangle \times \hat{B}_{\text{eff}}\right)\right)_n.$$  \tag{19}

or written as complete vector:

$$\frac{d}{dt} \langle \hat{S} \rangle = \left(\langle \hat{S} \rangle \times \hat{B}_{\text{eff}}\right) - \lambda \langle \hat{S} \rangle \times \left(\langle \hat{S} \rangle \times \hat{B}_{\text{eff}}\right).$$  \tag{20}

This equation is similar to the classical Landau-Lifshitz (LL) equation \[19\]:

$$\frac{d}{dt} \hat{S} = \hat{S} \times \hat{B}_{\text{eff}} - \lambda \hat{S} \times (\hat{S} \times \hat{B}_{\text{eff}}).$$  \tag{21}

A complete evidence of the previous statement and details of the calculation can be found in the supplementary of this publication \[34\].

Now, it is known that the LL equation will lead to unphysical results in the limit of a large damping $\lambda \gg 1$. The reason is that the precessional motion is not influenced by the damping. The equation which holds in the limit of a large damping is the Landau-Lifshitz-Gilbert (LLG) equation. In the case of the LLG equation both terms the precessional term as well as the relaxation term are influenced by the damping. The easiest way to obtain the LLG equation from the LL equation is to make the following transformation of the time $t$: $t \to t/(1 + \lambda^2)$. The same transformation in the case of Schrödinger equation \[1\] leads to:

$$i(1 + \lambda^2) \frac{d}{dt} |\psi(t)\rangle = (\hat{H} - i\lambda[\hat{H} - (\langle \hat{H} \rangle)]|\psi(t)\rangle.$$  \tag{22}

This equation can be seen as the quantum mechanical analog of the LLG equation:

$$\frac{d}{dt} \langle \hat{S} \rangle = \frac{1}{1 + \lambda^2} \langle \hat{S} \rangle \times \hat{B}_{\text{eff}} - \frac{\lambda}{1 + \lambda^2} \langle \hat{S} \rangle \times (\langle \hat{S} \rangle \times \hat{B}_{\text{eff}}).$$  \tag{23}

The classical LLG equation itself appears by replacing the spin expectation value $\langle \hat{S} \rangle$ by the classical spin $\hat{S}$.

### III. SINGLE SPIN VS. MULTI-SPIN SYSTEM

This could be the end of the story. However, there is one point which has not been discussed so far. In the classical description we assume a constant length of the spin: $|\langle \hat{S} \rangle| = 1$. The LLG equation at zero temperature just describes a precessional motion resp. relaxation due to an effective field $\hat{B}_{\text{eff}}$. In the quantum mechanical description we deal with the expectation values $\langle \hat{S} \rangle = \langle \psi | \hat{S} | \psi \rangle$ which strongly depend on the wave functions $|\psi\rangle$. The absolute value $|\langle \hat{S} \rangle|$ of these expectation values have not necessarily to be constant: $|\langle \hat{S} \rangle| \leq nS$. Furthermore, due to the time dependence of the wave function $|\psi(t)\rangle$, $|\langle \hat{S} \rangle|$ is also time dependent. This means that in general we cannot expect an agreement of the classical with the quantum mechanical spin dynamics. On the other hand, we find in textbooks the statement that we can expect a classical behavior, at least for a single spin in an external field and without damping \[22\]. This textbook statement of a semiclassical description of the spin dynamics is not totally wrong. In the case of single spins and in the case of linear excitations of spin system in the ferromagnetic ground state (spin wave excitation) the classical and the quantum mechanical description can lead to the same trajectories if the Hamiltonian is linear in $\hat{S}_n$ ($n$ stands for the lattice site and not for a spin component. For details see \[22\]).

To specify the description let us first assume a single spin which is in a pure state $|\psi(t)\rangle$. In this case the
density operator is given by Eq. (25) and we find $\text{Tr}(\hat{\rho}^2) = \text{Tr}(\hat{\rho}) = 1$. For comparison, in the case of a mixed state:

$$\hat{\rho} = \sum_i p_i |\psi_i\rangle\langle\psi_i|$$ (24)

we find $\hat{\rho}^2 \neq \hat{\rho}$, therefore $\text{Tr}(\hat{\rho}^2) < \text{Tr}(\hat{\rho}) = 1$. Then, we can write $\text{Tr}(\hat{\rho}^2)$ in the case of a single spin with $S = 1/2$:

$$\text{Tr}(\hat{\rho}^2) = \frac{1 + |\langle\hat{\sigma}\rangle|^2}{2} \leq 1.$$ (25)

A similar formula can be given for higher spin quantum numbers ($S > 1/2$) due to Eq. (25). However, in these cases it is impossible to give a geometric plot as for $S = 1/2$ (Bloch sphere).

$\text{Tr}(\hat{\rho}^2) = 1$ appears in the case of a pure state which corresponds to $|\langle\hat{\sigma}\rangle| = 1$ resp. $|\langle S\rangle| = \hbar/2$. In the case of a spin ensemble in a mixed state we have $\text{Tr}(\hat{\rho}^2) < 1$ corresponding to $|\langle S\rangle| < \hbar/2$. This means, in the case of a single spin in a pure state the norm of the expectation value $|\langle S\rangle|$ is constant and the dynamics can become classical [see Eq. (24)].

In the case of a multi-spin system the wave function is described by a product of the eigenstates of the single spins:

$$|\psi\rangle = |S_1m_1\rangle \otimes |S_2m_2\rangle \otimes \ldots \otimes |S_Nm_N\rangle.$$ (26)

Such a state is called product state. For example the ferromagnet state is described by a product state: $|\text{FM}\rangle = |\uparrow\ldots\uparrow\rangle = |\uparrow\rangle \otimes |\uparrow\rangle \otimes \ldots \otimes |\uparrow\rangle$.

However, product states are normally not the general states of a magnetic system. The normal state in a quantum mechanical system with more than one spin is a superposition of the product states (26):

$$|\psi\rangle = \sum_{m_1 \ldots m_N} c_{m_1m_2\ldots m_N} (|S_1m_1\rangle \otimes |S_2m_2\rangle \otimes \ldots \otimes |S_Nm_N\rangle).$$ (27)

The product states in this case cannot be separated which that we cannot write $c_{m_1m_2\ldots m_N} = c_{m_1}c_{m_2} \ldots c_{m_N}$. This means that we have a correlation between the spins which do not exist in classical physics. This phenomenon is called entanglement and leads to the fact that in the case of a two entangled spins a measurement on the first spin also affects the second spin. The same is true for more than two spins. In this case the measurement on one spin affects all spins. Only in the case of a product state the subsystems are not correlated and can be separated, which means that the measurement of a single spin in this case only affect this spin and do not change the wave functions of the other spins as in the case of entanglement.

Now, the expectation value $\langle \hat{S}_n \rangle$, where $n$ is the lattice site, can be calculated similar to a single spin by:

$$\langle \hat{S}_n \rangle = \langle \psi|\hat{S}_n|\psi\rangle,$$ (28)

where $|\psi\rangle$ is given by (26) or (27), or by:

$$\langle \hat{S}_n \rangle = \text{Tr} \left( \hat{\rho} \hat{S}_n \right).$$ (29)

In the following we assume a pure state. Therefore, the density operator of our multi-spin system $\hat{\rho}$ is defined by $\hat{\rho} = |\psi\rangle\langle\psi|$

Alternatively we can calculate the expectation value $\langle \hat{S}_n \rangle$ with aid of the reduced density operator $\hat{\rho}_m$ [33]:

$$\langle \hat{S}_n \rangle = \text{Tr}_n \left( \hat{\rho} \hat{S}_n \right) = \text{Tr}_n \left( \hat{\rho}_m \hat{S}_n \right),$$ (30)

where $\text{Tr}_n$ is the partial trace over the sub Hilbert space $\mathcal{H}_n$ and $\text{Tr}_{j \neq n}$ the partial trace over all the other sub Hilbert spaces: $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \ldots \otimes \mathcal{H}_N$. The advantage of using the reduced density operator $\hat{\rho}_m$ is that we have to deal with smaller matrices, which reduces the numerical effort.

It is easy to verify that the reduced density operator $\hat{\rho}_m$ is given by:

$$\hat{\rho}_m = \sum_{m_n} p_{m_n} |S_n m_n\rangle\langle S_n m_n|.$$ (31)

Eq. (31) clearly shows that the reduced density operator corresponds to a mixed state, the $p_{m_n}$ are the probabilities to find the system in the state $|S_n m_n\rangle$, even if the complete system is in a pure state $\hat{\rho} = |\psi\rangle\langle\psi|$

In the case of the product state (26) the reduced density operator is given by $\hat{\rho}_m = |S_n m_n\rangle\langle S_n m_n|$. Here, the reduced density operator $\hat{\rho}_m$ as well as the density operator of the complete system $\hat{\rho} = |\psi\rangle\langle\psi|$ are pure.

The consequences are as long as the system is described by a product state we find: $\langle \langle \hat{S}_n \rangle \rangle = \hbar S$. However, as mentioned before the normal states are superposition states which are entangled and not product states. In these cases we find $\langle \langle \hat{S}_n \rangle \rangle < \hbar S$ (see discussion before about the density operators of pure and mixed states).

The explicit value of $\langle \langle \hat{S}_n \rangle \rangle$ corresponds to the strength of the entanglement: no entanglement means $\langle \langle \hat{S}_n \rangle \rangle = \hbar S$ which is the maximal value and with entanglement $\langle \langle \hat{S}_n \rangle \rangle$ decreases and can become zero. Due to the fact that the entanglement depends on $|\psi\rangle$ and $|\psi\rangle$ can change with the time $t$, $\langle \langle \hat{S}_n \rangle \rangle$ can also change with the time.

Another way to quantify the entanglement is the von Neumann entropy:

$$S(\hat{\rho}_m) = -\text{Tr} (\hat{\rho}_m \log_2 \hat{\rho}_m),$$ (32)

where $\hat{\rho}_m$ is the reduced density matrix.

The von Neumann entropy is the extension of the classical Gibbs entropy concept to the quantum mechanics and can be seen as the quantum mechanical analog to the classical Shannon entropy [38] of the information technology.

In principle the von Neumann entropy is defined for any density matrix $\hat{\rho}$. In general, the von Neumann entropy proves if the system is in a pure or in a mixed state.
Therefore, it makes sense to use the reduced density matrix $\rho_m$, because in these cases a pure state corresponds to a product state, and therefore to no entanglement. In these cases we find $S(\rho_m) = 0$. A mixed state corresponds to an entangled superposition state. In these cases we find $0 < S(\rho_m) \leq 1$. The maximum value $S(\rho_m) = 1$ corresponds to $|\langle \hat{S}_n \rangle| = 0$. Furthermore, as before $|\langle \hat{S}_n \rangle|$, $S(\rho_m)$ is time dependent.

IV. NUMERICAL PROOF

In the previous section we have seen that only in the cases of a single spin or a spin ensemble which behaves like a single spin and in the cases of a linear excitation around the ferromagnetic ground state we can find a quantum mechanical spin dynamics similar to the classical spin dynamics. In these cases we have no entanglement and the absolute value $|\langle \hat{S} \rangle|$ stays constant. In the cases of entanglement this is not the case. To proof this statement computer simulations have been performed. In the previous publications only linear excitations [25] or single spins [27] have been investigated. In the following, we will discuss the magnetization reversal of a single spin as well as a linear excitation and a magnetization reversal of a trimer.

The Heisenberg Hamiltonian of our system is given by:

$$H = -J \sum_n \hat{S}_n \hat{S}_{n+1} - \mu_S \sum_n B_z \hat{S}_n^z + -\mu_S B_x(t) \hat{S}_1^x \quad (33)$$

The first term describes the nearest neighbor exchange interaction with ferromagnetic ($J > 0$) or antiferromagnetic ($J < 0$) coupling.

The second sum and third term describe couplings to external magnetic fields. In this case a static field in $z$-direction and a field pulse in $x$-direction acting on the first spin only:

$$B_x(t) = B_0 e^{-\frac{t-t_0}{\tau}} \quad (34)$$

This field pulse will be used to bring the system out of equilibrium and to start the reversal process or just for linear excitations.

For the moment we restrict ourself to a single spin [no exchange term in (33)]. The spin is initially oriented in $+z$ direction: $|\psi(t = 0)\rangle = |\uparrow\rangle$. The static external field in $-z$-direction. The field pulse is needed to break the symmetry and to initialize the magnetization reversal.

Fig. 1 shows the trajectories of $\hat{S}$ calculated with the Schrödinger equation (22) and for comparison the trajectory of the classical spin $S$ calculated with the classical Landau-Lifshitz-Gilbert equation. As expected, Fig. 1 shows a perfect agreement of both, the classical as well as quantum mechanical trajectories, which also means that $|\langle \hat{S} \rangle|$ is conserved. For a detailed discussion please see Sec. II and III.

Let us come to the trimer. All spins are aligned in a chain and we assume that there is no coupling between the first and the last spin. The Hamiltonian (33) is linear in $\hat{S}_n$ and therefore we can expect a classical behavior if we are close to the ferromagnetic ground state.

Fig. 2 shows the trajectories of three ferromagnetic coupled spins, excited by a tiny field pulse (linear excitation), with $S = 1$. The field pulse acts on the first spin only. In the initial configuration is: all spins are oriented in $+z$-direction, the direction of the external field $B_z$.

To show the agreement of the classical spins $S_n$ with the expectation values $\langle \hat{S}_n \rangle$ we have compared the curves of the first spin: it can be seen that both curves lie on top of each other which means that the expectation values behave classical. The comparison between classical and quantum mechanical trajectory of the other two spins show the same behavior (not shown).

As mentioned before such an agreement can be expected only for linear excitations of the ferromagnetic ground state, in this case $|FM\rangle = |\uparrow\uparrow\uparrow\rangle$. This is the
case within the simulation. This can be seen by the small amplitude of the $\langle \hat{S}_n^z \rangle$ and $\langle \hat{S}_n^y \rangle$ component. Furthermore, the simulation shows that only the basis state $|m_1 m_2 m_3\rangle = |m_1 m_2 m_3\rangle = |↑↑↑\rangle$ gives a relevant impact: $\langle \psi(t) | \psi(t) \rangle \approx 1$. All other basis states $|m_1 m_2 m_3\rangle$ are not occupied or just marginal with $\langle \psi(t) | \psi(t) \rangle < 0.01$. Furthermore, additional simulations show that with increasing $S$ the deviation from $\langle \psi(t) | \psi(t) \rangle$ increases. This becomes clear because with $S \to \infty$ we find the classical limit.

FIG. 3: Magnetization reversal for three ferromagnetic couple spins. a) $z$-component of the spin as function of time $t$, b) projection of the wave function $|ψ(t)\rangle$ to the basis states $|m_1 m_2 m_3\rangle$, c) precession motion of the second spin during the reversal process, d) spin length as function of time $t$. 
(S = 1/2, $J = 4$, $μSB_z = -2$, $μSB_y = 3.27$, $t_0 = 10$, $T_W = 0.02$, $λ = 0.1$)

FIG. 4: Von Neumann entropy $S(ρ_m)$ vs. time $t$, corresponding to the magnetization reversal of the three spin system presented in Fig. 3.

The situation changes if we leave the ferromagnetic ground state. Fig. 3 shows the magnetization reversal of three coupled spins with $S = 1/2$. The initial configuration is the same as before all three spins in $+z$-direction, however the external field is now $-z$-direction. Again, the field pulse excites the first spin only. The result is a stepwise magnetization reversal [see Fig. 3b]]. Each step corresponds to the occupation of one of the basis states $|m_1 m_2 m_3\rangle$ corresponding to $|+3/2\rangle = |↑↑↑\rangle$ (basis state with three spins up), $|+1/2\rangle = |↑↑↑\rangle$ (all basis states with two spins up), $|-1/2\rangle = |↓↓↓\rangle$ (all basis states with two spins down), and $|-3/2\rangle = |↓↓↓\rangle$ (basis state with three spins down) [see Fig. 3b]]. The oscillation of $\langle \hat{S}_1^z \rangle$ and $\langle \hat{S}_2^z \rangle$ around $\langle \hat{S}_2^z \rangle$ is a direct result of the field pulse acting on the first spin only and the exposed position of the second spin as the middle of this three spin cluster.

During the reversal process $\langle \hat{S}_n^z \rangle$ and $\langle \hat{S}_n^y \rangle$ [Fig. 3a] show a precessional motion of the spins similar to the magnetization reversal of the single spin before [see Fig. 1].

The most important result is shown in Fig. 3b]: the not conserved absolut value $|⟨\hat{S}_n⟩|$. This means, we cannot expect an agreement with the classical trajectories where we assume a constant spin length $|S_n| = 1$. As mentioned before $|⟨\hat{S}_n⟩| < hS$ means that the system is entangled, which can be seen also by Fig. 3b). The three spins are in a product state (FM) only at the beginning and at the end of the reversal process. In between, we see superpositions of the basis states $|m_1 m_2 m_3\rangle = |m_1 m_2 m_3\rangle$ which means entanglement.

To strengthen this message the von Neumann entropy

$$S(ρ_m) = -\text{Tr}(ρ_m \log_2 ρ_m) ,$$

for the reduced density operator $ρ_m$, corresponding with the Hilbert space of the first spin of our three spin system, has been calculated. For the details of the calculation please see the supplementary material 54.

Fig. 3 shows the von Neumann entropy $S(ρ_m)$ as function of time $t$. It can be seen that ferromagnetic states at the beginning and end: $|↑↑↑\rangle$ and $|↓↓↓\rangle$ show no entanglement. Furthermore, we see that the highest entanglement [max. $S(ρ_m)$] appears when the $|⟨\hat{S}_n⟩|$, $n \in \{1, 2, 3\}$, have their smallest values.

V. TEMPERATURE

The previous sections describe the quantum spin dynamics with energy dissipation at zero temperature. Within this section we discuss two possibilities to include temperature effects. The easiest way is to add to the Hamilton operator $H$ [Eq. 33] an additional stochastic field term:

$$\hat{H}_ξ = −\sum_n ξ_n \hat{S}_n .$$

$ξ_n = (ξ_x^n, ξ_y^n, ξ_z^n)$ is a stochastic field characterized by $⟨ξ_a^n(t)⟩ = 0$ and $⟨ξ_a^n(t)ξ_b^n(t')⟩ = Dδ_{a,b}δ(t − t')$, with $α, β \in \{x, y, z\}$, and lattice sites $n, m$. Depending on the prefactor $D$ the stochastic field can be used to describe temperature or quantum fluctuations 39.

The advantage of such an stochastic field is that this term is already a field term. This means that this
term behaves classical. In other words: the Heisenberg Hamiltonian $\hat{H} = -(\hat{B}_{\text{eff}} + \xi)\hat{S}$ inserted in the Schrödinger equation \( (22) \) immediately leads to the following Langevin equation which can be seen as the quantum mechanical analog of the stochastic Landau-Lifshitz-Gilbert equation \( [20, 41] \):

$$
\frac{d}{dt} \langle \hat{S} \rangle = \frac{1}{1 + \lambda^2} \left( \langle \hat{S} \rangle \times \hat{B}_{\text{eff}} - \frac{\lambda}{1 + \lambda^2} \langle \hat{S} \rangle \times (\langle \hat{S} \rangle \times \hat{B}_{\text{eff}}) \right) + \frac{1}{1 + \lambda^2} \langle \hat{S} \rangle \times \xi - \frac{\lambda}{1 + \lambda^2} \langle \hat{S} \rangle \times (\langle \hat{S} \rangle \times \xi) 
$$

(37)

Similar, the quantum mechanical analog of the stochastic Landau-Lifshitz can be derived using the same Heisenberg Hamiltonian together with the Schrödinger equation \( [1] \) or by making the same transformation we have used to derive the Schrödinger equation \( (22) \).

An alternative way to include temperature, where we assume that the system is already in equilibrium, is to use statistical operator \([35, 42]\):

$$
\hat{\rho}_{\text{Stat}} = \frac{e^{-\beta \hat{H}}}{\text{Tr}(e^{-\beta \hat{H}})},
$$

(38)

with $\beta$ the well known inverse temperature $\beta = \frac{1}{k_B T}$.

Then, the time dependence of $\hat{\rho}_{\text{Stat}}$, is given by:

$$
\hat{\rho}_{\text{Stat}}(t) = U(t) \hat{\rho}_{\text{Stat}}(0) U^+(t).
$$

(39)

$U(t)$ is the unitary operator

$$
U(t) = e^{-i\hat{H}t} e^{-\lambda \hat{H}t} e^{\lambda (\hat{H})t},
$$

(40)

which we have already seen in Eq. \( (2) \). At this point, we have to notice that Eq. \( (39) \) is a self-consistent equation, because the unitary operator $U(t)$ contains $\langle \hat{H} \rangle$ which has to be calculated with $\hat{\rho}_{\text{Stat}}$: $\langle \hat{H} \rangle = \text{Tr}(\hat{\rho}_{\text{Stat}} \hat{H})$. However, $\hat{\rho}_{\text{Stat}}$ already needs $\langle \hat{H} \rangle$ to be calculated. Alternatively, we can use \([35]\) in the Liouville equation \([1]\) to describe the dynamics.

VI. SUMMARY

In summary it has been show that the following non-Hermitian Hamilton operator $\hat{H} = \hat{H} - i\lambda \hat{H}$ inserted in the time dependent Schrödinger equation leads to an equation of motion similar to the classical Landau-Lifshitz Eq. \( (24) \). To show this the corresponding Liouville Eq. \([5]\) as well as Heisenberg Eq. \([17]\) have been derived and discussed.

It is known that the Landau-Lifshitz equation fails in the huge damping limit \([20]\). However, the Landau-Lifshitz-Gilbert (LLG) equation can be simply obtained from the Landau-Lifshitz equation by rescaling the time. The LLG equation itself shows the correct physics. The same rescaling has been used to derive the time dependent Schrödinger Eq. \( (22) \) which corresponds to the classical Landau-Lifshitz-Gilbert Eq. \( (24) \).

During the complete derivation and later in the manuscript the similarities and differences of the classical and quantum spin dynamics have been discussed. It has been shown that only for single spins with a Zeeman Hamiltonian $\hat{H} = -\hat{B} \cdot \hat{S}$ and in the case of a ferromagnetic multi-spin system we can expect a classical behavior, which means similar trajectories of the quantum mechanical expectation values $\langle \hat{S}_n \rangle$ and classical spins $S_n$. (The index $n$ stands for the $n$th spin.) In all other cases we expect a deviation of the trajectories of the expectation values $\langle \hat{S}_n \rangle$ from the classical behavior. The reasons are the appearance of additional terms of the order of $\hbar$ in the Heisenberg equation which disappear in the classical limit: $S \to \infty$ and $\hbar \to 0$ and in the case of a multi-spin system the appearance of entanglement. The entanglement itself is a pure quantum effect and also disappears in the classical limit.

All the results have been discussed theoretical with analytical calculations and proved with computer simulations. In all cases the theoretical estimated effects have been seen in the simulations.

In the last section of the manuscript two ways have been shown how to include temperature which has not been taken into account in the previous sections (Sec. II+IV). The first way is to add a random noise. This way allows us to investigate the dynamics under the influence of temperature as well as quantum fluctuations. The second way deals with the statistical operator. In this case fluctuations play no role. This way can be used if we are interested in system which are always in the thermodynamical equilibrium. This means, non-equilibrium effects cannot be described with this way.

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