

# We are IntechOpen, the world's leading publisher of Open Access books Built by scientists, for scientists

6,900

Open access books available

186,000

International authors and editors

200M

Downloads

Our authors are among the

154

Countries delivered to

TOP 1%

most cited scientists

12.2%

Contributors from top 500 universities



WEB OF SCIENCE™

Selection of our books indexed in the Book Citation Index  
in Web of Science™ Core Collection (BKCI)

Interested in publishing with us?  
Contact [book.department@intechopen.com](mailto:book.department@intechopen.com)

Numbers displayed above are based on latest data collected.  
For more information visit [www.intechopen.com](http://www.intechopen.com)



# Mesoscopic Modeling of Ferroelectric and Multiferroic Systems

Thomas Bose and Steffen Trimper

*Martin-Luther-University Halle, Institute of Physics  
Germany*

## 1. Introduction

Motivated by the progress of a multi-scale approach in magnetic materials the dynamics of the Ising model in a transverse field introduced by de Gennes (1963) as a basic model for a ferroelectric order-disorder phase transition is reformulated in terms of a mesoscopic model and inherent microscopic parameters. The statical and dynamical behavior of the Ising model in a transverse field is considered as classical field theory with fields obeying Poisson bracket relations. The related classical Hamiltonian is formulated in such a manner that the quantum equations of motion are reproduced. In contrast to the isotropic magnetic system, see Tserkovnyak et al. (2005), the ferroelectric one reveals no rotational invariance in the spin space and consequently, the driving field becomes anisotropic. A further conclusion is that the resulting excitation spectrum is characterized by a soft-mode behavior, studied by Blinc & Zeks (1974) instead of a Goldstone mode which appears when a continuous symmetry is broken, compare Tserkovnyak et al. (2005). Otherwise the underlying spin operators are characterized by a Lie algebra where the total antisymmetric tensor plays the role of the structural constants. Using symmetry arguments of the underlying spin fields and expanding the driving field in terms of spin operators and including terms which break the time reversal symmetry we are able to derive a generalized evolution equation for the moments. This equation is similar to the Landau Lifshitz equation suggested by Landau & Lifshitz (1935) with Gilbert damping, see Gilbert (2004). Alternatively, such dissipative effects can be included also in the Lagrangian written in terms of the spin moments and bath variables Bose & Trimper (2011). Due to the time reversal symmetry breaking coupling the resulting equation includes under these circumstances a dissipative equation of motion relevant for ferroelectric material. The deterministic equation is extended by stochastic fields analyzed by Trimper et al. (2007). The averaged time dependent polarization offers three modes below the phase transition temperature. The two transverse excitation energies are complex, where the real part corresponds to a propagating soft mode and the imaginary part is interpreted as the wave vector and temperature dependent damping. Further there exists a longitudinal diffusive mode. All modes are influenced by the noise strength. The solution offers scaling properties below and above the phase transition. The results are preferable and applicable for ferroelectric order-disorder systems.

A further extension of the approach is achieved by a symmetry allowed coupling of the polarization to the magnetization. The coupling is related to a combined space-time symmetry due to the fact that the magnetization is an axial vector with  $\vec{m}(\vec{x}, -t) = -\vec{m}(\vec{x}, t)$  whereas

the polarization is represented by a polar vector  $\vec{p}(-\vec{x}, t) = -\vec{p}(\vec{x}, t)$ . Multiferroic materials are characterized by breaking the combined space-time symmetry. Possible couplings are considered. Introducing a representation of spin fields without fixed axis one can incorporate spiral structures. Different to the previous system the ground state is in that case an inhomogeneous one. The resulting spectrum is characterized by the conventional wave vector  $\mathbf{q}$  and a special vector  $\mathbf{Q}$  characterizing the spiral structure.

Our studies can be grouped into the long-standing effort in understanding phase transitions in ferroelectric and related materials, for a comprehensive review see Lines & Glass (2004). To model such systems the well accepted discrimination in ferroelectricity of order-disorder and displacive type is useful as discussed by Cano & Levanyuk (2004). Both cases are characterized by a local double-well potential the depth of which is assumed to be  $V_0$ . Furthermore, the coupling between atoms or molecules at neighboring positions is denoted by  $J_0$ . The displacive limit is identified by the condition  $V_0 \ll J_0$ , i.e. the atoms are not forced to occupy one of the minimum. Instead of that the atoms or molecular groups perform vibrations around the minimum. The double-well structure becomes more important when the system is cooled down. The particle spend more time in one of the minimum. Below the critical temperature  $T_c$  the displacement of all atoms tends preferentially into the same direction giving rise to elementary dipole moments, the average of which is the polarization. The opposite limit  $V_0 \gg J_0$  means the occurrence of high barriers between the double-well structure, i.e. the particles will reside preferentially in one of the minimum. Above the critical temperature the atoms will randomly occupy the minimum whereas in the low temperature phase  $T < T_c$  one of the minimum is selected. The situation is sketched in Fig. 1. Following de Gennes (1963) the double-well structure can be modeled by a conventional Ising model where the eigenvalues of the pseudo-spin operator  $S^z$  specify the minima of the double-well potential. The dynamics of the system is described by the kinetic energy of the particles which leads to an operator  $S^x$ . Due to de Gennes (1963) and Blinc & Zeks (1972; 1974) the situation is described by the model Hamiltonian (TIM)

$$H = -\frac{1}{2} \sum_{\langle ij \rangle} J_{ij} S_i^z S_j^z - \sum_i \Omega S_i^x, \quad (1)$$

where  $S^x$  and  $S^z$  are components of spin- $\frac{1}{2}$  operators. Notice that these operators have no relation to the spins of the material such as  $KH_2P0_4$  (KDP). Therefore they are denoted as pseudo-spin operators which are introduced to map the order-disorder limit onto a tractable Hamiltonian. The coupling strength between nearest neighbors  $J_{ij}$  is assumed to be positive and is restricted to nearest neighbor interactions denoted by the symbol  $\langle ij \rangle$ . The transverse field is likewise supposed as positive  $\Omega > 0$ . Alternatively the transverse field can be interpreted as tunneling frequency. In natural units the time for the tunneling between both local minimums is  $\tau_t = \Omega^{-1}$  whereas the transport time between different lattice sites is given by  $\tau_i = (\hbar J)^{-1}$ . The high temperature limit is determined by  $\tau_t < \tau_i$  or  $\Omega > \hbar J$ . The tunnel frequency is high and the behavior of the system is dominated by tunneling processes. With other words, the kinetic energy is large which prevents the localization of the particles within a certain minimum. The low temperature limit is characterized by a long or a slow tunneling frequency or a long tunneling time  $\tau_t > \tau_i$ . The behavior is dominated by the coupling strength  $J$ .

Since already the mean-field theory of the model Eq. (1), see Stinchcombe (1973) and also Blinc & Zeks (1972), yields a qualitative agreement with experimental data, the model was increasingly considered as one of the basic models for ferroelectricity of order-disorder type

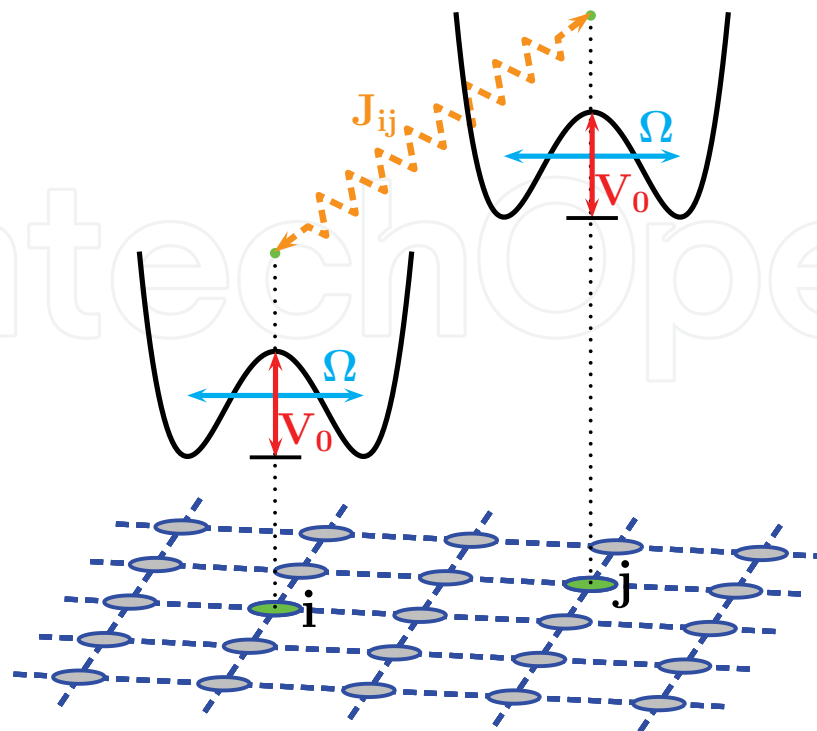


Fig. 1. Schematic representation of the physical situation in ferroelectric material.  $J_{ij}$  is the interaction between the atoms in the double-well potential at lattice site  $i$  and  $j$ ,  $\Omega$  is the tunneling frequency and  $V_0$  the height of the barrier.

as analyzed by Lines & Glass (2004); Strukov & Levnyuk (1998). Whereas the displacive type of ferroelectricity offers a mainly phonon-like dynamics, a relaxation dynamics is attributed to the order-disorder type by Cano & Levanyuk (2004). The Ising model in a transverse field allows several applications in solid state physics. Thus a magnetic system with a singlet crystal field ground state discussed by Wang & Cooper (1968) is described by Eq. (1), where  $\Omega$  plays the role of the crystal field. The model had been extensively studied with different methods by Elliot & Wood (1971); Gaunt & Domb (1970); Pfeuty & Elliot (1971), especially a Green's function technique was used by Stinchcombe (1971). It offers a finite excitation energy and a phase transition. A more refined study using special decoupling procedures for the Green's function investigated by Kühnel et al. (1977) allows also to calculate the damping of the transverse and longitudinal excitations as demonstrated by Wesselinowa (1984). Very recently Michael et al. (2006) have applied successfully the TIM to get the polarization and the hysteresis of ferroelectric nanoparticles and also the excitation and damping of such nanoparticles, compare Michael et al. (2007) and also the review article by Wesselinowa et al. (2010).

Despite the great progress in explaining ferroelectric properties based on the microscopic model defined by Eq. (1), the ferroelectric behavior should be also discussed using classical models. Especially, the progress achieved in magnetic systems, see Landau et al. (1980) and for a recent review Tserkovnyak et al. (2005), has encouraged us to analyze the TIM in its classical version capturing all the inherent quantum properties of the spin operators. The classical spin is introduced formally by replacing  $\vec{S} \rightarrow \vec{S}/(\hbar S(S+1))$  in the limit  $\hbar \rightarrow 0$

and  $S \rightarrow \infty$ . Stimulated by the recent progress in studying ferromagnets reviewed by Tserkovnyak et al. (2005), we are interested in damping effects, too. In the magnetic case the classical magnetic moments obey the Landau-Lifshitz equation, see Landau et al. (1980). It describes the precession of spins around a self-organized internal field, which can be traced back to the interaction of the spins. The reversible evolution equation can be extended by introducing dissipation which is phenomenologically proposed by Landau & Lifshitz (1935) or alternatively the so called Gilbert-damping is introduced by Gilbert (2004). Usadel (2006) has studied the temperature-dependent dynamical behavior of ferromagnetic nanoparticles within a classical spin model, while a nonlinear magnetization in ferromagnetic nanowires with spin current is discussed by He & Liu (2005). Even the magnetization of nanoparticles in a rotating magnetic field is analyzed by Denisov et al. (2006) based on the Landau-Lifshitz equation. The dynamics of a domain-wall driven by a mesoscopic current is inspected by Ohe & Kramer (2006) as well as the thermally assisted current-driven domain-wall was considered recently by Duine et al. (2007).

In the present chapter we follow the line offered by magnetic materials to extend the analysis to ferroelectricity accordingly. The main difference as already mentioned above is that in ferroelectric system the internal field is an anisotropic one and therefore, both the reversible precession and the irreversible damping are changed.

## 2. Model

In this section the model and the basic equation will be discussed. Especially the differences between isotropic magnets and anisotropic ferroelectrics are analyzed.

### 2.1 Hamiltonian

In this section we propose a classical Hamiltonian which is dynamical equivalent to the quantum case introduced in Eq. (1). The Hamiltonian is constructed in such a manner that it leads to the same evolution equations for the spins. The most general form is given by

$$H = \int d^d x \left( -\Omega_\mu S_\mu + \frac{1}{2} J_{\mu\nu\kappa\delta} \frac{\partial S_\mu}{\partial \kappa} \frac{\partial S_\nu}{\partial \delta} + \frac{1}{2} \Gamma_{\mu\nu} S_\mu S_\nu \right). \quad (2)$$

Here summation over repeated indices is assumed. If the system is symmetric in spin space the coupling tensor  $J$  is diagonal in the spin indices  $J_{\mu\nu\kappa\delta} = \delta_{\mu\nu} \tilde{J}_{\kappa\delta}$ . In case that spin and configuration space are independent one concludes the separation  $J_{\mu\nu\kappa\delta} = \hat{J}_{\mu\nu} \tilde{J}_{\kappa\delta}$ . The anisotropic TIM is obtained by assuming  $\vec{\Omega} = (0, 0, \Omega)$ ,  $\hat{J}_{\mu\nu} = J \delta_{\mu z} \delta_{\nu z}$ ,  $\tilde{J}_{\kappa\delta} = \delta_{\kappa\delta}$ , and  $\Gamma_{\mu\nu} = J z \delta_{\mu z} \delta_{\nu z}$ . Here  $z$  is the coordination number. The Hamiltonian reads now

$$H_f = \int d^d x \left( -\Omega S^x + \frac{J}{2} (\nabla S^z)^2 - J z S_z^2 \right). \quad (3)$$

The last equation represents the TIM on a mesoscopic level, i. e. the spin variables are spatiotemporal fields  $\vec{S}(\vec{x}, t)$ . The Hamiltonian Eq.(3) offers no continuous symmetry as the corresponding magnetic one. For that case the magnetic Hamiltonian is written in terms of spin fields  $\vec{\sigma}(\vec{x}, t)$  as Tserkovnyak et al. (2005)

$$H_m = \frac{K}{2} \int d^d x (\nabla \vec{\sigma})^2. \quad (4)$$

Here  $K$  designates the exchange coupling. The last Hamiltonian is invariant under spin-rotation. A further difference between the ferroelectric and the magnetic case is the form of the internal field and the underlying dynamics which obeys the mesoscopic equation of motion, compare Hohenberg & Halperin (1977):

$$\frac{\partial S_\alpha}{\partial t} = \{H, S_\alpha\}. \quad (5)$$

This equation will be discussed in the following subsection.

## 2.2 Poisson brackets

Because the Hamiltonian Eq. (2) is given in terms of classical fields the dynamics of the system has to be formulated using Poisson brackets. They are defined for two arbitrary functionals of an arbitrary field  $\phi$  by

$$\{A(\phi), B(\phi')\} = \int d^d x d^d x' \frac{\delta A}{\delta \phi_\alpha(x)} \{\phi_\alpha(x), \phi_\beta(x')\} \frac{\delta B}{\delta \phi_\beta(x')}.$$

In case that the arbitrary field  $\phi$  is realized by the components of spin fields we get due to Mazenko (2003)

$$\{A(S), B(S)\} = \int d^d x \epsilon_{\alpha\beta\gamma} S_\alpha(\vec{x}) \frac{\delta A}{\delta S_\beta(\vec{x})} \frac{\delta B}{\delta S_\gamma(\vec{x})}. \quad (6)$$

Here we have applied the Poisson brackets for angular momentum fields

$$\{S_\alpha(\vec{x}, t), S_\beta(\vec{x}', t)\} = \epsilon_{\alpha\beta\gamma} S_\gamma(\vec{x}, t) \delta(\vec{x} - \vec{x}').$$

According to Eq. (6) the spin field satisfies the evolution equation

$$\frac{\partial \vec{S}}{\partial t} = \vec{B} \times \vec{S}, \quad (7)$$

where the effective internal field  $\vec{B}$  is introduced by

$$B_\alpha(\vec{x}, t) = -\frac{\delta H_f}{\delta S_\alpha(\vec{x}, t)}. \quad (8)$$

Using the Hamiltonian Eq. (3) the vector of the internal field is given by

$$\vec{B} = (\Omega, 0, [Jz + J\nabla^2]S^z). \quad (9)$$

Eqs. (7)-(8) coincide with the quantum mechanical approach based on the Heisenberg equation of motions

$$i\hbar \frac{\partial S_r^\alpha}{\partial t} = [H, S_r^\alpha],$$

and the quantum model defined in Eq. (1), compare also the article by Trimper et al. (2007). Because the quantum model is formulated on a lattice we have performed the continuum limit. Eq. (7) describes the precession of the spin around the internal field  $\vec{B}$  defined in Eq. (8). Notice that the Hamiltonian should be invariant against time reversal. From here we conclude that the tunneling frequency  $\Omega$  or alternatively the transverse field is changed to  $-\Omega$  in case of  $t \rightarrow -t$ . As a consequence the self-organized internal field  $\vec{B}$  is antisymmetric under time



reversal. In the magnetic case, represented by the Hamiltonian in Eq. (4), the internal field is isotropic and is defined by

$$\vec{B}^{(m)} = K\nabla^2\vec{\sigma}. \quad (10)$$

Directly from Eq. (7) it follows that the spin length  $\vec{\sigma}^2$  or even  $\vec{S}^2$  is conserved which is reflected in the quantum language by the conservation of the total spin  $[H, \vec{S}^2]_- = 0$ . Vice versa one concludes from the conservation of any vector, that  $\dot{\vec{S}} \cdot \vec{S} = 0$ , i.e. the time derivative of the vector is perpendicular to the vector itself which is simply fulfilled by assuming  $\dot{\vec{S}} \propto \vec{A} \times \vec{S}$  for an arbitrary vector field  $\vec{A}$ . Insofar Eq. (7) is a consequence of the spin conservation. The same is valid for the spin field  $\vec{\sigma}$ .

### 2.3 Dissipation

Eq. (7) is a reversible equation, i.e. it is invariant against time reversal. As demonstrated in the next section Eq. (7) allows pseudo-spin-wave solutions. However, the excitation does not tend to restore a continuous symmetry, i.e. the Goldstone theorem, for details see Mazenko (2003), is not valid. Instead of that a soft mode behavior is observed. Normally, the excitation modes are damped. It is the aim of the present section to extend the evolution equation by including damping effects. From a microscopic point of view the damping can be traced back to scattering processes of spin-wave excitations with different wave vectors emphasized by Wesselinowa (1984) in second order of the interaction  $J$ . In principle this interaction effects are included in the microscopic Hamiltonian. Recently, Wesselinowa et al. (2005) have studied the influence of layer defects to the damping of the elementary modes in ferroelectric thin films. Likewise the analysis can be generalized for ferroelectric nanoparticles, where the interaction of those can also lead to finite life-times of the excitation modes as performed by Michael et al. (2007). Otherwise, the damping of pseudo-spin-waves can be originated by a coupling to lattice vibrations. Due to the coupling of the TIM to phonons the spin excitations can be damped as detected by Wesselinowa & Kovachev (2007). Generally one expects that due to attenuation the spin length is not conserved. On a mesoscopic level the inclusion of damping effects are achieved by a generalized evolution in the form

$$\frac{\partial \vec{S}(\vec{x}, t)}{\partial t} = \vec{B}(\vec{x}, t) \times \vec{S}(\vec{x}, t) + \vec{D}(\vec{S}). \quad (11)$$

The origin of the damping term  $\vec{D}$  is a pure dynamic one, i.e. all possible static parts should be subtracted. From Eq. (11) one finds

$$\frac{\partial \vec{S}^2}{\partial t} = \vec{D} \cdot \vec{S} < 0.$$

A non-trivial damping part is oriented into the direction of the effective field  $\vec{B}$ . Following Hohenberg & Halperin (1977) and using the approach discussed by Trimper et al. (2007) we make the ansatz

$$D_\alpha = -\Lambda_{\alpha\beta}(\vec{S})B_\beta. \quad (12)$$

In case the coefficient matrix  $\Lambda_{\alpha\beta}(\vec{S})$  is positive and independent of the spin field Eq. (11) corresponds to a pure relaxation dynamics for a non-conserved order parameter field. This fact reflects another difference to the magnetic case, where the internal field is defined in Eq. (10). The evolution equation for the Heisenberg spins  $\vec{\sigma}$  reads

$$\frac{\partial \vec{\sigma}(\vec{x}, t)}{\partial t} = \vec{B}^{(m)}(\vec{x}, t) \times \vec{\sigma}(\vec{x}, t) + \Lambda_{\alpha\beta} K \nabla^2 \vec{\sigma}.$$

Provided the coefficient matrix  $\Lambda_{\alpha\beta}$  is independent on  $\vec{\sigma}$  the damping effects are realized by spin diffusion and hence the order parameter is conserved according to the classification introduced by Hohenberg & Halperin (1977).

To proceed further in the ferroelectric model with non-conserved order parameter let us expand the coefficient matrix  $\Lambda_{\alpha\beta}(\vec{S})$  in terms of the spin field  $\vec{S}$ , where only terms are included which break the time reversal symmetry. Denoting the field independent part as  $\Lambda_{\alpha\beta}^{(0)}$  we get up to second order in  $\vec{S}$

$$\Lambda_{\alpha\beta}(\vec{S}) = \Lambda_{\alpha\beta}^{(0)} + \Lambda_{\alpha\beta\gamma\delta}^{(1)} S_\gamma S_\delta + O(\vec{S}^4). \quad (13)$$

Due to the spin algebra the tensor structure of the coefficients  $\Lambda$  are given in terms of the structure constant of the underlying Lie-group, i.e. the complete antisymmetric tensor  $\epsilon_{\alpha\beta\gamma}$  and unit tensor  $\delta_{\alpha\beta}$ . The zeroth order term is

$$\Lambda_{\alpha\beta}^{(0)} \propto \epsilon_{\alpha\mu\nu} \epsilon_{\beta\mu\nu}.$$

From here we define

$$\Lambda_{\alpha\beta}^{(0)} = \frac{1}{\tau_1} \delta_{\alpha\beta}, \quad (14)$$

where  $\tau_1$  plays the role of a relaxation time. Because the damping should be pointed to the direction of the effective field and consequently the vector  $\vec{D}$  is perpendicular to the propagating part  $\vec{B} \times \vec{S}$ . Summarizing these conditions we make the ansatz

$$\Lambda_{\alpha\beta\gamma\delta}^{(2)} = \frac{1}{2\tau_2} \left[ \epsilon_{\alpha\beta\rho} \epsilon_{\rho\gamma\delta} + \epsilon_{\alpha\gamma\rho} \epsilon_{\rho\beta\delta} + \epsilon_{\alpha\delta\rho} \epsilon_{\rho\beta\gamma} \right]. \quad (15)$$

In the conventional vector notation the complete equation of motion reads now

$$\frac{\partial \vec{S}}{\partial t} = \vec{B} \times \vec{S} - \frac{1}{\tau_1} \vec{B} - \frac{1}{\tau_2} \vec{S} \times (\vec{S} \times \vec{B}). \quad (16)$$

There appear two damping terms characterized by the relaxation times  $\tau_1$  and  $\tau_2$ , the determination of those is beyond the scope of a mesoscopic approach. They could reflect the coupling to other degrees of freedom and become of the order of microscopic spin-flip-processes. Eq. (16) reminds of the Landau-Lifshitz-Gilbert equation discussed in the ferromagnetic case, see Tserkovnyak et al. (2005). The differences to the magnetic case are the form of the internal field  $\vec{B}$  and the underlying symmetry. The consequences will be discussed in the next section.

### 3. Excitation spectrum

In this section we investigate the spectrum of collective pseudo-spin-wave excitations and their damping. The starting point is Eq. (16). Firstly we study the reversible precession part.



### 3.1 Soft mode

Because no continuous symmetry is broken one expects a soft mode behavior, see Blinc & Zeks (1974); Lines & Glass (2004), which is characterized by the temperature dependent excitation energy  $\varepsilon(\vec{q}, T)$  offering the following behavior

$$\lim_{T \rightarrow T_c} \varepsilon(\vec{q} = 0, T) = 0. \quad (17)$$

The situation is sketched schematically in Fig. 2 To compute the dispersion relation we insert

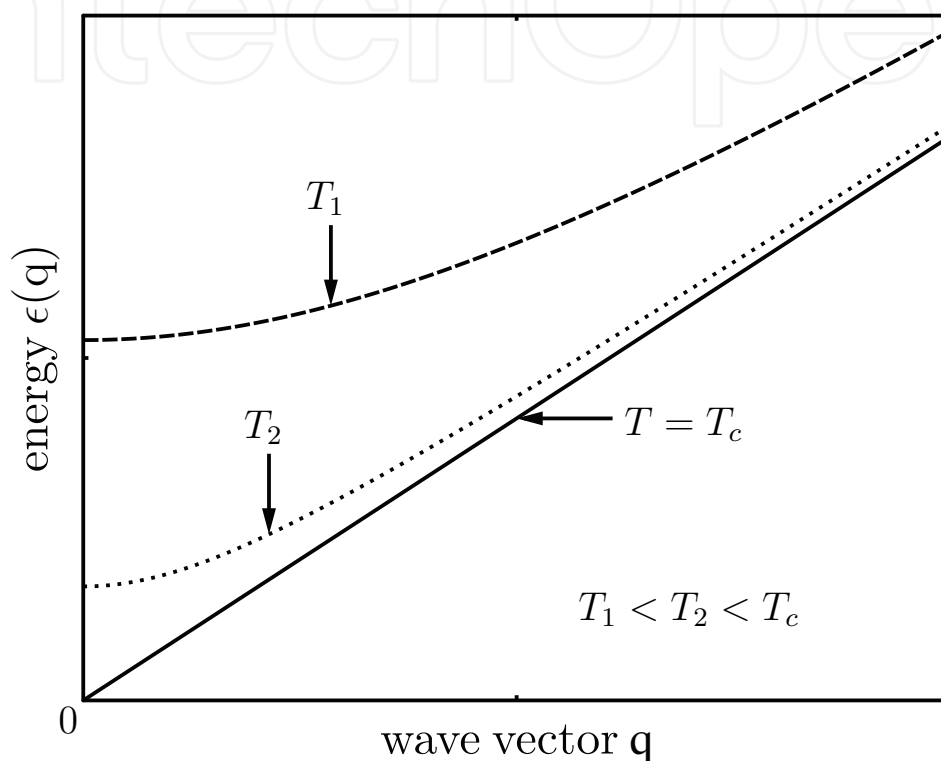


Fig. 2. Soft mode behavior: There is a gap for wave vector  $\vec{q} = 0$ , which tends to zero for  $T \rightarrow T_c$ , compare Eq. (17).

the internal field  $\vec{B}$  defined in Eq. (9) into Eq. (7). In the frame of linear spin-wave theory the spin field  $\vec{S}(\vec{x}, t)$  is splitted into a static and a dynamic part according to

$$\vec{S}(\vec{x}, t) = \vec{p}(\vec{x}) + \vec{\varphi}(\vec{x}, t), \quad (18)$$

where  $\vec{p}(\vec{x}) = (p_x, 0, p_z)$  is a time-independent but temperature-dependent vector in the  $x - z$  plane as suggested in Eq. (1). In case that  $\vec{p}$  is independent of the coordinates it describes the homogeneous polarization whereas for multiferroic material, for a review compare Wang et al. (2009), one finds a spiral structure of the form

$$\vec{p}(\vec{x}) = p_0 [\cos(\vec{Q} \cdot \vec{x}) \vec{e}_x + \sin(\vec{Q} \cdot \vec{x}) \vec{e}_y] + p_z \vec{e}_z. \quad (19)$$

Here  $\vec{Q}$  characterizes the spiral structure.

Inserting the ansatz made in Eq. (18) into Eq. (7) the field  $\vec{\varphi}$  obeys in spin-wave approximation

$$\dot{\vec{\varphi}} = \vec{B}_1 \times \vec{p} + \vec{B}_0 \times \vec{\varphi},$$

with  $\vec{B}_0 = (\Omega, 0, Jzp_z)$ , and  $\vec{B}_1 = (0, 0, J(\nabla^2 + z)\varphi_z)$ . The direction of the homogeneous polarization is given by  $\vec{p} \times \vec{B}_0 = 0$ . The last relation has two solutions

$$\begin{aligned} (i) \quad & p_z(T) \neq 0, \quad p_x = \frac{\Omega}{Jz} \quad \text{if } T \leq T_c \\ (ii) \quad & p_z = 0, \quad p_x(T) \neq \frac{\Omega}{Jz} \quad \text{if } T > T_c. \end{aligned} \quad (20)$$

Here the phase transition temperature is obtained by  $p_z(T = T_c) = 0$ . Moreover, the relation  $p_x(T_c) = \Omega/Jz$  should be fulfilled, i.e.  $p_x$  remains fixed and is temperature-independent below  $T_c$ . In a quantum language it means that the quantization axis is oriented within the  $x - z$ -plane in accordance with microscopic investigations, see for instance de Gennes (1963); Kühnel et al. (1977). In the frame of a multi scale approach the temperature dependence of  $p_x$  and  $p_z$  is calculated based upon the microscopic model Eq. (1). In the high temperature regime  $p_x$  decreases with increasing temperature which can be estimated to be  $p_x \propto \Omega/T$ , compare the book by Lines & Glass (2004). The quantity  $p_z$  offers a behavior like  $p_z \propto (-\tau)^\beta$  where  $\tau = (T - T_c)/T_c$  is the relative distance to the phase transition temperature and  $\beta \leq 1/2$  is the critical exponent of the polarization. The results are shown in Fig. 3. The subsequent analysis

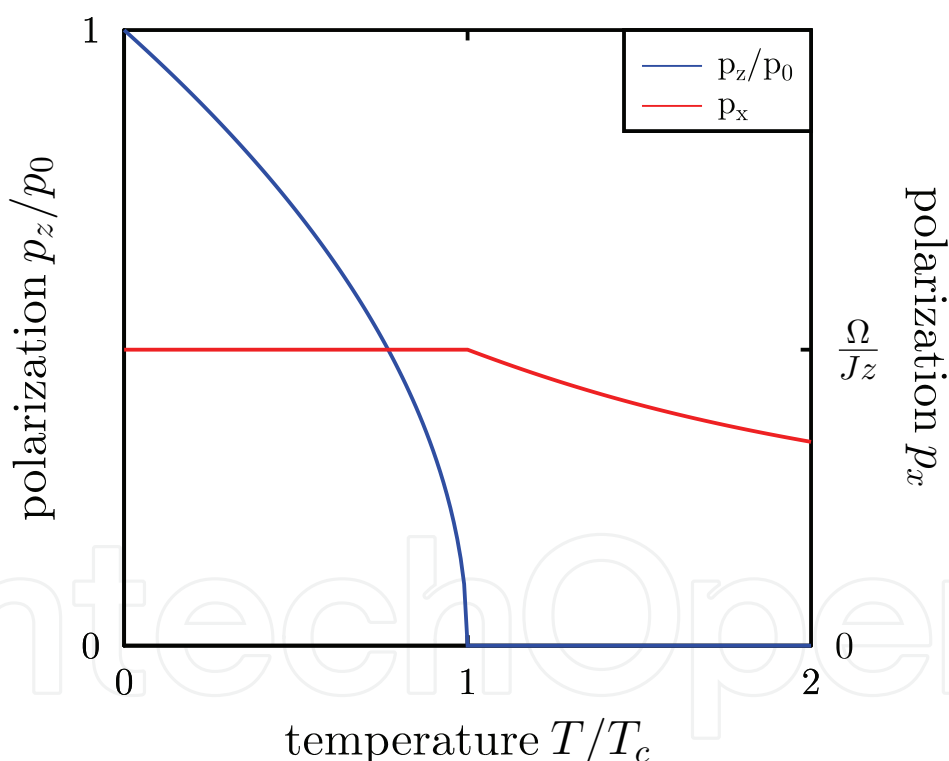


Fig. 3. Static polarization  $p_z(T)$  (blue line) and  $p_x(T)$  (red line) versus the ratio  $T/T_c$ . Whereas  $p_z$  vanishes at  $T_c$  according to a power law  $\propto (-\tau)^\beta$ ,  $p_x$  remains temperature independent for  $T < T_c$ .

is performed for the low and the high temperature phase separately. For  $T < T_c$ , i. e.  $p_z \neq 0$  one finds after Fourier transformation

$$\begin{aligned} \dot{\phi}_x(\vec{q}, t) &= -Jzp_z\varphi_y(\vec{q}, t), \quad \dot{\phi}_z(\vec{q}, t) = \Omega\varphi_y(\vec{q}, t) \\ \dot{\phi}_y(\vec{q}, t) &= Jzp_z\varphi_x(\vec{q}, t) - [\Omega - p_xJ\kappa(\vec{q})]\varphi_z(\vec{q}, t). \end{aligned} \quad (21)$$

Here we have used the abbreviation  $\kappa(\vec{q}) = z - q^2$ . Notice that the lattice constant  $a$  is set to unity and the approach is valid in the long wave length limit  $qa \ll 1$ . Notice that we set  $a = 1$ . A non-trivial solution of Eqs. (21) is given by  $\varphi_\alpha \propto \exp[i\varepsilon(\vec{q})t]$ . The eigenvalue of the coefficient matrix leads to the excitation energy  $\varepsilon_l(\vec{q})$ , which is in the low temperature phase dominated by the coupling  $J$  as pointed out already in the introduction. It results

$$\varepsilon_l(\vec{q}, T) = Jz \sqrt{p_z^2 + p_x^2 \frac{\vec{q}^2}{z}}. \quad (22)$$

This dispersion relation reveals the typical soft mode behavior characterized by Eq. (17) and depicted in Fig. 2. Such a behavior is in accordance to the microscopic behavior, see Kühnel et al. (1977); Stinchcombe (1973). The excitation field is found to be

$$\vec{\varphi}(\vec{q}, t) = \Phi_l(\vec{q}) \left( \frac{Jz p_z e^{i\pi/2}}{\varepsilon_l(\vec{q})}, 1, \frac{\Omega e^{-i\pi/2}}{\varepsilon_l(\vec{q})} \right) \exp[i\varepsilon_l(\vec{q})t], \quad (23)$$

where  $\Phi_l(\vec{q})$  is the amplitude of the excitation mode determined by the initial condition. The high temperature phase is characterized by  $p_z = 0$ . For that case one gets a similar dispersion relation as for  $T < T_c$  which can be written as

$$\varepsilon_h(\vec{q}, T) = \Omega \sqrt{\frac{p_x(T)}{p_x(T_c)} \frac{\vec{q}^2}{z} + \frac{p_x(T_c) - p_x(T)}{p_x(T_c)}}. \quad (24)$$

Above the critical temperature the excitation energy is dominated by the tunneling field  $\Omega$ . This result corresponds to the discussion in the introduction concerning the relevance of the different time scales. The dispersion relation Eq. (24) offers likewise a soft mode behavior due to  $p_x(T = T_c) = \frac{\Omega}{Jz}$  according to Eq. (20). Furthermore, the relation  $p_x(T)/p_x(T_c) < 1$  is fulfilled as one can observe also in Fig. 2. Making a Taylor-expansion of the second term in Eq. (24) the zero-wave vector mode satisfies in the vicinity of  $T_c$  the relation

$$\varepsilon_h(\vec{q} = 0) = \sqrt{\frac{Jz\Omega^2}{T_c^2} \left[ 1 - \left( \frac{\Omega}{zJ} \right)^2 \right]} (T - T_c)^{1/2}, \quad (25)$$

provided  $\Omega < Jz$ . In the opposite case a phase transition is suppressed at finite temperatures. The prefactor in front of the  $q^2$  term in the dispersion relation, Eq. (22) and (24), sometimes called as stiffness parameter remains finite at  $T_c$ . This result is also different to the magnetic case, where the stiffness constant tends to zero for  $T \rightarrow T_c$ . The spin wave field  $\vec{\varphi}(\vec{q})$  exhibits in the high temperature phase a similar form as for  $T < T_c$ , but one has to set  $p_z = 0$  and  $\varepsilon_l$  has to be replaced by  $\varepsilon_h$ . As expected the field  $\vec{\varphi}$  is continuous at  $T_c$ .

### 3.2 Dynamic scaling

In the vicinity of a second order phase transition a system is usually characterized by critical exponents and scaling relations, see Hohenberg & Halperin (1977). Especially there exist characteristic energies (propagating and relaxation modes) which fulfill

$$\varepsilon_c(\vec{q}, T) = q_c^{z_c} f_1(q\tilde{\xi}) \equiv \tilde{\xi}^{-z_c} f_2(q\tilde{\xi}). \quad (26)$$

Here  $z_c$  means the dynamic scaling exponent,  $\tilde{\xi}$  is the correlation length which behaves near to  $T_c$  as  $\tilde{\xi} \propto (\tau)^{-\nu}$  with the critical exponent  $\nu$  and  $\tau = (T - T_c)/T_c$ . As well  $f_1$  and  $f_2$  are

scaling functions which depend only on the combination  $q\zeta$ . The domain of wave vector and relative distance to the critical temperature  $\tau$  is due to Hohenberg & Halperin (1977) shown in Fig. 4. The critical regime denoted as region *I* is characterized by  $q\zeta \gg 1$  which is relevant

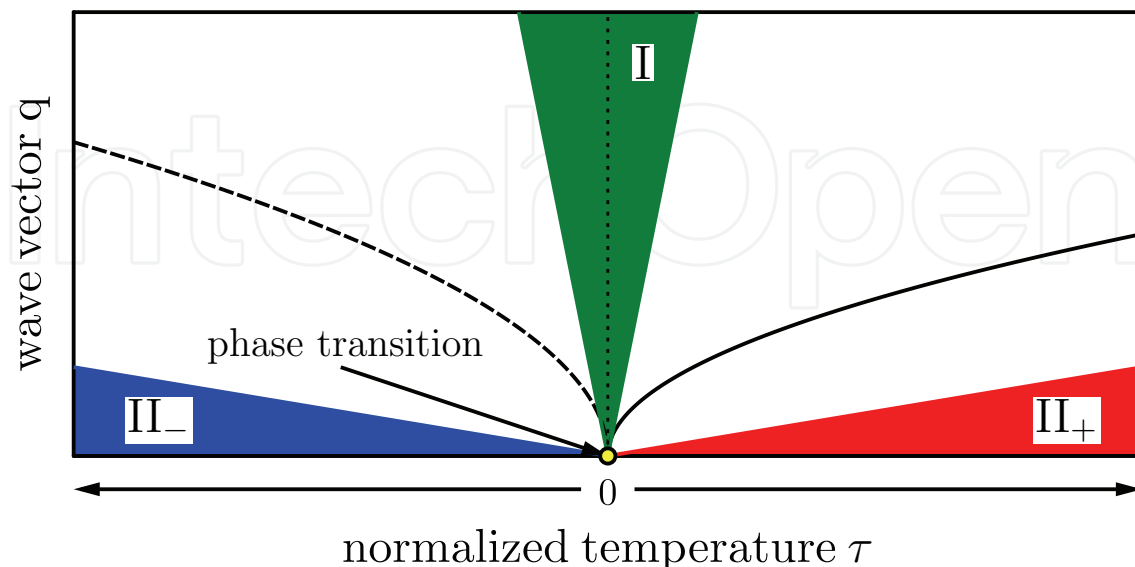


Fig. 4. Domain of wave vector versus  $\tau = (T - T_c)/T_c$ , *I* is the critical regime (green),  $II_{\pm}$  are the hydrodynamic regimes above (red) and below  $T_c$  (blue). The bold and the dashed line indicate the cross-over between the regimes.

for  $T \approx T_c$ . The two other regimes  $II_+$  and  $II_-$  are the hydrodynamic regimes relevant for  $T > T_c$  and  $T < T_c$ , respectively. Our model exhibits propagating modes denoted as  $\varepsilon_l$ , Eq. (22), and  $\varepsilon_h$ , Eq. (24). They play the role of the characteristic energy and obey the scaling form of Eq. (26). So we get in the low temperature phase

$$\varepsilon_l(\vec{q}, T) = qp_x(T)J\sqrt{z(1 + (q\zeta_l)^{-2})}. \quad (27)$$

From here we conclude the dynamical exponent  $z_c = 1$ , the correlation length below the phase transition  $\xi_l^{-2} = zp_z^2/p_x^2$  and the scaling function  $f_l(x) \propto \sqrt{1 + x^{-2}}$ . The critical exponents fulfill the relation  $\nu = \beta$ , which is in accordance with the scaling law  $z_c = \beta/\nu$ . A similar expression is found above  $T_c$  with the same dynamic exponent, but a different correlation length  $\xi_h^{-2} = z(p_x(T_c) - p_x(T))/p_x(T)$ .

### 3.3 Damping effect

For the complete Eq. (16) with damping we make the same ansatz as in Eq. (18) to find the complex dispersion relation  $\omega(\vec{q}, T)$ . In the low temperature phase  $T \leq T_c$  the system reveals three complex modes

$$\begin{aligned} \omega_{1,2}(\vec{q}, T) &= \pm\varepsilon_l(\vec{q}, T) - i\frac{\Gamma_{1l}(\vec{q}, T)}{2\tau_1} - i\frac{\Gamma_{2l}(\vec{q}, T)}{2\tau_2}, \\ \omega_3(\vec{q}, T) &= -i\frac{(Jzp_z)^2J\kappa(\vec{q})}{\varepsilon_l^2(\vec{q}, T)\tau_1} \equiv -i\omega_d(\vec{q}, T). \end{aligned} \quad (28)$$

The spin-wave field  $\vec{\varphi}(\vec{q}, t)$  introduced in Eq. (18) behaves as

$$\vec{\varphi}_{1,2}(\vec{q}, t) \propto \exp \left[ \left( \pm i\varepsilon_l - \left[ \frac{\Gamma_{1l}}{2\tau_1} + \frac{\Gamma_{2l}}{2\tau_2} \right] \right) t \right], \quad \varphi_3(\vec{q}, T) \propto \exp(-\omega_d(\vec{q}, T) t).$$

Whereas the modes  $\omega_{1,2}$  describe the propagation of pseudo-spin waves and their damping, the mode  $\omega_3 = -i\omega_d(\vec{q}, T)$  is a pure imaginary one, influenced only by  $\tau_1$ . Such a situation is also known for magnets, see Hohenberg & Halperin (1977) with two complex transverse modes and one diffusive longitudinal mode. Due to the different physical situation the pure imaginary mode  $\omega_3$  offers here a dispersion relation different to diffusion. The results in Eq. (28) are valid in the long wave length limit  $q \ll 1$  and in first order in  $\tau_{1,2}^{-1}$ . In this approximation the propagating part  $\varepsilon_l(\vec{q}, T)$  remains unchanged in Eq. (22). Higher order terms give rise to a slightly changed behavior. The finite life-time of the excitation is related to the temperature and wave vector dependent damping terms which read

$$\begin{aligned} \Gamma_{1l}(\vec{q}, T) &= \frac{J\kappa(\vec{q})\Omega^2}{z\varepsilon_l^2(\vec{q}, T)} q^2, \\ \Gamma_{2l}(\vec{q}, T) &= \frac{\varepsilon_l^2(\vec{q}, T) + (Jzp_z(T))^2 + \Omega^2}{Jz} \quad \text{with} \quad \kappa(\vec{q}) = z - q^2. \end{aligned} \quad (29)$$

At the critical point the damping is continuously as demonstrated in Trimper et al. (2007). While the life-time in the high temperature phase is only weakly temperature dependent, it depends on  $T$  in the low temperature regime via  $p_z$  which disappears at  $T_c$  according to  $p_z(T) \propto (-\tau)^\beta$  with a critical exponent  $\beta \leq 1/2$ . The temperature dependence of the excitation energy and the relevant life-time  $(\Gamma_{2l})^{-1}$  of the soft mode at  $\vec{q} = 0$  are depicted in Trimper et al. (2007). The damping function can be written in scaling form using the results obtained in subsection (3.2). For simplicity we assume  $\tau_1 \simeq \tau_2 \equiv \tau_0$ . Defining  $\gamma_{1l} = \Gamma_{1l}/2\tau_0$  and  $\gamma_{2l} = \Gamma_{2l}/2\tau_0$ . In the long wave length limit it results

$$\frac{2\tau_0\gamma_{1l}}{Jz} = (q\xi_l)^2 \quad \frac{2\tau_0\gamma_{2l}}{Jzp_x^2} = 1 + \frac{q^2}{z} \left[ 1 + 2(q\xi_l)^{-2} \right] \quad (30)$$

Whereas the excitation energy  $\varepsilon_l$  is dominated by a linear  $q$ -term, see Eq. (27), and disappears for  $T \rightarrow T_c$  at  $\vec{q} = 0$ , the damping is quadratic in  $q$ . In our case the life time remains fixed at  $T_c$ . Apparently one finds the total damping  $\gamma_l = \gamma_{1l} + \gamma_{2l}$  satisfies in the vicinity of the critical temperature

$$\gamma_l^{-1}(\vec{q}, T_c) < \gamma_l^{-1}(\vec{q}, T \leq T_c).$$

When the system is approaching the phase transition temperature, the elementary excitation decays more rapidly for wave vector  $\vec{q} \neq 0$ .

The corresponding damping parameters  $\Gamma_{1h}$  and  $\Gamma_{2h}$  can be also found in the high temperature limit characterized by  $p_z = 0$  and  $p_x \rightarrow 0$ , compare Fig. 3. The analytical expressions are presented in Trimper et al. (2007). In that case we obtain  $\varepsilon_h(\vec{q}, T \rightarrow \infty) = \Omega$ , i.e the mode is frozen in. A corresponding analysis for the damping shows that the system is overdamped with  $\varepsilon_h \ll \Gamma_{1h}$ .

The analysis can be performed likewise on a microscopic level using Eq. (1), cf. Michael et al. (2006). In that case a more refined Green's function technique enables us to calculate both the excitation energy and its damping. The temperature dependence of both quantities is in accordance to the present analysis and also in qualitative agreement with experimental results as shown by Michael et al. (2007).

#### 4. Stochastic equation

The model defined by Eq. (16) can be extended by introducing stochastic forces. To that aim we have two possibilities:

- (i) All the residual degrees of freedom, which are not taken into account so far, will be incorporated into the model as an additive noise. If this stochastic force is denoted as  $\vec{\eta}(\vec{x}, t)$  the evolution equation reads now

$$\begin{aligned} \frac{\partial \vec{S}}{\partial t} &= \vec{B} \times \vec{S} - \frac{1}{\tau_1} \vec{B} - \frac{1}{\tau_2} \vec{S} \times (\vec{S} \times \vec{B}) + \vec{\eta}(\vec{x}, t), \\ \langle \eta_\alpha(\vec{x}, t) \eta_\beta(\vec{x}', t') \rangle &= 2T \delta_{\alpha\beta} \delta(\vec{x} - \vec{x}') \delta(t - t'), \end{aligned} \quad (31)$$

where for simplicity a Gaussian white noise is supposed.

- (ii) A second realization is given by assuming that the effective field  $\vec{B}$ , see Eq. (8), is extended by a stochastic force, i.e.  $\vec{B}(\vec{x}, t) \rightarrow \vec{B}(\vec{x}, t) + \vec{\eta}(\vec{x}, t)$ . Such a situation leads to a multiplicative noise and is already discussed for a magnet in Usadel (2006) studying ferromagnetic resonance, and in Bose & Trimper (2010) including also colored noise.

Here we are interested in the model defined by Eqs. (31). The spin-wave fields obey in the low temperature phase the relation

$$\frac{\partial \varphi_\alpha(\vec{q}, t)}{\partial t} = W_{\alpha\beta}(\vec{q}) \varphi_\beta(\vec{q}, t) + \eta_\alpha(\vec{q}, t). \quad (32)$$

Here  $\mathbf{W}$  is a  $3 \times 3$  matrix

$$W_{\alpha\beta} = \begin{pmatrix} -\frac{m_z A_l}{\tau_2} & -A_l & \frac{m_z B_l q^2}{\Omega \tau_2} \\ A_l & -\frac{\Omega^2 + A_l^2}{Jz\tau_2} & -\frac{B_l q^2}{\Omega} \\ \frac{m_z \Omega}{\tau_2} & \Omega & -\frac{J\kappa(\vec{q})}{\tau_1} - \frac{B_l q^2}{Jz\tau_2} \end{pmatrix}$$

with the coefficients  $A_l = Jzp_z$  and  $B_l = \Omega^2/z$ . Eq. (32) is solved by the Green's function defined by

$$G_{\alpha\beta}(t - t') = \Theta(t - t') \left\langle \frac{\delta \varphi_\alpha(t)}{\delta \eta_\beta(t')} \right\rangle.$$

Here  $\Theta(t)$  is the Heavyside function. After Fourier transformation the Green's function is written in lowest order in  $\tau_{1,2}^{-1}$  as

$$G_{\alpha\beta}(\vec{q}, \omega) = \frac{g_{\alpha\beta}(\vec{q}, \omega)}{[\omega - \omega_1(\vec{q}, T)][\omega - \omega_2(\vec{q}, T)][i\omega + \omega_d(\vec{q}, T)]}, \quad (33)$$

where the excitation energies in the low temperature phase  $\omega_{1,2}$  and  $\omega_d$  are already introduced in Eqs. (28). The elements of the matrix  $g_{\alpha\beta}(\vec{q}, \omega)$  are given by

$$\begin{aligned} g_{11} &= -\omega^2 - i\omega \left[ \frac{\Omega + \varepsilon_l^2}{Jz\tau_2} + \frac{J\kappa(\vec{q})}{\tau_1} \right] + B_l q^2, & g_{22} &= -\omega^2 - i\omega \left[ \frac{\varepsilon_l^2}{Jz\tau_2} + \frac{J\kappa(\vec{q})}{\tau_1} \right], \\ g_{33} &= -\omega^2 - i\omega \frac{2A_l^2 + \Omega^2}{Jz\tau_2} + A_l^2, & g_{12} &= A_l \left[ i\omega - \frac{J\kappa}{\tau_1} \right] = -g_{21}, \\ g_{23} &= \frac{i\omega B_l q^2}{\Omega} = -\frac{B_l q^2 g_{32}}{\Omega^2}, & g_{13} &= \frac{B_l q^2}{\Omega} \left[ A_l - \frac{i\omega p_z}{\tau_2} \right] = \frac{B_l q^2 g_{31}}{\Omega^2}. \end{aligned} \quad (34)$$



The real correlation function is defined conventionally by

$$\langle \varphi_\alpha(\vec{q}, \omega) \varphi^\dagger(\vec{q}, \omega) \rangle = C_{\alpha\beta}(\vec{q}, \omega) (2\pi)^{d+1}.$$

Using the solution for  $\varphi$  in terms of Green's function in Eq. (33) and the relation for the excitation energy  $\omega_{1,2}^* = -\omega_{2,1}$  the correlation function reads

$$\begin{aligned} C_{\alpha\beta}(\vec{q}, \omega) &= \frac{2T c_{\alpha\beta}(\vec{q}, \omega)}{(\omega^2 - \omega_1^2)(\omega^2 - \omega_2^2)(\omega^2 + \omega_d^2)} \\ c_{\alpha\beta}(\vec{q}, \omega) &= g_{\alpha\mu}(\vec{q}, \omega) g_{\mu\beta}^*(\vec{q}, \omega) \end{aligned} \quad (35)$$

The coefficients of the correlation function  $c_{\alpha\beta}$  are obtained from the corresponding expressions in Eq. (34). A direct calculation shows that the fluctuation-dissipation theorem is fulfilled

$$C_{\alpha\beta}(\vec{q}, \omega) = \frac{2T}{\omega} \Im G_{\alpha\beta}(\vec{q}, \omega).$$

In the context of the linear spin-wave approximation the stochastic equations with additive noise term do not give more information as the conventional equations. The poles of the Green's function determine the excitation energy like in the microscopic case. The situation is different for a multiplicative noise where the effective field  $\vec{B}$  is supplemented by a stochastic force. This behavior is discussed for magnets by Bose & Trimper (2010).

## 5. Multiferroics

As already remarked there is a new class of materials, called multiferroics, see Eerenstein et al. (2006); Fiebig (2005); Van den Brink & Khomskii (2008), which are classified as materials possessing at least two ferroic orders such as ferromagnetic and ferroelectric order in a single phase. For a recent review consult Wang et al. (2009). In this section we present a mesoscopic model where the ferroelectric properties are described by the Hamiltonian Eq. (3) and the magnetic part by non-linear sigma model defined in Eq. (4). The total Hamiltonian for such a multiferroic system reads

$$H = H_f + H_m + H_{fm} \quad (36)$$

The coupling term should be invariant against time reversal symmetry and space inversion. Due to Mostovoy (2006) we use

$$H_{fm} = \int d^d x \lambda_{\alpha\beta\gamma\delta} S_\alpha \sigma_\beta \frac{\partial \sigma_\delta}{\partial x_\gamma}, \quad (37)$$

where the symmetry allowed coupling constant is

$$\lambda_{\alpha\beta\gamma\delta} = \lambda_1 \epsilon_{\alpha\beta\mu} \epsilon_{\mu\gamma\delta} + \lambda_2 \delta_{\alpha\beta} \delta_{\gamma\delta}.$$

In case the magnetization field  $\vec{\sigma}$  fulfills  $\nabla \cdot \vec{\sigma} = 0$ , see Landau & Lifshitz (1935), the coupling is

$$H_{fm} = \lambda_1 \int d^d x \vec{S} \cdot [\vec{\sigma} \times (\nabla \times \vec{\sigma})] \quad (38)$$

Using the same procedure as before, i.e. defining the effective fields for the magnetic and for the ferroelectric case, then the equations for the magnetic spin field  $\vec{\sigma}$  and the ferroelectric pseudo-spin field  $\vec{S}$  are given by the following expressions

$$\begin{aligned}\frac{\partial \sigma_\alpha}{\partial t} &= K(\nabla^2 \vec{\sigma})_\alpha + \lambda_1 \epsilon_{\alpha\beta\gamma} \sigma_\beta \left( \sigma_\mu \frac{\partial S_\gamma}{\partial x_\mu} - S_\mu \frac{\partial \sigma_\gamma}{\partial x_\mu} \right) \\ \frac{\partial S_\alpha}{\partial t} &= (\vec{B} \times \vec{S})_\alpha + \lambda_1 \left( \vec{S} \times (\vec{\sigma} \times \nabla \times \vec{\sigma}) \right)_\alpha.\end{aligned}\quad (39)$$

The internal field for the ferroelectric subsystem is defined in Eq. (9). Now let us discuss the excitation energies for the magnetic and the ferroelectric system which are coupled mutually due to the multiferroic effect. To this aim we set according to Eq. (18)

$$\vec{S}(\vec{x}, t) = \vec{p}(\vec{x}) + \vec{\varphi}(\vec{x}, t), \quad \vec{\sigma}(\vec{x}, t) = \vec{m}(\vec{x}) + \vec{\Phi}(\vec{x}, t).$$

For simplicity we consider excitations around a homogeneous ground state, i.e.  $\vec{p} = (p_x, 0, p_z)$  and  $\vec{m} = (0, 0, m_z)$ . The magnetization  $\vec{m}$  points in the z-direction. Here we consider the experimentally realized situation, compare the review article by Wang et al. (2009), that lowering the temperature the system undergoes firstly at  $T_c$  a phase transition into a ferroelectric phase characterized by  $p_z \neq 0$ ,  $p_x = \Omega/(Jz)$  as well as  $m_z = 0$ . This phase is observable in the temperature regime  $T_m \leq T < T_c$ , where  $T_m$  is the magnetic phase transition temperature. A further reducing of the temperature leads at  $T = T_m < T_c$  to a transition into the magnetic phase, characterized by  $m_z \neq 0$ . In the low temperature regime one observes the multiferroic phase with  $m_z \neq 0$ ,  $p_z \neq 0$  and  $p_x = \Omega/Jz$ . In this regime the excitation energy offers a dispersion relation which depends on the parameters of the ferroelectric subsystem ( $J, \omega$ ), the coupling strength of the magnetic system  $K$  as well as the mutual coupling constant  $\lambda_1$  between both systems. A tedious but straightforward calculation shows that the excitation energy of the ferroelectric system  $\varepsilon_l(\vec{q}, T)$  remains unchanged in first order expansion with respect to the coupling  $\lambda_1$ , i.e. in the interval  $T_m < T \leq T_c$  the system reveals a soft mode behavior characterized by the dispersion relation presented in Eq. (18). In the low temperature phase  $T < T_m$  we get in lowest order in  $\lambda_1$  an excitation energy of the multiferroic system in the following form

$$\varepsilon_{fm}^2(\vec{q}, T) = (Km_z(T)q)^2 \left[ (q_x^2 + (q_y + Q)^2 + q_z^2 - Q^2) \right]. \quad (40)$$

Here the parameter  $Q$  is defined by

$$Q = \frac{\lambda_1 \Omega}{2JKz}.$$

This parameter reflects the influence of the ferroelectricity in the multiferroic phase. In absence of a multiferroic coupling the dispersion relation yields the well known Goldstone mode of the magnetic system  $\varepsilon_m = Km_z q^2$ . The multiferroic mode  $\varepsilon_{fm}$  remains a Goldstone mode, i. e.  $\varepsilon_{fm}(\vec{q} = 0) = 0$ , because at the magnetic transition a continuous symmetry is broken. The wave vector  $Q$  indicates (probably) the presence of spiral structures, compare Tokura & Seki (2010). Notice that we have considered only excitations with respect to the homogeneous ground state characterized by  $\vec{p} = \text{const}$ . The result is altered in case one studies an inhomogeneous static state given by Eq. (19) for instance. This point deserves further studies.

## 6. Conclusions

In this chapter we have discussed a mesoscopic modeling of ferroelectric materials. There exists two limiting cases denoted as displacive and order-disorder ones. The last category is often discussed in terms of an Ising model in a transverse field. Such a quantum model can be studied using different techniques, especially Green's function methods. Otherwise ferroelectric systems offer a phase transition at finite temperatures. In this region the quantum effects are not relevant and therefore, a mesoscopic description should be adequate. The mesoscopic limit of the underlying quantum model is constructed in such a manner that the evolution equations coincides, namely those based on the Heisenberg equation of motion and on the Poisson bracket relations, respectively. The main effort in this region came from the analysis of magnetic materials. Motivated by several theoretical activities in that field, we have studied the basic model for describing the order-disorder transition in ferroelectrics. To that aim we have brought forward the concept of mesoscopic evolution equations with damping terms to one of the standard models for ferroelectricity. In doing so we followed our paper, see Trimper et al. (2007), which is modified and extended accordingly. Whereas the previous discussion was primarily focused on isotropic magnetic systems, we are able to derive the mesoscopic evolution equation for a ferroelectric system under quite general conditions as the behavior of the spin moments, a self-organized effective field and its behavior under time reversal symmetry as well as the underlying Lie group properties of the moments. In particular, we have demonstrated that the form of the damping terms is rather universal, although the realization of the effective field in ferroelectric systems is distinct from that of the ferromagnet ones. The reason consists of the different symmetry of the ferroelectric system. While the classical Heisenberg model reflects the isotropic symmetry, the Ising model in a transverse field is anisotropic. The differences are clearly indicated. Consequently the differences lead to a totally different dynamic behavior which is observed in both the reversible propagating part and its damping. Thus the ferroelectric mode becomes a massive one and the life-time of the elementary excitation offers another temperature dependence. In terms of a multi-scale approach the relevant incoming static quantities as the polarization are calculated using the microscopic model. Our approach allows the investigation of both the low and the high temperature phase. They are discussed within dynamic scaling theory. As a further step we are interested in systems where magnetic and polarization behavior is coupled leading to a new class of systems known as multiferroicity reviewed recently by Wang et al. (2009). Such systems are characterized by the occurrence of spiral structures manifested in an inhomogeneous ground state as shown in Eq. (19). In the quantum model this phenomena can be described by spin operators without fixed quantization direction, as studied by Michael & Trimper (2011). In this chapter we studied a simple model allowing a sequence of phases, namely for  $T > T_c$  the system is paraelectric as well as paramagnetic. Reducing the temperature the system offers a phase transition at  $T_c$  into a ferroelectric but paramagnetic phase. When the temperature is lowered further there is at  $T_m$  a transition into the magnetic phase which is due to the multiferroic coupling simultaneously characterized by the parameters of the ferroelectric and the magnetic system. The multiferroic dispersion relation suggests the occurrence of incommensurable structures which can be also interpreted as spiral structure. A related more detailed approach using the mesoscopic formulation is under progress.

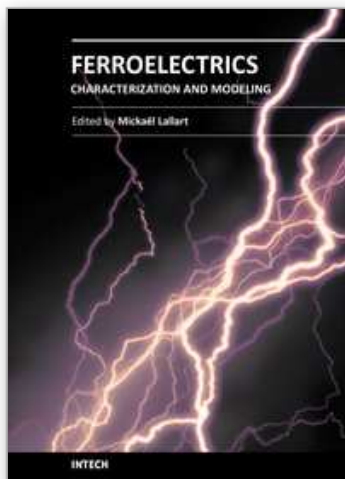
## 7. References

- Blinic, R. & Zeks, B. (1972). Dynamics of order-disorder-type ferroelectrics and anti-ferroelectrics, *Adv. Phys.* 21: 693.
- Blinic, R. & Zeks, B. (1974). *Soft modes in ferroelectrics and antiferroelectrics*, North-Holland, Amsterdam.
- Bose, T. & Trimper, S. (2010). Correlation effects in the stochastic Landau-Lifshitz-Gilbert equation, *Phys. Rev. B* 81(10): 104413.
- Bose, T. & Trimper, S. (2011). Lagrangian formulation of a dissipative magnetic system on a mesoscopic scale, *Euro. Phys. Lett. submitted*.
- Cano, A. & Levanyuk, A. P. (2004). Low-temperature structural phase transitions: Phonon-like and relaxation order-parameter dynamics, *Phys. Rev. B* 70: 064104.
- de Gennes, P. G. (1963). Collective motions of hydrogen bonds, *Solid State Communications* 1: 37.
- Denisov, S. I., Lyutyy, T. V. & Hänggi, P. (2006). Magnetization of nanoparticle systems in a rotating magnetic field, *Phys. Rev. Lett.* 97: 227202.
- Duine, R. A., Núñez, A. S. & MacDonald, A. H. (2007). Thermally assisted current-driven domain-wall motion, *Phys. Rev. Lett.* 98: 056605.
- Eerenstein, W., Mathur, N. D. & Scott, J. (2006). Multiferroic and magnetoelectric materials, *Nature* 442: 759.
- Elliot, R. J. & Wood, C. (1971). The Ising model with a transverse field. i. high temperature expansion, *J. Phys. C: Solid State Phys.* 4: 2359.
- Fiebig, M. (2005). Revival of the magnetoelectric effect, *J. Phys. D: Appl. Phys.* 38: R123.
- Gaunt, D. S. & Domb, C. (1970). Equation of state of the Ising model near the critical point, *J. Phys. C: Solid State Phys.* 3: 1442.
- Gilbert, T. L. (2004). A phenomenological theory of damping in ferromagnetic materials, *IEEE Trans. Magn* 40: 3343.
- He, P.-B. & Liu, W. M. (2005). Nonlinear magnetization dynamics in a ferromagnetic nanowire with spin current, *Phys. Rev. B* 72: 064410.
- Hohenberg, P. C. & Halperin, B. I. (1977). Theory of dynamic critical phenomena, *Rev. Mod. Phys.* 49: 435–479.
- Kühnel, A., Wendt, S. & Wesselinowa, J. (1977). Dynamic behaviour of the Ising model in a transverse field, *physica status solidi (b)* 84: 653.
- Landau, L. D. & Lifshitz, E. M. (1935). On the theory of the dispersion of magnetic permeability in ferromagnetic bodies, *Zeitschr. d. Sowjet.* 8: 153.
- Landau, L. D., Lifshitz, E. M. & Pitaevski, L. P. (1980). *Statistical Physics, Part 2*, Pergamon, Oxford.
- Lines, M. E. & Glass, A. (2004). *Principles and Applications of Ferroelectrics and Related Materials*, Clarendon Press, Oxford.
- Mazenko, G. F. (2003). *Fluctuations, order, and defects*, John Wiley & Sons. Inc Hoboken, New jersey.
- Michael, T. & Trimper, S. (2011). The excitation spectrum of multiferroics at finite temperatures, *Phys. Rev. B accepted*.
- Michael, T., Trimper, S. & Wesselinowa, J. M. (2006). Size and doping effects on the coercive field of ferroelectric nanoparticles: A microscopic model, *Phys. Rev. B* 74: 214113.
- Michael, T., Trimper, S. & Wesselinowa, J. M. (2007). Size effects on static and dynamic properties of ferroelectric nanoparticles, *Phys. Rev. B* 76: 094107.
- Mostovoy, M. (2006). Ferroelectricity in spiral magnets, *Phys. Rev. Lett.* 96: 067601.

- Ohe, J.-i. & Kramer, B. (2006). Dynamics of a domain wall and spin-wave excitations driven by a mesoscopic current, *Phys. Rev. Lett.* 96: 027204.
- Pfeuty, P. & Elliot, R. J. (1971). The Ising model with a transverse field. ii. ground state properties, *J. Phys. C: Solid State Phys.* 4: 2370.
- Stinchcombe, R. B. (1971). Ising model in a transverse field. ii. spectral functions and damping, *J. Phys. C: Solid State Phys.* 6: 2484, 2507.
- Stinchcombe, R. B. (1973). Ising model in a transverse field, *J. Phys. C: Solid State Phys.* 6: 2459.
- Strukov, B. A. & Levnyuk, A. P. (1998). *Ferroelectric Phenomena in Crystals*, Springer, Berlin.
- Tokura, Y. & Seki, S. (2010). Multiferroics with spiral spin order, *Adv. Mater.* 22: 1554.
- Trimper, S., Michael, T. & Wesselinowa, J. M. (2007). Ferroelectric soft modes and Gilbert damping, *Phys. Rev. B* 76: 094108.
- Tserkovnyak, Y., Brataas, A., Bauer, G. E. W. & Halperin, B. I. (2005). Nonlocal magnetization dynamics in ferromagnetic heterostructures, *Rev. Mod. Phys.* 77: 1375–1421.
- Usadel, K. D. (2006). Temperature-dependent dynamical behavior of nanoparticles as probed by ferromagnetic resonance using Landau-Lifshitz-Gilbert dynamics in a classical spin model, *Phys. Rev. B* 73: 212405.
- Van den Brink, J. & Khomskii, D. (2008). Multiferroicity due to charge ordering, *J. Phys.: Condens. Matter* 20 (2008) 434217 (12pp) 20: 434217.
- Wang, K. F., Liu, J. M. & Ren, Z. F. (2009). Multiferroicity: the coupling between magnetic and polarization order, *Adv. Phys.* 58: 321.
- Wang, Y.-L. & Cooper, B. R. (1968). Collective excitations and magnetic ordering in materials with singlet crystal-field ground state, *Phys. Rev.* 172: 539–551.
- Wesselinowa, J. M. (1984). Damping of the transverse and longitudinal excitations of the Ising model in a transverse field, *physica status solidi (b)* 121: 317.
- Wesselinowa, J. M. & Kovachev, S. (2007). Hardening and softening of soft phonon modes in ferroelectric thin films, *Phys. Rev. B* 75: 045411.
- Wesselinowa, J. M., Michael, T. & Trimper, S. (2010). *Handbook of Nanophysics Vol.4*, Taylor & Francis, London, Editor: Klaus Sattler.
- Wesselinowa, J. M., Trimper, S. & Zabrocki, K. (2005). Impact of layer defects in ferroelectric thin films, *J. Phys.: Cond. Mat* 17: 4687.

IntechOpen





## **Ferroelectrics - Characterization and Modeling**

Edited by Dr. Mickaël Lallart

ISBN 978-953-307-455-9

Hard cover, 586 pages

**Publisher** InTech

**Published online** 23, August, 2011

**Published in print edition** August, 2011

Ferroelectric materials have been and still are widely used in many applications, that have moved from sonar towards breakthrough technologies such as memories or optical devices. This book is a part of a four volume collection (covering material aspects, physical effects, characterization and modeling, and applications) and focuses on the characterization of ferroelectric materials, including structural, electrical and multiphysic aspects, as well as innovative techniques for modeling and predicting the performance of these devices using phenomenological approaches and nonlinear methods. Hence, the aim of this book is to provide an up-to-date review of recent scientific findings and recent advances in the field of ferroelectric system characterization and modeling, allowing a deep understanding of ferroelectricity.

### **How to reference**

In order to correctly reference this scholarly work, feel free to copy and paste the following:

Thomas Bose and Steffen Trimper (2011). Mesoscopic Modeling of Ferroelectric and Multiferroic Systems, *Ferroelectrics - Characterization and Modeling*, Dr. Mickaël Lallart (Ed.), ISBN: 978-953-307-455-9, InTech, Available from: <http://www.intechopen.com/books/ferroelectrics-characterization-and-modeling/mesoscopic-modeling-of-ferroelectric-and-multiferroic-systems>

**INTECH**  
open science | open minds

### **InTech Europe**

University Campus STeP Ri  
Slavka Krautzeka 83/A  
51000 Rijeka, Croatia  
Phone: +385 (51) 770 447  
Fax: +385 (51) 686 166  
[www.intechopen.com](http://www.intechopen.com)

### **InTech China**

Unit 405, Office Block, Hotel Equatorial Shanghai  
No.65, Yan An Road (West), Shanghai, 200040, China  
中国上海市延安西路65号上海国际贵都大饭店办公楼405单元  
Phone: +86-21-62489820  
Fax: +86-21-62489821



© 2011 The Author(s). Licensee IntechOpen. This chapter is distributed under the terms of the [Creative Commons Attribution-NonCommercial-ShareAlike-3.0 License](https://creativecommons.org/licenses/by-nc-sa/3.0/), which permits use, distribution and reproduction for non-commercial purposes, provided the original is properly cited and derivative works building on this content are distributed under the same license.

IntechOpen

IntechOpen