

## Ferroelectric soft modes and Gilbert damping

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Motivated by the progress of a multiscale approach in magnetic materials, the dynamics of the Ising model in a transverse field as a basic model for ferroelectric order-disorder phase transition is reformulated in terms of a mesoscopic model and inherent microscopic parameters. The dynamics is governed by a reversible propagating part giving rise to excitation energy which offers a soft mode behavior at the critical temperature. The lifetime of the excitation is obtained by including damping terms which are derived under the condition of breaking the time reversal symmetry due to dissipation. The final dynamical equation reminds of the Gilbert damping appearing for an isotropic ferromagnet, but with an anisotropic effective field and consequently a different physical behavior. The temperature dependence of the excitation energy and its lifetime is discussed. The model is extended by including an additive noise term which modifies the excitation spectrum.

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### I. INTRODUCTION

The analysis of the Ising model in a transverse field (TIM) dates back to the early 1960s, where de Gennes<sup>1</sup> studied the model to elucidate the order-disorder transition in some double-well ferroelectric systems such as  $\text{KH}_2\text{PO}_4$  (KDP).<sup>2,3</sup> Since the mean-field theory<sup>4</sup> (see also Ref. 3) already gave a qualitative agreement with experimental data, the model was increasingly considered as one of the basic models for ferroelectrics of order-disorder type.<sup>5,6</sup> Whereas the displacive-type ferroelectric offers a mainly phononlike dynamics, a relaxation dynamics is attributed to the order-disorder type.<sup>7</sup> The model Hamiltonian for the second class is

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

where  $S^x$  and  $S^z$  are components of spin- $\frac{1}{2}$  operators. The coupling strength between nearest neighbors  $J_{ij}$  is assumed to be positive and likewise the transverse field is also positive,  $\Omega > 0$ . The symbol  $\langle ij \rangle$  means summation over all pairs of nearest neighbors. 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<sup>8</sup> is described by Eq. (1), where  $\Omega$  plays the role of the crystal field. The model had been extensively studied with different methods in Refs. 9–11, especially a Green's function technique.<sup>12</sup> It offers a finite excitation energy and a phase transition. A more refined study using special decoupling procedures for the Green's function<sup>13</sup> allows also the calculation of the damping of the transverse and longitudinal excitations.<sup>14</sup> Very recently, we have applied successfully the TIM to get the polarization and the hysteresis of ferroelectric nanoparticles<sup>15</sup> and also the excitation and damping of such nanoparticles.<sup>16</sup> Despite the great progress in explaining ferroelectric properties based on the microscopic model in Eq. (1), the system should be studied by using classical spin vectors as in the corresponding magnetic case.<sup>17</sup> The aim of the present paper is to analyze the TIM in its classical ver-

sion capturing all the inherent quantum properties of the spin operators. Additionally, we are interested in damping effects. Such an interest is also stimulated by the recent progress in studying ferromagnets, where the classical magnetic moments are assumed to obey the Landau-Lifshitz equation<sup>17</sup> and damping effects are included by the so called Gilbert damping (see. Ref. 18). The temperature-dependent dynamical behavior of ferromagnetic nanoparticles is studied within a classical spin model,<sup>19</sup> while a nonlinear magnetization in ferromagnetic nanowires with spin current is discussed in Ref. 20. Even the magnetization of nanoparticles in a rotating magnetic field is analyzed, based on the Landau-Lifshitz equation.<sup>21</sup> The dynamics of a domain wall driven by a mesoscopic current<sup>22</sup> as well as the thermally assisted current-driven domain wall<sup>23</sup> were considered recently. In the present paper, we derive under rather general assumptions the damping part of the evolution equation which is similar to the Gilbert damping. However, a totally different effective field occurs in comparison to magnetic materials. Insofar our approach is a multiscale one based on a mesoscopic equation of motion, capturing the algebraic properties of the quantum model, and on microscopic parameters of the underlying quantum system.

### II. SOFT MODE WITHIN THE CLASSICAL APPROACH

The model under consideration is the TIM with the Hamiltonian defined in Eq. (1). The spin operators obey the equation of motion

$$i\hbar \frac{\partial S_r^\alpha}{\partial t} = [H, S_r^\alpha]. \quad (2)$$

Using the Hamiltonian and Eq. (2), we get

$$\frac{\partial S_r^x}{\partial t} = - \sum_{j(r)} J_{rj} S_j^z S_r^y, \quad \frac{\partial S_r^y}{\partial t} = - \Omega S_r^z + \sum_{j(r)} J_{rj} S_j^z S_r^x,$$

$$\frac{\partial \vec{S}_r^z}{\partial t} = +\Omega \vec{S}_r^y. \quad (3)$$

The effective field is defined by

$$\vec{h}_r^\alpha = -\frac{\delta H}{\delta \vec{S}_r^\alpha}.$$

The changeover to the classical limit  $\vec{S}_r \rightarrow \vec{S}_r \hbar S(S+1)$  is carried out by  $\hbar \rightarrow 0$  and  $S \rightarrow \infty$ . The discrete equation of motion for the corresponding vector field  $\vec{S}_r(t)$  reads

$$\frac{\partial \vec{S}_r}{\partial t} = \vec{h}_r \times \vec{S}_r \quad \text{with } \vec{h}_r = \left( \Omega, 0, \sum_{j(r)} J_{rj} S_j^z \right). \quad (4)$$

Within the classical limit, the spin vector has a spatially fixed length  $\vec{S}^2$  reflecting the conservation of the spin operator  $\vec{S}^2$  by  $[H, \vec{S}^2]=0$ . In general, the length can be a function of the temperature. Further, the equation of motion can be written in a continuous description which should be adequate especially nearby to the phase transition in the form

$$\frac{\partial \vec{S}(\vec{x}, t)}{\partial t} = \vec{h}(\vec{x}, t) \times \vec{S}(\vec{x}, t). \quad (5)$$

The effective field is also expressed in a continuous approximation as

$$\vec{h}(\vec{x}, t) = (\Omega, 0, J\kappa S^z(\vec{x}, t)) \quad \text{with } \kappa = a^2 \nabla^2 + z, \quad (6)$$

where  $J$  is the coupling strength between the  $z$  nearest neighbors and  $a$  is the lattice spacing in a simple cubic lattice. This relation follows from

$$\sum_{j(r)} J_{rj} S_j^z \equiv \sum_{j(r)} J_{rj} (S_j^z - S_j^z + S_j^z) \approx J(a^2 \nabla^2 + z) S^z(\vec{x}).$$

Let us emphasize that due to the TIM, Eq. (1), the effective field  $\vec{h}$  is an anisotropic one, while in the Heisenberg model the effective field is isotropic.<sup>18</sup> In order to solve the evolution equation (5), we make the ansatz  $\vec{S}(\vec{x}, t) = \vec{m}(\vec{x}) + \vec{\varphi}(\vec{x}, t)$ , where  $\vec{m}(\vec{x}) = m_x \vec{e}_x + m_z \vec{e}_z$  is a time-independent but temperature-dependent vector in the  $x$ - $z$  plane as suggested by Eq. (1). In the case that  $\vec{m}$  is spatially independent, it describes the homogeneous polarization. In first order, the fluctuating field  $\vec{\varphi}$  obeys

$$\dot{\vec{\varphi}} = \vec{h}_1 \times \vec{m} + \vec{h}_0 \times \vec{\varphi},$$

with  $\vec{h}_0 = (\Omega, 0, Jzm_z)$  and  $\vec{h}_1 = (0, 0, J\kappa\varphi_z)$ . In deriving the last result, we have used  $\vec{m} \times \vec{h}_0 = 0$ , which defines the direction of the homogeneous polarization. The last relation gives rise to the two solutions

$$(i) \quad m_z(T) \neq 0, \quad m_x = \frac{\Omega}{Jz} \quad \text{if } T < T_c,$$

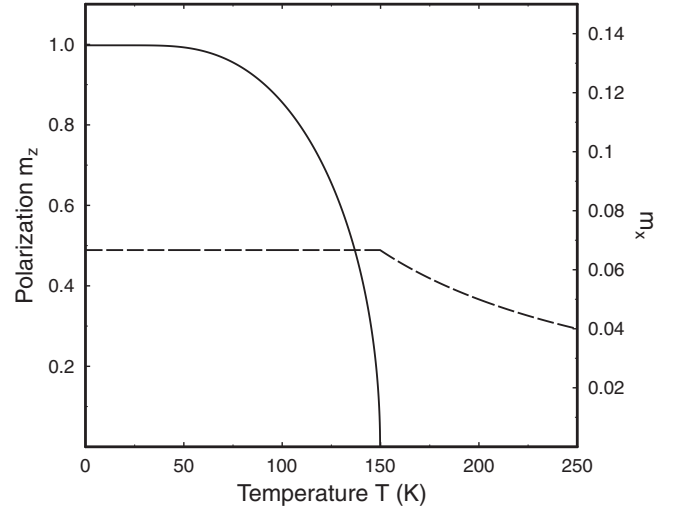


FIG. 1. Temperature dependence of  $m_z(T)$  (solid line) and  $m_x(T)$  (dashed line) based on the microscopic model with  $\Omega=10$  K and  $J=25$  K.

$$(ii) \quad m_z = 0, \quad m_x(T) \neq \frac{\Omega}{Jz} \quad \text{if } T > T_c. \quad (7)$$

In the low temperature regime, the  $x$  component of the polarization is temperature independent. At  $T_c$ , it results to  $m_x(T_c) = \Omega/Jz$ . In the high temperature regime,  $m_x$  decreases with increasing temperature. In terms of a multiscale approach, the temperature dependence of  $m_x$  and  $m_z$  is calculated using the microscopic model [Eq. (1)]. In mean-field approximation, one gets  $m_x(T) = \tanh \frac{\Omega}{T}$ . The results are shown in Fig. 1. Notice that a finite phase temperature is only realized if  $\Omega < Jz$ .

Now let us discuss the low temperature phase  $T < T_c$ . The fluctuating field satisfies for finite  $m_z \neq 0$  the coupled equations

$$\dot{\varphi}_x(\vec{q}, t) = -Jzm_z\varphi_y(\vec{q}, t), \quad \dot{\varphi}_z(\vec{q}, t) = \Omega\varphi_y(\vec{q}, t),$$

$$\dot{\varphi}_y(\vec{q}, t) = Jzm_z\varphi_x(\vec{q}, t) - [\Omega - m_x J\kappa(\vec{q})]\varphi_z(\vec{q}, t). \quad (8)$$

Here, we have used the Fourier transformed  $\kappa(\vec{q}) = z - (a\vec{q})^2$ , whereas the approach is only valid in the long wavelength limit  $aq \ll 1$ . The set of equations (8) allows a nontrivial solution  $\varphi \propto \exp[i\varepsilon(\vec{q})t]$  if the excitation energy  $\varepsilon_l(\vec{q})$  obeys

$$\varepsilon_l(\vec{q}, T) = \sqrt{A_l^2 + B_l q^2},$$

$$A_l(T) = Jzm_z, \quad B_l = \frac{a^2 \Omega^2}{z}. \quad (9)$$

The excitation energy below the critical temperature is dominated by the coupling  $J$ ,

$$\varepsilon_l(\vec{q}) = Jz \sqrt{m_z^2 + m_x^2 \frac{a^2 q^2}{z}},$$

and the dispersion relation [Eq. (9)] reveals the typical soft mode behavior,

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

in accordance with the microscopic behavior.<sup>4,12</sup> In a scaling form, the dispersion reads

$$\varepsilon_l(\vec{q}, \xi_c) = \xi_c^{-1} f_l(q \xi_c),$$

where  $\xi_c$  is the correlation length,  $f_l(x) \propto \sqrt{1+x^2}$  is the scaling function, and the critical exponents fulfill  $\nu = \beta$ . The evolution equations for the fluctuating field can be solved, leading to

$$\vec{\varphi}(\vec{q}, t) = R_l(\vec{q}) \left( \frac{J_z m_z e^{i\pi/2}}{\varepsilon_l(\vec{q})}, 1, \frac{\Omega e^{-i\pi/2}}{\varepsilon_l(\vec{q})} \right) \exp[i\varepsilon_l(\vec{q})t], \quad (10)$$

where  $R_l(\vec{q})$  is the amplitude of the excitation mode determined by the initial condition. A phase shift appears between the different components. Making the same approach for the high temperature phase with  $m_z=0$ , the dispersion relation offers the same structure as below  $T_c$ , however, with different coefficients,

$$\varepsilon_h(\vec{q}) = \sqrt{A_h^2 + B_h \vec{q}^2},$$

$$A_h^2 = \Omega[\Omega - m_x(T)J_z], \quad B_h = m_x(T)Ja^2\Omega. \quad (11)$$

Above the critical temperature, the excitation energy is dominated by the tunneling energy  $\Omega$  and reads

$$\varepsilon_h(\vec{q}) = \Omega \sqrt{\frac{m_x(T)}{m_x(T_c)} \frac{a^2 \vec{q}^2}{z} + \frac{m_x(T_c) - m_x(T)}{m_x(T_c)}}.$$

Notice that in the high temperature phase, the relation  $m_x(T)/m_x(T_c) < 1$  is fulfilled as one can also observe in Fig. 1. The fluctuation field  $\vec{\varphi}(\vec{q})$  exhibits a similar form as for  $T < T_c$ , but setting  $m_z=0$  and replacing  $\varepsilon_l$  by  $\varepsilon_h$ . Thus, the field  $\vec{\varphi}$  is continuous at the phase transition. The dispersion relations, given by Eq. (11), show likewise a soft mode behavior because the critical temperature  $T_c$  is defined by  $m_x(T=T_c) = \frac{\Omega}{J_z}$  according to Eq. (7). In the vicinity of  $T_c$ , it results to

$$A_h^2 = J_z \Omega [m_x(T_c) - m_x(T)] \simeq -J_z \Omega \frac{dm_x(T_c)}{dT} (T - T_c).$$

Combined with the mean-field result  $m_x = \tanh(\frac{\Omega}{T})$ , the mode at  $\vec{q}=0$  satisfies

$$\varepsilon_h(\vec{q}=0) = \sqrt{\frac{J_z \Omega^2}{T_c^2} \left[ 1 - \left( \frac{\Omega}{zJ} \right)^2 \right]} (T - T_c)^{1/2}. \quad (12)$$

This relation is only valid provided that  $\Omega < Jz$ . In the opposite case, there is no phase transition at finite temperatures. Furthermore, the stiffness constant  $B_h$  depends on the temperature via  $m_x(T)$  and remains finite at  $T_c$  with  $B(T_c) = \frac{\Omega^2 a^2}{z}$ .

### III. DAMPING EFFECT

Now let us generalize the equation of motion [Eq. (5)] by including damping effects. Microscopically, there is a great diversity of the origin of damping effects. An intrinsic reason

for damping effects might be the mutual interaction between the excitation modes for different wave vectors. This has been demonstrated within the TIM in Ref. 14 in second order of the coupling strength  $J$ . In that case, the Green's function offers poles, the imaginary part of which has been considered as the damping of the elementary excitation. Recently, we have studied within the TIM the influence of layer defects to the damping of the elementary modes in ferroelectric thin films.<sup>24</sup> The analysis can be generalized for ferroelectric nanoparticles, where the interaction of those can also lead to finite lifetimes of the excitation modes.<sup>16</sup> Likewise, the damping effects of the excitation modes can be originated by a coupling to phonons. Due to the interaction of the pseudospin excitations with the phonon modes, there results a damping of the excitation modes which is shown recently in Ref. 25. The intention of the present paper is to discuss the general form of the evolution equation [Eq. (5)] with additional damping part. As mentioned above, this can be achieved by taking into account the intrinsic interaction of the modes or by a coupling to additional degrees of freedom such as defects or phonons. As the result, we expect that Eq. (5) has to be supplemented by a damping term  $\vec{D}$ , resulting in

$$\frac{\partial \vec{S}(\vec{x}, t)}{\partial t} = \vec{h}(\vec{x}, t) \times \vec{S}(\vec{x}, t) + \vec{D}(\vec{S}). \quad (13)$$

The damping term  $\vec{D}$  has a pure dynamical origin, so possible static parts in the final equation [see Eq. (17)] should be subtracted. Although due to the spin wave damping the length of  $\vec{S}$  is not conserved, one concludes that the a non-trivial damping part is oriented into the direction of the effective field  $\vec{h}$ . Obviously, the damping fulfills  $\vec{D} < 0$ , i.e.,

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

Following the general concept of phase transitions,<sup>26</sup> let us make the ansatz

$$D_\alpha = -\Lambda_{\alpha\beta}(\vec{S}) h_\beta. \quad (14)$$

In the case of a positive definite matrix  $\Lambda_{\alpha\beta}$ , independent of  $\vec{S}$ , the last relation corresponds to the conventional relaxation dynamics for a nonconserved quantity. To get higher order terms, one can expand the matrix  $\Lambda_{\alpha\beta}$  in powers of  $\vec{S}$  leading to

$$\Lambda_{\alpha\beta} = \Lambda_{\alpha\beta}^{(0)} + \Lambda_{\alpha\beta\gamma}^{(1)} S_\gamma + \Lambda_{\alpha\beta\gamma\delta}^{(2)} S_\gamma S_\delta + O(\vec{S}^3). \quad (15)$$

The expansion parameters, denoted by  $\Lambda$ , will be determined in accordance with the behavior under time reversal and the underlying Lie group properties of the spin vectors  $\vec{S}$ . Whereas the propagating part of the equation of motion, Eq. (5) is invariant under the instantaneous change  $t \rightarrow -t$ ,  $\vec{S} \rightarrow -\vec{S}$ , and  $\vec{h} \rightarrow -\vec{h}$ , the damping part  $\vec{D}$  should break the time reversal invariance. Due to this requirement and the fact that  $\vec{D} \propto \vec{h}$ , we get

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

where  $\tau_1$  plays the role of a relaxation time. The breaking of time reversal symmetry is only realized if the linear term in Eq. (15) disappears. The structure constants of the symmetry group of  $\vec{S}$  are essentially given by the complete antisymmetric tensor  $\epsilon_{\alpha\beta\gamma}$ . Further, the damping should be pointed to the direction of the effective field and consequently the vector  $\vec{D}$  is perpendicular to the propagating part  $\vec{S} \times \vec{h}$ . Summarizing these conditions, let us make the ansatz

$$\Lambda_{\alpha\beta\gamma}^{(1)} = b \epsilon_{\alpha\beta\gamma},$$

$$\Lambda_{\alpha\beta\gamma\delta}^{(2)} = \frac{1}{2\tau_2} [\epsilon_{\alpha\beta\rho} \epsilon_{\rho\gamma\delta} + \epsilon_{\alpha\gamma\rho} \epsilon_{\rho\beta\delta} + \epsilon_{\alpha\delta\rho} \epsilon_{\rho\beta\gamma}]. \quad (16)$$

The form of  $\Lambda_{\alpha\beta\gamma}^{(1)}$  with an arbitrary parameter  $b$  guarantees that a linear term does not occur. In the conventional vector notation, the complete equation of motion now reads

$$\frac{\partial \vec{S}}{\partial t} = \vec{h} \times \vec{S} - \frac{1}{\tau_1} \vec{h} - \frac{1}{\tau_2} \vec{S} \times (\vec{S} \times \vec{h}). \quad (17)$$

Two damping terms arise with the prefactors  $\tau_1$  and  $\tau_2$ . Although the determination of both parameters is beyond the scope of our mesoscopic approach, they should be of the order of a microscopic flip process and become of the same order,  $\tau_1 \approx \tau_2$ . They reflect the influence of the interaction between the excitations or the coupling to other degrees of freedom as discussed before. The last equation is similar to the Landau-Lifshitz equation with Gilbert damping. In contrast to the isotropic ferromagnetic case, the effective field  $\vec{h}$  is in our case an anisotropic one directed in the  $x$ - $z$  plane. As a consequence, the dispersion relations for the excitation energy, Eqs. (9) and (11), are likewise different in comparison to the magnetic case. While isotropic magnetic systems offer a gapless Goldstone mode here due to the transverse field, the dispersion relation becomes soft only for  $T \rightarrow T_c$ .

Making the same procedure as before, we find in the high temperature phase the dispersion relation of the form

$$\omega_h(\vec{q}) = \varepsilon_h(\vec{q}) + i \frac{\Gamma_{1h}(\vec{q})}{2\tau_1} + i \frac{\Gamma_{2h}(\vec{q})}{2\tau_2},$$

$$\Gamma_{1h}(\vec{q}) = J\kappa(\vec{q}), \quad \Gamma_{2h}(\vec{q}, T) = m_x(T)[2\Omega - J\kappa(\vec{q})m_x(T)]. \quad (18)$$

The result is valid in the long wavelength limit and in first order in  $\tau^{-1}$ . The propagating part  $\varepsilon_h(\vec{q})$ , written in Eq. (18), remains unchanged in first order in  $\tau^{-1}$ . Higher order terms give rise to a slightly changed behavior. The appearance of the imaginary parts is related to damping effects, and the fluctuating field offers a behavior like

$$\vec{\varphi}(\vec{q}, t) = R(\vec{q}) \exp \left[ i\varepsilon(\vec{q}) - \frac{\Gamma_1(\vec{q}, T)}{2\tau_1} - \frac{\Gamma_2(\vec{q}, T)}{2\tau_2} \right] t. \quad (19)$$

The inverse function  $\Gamma^{-1}$  plays the role of the lifetime of the excitation energy. In the high temperature phase,  $\Gamma_{1h}$  is tem-

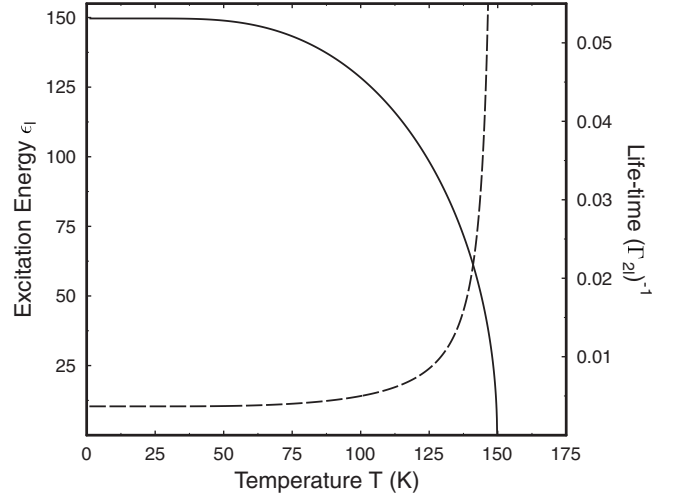


FIG. 2. Excitation energy  $\varepsilon(\vec{q}=0)$  (solid curve) and the lifetime  $(\Gamma_{2l})^{-1}$  (dashed curve) at  $\vec{q}=0$  as function of the temperature at  $\Omega = 10$  K and  $J = 25$  K.

perature independent; however, it is dominated by the exchange coupling  $\Gamma_{1h} \approx Jz$ . The damping function  $\Gamma_{2h}$  offers a weak temperature dependence and it is dominated by the tunneling energy  $\Omega$  with  $\Omega < Jz$ . One gets

$$\Gamma_{2h}(\vec{q}, T = T_c) > \Gamma_{2h}(\vec{q} = 0, T = T_c) = \frac{\Omega^2}{Jz}.$$

A similar relation is also valid for  $T > T_c$ , i.e., the damping is enhanced for short wavelength accurately as the excitation energy. The situation is drastically changed for  $T \leq T_c$ . Likewise, the dispersion relation  $\omega_l(\vec{q}, T)$  offers a real and an imaginary part according to Eq. (18). The real part  $\varepsilon_l(\vec{q}, T)$  remains unchanged in lowest order of  $\tau^{-1}$  and is given by Eq. (9). It characterizes the excitation energy. The finite lifetime of the excitation is related to the temperature and wave vector dependent damping terms. We get

$$\Gamma_{1l}(\vec{q}, T) = J\kappa(\vec{q}) \left[ 1 - \frac{A_l^2}{\varepsilon_l^2(\vec{q})} \right] \equiv \frac{J\kappa(\vec{q})B_l}{\varepsilon_l^2(\vec{q})} q^2, \quad (20)$$

$$\Gamma_{2l}(\vec{q}, T) = \frac{\varepsilon_l^2(\vec{q}) + A_l^2 + \Omega^2}{Jz} \quad \text{with } \kappa(\vec{q}) = z - (a\vec{q})^2.$$

At the critical point, the damping is continuous, i.e., for instance,  $\Gamma_{1l}(\vec{q}, T_c) = \Gamma_{1h}(\vec{q}, T_c)$ . While the lifetime in the high temperature phase is only weakly temperature dependent, it depends on  $T$  in the low temperature regime via  $m_z$  which disappears at  $T_c$  with a critical exponent  $\beta \leq 1/2$ . The temperature dependence of the excitation energy and the relevant lifetime  $(\Gamma_{2l})^{-1}$  of the soft mode at  $\vec{q}=0$  are depicted in Fig. 2. Whereas the excitation energy  $\varepsilon_l$  disappears for  $T \rightarrow T_c$  at  $\vec{q}=0$ , the lifetime  $(\Gamma_{2l})^{-1}$  increases strongly at the phase transition but remains fixed at  $T_c$ . Apparently, one finds



$$\Gamma_{1l}^{-1}(\vec{q}, T_c) < \Gamma_{1l}^{-1}(\vec{q}, T),$$

i.e., the life of the excitation is shorter at the critical temperature as in the low temperature regime. When the system is approaching to the phase transition temperature, the elementary excitation decays more rapidly for wave vector  $\vec{q} \neq 0$ . In view of  $\tau_1 \approx \tau_2$ , one can introduce a total damping constant  $\Gamma_l(\vec{q}, T) = \Gamma_{1l}(\vec{q}, T) + \Gamma_{2l}(\vec{q}, T)$ . In the vicinity of the critical temperature and the long wave limit, it results to

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

The total lifetime is likewise reduced for  $(a\vec{q})^2 \ll 1$  where both damping terms in Eq. (17) contribute to the lifetime of the excitation. A simple power counting reveals that the damping part with  $\tau_1$  is of first order in  $\vec{S}$ , whereas the second part is of second order in  $\vec{S}$  and consequently it is of the same order as the propagating part  $\vec{h} \times \vec{S}$ .

Whereas the present calculations are performed on a mesoscopic level, one can also analyzed the properties of ferroelectric nanoparticles using the microscopic Hamiltonian defined by Eq. (1).<sup>15</sup> 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 with the present analysis and also in qualitative agreement with experimental results.<sup>16</sup>

#### IV. STOCHASTIC EQUATION

To refine the model further, let us include all the residual degrees of freedom, not taken into account so far, in a stochastic force  $\vec{\xi}(\vec{x}, t)$ . Then, Eq. (17) is supplemented by a noise term,<sup>26</sup> leading to the final form

$$\begin{aligned} \frac{\partial \vec{S}}{\partial t} &= \vec{h} \times \vec{S} - \frac{1}{\tau_1} \vec{h} - \frac{1}{\tau_2} \vec{S} \times (\vec{S} \times \vec{h}) + \vec{\xi}(\vec{x}, t), \\ \langle \vec{\xi}_\alpha(\vec{x}, t) \xi_\beta(\vec{x}', t') \rangle &= 2T \delta_{\alpha\beta} \delta(\vec{x} - \vec{x}') \delta(t - t'). \end{aligned} \quad (21)$$

Even such an additive noise term should influence the damping part apparently. Alternatively, one could also discuss a stochastic field which leads to a multiplicative noise. That situation has been considered in Ref. 19 studying ferromagnetic resonance. The influence of a rotating magnetic field is analyzed in Ref. 21. In the framework of the TIM, the situation is more complicated and should be considered separately. Making the same ansatz as before,  $\vec{S} = \vec{m} + \vec{\varphi}$ , Eq. (21) reads in the low temperature phase

$$\frac{\partial \varphi_\alpha(\vec{q}, t)}{\partial t} = Y_{\alpha\beta}(\vec{q}) \varphi_\beta(\vec{q}, t) + \xi_\alpha(\vec{q}, t). \quad (22)$$

Here  $\mathbf{Y}$  is a  $3 \times 3$  matrix,

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

where the coefficients  $A_l$  and  $B_l$  are defined in Eq. (9). From here, we obtain the Green's function via

$$G_{\alpha\beta}(t, t') = \left\langle \frac{\delta \varphi_\alpha(t)}{\delta \xi_\beta(t')} \right\rangle, \quad t > t'.$$

After performing Fourier transformation, the Green's function is simply

$$\mathbf{G}(\vec{q}, \omega) = -[i\omega \mathbf{I} + \mathbf{Y}(\vec{q})]^{-1}.$$

As the result, the Green's function is written in lowest order in  $\tau$  as

$$G_{\alpha\beta} = \frac{g_{\alpha\beta}(\vec{q}, \omega)}{[\omega + \omega_l(\vec{q})][\omega - \omega_l^*(\vec{q})][\omega - \omega_d(\vec{q})]},$$

$$\omega_l(\vec{q}) = \varepsilon_l(\vec{q}) + i \frac{\Gamma_{1l}(\vec{q})}{2\tau_1} + i \frac{\Gamma_{2l}(\vec{q})}{2\tau_2}, \quad \omega_d(\vec{q}) = \frac{\Gamma_1(\vec{q}) A_l^2}{\tau_1 [\varepsilon_l^2(\vec{q}) - A_l^2]}. \quad (23)$$

The influence of the noise is twofold. The dispersion relations of the low temperature phase, obtained already in Eqs. (9) and (20), are reconfirmed as the complex poles  $\omega_l(\vec{q})$  and  $\omega_l^*(\vec{q})$  of the Green's function. Otherwise, there appears an additional pure imaginary pole  $\omega_d(\vec{q})$ . This mode is a dissipative one which is originated by the stochastic force. In lowest order in  $\tau^{-1}$ , the mode is only influence by  $\tau_1$ . The matrix elements are given by

$$\begin{aligned} g_{11} &= -\omega^2 - i\omega \left[ \frac{\Omega + \varepsilon_l^2}{J_z \tau_2} + \frac{J\kappa(\vec{q})}{\tau_1} \right] + B_l q^2, \\ g_{22} &= \omega^2 - i\omega \left[ \frac{\varepsilon_l^2}{J_z \tau_2} + \frac{J\kappa(\vec{q})}{\tau_1} \right], \\ g_{33} &= -\omega^2 - i\omega \frac{2A_l^2 + \Omega^2}{J_z \tau_2} + A_l^2, \\ g_{12} &= A_l \left[ i\omega - \frac{J\kappa}{\tau_1} \right] = -g_{21}, \quad g_{23} = \frac{i\omega B_l q^2}{\Omega} = -\frac{B_l q^2 g_{32}}{\Omega^2}, \\ g_{13} &= \frac{B_l q^2}{\Omega} \left[ A_l - \frac{i\omega m_z}{\tau_2} \right] = \frac{B_l q^2 g_{31}}{\Omega^2}. \end{aligned} \quad (24)$$

To illustrate the influence of the noise term, the special case  $m_z = 0$  and the inclusion of damping proportional to  $\tau_1^{-1}$  in Eq. (17) are considered. The coupled set of equations for the time-dependent part  $\vec{\varphi}(\vec{q}, t)$  reads

$$\dot{\varphi}_x = \xi_x,$$

$$\begin{aligned}\dot{\varphi}_y &= [m_x J \kappa(\vec{q}) - \Omega] \varphi_z + \xi_y, \\ \dot{\varphi}_z &= \Omega \varphi_y - \frac{1}{\tau_1} J \kappa(\vec{q}) \varphi_z + \xi_z.\end{aligned}\quad (25)$$

The first equation can be immediately solved. It results to

$$\langle \varphi_x^2(\vec{x}, t) \rangle = \varphi_x^2(\vec{x}, 0) + 2Tt. \quad (26)$$

Due to the stochastic force, the  $x$  component of the fluctuating field offers a diffusive behavior. The remaining Green's function is then a  $2 \times 2$  matrix,

$$\mathbf{G}(\omega, \vec{q}) = \frac{1}{[\omega - \omega_h^*(\vec{q})][\omega + \omega_h(\vec{q})]} \times \begin{pmatrix} i\omega - \frac{\Gamma_{1h}(\vec{q})}{\tau_1} & \Omega - m_x J \kappa(\vec{q}) \\ -\Omega & i\omega \end{pmatrix}. \quad (27)$$

The poles of this function are already given in Eq. (18). The Ising model in a transverse field shows cross correlation which is also visible in the correlation function defined by

$$C_{\alpha\beta}(\vec{q}, \omega) = \langle \varphi_\alpha(\vec{q}, \omega) \varphi_\beta^\dagger(\vec{q}, \omega) \rangle. \quad (28)$$

The fluctuation-dissipation theorem is fulfilled,

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

The correlation function follows

$$\mathbf{C} = \frac{2T}{[\omega^2 - \varepsilon_h^2(\vec{q})]^2 + \left(\frac{\Gamma_{1h}(\vec{q})}{\tau_1}\right)^2} \times \begin{pmatrix} \omega^2 - \varepsilon_h^2(\vec{q}) + \left(\frac{\Gamma_{1h}(\vec{q})}{\tau_1}\right)^2 & -\frac{\Gamma_{1h}(\vec{q})}{\tau_1} [\Omega - m_x J \kappa(\vec{q})] \\ -\frac{\Gamma_{1h}(\vec{q})}{\tau_1} \Omega & \omega^2 - \varepsilon_h^2(\vec{q}) \end{pmatrix}. \quad (29)$$

In our context, the stochastic equations with an additive noise term do not give more information as the conventional

equations. The situation is different for a multiplicative noise where, for instance, the effective field  $\vec{h}$  is supplemented by a stochastic force. This behavior will be discussed elsewhere.

## V. CONCLUSIONS

Motivated by several theoretical activities in describing damping effects in magnetic materials, we have studied a 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 ferroelectrics. 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 such as the behavior of the moments and the effective field under time reflection 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. Consequently, this leads to a totally different dynamical behavior which is observed in both the reversible propagating part and in its damping. Thus, the ferroelectric mode becomes a massive one and the lifetime of the elementary excitation offers another temperature dependence. In terms of a multiscale approach, the relevant incoming static quantities such as the polarization are calculated using the microscopic model. Our approach allows the investigation of both the low and the high temperature phase. The model seems also appropriate to discuss the properties of ferroelectric nanoparticles as discussed in Refs. 15 and 16.

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