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A method for the numerical simulation of the thermal magnetization fluctuations in micromagnetics

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Abstract. A new method for the numerical modelling of the thermal fluctuations in micromagnetic systems is presented. The approach is based on the set of stochastic Langevin equations, which are derived from the energy expression for the system studied. The correlation matrix of the corresponding random forces required to perform numerical simulations is evaluated using the fluctuation-dissipation theorem following a transformation to the normal coordinates. The method is tested for the finite 1D chain of classical magnetic moments. The temperature dependence of the average magnetization deviation $\Delta M/M(0)$ exhibits good agreement with analytical theory.

1. Introduction

The collective magnetic excitations in ferromagnetic materials are responsible for a variety of different phenomena, like spin waves, superparamagnetism and the magnetic after-effect. The micromagnetic equilibrium states can be metastable and thermally induced irreversible transitions may occur over energy barriers arising from the crystal and the magnetostatic anisotropy.

A theoretical study of the thermally activated remagnetization processes for a fine single-domain particle was carried out by Brown [1,2]. The thermal agitation forces were represented by a 'random-field' term. The Gilbert equation of motion for the magnetization was then replaced by a Langevin equation and an analytical treatment was possible close to any stationary points where this equation could be linearized.

Most micromagnetic systems, however, have a rather large number of degrees of freedom, so a numerical approach is required. In sections 2 and 3 we present such a method for the simulation of small magnetization fluctuations about some local equilibrium. As a simple test, we applied the method to a finite 1D chain of classical spins to compare our data with analytical results obtained from the spin-wave theory. The implementation and the discussion of this application is described in section 4.

2. Theory

Consider a closed system at equilibrium that is subdivided into a large number of subsystems. Let x_i be a set of classical variables that describe the deviation of the subsystems from equilibrium ($\overline{x_i} = 0$). We consider quasistationary [3] fluctuations of x_i from their mean

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values and represent them as a column vector x. We assume that the vector x characterizes a definite state of partial equilibrium. This means that the relaxation time for the establishment of internal thermodynamic equilibrium within the subsystems is much less than the time required to reach the equilibrium state for the system as a whole (quasistationarity).

The macroscopic equations of motion involving those variables are in general non-linear ($dx_i/dt = f(x_j)$). If the values x_i are sufficiently small, we can expand the time derivatives in powers of x_i retaining only the linear terms. We then obtain a system of linear differential equations describing the relaxation of small deviations in the absence of any thermal perturbations [3]:

$$\frac{dx_i}{dt} = \sum_j L_{ij} x_j \tag{1}$$

or in matrix notation

$$\frac{dx}{dt} = \mathbf{L}x. \tag{2}$$

To derive the set of Langevin equations, we must express (1) in the form

$$\frac{dx_i}{dt} = -\sum_j \gamma_{ij} X_j + f_i. \tag{3}$$

Here X_j are thermodynamically conjugate variables defined by [3]

$$X_j = -\frac{\partial S}{\partial x_j} \tag{4}$$

where S is the entropy. For a closed system consisting of a body in an external medium, equation (4) can be written as [4]

$$X_j = \frac{1}{kT}\frac{\partial E}{\partial x_j} = X_j(x_i) \tag{5}$$

where E is the free energy of the body expressed in terms of x_j.

The coefficients γ_{ij} in (3) are the kinetic coefficients and the variables f_i represent random forces responsible for the spontaneous fluctuations. The statistical properties of these random forces are specified to be compatible with the known correlation properties of the fluctuations x_i:

$$\langle f_i(t)\rangle = 0 \qquad \langle f_i(t) f_j(0)\rangle = \left(\gamma_{ij} + \gamma_{ji}\right)\delta(t). \tag{6}$$

The second expression in (6) is a simple form of the fluctuation-dissipation theorem [5].

To evaluate the variables X_j we expand the free energy E about the equilibrium value E_0 up to the second power of small quantities x_i. First order terms in this expansion vanish and we obtain

$$E = E_0 + \frac{1}{2}\sum_{i,j} A_{ij} x_i x_j = E_0 + \frac{1}{2} x^T \mathbf{A} x. \tag{7}$$

In our case the symmetric energy matrix $\mathbf{A}$ can be evaluated from the micromagnetic energy expression. Due to the interactions between the different subsystems (exchange and magnetostatic interactions between the magnetic moments), the matrix $\mathbf{A}$ is non-diagonal. For this reason, the thermodynamically conjugate variables X_i are not simply proportional to the corresponding x_i but are given by

$$X_i = \frac{1}{kT}\sum_j A_{ij}x_j. \tag{8}$$

In principle, one can solve the system (8) to calculate the variables x_j as a function of X_i and then substitute the result into (1) to obtain the desired form (3). It is also useful, however, to perform a transformation to the normal coordinates of the system where the energy matrix is diagonal since it is then possible to obtain information about the system normal modes.

A transformation $\boldsymbol{x} = \mathbf{Q}\boldsymbol{y}$, or $\boldsymbol{y} = \mathbf{Q}^T\boldsymbol{x}$ can be performed using an orthogonal matrix $\mathbf{Q}$ chosen in such a way that the matrix $\mathbf{D} = \mathbf{Q}^T\mathbf{A}\mathbf{Q}$ is diagonal:

$$E = E_0 + \frac{1}{2}\boldsymbol{x}^T\mathbf{A}\boldsymbol{x} = E_0 + \frac{1}{2}\boldsymbol{y}^T\mathbf{Q}^T\mathbf{A}\mathbf{Q}\boldsymbol{y} = E_0 + \frac{1}{2}\boldsymbol{y}^T\mathbf{D}\boldsymbol{y} = E_0 + \frac{1}{2}\sum_i D_{ii}y_i^2. \tag{9}$$

The variables y_i represent the amplitudes of the normal modes and in the new coordinate system, the thermodynamically conjugate variables are proportional to the corresponding displacements:

$$Y_i = \frac{1}{kT}\frac{\partial E}{\partial y_i} = \frac{D_{ii}}{kT}y_i. \tag{10}$$

Applying the same orthogonal transformation to the linearized equations of motion and adding random forces to the right side, we obtain

$$\frac{\mathrm{d}y_i}{\mathrm{d}t} = \sum_j K_{ij}y_j + f_i \tag{11}$$

where the matrix $\mathbf{K}$ is given by $\mathbf{K} = \mathbf{Q}^T\mathbf{L}\mathbf{Q}$. Substituting (10) into (11) we obtain a multivariate Langevin equation of the form

$$\frac{\mathrm{d}y_i}{\mathrm{d}t} = kT\sum_j \frac{K_{ij}}{D_{jj}}Y_j + f_i = -\sum_j \gamma_{ij}Y_j + f_i. \tag{12}$$

The statistical properties of the random forces are then given by

$$\langle f_i(t)\rangle = 0$$

$$\langle f_i(0)f_j(t)\rangle = (\gamma_{ij} + \gamma_{ji})\,\delta(t) = -kT\left(\frac{K_{ij}}{D_{jj}} + \frac{K_{ji}}{D_{ii}}\right)\delta(t) = \mu_{ij}\,\delta(t). \tag{13}$$

3. Numerical simulations

Equation (13) is not suitable for numerical simulations because of the presence of the delta function. Integrating over a finite time interval Δt, we obtain a set of finite-difference Langevin equations in the normal coordinates:

$$y_i(t + \Delta t) = y_i(t) + \sum_j K_{ij} y_j \, \Delta t + F_i. \tag{14}$$

The statistical properties of the random variables F_i can be deduced from (12):

$$\langle F_i \rangle = 0 \qquad \langle F_i F_j \rangle = \mu_{ij} \, \Delta t. \tag{15}$$

The problem of the optimal choice for the time step Δt should be considered separately for each concrete system. Here we only mention that it obviously should be much larger than the typical correlation time for the random forces [3]:

$$\Delta t \gg \frac{\hbar}{kT}. \tag{16}$$

The statistical properties of the collective excitations of the magnetization can be calculated using the following procedure.

(i) The equilibrium state is determined using any standard method of numerical micromagnetics (see, for example, [6, 7]). For this equilibrium state, the matrices **L**, **A** and the corresponding orthogonal transformation matrix **Q** are evaluated.

(ii) The correlation matrix of the random forces μ is then evaluated.

(iii) The vector x of the moment deviations from equilibrium is initialized as $x = 0$.

(iv) The vector of normal coordinates $y = \mathbf{Q}^T x$ is evaluated.

(v) The set of Langevin finite-difference equations (14) is used to update the normal coordinates $y(t) \rightarrow y(t + \delta t)$. This step is performed several hundred times before starting measurements of the physically interesting quantities (to bring the system into thermal equilibrium).

(vi) The vector $x(t + \delta t) = \mathbf{Q}y(t + \delta t)$ of moment deviations at successive time intervals is used to evaluate the average of physical quantities of interest (e.g. the average magnetization).

4. Implementation of the numerical model

The method described in sections 2 and 3 is now applied to a finite 1D chain of N classical spins in order to test its validity. The length of the chain is taken to be smaller than the coherence length [8] so that ferromagnetic order is preserved. For this simple system even the dynamical properties can be studied successfully by numerical methods [9, 10, 11], but here we focus our attention on thermodynamic quantities like the average magnetization, so that our results can be compared with analytical theory.

The spins at the end of the chain are here considered to be fixed. For sufficiently low temperatures ($T \ll T_c$) the equilibrium magnetization is near the saturation value: $\langle M_z(T) \rangle \simeq M_s$. A natural choice for the thermodynamic variables of the theory is the spin components (S_i^x, S_i^y, $i = 2, \ldots, N - 1$), since their ensemble and time averages vanish.

These constitute a set of $2(N-2)$ degrees of freedom that can support $2(N-2)$ normal modes.

The motion of the spins in the absence of thermal excitations is described by the non-linear Landau–Lifshitz differential equation:

$$\hbar \frac{\mathrm{d}\boldsymbol{S}_i}{\mathrm{d}t} = \boldsymbol{\mu}_i \times \boldsymbol{B}_i + \alpha\left[\hat{\boldsymbol{\mu}}_i \times \left(\boldsymbol{\mu}_i \times \boldsymbol{B}_i\right)\right] \tag{17}$$

where $\boldsymbol{\mu}_i$ is the magnetic moment of the spin at site i, $\boldsymbol{B}_i$ is the local effective field and α denotes a dissipation constant.

Equation (2) for our system takes the form

$$\begin{aligned} \frac{\mathrm{d}S_i^x}{\mathrm{d}t} &= \sum_j L_{ij}^{xx} S_j^x + \sum_j L_{ij}^{xy} S_j^y \\ \frac{\mathrm{d}S_i^y}{\mathrm{d}t} &= \sum_j L_{ij}^{yx} S_j^x + \sum_j L_{ij}^{yy} S_j^y \end{aligned} \tag{18}$$

where the matrix $\mathbf{L}$ can be obtained in the limit of small excitations ($S_i^x, S_i^y \ll S$) by linearization of (17):

$$\begin{aligned} L_{ij}^{xx} &= -\frac{2JS\alpha}{\hbar}(2\delta_{i,j} - \delta_{i-1,j} - \delta_{i+1,j}) \\ L_{ij}^{yx} &= \frac{2JS}{\hbar}(-2\delta_{i,j} + \delta_{i-1,j} + \delta_{i+1,j}) \\ L_{ij}^{xy} &= \frac{2JS}{\hbar}(2\delta_{i,j} - \delta_{i-1,j} - \delta_{i+1,j}) \\ L_{ij}^{yy} &= -\frac{2JS\alpha}{\hbar}(2\delta_{i,j} - \delta_{i-1,j} - \delta_{i+1,j}). \end{aligned} \tag{19}$$

The spins are coupled by the Heisenberg exchange interaction. The energy can be expanded as in (7):

$$E = E_0 + \frac{1}{2}\sum_{i,j}[A_{ij}^{xx} S_i^x S_j^x + A_{ij}^{xy} S_i^x S_j^y + A_{ij}^{yx} S_i^y S_j^x + A_{ij}^{yy} S_i^y S_j^y] \tag{20}$$

to obtain the elements of matrix $\mathbf{A}$:

$$A_{ij}^{xy} = A_{ij}^{yx} = 0 \qquad A_{ij}^{xx} = A_{ij}^{yy} = 2J[2\delta_{i,j} - \delta_{i,j-1} - \delta_{i,j+1}] \tag{21}$$

with the orthonormal eigenvectors in the form of standing spin waves

$$S_p^x, S_p^y = C\sin(kpa) \tag{22}$$

where C is a normalization constant and the wavevector k takes discrete values determined by the fixed boundary condition (a is the lattice constant):

$$k = \frac{\pi}{(N-1)a}, \frac{2\pi}{(N-1)a}, \ldots, \frac{(N-2)\pi}{(N-1)a}. \tag{23}$$

The computed eigenvalues D_{ii} coincide with an analytical expression:

$$D_{ii} = 4J[1 - \cos(k_i a)] = \hbar\omega_i / S \tag{24}$$

where k_i are given by (23). The eigenvalues are related to the energy $\hbar\omega_i$ of the eigenmodes through the magnon dispersion relation [12]. There is twofold degeneracy, since the eigenvalues can acquire only $N-2$ discrete values whereas there are $2(N-2)$ eigenvectors.

The matrix of the kinetic coefficients defined by (12) is antisymmetric

$$\gamma_{ij} = 0 \qquad \text{if } D_{ii} \neq D_{jj}$$
$$\gamma_{ij} = -\gamma_{ji} \qquad \text{if } D_{ii} = D_{jj}$$

which is consistent with Onsager's principle of the reciprocity in the mutual interference of two simultaneous irreversible processes in the presence of a magnetic field [13].

It is clear from (13) that all the non-diagonal elements in the correlation matrix of the random forces vanish and the fluctuations are statistically independent. For this reason, it is possible to employ those results of the fluctuation theory applicable to a single variable only [13].

$$\langle y_i^2 \rangle = \frac{kT}{D_{ii}}$$
$$\langle y_i(0) y_i(t) \rangle = \frac{kT}{D_{ii}} e^{K_{ii}|t|}$$
$$\langle f_i(0) f_i(t) \rangle = -2\frac{K_{ii}}{D_{ii}} kT\, \delta(t). \tag{25}$$

The first expression in (25) is a statement of the principle of equipartition of thermal energy $kT/2$ between the modes. From the second expression we obtain a relation for the relaxation times τ_i of the modes:

$$\tau_i = -\frac{1}{K_{ii}} \tag{26}$$

An analytic expression for τ_i is also obtained by assuming a solution of the form $S_p^x = Ae^{ikpa}e^{-t/\tau}$ in the linearized equations of motion:

$$\tau_i = \frac{1}{\alpha\omega_i}. \tag{27}$$

Using (24)–(27) we obtain

$$K_{ii} = -\frac{\alpha S}{\hbar} D_{ii} \qquad \langle f_i(0) f_i(t) \rangle = \frac{2\alpha kTS}{\hbar}\delta(t). \tag{28}$$

The correlation function of the random forces is therefore identical for all modes and is similar in form to the expression obtained by Brown [1] for a single particle.

The mean square amplitude of the normal modes is independent of the dissipation constant α. It is therefore convenient and necessary to choose α such that the timestep Δt in the Langevin equation (equation (14)) satisfies the condition

$$\Delta t \ll \frac{1}{\alpha\omega_{i,\max}} = \tau_{i,\min}. \tag{29}$$

The thermal average occupation of the modes is given by the Bose distribution $1/(e^{\hbar\omega_i/kT} - 1)$ from which we determine a maximum frequency $\omega_{max} = 10kT/\hbar$ above which the modes are unlikely to contribute significantly to the magnetization fluctuations.

The simulations of long-wavelength excitations require orthogonal transformations of matrices of excessively large dimensions. These can be avoided in our case since the eigenmodes are sinusoidal and a simple analytic expression relates the fluctuation of the magnetization $\Delta M/M(0)$ to the amplitude y_i of the modes:

$$\frac{\Delta M}{M(0)} = \sum_i \frac{1}{2}\frac{y_i^2}{N}. \tag{30}$$

The thermal excitations of the magnetization were simulated as follows. The diagonal elements of the matrices **D** and **K** were evaluated from (23), (24) and (28) respectively. The non-diagonal elements of matrix **K** were ignored since they do not influence the statistical behaviour of the system. The random variables F_i were obtained from (13) and (15) using the G05DDF NAG numerical routine. Starting with the spins in perfect alignment with the field ($y_i = 0$), the set of Langevin equations (14) was used to update the amplitudes of the normal modes y_i and (30) was used to evaluate the magnetization. This procedure avoids the necessity for diagonalization of the matrix **A** and the orthogonal transformations required by the algorithm in section 3, but yields identical results.

The thermal average of the magnetization of a chain of 100 spins was computed as a function of temperature and is shown with the associated rather small statistical errors in figure 1. The numerical data are in excellent agreement with spin-wave theory, as is indicated by the curve on the same figure obtained by taking the sum over all the spin-wave modes [12]:

$$\frac{\Delta M}{M(0)} = \frac{1}{NS}\sum_i \frac{1}{e^{\hbar\omega_i/kT} - 1}. \tag{31}$$

Although (31) is derived from quantum statistics, the dominant contribution to $\Delta M/M(0)$ arises from modes for which the classic limit is valid ($\hbar\omega_i \ll kT$), as will be discussed below. It was not necessary, therefore, to modify the basic numerical approach which is based on classical ideas of fluctuation theory.

In the low-temperature limit, the change in the magnetization in figure 1 is exponentially small as a result of the energy gap in the finite system. In the high-temperature limit, the linear dependence of $\Delta M/M(0)$ on temperature is interpreted physically as follows. The contribution of a long-wavelength mode ($\hbar\omega_i/kT \ll 1$), given by (31), is $\Delta M_i \propto kT/\hbar\omega_i$ and is proportional to temperature. The contribution of such modes varies according to (24) as $1/k^2$ whereas the distribution density of the modes in one dimension is independent of frequency ($D(k) = 2a/\pi$). The total contribution is therefore dominated by a small number of long-wavelength modes and is therefore linearly dependent on temperature.

5. Discussion

In strongly coupled ferromagnetic systems, the modes of thermal excitation are likely to have a long wavelength. The spontaneous fluctuations are spatially correlated and it is therefore of advantage to perform a transformation to the normal coordinates of a system. This transformation provides information concerning the normal oscillation modes.

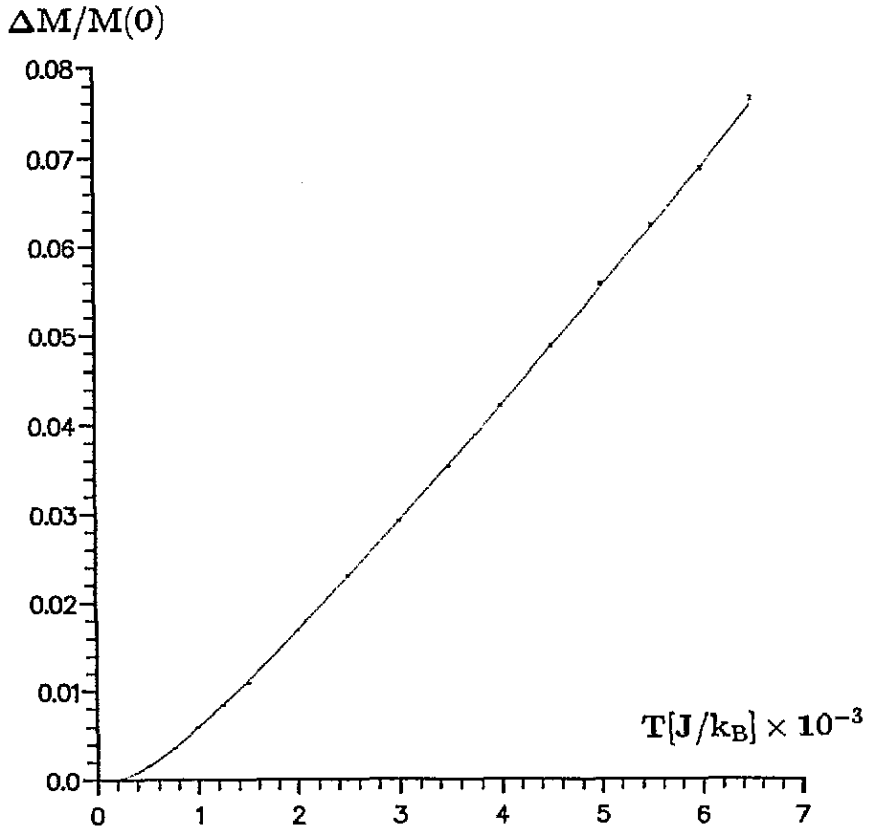

Figure 1. The average magnetization change $\Delta M/M(0)$ as a function of temperature.

The numerical method used requires knowledge only of the equilibrium magnetization configuration in the absence of thermodynamic fluctuations and the micromagnetic energy expression. The main limitation is that the fluctuations are sufficiently small that the equations of motion for the magnetization are linearizable and the fluctuation-dissipation theorem is applicable. The theory is also restricted to quasistationary fluctuations [3] that do not retain a memory of the history of any externally applied fields and satisfy the criterion for Brownian motion. For a given equilibrium state the correlation matrix of the thermal agitation forces is evaluated and the collective excitations are simulated using a set of Langevin equations.

The main advantage of the numerical method is that it allows the construction of a physical realization of the time dependence of multivariate magnetic systems. Time does not play the role of a label characterizing the sequential order of generated states, as is the case in the Monte Carlo method, but is related to physical time.

In principle, it is possible to construct a model of the thermal fluctuations without a transformation to the normal coordinates; however, the transformation is necessary since it provides an estimate for the maximum timestep Δt that should be employed in the finite-difference Langevin equations. The optimal timestep is related to the maximum eigenfrequency and when it is exceeded there will be an error in the simulation of the high-frequency modes of excitation. The transformation is also useful since the lowest eigenvalue

provides a measure of the stability of the equilibrium state. When it vanishes the associated eigenmode represents the initial mode of magnetic reversal to a new equilibrium state.

When the spectrum of eigenfrequencies is wide, a difficulty arises, in that the number of iterations required to simulate the low-frequency excitations may be too large, since the timestep is determined by the maximum frequency. In this case, a detailed study of the relative contribution of the different modes is necessary and various approximations might be possible. For example, if one is interested in the behaviour of the system only over a long timescale, the contribution of the high-frequency modes could possibly be averaged out by the method of adiabatic elimination of fast variables used in the theory of stochastic processes [14]. Alternatively, if only the equilibrium properties of a system are of interest, the normal modes may be treated as being decoupled from one another and only their average amplitude needs to be determined.

Since the transformation to the normal modes involves matrices whose dimension is determined by the number of variables in the system, a further difficulty arises in that the computational time required may be too long. This imposes, in practice, an upper limit to the size of the system studied, estimated to be currently of the order of few hundred degrees of freedom.

The method is clearly applicable to the study of the equilibrium properties of magnetic systems. A test was carried out in the present study on a chain of spins with fixed boundary conditions in the ferromagnetic range and it was shown that the method is consistent with the prediction of spin-wave theory. Potential applications also include for example the study of the equilibrium thermal excitations of the magnetization in fine ferromagnetic particles that result in the reduction of the magnetic splitting of the Mössbauer spectrum [15].

The current objective is to extend the method to the study of non-linear collective excitations in metastable systems that result in the thermal activation of the magnetization over an energy barrier. The modelling of the thermal activation process clearly requires a good understanding of the magnetic response of the system in the limit of small 'linear' excitations. The Fokker–Planck and the Langevin methods represent two alternative but equivalent techniques for evaluating the characteristic relaxation time of an activation process; however, for multivariate systems the Langevin method is probably simpler to implement [14].

Acknowledgments

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References

[1] Brown Jr W F 1963 *Phys. Rev.* **130** 1677
[2] Brown Jr W F 1979 *IEEE Trans. Magn.* **MAG-15** 1196
[3] Landau L D and Lifshitz E M 1980 *Statistical Physics* (Oxford: Pergamon) ch 12
[4] Landau L D and Lifshitz E M 1980 *Statistical Physics* (Oxford: Pergamon) p 120
[5] Callen H B and Welton T A 1951 *Phys. Rev.* **83** 34
[6] Nakatani Y, Uesaka Y and Hayashi N 1989 *Japan. J. Appl. Phys.* **28** 2485
[7] Schabes H and Bertram H M 1988 *J. Appl. Phys.* **64** 1347
[8] Reiter G and Sjölander A 1980 *J. Phys. C: Solid State Phys.* **13** 3027
[9] Balcar E and Loveluck J M 1982 *J. Phys. C: Solid State Phys.* **15** 4533
[10] Hendriksen P V, Linderoth S and Lindgard P A 1992 *J. Magn. Magn. Mater.* **104-107** 1577

[11] Shirakura T, Matsubara F and Inawashiro S 1990 *J. Phys.: Condens. Matter* **2** 2231
[12] Kittel C 1953 *Introduction to Solid State Physics* (New York: Wiley) ch 15
[13] Onsager L 1931 *Phys. Rev.* **37** 405
[14] Gardiner C W 1983 *Handbook of Stochastic Methods* (Berlin: Springer) ch 6
[15] Mørup S 1983 *J. Magn. Magn. Mater.* **37** 39