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Application of computer algebra systems (CAS) to symbolic construction of coupled equations for magnetic susceptibility of amorphous systems with different coordination numbers

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Abstract

We present the application of computer algebra systems to symbolic construction of two coupled systems of equations obtained from the exact Callen equation for a set of magnetizations and relevant magnetic susceptibilities in the case of complex amorphous ternary and binary diluted alloys like $(A_pB_{1-p})_xC_{1-x}$ with concentrations p and x, and different coordination numbers. The present paper is an extension of our previous one (Annales UMCS Informatica AI 5, 2006, 93) where the systems of polynomial equations for spontaneous magnetizations without external magnetic field have been obtained. Now, we introduce the external magnetic field and determine with the use of CAS full system of equations for both local magnetic susceptibilities and local magnetizations concerning all components of the complex magnetic systems. Finally, the numerical solutions of constructed coupled equations are found and discussed. The special attention is paid to the ferromagnetic region where the existence of low-temperature ordering transition, below the usual Curie phase transition, is searched as an interesting phenomenon from the technical point of view. The presented CAS added description can be understood as automatic constructor-simulator of relevant properties of amorphous alloys when the parameters of the system in question form an input to the described CAS-package.

1. Introduction

One of the most accurate methods of the Ising spin magnetic materials description is the Matsuaira approximation, which is mostly useful for the description of the binary and ternary alloys [1]. The successive levels of this method can give us the system of coupled equations for magnetization curves, correlation functions and thus the Cure temperature and critical temperature, so called Curie temperature [2,3]. The starting point for these calculations is well known exact Callen equation (CE) for the mean value of spin operator (in

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thermodynamic sense) which, however, in its compact form is not executable from the numerical point of view [4]. The problem was presented in our previous paper [3]. There, we showed the application of computer algebra system (CAS) to symbolic construction of the system of polynomial equations for spontaneous magnetizations describing the properties of stochastic magnetic systems with an external magnetic field not included. On the other hand, the interesting feature of magnetic systems is just their response to the external magnetic field. This response is usually determined in terms of magnetic susceptibility defined as the derivative of magnetization over the external magnetic field parameter taken into account.

Below, we extend our previous description and show the application of CAS to symbolic construction of the systems of multi-variable polynomial equations describing the properties of stochastic magnetic systems interacting with the external magnetic field. We perform the averaging procedure by using the so called integral operator method in the lowest approximation level (first Matsudaira approximation) and obtain the expansion of the CE with the external field included to a simpler polynomial form. Obviously, the equations for magnetic susceptibilities are derived as well by using the CAS symbolic calculations. Finally, these equations are linear with the coefficients dependent on all magnetizations of the system in question. Thus, all equations, these nonlinear for magnetizations as well as those linear for susceptibilities, should be solved simultaneously, at least in the ferromagnetic phase domain means below the critical temperature.

The particular advantage coming from the CAS application in symbolic derivation of specific long-term coefficients in CE is even more visible in the present case (with the external field included) than previously presented in our paper [3]. Now, both odd and even terms in polynomial equations for magnetisations are present while the form of all temperature coefficients is more complicated due to the existence of field parameter. Moreover, the complexity of expressions grows up quickly with the coordination number and spin value of magnetic components, as shown before. Thus, we finally conclude that the correct symbolic expansion of CE with the external magnetic field even in the simplest case of complex amorphous multicomponent structures would be not possible without CAS added construction. The symbolic treatment with the addition CAS packages like Mathematica [5] presented below is indispensable.

2. Outline of the model

We consider stochastic magnetic alloy structure like amorphous $(A_pB_{1-p})_xC_{1-x}$ with concentrations p and x of respective components A, B and C each possessing different coordination number, number of the nearest neighbours (see

Fig. 1). The system is immersed in the external magnetic field h and thus described with spin-1/2 Ising Hamiltonian leading to the exact Callen equation

$$\langle S_i^p \rangle_{T,\,c} = \langle Tanh(E_p(i;h)/k_B T) \rangle_{T,\,c}\,, \tag{1}$$

with the effective field operator defined by

$$E_p(i;h) = \sum_{r=A,B} \sum_{j\in i;}^{z_p} \xi_j^r J_{ij}^{pr} S_j^r + h\,, \tag{2}$$

where $p = A, B, \ldots$ (type of system component with p-spin S^p), $<\ldots>_{T,c}$ means both thermodynamic and configuration averaging procedure. $E_p(i; h)$ stands for the magnetic energy related to the i-site occupied by p-component when interacting with z_p neighbouring j-site with exchange energy J occupied by r-component in the presence of external magnetic field h. Amorphous crystallographic structure is modelled applying the stochastic occupation operator technique with a completeness rule ($p \neq r$):

$$\xi_j^r + \xi_j^p = 1\,, \text{ for } \xi_j^r = 0,1\,. \tag{3}$$

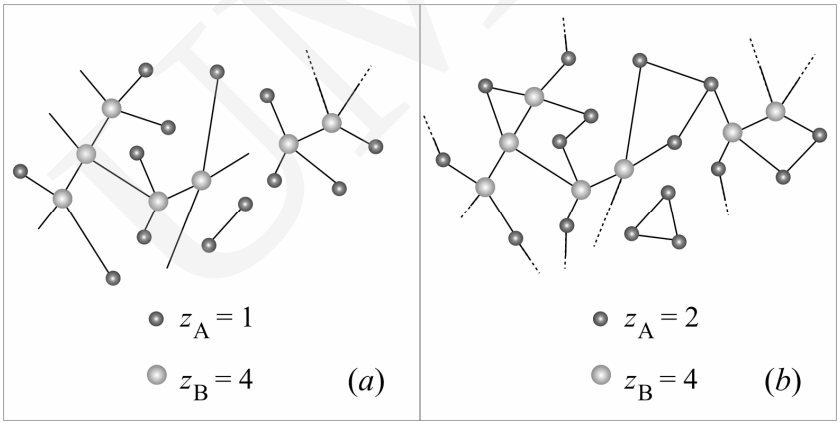

Fig. 1. Two schemes of binary alloy structures discussed in the paper for: (a) $c_A = 0.65$, $c_B = 0.35$ and $z_A = 1$, $z_B = 4$, (b) $c_A = 0.7$, $c_B = 0.3$ and $z_A = 2$, $z_B = 4$, respectively

The additional field dependent term in (2) (so called Zeeman energy) introduces essential difficulties in calculated coefficients of equations for magnetizations in respect our previous results in [3]. However, this term lets us determine the zero-field magnetic susceptibility for each of the magnetic components from the simple thermodynamic definition:

$$\chi_p(T) = \left. \frac{\partial \left\langle S_j^p \right\rangle_{T,c}}{\partial h} \right|_{h\to 0}\,. \tag{4}$$

The exact CE (1) may be easily transformed to the simplest molecular field form by shifting the averaging procedure $<\ldots>_{T,c}$ to the argument of transcendent hyperbolic tangent, however, this approximation is the most crude one and unfortunately gives non-physical results when speaking about stochastic or even diluted alloys [2,6]. Instead, we apply the integral operator method according to which CE transforms into the multi-variable polynomial equation after simple but very tedious algebra. This approach leads us to proper results for values of critical temperature and critical concentration in respective mixed-spin systems. The later becomes quick and rather easy with the use of symbolic CAS treatment.

The integral representation of Dirac-delta function allows us to rewrite CE (1) in the numerically tractable form

$$\langle S_i^p \rangle_{T,c} = \int \langle \delta(x - E_p(i;h)/k_B T) \rangle_{T,c} Tanh(x)\, dx\,, \tag{5}$$

and further

$$\left\langle S_k^p \right\rangle_{T,c} = \int \Gamma\{\left\langle \exp[-itE_p(k;h)/k_B T] \right\rangle_{T,c}\}\, Tanh(x)\, dx\,, \tag{6}$$

where we have used the Fourier transform $\Gamma\{\ldots\}$ to simplify the CAS implementation in a similar way as discussed in [3]. In particular, we have to transform the complex exponential in (6) into the sum of Dirac-delta functions according to (2) and the relation

$$\exp[-itE_p(k;h)/k_B T] = \prod_{r=A,B,\ldots} \left\{1 - c_r + c_r Cos\left(J^{pr}/k_B T\right) - im_r Sin\left(J^{pr}/k_B T\right)\right\}^{z_p} * \left[Cos\left(h/k_B T\right) - iSin\left(h/k_B T\right)\right] \tag{7}$$

where $m_r = c_r \left\langle S_k^r \right\rangle_{T,c}$ is the magnetization and $c_r = \left\langle \xi_k^r \right\rangle_c$ denotes the concentration of *r*-component in the alloyed magnetic structure $(A_pB_{1-p})_xC_{1-x}$ (*r* = A, B, …).

3. CAS implementation

Equation (6) is still exact while in relation (7) we have already neglected all spin-spin correlations of next nearest neighbours in a similar way as in our paper [3]. Then, the product in (7) has to be expanded into the polynomials of magnetizations m_A, m_B, and so on, with the powers related to the respective coordination numbers z_p ($p = A, B, \ldots$). Here, we apply CAS symbolic expansion, in the frame of *Mathematica* package [5], for bulk binary alloys with z_A = 1, 2, 3 *and* z_B = 3 or 4 in both cases of pure and diluted structures (with additional non-magnetic component *C* not shown in Fig. 1).

Bulk binary alloy structure ($z_A = 1, 2, 3$ and $z_B = 4$)

To derive the equations for *A* and *B*-sublattice magnetisations: *ma* and *mb*, we apply *Expand* and *TrigReduce* commands which transform trigonometric functions as rational functions of exponentials:

$$\begin{aligned} rma = Expand[((cA\ Cos[kAA\ t] - I\ ma\ Sin[kAA\ t] + cB)\hat{}\ zA) \\ *(cB\ Cos[kAB\ t] - I\ mb\ Sin[kAB\ t] + cA)\hat{}\ zA) \\ *(Cos[t*h] - I\ Sin[t*h])]. \end{aligned} \tag{8a}$$

$$\begin{aligned} rmb = Expand[((cB\ Cos[kBB\ t] - I\ mb\ Sin[kBB\ t] + cA)\hat{}\ zB) \\ *(cA\ Cos[kAB\ t] - I\ ma\ Sin[kAB\ t] + cB)\hat{}\ zB) \\ *(Cos[t*h] - I\ Sin[t*h])]. \end{aligned} \tag{8b}$$

$$rma1 = TrigReduce[rma], \tag{9a}$$

$$rmb1 = TrigReduce[rmb]. \tag{9b}$$

As a result we obtain the most compact form of integrals in (6) now with an additional factor dependent on external magnetic field in comparison with our previous results in [3]. For example we show one of the coefficients, namely that of length equal to 120 components, by *ma mb*^4:

$$wma1mb4 = Coefficient[rmb1, ma, mb1\hat{}4], \tag{10a}$$

$$\begin{aligned} &-\tfrac{3}{32} Cos(ht - 4kAA\ \ t)\ \ cA\hat{}3 + \tfrac{3}{32} Cos(ht + 4kAA\ \ t)\ \ cA\hat{}3 + \\ &\tfrac{3}{32} iSin(ht - 4kAA\ \ t)\ \ cA\hat{}3\ \ - \tfrac{3}{32} iSin(ht + 4kAA\ \ t)\ \ cA\hat{}3 + \\ &-\tfrac{9}{8}\ \ Cos(ht - 2kAA\ \ t)\ \ cA\ cB\hat{}2 + \tfrac{9}{8}\ \ Cos(ht + 2kAA\ \ t)\ \ cA\ cB\hat{}2 + \ldots + \\ &\tfrac{3}{32}\ \ Cos(ht + 3kAA\ \ t + 4kAB\ \ t)\ \ cA\hat{}2\ cB - \tfrac{3}{32} i\ \ Sin(ht + 3kAA\ \ t - 4kAB\ \ t)\ \ cA\hat{}2\ cB + \ldots + \\ &\tfrac{1}{64}\ \ Cos(ht - 4kAA\ \ t + 4kAB\ \ t)\ \ cA\hat{}3\ \ - \tfrac{1}{64} i\ \ Sin(ht - 4kAA\ \ t + 4kAB\ \ t)\ \ cA\hat{}3 + \\ &\tfrac{1}{64}\ \ Cos(ht + 4kAA\ \ t + 4kAB\ \ t)\ \ cA\hat{}3\ \ - \tfrac{1}{64} i\ \ Sin(ht + 4kAA\ \ t + 4kAB\ \ t)\ \ cA\hat{}3. \end{aligned} \tag{10b}$$

where k_{AA}, k_{AB}, k_{BB} and t are related to exchange integrals J_{AA}, J_{AB}, J_{BB} and temperature parameter $(k_BT)^{-1}$, respectively. Length of other coefficients varies from 50 for *ma*^4 *mb*^4 term up to 378 for magnetization independent term *ma*^0 *mb*^0, which now, however, plays its important role in calculated susceptibilities (while previously in [3] for $h = 0$ had no importance as giving zero contribution to spontaneous magnetization).

Let us find all the coefficients w1[ia,ja] in expression (8b) each standing by terms $ma\hat{}\,ia * mb\hat{}\,ja$, respectively:

Do[w1[ia,ja]=

Coefficient[*Coefficient*[*rmb*1,*ma*,*ia*],*mb*,*ja*], {*ia*,0,4},{*ja*,0,4}]. (11)

Next, we use the available *Fourier'Transform* package to perform the integral operator technique:

$$<< Calculus\ 'FourierTransform'. \tag{12}$$

Then, all the coefficients f1[i1,j1] in expression (6) are found by successive commands

Do[*f*[*i*1,*j*1]=*Expand*[
FourierTransform[*w*1[*i*1,*j*1],*t*,*w*] *Sqrt*[1/(2Pi)]],{*i*1,0,4},{*j*1,0,4}], (13a)

Do[*bb*[*i*1,*j*1]=
Integrate[*f*[*i*1,*j*1] *Tanh*[*w*], {*w*,-*Infinity*, *Infinity*}],{*i*1,0,4},{*j*1,0,4}] (13b)

Finally, we obtain the system of equations for magnetizations in the expanded form:

*equ*1=*ma*==cA (Sum[*aa*[[*i*1,*j*1]] *ma*^*i*1 *mb*^*j*1, {*i*1,0,1}, {*j*1,0,1}]), (14a)

*equ*2=*mb*==*cB* (Sum[*bb*[[*i*1,*j*1]] *ma*^*i*1 *mb*^*j*1, {*i*1,0,4}, {*j*1,0,4}]). (14b)

Next, according to (4) we derive the equations for magnetic susceptibilities applying the possibility of symbolic derivative of equations (14) over the field parameter *h* under the condition that *ma* and *mb* symbols are non constant:

```
eqchia=D[equ1,h,NonConstants→{ma,mb}],                    (15a)
eqchib=D[equ2,h,NonConstants→{ma,mb}].                    (15b)
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and

```
eqchia=eqchia/.{D[ma,h,NonConstants→{ma,mb}]→chia,D[mb,h,N
onConstants→{ma,mb}]→chib,h→0},                           (16a)
eqchb=eqchib/.{D[ma,h,NonConstants→{ma,mb}]→chia,D[mb,h,No
nConstants→{ma,mb}]→chib,h→0}.                            (16b)
```

The complete equations for *ma*, *mb*, *chia*, and *chib* in (14) and (16) should be solved simultaneously for each temperature with all concentrations and exchange couplings given in advance. In Figs. 2 and 3, we show the numerical results for $z_A = 1$, $z_B = 4$, and $z_A = 2$, $z_B = 4$, respectively. The set of parameters in each case is following: (1) $c_A = 0.8$, $c_B = 0.2$ and $J_{AB} = 1.2J_{AA}$, $J_{BB} = 1.5\ J_{AA}$; (2) $c_A = 0.5$, $c_B = 0.5$ and $J_{AB} = 1.2J_{AA}$, $J_{BB} = 5.0\ J_{AA}$; (3) $c_A = 0.2$, $c_B = 0.8$ and $J_{AB} = 2.0J_{AA}$, $J_{BB} = 5.0\ J_{AA}$.

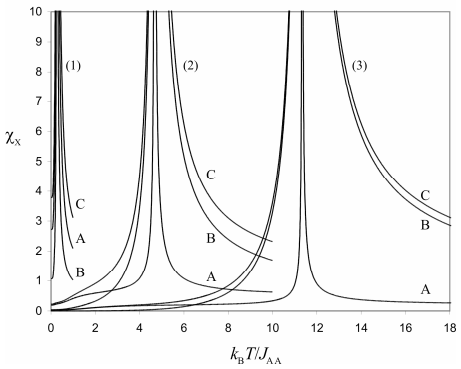

Fig.2. Magnetic susceptibility χ_X (X = A, B; $\chi_C = \chi_A + \chi_B$) vs. reduced temperature k_BT/J_{AA} for non-diluted ($x = 1$) amorphous structure $(A_pB_{1-p})_xC_{1-x}$ with $z_A = 1$, $z_B = 4$, and three sets of parameters described above in the text

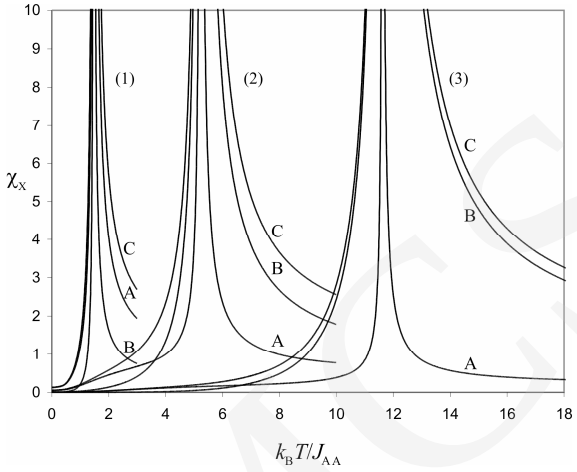

Fig.3. Magnetic susceptibility χ_X (X = A, B; $\chi_C = \chi_A + \chi_B$) vs. reduced temperature $k_B T/J_{AA}$ for non-diluted ($x = 1$) amorphous structure $(A_pB_{1-p})_xC_{1-x}$ with $z_A = 2$, $z_B = 4$, and three sets of parameters described above in the text

Bulk diluted binary alloy structure ($z_A = 3$ and $z_B = 3$)

Similar CAS treatment of equations for magnetic binary systems with additional dilution effects (see also [3]) gives numerical results for magnetic susceptibilities shown in Figs. 4 and 5. The set of parameters in Fig. 4 is following: (1) $c_A = 0.5$, $c_B = 0.1$, $c_C = 0.4$ and $J_{AB} = 1.2J_{AA}$, $J_{BB} = 1.5\ J_{AA}$; (2) $c_A = 0.1$, $c_B = 0.5$, $c_C = 0.4$ and $J_{AB} = 2.0J_{AA}$, $J_{BB} = 5.0\ J_{AA}$; where c_C denotes the concentration of non-magnetic component.

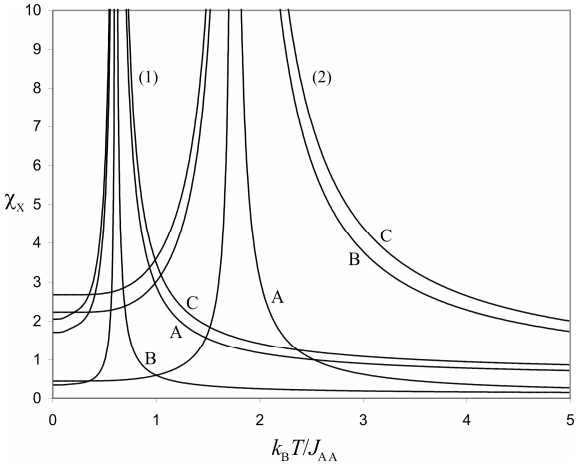

Fig. 4. Magnetic susceptibility χ_X (X = A, B; $\chi_C = \chi_A + \chi_B$) vs. reduced temperature $k_B T/J_{AA}$ for diluted ($x = c_C$) binary amorphous structure $(A_pB_{1-p})_xC_{1-x}$ with $z_A = z_B = 3$, and two sets of parameters described above in the text

The set of parameters in Fig. 5 is the following: (1) $c_A = 0.1$, $c_B = 0.4$, $c_C = 0.5$ and $J_{AB} = 1.2J_{AA}$, $J_{BB} = 50\ J_{AA}$; (2) $c_A = 0.05$, $c_B = 0.5$, $c_C = 0.45$ and $J_{AB} = 0.1J_{AA}$, $J_{BB} = 5.0\ J_{AA}$ - this describes the special case of paramagnetic phase.

Conclusions

The extension of previously presented CAS added results for spontaneous magnetization, now also taking into account the external magnetic field contribution, is presented. The symbolic expansion of Callen equations gives us the system of four coupled linear-nonlinear algebraic equations. The present paper shows a power of CAS application to formal reconstruction of these equations for mean values of magnetisation and susceptibility in both binary alloy and diluted structures. In the frame of the mathematical formulation of the symbolic expansion we have used mainly the available Fourier'Transform package to perform the integral operator technique and TrigReduce command which allows for algebraic manipulation of trigonometric functions as rational functions of exponentials. The symbolic derivative of complex expressions with the rules of non-constant variables was also applied. Finally, it has been shown, that amorphous magnetic systems with the assumed distribution of structural parameters like partial coordination numbers can be also easily studied with similar CAS procedures in the vicinity of external magnetic field.

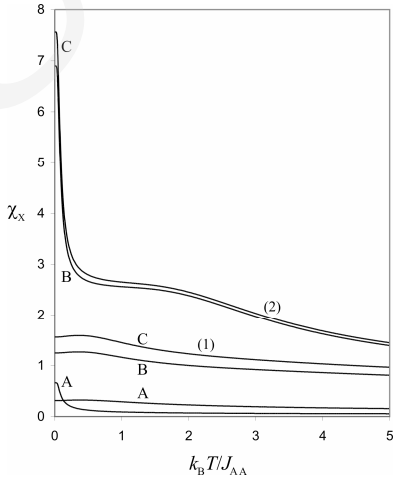

Fig. 5. Magnetic susceptibility χ_X (X = A, B; $\chi_C = \chi_A + \chi_B$) vs. reduced temperature k_BT/J_{AA} for diluted ($x = c_C$) binary amorphous structure $(A_pB_{1-p})_xC_{1-x}$ with $z_A = z_B = 3$, and two sets of parameters described above in the text

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