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TRANSDISCIPLINARY ASPECTS OF DIFFUSION AND MAGNETOCALORIC EFFECT

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Abstract

The modeling of magnetocaloric effect (MCE) based on quasiparticle formalism was used to show a possibility to increase our knowledge of diffusion and phase transitions by a transdisciplinary scientific approach. Generalized understanding of diffusion and of some phase transitions was suggested. New relations between MCE and elastic parameters of materials, obtained from modeling procedure, were presented.

The paper contains also the short discussion of a necessity to use hypercomplex mathematics in modeling of magnetic processes and specifically in a modeling of MCE. Some remarks concerning nanomaterials are added.

Keyword: diffusion, magnetocaloric effect, phase transition, transdisciplinarity

Introduction

The study of magnetocaloric effect (MCE) has become important from the technological point of view, which, in the last decade, has initiated the boom aimed to its deeper investigation [1–13, 19]. The search for materials with a big enough MCE within technologically interesting temperatures intervals is impressive.

MCE is the special type of diffusion and can be seen as a transfer of energy between collective excitations of magnetic and elastic structure of materials. The behavior of collective excitations can be effectively represented by quasiparticles [14]. Quasiparticles are products of the formalism of second quantisation and they are characterized with the quantum of energy, which is necessary for their creation, and with their wave vector. In the case of the weak magnetoelastic interaction MCE is a transfer of energy between the magnons and phonons. In the case of stronger (but not very strong) magnetoelastic interaction the energy flows between such a comprehended quasiparticles that are only similar to magnons, and phonons (quasimagnons and quasiphonons).

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Our study of MCE will be restricted on the adiabatically-isolated systems. The entropy is supposed to be composed from the contribution of both the magnons and the phonons. The requirement of constant entropy provides us with the functional dependence of temperature as a function of varying external magnetic field. It is, however, not the only way how to get MCE. For example, we can consider the degree of correlation in the system describable by Green's functions as a constant parameter. The dependence of Green's function on temperature and magnetic field can be then used for finding of MCE.

The growing interest for MCE has consequence impacts to various sciences. For example, in mathematics there are tested new mathematical tools – even beyond the scope of classical mathematics. We believe that better and more interesting results concerning MCE could be reached with the help of hypercomplex mathematics – quaternions or multivectors, which are now reappearing in physical applications.

Some modeling aspects of MCE

We already published some results of our modeling of MCE [2, 8]. This paragraph will mostly contain some supplementary remarks to sketch the modeling procedure to make the following text about diffusion and phase transitions more understandable. Our calculations were done by a standard Heisenberg method of commutation of magnon and phonon operators with the Hamiltonian. It provided us with equations for time derivations of quasiparticle operators (in the Heisenberg representation). We obtained 8 equations with more than 8 unknown operators. Our decoupling (simplification approximations) included the neglecting of nonlinear terms. The condition of solubility of our system of homogeny equations gave us secular equation of 8^{th} order for the energies for 8 quasiparticle modes. We decided to expect two quasiparticles modes of magnon type, with the quadratic dependence of energy on wave vector, and 6 quasiparticle modes of phonon type with the energies depending linearly on wave vectors. The approximate diagonalisation of our Hamiltonian was possible only for some special directions (parallel and perpendicular to the anisotropy axis) and we received for those directions analytical terms for corresponding quasiparticle energies.

The usage of a proper mathematical formalism is thus very important. For the study of MCE it appears to us as that a most suitable approach is the formalism of quasiparticles. We expect that such an approach is intimately connected with the physics of relevant thermodynamic procedures [12, 13]. The application of the method of second quantisation to the mathematical modeling of MCE has, however, some partial problems. Crucial is the proper choice of the Hamiltonian, especially the choice of the term corresponding to the magnon-phonon interaction. We are trying now to find a better mathematical expression for the contribution of magnetoelastic energy in the special materials. In connection with it appears to us as promising an exploitation of hypercomplex mathematics. We turned our attention, for example, to the indexes of annihilation and creation operators for magnons and phonons. As indexes of creation and annihilation operators for magnons are usually used vectors, but it seems to us that, especially in the case of magnons, it is worth of trying to use some higher multivectors – for example bivectors. The same can be valid for quasiparticle operators describing the collective excitations of vortexes in superconductors of second type. The usage of proper higher multivectors makes formalism more transparent for important physical connotations and also it is possible to avoid some confusion – for example the peculiarity of polar and axial vectors.

Our Hamiltonian (*H)* was composed from three parts: magnon term, phonon term and the term $H^{\mathrm{magnetoelastic}}$ describing the magnon – phonon interaction. For the latter term we have used the simplest mathematical expression combining together the elasticity of a crystalline lattice and magnetic moments. We supposed that the magnetoelastic energy is proportional to the numbers of interacting quasiparticles, i.e.,: $\mathrm{H}^{\mathrm{magnetoelastic}} = gM_iM_ku_{ik}$ (where g is magnetoelastic constant, u_{ik} is tensor of deformation for positions i and k).

In our modeling of MCE we considered only the case of thermally isolated material (adiabatic isolation with the constant total entropy of the system) and it had to be done numerically. We used the standard formula for entropy of quasiparticle gas [18].

$$S=\sum_{\alpha}\int_{k,\alpha}[(1+n_{k,\alpha})\ln(1+n_{k,\alpha})-n_{k,\alpha}\ln(n_{k,\alpha})]k^{2}\mathrm{d}k$$

The change of particular entropy terms made by an application of external magnetic field had to be compensated by the change of temperature. S is the total entropy for the system of quasiparticle modes, $n_k = n_{k,}$ (T, H) are the numbers of quasiparticles which can be functions of temperature T and external magnetic field H. Index k denotes the wave vector and is the index of quasiparticle mode (quasimagnons or quasiphonons).

The self-consistent numerical calculations provided us with the temperature for which the total entropy of system is unchanged and equal to the total entropy before the application of magnetic field. The dependence of this temperature on external magnetic field $T=T(H)$ is than the actual MCE.

Our modeling predicts in the vicinity of some magnetic phase transitions not only the increase of MCE but also the change of its sign. Our modeling included also the study of crystalline anisotropy of materials illustrated in Fig. 1. The energy of our quasiphonons depends on the transversal or longitudinal speed of sound and we found the local extreme of MCE for the ratio of longitudinal and transversal speed of sound c near the value 1.4. We were happy to see that this number corresponds to the value of $c^{\mathrm{longitudinal}}/c^{\mathrm{transversal}}$ realistic in specific materials.

Our calculated quasiparticle energies are approximatively valid only for the small values of wave vectors, but this constrain is compensated in the process of numerical calculation because the quasiparticles with the bigger wave vector have also relatively higher energy and therefore the probability of their appearance exponentially decreases. In our modeling the quasiparticle energy should be small in comparison with the thermal energy per atom ($\sim k_BT$ where k_B is the Boltzman constant and T is the temperature) and therefore our calculations do not fit for very low temperatures. Actually, we made our calculations for temperatures around 20 K.

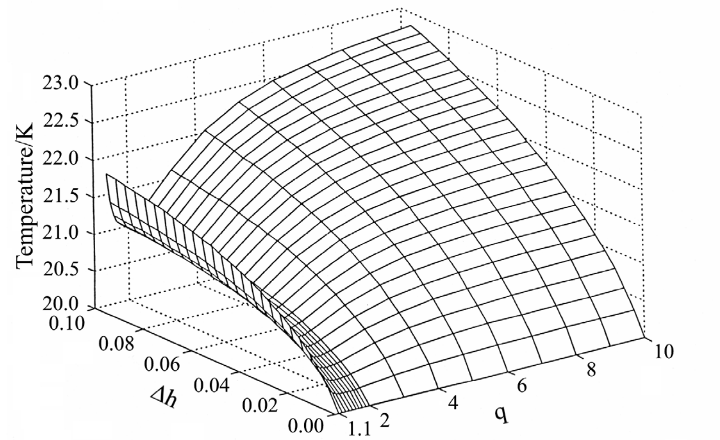

Fig. 1 Dependence of the temperature on the external magnetic field (MCE) and on the ratio of longitudinal and transversal speed of sound. It is based on the self-consisted computations similar to computations made in [3]. T is the temperature in K, h H–H^{crit})/ H^{crit} is a relative distance from the phase transition, H is external magnetic field, for H^{crit} is the magnetisation of sample turned from the easy direction into the hard direction, $q=c^{longitudinal}/c^{transversal}$ is the speed ratio where c the speed of sound. Note that there is the change of sign of magnetocaloric effect in the instant of phase transition

Some remarks to nanomagnetic materials

In the center of our special interest there are artificially produced nanomagnetic materials. The research of nanomagnetic materials is now in the focal point for many laboratories. From the point of view of our MCE modeling nanomagnetic materials possess encouraging properties.

Decoherence of longer wavelengths in nanomagnetic structures is smaller than in normal crystalline material. (The coherent behavior is possible if the wavelength is longer than the smallest distance in the medium. In nanomagnetic materials is this minimal wavelength 10 or 10000 times longer than in normal crystals.) The number of allowed wavelengths in nanomagnetic materials is restricted. The resonance condition for transfer energy between magnons and phonons can be better adjusted.

The Debye temperature in nanomagnetic materials is higher comparatively to other materials and therefore the entropy term for thermal lattice vibrations has a magnitude comparable to the entropy term for magnons. On the boundaries of anisotropic nano-grains could appear thermal gradients and elastic stresses. Some nanomagnetic materials are even transparent for wavelengths comparable with the size of nanomagnetic clusters and photoelastic method of observation of elastic stresses could be used.

There are indications that dipole-dipole interaction starts to be more important in nanomaterials than in normal, more homogenous materials. The study of anisotropy of sound velocities can also bring interesting and even practical results.

Diffusion as a transdisciplinary concept

Diffusion is a good example to illustrate the possibility of transdisciplinary scientific attitude. Diffusion is possible to meet in many scientific disciplines [19], but the content of concept could be surprisingly different. Diffusion of gas through a membrane is the usual type of diffusion. MCE is usually understood as a non-local and non-coherent transfer of energy between magnons and phonons. It is also considered as a specific type of diffusion but certainly much less usual. It is not the traditional flow of heat through a sample but the transfer of energy accomplished at the same time in the whole volume of magnetic material. Such process cannot be described just by a normal procedure of heat diffusion through a real body/space. For MCE we need some other, more sophisticated, type of diffusion (one suggestion could be a diffusion in the space based on the wave vectors).

There are some even more non-orthodox imaginations of diffusion. For example, the basic equation of quantum mechanics – Schrödinger equation – can be also considered as an equation for a diffusion of amplitudes of probability to find a particle in the specific place and specific time. Schrödinger discovered his equation to support the idea of universality of dual, particle-like and wave-like, character of matter. The new interpretation of Schrödinger equation, as an equation describing a diffusion – diffusion of probability amplitudes, is mostly known from the Feynman's lectures given few years after the Schrödingers discovery [1, 9]. It is worth noting that the idea of Feynman argumentation appeared even few years before Schrödinger's discovery. In connection with the search for the 'nature's natural numbers' Steiner suggested in his lectures for scientists and teachers [4], given in Stuttgart in the year 1920, the formally same equation as that given by Schrödinger. The diffusion equation could be written in the following form:

$$\frac{\partial\Theta}{\partial t}=\kappa\frac{\partial^2\Theta}{\partial x^2}$$

It can be in use as an equation for normal diffusion (or the heat conductivity equation), but it can be also the equation for diffusion of probability amplitudes of objects from a realm of quantum physics. The principal difference makes the constant . Putting the 'real number' for means to lay emphasis on the 'normal' diffusion (or thermal conductivity) while the 'imaginary number' replaced for leads to the quantum-mechanical equation. In the first case is Θ a normal density (or the heat flow) and in the second case Θ is related to the change of an amplitude of probability that the quantum particle is possible to find in the specific place *x* and specific time *t*.

It is worth of remark that Steiner proceeded in the 'search for the nature's natural numbers' even further on and considered a hypercomplex number to be used for the constant κ. He suggested that in such a particular case, the new equation could be useful in some specific applications, as is biodynamic. In fact, the hypercomplex numbers are now being of help in order to avoid mathematical difficulties while modeling human's knee kinematics [5] and they are also very promising in the construction of mathematic models of skin [6].

We think that a contemplative synthesis of mentioned modification of diffusion can enrich the present knowledge and interpretation [8, 9, 16].

Phase transitions and transdisciplinary aspect of MCE

We already suggested in the previous part of this paper that the concept of phase transition is also strongly transdisciplinar. One from the results of our modeling of MCE, which is closely connected with the diffusion of heat and with MCE, is that (in our model) the energy of one from phonon-like modes (for direction parallel or perpendicular to the anisotropy axis) is going to zero by approaching to the phase transition. We considered the phase transition of second order, which appears by the rotation of magnetization from the easy anisotropic direction into the hard direction. The driving force for rotations was a growing external magnetic field.

Our model predicted the anomalous behavior of MCE by approaching to the above considered phase transition and our theoretical forecast is now going to be partially confirmed by new experiments [7]. MCE was recently measured in nano-magnetic materials in the vicinity of magnetic phase transition of second order. The phase transition in quoted experiment and the one in our model are very similar. External magnetic field is turning magnetization of sample from the easy direction of magnetic anisotropy into the hard direction. In agreement with our expectations there was observed the significant increase of magnetocaloric effect in the vicinity of this phase transition. The existence of an easily excitable mode supposed in our model can explain the magnitude and even the change of MCE sign. The appearance of easily excitable mode by approaching to phase transition could be, however, a more general transdisciplinary phenomenon.

This belief can be supported with a possibility of a similar magnetocaloric behavior in superconductors in the neighborhood of phase transition from superconductivity to normal conductivity. Phase transition in superconductors of second type is made by the grow of external magnetic field to the critical value. We made modeling calculations based on the supposition of a transfer of energy between collective excitations of vortexes and thermal phonons in the superconducting material [2]. Experimental confirmation of this expectation could be even more interesting and important [10]. We also recently learned that such ideas are now going to be practically used in the so-called 'thermal machine' where the standard working medium (water) is replaced by superconductor [11]. The phase transition from superconductivity to normal conductivity and vice versa is realized by the change of distance between sample and the space with strong magnetic field. The change of sign of MCE produced by passing through the phase transition is than rhythmically used for engine-like cycling process [11, 12]. Transdisciplinary scientific attitude can be seen here as a driving force leading possibly not only to better knowledge but also to futuristic machines.

Conclusions

The magnetocaloric effect (MCE) is one of the physical topics, which fit very well not only to the standard framework of thermodynamics and applied thermal analysis but also to broader transdisciplinary activities. The study of MCE can bring a new light into understanding of such phenomena as phase transitions and collective excitations. It makes possible to study mechanisms responsible for a realization of phase transitions – for example the appearance of a new quasiparticle mode with very low energy near phase transitions. The label transdisiplinarity belongs here not only to MCE but to phase transitions and collective excitations as well. Modifications of those concepts are possible to find in many scientific disciplines [15] – mathematics, biology, social sciences or even in philosophy.

The idea of transfer of energy between different modes of collective excitations has also the transdisciplinary meaning and it can be exploited in different fields of scientific effort (even such as economy or sociology). It is surprising how relatively easy is possible to reinstall into nonphysical disciplines such basic concepts as quantisation of energy of collective excitations, definition of their wave length, relaxation times, effective mass or the appearance of easy excitable modes near some phase transitions.

The modeling of MCE based on quasiparticle formalism was used to show a possibility to increase our knowledge by a transdisciplinary scientific approach. Generalized understanding of diffusion and some phase transitions was suggested.

New relations between MCE and elastic parameters of materials, obtained from modeling procedure, were presented. The paper also contains the short discussion of a necessity to use hypercomplex mathematics in modeling of magnetic processes and specifically in a modeling of magnetocaloric effect.

Authors of the paper are now working on the more precise modeling of MCE for a specific, partly artificial material (collaboration with the laboratory of G. Kozlowski at Wright University, Dayton USA) where some new remarks concerning nanomaterials are added [17].

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References

1 R. P. Feynman, R. B. Leighton and M. Sands, 'The Feynman Lectures on Physics' (Addison-Wesley publishing Company 1966), R. P. Feynman 'Feynman Lectures', Vol. 3, p. 16 and QED The Strange Theory of Light and Matter (third lecture).
2 T. Svobodny and Z. Kalva, Phys. Stat. Sol.(b), 208 (1998) 187.
3 Z. Kalva and P. Mánek, Acta Physica Polonica, A3 (2000) 407.
4 D. Hardorp and V. Pinkall, Math. Phys. Korrespondenz, 201 (2000) 16.

5 S. Schreiber, 'The displacement workspace of the human knee' Dissertation, Darmstadt D17, 1997 or A. T. Yang 'Application of Quaternion Algebra and Dual Numbers to the Analysis of Spatial Mechanisms', Dissertation Columb. Univ. N.Y. Mic. 64-2804.
6 P. Gschwind, 'Mass, Zahl und Farbe' Mathematisch-Astronomische Blätter, Band 23, Phil.-Anth. Verlag Goetheanum, Dornach, Schweiz 2000.
7 X. X. Zhang, H. L. Wei, Z. Q. Zhang and L. Zhang, Phys. Rev. Lett., 87 (2001) 157203/1-4.
8 Z. Kalva, Acta Physica Slovaca, 46 (1996) 651.
9 J. Šesták, 'Heat, Thermal Analysis and Society', Nucleus, Hradec Kralove 2004.
10 K. Kakuyanagi and Ken-ichi Kumagai, Phys. Rev., B65 060503(R).
11 P. D. Keefe, 'Coherent magneto-caloric effect superconductive heat engine process cycle', US Patent 4 638 194 (1987).
12 P. D. Keefe in D. P. Sheeham (Ed.), 'Quantum limits to the second thermodynamic law', Proceedings by the American Institute, Melville, New York 2002.
13 P. Lipavský, K. Morawetz and V. Špička, 'Kinetic equations for strongly interacting dense Fermi systems', EDP Science, France 2001 (Annales Phys., Vol. 26, No. 1).
14 L. P. Landau, Sov. Phys. JETP, 3 (1957) 920 and 5 (1957) 101.
15 I. M. Havel, 'Longing for unified knowledge' CTS report No. CTS-97-04, UK Praha 1997.
16 Z. Kalva and J. Šesták, 'Heat diffusion from a more general perspective and the magnetocaloric effect in superconducting and also nanomagnetic materials', 9th CCTA – Symposium on thermodynamics and structure, Zakopane, Poland 2003, CD.
17 J. Ulner and Z. Kalva, to be published.
18 R. Kubo, 'Statistical Mechanics', North-Holland, Amsterdam 1965.
19 J. Šesták, J. Therm. Anal. Cal., 69 (2002) 113.