Purpose of the visit

During my visit of the Department of Physics at Loughborough University I wrote a paper together with Prof. F.V. Kusmartsev entitled

MAGNETIC QUANTUM CELLULAR AUTOMATA

We both were invited speakers at the

XXVIII International Workshop on Condensed Matter Theories

St. Louis, Mo, USA, September 2004

The article is included in this report (except one figure, since it exceeds 5 MB) It will appear in the series

Condensed Matter Theories, Vol. **20**, Nova Science Publisher, N.Y.

I also finished my individual contribution for the book of the conference proceedings with the title

FRACTAL PROPERTIES OF SMALL MAGNETIC PARTICLES AND MAGNETIC MULTILAYERS: AN EXACTLY SOLVABLE MODEL

The focus of this contribution is an analytical study of the energy landscape of the Hamiltonian based on a piecewise quadratic potential such that the corresponding variational equations are piecewise linear. In contrast to widely used highly non-linear on-site potentials with a quadratic maximum all physical quantities of interest can be studied analytically.

Future collaboration with host institution

The collaboration Vienna-Loughborough with Prof. Kusmartsev will be continued during this year. Both above papers will be the basis for more detailed publications of this subject and future collaborations.

MAGNETIC QUANTUM CELLULAR AUTOMATA

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1. INTRODUCTION

Recently Cowburn and Welland have proposed to use a chain of magnetic nanoparticles deposited on a nonmagnetic substrate as a room temperature Magnetic Quantum Cellular Automata (MQCA) [1-2]. Such automata made of magnetic dots are capapable of data handling. The silicon microchip, the single electron transistor (SET) seems set to generate the next revolution in data processing and storage. Arrangements of SETs have recently shown their ability to perform logic operations. They were called Quantum Cellular Automata (QCA) because they use quantum mechanical tunnelling of charge between quantum dots to change logic state. However, currently, unless the SET dots are less than 2 nm across, the electronic QCA will only work at millikelvin temperatures. Now the attention is focused to magnetic QCAs instead, which can operate at room temperatures. The MQCA networks are built up of magnetic dots, which are made from a common magnetic alloy on a silicon substrate. And indeed it was found that the MQCA was able to work at room temperature[1,2]. Each dot of the MQCA is 110 nm across and 10 nm thick with a pitch of 135 nm. The quantum mechanical interactions in a magnetic QCA are exchange interactions between spins in a single dot, forming a single giant classical spin. The direction of the dot's magnetization vector is supposed to indicate a logic state. Magnetostatic interactions between nearest neighbours along the chain of dots allow the propagation of information, but also force the magnetization to point along the direction of the chain, to either the left or the right, producing a natural binary logic system. The logic state can be set by applying a single magnetic pulse at the input dot. Oscillating magnetic fields can then reverse the magnetic state of the chain of dots, changing the logic state, as a magnetic soliton propagates along the chain. This soliton or better to say the kink, like a domain wall in a bulk material, separates regions of left and right magnetization. In theory, solitons propagate without loss, but small fluctuations in the shape of the dots will cause a soliton to dissipate energy as it propagates. To minimize losses requires an accuracy on dot circularity of better than 5%. It is a far less stringent requirement than that for electronic QCAs, and easily achievable. Due to the special energy structure the magnetic QCAs can be made also very stable against data errors caused by thermal fluctuations, even down to dot diameters of 20 nm. Integration densities could reach 250 000 million/cm^2 with only about 1 W of typical power dissipation and across-chip clock frequencies of up to 100 MHz. We believe that the magnetic QCA "has enormous potential" to meet the requirements of digital processing of the future[1].

Cowburn et al have realized various linear chains where all particles were ferromagnetically and anti-ferro-magnetically coupled. The magnetic moments were then oriented along or perpendicular to the the chain. The orientation of the magnetic moments has been controlled by a deposition of a first particle of the chain which was different (larger or elongated) than other particles. Normally this first particle had a distinguished ellipsoidal or cigar shape while in other papers all particles had an elliptic shape oriented in the same direction. In Ref. [1] it could be shown that by slightly biased, pulsed magnetic field the magnetic moments associated with these individual particles are flipped coherently, comparable to a "domino" effect. The experimental studies have revealed that such a chain has all properties needed to form a quantum cellular automata indeed. Usually in such automata each basic element has two states which are related to the bit information forming a digital structure. That is each such element takes the values ± 1. In the magnetic automata the value +1 corresponds to one spin orientation of the single particle, while the value -1 corresponds to the opposite spin orientation. The MQCA is consists of gates built up from chains made of small magnetic particles. For example, Fig. 1 depicts the AND gate constructed from two perpendicular chains made of small magnetic particles. By fixing the input A to zero, this device made of the crossed chains performs the boolen logic operation *AND*, while fixing the input A to the value one, the spin down orientation, we force this gate operate in the mode *OR*.

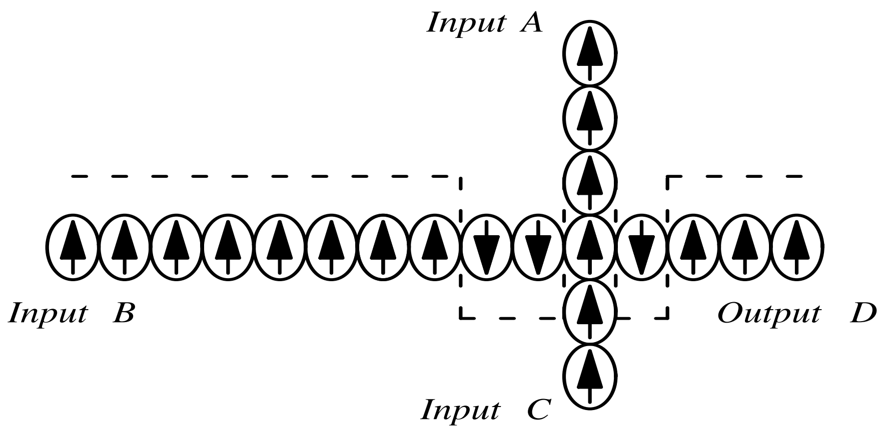

Figure 1. Operational AND gate made of small magnetic particles in MQCA, The vertical chain is the control chain with two inputs Input A and Input C. The information signal (Input B) is processing along the horizontal chain. The dashed line corresponds to the signal, which consists of four domain walls propagating along the horisontal chain.

Obviously if all spins are originally ferromagnetically oriented, then the switch of one element or a spin flip in such a chain corresponds to a creation of two domain walls(domain and anti-domain walls). In order to describe a formation of domain walls and other magnetic structures in microscopic systems made of the small magnetic nanoparticles we have proposed here a theoretical model. In particular, using this model we have investigated the formation of the domain structures in a linear chain and in other small multi-particle clusters.

We have investigated this model in detail considering arrays of a few and many nanoparticles, and shown that besides MQCA they also have potential for sensor applications and magnetic data storage. In particular we show that such systems have a very complex nontrivial magnetic behaviour. There different nontrivial structures displaying fractal features may be formed. That is with increasing particle number the system behaviour, ie the values of magnetic moments, the energy spectrum, coercive forces, hysteresys loops may display the features of a fractal. The formation of these fractal structures is mostly related to the discrete nature of the systems made of small particles and does not depend of the specific models which we have been considering. Therefore the phenomenon of the fractal creation has a very general character and must be taken into account in a design of any MQCA system made of small particles and having a potential for important applications.

For an illustration of the fractal formation in the present work we consider one of these systems made of small particles, namely, a linear chain. Such system can be and has been already produced from small ferromagnetic particles made, for example, of Fe (see, also, Ref.[1-3]. If all spins within a single particle are ferro-magnetically ordered, then each particle may be considered as having a single classical spin $\vec{S}$. The value of $\vec{S}$ may be well described by a model of a classical spin. Then the chain of magnetic particles having a disk or elliptic shape can be described by a model of interacting classical spins, that is the Hamiltonian has the form:

$$H = \sum_{<i,j>} J_{ij} \vec{S}_i \vec{S}_j - \sum_i \vec{H} \vec{S}_i + \sum_{i\alpha} K_\alpha S_{i\alpha}^2$$

Here we assume that magnetic moments associated with individual disks are interacting via exchange and dipole-dipole interactions characterised by the constants J_{ij}, which also depend on the orientation of the appropriate moments $\vec{S_i}$ and $\vec{S_j}$, where $\vec{S} = (S_x, S_y, S_z)$;. Each disk is characterised by anisotropy constants K_α, where $\alpha = x, y, z$. We also assume that the disks are located on the (x,y) plane of a substrate, so that the z-axes is perpendicular to the disk plane. Then the value of the configurational anisotropy constant K_z associated with the disk shape is the largest. That is it is much larger than the constants of the in plane anisotropy, K_x and K_y, ie $K_z/K_x >> 1$ and $K_z/K_y >> 1$ as well as $K_x >> K_y$.

Assuming that within each particle all magnetic moments are ferromagnetically aligned but with an orientation differing from particle to particle, the system can be modelled as a collection of N elementary classical magnetic moments and can be described by a classical Hamiltonian that is discrete in space. For the disk shape particle the value of $\vec{S_i} = (s\cos(x_i), s\sin(x_i), 0)$. Below we use unites where $s = 1$.

Then, the total energy of such a spin chain is given by the N-particle Hamiltonian

$$H = \sum_{i=1}^{N} \left(-J \cos(x_i - x_{i-1}) - h \cos(x_i - \beta) + \frac{K}{2} \sin^2(x_i) \right) \quad (1)$$

where periodic boundary conditions are imposed. Here, the variables x_i specify the angles between the magnetizations of the individual particles and the axis of symmetry of individual single particles. The variety of possible spatial magnetic structures stems from a competition between three forces that leads to locally stable spatially modulated structures. The first is the inter-particle exchange energy, favouring uniform magnetization configurations. It is usually very small in comparison with dipole-dipole coupling constant J. Depending on the orientation of the magnetic moments of interacting particles J may take positive or negative values. Supposed that the magnetic moments of all particles are oriented perpendicular to the chain due to the shape anisotropy, the value of J is chosen to be antiferromagnetic, ie $J < 0$ and set to unity. Second, the Zeeman energy defined by the strength of an external magnetic field h, favouring the alignment of the moments along the field direction. Third, the shape anisotropy energy defined by a suitable multi-well potential favouring collinear structures along preferred directions. In our case this symmetry axes is oriented perpendicular to the horisontal chain direction. The quantity β defines the angle between the reference symmetry axis of individual particles and the external magnetic field, while the quantity K specifies the strength of the particle anisotropy. Besides the energy, another important macroscopic quantity of interest is the total magnetization M taken along the direction of the reference axis or along magnetic field. Defined as

$$M = \frac{1}{N} \sum_{i=1}^{N} \cos(x_i - \beta) \quad (2)$$

this quantity specifies an average over the magnetic moment directions of the individual magnetic particles with respect to magnetic field orientation. Locally stable equilibrium configurations obey the set of N nonlinear coupled equations

$$-\sin(x_i - x_{i-1}) - \sin(x_i - x_{i+1}) + h \sin\,(x_i - \beta) + \frac{K}{2} \sin(2x_i) = 0 \quad i = 1, 2, ..., N \quad (3)$$

However, an N-dimensional vector $\mathbf{x}^* = (x_1^*, x_2^*, ..., x_N^*)$ satisfying Eq.(3) specifies a local minimum of the Hamiltonian only if the eigenvalues of the Hessian $(\frac{\partial^2 \mathbf{H(x)}}{\partial x_i \partial x_j})_{|\mathbf{x}=\mathbf{x}^*}$ are all positive. When the diagonal entries dominate, which is always the case for $U''(x_i^*) > 0$ Gershgorin's disk theorem provides a simple and sufficient stability condition.

2. CONFIGURATIONAL SPACE OF MQCA

Magnetic sub-micron particles are typically characterized by a high value of the anisotropy constant K associated with their shapes. It is normally much larger than the absolute value of the exchange interaction J. The large number of experimentally possible observed locally stable spatial structures in the magnetic chains is a simple consequence of the variety of possible magnetic domain structures. Magnetic domains and solitons result from the balance of several competing energy contributions, where the system tries to compromise between all the competing forces. When the three control parameters H, K and β vary, the energy balance is changed such that a rearrangement of the domain structure can take place. This is mainly attributed to the motion of domain walls, separating adjacent domains. At high fields, the MQCA is everywhere magnetized along the applied field direction such that we have only one big domain governing the whole system. In order to determine the exact number of locally stable spatial structures we first consider the system at zero magnetic field H, where Eq. (3) reduces to

$$-\sin(x_i - x_{i-1}) - \sin(x_i - x_{i+1}) + \frac{K}{2}\sin(2x_i) = 0 \qquad i = 1, 2, ..., N \tag{4}$$

This set of equations has exactly 2^N distinct solutions consisting of "binary" strings $\mathbf{x}^* = (x_1^*, x_2^*, ..., x_N^*)$ with $x_i^* \in \{0, \pi\}$. According to Gershgorin's theorem they can be shown to be locally stable for sufficiently large values of K. However due to internal symmetries within the strings $(x_1^*, x_2^*, ..., x_N^*)$ the corresponding energies as well as the total magnetizations M are highly degenerate. The number of nonequivalent strings can be determined by the action of the dihedral group D_N consisting of N translations $(x_s \rightarrow x_{s+i})$ and N mirror reflections $(x_{s+i} \rightarrow x_{s-i})$ with respect to all symmetry axes. With the aid of Redfield-Pòlya theory one can show that their number behaves asymptotically as $\frac{1}{N}2^{N-1}$ with increasing N [4-5]. Accordingly, the energy landscape in which the system evolves is expected to exhibit an extremely complicated multi-valley structure with an exponentially increasing number of local minima and saddle points that also allows the appearance of structural disorder.

3. MODELLING OF FRACTAL FEATURES OF MQCA

Usually any magnetic system is characterised by a dependence of the total magnetisation on the magnetic field. Such dependence obtained with increasing and decreasing magnetic field is known as hysteresis loop. The MQCA is of course characterised by its own hysteresis loop as well. However this hysteresis loops reveals many additional features. In fact the MQCA has not only one but many hysteresis loops with different coercive forces. The existence of these loops is related to the main character of the MQCA work or to the basic elements of MQCA. These elements are locally stable spin up and down configurations associated with +1 and -1 units. So the MQCA operates with such configurations and they are locally stable. The application of a magnetic field will destabilise such a configuration and different configurations will have different critical field for the instability.

Since the total set of all possible values of magnetic moments associated with individual particles of the chain forms a fractal we expect that the total magnetisation will be also characterised by fractal structures. Indeed, below we have calculated the magnetisation as a function of the applied external magnetic field as well as the associated hysteresis loop. The dependence of the total magnetisation on external magnetic field is presented on the Fig. 2. One can see from this Figure that this dependence is multivalued. Indeed the possible values of the total magnetisation form a fractal. Thus the possible hysteresis loops of MQCA could be be presented as some kind of a Cantor set.

Since the nonlinear set Eq. (3) cannot be decoupled in general we will not able to find analytical solutions, except for some simple cases. For the numerical evaluation we use standard iterative gradient descent methods in order to find the local energy minima. Here the asymptotic binary configurations $\mathbf{x}^*$ introduced in section 2 serve as initial configuration for our iteration procedure such that one can systematically calculate all nonequivalent solutions.

Provided that H/K is sufficiently small, the implicit function theorem then allows for the existence of solutions of Eq. (3) in terms of a power series expansion about the asymptotic strings $\mathbf{x}^*$, where the first order correction term is proportional to H/K. We now solve the nonlinear system Eq. (3) and calculate all possible magnetizations M as a function of the external magnetic field H for fixed values of K and β. Fig. 2 shows all magnetizations M which can be reached in various ways depending on the initial condition. We observe that the magnetization, considered as the output, is a multi-valued function of the magnetic field H. Fig. 2 also suggests that a variety of different hysteresis loops are theoretically possible [6]. In particular, the magnetization M as a function of the field is not necessarily smooth but can increase in steps. This fundamental mechanism giving rise to a series of minute jumps in the magnetization is the so-called Barkhausen effect [7]. It was discovered in 1919 and gave first experimental evidence of these magnetic instabilities.

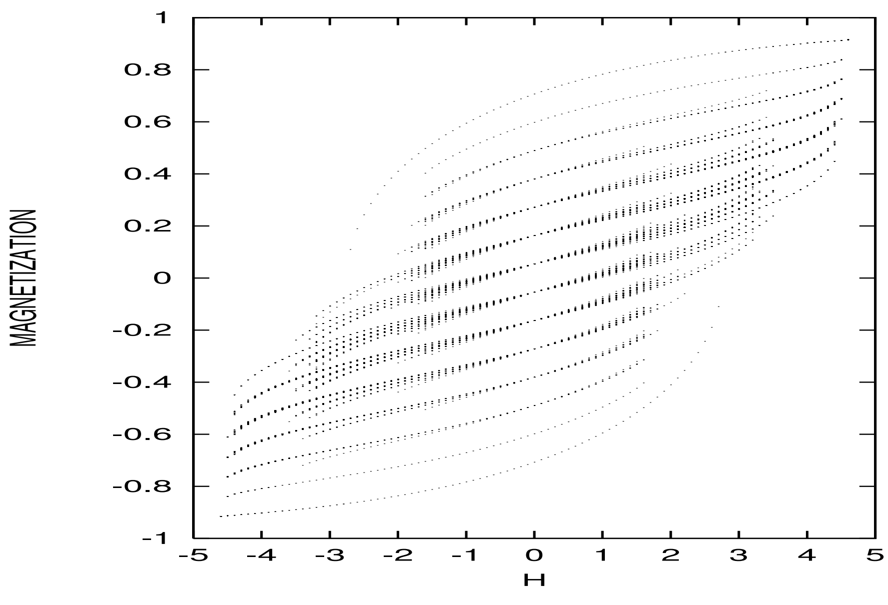

Figure 2. Distribution of all possible total magnetizations M as a function of the magnetic field H for $K = 5.5$, $N = 13$ and $\beta = \frac{\pi}{4}$.

Note that a specific domain structure corresponds to the system being trapped in one of these local energy minima. If thermal fluctuations are neglected and the energy barriers separating this minimum from neighbouring ones are large enough, the system will indefinitely remain in such a metastable state. However, a slight change of the strength of the applied field H can easily destabilise a specific domain structure. It is sufficient that a local minimum of the energy landscape is transformed into a saddle point such that the system can evolve toward some other metastable configuration. These rearrangements can be quite localized in space or may involve even the whole domain structure.

To understand the distribution of the total magnetisation presented in Fig. 2 let us consider the distribution of all possible magnetic moment directions $\vec{S}$ which can take individual dots under influence of magnetic field. It is also useful to compare the results presented in Fig. 2 with the distribution of the energy values associated with different locally stable spin configurations and how this energy spectrum is changing as a function of the magnetic field H. Such distributions, somewhat reminiscent of Cantor-set structures, are depicted in Fig. 3 and Fig. 4, respectively.

Figure 3. Distribution of the magnetic moment directions as a function of H for $\beta = \frac{\pi}{4}$, and $K = 5.5$. The number of particles in the horizontal chain is equal to $N = 13$.

In this distribution we see a number of branches. The most dense pack of branches is arising in the vicinity of zero magnetic field. Each line from these branches corresponds to a specific domain configuration, which is locally stable. With increasing (or decreasing) magnetic field some of these configurations associated with shallower minima will disappear. The shallower minimum, the faster the particular domain configurations disappears. The domain walls always disappear in pairs (see,Fig.1). The least locally stable state corresponds to a bound state of the two domain walls located as close as possible. In a previous paper we called such a state a "soliton". The disppearence of the two domain wall configurations as well as other least stable configuration are also seen in the energy spectrum (see, Figure 4). Figure 4, the "crab", shows that there are seven branches in the energy spectrum. Each energy level corresponds to a configuration consisting of 0,2,4,6,8,10 or 12 domain walls. For example, depending on the Input on AC chain on the MQCA gate there are two or 4 domain wall configurations, see, Fig.1. Provided that the moments on the AC chain are up-spin oriented, we have 4 domain walls. When the moments on the AC chain are be spin-down oriented, we had only two domain walls on the gate. For the horizontal chain, BD, the number of particles is equal to $N = 13$. This means that there are following configurations: two fully polarized states which could be classified with the use of the total absolute value of magnetisation multiplied by the number of particles $L = NM$, ie here we have $L = 13$. These states arise at high magnetic field only. There are branches associated with two, four, six domain walls and further up to 12 domain walls. Accordingly, the energy spectrum depicted in Fig. 4 has 7 branches corresponding to 14 hysteresis branches presented in Fig. 2 Each branch corresponds to the following number associated with the value of the total magnetization multiplied by number of particles $L = MN$, $L = (-13, -11, -9, -7, -5, -3, -1, 1, 3, 5, 7, 9, 11, 13)$. Of course the number L is used as a classification number. The exact value of the total magnetization of the system is presented in Fig.2

Each of this branch corresponds to distinct magnetic moments associated with different configurations having the same fixed number of domains. Varying the magnetic field the degenerate energy levels split and lead to the spectrum presented in

Fig. 4.

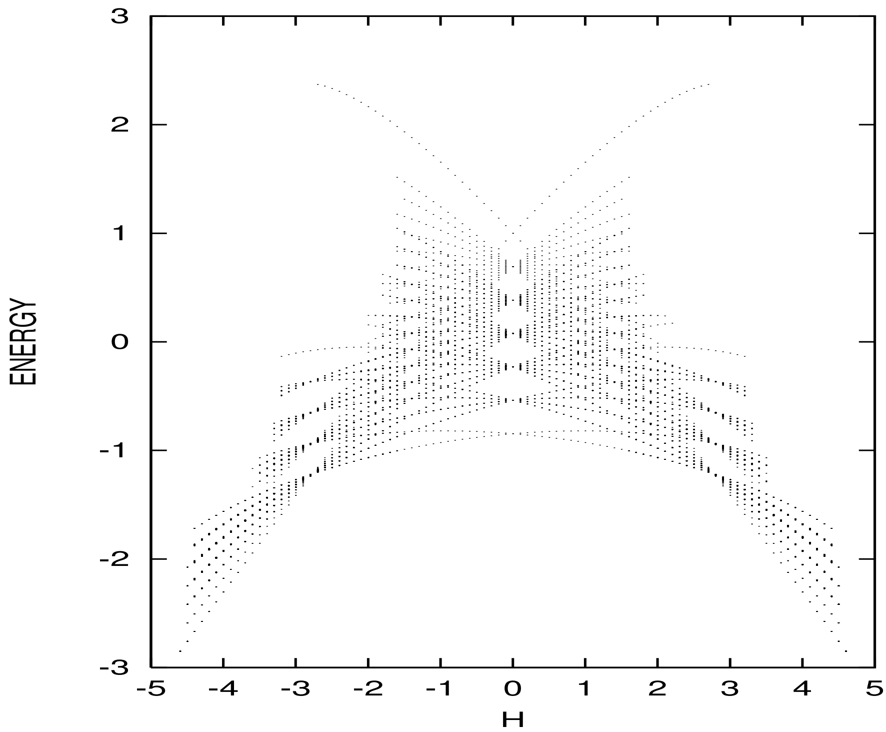

Figure 4. Energy spectrum as a function of h for $\beta = \frac{\pi}{4}$ and $K = 5.5$. The number of particles in the horizontal chain is equal to $N = 13$.

In order to get some more insight how these structures evolve, we analyse the distribution of the microscopic variables, the magnetic moment vectors (directions). Effectively we consider only a projection on the vertical axes. For fixed value of the magnetic field h we first calculate all possible magnetic moment formations as the length N of the chain is varied. With increasing number of particles the magnetic moment spectrum for moments associated with the asymptotic value 0 evolves in terms of tripling and quadrupling of spectral substructures. Fig. 5 illustrates how the spectrum grows in a quasi self-similar manner, where structures replicate themselves on successively smaller scales with respect to their statistical properties. Triplets split into a quadruplet surrounded by two triplets, while quadruplets split into four quadruplets.

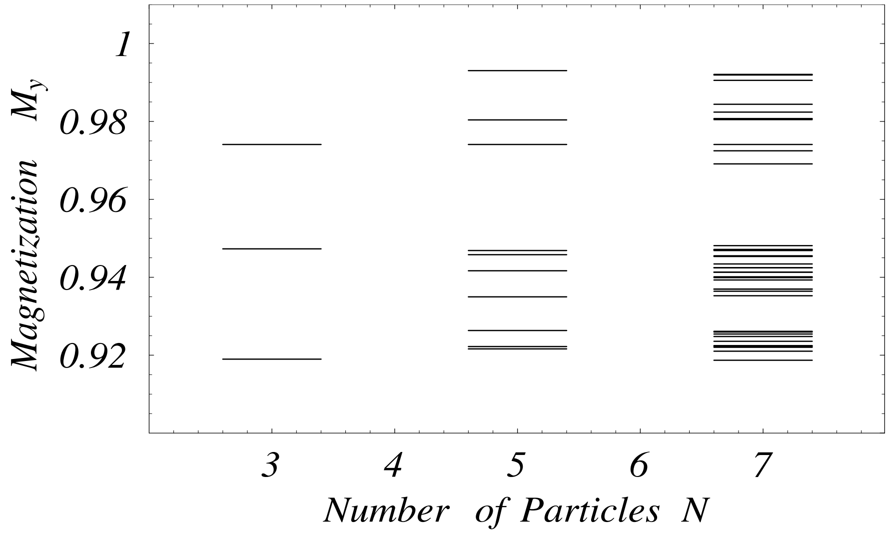

Figure 5. The values of the projection on the vertical axes of the magnetic moment vectors for $N = 3$, $N = 5$ and $N = 7$ for $h = 1$, $K = 8$, and $\beta = \frac{\pi}{4}$

For $N = 3, 5, 7$ we have $3, 10$ and 36 spectral lines, respectively, see Figure 5. For moments associated with the asymptotic value π the situation is statistically the same. Note however that the spectrum is not self-similar in the strict sense. For $N = 1, 2, ...$ the total number of distinct magnetic moments is given by the sequence $\{1, 2, 3, 6, 10, 20,\ 36, 72, 136, 272,\ 528, 1056,\ 2080, 4160, 8256, 16512, ...\}$ [5]. It is interesting to note that this sequence also specifies the number of all possible N-bead black-white reversible strings, a colouring problem in combinatorical mathematics. An estimate for the fractal dimension with the aid of a box counting algorithm gives the value $d_f = 0.61$ compared to $d_f = 0.538$ for the logistic map at the critical accumulation point for period doubling. With increasing strength of the anisotropy parameter the fractal dimension d_f tends logarithmically to zero. Note that also the Barkhausen effect exhibits fractal properties at sufficiently low domain wall velocity. Moreover, it has been shown that its self-similar properties are in fact associated with random Cantor dust of a fractal dimension depending on the strength of the magnetic field h [8].

DISCUSSION AND SUMMARY

The Cantor set of the total magnetization presented in the Fig. 2 may be detected in experiments with the use of the fast cooling rates at different field strength. At the fast cooling a random configuration formed at high temperatures will be associated with one of the metastable states and therefore at low temperatures it will be frozen and corresponds to one specific value of the fractal presented in the Fig.2. Since at high temperatures any state does not correspond to a specific deep minimum. Then all type of configurations will be formed. With fast cooling these configurations could be frozen into one of the configurations of the multi valley energy landscape which will be revealed with the measured values of the total magnetization, which set forms a fractal.

Thus, our studies led us to amazing results: Namely the spatial structures of domains in a chain made of small magnetic particles in in MQCA gates show a selfsimilarity of the fractal. Such spatial distribution of magnetic moments associated with different particles is a difficult task to measure on experiments although the modern technique, like STM and AFM as well as the Kerr rotation may allow to fullfill such a task. However, from the point of view of MQCA operational properties, the fractal structure found can have a strong impact. The energy landscape associated with the creation of domains and fractal values of the total magnetization, may further stabilize the work of MQCA. Because the energy surface consists of many locally stable minima separated by large barriers the MQCA may operate as data storage. Each of these minima corresponds to the state with some fixed number of domains or domain walls. Even if such a number is fixed he states associated with different configurations or rearrangement of these domains will correspond to different or the same minima. This is the situation, which is precisely arising in glassy system. Such shape of the energy landscape led us to the conclusion that the systems formed from magnetic particles is a some kind of magnetic glass associated with the creation of domains. We propose to make a detailed experimental investigation of the MQCA systems made of small magnetic particles to identify this glassy character and fractal features of their domain structure as well as influence of the fractal structure on the operation of teh MQCA. In this respect it might be useful to measure the magnetization at zero field as well as in cooled regimes as commonly practiced in experiments on spin glasses. Due to these above described energy landscapes the corresponding magnetic structures at very low temperatures are very stable with respect to thermal as well as to quantum fluctuations. To reveal these fractals the experiments associated with fast cooling should be set up. The repetition of the fast cooling from high temperatures at different magnetic field may drive the system to settle in the different valley of the energy landscape. The measuring of the total magnetization at the each lap of cooling with the same and different cooling rates may provide the set of numbers which can reminicent some bits of a fractal. The latter will depend on the shape and the number of particles of which the nanostructure is formed. Since the different clusters will be associated with the different fractals then in general these studies may lead to a development of the new type of the spectroscopy where with the aid of the fast cooling magnetization measurements the structure of small clusters may be identified.

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