Molecular Magnetic Quantum Cellular Automata

(Molecular MQCAs)

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ABSTRACT

This report examines a specific nanoscale computing technology, namely Magnetic Quantum Cellular Automata (MQCA) systems. It provides estimates of the temperature stability and operating speed as a function of the device size, together with estimates of how such systems might behave if the device sizes could be scaled down to molecular dimensions.

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14. ABSTRACT

This report results from a contract tasking University College London as follows: The contractor shall conduct theoretical analyses and computer modeling of magnetic quantum cellular automata systems and devices, at both the mesoscopic and molecular scale, with the goal of providing an original concept significantly different from other proposed nanodevices, offering the prospects of molecular-scale with relative ease of fabrication, and uses fabrication techniques which would be compatible with magnetic ultra-high density data storage devices. Performance enhancement and limitations will be predicted using the theoretical models.

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1. INTRODUCTION

As Moore's law for the continued size downscaling and speed upscaling of conventional CMOS transistor technology approaches its end, so more and more effort is being devoted to trying to develop possible device technologies and system architectures, that might allow improvements in computing logic and memory performance to continue. Many such devices and architectures have been, and are being, examined. This report considers only one such device and one architecture, namely bistable magnetic elements and magnetic quantum cellular automata (MQCA) systems.

In an MQCA system, every cell is supposed to evolve into a stable state that is determined by the properties of the neighboring cells (and perhaps by external fields). Arrays of MQCA cells can be seen as computing circuits, where the state of an array is mapped to a computation. The potential advantages of this concept over conventional transistor-based logic are:

- high speed,
- insensitivity to electrical disturbances and cosmic rays,
- ease of fabrication,
- very good scaling potential (possibly down to molecular size),
- room temperature operation and low power.

Unfortunately these advantages do not as yet all exist in the same device.

Quantum cellular automata based on electronic interactions (EQCAs) have been studied for more than a decade, but *magnetic* QCAs were first described only in 2000. These used lithographically-defined magnetic elements, with typical sizes of ~100 nm, and made of the magnetically soft material supermalloy. The possibility has recently arisen, that molecular-sized magnetic elements might be used instead, with a concomitant increase in device density by a factor of more than a thousand. This was the driving force behind the proposal that led to the study whose results are reported here.

Cost constraints meant that a total of only about 2.5 person-months could be devoted to the study. It was therefore quite limited in extent, but some clear results and conclusions can already be drawn. There were two complementary aims. The first was to see what the performance of 'conventional' magnetic quantum cellular systems, using lithographically defined devices, might be if they could be miniaturised. The second aim was to see what the performance might be achievable using a new magnetic logic nanodevice, which would be molecular level in scale. Both the 'lithographic scale' and the 'molecular scale' devices are related to spintronic devices, but they are significantly different both in their operation and in the materials that are used. The outcome of the study was to be a short report containing, amongst other things, an assessment of the performance envelope of systems using these devices, in terms of the tradeoff between operating speed, reliability, size and operating temperature. This document is that report.

2. BACKGROUND

The concept of cellular automata systems began in 1956, with publications by von Neumann and Codd [Codd 1956], but the idea only became widely known in 1971, when John Conway described the game of Life, where a regular grid of cells, each interacting with its nearest neighbors and obeying very simple rules, produced extremely complicated results (see Figure 1).

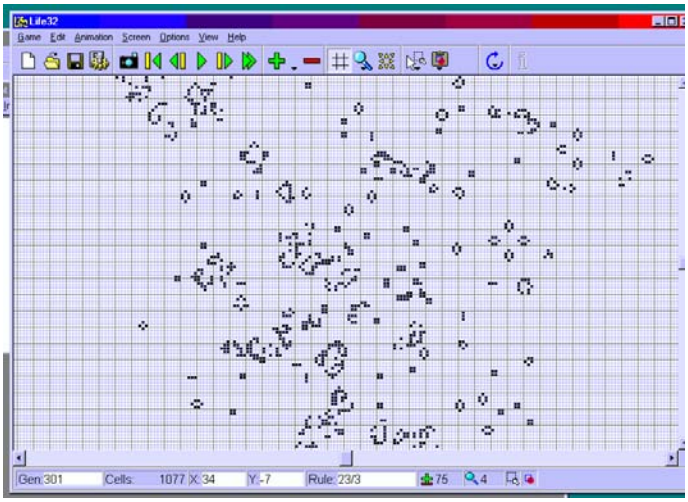


Figure 1: An instant in the evolution of a pattern using the cellular automaton system 'Life' (ref. [Life32]).

'Life' is an example of a system which is in principle capable of universal computation, but it was shown (in 1973, by students at MIT) that it would not be much use in practice – a simple logic gate would need perhaps 1000 by 1000 cells. However, if one is allowed to control the placement of the cells – that is, if the completely regular mesh arrangement is abandoned - then more efficient systems become possible.

2.1 Electronic QCAs

Implementations of QCAs as electronic systems, encoding logic states by means of the spatial distribution of electric charges within a cell, were described some years ago [Lent and Tougaw 1996, Lent and Tougaw 1997, Porod *et.al.* 1999]. The mutual cell interactions are used to propagate and compute binary information. Every EQCA system is supposed to evolve into a ground state determined by the polarisation of edge cells (and possible external electrostatic fields).

A typical EQCA cell design consists of four quantum-dots [Lent and Tougaw 1997], see Fig. 2. The cells are electro-neutral (but have two free electrons), and can be in a polarized or non-polarized state, depending on the tunnelling potential between quantum wells. There are two polarized states due to Coulomb repulsion between electrons, which can be used for representing binary information.

Work on EQCAs is still mainly theoretical, and only a few experimental devices have been fabricated [Csurgay and Porod 2001], although the fabrication of quantum dots (which are

the basic elements of solid-state EQCAs) is well developed. An experimental demonstration of a four-dot EQCA cell has been reported [Orlov *et al* 2000]. The device was composed of four metal dots (a pair of dots connected via a tunnel junction and capacitatively coupled to another dot pair) and operated at temperatures below 50mK.

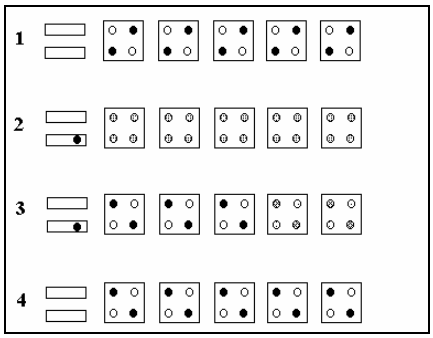


Figure 2. Four stages of the process of signal propagation in an array of EQCA. Individual cells are represented by a square, with four (quantum) wells (circles). Full circles represent wells occupied by an electron.

There are currently only a few functional EQCA circuit designs in the literature. Some fundamental circuit elements have been proposed: binary wire (Fig. 2), fan-out, inverter and majority gate. A logic gate based on a four-dot EQCA has been experimentally realized [Amlani *et al* 1999], where AND and OR logic functions were demonstrated by operating a single majority gate. A clocked EQCA two-stage shift register was recently demonstrated [Orlov *et al* 2003]. An EQCA memory design has been proposed by Berzon and Fountain [Berzon and Fountain 1999], and a one-bit full adder design has been proposed by Lent and Tougaw [Lent and Tougaw 1996], see Fig.3. Adiabatic clocking is necessary for correct circuit operation, providing circuit directionality and for preventing thermodynamic effects which might cause the system to finish up in an undesirable metastable state rather than the lowest-energy ground state.

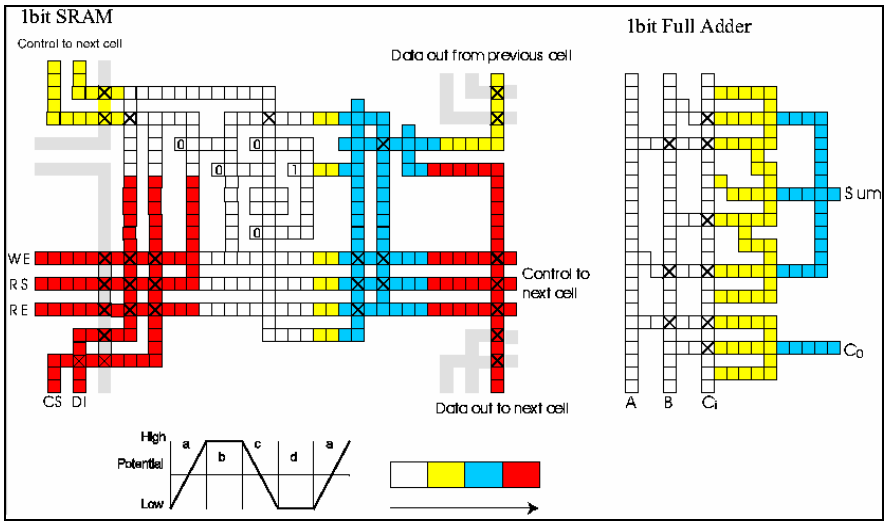


Figure 3. Proposed designs for one-bit SRAM [Berzon and Fountain 1999**] and 1 bit full adder [**Lent and Tougaw 1996**]. The four phase clock (provided in the form of the tunnelling potential with a ramp wave-form) is shown at the bottom of the figure. WE=Write Enable, RE=Read Enable, RS=Row Select, CS=Column Select, DI=Data In. Cells labeled X represent a wire crossover.**

There has been considerable work on the physics of EQCAs. In addition, several circuit models have been developed [e.g. Nikolic *et al* 2001], but they are still incomplete at the moment. However, there are several simulation packages which enable EQCA circuit analysis at either basic, quantum-mechanical level, or functional, logic level [Nikolic *et al* 2003]. A high level simulation tool, such as SQUARES [Berzon and Fountain 1999] allows simulations of large assemblies of EQCAs but only at a logical level, see Fig. 4.

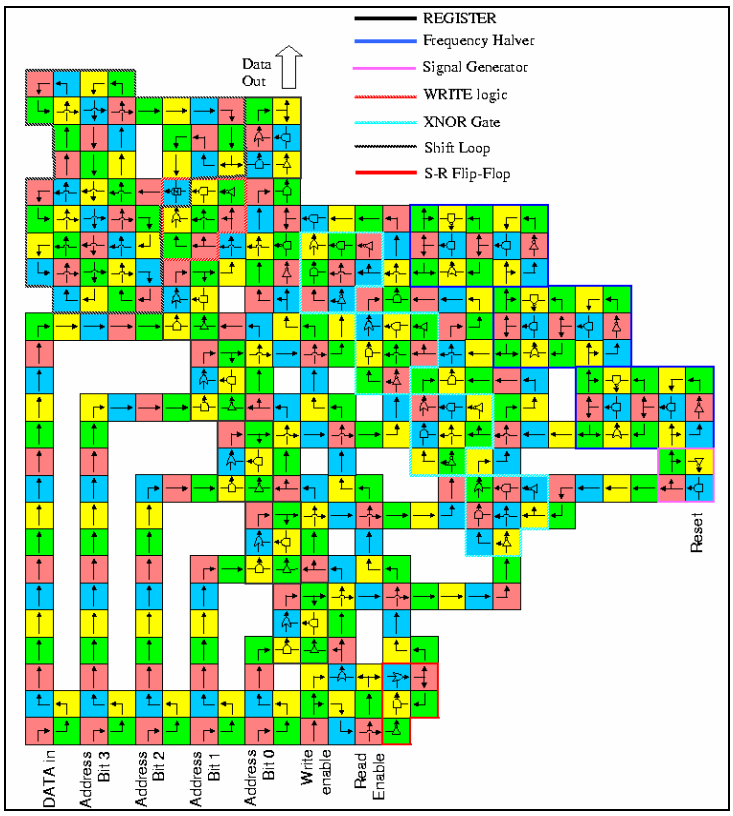


Figure 4. Four-bit memory and shift register: each block contains 5x5 EQCA elements.

The EQCA concept has sometimes been described as a 'computation without current'. However, it does not appear to be possible to avoid using some sort of power-dissipating conventional electronics to provide clocking for an EQCA system, which is essential for synchronized computing and for introducing directionality into EQCA dynamics. EQCA designs might be useful as a circuit architecture for molecular chips, since the EQCA concept is potentially viable at the molecular level [Macucci *et.al.* 2001, Lent and Isaksen 2003]. Apart from the general problem of (currently) needing very complex structures for solving real-life logic or memory structures (Figures 3 and 4), one particular problem with EQCAs at present is that they need a very low operational temperature and relatively slow speed [Niemier and Kogge 2001], determined by the adiabatic transition of an electronic system into the ground state. However, the electronic QCA concept has been examined at the molecular level, especially the idea of using EQCAs for quantum computing [Twamely 2003].

2.2 Magnetic QCAs

It comes as a natural idea that CA cells could be small magnets, where the direction of the cell magnetic moment can represent a logical '1' or '0' state. For example the CA cell could be a piece of a ferromagnetic material, Fig. 5.

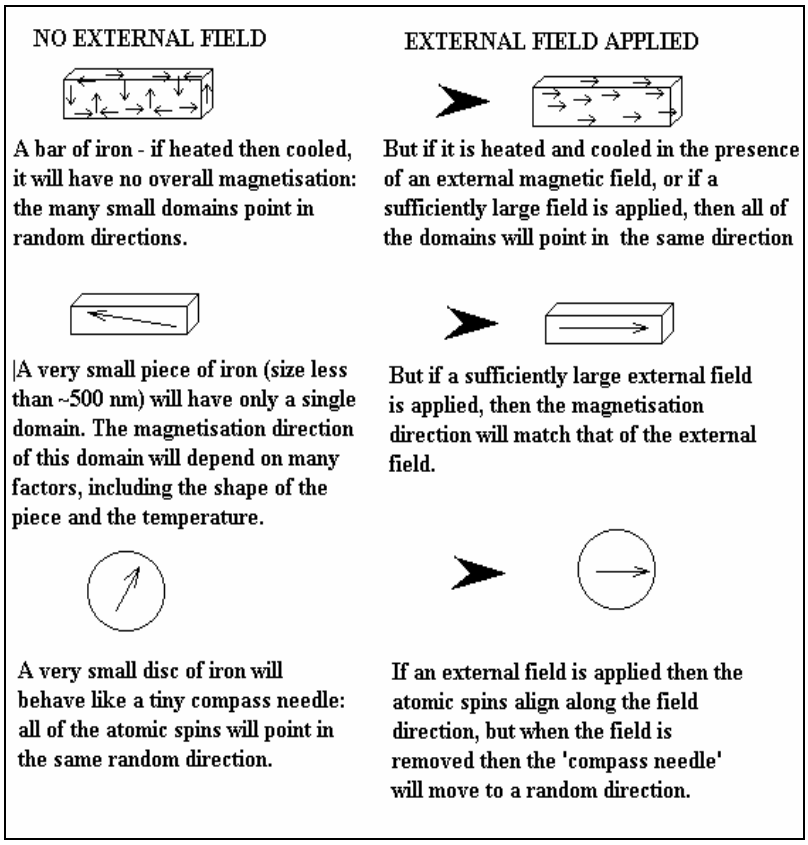


Figure 5. If an MQCA cell were a piece of iron, how would it work?

Magnetic QCAs (MQCAs) rely on a property of very small ferromagnetic structures (nanomagnets), namely that the electronic spins act coherently as a 'giant spin' [Cowburn *et.al.* 1999]. The word 'quantum' (in QCA) here refers to the quantum mechanical nature of the short-range exchange interaction, which tends to align the spins of neighboring atoms, and wins over the competing, longer range, classical dipole-dipole (magnetostatic) interaction.

Cowburn and Welland [Cowburn and Welland 2000] demonstrated the first MQCA system, in the form of a `wire' of 69 magnetic QCA `dots', Fig. 6(a). The elements were fabricated from a 10nm thick Supermalloy (with composition $Ni_{80}Fe_{14}Mo_5X_1$, where X is some other metal), each 110nm in diameter. The 'wire' had an elongated input dot and a set of circular dots. The propagation of a binary signal down the wire was shown to be possible with the assistance of external magnetic field (shown in Fig. 6 with large arrows). Binary signal propagation has been demonstrated at *room temperature*. However, very quickly several problems were identified in connection with this proposal:

1. circular cells offer no intrinsic spin directionality, hence it is hard to implement more complex structures,
2. a driver signal with an appropriate polarity needed, but generally it cannot be predicted in advance what that would be, and
3. poor packing density of the MQCA discs - not enough to give significant advantage over CMOS in logic applications.

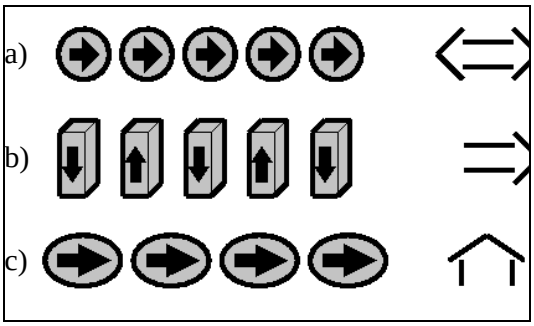


Figure 6. Proposed MQCA designs: (a) circular (nano)magnetic dots [Cowburn and Welland 2000]**, (b) antiferromagnetically coupled bar (nano)magnets,** [Csaba et al 2002] **and (c) ellipsoid discs** [Parish & Forshaw 2003]**.**

An alternative arrangement of magnetic nanodots has been proposed by [Csaba *et al* 2002], shown in Fig. 6(b). They demonstrated in a computer simulation that their proposed system of antiferromagnetically coupled magnets could be used for digital information processing. They also created a SPICE macromodel simulator for simulation of interacting nanomagnet arrays, which could also be used in the case when these arrays are embedded in microelectronic circuits. The SPICE simulation tool for nanomagnetic arrays is important for the simulation and design of logic gates and structures of higher complexity.

Another alternative magnetic cellular automata system was proposed by Parish and Forshaw [Parish and Forshaw 2003], and was called a 'bistable MQCA' (BMQCA). Here the basic cell is in the shape of a planar ellipse, Fig.6(c). As the illustrative analysis in Fig. 7 shows, it would be desirable if only two directions are energetically favorable in the cell, which is possible to arrange either through shape anisotropy, or magnetostatic interactions between the dots. The shape anisotropy provides two stable ground states, see Fig. 7, hence each particle can store binary information. The bistability of the BMQCA allows the implementation, not only of planar wires (either ferromagnetically or antiferromagnetically coupled) but also of vertical wires and majority gates, Fig. 8.

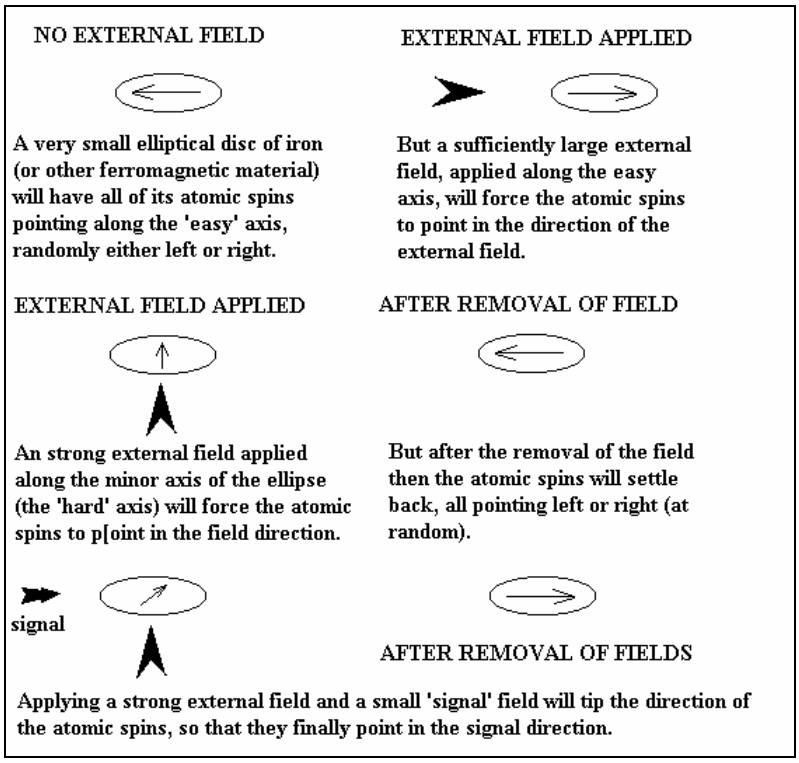


Figure 7. Shape anisotropy provides desirable binary coding in MQCA cells.

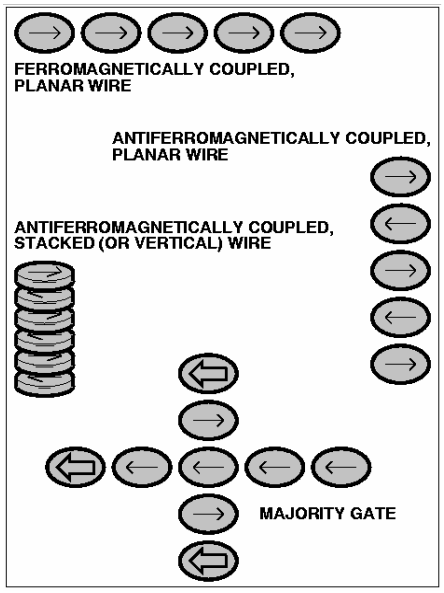


Figure 8. Possible BMQCA wire designs and majority gate design.

Fig. 9 illustrates the basic principles of BMQCA operation, using a planar ferromagnetic wire of nanomagnetic elements. The direction of the magnetization of each element is represented by a single spin vector, which in the absence of an external magnetic field is parallel to the long axis of the ellipse (in this instance, the ± *x*-direction). The application of a slowly-varying external *adiabatic clock field* parallel to the hard axis (+*y* direction) forces all of the spins to rotate and eventually align with the driving field when it reaches a sufficiently large value (typically a few hundred oersteds). An input signal (illustrated at the left of Fig. 9) is applied when the clock field reaches its maximum value. As the clock field is slowly reduced to zero, the spins interact in such a way that the final state of the wire has all of them pointing in the same direction as the input signal.

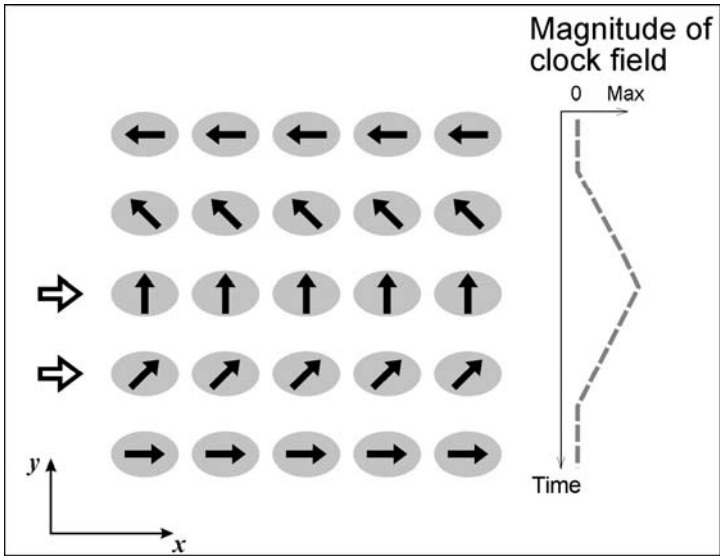


Figure 9. Adiabatic clocking of a five element BMQCA wire. The time dependence of the clocking magnetic field (which is pointing along the *y*-axis) is shown on the right. The input signal is illustrated with two arrows on the left.

Perhaps a better description of the wire operation would be a magnetic soliton propagation, shown in Fig. 10. The magnetic solitons carry information through the MQCA networks [Cowburn and Welland 2000], but the alternating external magnetic field is needed to set the cells into their neutral positions and to provide synchronization in the network.

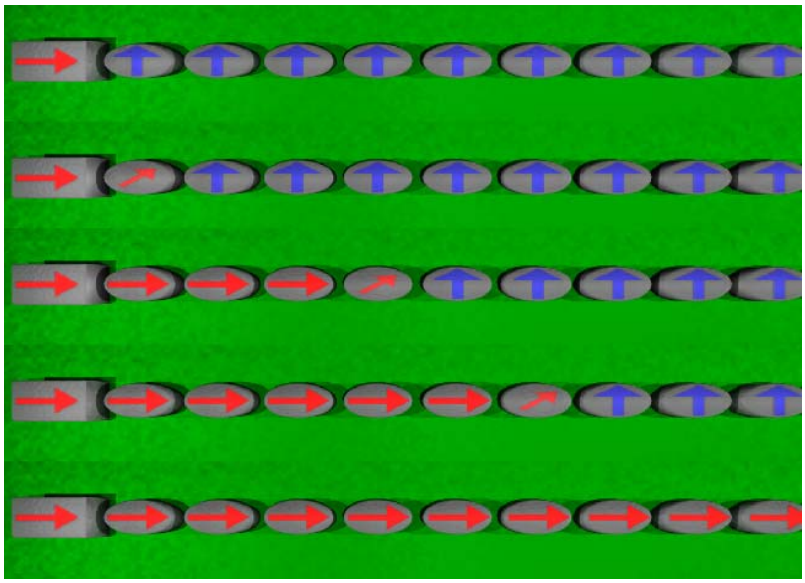


Figure 10. Propagation of a magnetic soliton.

Although the BMQCA concept has solved some of the deficiencies of the MQCA system proposed by Cowburn and Welland, many problems remain, such as:

- a full assessment of the maximum processing speed,
- a full assessment of system power dissipation
- ensuring that the system does not become locked in a non-ground metastable state, and
- ensuring that the clocking fields of adjacent devices do not interfere with one another.

The question of the processing speed is connected to the requirement for adiabatic evolution of the system (which in essence means that the external fields must change relatively slowly, so that the system always remains in near-equilibrium). Adiabatic evolution in turn is linked to the third problem: the undesirable event of the system becoming stuck in a metastable state, i.e. the magnetic soliton stops before reaching the end of line. Although QCA systems are nominally very low power devices, since the flip of a magnetic moment should involve only a very small power dissipation, there still remains the question of the power dissipation in the system which has to generate the rapidly-oscillating, magnetic clocking field.

Hence, it was therefore an obvious idea to examine the properties of an MQCA system if the magnetic cells are reduced in size down to the nanometre range. The smallest individual magnets are *molecular* magnets, which are described in the next section. Here we wish to consider whether they offer any possibilities for extending the performance envelope of MQCAs.

3. MOLECULAR MAGNETS

During the 1990s certain molecules were discovered to show ***permanent magnetisation*** and ***magnetic hysteresis*** [Sessoli *et.al.* 1993a and 1993b]**.** This was shown to be a purely one-molecule phenomena. Investigations have shown that these molecular magnets have a high spin ground state and high zero-field-splitting. These properties lead to an energy barrier at low temperatures, and such a system can be trapped in one of the high-spin states. A prototype of a single molecule magnet is the Mn_{12} – acetate molecule [Mertes et.al. 2003], see Fig. 11.

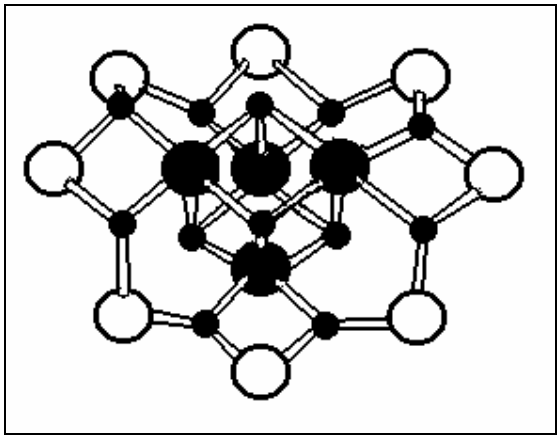


Figure 11. The $Mn_{12}O_{12}$ core of the Mn_{12} –acetate $Mn_{12}O_{12}(CH_3COO)_{16}(H_2O)_4$ molecule. The small spheres represent oxygen atoms, the large spheres manganese. The four large black spheres are Mn^{3+} ions and have spin s = 3/2 each (combined: S=6), while the eight large outer spheres are Mn^{4+} ions and has s = 2 (S=16, antiparallel to the 3/2 spins); thus the total spin is S = 10. This inner core is surrounded by methyl groups, and also (in bulk crystals) by acetic acid molecules and by water of crystallisation.

The magnetisation properties of the Mn_{12}-ac molecule are shown in Fig. 12. Two important properties of magnetic molecules follow from Fig. 12, namely high saturation fields, and the need to use very low temperatures before the onset of (in this case undesirable effect of) 'superparamagnetism' (T = 4.2K case in Fig. 12).

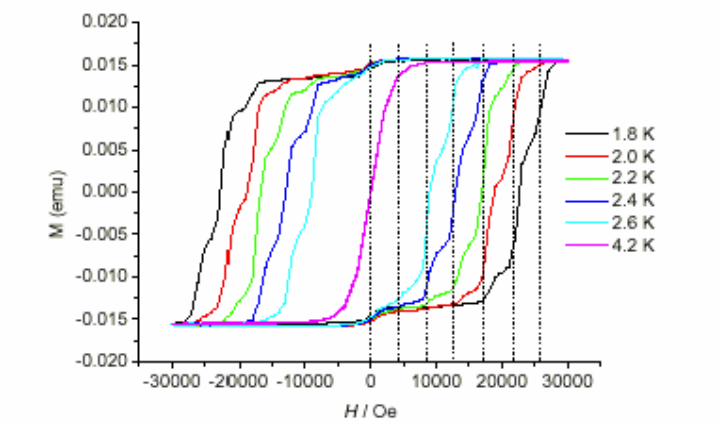
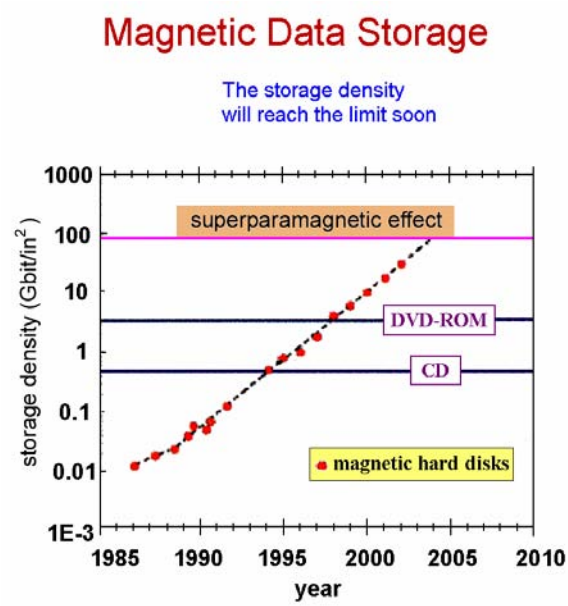


Figure 12. Hysteresis curve for the Mn_{12} –acetate molecule.
(Graph taken from: http://www.pi1.physik.uni-stuttgart.de/indexjs.html)

There are a few dozen molecular magnetic systems that are known today. They are based on exchange-coupled clusters of four to about thirty magnetic ions, usually from the first period of the transition metals, such as Mn, Fe, Cu, Ni, Co etc. The spin values (i.e. the total magnetization) of molecular magnets are of the order of ten electron spin units. This makes them exhibit some interesting properties, which lie between the properties of a bulk magnet with an enormous magnetic moment (which can be described in a classical framework) and the properties of a single electronic spin.

Magnetic molecules are being investigated for their possible use as conventional magnetic data storage devices. The ultimate limit of data storage would be: one molecule = one bit. The theoretical data density in that case would be enormous, ~100 Tbit/in^2, which is about 3-4 orders of magnitude above current technological limits.



(Graph taken from: http://www.quantchem.kuleuven.ac.be/~vladimir/research.html)

Single-molecule magnets are also of great scientific interest because they exhibit various quantum-related phenomena (such as quantum tunneling of the magnetization), which suggests the possible application of single-molecule magnets in quantum computing.

Quantum mechanical tunneling processes can alter the magnetization of molecules. This effect, in principle, represents a disadvantage for information storage. However, there are some ideas about how to influence and control the quantum tunneling. Wernsdorfer et. al. have developed and studied a system of two single-molecule magnets coupled antiferromagnetically in a dimer [Wernsdorfer *et.al.* 2002]. The quantum tunneling of magnetization in the dimer was different from that of the individual single-molecule magnets. The exchange interaction between two molecules' total spins can suppress the tunnelling at zero magnetic field and hence restore the information storage ability in the dimer. In addition, the possibility of having the ground state as the combination of two entangled states makes it a possible candidate for a qubit, which is a crucial step in building future quantum computers. The idea to use pairs of magnetic dipoles, i.e. magnetic quadrupoles, was originally proposed by Forshaw et.al., but for the case of nanomagnets, which utilised classical magnetostatic interaction between the magnets.

Another potential problem with molecular magnets is that, for the single-molecule magnet structures discovered so far, magnetization is retained only at very low temperatures (below liquid helium temperature) for zero external magnetic field (e.g. see Fig. 12). Furthermore, since the magnetostatic interaction between the neighboring molecules is very weak, the 'bulk' type magnetization as a collective phenomenon is very quickly destroyed by thermal fluctuations.

There are many other interesting phenomena associated with these molecules that we only comment on here very briefly. In addition to the electronic spins, there are *nuclear* spins which can produce a variety of additional effects (and which may prove useful for the purposes of quantum computing, as opposed to the quasi-conventional logic systems considered in this report). Completely separate phenomena are associated with the fact that, although individual molecules show magnetic effects, other magnetic phenomena occur when the molecules are assembled into crystals: coupling between the individual magnetic moments occurs and various cooperative bulk effects take place.

How might these individually-magnetised molecules be used in magnetic quantum cellular systems, and what would their performance be, especially with regard to temperature? In brief, we suppose that individual molecules may eventually be used as MQCA elements. Thus, for example, the line of elliptical supermalloy element in Figure 8 would be replaced by individual magnetic molecules, which it is hoped would interact in a similar way to their much larger supermalloy counterparts. However, we wish to emphasize that this report does *not* concern itself with the technological aspects of how the individual molecules would be fixed in the correct positions on some substrate, in order to form the desired circuit layout. We are interested here only in trying to produce quantitative estimates of whether the basic physical phenomenon of magnetic interaction between closely-spaced molecules might (or might not) have properties which could lead to technologically useful computing performance.

One of many problems which have to be faced is that it is difficult to produce reliable mathematical models or computer simulations of these molecules and their properties (for example, see the excellent review in [Postnikov *et. al*. 2004]). However, good progress has been made and reasonable agreement between experiment and theory is starting to appear, but the simulation software is typically very complicated, in order to handle the many complicated quantum mechanical effects that are associated with changes in the molecular configuration, multi-electron interactions, resonant tunneling etc.

In this study we have made no attempt to model these very complicated effects. Instead, we have used a hugely simplified model, which is essentially classical in its phenomenology. Our justification for this is as follows.

Although existing molecular magnets are very complicated structures, which exhibit many complicated quantum mechanical phenomena, their most outstanding characteristic is that they exhibit magnetic anisotropy. That is, their preferred magnetisation direction is parallel (or antiparallel) to a fixed axis, which is determined by the structure of the molecule. It is this property which might make them suitable candidates for use in MQCAs: if these molecules could be deposited, for example in a line, so that their preferred magnetisation directions were all parallel, then one would have a structure which at first sight would look like a miniature version of the line of elliptical elements illustrated in Figure 9.

There are several big differences between the line of molecules and the line of elliptical supermalloy elements. The internal magnetic structure of the ~100 nm-sized supermalloy elements is determined by a complex interplay between quantum mechanical exchange forces, which typically act between the electrons in nearest-neighbor atoms, and the longer-range 'classical' magnetic dipole-dipole interaction, which extends over all of the atoms in the element. However this complex internal behavior can be modeled relatively simply when only the external properties of the element are of interest. In particular, it is possible to describe the magnetic properties of the element as if it consisted of a single 'giant spin', which preferentially points parallel (or antiparallel) to the long axis – the 'easy axis' - of the ellipse. These two low-energy states are separated by an energy barrier, whose magnitude can be estimated by detailed simulation of the internal magnetic structure of the elements. This barrier corresponds to the situation where the giant spin of the element is forced to point along the minor axis of the ellipse, i.e. 'north' or 'south' in Figures 9 or 10. One other major factor, which cannot be ignored, is the effect of temperature. Increasing the temperature has two main effects. The direction of the giant spin fluctuates: if the energy imparted to the system by thermal fluctuations is sufficiently large, then the magnetisation of the element can flip backwards and forwards over the energy barrier. This is, of course, extremely undesirable. At still higher temperatures the giant spin starts to decohere as the individual electronic spins begin to fluctuate more and more. Eventually, at the Curie temperature, the giant spin effect is lost (the Curie temperature for supermalloy is many hundreds of degrees Celsius).

The typical size of the elliptical supermalloy elements might be ~150 nm, and the center-to-center separation would be only very slightly larger – perhaps 170 nm. A line of such elements can be simulated using exchange forces and dipole-dipole coupling for intra-element behavior, and using just dipole-dipole coupling for inter-element effects. The presence of any external magnetic fields would, of course, affect the internal structure of the elements and hence the overall behavior of any assembly of such elements.

The situation for molecular-sized elements would at first sight seem to be completely different. The elements would now be ~1 nm in size, and their center-to-center separation would be only very slightly larger – perhaps 1.1 nm. The internal structure of the molecules would be dominated by exchange forces, and the dipole-dipole coupling between molecules would be much smaller in magnitude. It might therefore be thought that the magnetic behavior of a line of such molecular-sized elements would have to be described using a purely quantum-mechanical formalism. This is strictly correct, but it have been noted by experimenters that these molecules behave (to a first order) as if they were independent, even when large numbers of them are assembled into a crystal. We suggest that this behavior is analogous to what has been observed (or simulated) with arrays of supermalloy elements. The internal structure of individual molecular magnets is relatively little affected by the presence of neighboring elements. Each molecule behaves (to a first approximation) like a single giant spin, whose direction can be influenced most easily by the application of a large external magnetic field, as shown in Fig. 12. In the absence of an external field, neighboring molecules in a crystal will still interact through dipole-dipole interactions, but the relatively low strength of these interactions mean that they will be easily disrupted by thermal fluctuations. It will therefore be necessary to operate molecular MQCA structures at low temperatures, at least for existing molecules. One of the aims is to try to achieve new molecular structures which would exhibit giant spin effects at room temperature.

Although the detailed magnetic behavior of these molecules is very complicated, it is nevertheless true that they exhibit hysteresis loops, in a similar manner to more conventional

magnetic storage elements or supermalloy elements with shape anisotropy. It is therefore possible in principle to model their use in MQCA structures, using a simulation program. The simulator, which is described briefly in the next section, does not take into account the effects of quantum tunneling of magnetization (which show themselves through the presence of steps in the magnetization curves in Figure 12). The results of the simulation program will therefore be optimistic for molecular magnets, but they can provide useful information, in the form of an upper bound to the performance of MQCA systems using molecular-scale elements.

4. DESCRIPTION OF SIMULATOR

The theory of micromagnetics is well established [Aharoni 1996], but is too complex and computationally demanding to be an efficient tool in analysing arrays of micromagnets. Many numerical micromagnetic simulators have been developed but their reliability for any arbitrary case has been questioned [Aharoni 2001]. One of the more widely used simulators is OOMMF (Object Orientated Micromagnetic Framework, mainly developed at NIST) which is in the public domain [oommf]. The simulator that was used in this study to assess the performance of quantum cellular automata is called *Nanomag*. It was developed during Ph.D. research by M. Parish, with M. Forshaw and K. Nikolic acting as supervisor and second supervisor respectively. Full details are available in the thesis [Parish 2003], and extracts are contained in [Parish and Forshaw 2003, Parish and Forshaw 2004]. It uses a different theoretical basis from OOMMF.

4.1 Nanomag

The simulator uses Monte Carlo/Metropolis methods to estimate the detailed magnetic structure of small (< 500 nm), arbitrarily-shaped, magnetic elements, as a function of any applied external magnetic field, temperature and time. Because of the discrepancies between simulation and experiment that had been found with many other simulators, great care was taken to ensure that simulations were carried out using only those operating conditions and parameters that gave valid results. These correspond to those needed to model the behavior of the MQCAs considered in this report.

Individual elements were modelled at high spatial resolution (for example, a 100 x 50 x 10 nm element could be modelled using 2x2x2 nm cells). The most significant quantity that could be determined from the high-resolution simulations was the energy barrier that separates the two minimum-energy magnetic states that typically exist in zero external field for elongated elements, or those having a dominant 'easy axis' for alignment of the element magnetisation. Once this energy barrier value had been determined for a given element shape and anisotropy, it was then possible to use a low-resolution model of the element, represented now by only a single spin. The 'low resolution' element could then be replicated as many times as necessary, in any spatial configuration such as a 'wire' or a majority gate. The response of arrays of elements to the effects of varying external fields, temperature and time could then be determined with relative ease. In the present study, time constraints meant that only short 'wires' could be examined in any detail, but such structures have long been used to assess the performance of quantum cellular automata, whether electronic or magnetic.

5. RESULTS

All of the simulations were devoted to examining the behavior of 'wires' with ten active elements and a single input signal element. The system analysed is shown schematically in Fig. 9. Most of the simulation time was spent examining elliptical elements (with magnetic properties equivalent to those of supermalloy), and in trying to assess what parameter values were needed to achieve reliable switching of the whole wire, as a function of the 'clock speed' of the driving field (oriented along the +y direction), the temperature, and the cell dimensions (which determine the energy barrier that separates the two stable states of each element). If the energy barrier is low at any given temperature, then thermal fluctuations will often cause the elements of the wire to settle into a metastable state, where some point left and some point right, rather than into the desired lowest-energy state where they all point in the same direction as the input signal element. False states also occur if the driving field changes too quickly ('non-adiabatically'): some elements do not have time to move in a quasi-steady state equilibrium with the driving field, the fields from neighboring or more distant elements, and the fluctuations in direction caused by thermal disturbances such as phonons. It would clearly be possible to develop a theory that predicts the relation between these competing effects, but this has not been done yet.

Figure 13 illustrates how the total magnetisation of a wire varies with time, over two cycles of the driving field. M_y represents the y-component of the wire magnetisation, summed over all of the wire elements and normalised to unity. When M_y is zero then all of the elements point either left or right, i.e. either parallel to the input signal direction or antiparallel to it. When M_y reaches the value 1.0 then all of the spins in the wire point along the +y direction ('north'). The driving field magnitude was modelled as a simple linear ramp-up, followed by a linear ramp-down to zero (as shown in Fig. 9), and then repeated over each succeeding cycle. In this example it is clear that the driving field is sufficient to saturate M_y over about half of the cycle: this phase of the cycle could be shortened significantly.

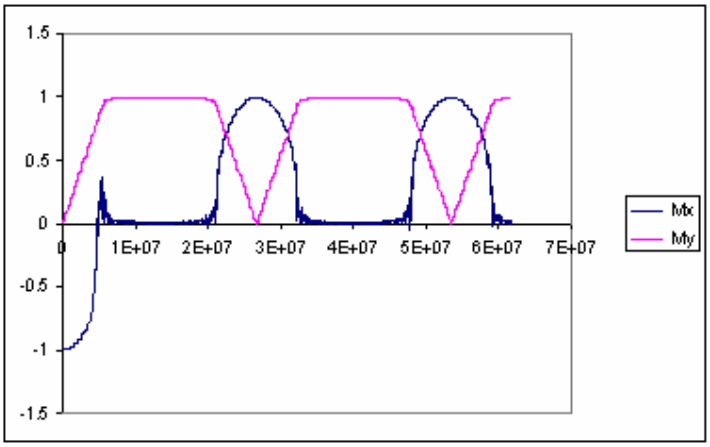


Figure 13. The simulated time response of a 10-cell BMQCA wire, under the influence of an external (magnetic) clocking field and an input dot with magnetization oriented in the +x direction. The vertical axis is the (normalised) magnetisation of the whole wire, with M_x denoting the along-wire magnetisation, and M_y the magnetisation component that is perpendicular to the wire axis. The cells are modeled as elliptical discs of size 5x3 nanometres and 1nm thickness, with the (centre-to-centre) separation of 6nm. The clock frequency is 60 kHz, the temperature is 0.5 K. The total time displayed is approximately 40 microseconds.

Figure 13 also shows how the along-wire magnetisation component M_x varies with time. At time t = 0, the value of M_x is –1, i.e. all of the wire elements point along the –x direction, and opposite to the direction of the input signal element (which will point along the +x direction). This initial state was deliberately chosen to show how, as the driving field forces all of the spins to point north, so the east-west component M_x is driven towards zero. However, thermal fluctuations cause the spins to wobble slightly, and this is most clearly seen when the spins are all pointing nearly north. As the driving field H_y increases, so the effect of the thermal fluctuations is suppressed, but they increase once more when H_y starts to decrease back to zero. As M_y comes out of saturation, so M_x is affected by the presence of the signal field, and it increases towards the desired value of +1. This sequence is carried out once more during the second cycle of the driving field: the wire has successfully switched on both occasions.

Figure 14 illustrates what happens when the system parameters remain the same but the frequency of the clocking field increases. It can be seen that at the end of the first cycle M_x does not tend to the value +1, but stays near zero. A similar effect occurs in the eleventh cycle, but here M_x is approximately –0.2.

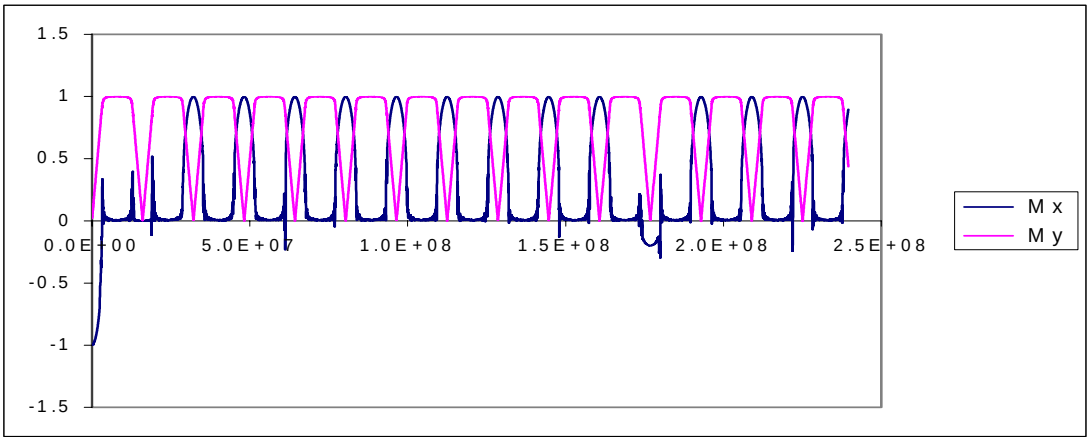


Fig. 14. The time response of the same system as in Fig. 13, but for higher frequency (110 kHz).

An M_x value of zero indicates that there are one or more kinks in the magnetisation directions of the elements of the wire, and in total - half point left, half point right. Usually there is only one kink in short wires, but there may be more at high temperatures. In the cycle 11, M_x ~ -0.2, and six of the ten elements point left (m_x, the magnetisation of an individual element, equals -1) and four point right (m_x = +1). The signal fails to propagate successfully in these two cycles. Figure 15 shows more cycles from the same sequence.

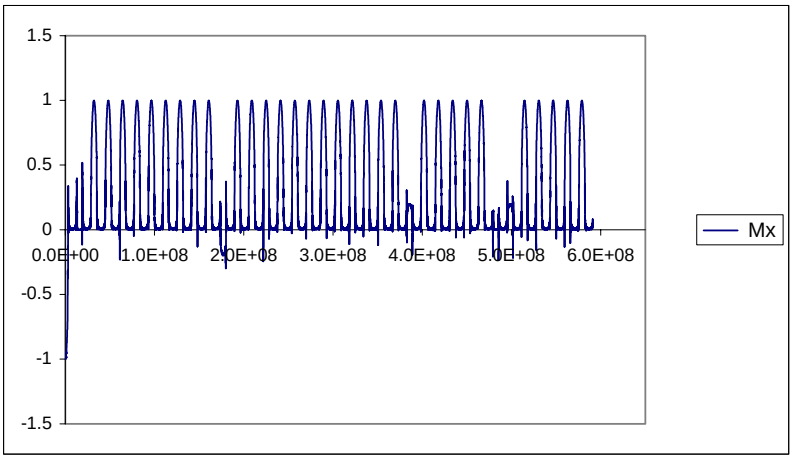


Figure 15. As for previous plot, but showing more cycles. Only M_x shown for simplicity.

The stability requirements for MQCA elements are much the same as those for data storage elements. Each element should be stable enough to withstand thermal fluctuations which might cause the spin of any element to flip into the wrong direction. It is relatively straightforward to show that the energy barrier that separates the two low-energy states has to be in the range ~50 to ~100 kT , where T is the absolute temperature and k is Boltzmann's constant. The multiplying factor will depend on exactly how many elements there are in a system, and for how long they should remain stable (e.g. 1 year or 10 years). For molecular magnets the additional possibility of quantum tunneling will have to be taken into consideration: such effects are not considered in this report.

For supermalloy elements, this energy barrier is produced by making them in the form of thin elliptical discs, which produces the so-called shape anisotropy. The lowest-energy states occur when the electronic spins all point along the long axis of the ellipse. A magnetic field has to be applied to force the spins to rotate (in the plane of the ellipse) so that they point along the short axis. The field that is needed to do this, which can be called the hard axis saturation field H_s , is related to the energy barrier height, ΔE, by

$$H_s = 2\,\Delta E / m \qquad (1)$$

where m is the total magnetisation of the element. It should be noted that there is another, even higher, energy barrier which corresponds to all of the electron spins pointing out of the plane of the ellipse (i.e. out of the plane of the paper in Figure 9). If the thickness of the ellipse is less than the length of its minor axis then this energy barrier has no effect on the dynamics of the element, but its presence will eventually have to be taken into account when carrying out detailed simulations of magnetic molecules, which have much more complicated shapes and hence more complicated anisotropy energies.

The exact magnitude of ΔE is a complicated function of the shape of the magnetic element, but for simple structures, such as that shown in Figure 16, one can obtain a good first-order approximation. Consider the bar magnet shown in Figure 16.

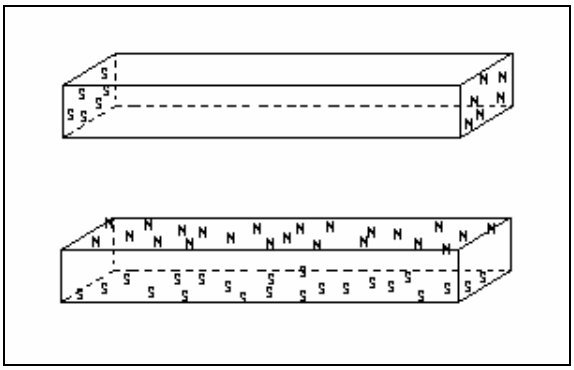


Figure 16. A bar magnet magnetised along its 'easy' axis (top) and 'hard' axis (bottom). The N and S symbols represent uncompensated north and south magnetic poles. The system illustrated in the upper picture has a much lower free energy than that in the lower picture. Energy has to be provided to push the system from the upper state to the lower one.

If the magnet length is less than ~100 nm, then the electron spins all line up in approximately the same direction. The magnet will behave as if it has uncompensated north and south monopoles on the two end faces, because this is (approximately) the lowest-energy configuration. If an external magnetic field is used to force all of the spins to point up, then there will be a greatly-increased number of uncompensated north and south poles. The extra energy associated with this metastable configuration is directly proportional to the extra number of uncompensated poles that are generated, which is proportional to the difference in area of the top and end faces of the magnet. If we assume that the thickness of the end faces is small in comparison with the length or breadth of the top (and bottom) faces, then the energy difference (the energy barrier ΔE) is simply proportional to the area LW of the top face, where L is the length and W is the width. However, the total magnetisation m is proportional to the *volume* LWD of the element, where D is the depth (thickness). Therefore

$$H_s = 2\,\Delta E / m \propto 1/D \qquad (2)$$

- the saturation field *increases* undesirably as the magnet is reduced in size. However ΔE, which should ideally remain constant, at ~50 to ~100 kT is (approximately) proportional to the area LW of the top face:

$$\Delta E \propto m/D \propto LW$$

Thus miniaturising the bar magnet (reducing LW), will adversely affect its thermal stability.

We assumed a bar magnet in the analysis above, but a similar analysis can be carried out for the elliptical elements of the BMQCA, where the saturation field has to be applied in the plane of the ellipse. The implications in both cases are that:

Elliptical or rectangular elements made of supermalloy that are much smaller than ~100 nm will not be sufficiently stable at room temperature, to be used either as data storage elements or as elements for use in magnetic quantum cellular automata systems.

This conclusion is confirmed by the simulation results previously presented in [Parish 2003] and by the additional simulations (an example of which is shown in Figures 13 – 16) carried out during this study. It is also consistent with results obtained by research carried out by other workers into the stability of elements for data storage.

This seems to imply that it will be impossible to make MQCA systems with elements that are smaller than ~100 nm? However, thanks to the discovery of molecular nanomagnets, it appears there may be a way round the problem. The discussion above was presented in terms of shape anisotropy, and it was assumed that the internal structure of the bar magnet or elliptical element was essentially isotropic and homogeneous. However, it may be possible in molecular magnets to have a sufficiently inhomogenous and anisotropic molecular environment for the energy barrier ΔE to be determined by intra-molecular anisotropy, instead of the conventional shape anisotropy described above. It may eventually be possible to design a magnetic molecule in such a way that its anisotropy energy is comparable with ~50 to ~100 kT, for T = 300 K. Whether this can be achieved is outside the terms of reference of this short study, but it is pertinent to note that a *lot* of people are looking at molecular magnets. However, at present, with molecules such as Mn_{12}-ac, the energy barrier is very small – about 10^{-22} joules – which represents 1 kT when T ~ 10 K, and 50 kT when T ~ 0.5 K. There is still a long way to go before a molecular magnetic quantum cellular automata system could be operated at any higher temperature than one degree above absolute zero.

6. DISCUSSION

The results of the simulations and analyses of the previous pages can be summarised in the diagram below (Figure 17). The horizontal axis denotes the characteristic size of an individual magnetic QCA element, and the vertical axis denotes temperature in degrees K. The diagram is intended to show where different types of MQCA systems might be feasible, but it can equally be taken (approximately) as showing suitable regions for *data storage* elements.

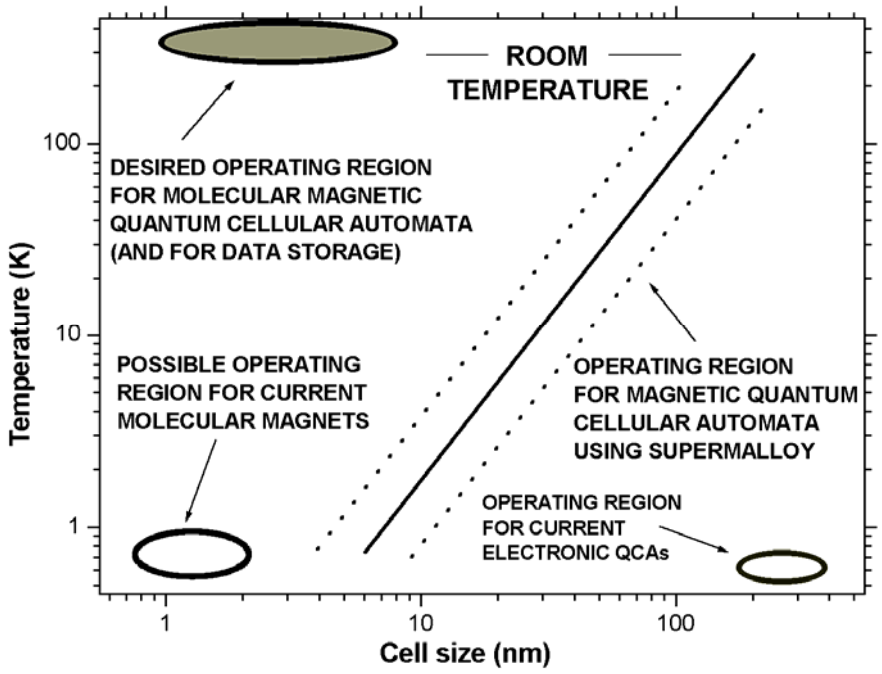


Figure 17. Comparison of operating regimes for different types of quantum cellular automata. 'Cell size' denotes the characteristic largest dimension of individual QCA elements. The separation between individual elements would typically be about 10% of this characteristic size. One should note that this diagram is annotated with the aim of assessing the potential usefulness of magnetic QCA systems, but that essentially the same diagram could be used to describe the potential capabilities for *data storage* (in future hard disks etc.).

Cowburn and Welland have already demonstrated an MQCA system, with 69 elements working at room temperature – the top right-hand end of the black diagonal line. One would like to be able to have an MQCA system which operates at room temperature (or above), with element sizes of a few nm or less, as shown by the shaded region at the top left. Molecular magnets are possible candidates for use in future MQCA systems, but at present their magnetic properties are such that they would only be stable at very low temperatures of less than 1 K (bottom left). MQCA systems, based on the elliptical elements described earlier, could in principle operate anywhere along the solid diagonal line. The two dashed lines are intended to show that there are approximations in the simulation calculations which introduce uncertainties of ~30% in the predictions. In addition, it may be possible to find materials with better properties than supermalloy, which would move the solid diagonal line

(favourably) to the left. We have not carried out simulations of MQCA systems using the magnetic elements described in [Csaba et al. 2003], but it is probable that the stability of their MQCA elements would also lie within the bounds of the two dashed lines.

For completeness, we have included (at the bottom right) the size and operating temperature of the experimental *electronic* QCA element [Csurgay and Porod 2001]. It is quite possible that molecular-sized EQCA elements may be achievable in the future: this would in principle move the operating region for EQCAs over to the left of the diagram. However, it is not clear what the operating temperature of molecular-sized EQCAs might be.

We now comment briefly on the operating speed of MQCAs. It is certainly the case that a single MQCA element could switch at several hundred MHz or even a little higher, with the limit being due to the need to dampen the precession of the spins during the clocking cycle. However, when several or many such elements are coupled together to form some sort of circuit (a wire, a logic gate etc.) then it has been shown that the system speed drops dramatically (the ten-element wire in Figures 14 and 15 failed at ~110 kHz). Simulation results in [Parish 2003] suggested that frequencies of perhaps less than 1 MHz might be the maximum achievable by careful adjustment of system parameters, but it must be emphasised that the Nanomag simulator includes time-dependence in a complicated way, and that it *may* be possible to run at higher speeds. It is nevertheless definitely the case that the need to use adiabatic clocking requires a dramatic reduction in the clock speed below the hundreds of MHz referred to above. The clock speeds for molecular MQCA elements are unlikely to be much different from those for elliptical supermalloy elements, because the same precession effects will affect one spin or a million spins.

7. CONCLUSIONS AND RECOMMENDATIONS

The conclusions that may be drawn from this short study are the following:

Magnetic quantum cellular automata (MQCA) systems using ferromagnetic elements composed of supermalloy or similar materials will only operate at room temperature if the size of the elements is of the order of 100 nanometers.

The thermal stability requirements for MQCA elements are similar to those for magnetic data storage elements. It should therefore be possible in many cases to use research results for data storage to guide research into MQCA systems.

At present magnetic molecules are only thermally stable at temperatures of 1 K or less. Thus MQCA systems using *existing* magnetic molecules would not have many practical applications.

If, in the future, magnetic molecules can be designed and made, so that they are stable at or above room temperature, then they would be potential candidates for use in both data storage and magnetic quantum cellular automata systems.

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