ABSTRACT

MONTE CARLO SIMULATIONS OF SHAPE DEPENDENCE IN MAGNETIC ANTIDOT ARRAYS

By Brian Weir

The objective of this project is to determine the effect of antidot shape and density on the magnetic ordering of two-dimensional antidot lattices. With Monte Carlo modeling software, this lattice may be tested using order parameter and susceptibility as functions of temperature, anisotropy and external magnetic fields. The ordering temperature is observed to increase as inter-antidot spacing increases and antidot size decreases. Other correlations to ordering temperature follow when multiple different fields are applied. Additionally, artifacts are found to appear in the magnetization graphs of antidot lattices with an external field bias perpendicular to the axis of anisotropy.
MONTE CARLO SIMULATIONS OF SHAPE DEPENDENCE IN MAGNETIC ANTIDOT ARRAYS

A THESIS

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1. Introduction

Development of micromagnetic systems and technologies is of great interest. Using domain-scale control over magnetic films and alloys, a variety of new technologies has been developed for sensors, data storage, processing and other applications. Current research is in devices called quantum dots and magnetic antidots\(^1\). These devices exploit the unique effects of imprinting nano-scale plateaus and holes, respectively, into thin films of primarily magnetic alloys. While production techniques advance to catch up with this new technology, theoretical modeling is increasingly important for research into these devices. Applications for magnetic antidots are currently being investigated and include high-density, high-stability data storage media, micro-sensors and other similar devices.

Already a common subject in statistical mechanics, micromagnetic systems lend themselves well to computer modeling techniques. Computer simulations, such as the popular OOMMF program\(^2\), allow researchers to predict the effect of particular material parameters and environmental variables on a complex magnetic system as well as visualize the system itself. It can be compiled in multiple environments, is easily expanded, adaptable to three-dimensional lattices and has an efficient graphical interface. In addition to outputting the many parameters of the system, it can also display images of the system with spin vectors, streamlines and magnetization magnitudes shown in false color. However, a weakness of this and other modern techniques is that they assume temperature has no effect. The calculations are done for a temperature of 0 K and therefore cannot examine the temperature dependence of the magnetization. Additionally, as temperature increasingly becomes a factor in modern micromagnetic technology, such as in the rapid approach of magnetic storage media to the superparamagnetic limit, improvements on simulation software are necessary.

Fortunately, Monte Carlo algorithms ease the transition to variable-temperature systems and allow their results to be applied to a wide range of theoretical and real-world systems. Using variable-temperature code, the purpose of this research is to investigate the effect of antidot geometry on properties such as ordering temperature and susceptibility, as well as large and small scale magnetization stability.
2. Background

2.1. Computer simulations of micromagnetic systems

2.1.1. Thermodynamics

The basis of some computer simulations in physics comes from statistical mechanics, developed in the late 19th century by some of the greatest scientists of the era. Among them were J. Willard Gibbs, Ludwig Boltzmann and James Clerk Maxwell. The basis of statistical mechanics is the idea that a physical system can be described as an ensemble of many smaller systems. This became a new way of discussing another branch of physics where small scale events cause large scale phenomena, known as thermodynamics. Thermodynamics specifically covers phenomena to which heat and temperature are central, and although statistical mechanics is not restricted as such, it works just as well for it.

The modern formulation of thermodynamics, central to statistical mechanics, is based around the canonical ensemble partition function:

\[ Z = \sum_{\{\{x_i\}\}} e^{-\beta H} \]  

(1)

Here, \( \beta = 1/k_B T \), \( H \) is the Hamiltonian of the system, and the sum is over all the states of the system. This function, \( Z \), is a normalizing factor for a system that follows a Boltzmann distribution. This describes the distribution of the energy states for particles in thermodynamic equilibrium. Depending on the ‘temperature,’ \( \beta \), and the ‘energy,’ \( H \), a particle will fall into a particular energy state with a particular probability. For a system of particles whose energy state is determined by their magnetic spin moments, the canonical partition function describes the probability of an atom’s particular spin state occurring, given a particular energy and temperature.

2.1.2. Simulation techniques

In the investigation of near-atomic scale systems, statistical mechanical techniques have led the way. Modern use of these techniques often takes the form of Monte Carlo algorithms in computer simulations. Continual advances in this field allow for the modeling of many important and non-trivial systems that cannot be solved explicitly, including micromagnetic systems in particular.

Monte Carlo techniques are used primarily for thermodynamic systems as they generate an ensemble of states of the system from which a range of quantities can be
calculated. A large factor of this generation is in importance sampling, where certain random numbers have a greater effect than others. Models range in complexity from the simple Ising model to more complex two- and three-dimensional spin models, such as the XY- and Heisenberg models, respectively. In the XY-model, random numbers are compared to the partition function of each lattice site and if the number is larger then a new state for that site is chosen. These models correspond well to precise experimental results due to their abstraction to dependence on just the basic physics of the system.

The simplest way of describing a system of spins is as a two-state system – up, or down. The model that describes a system in these terms is called the Ising model, named for its creator Ernst Ising. Although a one-dimensional spin seems a bit unrealistic at first, the model does map relatively well to real systems.

However, it is common to use a spin model that is a closer approximation of real systems by increasing the spin dimensionality. Thus, in the XY- or planar rotator model, the simulated magnetic spin moments are allowed to rotate freely in two dimensions rather than the single dimension they are limited to in the Ising model. As recent experiments have shown, this increase in detail allows XY-model simulations to compare well to experimental results for thin films.

Having established the application of statistical mechanics to the technique of computer modeling, there are several algorithms available for the task. These algorithms use the Monte Carlo method which suggests that physical systems can be studied by using random or pseudo-random numbers. Simply stated, the basic form of the method used here compares these random numbers to a probability to determine the state of a system.

The algorithm primarily used to implement our XY-model is the Metropolis algorithm. This algorithm uses single-spin-flip dynamics to generate states for a system. The algorithm compares the energy of each spin individually to its energy were it to rotate to a new, random direction. This leads to the unique characteristic of this algorithm, which is that it chooses whether a spin rotates or not by a specific acceptance ratio: for $\Delta E > 0$, it will change state with a probability of $P = e^{-\beta \Delta E}$, and $P = 1$ for any other value of $\Delta E$, where $\Delta E = E_{\text{new}} - E_{\text{original}}$ and $\beta$ is $1/k_BT$. As we can see, in this model the probability is proportional to the canonical partition function from thermodynamics, but here, we can replace $H$ with $\Delta E$ in that equation by taking a ratio of the Boltzmann factor. This same algorithm can be applied to the XY-model by comparing the initial energy of each spin to the energy of a new state, but now the flip is a random rotation in the XY plane.
2.2. Properties of magnetic materials

2.2.1. Structure and properties

In order to discuss a system, one must have a basis of properties and parameters with which to work. For a micromagnetic system in particular, the first variables one must be concerned with are the magnetic spin moment, $\vec{S}_i$, and the interaction parameter or exchange constant, $J$. Spin moments in two dimensions have x and y components that range from a maximum of 1 to a minimum of -1. The exchange constant is actually shorthand for the exchange integral$^{10}$,

$$J_{12} = \int \psi_a^*(1) \psi_b(2) H \psi_a(2) \psi_b^*(1) d\tau$$

(2)

In this, the $\psi$ variables are the state wave functions of the atom and $H$ is the Hamiltonian of the system. This quantum mechanical effect describes the interaction between spins in neighboring atoms. Using this strength of interaction and values for the spin moments, we can define the exchange energy of this system to be$^{10}$:

$$E = -J \sum_{nn} \vec{S}_i \cdot \vec{S}_j$$

(3)

Here, $\vec{S}_i$ is the magnetic spin moment; $J$ is the exchange energy from above and our summation is over ‘nn,’ or all of the nearest-neighbor pairs in the system. It is important to note that this is over sets of neighbors, not just the neighbors of a single spin. We are not necessarily limited to including just the nearest neighbors but they are often sufficient. We can extrapolate from this that for a large system of atoms, the total energy of that system would be the sum of the exchange energies of each atom.

To simulate a thin film antidot lattice we will establish two-dimensional square lattice. Following that, the next step is to determine a parameter that describes the large-scale orientation of the atoms in our system. In magnetic systems, we define one such parameter, the order parameter - the absolute value of the magnetization, the net direction and magnitude of the magnetic moments of the system, such that$^{11}$:

$$\langle O \rangle = |\vec{M}| = \frac{\sum_i \vec{S}_i}{N} = \frac{\sqrt{(\sum_i S_{ix}})^2 + (\sum_i S_{iy})^2}{N}$$

(4)

Here, $\vec{S}_i$ is again the magnetic spin moment of a location, $N$ is the total number of locations and $O$ has a magnitude that ranges from 0 to 1. For magnetic materials, the locations do not have to be individual atoms; they can be groups of atoms with an internally constant spin. The effect of this coupling of atoms to each other can be seen in higher-order effects such as this one.

Other than order parameter, there are several other derived parameters; the extrema of which are useful for determining the temperature at which the ordering of the
system drops suddenly, i.e. the critical temperature. The magnetic susceptibility is defined as:

\[ \chi = \frac{N\langle O^2 \rangle - \langle O \rangle^2}{k_B T} \quad (5) \]

This quantity measures the fluctuations in the order parameter and is usually observed in the context of the presence of an external field. Another useful property is the specific heat capacity:

\[ C_v = \frac{\langle E^2 \rangle - \langle E \rangle^2}{Nk_B T^2} \quad (6) \]

Here, \( E \) is the total energy of the system. Similar to the susceptibility, it shows the fluctuations in the energy of the system. Graphs of the susceptibility and heat capacity with temperature should have maxima at the inflection points of the graphs of the order parameter and energy, respectively.

### 2.2.2. Anisotropy, dipolar field and the Zeeman effect

In real systems, there are additional effects that affect the ordering of the system. These effects take the form of additional terms can be added directly to the energy Hamiltonian of each spin in the system. The total energy used here is as follows:

\[ E = -J \sum_{m} \mathbf{S}_i \cdot \mathbf{S}_j - \sum_{i} K_2 \mathbf{S}_i^2 - \sum_{i} \mathbf{H}_{\text{ext}} \cdot \mathbf{S}_i - \sum_{i} \mathbf{H}_{D} \cdot \mathbf{S}_i \quad (7) \]

The first term is the spin-spin exchange energy from before, known as ‘nearest neighbor’ coupling, where the energy of a spin site of the system is determined by its exchange with the closest neighboring spins. Typically the factor \( J \) in the first term is given a value of 1 and other constants are scaled accordingly, such as the temperature which is referred to by the dimensionless quantity, \( k_B T/J \). This allows for the system to be described in terms of dimensionless magnitudes and be generalized to any real world system.

The second term is the uniaxial anisotropy energy, due to the crystalline structure of a material that defines a preferred axis of magnetization. It is taken arbitrarily here to be along the x-axis and its magnitude is set by the factor \( K_2 \).

The third term is the Zeeman coupling energy, the magnitude of paramagnetic behavior in a material. This is the tendency of the magnetization of a material to align with an external magnetic field, the magnitude of which is set by the external magnetic field, \( H_{\text{ext}} \). This field acts much like the anisotropy, in that the axis and direction of that field is of lower energy than other directions, causing the magnetization to prefer to fall
along it.

The effective magnetic field generated by the other spins in the lattice gives us our fourth term in Equation 7 called the dipolar field\(^{13}\). A rigorous discussion of this term and its derivation can be found in Appendix 2.

### 2.2.3. Transitions and pseudo-transitions

For our system, the change in the state of magnetic order is indicated by the inflection point of the graph of the order parameter. In many systems, this is a phase transition, similar to the point at which water freezes. Phase transitions usually occur when a system undergoes spontaneous symmetry breaking and changes from one distinct state to another.

Phase transitions are very specific phenomena, and types of such transitions are classified into orders\(^{14}\). The example of water transitioning from liquid to solid in freezing would be a first-order phase transition. In this transition, the material transfers or absorbs a fixed amount of energy, which leads to an intermediate mixed state. A second-order phase transition has no associated latent heat like a solid-liquid first-order transition would, but it does have a transition from a state of order to one of disorder at a critical temperature. In ferromagnetic systems, this critical temperature occurs at the Curie point\(^{15}\), the point at which a material loses its ability to hold its own net magnetic order.

However, a two-dimensional system such as a magnetic thin film has additional complications that do not allow this transition. The Mermin-Wagner theorem\(^{16,17}\) states that two-dimensional systems with a continuous symmetry cannot have a broken symmetry at finite temperature. As this applies to our system, spins in two dimensions are continuously symmetric as they rotate around an infinite range of directions, thus it cannot truly undergo a second order transition.

However, all is not lost – even systems with continuous symmetry can experience local disorder. This local transition is classified as an infinite-order transition called the Kosterlitz-Thouless transition\(^{18,19,20,21}\). This transition occurs when a continuous system shifts from a high-order state to one that prefers locally disordered states, known as vortices. These vortices are stable but are of high disorder and their appearance occurs with specific temperature dependence in a two-dimensional system. However, even this transition breaks down if external fields are added, so any transition we observe in such a two-dimensional system is not necessarily a ‘true’ transition. This transition is a sort of pseudo-phase transition, as it is not formally defined, but we can still use it to evaluate each state and the entire ensemble. We can thus define an ‘ordering temperature\(^{22}\) that occurs at the peak of the susceptibility, below which the system becomes more ordered.
3. Magnetic antidots

3.1. Background

Magnetic antidots are formed by creating a mesh of holes into a magnetic film. The immediate effect of this is similar to introducing a highly ordered impurity into the material. The antidots form gaps in between the magnetic sites and disrupt long-range ordering. As the size, shape and pattern of the antidots disrupts the symmetry of the lattice, every combination of those variables has a unique effect on the magnetic properties of the lattice.

3.2. Derivation of theoretical parameter ranges

It is important to characterize what the sizes of the experimental equivalents of our lattice sites might be. Our antidots sit in a two-dimensional square lattice of a particular length and width and each lattice site is considered to contain many atoms. In an experimental paper by C.T. Yu, et al.\textsuperscript{23}, the antidots they used were about 1.26x1.26 μm and a similar paper by P. Vavasori, et al.\textsuperscript{24} used 1.5x1.5 μm antidots. Smaller antidots were used by I. Guedes, et al.\textsuperscript{8} with dimensions 200x800x60nm. In a theoretical paper by L. Lopez-Diaz, et al.\textsuperscript{25}, the size of an antidot was taken to be 20nm in size, although other reasonable sizes include 10 and 5 nm. This is much smaller than the experimental values given by Yu and Guedes, but still reasonable and easier to work with.

In order to collect data on reasonably-sized systems and given the limitations of computer speed, we took the length of one side of a lattice site to be 20nm. For a 222 lattice, this would make our antidots 40x40nm in size. See Section 4.1 for discussion of this lattice.

Lopez-Diaz\textsuperscript{25} also quotes several other experimental parameters that define their system which include the anisotropy, $K_2$, and the exchange stiffness constant, $C$. It can be shown that the exchange stiffness\textsuperscript{1} is related to the exchange constant $J$ by\textsuperscript{26}:

$$C = \frac{2JS^2c}{a}$$

(8)

Here, $a$ is the length of the edge of the lattice site, $S$ is the associated magnetic moment and $c$ is 1, 2 or 4 for simple, bcc or fcc cubic lattices\textsuperscript{27}, respectively. Since we are making only order-of-magnitude calculations, we will take $c$ and $S$ to be 1. This simplification gives us $J$ in terms of $C$:

$$J = \frac{aC}{2}$$

(9)
According to Lopez-Diaz\textsuperscript{25}, $C$ for permalloy is 1.3x10\textsuperscript{-6} erg/cm, so this gives us a value for $J$ of 10\textsuperscript{-19} J. This is larger than the interatomic $J$, but since our cell has a fairly large area and thus contains many atoms, this is unsurprising. We can use this value next to take a ratio of $J$ to the anisotropy, $K_2$.

Lopez-Diaz\textsuperscript{25} gives an anisotropy value of 5x10\textsuperscript{2} J/m\textsuperscript{3} which we can convert to the same units as $J$ with the relation $E_k = K_2 * V$ where $V$ is the volume of the cell. For our cell, we will take the thickness to be 40nm, giving us a total volume of 1.6x10\textsuperscript{-23} m\textsuperscript{3}. Multiplying these values gives us the anisotropy energy of 8.0x10\textsuperscript{-21} J. This leaves us with the ratio $K_2/J = 0.08$. This is close to the relative anisotropy magnitude of 0.10 that we use in our model.

Next is the external magnetic field, and to compare our Zeeman energy to our exchange energy, we use the following relation:

$$E_{ext} = \vec{H}_{ext} \vec{S}$$  \hspace{1cm} (10)

Here, $\vec{S}$ is our spin moment, except that it includes all the spin moments of the lattice site. For iron, this is about $(5\mu_B)*N$, where the moment of an iron atom is about 5 Bohr magnetons and N is the number of atoms. If we use the volume of our lattice site to get a value for $\vec{S}$ and take $E_{ext}$ to be on the order of 0.1$J$, we can to solve Equation 10 for $\vec{H}_{ext}$. This gives us the value of about 10\textsuperscript{3} G, which reasonable since lab fields can reach over 10\textsuperscript{4} G.

Finally, we must take into account our dipolar energy. Lopez-Diaz\textsuperscript{25} uses this energy but does not give a value, so we will have to make an order of magnitude comparison on our own. Appendix 2 covers the derivation of this term and due to its considerable variability, we will make the assumption that it is on the order of the anisotropy and external field for the purposes of this project.
4. Initial simulations with magnetic antidots

4.1. The square 222 lattice

The simplest form of a magnetic antidot array would be one with symmetric, square antidots. A segment of such an array can be seen here:

![Figure 1 - Segment of a 222 lattice with unit cell](image)

In the above diagram, the black spaces are antidots while the empty white squares are lattice sites with individual magnetic spin moments. Also shown in the bordered and numbered area is what we will define to be a unit cell. A lattice to be studied can be thought of as a pattern of larger ‘cells’ which include an antidot and the lattice sites that border it, and these cells are repeated to form the lattice. In the case of square antidots, we can use the dimensions of a unit cell to classify each lattice pattern, using a naming convention of $abc$, where $a$ is the length of one side of the antidot and $b$ & $c$ are the space from one antidot to the next along the x- and y-axes, respectively. Thus, the lattice described in Figure 1 as ‘222’ would consist of 2x2 antidots, spaced 2 sites apart in either direction. In our simulations, the region of computation used is 10x10 unit cells in size and they are run for at least a total of $5 \times 10^5$ Monte Carlo steps per spin (MCSS).
Figure 2 – Example of reproducibility of results using the 222 lattice

Figure 2 above illustrates the reproducibility of our results, using two runs of the 222 lattice with different random number seeds. As we can see, the error is on the order of the size of the symbols of the lines, so for that reason we will leave out including error bars on the graphs used here.

Figure 3 – Order parameter (OP), heat capacity (C) and susceptibility (X) parameters for the 222 lattice with ordering temperature and ordering width
Figure 3 above shows the order parameter, heat capacity and susceptibility of the 222 lattice. As you can see, their inflection points are aligned at the same temperature, the ordering temperature, as indicated by the vertical line on the graph. We can also define a parameter called the ‘ordering width’ as the temperature (kT/J) between order parameter magnitudes of 0.7 and 0.1, shown by the horizontal arrow on the figure. These values were chosen arbitrarily because they appear to fall where the curve flattens out. This value is also approximately the width of the susceptibility curve, but not full width at half maximum. This parameter allows us to quantitatively characterize the steepness of the ordering curves of various systems. Numerical values for these two parameters are given in Appendix 1. The properties of this system will serve as a baseline value to compare to other systems.

**Figure 4 – Order parameter as a function of temperature for the 222 lattice in the presence of an external field**

Figure 4 shows order parameter as a function of temperature for three magnitudes of the external field as applied to our 222 magnetic antidot lattice. In this case, the field is in the positive x-direction, although due to the symmetry of the system, an alignment in the y-direction would give the same results. As we can see, the addition of an external field shifts the ordering temperature higher and reduces the slope of the curve. The effect of the field is to give the spins of the system a preferred direction and reduce the effect of thermal energy on the orientation of the magnetization.
In Figure 5, we see the effect of several magnitudes of the anisotropy field along the x-axis. The anisotropy is uniaxial in nature and therefore has no preferred direction along that axis. As we can see, similar to the application of an external magnetic field, the anisotropy causes the system to be more stable with ordering temperature increasing as anisotropy magnitude increases. However, unlike the magnetic field it makes the curve steeper instead of shallower and has a much weaker effect on the ordering temperature.

Figure 6 – Order parameter as a function of temperature for the 222 lattice with the presence of both an external field and magnetocrystalline anisotropy
Since the magnetic field appears at first to have a significantly larger effect on the ordering temperature, we take a look at the combination of their effects in Figure 6. We see that the highest ordering temperature occurs when $K_2$ and $H$ are along the same axis, followed by the case with only the external field. The addition of anisotropy of equal magnitude appears to have little effect on the system under an external field. Since the energy terms for $K_2$ and $H$ are different, we are only making an order-of-magnitude estimate, but it is sufficient to demonstrate their relative effects.

Now we will include the last part of our energy term, the dipolar field. Given its place in our equation, it serves to reduce the total energy of the system and preserve order. Thus, we can see in Figure 7 that increasing the dipolar field shifts the magnetization curve and associated ordering temperature to higher temperatures. Note here that $D$ refers to a dipolar field magnitude that we input into our system. Further discussion of this is in Appendix 2.

![Figure 7 – Order parameter as a function of temperature for the 222 lattice with the presence of a dipolar field](image)
4.2. Effect of size on a square antidot lattice

Now that we have taken a look at the basic properties and field effects of the 222 lattice, we can take a look at the effect of changing the geometry of the system. First, we begin by expanding the size of the antidots but keeping their x-y spacing constant. Unit cells of these lattices can be found in Appendix 3.

![Graph](image)

**Figure 8 – Order parameter as a function of temperature for the 222, 422 and 622 lattices**

In Figure 8, we see that by increasing the antidots’ size, we lower the ordering temperature a noticeable amount. Although the immediate effect increases the total number of spin sites in the unit cell, it really just increases the number of sites that have few neighbors. As we can see in Figure 1, the sites in unit cell regions 1 and 3 have only three neighbors while the sites in region 2 have four. Such sites with three neighbors are less easily influenced by their neighbors than are sites with four neighbors. Thus with the number of those sites with three neighbors increased, from 8 to 16 between the 222 and 422 cases, the overall stability of the system drops.
5. Effects of rectangular antidots

5.1. Ordering of rectangular antidots

Rectangular antidots act very similarly to square ones except that they break the x-y symmetry of the square lattice. We will keep the same symmetric spacing between the dots like in the square lattice as follows:

![Figure 9 – Segment of a 4222 lattice with unit cell](image_url)

Figure 9 shows a portion of a 4222 rectangular antidot lattice with the unit cell area and the regions of the cell numbered. Consequently, the convention for a lattice with rectangular antidots consists of 4 numbers now, the first two of which are the x and y dimensions of the antidot and the second two are the x and y spacing, respectively.

![Figure 10 – Order parameter as a function of temperature for the 422, 6222 and 8224 lattices; K₂=0, H=0, D=0](image_url)
The first comparison to make with the rectangular antidots is to see if changes that occur are related to the geometry of the antidot itself. Figure 10 shows the magnetization curves of the 422 (4422), 6222 and 8224 systems. Unit cells of these lattices can be found in Appendix 3. The spacing for the last one is different in order to keep the square shape of the lattice, a convention we will later drop, but one that has no effect on the ordering. The correlation between these is that the antidots in 422 and 6222 lattices share the same perimeter (12), and the 422 and 8224 share the same antidot area (16). From what we can see, the magnetizations of the 8224 and 422 lattices are quite different, making area correlation unlikely, although 8222 data would make for a better comparison. This would make the spacing between the antidots equal to that of the 422 and 6222 systems, resulting in a clear comparison. As we saw in Figure 8, the x- and y-dimensions of the antidots at constant spacing determine the number of sites with 3 and 4 neighbors and that this affects the order parameter. Here, our 422 and 6222 both have 16 sites in the entire unit cell with three neighbors and four with four, resulting in their similar ordering temperatures.

![Figure 11](image)

**Figure 11 – Order parameter as a function of temperature for 4x1 rectangular antidot lattices; K_z=0, H=0, D=0**

Next, Figure 11 shows the relative magnetization curves of a series of rectangular lattices that vary the spacing between the antidots. Again, unit cells of these lattices can be found in Appendix 3. The ordering temperature of the 4114 lattice appears to fall between the other two at about 0.70, with the 4122 with a slightly lower ordering.
temperature at 0.65 and the 4124, with the largest inter-antidot spacing of the three, holding a much larger ordering temperature at 0.75. However, rectangular antidots of one site in width versus four in length are insufficiently realistic; more in line with real systems are the wider rectangular antidots whose results are shown in Figure 12.

![Figure 12](image)

**Figure 12 – Order parameter as a function of temperature for 4x2 rectangular antidot lattices; $K_z=0$, $H=0$, $D=0$**

Here in Figure 12 we have a series of wider rectangular systems. Both the 4224 and 4242 lattices are similar to the 222 in terms of ordering temperature and width. It is a curious thing to note that despite the asymmetry of the system, it made little difference whether the x- or y- spacing was increased from the 4222 lattice. It is also interesting to note that the larger y-spacing affects the ordering temperature more than the larger x-spacing.

In addition to just affecting the ordering temperature as we have seen, the degree to which increasing fields affect our system is in turn affected by the shape of the antidots as well. As we see in Figures 13 and 14, the 4222 lattice behaves differently from the 222 when anisotropy is applied. This is likely due to the shape anisotropy induced by the rectangular antidots in the 4222 lattice.
Figure 13 – Order parameter as a function of temperature for the 4222 lattice with the presence of magnetocrystalline anisotropy

In Figure 14, we have a more detailed comparison of the anisotropy effects using data from Figures 5 and 13. As we see, the 4222 lattice with anisotropy of 0.1 has a similar ordering temperature as the 222 lattice with no anisotropy, but the ordering width is smaller by 0.1 so this is probably coincidental. The important thing to note is that at equal anisotropy, the 4222 always has a lower ordering temperature than the 222 due to the shorter spin site-to-spin site correlation length.

Figure 14 – Order parameter as a function of temperature for the 222 and 4222 lattices with the presence of magnetocrystalline anisotropy
In comparing the effect of several antidot sizes with an applied anisotropy of 0.1 as shown in Figure 15, we see a change in the typical patterns with the 4222 at the lowest ordering temperature followed not by the 222 but rather the 4122 lattice, and with the 4244 lattice again at the highest temperature. It also appears that the 4122 and 4244 curves have a narrower width than those of the 222 and 4222 lattices.

Figure 15 – Order parameter as a function of temperature for the 222, 4122, 4222 and 4244 lattices with the presence of magnetocrystalline anisotropy of magnitude 0.10

Comparing Figure 16 to the 222 results of Figure 4, we see that the external field has a much more significant effect on the rectangular antidot lattice. In particular, an external field of 0.10 raises the ordering temperature by 0.30 and the ordering width by 0.50. In this case, the field is along the x-axis which is also the long axis of the antidots.

Figure 16 – Order parameter as a function of temperature for the 4222 lattice in the presence of an external magnetic field
When varying the antidot size and spacing with an external field of 0.1, we see the curves of Figure 17 arranged in the same order as in the size comparisons with anisotropy. Again, the 4244 lattice has a much larger ordering temperature than the other systems as the increased spacing greatly increases the number of sites with four neighbors as well as the spin site-to-spin site correlation length.

![Graph showing order parameter as a function of temperature for different lattices](image)

**Figure 17 – Order parameter as a function of temperature for the 222, 4122, 4222 and 4244 lattices in the presence of an external magnetic field of magnitude 0.10**

Another thing to note, however, is that despite the lack of x-y symmetry with the rectangular antidots as we see in Figure 8, the results for systems with just an external magnetic field are the same whether the external field is along the x or y axis. We can see this for the 4222 lattice in Figure 18. This breaks with the initial assumption that the antidot x-y symmetry breaking would have a significant effect on the axis-dependent anisotropy and magnetic fields.
As with the 222 lattice, we again see in Figure 19 that the 4222 system with anisotropy by itself loses its ordering at a significantly lower temperature than one with a magnetic field. We also see that the system with both anisotropy and magnetic field has only a slightly higher ordering temperature by 0.10 and the same ordering width as the one with only the external field. Here, the anisotropy goes as $S_x^2$ rather than just $S_x$ for the magnetic field. Thus, as the spins deviate from the preferred direction due to thermal fluctuations, the strength of the anisotropy field drops much faster than that of the external magnetic field. The uniaxial nature of the anisotropy rather than the unidirectional nature of the field likely plays a role, but further study is needed.
The effect of the dipolar field on the rectangular 4222 lattice as shown in Figure 20 is similar to that of the 222 of Figure 7 above but with a steeper slope of the magnetization curves. Additionally we can see that the D=0.25 curve will not reach a magnetization of 1 at 0 temperature but will rather have an inherent disorder as a result of the strong dipolar field. This low-temperature effect is discussed further in Appendix 2.

![Graph showing order parameter as a function of temperature for the 4222 lattice with the presence of a dipolar field, K2=H=0](image)

**Figure 20 – Order parameter as a function of temperature for the 4222 lattice with the presence of a dipolar field, K2=H=0**

What we see in Figure 21 when we keep the dipolar constant but vary the size and shape of the antidots is again similar to the effect of varying the field magnitude. The low ordering width of the curves appears more like the shape with anisotropy, implying that the dipolar field induces a shape anisotropy. With this as an introduction, we will continue to compare the effects of varying both fields and antidot geometry.
5.2. Effect of a perpendicular magnetic field

If we were to take the system of Figure 19 and rotate the direction of our magnetic field by 90° so that it is perpendicular to the axis of the anisotropy, we get an interesting result that we see in Figure 22 - an additional inflection point appears in the perpendicular case. To determine a source of this effect, extracting more information than just the order parameter is necessary.
We need to determine whether or not this effect is limited to antidot systems. Figure 23 provided by P. Scholten shows us a pure lattice with no antidots. Here the x- and y-components of the order parameter are plotted and we see that the effect appears here just as well as with the antidots. The axis of ordering appears to coincide with a transition of magnetization direction from the x to the y axis. This is demonstrated as the point at which x- and y-components of the order parameter have inflection points is also an extra peak in the graph of the susceptibility.

![Graph](image)

Figure 23 – Order parameter as a function of temperature for the pure lattice in the presence of an external magnetic field perpendicular to the axis of magnetocrystalline anisotropy, both of magnitude 0.10

The appearance of the inflection point and the transition of ordering axis is reproducible, occurring in both heating and cooling and being independent of the initial direction of the magnetization. Since the inflection point is not unique to magnetic antidot systems, the next step is to investigate the extent to which the antidots affect the appearance of the inflection point.
Figure 24 – Order parameter as a function of temperature for the 222, 4122, 4222 and 4244 lattices in the presence of an external magnetic field perpendicular to the axis of magnetocrystalline anisotropy, both of magnitude 0.10

In Figure 24, we see that the ordering curves for most of our lattices are very similar, except for the 4244 lattice which again is the most strongly affected as in Figure 21. Due to the larger spacing, the 4244 lattice has both more total spin sites and a longer coherence length between lattice sites out of the systems we are looking at, and so any large-scale effects such as this one will occur more distinctly.
In Figure 25, we see the ordering curves for our lattices, this time with the dipolar field as well such that $K_2=H=D=0.10$. The lowest temperature inflection point occurs for the 222 lattice, followed by a steep drop for the 4222. The drops in order parameter for the 4122 and 4244 systems occur at about the same temperature. However, the drop is much steeper, corresponding to a larger peak of the susceptibility, for the 4122 than for the 4244. The additional dipolar field does not to appear to have affected the 222 lattice much, or even the 4244 for that matter, but the 4222 and 4122 have their inflection points occur at temperatures higher by 0.20 and 0.30, respectively, than without the dipolar field.

Figure 25 differs from the system of Figure 24 for all systems with merely the addition of the dipolar field. The 222 and 4244 systems have changed only slightly, with their respective inflection points growing slightly wider. However, the inflection points of the 4122 and 4222 systems have shifted to higher temperatures and their respective changes in order are more significant.
Looking deeper into the effect of the dipolar energy on systems with other additional fields, Figure 26 shows three combinations for the 222 lattice. Here, the system with a perpendicular field but no anisotropy has no additional inflection point. We can also see the slight shift of the ordering to higher temperatures more clearly than in Figure 23. We also include a system with anisotropy and dipolar field but no magnetic field to be certain the appearance of this inflection point is related to the magnetic field.
Figure 27– Order parameter as a function of temperature for the 4222 lattice in the presence of an external magnetic field perpendicular to the axis of magnetocrystalline anisotropy and a dipolar field of varying magnitudes

Similar to Figure 26 is Figure 27 above. Here, the system with anisotropy and perpendicular field is not very different from the system with a dipolar field with perpendicular field. This is very different from the 222 case since not only does having all three fields on create a significant change, but we also get the inflection point without magnetocrystalline anisotropy. As in Figure 24, there is no inflection without the magnetic field; and as we saw in Figure 21, that magnetic field must also be perpendicular to the long axis of the antidots.

Figure 28 – Order parameter as a function of temperature for the 222 lattice in the presence of an external magnetic field in the y-direction and a dipolar field of equal and increasing magnitude
In Figure 28, we look more closely at the 222 lattice without anisotropy and observe as the external field and dipolar field vary at equal magnitude. The ordering temperature and the ordering width increase as the magnitude increase, similar to the change shown in Figure 4 from an increasing magnetic field. The lack of the additional inflection point seen since Figure 21 seems to indicate at first that, for square antidots, the cause may be found in an interaction between the anisotropy and magnetic field.

Figure 29 – Order parameter as a function of temperature for the 4222 lattice in the presence of an external magnetic field perpendicular to the antidot direction and a dipolar field of equal and increasing magnitude

As we see in Figure 29, as in Figure 28, for the 4222 lattice that we get that extra inflection point without anisotropy to our system so long as dipolar field is included. It is interesting to see that increasing the magnitude of both fields causes the inflection to be steeper along with the increased ordering temperature and ordering width that accompanies an increase in external magnetic field.
Figure 30 – Order parameter as a function of temperature for the 4222 lattice in the presence of an external magnetic field perpendicular to the antidot direction and magnetocrystalline anisotropy

In Figure 30, we lower the magnitude of the fields even further to see how subtle the effect is. Here we see that the system with a magnetic field of 0.10 and the anisotropy of 0.05 does not appear to have any inflection at all, and for the system with a magnetic field of 0.05, the anisotropy of 0.10 seems to cause a slight dip, but not noticeably. In order to be certain we must take a look at the susceptibility of each graph, noting that inflection points in the graph of the order parameter occur at maxima of the susceptibility graph.

Figure 31 – Order parameter and susceptibility as a function of temperature for the 4222 lattice at $K_2=0.05$, $H=0.10(90)$, $D=0.00$
First in Figure 31, we look at the system with $K_2=0.05$, $H=0.10$ and see that it has only one maximum. This seems to indicate that either the anisotropy is too weak or it is being overwhelmed by the magnetic field.

To be certain, we look at the $K_2=0.10$, $H=0.05$ case in Figure 32. Here we do get an extra peak at a point that would have been difficult to spot visually on the graph. This indicates that only a small external magnetic field relative to the magnitude of the anisotropy or dipolar field is necessary for the effect.

![Figure 32](image)

**Figure 32** – Order parameter and susceptibility as a function of temperature for the 4222 lattice at $K_2=0.10$, $H=0.05(90)$, $D=0.00$

### 5.3. Unit cell statistics

As we saw in Figure 23, an indicator of the inflection point seems to be a transition from x- to y-ordering. Looking at Figure 9, each region of the unit cell differs in the number of total sites and the number of sites with only three neighbors, so this could be a source of the ordering direction transition. We will examine the small-scale effects of this ordering transition by taking some statistical counts of magnetizations around an antidot. To do this, we make a histogram of the x- and y-components for all spins in each given unit cell region. Data are collected for all unit cells for each lattice pass and are averaged over all the unit cells. These data are then normalized to compensate for the variation in the sizes of the regions.

Here in Figure 33 is the 4222 $K_2=0.10$, $H=0.1(90)$, $D=0$ system again, now showing the frequency of magnetization directions for the last temperature before the inflection point, $kT/J = 0.30$. The spins are generally weighted in the positive y-direction with the x-components pretty evenly distributed. Given our earlier results with this system, it is unsurprising that the spins prefer to be along the axis of the dominant external field direction.
Figure 33 – Magnetization population as a function of average magnetization energy for the X and Y components of unit cell regions 1, 2 and 3 for the 4222 lattice, K₂=0.10, H=0.1(90), D=0; kT/J=0.30
In Figure 34, we look closer at the peaks on the positive side of Figure 33 and can see a slight difference between the three regions of spin sites in a unit cell. Region 3 appears to be the most strongly aligned, followed by regions 1 and 2 in that order. The spins in region 2 are bordered only by other spins, not antidots, so they will understandably be more influenced by other spins, thus resulting in a lower number of spins in the favored direction, on average. This ordering shows that the inflection point falls entirely within the y-dominated region of the magnetization, so the full range of this effect must fall at lower temperatures than we initially expected.

Figure 34 – Close zoom of the positive magnetization peak of the population graphs for the regions of the 4222 lattice, K₂=0.10, H=0.1(90), D=0; kT/J=0.30

Similar to Figure 33, Figure 35 shows the 4222 lattice with K₂=0.10, H=0.1(90), D=0, but now we are looking at kT/J=0.60, the temperature immediately following the inflection. Although still in the y-dominated regime, this data shows the shift from the start to the end of the inflection point, rather from x- to y-ordering. The unit cell regions differ in their magnetization some, though the y-components are more frequently oriented in the preferred direction than their counterparts at the lower temperature. Also, the distribution of orientations in the x-direction appears to be more uniform than in the lower temperature system as well, but with sharper peaks at either end of the distribution.
Figure 35 – Magnetization population as a function of average magnetization energy for the X and Y components of unit cell regions 1, 2 and 3 for the 4222 lattice, $K_z=0.10$, $H=0.1(90)$, $D=0$; $kT/J=0.60$
Figure 36 again gives us a zoomed-in view of the peaks on the positive end of the magnetization scale. Here, unlike for the lower temperature system, the ranking of the x- and y-components is not the same. For the x-components, region 2 has the most, followed by regions 1 and 3; the reverse order of the lower temperature system. However the y-components are ranked as region 3 with the most, followed by regions 1 and 2, same as for the lower temperature.

\[\text{Graph showing magnetization scale with counts for different regions.}\]

5.4. Summary of results

In the process of this research, several significant observations have been made. First, we can see in Figure 7 that as we increase antidot size, we lower the ordering temperature and the ordering width thus reducing the overall order of the system. Similarly, we see in Figure 11 that increasing the spacing between the antidots increases the ordering temperature while lowering the ordering width. This reproduces earlier results by P. Scholten\textsuperscript{13} and establishes the accuracy of this method.

We can see in Figures 4, 7 and 5, respectively, that applying an external field or dipolar field to a 222 antidot lattice will increase both the ordering temperature and the ordering width, while anisotropy will reduce the ordering width while increasing the ordering temperature. In Figures 13, 16 and 20 we see that the same relations occur for the 4222 rectangular antidot lattices. When we combine the magnetic field and the anisotropy along the same axis as in Figure 6, the ordering temperature and width are
only slightly greater than for a system with only an external magnetic field.

As we see in Figure 22, rotating the direction of the magnetic field perpendicular to the axis of the anisotropy in a 4222 lattice causes an additional inflection point to occur before the ordering temperature, as well as increasing the ordering temperature and width slightly. In Figure 26, we see that the same is true for the 222 lattice, but that the inflection does not occur without anisotropy. However, Figures 27 and 29 show that the 4222 lattice has an inflection point so long as there is a magnetic field perpendicular to the long axis of the antidots and any anisotropy or dipolar field. Figures 30, 31 and 32 show that a near-zero magnetic field with a larger anisotropy still produces the effect, but a large field and small anisotropy removes it. Finally, Figures 34 and 36 show little difference in magnetization between the regions of the unit cell, but the ordering of the regions in the y-direction were different at each temperature.
6. Conclusions

6.1. Conclusion

As a result of our investigations we can see the effects of several variables on the ordering of magnetic antidot systems. Using a system of rectangular rather than square antidots while keeping other fields constant lowers the ordering temperature and reduces the ordering width, even with additional fields of varying magnitudes. Reducing the spacing of these antidots lowers the ordering temperature and width even further, suggesting reasonably that there is a limit to the density of magnetic antidots in a system, similar to the superparamagnetic limit for ferromagnetic grain density per cell. When an external magnetic field is applied perpendicular to the anisotropy axis present in an antidot lattice, an unusual inflection in the magnetization occurs before the ordering of the system would otherwise begin to drop. This same inflection occurs when the external field is perpendicular to the long axis of a rectangular antidot lattice with a dipolar field or anisotropy present. This seems to imply that rectangular antidots induce an effect similar to anisotropy along their long axis and this coincides with experimental results.

6.2. Future work

As one project comes to a close, there are often many doors still left unopened. For one, the detailed ordering within a unit cell and its regions is still not clear. Future work will seek to answer this question, as well as attempt to formulate a quantitative correlation between the geometry of the antidots and the ordering of the system.

One of the additional features that would be useful to add would be to collect visual snapshots of the system at regular intervals of Monte Carlo steps. The current statistics used in this project average over the entire lattice and do so only after all of the Monte Carlo steps for that temperature have been completed. This glosses over a lot of the changes that can occur in the ordering as the steps are completed and we could learn much more by looking into this. Additionally, two useful effects that are not covered here are the correlation length and the vorticity. The correlation length gives a quantitative value for the distance at which lattice sites can affect each other. This value is also directly related to the ordering, so it can be useful to give even more detail about ordering transitions that occur in our systems. As for the vorticity, it quantitatively describes the circulation of a system of rigidly rotating elements. Initially this was a concept from fluid dynamics, but since the elements of 2-dimensional spin models also rotate rigidly it applies here too. The formation and loss of vortices in a lattice of elements is central to ordering transitions and so calculating these values could provide further insight into the
change in the ordering that we see in antidot lattices. Finally, some tests into staggering the antidot placement could show new effects as a different way of varying the geometry of the lattice.
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Appendix 1 – Table of available data

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Appendix 2 – Dipolar field

Even without an external field or anisotropy, lattice sites prefer to be aligned with one another due to their exchange coupling. The effective magnetic field generated by the other spins in the lattice is called the dipolar field, and we see it as the last term in Equation 7 here:

\[
E = -J \sum_{nn} \sum_{i,j} \mathbf{S}_i \cdot \mathbf{S}_j - \sum_i K_2 \cdot S^2_i - \sum_i \mathbf{H}_{\text{ext}} \cdot \mathbf{S}_i - \sum_i \mathbf{H}_D \cdot \mathbf{S}_i
\]  

(7)

In this equation \( \mathbf{H}_D \) is the dipolar field (but has units of energy since \( \mathbf{S} \) is dimensionless) and includes several terms, the derivation of which is as follows:

We begin with an expression for the magnetic intensity of a volume \( \Delta v \) of material, and for a system with current density \( J(\mathbf{r}) \) of zero, our expression simplifies to\(^{29}\):

\[
\nabla \phi^* = \frac{1}{4\pi} \int \frac{\mathbf{M} \, d\mathbf{r}'}{||\mathbf{r} - \mathbf{r}'||} \quad \text{and} \quad \nabla \phi^* = \frac{1}{4\pi} \int \frac{\mathbf{\sigma} \, \mathbf{n} \, d\mathbf{a}'}{||\mathbf{r} - \mathbf{r}'||}
\]

(13)

Here, \( \mathbf{\sigma} \) is the surface density of magnetic pole strength, \( \mathbf{\sigma} \), and \( \mathbf{n} \), are, respectively, as follows:

\[
\mathbf{\rho}_M(\mathbf{r}') = -\mathbf{\nabla} \cdot \mathbf{M}(\mathbf{r}')
\]

(14)

\[
\mathbf{\sigma}_M(\mathbf{r}') = \mathbf{\tau}(\mathbf{r}') \cdot \mathbf{n}
\]

(15)

We note that in these expressions, \( \mathbf{\tau}(\mathbf{r}') \) is the local magnetization and \( \mathbf{n} \) is the normal unit vector to our pole density surfaces \( d\mathbf{a}' \). Since we are considering a thin film with \( \mathbf{\tau}(\mathbf{r}') \) in the x-y plane, our ‘thickness’ in the z-direction will be constant. The result of this is that we will only consider pole densities in the x-z and y-z planes, and our unit vector will be normal to those planes.

Consider one of the spins in our system to be at the origin. We want to calculate \( \mathbf{H}(\mathbf{r}) \) at this site due to the magnetization associated with a nearby lattice point. Recall that each of our spins corresponds to a volume containing many atoms. For each of these spin volumes, \( \mathbf{\tau}(\mathbf{r}') \) is constant, thus \( \mathbf{\rho}_M=0 \).

Now, we can simplify \( \mathbf{H}(\mathbf{r}) \) down to the following:

\[
\mathbf{H}(\mathbf{r}) = \frac{1}{4\pi} \nabla \int_S \left( \mathbf{\tau}(\mathbf{r}') \cdot \mathbf{n} \right) \, d\mathbf{a}'
\]

(16)
Note here that $\tilde{H}(\vec{r})$ is due to a single spin volume. We will expand $(\vec{r} - \vec{r}')$ and simplify further to get the following,

$$
\tilde{H}(x, y) = \frac{(\vec{M}(x', y') \cdot \vec{n})}{4\pi} \sqrt{\int_S \left[ (x - x')^2 + (y - y')^2 \right]^{\frac{1}{2}} da'}
$$

(17)

We consider the lattice sites in our model to be square, so the surface integral here will be along the vertical surfaces of the site in question while $x'$ and $y'$ will be the horizontal coordinates of the points on the surface.

To compute the integral, we will take it over the ranges $x_{\text{min}} \to x_{\text{max}}$ and $y_{\text{min}} \to y_{\text{max}}$, where the minimum is the coordinate of the closest corner and the maximum is the furthest corner as we see in Figure 38 below. This will cause us to have to separate our integral into four parts – one along each edge of the site of interest with two constant coordinates. Thus, we will get two along $x_{\text{min}} \to x_{\text{max}}$, at constant $y_{\text{min}}$ and $y_{\text{max}}$ respectively; and two along $y_{\text{min}} \to y_{\text{max}}$ at constant $x_{\text{min}}$ and $x_{\text{max}}$, respectively.

Figure 37 – Diagram of the evaluation of a vertical segment along a fifth-nearest-neighbor site

Now, we will separate our equation into $x$- and $y$-components:

$$
\tilde{H}(x, y) = \frac{(\vec{M}(x', y') \cdot \vec{n})}{4\pi} \sqrt{\int_{x_{\text{min}}'}^{x_{\text{max}}'} \left[ (x - x')^2 + (y - y')^2 \right]^{\frac{1}{2}} dx'}
\quad + \int_{y_{\text{min}}'}^{y_{\text{max}}'} \left[ (x - x')^2 + (y - y')^2 \right]^{\frac{1}{2}} dy'
$$

(18)

The integrals are in the form of the inverse hyperbolic sine so they can be evaluated, yielding the following step in our calculation:
\[ \vec{H}(x, y) = \frac{MW}{4\pi} \nabla \left[ \sinh^{-1}\left( \frac{x - x'}{y - y'} \right) \bigg|_{x'_{\min}}^{x'_{\max}} + \sinh^{-1}\left( \frac{y - y'}{x - x'} \right) \bigg|_{y'_{\min}}^{y'_{\max}} \right] \]  

Since there is no variation in the z-direction, we can call pull that out of the leading term and call it a constant width \( W \). At this point we note for our simplification that \( x \) and \( y \) are both zero given that we want to compute \( \vec{H} \) at the origin. We continue the derivation of the term above, and give the four parts of the resulting equation separately for clarity. Here, \( y_m \) is the y-coordinate of the given horizontal edge, while \( x_m \) is the x-coordinate of the given vertical edge. We begin with the x-component of the field induced by the horizontal segments, leaving off the prime notation for clarity:

\[ H_{\text{horiz}, x} = \frac{MW}{4\pi} \left[ \frac{1}{|y_m|} \left( \frac{x_{\max}}{y_m} \right)^2 + 1 \right]^{\frac{1}{2}} \left[ \frac{1}{|y_m|} \left( \frac{x_{\max}}{y_m} \right)^2 + 1 \right]^{\frac{1}{2}} \]  

(20)

This is followed subsequently by the y-components of the horizontal segments:

\[ H_{\text{horiz}, y} = \frac{MW}{4\pi} \left[ \frac{x_{\max}}{y_m^2} \left( \frac{x_{\max}}{y_m} \right)^2 + 1 \right]^{\frac{1}{2}} \left[ \frac{x_{\max}}{y_m^2} \left( \frac{x_{\max}}{y_m} \right)^2 + 1 \right]^{\frac{1}{2}} \left[ -\frac{y_m}{|y_m|} \right] \]  

(21)

Similarly, here is the x-component of the field induced by the vertical segments:

\[ H_{\text{vert}, x} = \frac{MW}{4\pi} \left[ \frac{y_{\max}}{x_m^2} \left( \frac{y_{\max}}{x_m} \right)^2 + 1 \right]^{\frac{1}{2}} \left[ \frac{y_{\min}}{x_m^2} \left( \frac{y_{\min}}{x_m} \right)^2 + 1 \right]^{\frac{1}{2}} \left[ -\frac{x_m}{|x_m|} \right] \]  

(22)

Finally, we have the y-component of the field of the vertical segments:
The complexity of these terms highlights the efficacy of computer modeling techniques. For the magnitudes of these geometric factors $H$, we make the assumption that the length of an edge of a lattice site is 1 and make our calculations from there. It should be noted that the $H_{\text{vert},x}$ and $H_{\text{horiz},y}$ magnitudes could be negative for edges that occur where $y$ or $x$ is negative, respectively. Thus, the terms $\left[\frac{-x_m}{|x_m|}\right]$ and $\left[\frac{-y_m}{|y_m|}\right]$, respectively, compensate for that. Thus we are left with a final equation for our dipolar energy, shown simplified here with $\tilde{M}(x, y)$ in terms of $\tilde{S}_x$ and $\tilde{S}_y$:

$$\tilde{H}_{\text{dmag}} = D\left[\tilde{S}_x \left(\tilde{H}_{\text{horiz},x} + \tilde{H}_{\text{vert},x}\right) + \tilde{S}_y \left(\tilde{H}_{\text{horiz},y} + \tilde{H}_{\text{vert},y}\right)\right]$$

The constant $D$ used here is a scaling factor as utilized in the code for this project, the magnitude of which we use to refer to the strength of the field in our data.

Now that we know the dipolar field at the origin due to a lattice site, we will extend this to include all sites up to fifth-nearest-neighbors as shown in Figure 38. The reason that we limit ourselves to the fifth nearest neighbors is that we found that each of these $\frac{4\pi H}{MW}$ factors have a magnitude that does not exceed approximately 2 for the nearest neighbors and diminishes over distance. The sites in Figure 38 are labeled in order of neighbor distance from the center site and each pair of line segments in the figure represents the pole density of each site that borders that segment. Note that not all of the edges are included, only those that are bordered on either side by a neighbor. The magnetization of each edge is the sum of the components along that axis of both sites that share it. This will exclude the magnetization of the central site $S$ because a site with a magnetization cannot demagnetize itself, so the edges of that site will only include the magnetization of the sites that share them.
Figure 38 – Diagram of the up to the fifth-nearest-neighbors, centered at a site \( S \)

Additionally, it has been shown in experimental and theoretical work\(^{28} \) that a system of rectangular antidots experiences a shape-induced anisotropy when in the presence of a dipolar field. Figure 39 shows a 4222 lattice with the spins of each neighbor site around \( S \) shown in their low-temperature alignment along the x-axis. The magnetization of \( S \) is also in the same direction. Looking at the effect of the dipolar field, \( S \) will see no magnetic poles formed by sites in unit cell regions two and three. This is because the pole density along an edge from one of those sites would be equal and opposite to the density from the site that shares that edge.

Figure 39 – A diagram showing poles forming as a result of the dipolar field in a 4222 lattice

However, the sites in unit cell region one will form poles where they meet the antidots, as shown by the thick lines in Figure 39. A ‘north’ pole will form at the head of the spin moment vector and a ‘south’ pole will form at the tail of that vector. The resulting magnetic field will not be parallel to the spin at \( S \). The net result of this effect is that at a strong enough magnitude, the dipolar field will cause some disorder, even at low or zero temperature. However, at higher temperatures, the spins will not be aligned and other poles will form, reducing this ‘demagnetization’ effect of the dipolar field.
Appendix 3 – Unit cell diagrams

Figure 40 – The 222 unit cell

Figure 41 – The 422 unit cell

Figure 42 – The 622 unit cell

Figure 43 – The 6222 unit cell
Figure 44 – The 8224 unit cell

Figure 45 – The 4122 unit cell

Figure 46 – The 4124 unit cell

Figure 47 – The 4114 unit cell
Figure 48 – The 4222 unit cell

Figure 49 – The 4224 unit cell

Figure 50 – The 4242 unit cell

Figure 51 – The 4244 unit cell
Appendix 4 – Monte Carlo simulation code

PROGRAM Domcalc
************************************************************************
* Magnetic antidot simulation - XY Model v.6.1                        *
* ---------------------------------------------------------------------- *
* This code is an variation of the XY model, metropolis algorithm.     *
* It simulates the time-evolution of an array of variable spin        *
* elements at various temperatures with periodic antidots.           *
************************************************************************
* This version includes the following features:                      *
* Energy & magnetization effects to the first nearest neighbor        *
* Susceptibility, heat capacity & 4th order cumulant                 *
* Demagnetization, external field & anisotropy are enabled            *
* Magnetization statistics of subdomains                             *
* flip frequency monitoring                                          *
************************************************************************
************************************************************************
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* 02111-1307 USA                                                      *
************************************************************************
Define initial variables
   INTEGER ITRNUM, L, K, DLOOP, NEG, I, J, RNGSED, N, SINC
   INTEGER STPNUM, Q, T, TP, IDX, MSNAP, LX, LY
C Define array variables
   REAL*8 EX, EY, SX(10000), SY(10000), NNX, NNY
C Define calculation variables
   REAL*4 RAND, TMPSTP
   REAL*8 TMPKTJ, OP, ENET, M, PROB, ENETT
   REAL*8 P1, TWOP1
   CHARACTER*12 FNAME, LVAR
   LOGICAL MFLIP, TMPFLIP, CTFLIP
   DIMENSION ENET(6000000), OP(6000000)
C Define variables for susceptibility, heat capacity and cumulant
REAL*8 X, C, SUMOP, SUMMAG, SUME, SQE, SQOP, U, SQQP
REAL*8 ENSUM, MOPSUM, CEN, COP, SQNOP, RANOP, SUMX, SQX
REAL*8 MX, MY, SX2, SY2, E1, DE, E
REAL*8 SQENET(6000000)

C Define quantum anti-dot properties
INTEGER DOTX, DOTY, SPACX, SPACY
INTEGER NN, SN, NT
COMMON /DOT/ DOTX, DOTY, SPACX, SPACY
COMMON /NN/ LX, LY, NN(10000,4)
COMMON /NN2/ SX, SY, SN(100000)
COMMON /EN/ ENET, SQENET, K

C Define complex Hamiltonian variables
REAL*8 HEXTX, HEXTY, D, EISO, ISODIR, HANGL, HEXT
COMMON /VAR/ EISO, HEXTX, HEXTY

C Extra info variables
REAL*4 RND1, RND2
REAL*8 SX1, SY1
INTEGER CHANGE(100000)
REAL*8 MBIN1X(110), MBIN1Y(110), MBIN2X(110)
REAL*8 MBIN2Y(110), MBIN3X(110), MBIN3Y(110)
REAL*8 MBIN1(110), MBIN2(110), MBIN3(110)
REAL*8 X1, X2, X3, BINSIZE(110)
COMMON /DOM1/ BINSIZE, MBIN1, MBIN1X, MBIN1Y, MBIN2, MBIN2X, MBIN2Y,
% MBIN3, MBIN3X, MBIN3Y, X1, X2, X3, TMPKTJ, ITRNUM, NT

C Define demagnetization calculation variables
REAL*8 DMA(10000, 10), DMB(10000, 10), DMC(10000, 10), DMD(10000, 10),
% DME(10000, 10)
REAL*8 MXA(10000, 10), MXB(10000, 10), MXC(10000, 10), MXD(10000, 10),
% MXE(10000, 10)
REAL*8 MYA(10000, 10), MYB(10000, 10), MYC(10000, 10), MYD(10000, 10),
% MYE(10000, 10)
REAL*8 DMAG, HDMAG
REAL*8 DMDISTH(20,2), DMDISTV(20,2)
INTEGER IDM
COMMON /DMG/ DMA, DMB, DMC, DMD, DME,
% MXA, MXB, MXC, MXD, MXE,
% MYA, MYB, MYC, MYD, MYE
COMMON /DMG2/ DMAG, HDMAG, IDM
COMMON /DIST/ DMDISTH, DMDISTV

C More variables for spin pictures
INTEGER NPASSPICT, ANS5, IP, ANS4, ANS3
CHARACTER*12 FSPINPICT

C CHANGE tracks how often a site flips
C Ask for user defined variables
C Define the array
   PRINT *, 'Enter array length: '
   READ (*,*) LX
   PRINT *, 'Enter array width: '
   READ (*,*) LY

C set initial values
   ANS5 = 0
   ANS4=0
   ANS3=0
   IP = 0
   ITRNUM = 1
   N = LX*LY
   NT = N
   ENETT = -2*N
   TMPNUM = 20
   PI = 3.141592653589793d0
   TWOPI = 2.0D0*PI
   HEXT = 0
   EISO = 0
   DMAG = 0
   IDM = 1
   fspinpict = 'spins.txt'

C Initialize the entire array to initial energy, +1
   DO 10 I = 1, N
      SX(I) = 1
      SY(I) = 0
      SN(I) = 1
      CHANGE(I) = 0
   C NOTE: I is used for columns while J is used for rows
   10    CONTINUE

C Initialize the bins for unit cell statistics
   DO I = 1, 102
      MBIN1X(I) = 0
      MBIN1Y(I) = 0
      MBIN1(I) = 0
      MBIN2X(I) = 0
      MBIN2Y(I) = 0
      MBIN2(I) = 0
      MBIN3X(I) = 0
      MBIN3Y(I) = 0
      MBIN3(I) = 0
   c Store statistics in 'bins'
c   bins range from '-1' to '1'
end do

C Call NEARBR to initialize the nearest neighbor array
call nearbr

C Ask for file
print *, 'Name the file to record to'
read (*) fname
close (unit = 1)

C Ask for multiple temperatures
print *, 'Run a range of temperatures? (Y/N)'
read (*,*) lvar
if (lvar .eq. 'y') then
  tmpflip = .true.
  print *, 'Enter initial temperature in kT/J'
  read (*,*) tmpktj
  print *, 'Enter temperature step size'
  read (*,*) tmpstp
  print *, 'How many steps?'
  read (*,*) stpnum
else
  tmpflip = .false.
  print *, 'Enter temperature in kT/J'
  read (*,*) tmpktj
  tmpstp = 0
  stpnum = 1
endif

C Ask for anti-dot generation
print *, 'Use anti-dots? (Y/N)'
read (*,*) lvar
if (lvar .eq. 'y') then
  print *, 'Use square dots?'
  read (*,*) lvar
  print *, 'Dot diameter (X)?'
  read (*,*) dotx
  if (lvar .eq. 'y') then
    doty = dotx
  else
    print *, 'Dot height (y)?'
    read (*,*) doty
  endif
else
  print *, 'Dot X spacing?'
READ (*,*) SPACX
PRINT *, 'Dot Y spacing?'
READ (*,*) SPACY
CALL DOTGEN

NT = 0
ENETT = 0

DO  I = 1, N
    NT = NT + SN(I)
    ENETT = ENETT - SN(I)*(SN(NN(I, 1)) + SN(NN(I, 2)))
END DO
END IF

E = ENETT
EI = ENETT

PRINT *, 'Enter number of passes'
READ (*,*) ITRNUM
PRINT *, 'Enter RNG seed'
READ (*,*) RNGSED
C This allows the system to reach some equilibrium before recording data
PRINT *, 'Skip how many passes before recording?'
READ (*,*) DLOOP
C Ask for complex Hamiltonian variables
PRINT *, 'Use anisotropy? (y/n)'
READ (*,*) LVAR
IF (LVAR .EQ. 'y') THEN
    PRINT *, 'Anisotropy energy?'
    READ (*,*) EISO
C    PRINT *, 'Direction of the anisotropy? (+1/-1)'
C    READ (*,*) ISODIR
ELSE
    EISO = 0
END IF

PRINT *, 'Use external field? (y/n)'
READ (*,*) LVAR
IF (LVAR .EQ. 'y') THEN
    PRINT *, 'Enter the magnitude of the field'
    READ (*,*) HEXT
    PRINT *, 'Enter the angle of the field'
    READ (*,*) HANGL
    HANGL = (HANGL * PI) / 180
    HEXTX = HEXT*DCOS(HANGL)
    HEXTY = HEXT*DSIN(HANGL)
ELSE

HEXT = 0
END IF

PRINT *, 'Include demagnetization? (y/n)'
READ (*,*) LVAR
IF (LVAR .EQ. 'y') THEN
  PRINT *, 'Enter the magnitude of the field'
  READ (*,*) DMAG
CALL the remaining 4 nearest neighbor arrays
  CALL NEARBR2
  CALL NEARBR3
  CALL NEARBR4
  CALL NEARBR5
ELSE
  DMAG = 0
END IF

write(*,*) 'Print out spin pictures?'
READ (*,*) LVAR
IF (LVAR .EQ. 'y') THEN
  ANS5 = 1
  write(*,*) 'Enter lattice pass number for pictures:'
  read(*,*) npasspict
  IP = NPASSPICT
  fspinpict = 'spins.txt'
else
  ANS5 = 0
endif

write(*,*) 'Record flip-rate statistics?'
READ (*,*) LVAR
IF (LVAR .EQ. 'y') THEN
  ANS4 = 1
  else
  ANS4=0
end if
write(*,*) 'Record domain data?'
READ (*,*) LVAR
IF (LVAR .EQ. 'y') THEN
  ANS3 = 1
  else
  ANS3=0
end if
* Write additional information to file:
  OPEN (UNIT = 1, FILE = 'data.txt')

C Write parameters
WRITE (1, *) 'Lattice size:', LX, 'x', LY
WRITE (1, *) 'Number of passes:', ITRNUM
WRITE (1, *) 'Number of skipped passes:', DLOOP
WRITE (1, *) 'Number generator seed:', RNGSED

C Write dot parameters
WRITE (1, *) 'Antidot geometry:', DOTX, DOTY, SPACX, SPACY

C Write variables
WRITE (1, *) 'Anisotropy Magnitude:', EISO
WRITE (1, *) 'External Field Magnitude:', HEXT
WRITE (1, *) 'External Field Angle:', HANGL
WRITE (1, *) 'Demagnetization Magnitude:', DMAG

C Write output headings
CLOSE(UNIT = 1)
OPEN (UNIT = 1, FILE = FNAME)
WRITE (1, 15) 'TMPKTJ', 'OP', 'X', 'M', 'MX', 'MY'
15 FORMAT(6(5X, A6))

C Prepare domain data
IF(ans3 .eq.1) then
  close(unit=1, status='save')
  OPEN (UNIT = 1, FILE = 'domain.txt')
  WRITE (1, 16) 'Bin', 'OP1', 'M1X', 'M1Y', 'OP2', 'M2X',
  'M2Y', 'OP3', 'M3X', 'M3Y', 'X1', 'X2', 'X3'
16 FORMAT(13(5X, A6))
  close(unit=1, status='save')
  open(unit=1, file=fname, STATUS='OLD')
end if

C Prepare spin statistics data
IF(ans3 .eq.1) then
  close(unit=1, status='save')
  OPEN (UNIT = 1, FILE = fspinpict)
  write(1,17) 'i,','sn(i),','sx(i),','sy(i),'
17 FORMAT(10(5X, A6))
  close(unit=1, status='save')
  OPEN (UNIT = 1, FILE = FNAME, STATUS = 'OLD')
end if

C RAN2 requires a negative seed, so we'll just correct it instead of asking
RNGSED = -ABS(RNGSED)

PRINT *, 'Randomizing system, please wait...'
Here's a loop to start up with DLOOP skipped passes

DO K=1, DLOOP

DO 30 I=1, N
  IDM = I
  SX1 = SX(I)
  SY1 = SY(I)

C Make sure holes are not counted
IF (SN(I) .EQ. 1) THEN
  NNX = 0
  NNY = 0
  DO J=1, 4
    NNX = NNX + SX(NN(I, J))
    NNY = NNY + SY(NN(I, J))
  END DO

CALL RAN2(RNGSED, RAND)
RND1 = RAND
SX2 = DCOS(RND1*TWOPI)
SY2 = DSIN(RND1*TWOPI)
EX = SX2*NNX
EY = SY2*NNY
CALL DMAGC
EI = -(NNX*SX(I) + NNY*SY(I))
%  -EISO * (SX(I)**2)
%  -HEXTX*SX(I) -HEXTY*SY(I)
%  -HDMAG
SX(I) = SX2
SY(I) = SY2

CALL DMAGC
E = -(EX + EY)
%  -EISO * (SX(I)**2)
%  -HEXTX*SX(I) -HEXTY*SY(I)
%  -HDMAG
DE = E - EI

IF (DE .LT. 0) THEN
  SY(I) = SY2
  SX(I) = SX2
  ENETT = ENETT + DE
ELSE
  CALL RAN2(RNGSED, RAND)
IF (RAND .LE. EXP(-DE / TMPKTJ)) THEN
   SY(I) = SY2
   SX(I) = SX2
   ENETT = ENETT + DE
ELSE
   SX(I) = SX1
   SY(I) = SY1
END IF
END IF
END IF
30 CONTINUE
ENDDO

********************
C We begin our temperature outer loop now
DO Q = 1, STPNUM
   PRINT *, 'Evaluating temperature', TMPKTJ
   ********************
C Reset sums before starting next temperature
   SUMMAG = 0
   SUMOP = 0
   SUME = 0
   SQOP = 0
   SQE = 0
   SQQOP = 0
   ********************
C Now we evaluate the system ITRNUM times
   DO K = 1, ITRNUM
   C K is a placeholder variable
   C Here begins the logic loop for evaluating each item
   C we will use row-wise processing because its easier for neighbors
   C We include nearest-neighbors here, but
   DO 20 I=1,N
      IDM = I
      SX1 = SX(I)
      SY1 = SY(I)
      C Make sure holes are not counted
      IF (SN(I) .EQ. 1) THEN
         NNX = 0
         NNY = 0
         DO J=1,4
         END DO 20

NNX = NNX + SX(NN(I,J))
NNY = NNY + SY(NN(I,J))

END DO

C Now, we evaluate the energy

CALL RAN2(RNGSED, RAND)
RND1 = RAND
SX2 = DCOS(RND1*TWOP1)
SY2 = DSIN(RND1*TWOP1)

EX = SX2*NNX
EY = SY2*NNY

CALL DMAGC
EI = -(NNX*SX(I) + NNY*SY(I))
% -EISO * (SX(I)**2)
% -HEXTX*SX(I) - HEXTY*SY(I)
% -HDMAG
SX(I) = SX2
SY(I) = SY2

CALL DMAGC
E = -(EX + EY)
% -EISO * (SX(I)**2)
% -HEXTX*SX(I) - HEXTY*SY(I)
% -HDMAG
DE = E - EI

C call random number here. RAND is a number from 0->1
C for high temperatures, S is more likely to flip

C allow for temperature effects here

IF (DE .LT. 0) THEN
SY(I) = SY2
SX(I) = SX2
ENETT = ENETT + DE
CHANGE(I) = CHANGE(I) + 1
ELSE
CALL RAN2(RNGSED, RAND)
IF (RAND .LE. EXP(-DE / TMPKTJ)) THEN
SY(I) = SY2
SX(I) = SX2
ENETT = ENETT + DE
CHANGE(I) = CHANGE(I) + 1
ELSE
SX(I) = SX1
SY(I) = SY1
END IF
ENDIF
END IF

20 CONTINUE
C Resolve Magnetization, $M = \frac{POS - NEG}{MSIZE^2}$

$M = 0$
$MX = 0$
$MY = 0$

DO $I = 1, N$
\quad MX = MX + SX(I)$
\quad MY = MY + SY(I)$
END DO

$M = \sqrt{MX^2 + MY^2}$
$M = M / NT$

C The order parameter is the absolute value of the magnetization
$OP(K) = \text{ABS}(M)$

C Set the Energy and Order Parameter averages now
$SUMMAG = SUMMAG + M$
$SUMOP = SUMOP + OP(K)$
$SQOP = SQOP + OP(K)*OP(K)$
$SQQOP = SQQOP + OP(K)*OP(K)**4$

C Recalculate energies for the full lattice
$E = 0$
$SUME = 0$
$SQE = 0$
$ENET(K) = 0$
$SQENET(K) = 0$

DO $I = 1, N$
\quad IDM = I$
\quad NNX = 0$
\quad NNY = 0$
\quad DO $J = 1, 2$
\quad \quad NNX = NNX + SX(NN(I, J))$
\quad \quad NNY = NNY + SY(NN(I, J))$
\quad END DO
\quad CALL DMAGC
\quad E = - (NNX*SX(I) + NNY*SY(I))$
\quad \% -EISO * (SX(I)**2)$
\quad \% -(HEXTX*SX(I) + HEXTY*SY(I))$
\quad \% -HDMAG
\quad ENET(K) = ENET(K) + E$
\quad SQENET(K) = SQENET(K) + E*E$

C this ends the energy recalculation here
END DO

C take spin picture data if necessary
if(ans5.eq.1) then
   if((K/NPASSPICT).eq.0) then
      close(unit=1,status='save')
      open(unit=1,file=fsinpict, STATUS='OLD')
      do i=1,N
         write(1,42) i,sn(i),sx(i),sy(i)
      enddo
      close(unit=1,status='save')
      open(unit=1,file=fname, STATUS='OLD')
   endif
endif

IF(ANS3.EQ.1) THEN
   CALL DOMAIN
end if

C this ends the iteration loop here, K
ENDDO

DO K=1, ITRNUM
   SUME = SUME+ENET(K)
   SQE = SQE+ENET(K)*ENET(K)
END DO
SUME = SUME/ITRNUM
SQE = SQE/ITRNUM

********************
C Calculate the susceptibility, heat capacity and cumulant
X = (NT / TMPKTJ) * ( (SQOP/ITRNUM) - (SUMOP/ITRNUM)**2 )
C = ( (SQE) - (SUME)**2 ) / (NT * TMPKTJ * TMPKTJ )
U = 1 - ( (SQQOP/ITRNUM) / (3 * ((SQOP/ITRNUM)**2)) )

C Store data per temperature
OPEN (UNIT = 1, FILE = FNAME, STATUS='OLD')
WRITE (1, 70) TMPKTJ, (SUMOP/ITRNUM), X, M, MX, MY
70 Format(6(2X, E12.5))

C Print domain data
IF(ANS3.EQ.1) THEN
   close(unit=1,status='save')
   OPEN (UNIT = 1, FILE = 'domain.txt', STATUS='OLD')
   DO I =1,101
      WRITE (1, 72) BINSIZE(I), ABS(MBIN1(I)), MBIN1X(I), MBIN1Y(I),
                                 % ABS(MBIN2(I)), MBIN2X(I), MBIN2Y(I), ABS(MBIN3(I)),
                                 % MBIN3X(I), MBIN3Y(I), X1, X2, X3
72  Format(13(2X, E12.5))
**Routine NEARBR:**

*NEARBR*: a nearest-neighbor indexing array subroutine

**Subroutine NEARBR**

**C** Site number is the lattice location, 1-N

**C** nnidx is the nn location, 1-4 clockwise

**INTEGER I, J, WX, WY, NR**

**COMMON /NN/ WX, WY, NR(10000, 4)**

**C** Here, W corresponds to L, and NR() to NN()

**DO I = 1, WX*WY**

**C** Set locations of nearest neighbors

**NR(I, 1) = I - WX**

**NR(I, 2) = I + 1**

**NR(I, 3) = I + WX**

**NR(I, 4) = I - 1**

**C** Correct if an edge

**C** right side

**IF (MOD(I, WX) .EQ. 0) THEN**

**NR(I, 2) = I - WX + 1**

**C** left side

**ELSE IF (MOD((I-1), WX) .EQ. 0) THEN**

**NR(I, 4) = I + WX - 1**

**END IF**

**C** Top
IF (I .LE. WX) THEN
   NR(1, 1) = 1 + WX*(WY-1)
C    Bottom
ELSE IF (I .GT. WX*(WY-1)) THEN
   NR(1, 3) = 1 - WX*(WY-1)
END IF
END DO

RETURN
END

************************************************************************
* DOTGEN: an anti-dot generator
************************************************************************

SUBROUTINE DOTGEN

INTEGER A, B, C, D
INTEGER NUMX, NUMY, VAR
INTEGER X, Y, SPX, SPY
INTEGER L, NN
REAL*8 SX, SY
INTEGER SN

COMMON /DOT/ X, Y, SPX, SPY
COMMON /NN/ LX, LY, NN(10000,4)
COMMON /NN2/ SX(10000), SY(10000), SN(100000)

VAR = 0
NUMX = INT( LX / (X + SPX) )
NUMY = INT( LY / (Y + SPY) )
PRINT *, "Generating holes..."

C All dots begin in the upper left corner
C Take each point in the original dot and copy it at regular intervals
DO A = 1, Y
   C Repeat each y point in the first dot NUMY times
   DO B = 1, NUMY
      C Now, repeat each x point NUMX times
      DO C = 1, X
         DO D = 1, NUMX
            VAR = (A + (B-1)*(Y+SPY) -1)*LX + C + (X+SPX)*(D-1)
            SN(VAR) = 0
            SX(VAR) = 0
            SY(VAR) = 0
         END DO
      END DO
   END DO
END DO

68
SUBROUTINE RAN2(idum, rn)

PARAMETER (IM1=2147483563, IM2=2147483399, AM=1./IM1,
& IMM1=IM1-1, IA1=40014, IA2=40692, IQ1=53668, IR1=12211,
& IR2=3791, NTAB=32, NDIV=1+IMM1/NTAB,
& EPS=1.2e-7, RNMX=1.-EPS)

INTEGER idum2, j, k, iv(NTAB), iy
SAVE iv, iy, idum2
DATA idum2/123456789/, iv/NTAB*0/, iy/0/

IF(idum.LE.0) THEN !initialize
      idum=MAX(-idum,1)
      idum2=idum
      DO j=NTAB+8,1,-1
         k=idum/IQ1
         idum=IA1*(idum-k*IQ1)-k*IR1
         IF(idum.LT.0) idum=idum+IM1
         IF(j.LE.NTAB) iv(j)=idum
      END DO
      iy=iv(1)
   END IF

k=idum/IQ1 !start here when not initializing
   idum=IA1*(idum-k*IQ1)-k*IR1
   IF(idum.LT.0) idum=idum+IM1
   k=idum2/IQ2
   idum2=IA2*(idum2-k*IQ2)-k*IR2
   IF(idum2.LT.0) idum2=idum2+IM2
   j=1+iy/NDIV
   iy=iv(j)-idum2
   iv(j)=idum
   IF(iy.LT.1) iy=iym+1
   rn=MIN(AM*iy, RNMX)

RETURN
END

************************************************************************

* RAN2: a random number generator that actually works *
************************************************************************


Parameter (IM1=2147483563, IM2=2147483399, AM=1./IM1,
 & IMM1=IM1-1, IA1=40014, IA2=40692, IQ1=53668, IR1=12211,
 &  IR2=3791, NTAB=32, NDIV=1+IMM1/NTAB,
 &  EPS=1.2e-7, RNMX=1.-EPS)
* DOMAIN: A domain magnetization tracking subroutine

************************************************************************
SUBROUTINE DOMAIN

INTEGER X, Y, SPX, SPY
INTEGER I, J, K, A, B
INTEGER LX, LY, NN
REAL*8 SX, SY
REAL*8 MX1, MY1, MX2, MY2, MX3, MY3
REAL*8 M1, M2, M3
REAL*8 MBIN1X(110), MBIN1Y(110), MBIN2X(110)
REAL*8 MBIN2Y(110), MBIN3X(110), MBIN3Y(110)
REAL*8 MBIN1(110), MBIN2(110), MBIN3(110)
REAL*8 BINSIZE(110)
INTEGER SN, NT
REAL*8 SQOP1, SQOP2, SQOP3
REAL*8 X1, X2, X3, TMPKTJ, S1, S2, S3

COMMON /DOT/ X, Y, SPX, SPY
COMMON /NN/ LX, LY, NN(10000, 4)
COMMON /NN2/ SX(10000), SY(10000), SN(100000)
COMMON /DOM1/ BINSIZE, MBIN1, MBIN1X, MBIN1Y, MBIN2, MBIN2X, MBIN2Y,
% MBIN3, MBIN3X, MBIN3Y, X1, X2, X3, TMPKTJ, ITRNUM, NT

A = 0
B = 0
MX1 = 0
MY1 = 0
MX2 = 0
MY2 = 0
MX3 = 0
MY3 = 0
S1 = 0
S2 = 0
S3 = 0
J = 1
X1 = 0
X2 = 0
X3 = 0
K = 0
C outer loop checks each row
   do I=1, LY
      c   A is the first location of the current row
         A = (I-1)*LX + 1
      c inner loop checks each cell in the row
         do J=1, LX
            c   B is the current location in the lattice
               B = (I-1)*LX + J
            IF (SN(A) .EQ. 0) THEN
               c       this is a row with a hole
               c       hole rows contain holes (#4) and cell #1
               IF (SN(B) .EQ. 1) THEN
                  MX1 = SX(B)
                  MY1 = SY(B)
                  M1 = SQRT(MX1**2 + MY1**2)
                  DO K = 1, 101
                     IF (M1 .GE. BINSIZE(K) .AND. M1 .LT. BINSIZE(K+1)) THEN
                        MBIN1(K) = MBIN1(K)+1
                     END IF
                  END DO
               ELSE
                  END IF
               ELSE
                  c       this is a row without a hole
                  c       non-hole rows contain cell #s 2 & 3
                  IF (SN(J) .EQ. 0) THEN
                     MX3 = SX(B)
                     MY3 = SY(B)
                     M3 = SQRT(MX3**2 + MY3**2)
                     DO K = 1, 101
                        IF (M3 .GE. BINSIZE(K) .AND. M3 .LT. BINSIZE(K+1)) THEN
                           MBIN3(K) = MBIN3(K)+1
                        END IF
                     END DO
                  ELSE
                     END IF
                  ELSE
                     END IF
                  END DO
                  ELSE
                     x2 = SX(B)
                     MY2 = SY(B)
M2 = SQRT(MX2**2 + MY2**2)
DO K = 1,101
    IF (M2 .GE. BINSIZE(K).AND. M2 .LT. BINSIZE(K+1)) THEN
        MBIN2(K) = MBIN2(K)+1
    END IF
    IF (MX2 .GE. BINSIZE(K).AND. MX2 .LT. BINSIZE(K+1)) THEN
        MBIN2X(K) = MBIN2X(K)+1
    END IF
    IF (MY2 .GE. BINSIZE(K).AND. MY2 .LT. BINSIZE(K+1)) THEN
        MBIN2Y(K) = MBIN2Y(K)+1
    END IF
END DO
END IF
END IF
RETURN
END

*************************************************************************
* NEARBR2: A 2nd nearest neighbor arranging subroutine               *
*                                                                *
*************************************************************************
SUBROUTINE NEARBR2

INTEGER A, B, C, D
INTEGER NUMX, NUMY, VAR
INTEGER X, Y, SPX, SPY
INTEGER L, NN
INTEGER SN, I, J, N
REAL*8 SX, SY
REAL*8 DMA(10000,10), DMB(10000,10), DMC(10000,10), DMD(10000,10),
% DME(10000,10)
REAL*8 MXA(10000,10), MXB(10000,10), MXC(10000,10), MXD(10000,10),
% MXE(10000,10)
REAL*8 MYA(10000,10), MYB(10000,10), MYC(10000,10), MYD(10000,10),
% MYE(10000,10)
REAL*8 DMAG, HDMAG, U

COMMON /DOT/ X, Y, SPX, SPY
COMMON /NN/ LX, LY, NN(10000,4)
COMMON /NN2/ SX(10000), SY(10000), SN(10000)
COMMON /DMG/ DMA, DMB, DMC, DMD, DME,
% MXA, MXB, MXC, MXD, MXE,
% MYA, MYB, MYC, MYD, MYE
COMMON /DMG2/ DMAG, HDMAG
I = 1
J = 1
N = LX*LY

C Designations for neighbor locations follow this pattern:
c DM[position]([location], [site number])
c where position is A-E in order of neighbor distance
c and location is in order, clockwise from the top
c and distance is edge distance

C Convert 1st nearest neighbors to new format
DO I=1,N
   DMA(I,1) = NN(I,1)
   DMA(I,2) = NN(I,2)
   DMA(I,3) = NN(I,3)
   DMA(I,4) = NN(I,4)
   DO J = 5,8
      DMA(I,J) = 0
   ENDDO
ENDDO

C Record the site location of each neighbor
DO I=1,N
   DMB(I,1) = I - LX + 1
   DMB(I,2) = I + LX + 1
   DMB(I,3) = I + LX - 1
   DMB(I,4) = I - LX -1

C Correct the neighbor locations
C   top
   IF (I .LE. LX) THEN
      DMB(I,1) = DMB(I,1) + N
      DMB(I,4) = DMB(I,4) + N
   ENDF
C   bottom
   IF (I .GT. LX*(LY-1)) THEN
      DMB(I,2) = DMB(I,2) - N
      DMB(I,3) = DMB(I,3) - N
   ENDF
C   left side
   IF (MOD((I-1),LX) .EQ. 0) THEN
      DMB(I,4) = DMB(I,4) + LX
      DMB(I,3) = DMB(I,3) + LX
   ENDF
C   right side
   IF (MOD(I,LX) .EQ. 0) THEN
      DMB(I,1) = DMB(I,1) - LX
      DMB(I,2) = DMB(I,2) - LX
* NEARBR3: A 3rd nearest neighbor arranging subroutine *
*
************************************************************************
SUBROUTINE NEARBR3

INTEGER A, B, C, D
INTEGER NUMX, NUMY, VAR
INTEGER X, Y, SPX, SPY
INTEGER L, NN
INTEGER SN, I, J, N
REAL*8 SX, SY
REAL*8 DMA(10000, 10), DMB(10000, 10), DMC(10000, 10), DMD(10000, 10),
% DME(10000,10)
REAL*8 MXA(10000, 10), MXB(10000, 10), MXC(10000, 10), MXD(10000, 10),
% MXE(10000,10)
REAL*8 MYA(10000, 10), MYB(10000, 10), MYC(10000, 10), MYD(10000, 10),
% MYE(10000,10)
REAL*8 DMAG, HDMAG, U

COMMON /DOT/ X, Y, SPX, SPY
COMMON /NN/ LX, LY, NN(10000,4)
COMMON /NN2/ SX(10000), SY(10000), SN(100000)
COMMON /DMG/ DMA, DMB, DMC, DMD, DME,
% MXA, MXB, MXC, MXD, MXE,
% MYA, MYB, MYC, MYD, MYE
COMMON /DMG2/ DMAG, HDMAG

I = 1
J = 1
N = LX*LY

C Designations for neighbor locations follow this pattern:
c DM[position][location]. [site number])
c where position is A-E in order of neighbor distance
c and location is in order, clockwise from the top
c and distance is edge distance

C Record the site location of each neighbor
DO 1=1,N
    DMC(I, 1) = I - 2*LX
    DMC(I, 2) = I + 2
    DMC(I, 3) = I + 2*LX
1    CONTINUE
DMC(1,4) = 1 - 2

C Correct the neighbor locations
C
top
IF (I . LE. 2*LX) THEN
   DMC(1,1) = DMC(1,1) + N
ENDIF
C
bottom
IF (I . GT. (N - 2*LX)) THEN
   DMC(1,3) = DMC(1,3) - N
ENDIF
C
left side
IF (MOD((I-1),LX) .EQ. 0) THEN
   DMC(1,4) = DMC(1,4) + LX
ELSE IF (MOD((I-2),LX) .EQ. 0) THEN
   DMC(1,4) = DMC(1,4) + LX
ENDIF
C
right side
IF (MOD(I,LX) .EQ. 0) THEN
   DMC(1,2) = DMC(1,2) - LX
ELSE IF (MOD((I+1),LX) .EQ. 0) THEN
   DMC(1,2) = DMC(1,2) - LX
ENDIF

ENDDO

RETURN
END

************************************************************************
* NEARBR4: A 4th nearest neighbor arranging subroutine
*                      *
************************************************************************

SUBROUTINE NEARBR4

INTEGER A, B, C, D
INTEGER NUMX, NUMY, VAR
INTEGER X, Y, SPX, SPY
INTEGER L, NN
INTEGER SN, I, J, N

REAL*8 SX, SY
REAL*8 DMA(10000,10), DMB(10000,10), DMC(10000,10), DMD(10000,10),
   % DME(10000,10)
REAL*8 MXA(10000,10), MXB(10000,10), MXC(10000,10), MXD(10000,10),
   % MXE(10000,10)
REAL*8 MYA(10000,10), MYB(10000,10), MYC(10000,10), MYD(10000,10),
   % MYE(10000,10)
REAL*8 DMAG, HDMAG, U

COMMON /DOT/ X, Y, SPX, SPY
COMMON /NN/ LX, LY, NN(10000, 4)
COMMON /NN2/ SX(10000), SY(10000), SN(100000)
COMMON /DMG/ DMA, DMB, DMC, DMD, DME,
% MXA, MXB, MXC, MXD, MXE,
% MYA, MYB, MYC, MYD, MYE
COMMON /DMG2/ DMAG, HDMAG

I = 1
J = 1
N = LX*LY

C Designations for neighbor locations follow this pattern:
  c  DM[position]([location], [site number])
  c where position is A-E in order of neighbor distance
  c and location is in order, clockwise from the top
  c and distance is edge distance

C Record the site location of each neighbor
  DO I = 1, N
      DMD(I, 1) = I - 2*LX + 1
      DMD(I, 2) = I - LX + 2
      DMD(I, 3) = I + LX + 2
      DMD(I, 4) = I + 2*LX + 1
      DMD(I, 5) = I + 2*LX - 1
      DMD(I, 6) = I + LX - 2
      DMD(I, 7) = I - LX - 2
      DMD(I, 8) = I - 2*LX - 1
  
C Correct the neighbor locations
  top
    IF (I .LE. LX) THEN
        DMD(I, 1) = DMD(I, 1) + N
        DMD(I, 2) = DMD(I, 2) + N
        DMD(I, 7) = DMD(I, 7) + N
        DMD(I, 8) = DMD(I, 8) + N
    ENDIF
    IF ((I .GT. LX) .AND. (I .LE. 2*LX)) THEN
        DMD(I, 1) = DMD(I, 1) + N
        DMD(I, 8) = DMD(I, 8) + N
    ENDIF
  
C bottom
    IF (I .GT. LX*(LY-1)) THEN
        DMD(I, 3) = DMD(I, 3) - N
        DMD(I, 4) = DMD(I, 4) - N
        DMD(I, 5) = DMD(I, 5) - N
        DMD(I, 6) = DMD(I, 6) - N
    ENDIF
    IF ((I .GT. LX*(LY-2)) .AND. (I .LT. N-LX)) THEN
        DMD(I, 4) = DMD(I, 4) - N
    ENDIF

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DMD(1,5) = DMD(1,5) - N

ENDIF

C

left side

IF (MOD((I-1), LX) .EQ. 0) THEN
  DMD(1,5) = DMD(1,5) + LX
  DMD(1,6) = DMD(1,6) + LX
  DMD(1,7) = DMD(1,7) + LX
  DMD(1,8) = DMD(1,8) + LX
ENDIF

IF (MOD((I-2), LX) .EQ. 0) THEN
  DMD(1,6) = DMD(1,6) + LX
  DMD(1,7) = DMD(1,7) + LX
ENDIF

C

right side

IF (MOD((I+1), LX) .EQ. 0) THEN
  DMD(1,1) = DMD(1,1) - LX
  DMD(1,2) = DMD(1,2) - LX
  DMD(1,3) = DMD(1,3) - LX
  DMD(1,4) = DMD(1,4) - LX
ENDIF

IF (MOD((I+1), LX) .EQ. 0) THEN
  DMD(1,2) = DMD(1,2) - LX
  DMD(1,3) = DMD(1,3) - LX
ENDIF

ENDDO

RETURN
END

*************************************************************************
* NEARBR5: A 5th nearest neighbor arranging subroutine                *
*                                                                      *
*************************************************************************

SUBROUTINE NEARBR5

INTEGER A, B, C, D
INTEGER NUMX, NUMY, VAR
INTEGER X, Y, SPX, SPY
INTEGER L, NN
INTEGER SN, I, J, N

REAL*8 SX, SY
REAL*8 DMA(10000, 10), DMB(10000, 10), DMC(10000, 10), DMD(10000, 10),
  % DME(10000, 10)
REAL*8 MXA(10000, 10), MXB(10000, 10), MXC(10000, 10), MXD(10000, 10),
  % MXE(10000, 10)
REAL*8 MYA(10000, 10), MYB(10000, 10), MYC(10000, 10), MYD(10000, 10),
  % MYE(10000, 10)
REAL*8 DMAG, HDMAG, U
COMMON /DOT/ X, Y, SPX, SPY
COMMON /NN/ LX, LY, NN(10000,4)
COMMON /NN2/ SX(10000), SY(10000), SN(100000)
COMMON /DMG/ DMA, DMB, DMC, DMD, DME,
% MXA, MXB, MXC, MXD, MXE,
% MYA, MYB, MYC, MYD, MYE
COMMON /DMG2/ DMAG, HDMAG

I = 1
J = 1
N = LX*LY

C Designations for neighbor locations follow this pattern:
c DM[position][[location], [site number]]
c where position is A-E in order of neighbor distance
c and location is in order, clockwise from the top
c and distance is edge distance

C Record the site location of each neighbor
DO I=1,N
    DME(I,1) = I - 2*LX + 2
    DME(I,2) = I + 2*LX + 2
    DME(I,3) = I + 2*LX - 2
    DME(I,4) = I - 2*LX - 2
END DO

C Correct the neighbor locations
C
top
IF (I .LE. LX) THEN
    DME(I,1) = DME(I,1) + N
    DME(I,4) = DME(I,4) + N
ENDIF
IF ((I .GT. LX) .AND. (I .LE. 2*LX)) THEN
    DME(I,1) = DME(I,1) + N
    DME(I,4) = DME(I,4) + N
ENDIF

C bottom
IF (I .GT. LX*(LY-1)) THEN
    DME(I,2) = DME(I,2) - N
    DME(I,3) = DME(I,3) - N
ENDIF
IF ((I .GT. LX*(LY-2)) .AND. (I .LT. N-LX)) THEN
    DME(I,2) = DME(I,2) - N
    DME(I,3) = DME(I,3) - N
ENDIF

C left side
IF (MOD((I-1),LX) .EQ. 0) THEN
    DME(I,3) = DME(I,3) + LX
    DME(I,4) = DME(I,4) + LX
ENDIF
ENDIF
IF (MOD((I-2),LX) .EQ. 0) THEN
  DME(I,3) = DME(I,3) + LX
  DME(I,4) = DME(I,4) + LX
ENDIF
C right side
IF (MOD(I,LX) .EQ. 0) THEN
  DME(I,1) = DME(I,1) - LX
  DME(I,2) = DME(I,2) - LX
ENDIF
IF (MOD((I+1),LX) .EQ. 0) THEN
  DME(I,1) = DME(I,1) - LX
  DME(I,2) = DME(I,2) - LX
ENDIF
ENDDO
RETURN
END
************************************************************************
* DMAGC: A demagnetization calculator to the 5th nearest neighbor      *
*            *                                                        *
************************************************************************
SUBROUTINE DMAGC

INTEGER A, B, C, D
INTEGER NUMX, NUMY, VAR
INTEGER X, Y, SPX, SPY
INTEGER L, NN
INTEGER SN, I, J, K, N, IDM
REAL*8 SX, SY
REAL*8 DMA(10000,10), DMB(10000,10), DMC(10000,10), DMD(10000,10),
% DME(10000,10)
REAL*8 MXA(10000,10), MXB(10000,10), MXC(10000,10), MXD(10000,10),
% MXE(10000,10)
REAL*8 MYA(10000,10), MYB(10000,10), MYC(10000,10), MYD(10000,10),
% MYE(10000,10)
REAL*8 DMDISTH(20,2), DMDISTV(20,2)
REAL*8 DMAG, HDMAG, UHX, UHY, UVX, UVY
REAL*8 X1, Y1, X2, Y2
REAL*8 MNETH(10000,20), MNETV(10000,20)

C Variables are named where the MX series is the magnetization x-components
C and the MY series is the magnetization y-components of the neighbors
C DMDIST records the magnitude of the distances to each neighbor
C positive and negative signs will be added later to make the data more manageable
COMMON /DOT/ X, Y, SPX, SPY
COMMON /NN/ LX, LY, NN(10000, 4)
COMMON /NN2/ SX(10000), SY(10000), SN(100000)
COMMON /DMG/ DMA, DMB, DMC, DMD, DME,
% MXA, MXB, MXC, MXD, MXE.
% MYA, MYB, MYC, MYD, MYE
COMMON /DMG2/ DMAG, HDMAG, IDM
COMMON /DIST/ DMDISTH, DMDISTV

I = IDM
J = 1
K = 1
N = LX*LY
UXH = 0
UYH = 0
UXV = 0
UYV = 0
HDMAG = 0

C record the component of the magnetization of each neighbor from its site
IF (DMAG .ne. 0) THEN
   DO J = 1, 4
      MXA(I, J) = SX(DMA(I, J))
      MYA(I, J) = SY(DMA(I, J))
      MXB(I, J) = SX(DMB(I, J))
      MYB(I, J) = SY(DMB(I, J))
      MXC(I, J) = SX(DMC(I, J))
      MYC(I, J) = SY(DMC(I, J))
      MXD(I, J) = SX(DMD(I, J))
      MYD(I, J) = SY(DMD(I, J))
      MXE(I, J) = SX(DME(I, J))
      MYE(I, J) = SY(DME(I, J))
   END DO
   DO J = 5, 8
      MXD(I, J) = SX(DMD(I, J))
      MYD(I, J) = SY(DMD(I, J))
   END DO
C For the purpose of organization, we'll reorder these
C into the sums we will use in our calculation
C This section will be very long
MNETH(I, 1) = -MYE(I, 4) + MYD(I, 7)
MNETH(I, 2) = -MYD(I, 8) + MYB(I, 4)
MNETH(I, 3) = -MYC(I, 1) + MYA(I, 1)
MNETH(I, 4) = -MYD(I, 1) + MYB(I, 1)
MNETH(I, 5) = -MYE(I, 1) + MYD(I, 2)
MNETH(I, 6) = -MYD(I, 7) + MYC(I, 4)
MNETH(I, 7) = -MYB(I, 4) + MYA(I, 4)
MNETH(I, 8) = -MYA(I, 1) + SY(I)
MNETH(I, 9) = -MYB(I, 1) + MYA(I, 2)
MNETH(I, 10) = -MYD(I, 2) + MYC(I, 2)
MNETH(I, 11) = -MYC(I, 4) + MYD(I, 6)
MNETH(I, 12) = -MYA(I, 4) + MYB(I, 3)
MNETH(I, 13) = -SY(I) + MYA(I, 3)
MNETH(I, 14) = -MYA(I, 2) + MYB(I, 2)
MNETH(I, 15) = -MYC(I, 2) + MYD(I, 3)
MNETH(I, 16) = -MYD(I, 6) + MYE(I, 3)
MNETH(I, 17) = -MYB(I, 3) + MYD(I, 5)
MNETH(I, 18) = -MYA(I, 3) + MYC(I, 3)
MNETH(I, 19) = -MYB(I, 2) + MYD(I, 4)
MNETH(I, 20) = -MYD(I, 3) + MYE(I, 2)

MNETV(I, 1) = MXE(I, 4) - MXD(I, 8)
MNETV(I, 2) = MXD(I, 8) - MXC(I, 1)
MNETV(I, 3) = MXC(I, 1) - MXD(I, 1)
MNETV(I, 4) = MXD(I, 1) - MXE(I, 1)
MNETV(I, 5) = MXD(I, 7) - MXB(I, 4)
MNETV(I, 6) = MXB(I, 4) - MXA(I, 1)
MNETV(I, 7) = MXA(I, 1) - MXB(I, 1)
MNETV(I, 8) = MXB(I, 1) - MXD(I, 2)
MNETV(I, 9) = MXC(I, 4) - MXA(I, 4)
MNETV(I, 10) = MXA(I, 4) - SX(I)
MNETV(I, 11) = SX(I) - MXA(I, 2)
MNETV(I, 12) = MXA(I, 2) - MXC(I, 2)
MNETV(I, 13) = MXD(I, 6) - MXB(I, 3)
MNETV(I, 14) = MXB(I, 3) - MXA(I, 3)
MNETV(I, 15) = MXA(I, 3) - MXB(I, 2)
MNETV(I, 16) = MXB(I, 2) - MXD(I, 3)
MNETV(I, 17) = MXE(I, 3) - MXD(I, 5)
MNETV(I, 18) = MXD(I, 5) - MXC(I, 3)
MNETV(I, 19) = MXC(I, 3) - MXD(I, 4)
MNETV(I, 20) = MXD(I, 4) - MXE(I, 2)

C Calculate the net demagnetization effect on the site.
C note that the magnetization is the sum of the neighbors
C on either side of the edge being considered
C 20 horizontal and 20 vertical edges

DO J = 1, 20
C sum the horizontal edges, x components
UXH = UXH + MNETH(I, J)*DMDISTH(J, 1)
C sum the horizontal edges, y components
UYH = UYH + MNETH(I, J)*DMDISTH(J, 2)
C sum the vertical edges, x components
UXV = UXV + MNETV(I, J)*DMDISTV(J, 1)
C sum the vertical edges, y components
UYV = UYV + MNETV(I, J)*DMDISTV(J, 2)
END DO

return the scaled demagnetization energy

HDMAG = DMAG * (SX(I)*(UXH+UXV)+SY(I)*(UYH+UYV))
END IF
RETURN
END

************************************************************************
* DMDIST: A neighbor distance calculator     *
*           *
************************************************************************
SUBROUTINE DMDIST

INTEGER A, B, C, D
INTEGER NUMX, NUMY, VAR
INTEGER X, Y, SPX, SPY
INTEGER L, NN
INTEGER SN, I, J, K, N
REAL*8 SX, SY
REAL*8 DMA(10000, 10), DMB(10000, 10), DMC(10000, 10), DMD(10000, 10),
% DME(10000, 10)
REAL*8 MXA(10000, 10), MXB(10000, 10), MXC(10000, 10), MXD(10000, 10),
% MXE(10000, 10)
REAL*8 MYA(10000, 10), MYB(10000, 10), MYC(10000, 10), MYD(10000, 10),
% MYE(10000, 10)
REAL*8 DMDISTH(20, 2), DMDISTV(20, 2)
REAL*8 UHX, UHY, UVX, UVY
REAL*8 X1, Y1, X2, Y2

COMMON /DOT/ X, Y, SPX, SPY
COMMON /NN/ LX, LY, NN(10000, 4)
COMMON /NN2/ SX(10000), SY(10000), SN(100000)
COMMON /DIST/ DMDISTH, DMDISTV

x1=0
x2=0
y1=0
y2=0
N = LX*LY
C Record the distances to each neighbor edge
C the distance array is in order like the lattice array
C note that the distances are the same for several edges;
C this is due to symmetry
C Also, x1 and y1 are Xmax and Ymax, respectively
C As such, x2 and y2 are thus Xmin and Ymin
C note that to simplify data use, we are calculating the distance
C component of the demagnetization energy here instead of just
C recording x1,x2,y1,y2
C this makes the later calculation much simpler to follow
C also the index L in DMDISTH(K,L) is the component, i.e. 1=x, 2=y

C First calculate the distances for the horizontal components
  Y1 = 1.5
  DO J = 1,4
    X1 = -2.5
    DO I = 1,5
      X2 = X1 + 1
      K = 5*(J-1)+I
      DMDISTH(K,1) = (ABS(y1)**(-1))*((x2/y1)**2+1)**(-0.5D0)
%      -(ABS(y1)**(-1))*((x1/y1)**2+1)**(-0.5D0)
      DMDISTH(K,2) = (-x2/(y1**2))*((x2/y1)**2+1)**(-0.5D0)
%      +(x1/(y1**2))*((x1/y1)**2+1)**(-0.5D0 )*(y1/abs(y1))
      c the term (y1/abs(y1)) corrects for vector direction
      X1 = X2
    END DO
    Y1 = Y1 - 1
  END DO

C Now calculate the vertical segments
  Y1 = 1.5
  DO J = 1,5
    Y2 = Y1 + 1
    X1 = -1.5
    DO I = 1,4
      K = 4*(J-1)+I
      DMDISTV(K,1) = (-(y2/(x1**2)))*((y2/x1)**2+1)**(-0.5D0)
%      +(y1/(x1**2))*((y1/x1)**2+1)**(-0.5D0) )*(x1/abs(x1))
      DMDISTV(K,2) = (ABS(x1)**(-1))*((y2/x1)**2+1)**(-0.5D0)
%      -(ABS(x1)**(-1))*((y1/x1)**2+1)**(-0.5D0)
      X1 = X1 + 1
    END DO
    Y1 = Y1 - 1
  END DO
  RETURN
END

************************************************************************