Ising_Model_ACarbone

April 14, 2021

1 Aim

This computational lab will investigate the spin alignment behaviour of a lattice using the Ising Model, its effect on quantities including magnetisation, magnetic susceptibility, and energy. I also demonstrate calculating this particular model's critical temperature T_C.

2 Core Experiments

2.1 Hot vs Cold Start

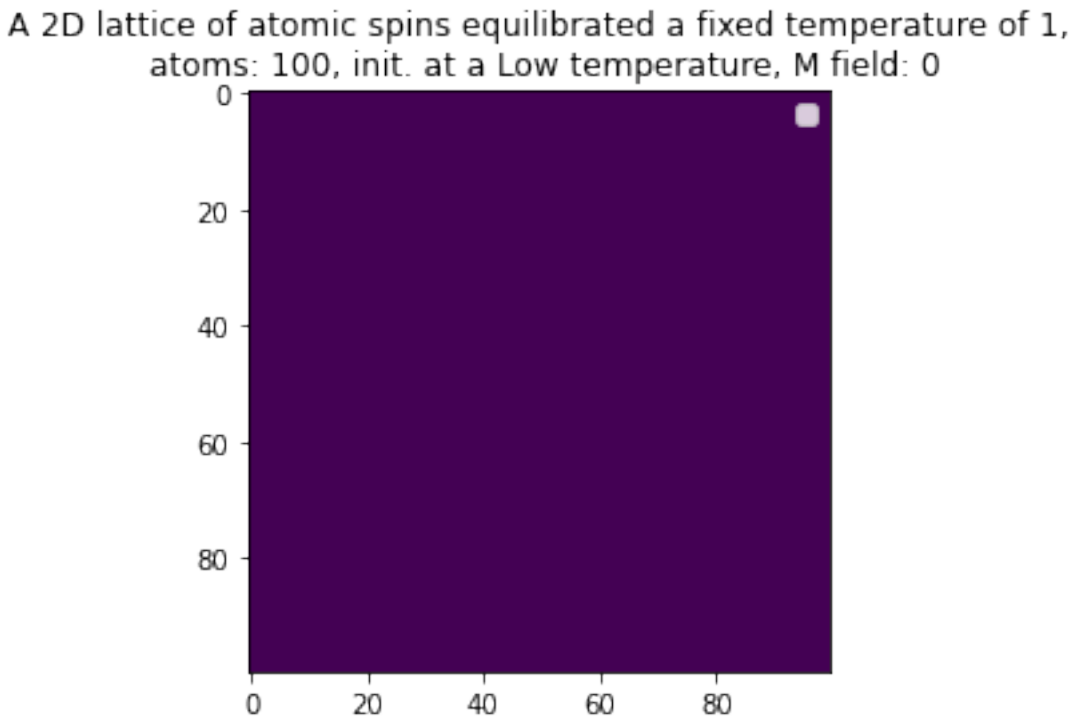
In this Ising Model, a cold start is whereby all the spins are initially aligned, that is all the spins start as $+1$. Conversely a hot start is where the spins start randomly using Python's `random.choice()` function, which randomly selects with equal probability between a spin of $+1$ or -1.

The following two figures plot the initial spin state of a 100x100 lattice by setting `steps=0`.

[51]:
```
# Import Ising Model
import Ising_model_v2 as model
```

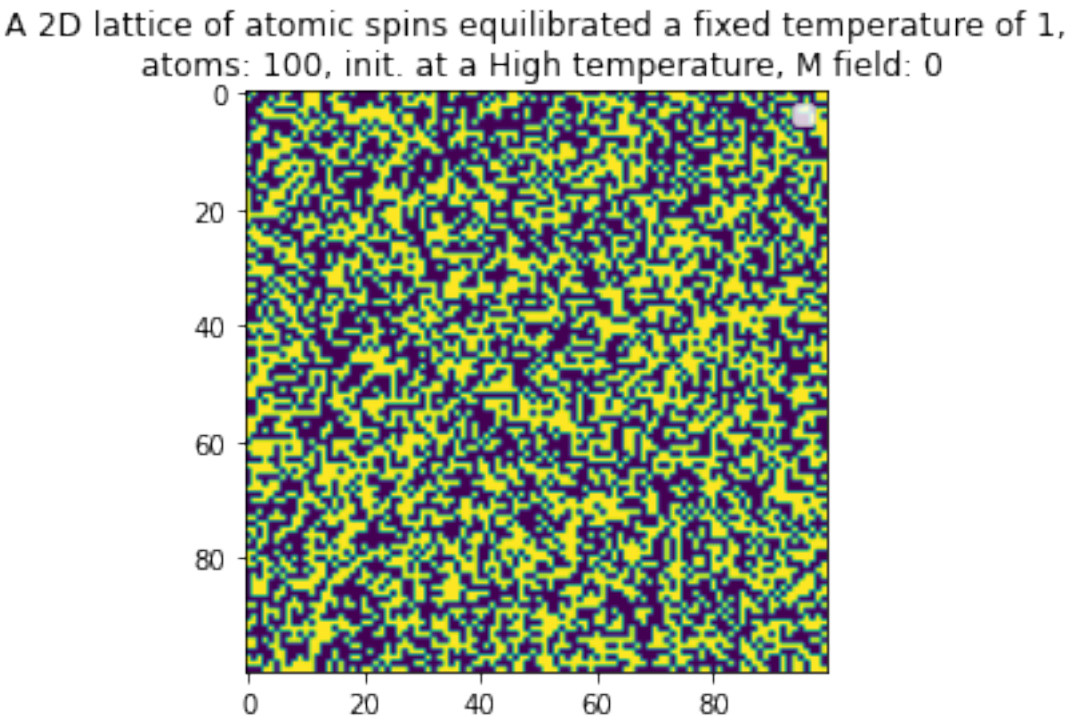
[2]:
```
exp1_cold_demo = model.plots(N=100, start='Low', steps=0)
exp1_cold_demo.lattice()
exp1_cold_demo.show()
```

```
No handles with labels found to put in legend.
```



[3]:
```
exp1_hot_demo = model.plots(N=100, start='High', steps=0)
exp1_hot_demo.lattice()
exp1_hot_demo.show()
```

```
No handles with labels found to put in legend.
```



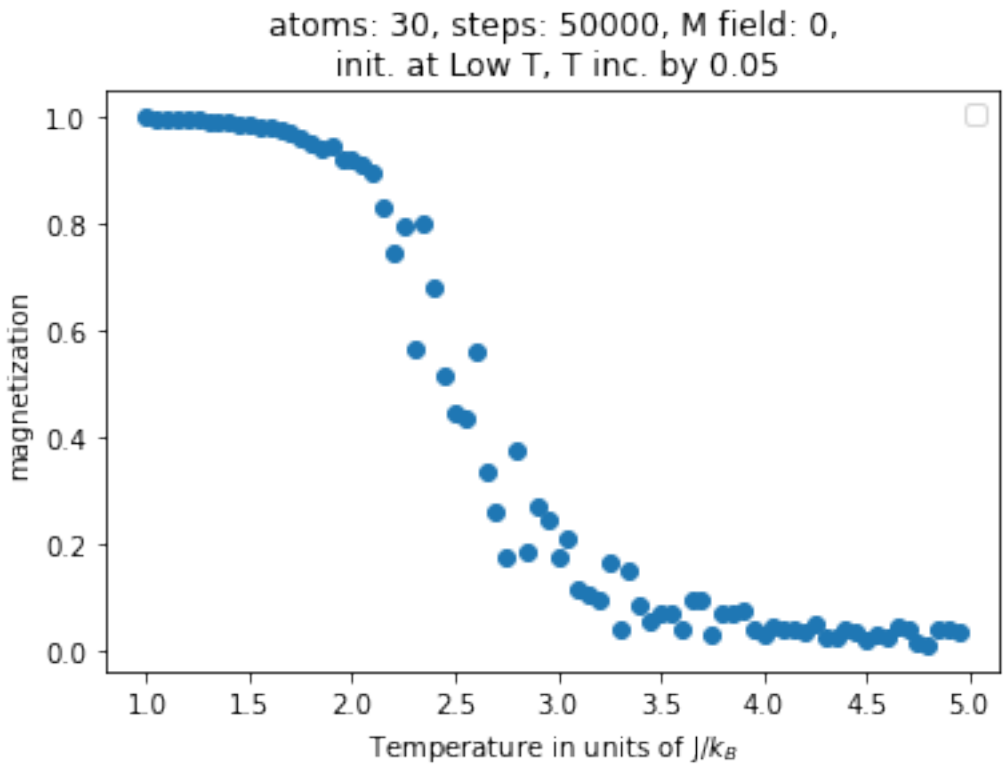
One can observe that the cold start has all spins set to +1 (dark) and the hot start seems to be randomly set.

In the Extensions section however I suggest this may not as random as one might think.

Addressing Question 1. Next I plot the magnetisation vs temperature for 30x30 lattices for both cold and hot starts.

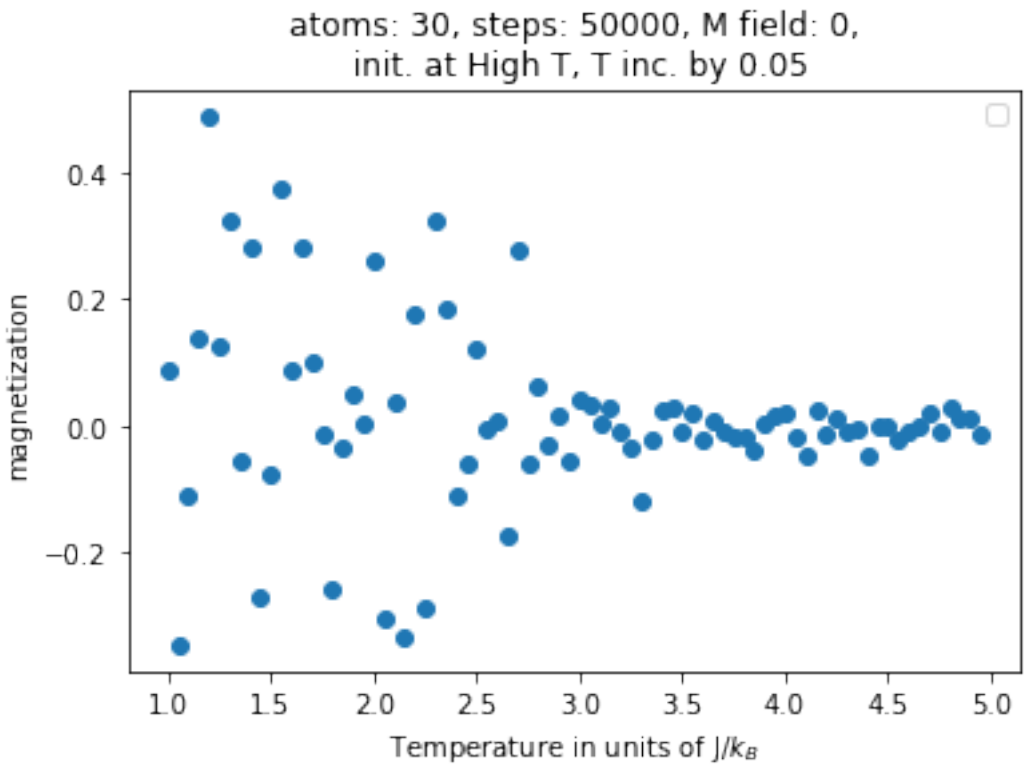
[4]:
```
exp1_cold = model.plots(N=30, start='Low', inc=0.05, x0=1, x1=5, T=1)
exp1_cold.mag()
exp1_cold.show()
```

```
No handles with labels found to put in legend.
```



[5]:
```
exp1_hot = model.plots(N=30, start='High', inc=0.05, x0=1, x1=5, T=1)
exp1_hot.mag()
exp1_hot.show()
```

```
No handles with labels found to put in legend.
```



Comparing the hot and cold starts, it is clear that the initial conditions of the cold start far more strongly defines the initial magnetisation than that of the hot start.

This is because as the model iterates over the Metropolis algorithm for the cold start model, almost no spins flip as it would lead to an increase in the total energy, and those that do flip randomly soon therafter flip back to decrease the total energy. The hot start model however has no clearly defined domains initally and so spins do not settle on an obvious initial equilibrium. One may consider this hot start model as 'highly volatile' in its magnetisation initially.

Of course as the temperature increases, the chaotic nature of the thermal effects dominate and so the magnetisation tends to zero.

Note also for the cold start the transition phase between the ordered and chaotic states, or rather ferromagnetic and paramagnetic states.

2.2 Susceptibility vs Temperature

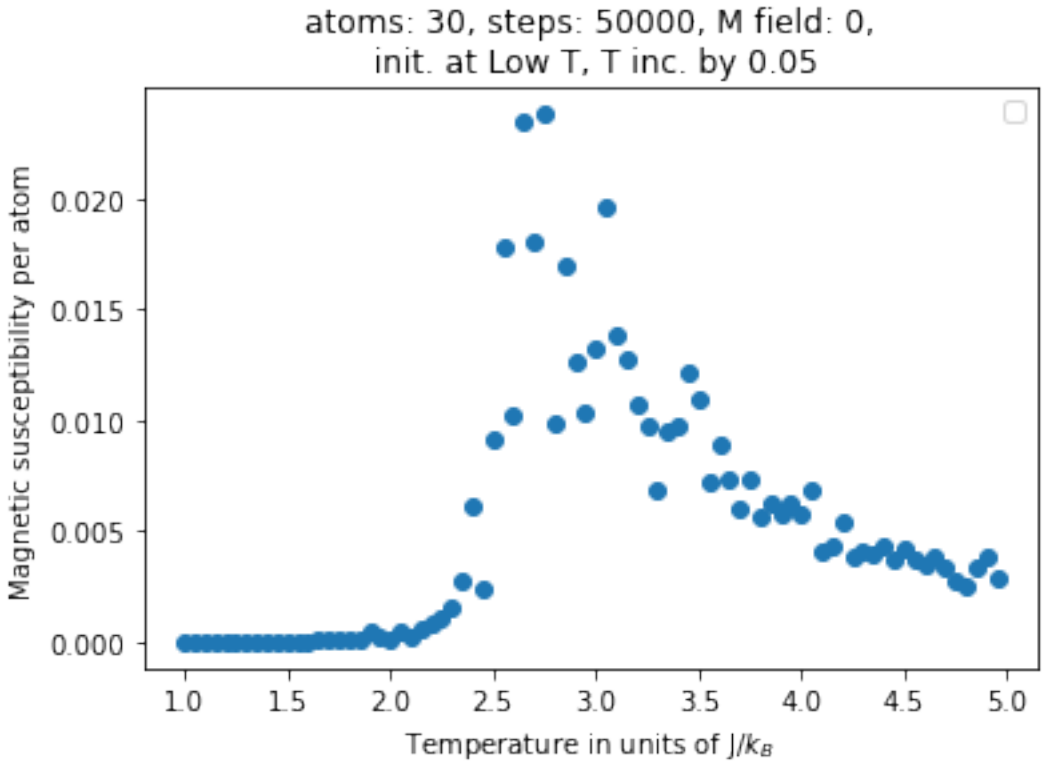
Magnetic susceptibility χ is the ratio of magnetisation to an applied magnetic field. i.e. $\mathbf{M} = \chi\mathbf{H}$.

This may in the context of this model be considered as *how susceptible is the lattice's magnetisation (spin distribution) to an applied magnetic field.* This model calculates this

Here I plot the magnetic susceptibility per atom against temperatue for a cold start for temperatures $T = \{1 : 0.05 : 5\}$.

[6]:
```
exp2 = model.plots(N=30, start='Low', inc=0.05, x0=1, x1=5, T=1)
exp2.mag_sus()
exp2.show()
```

```
No handles with labels found to put in legend.
```



One may observe that initially the suceptibility is zero. This is because all the spins are +1, and so the lattice's magnetisation is highly resistant to change due to an applied magnetic field.

Most importantly however is the magnetic susceptibility peaks at the critical temperature. This may be considered as the point where there is equal influence of ordered domains and chaotic spin distributions, and so an applied magnetic field will have the greatest influence on the final magnetisation.

This critical temperatue of course is a useful value to know, for instance if someone wanted to perform an experiment where the lattice is at maximum magnetisation.

Addressing Question 3. Calculating T_C

The critical temperature is also known as the Curie temperature, which by the Curie Weiss law may describe

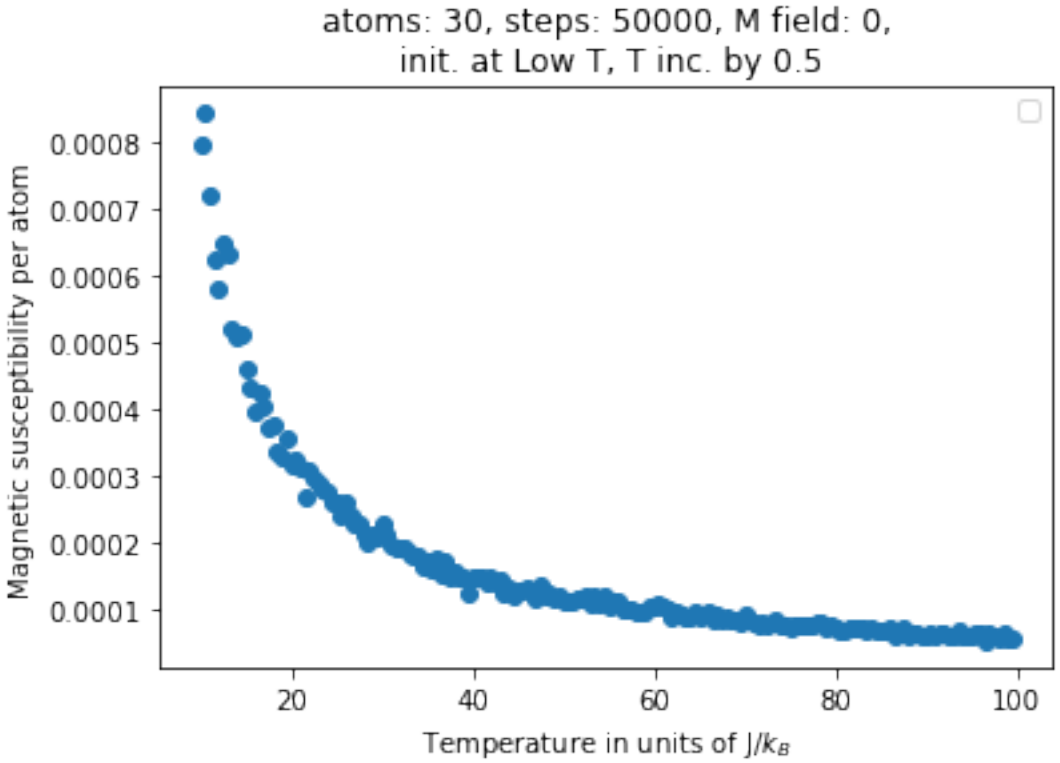
$$\chi = \frac{C}{T - T_C}$$

for $T >> T_C$, where C is the material-specific Curie constant.

From previous plots it is clear $T_C \approx 1.5\, J/k_B$, so what I propose is to curve fit the above equation for the magnetic susceptibility results over $T = [10, 100]$. This will return C and T_C. The uncertainty can be considered as the standard deviation obtained from `curve_fit`'s covariance matrix.

[83]:
```
exp2_T_C = model.plots(N=30, start='Low', inc=0.5, x0=10, x1=100, T=1)
exp2_T_C.mag_sus()
exp2_T_C.show()
```

```
No handles with labels found to put in legend.
```



[91]:
```
from scipy.optimize import curve_fit
import numpy as np

# Function to fit
def curie_weiss_law(T, T_C, C):
    chi = C/(T-T_C)
    return chi

T = np.arange(exp2_T_C.x0, exp2_T_C.x1, exp2_T_C.inc)

params, covar = curve_fit(curie_weiss_law, T, exp2_T_C.data, p0=[2.5, 1]) # Fit␣
 ↪the raw data
```

```
print(f'T_C = {params[0]:.2f} +/- {np.sqrt(covar[0][0]):.2f} J/k_B')
```

```
T_C = 3.44 +/- 0.10 J/k_B
```

So the critical temperature from this method is said to be $T_C = 3.44 \pm 0.10 J/k_B$, which is slightly greater than what might be expected from the previous plot. This may be because this simple model fails to adhere by the Curie-Weiss Law.

Instead opting for the simple method of obtaining T_C from the maximum magnetic susceptibility yields

[99]:
```
T_simple = np.arange(exp2.x0, exp2.x1, exp2.inc)
T_C_simple = T_simple[np.argmax(exp2.data)]
print(f'T_C = {T_C_simple:.2f} +/- {exp2.inc:.2f} J/k_B')
```

```
T_C = 2.40 +/- 0.05 J/k_B
```

where the uncertainty was considered to be the temperature divisions, which of course may be reduced by improving the temperature resolution.

It is hard to settle on the discrepency between these two values and would benefit from further investigation.

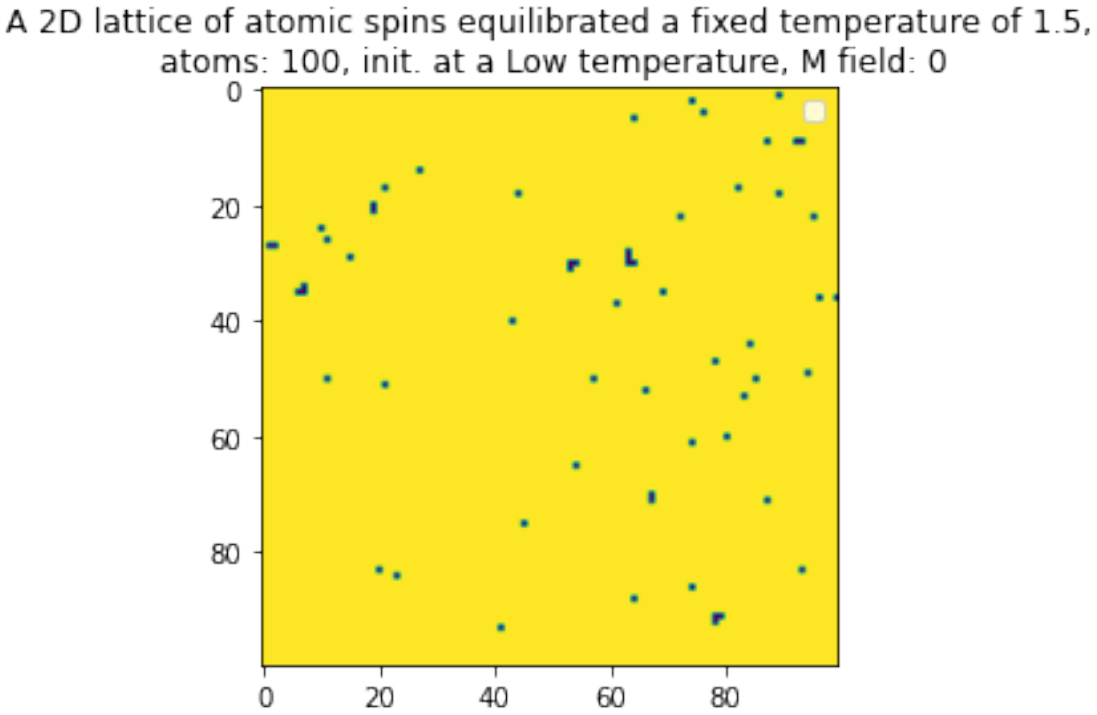
2.3 Spin Distributions and Temperature

Addressing Question 3. Next I plot the spin distributions for both cold and hot starts for temperatures $T = 1.5, 2, 3.5$, and 4.

First let us look at the cold start.

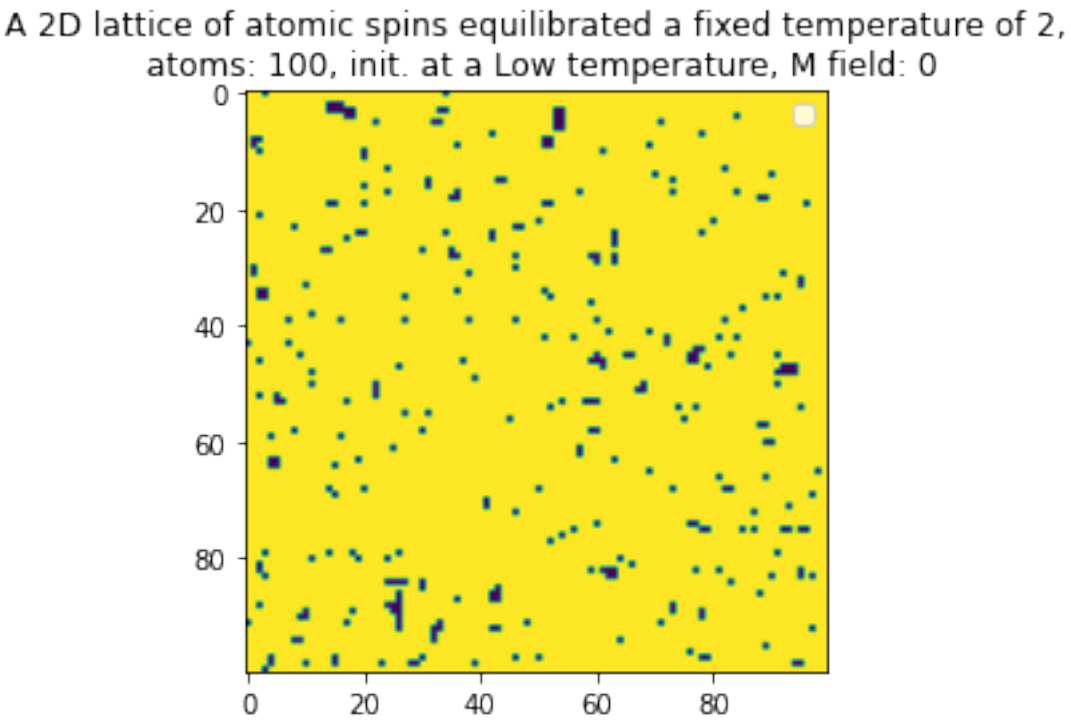
[27]:
```
exp3_cold_1p5 = model.plots(N=100,start='Low',inc=0.1,T=1.5)
exp3_cold_1p5.lattice()
exp3_cold_1p5.show()
```

```
No handles with labels found to put in legend.
```



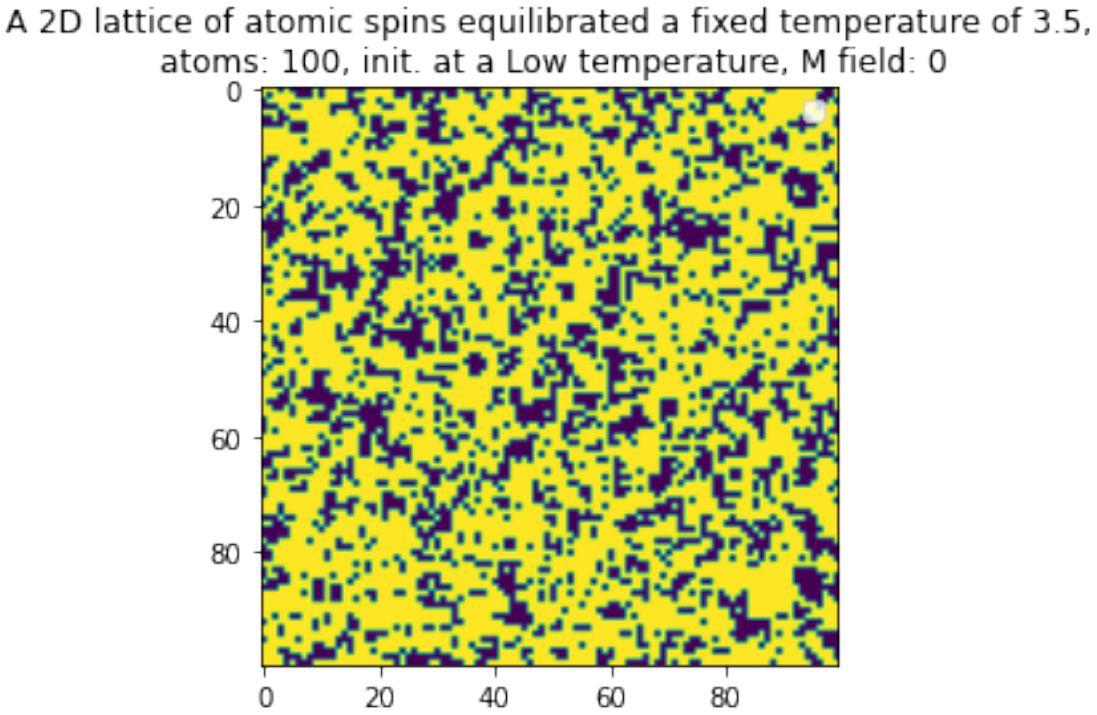
[28]:
```
exp3_cold_2=model.plots(N=100,start='Low',inc=0.1,T=2)
exp3_cold_2.lattice()
exp3_cold_2.show()
```

```
No handles with labels found to put in legend.
```



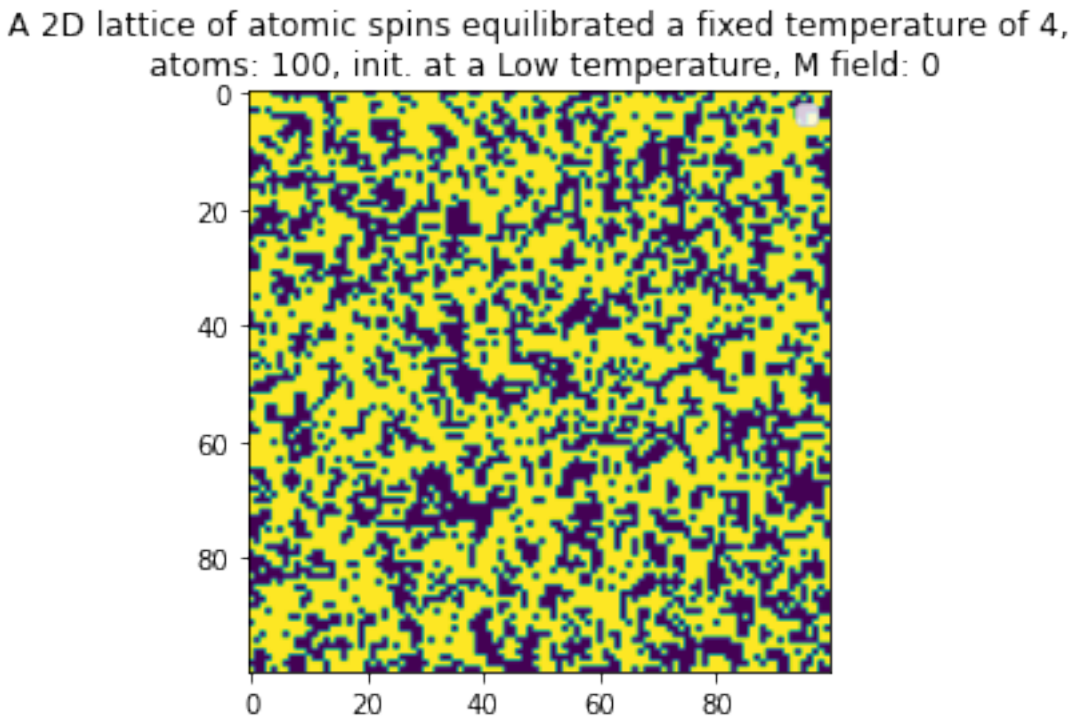
[29]:
```
exp3_cold_3p5=model.plots(N=100,start='Low',inc=0.1,T=3.5)
exp3_cold_3p5.lattice()
exp3_cold_3p5.show()
```

```
No handles with labels found to put in legend.
```



[30]:
```
exp3_cold_4=model.plots(N=100,start='Low',inc=0.1,T=4)
exp3_cold_4.lattice()
exp3_cold_4.show()
```

```
No handles with labels found to put in legend.
```

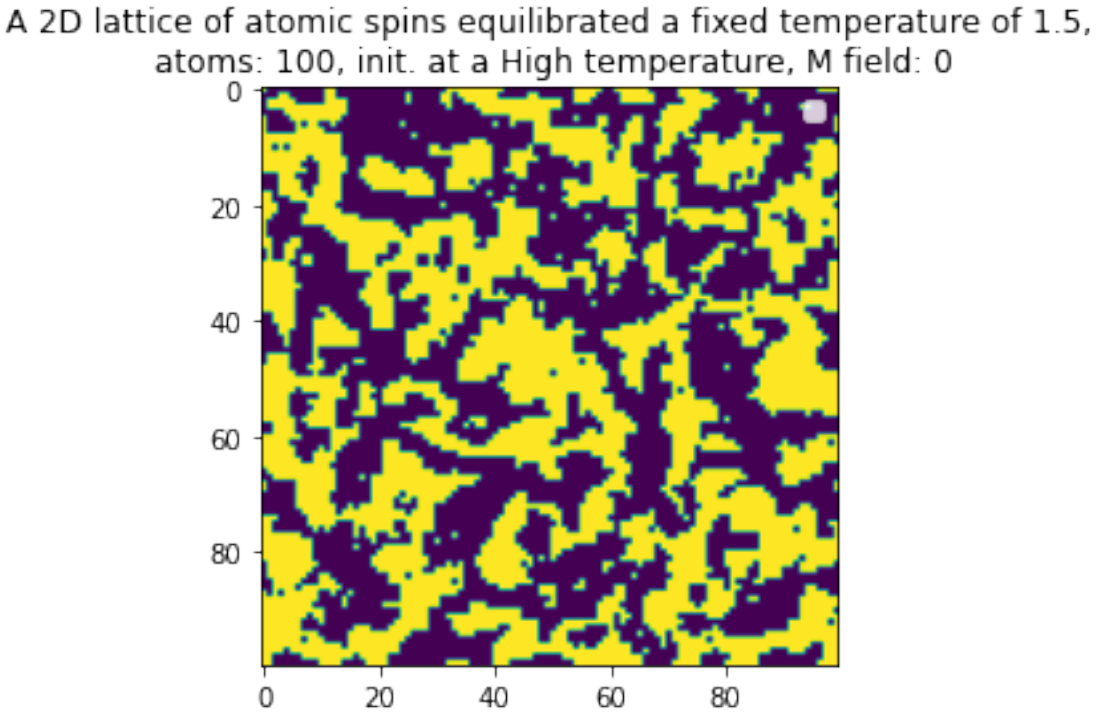


As expected, and illustrated in the Experiment 1, the cold start begins with ultimately all spins +1. As the temperature increases however, the chaotic thermal effects cause spins to become more random, thus breaking up the once ordered, largely homogoneous, domain.

Now looking to the hot start.

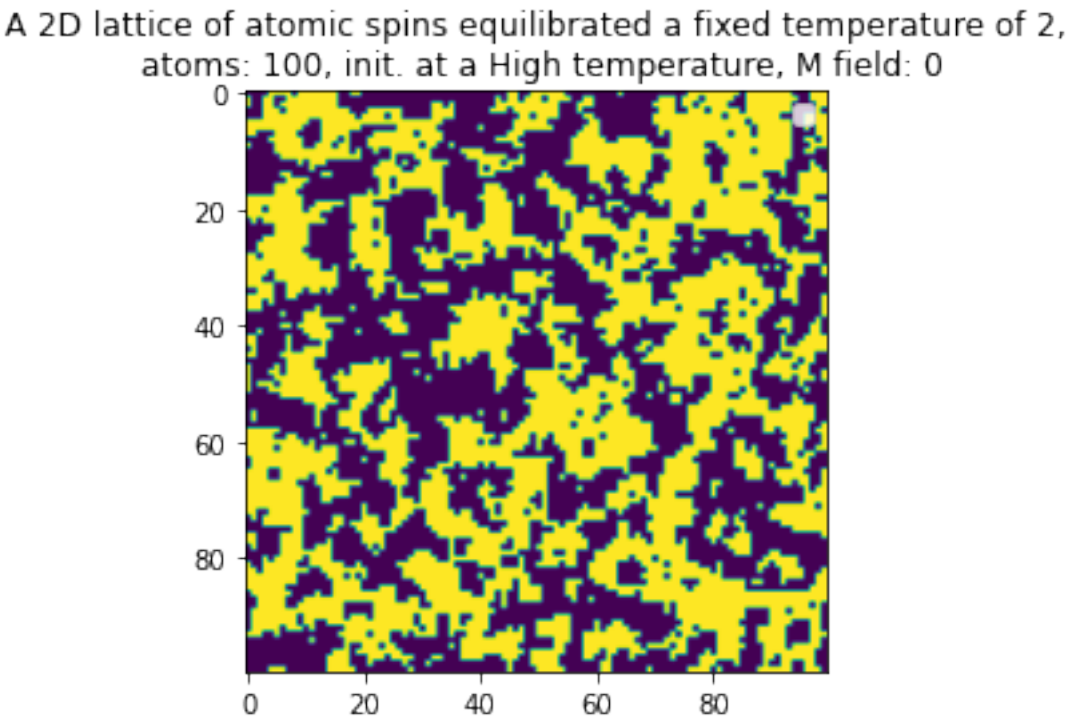
[23]:
```
exp3_hot_1p5=model.plots(N=100,start='High',inc=0.1,T=1.5)
exp3_hot_1p5.lattice()
exp3_hot_1p5.show()
```

```
No handles with labels found to put in legend.
```



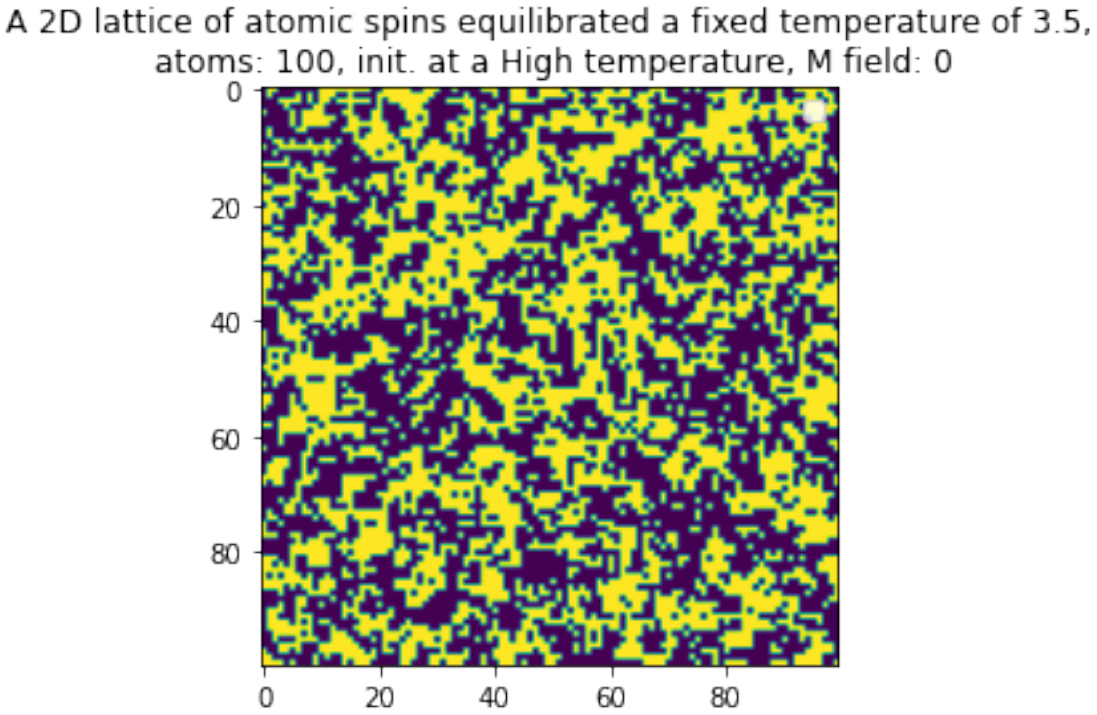
[24]:
```
exp3_hot_2=model.plots(N=100,start='High',inc=0.1,T=2)
exp3_hot_2.lattice()
exp3_hot_2.show()
```

```
No handles with labels found to put in legend.
```



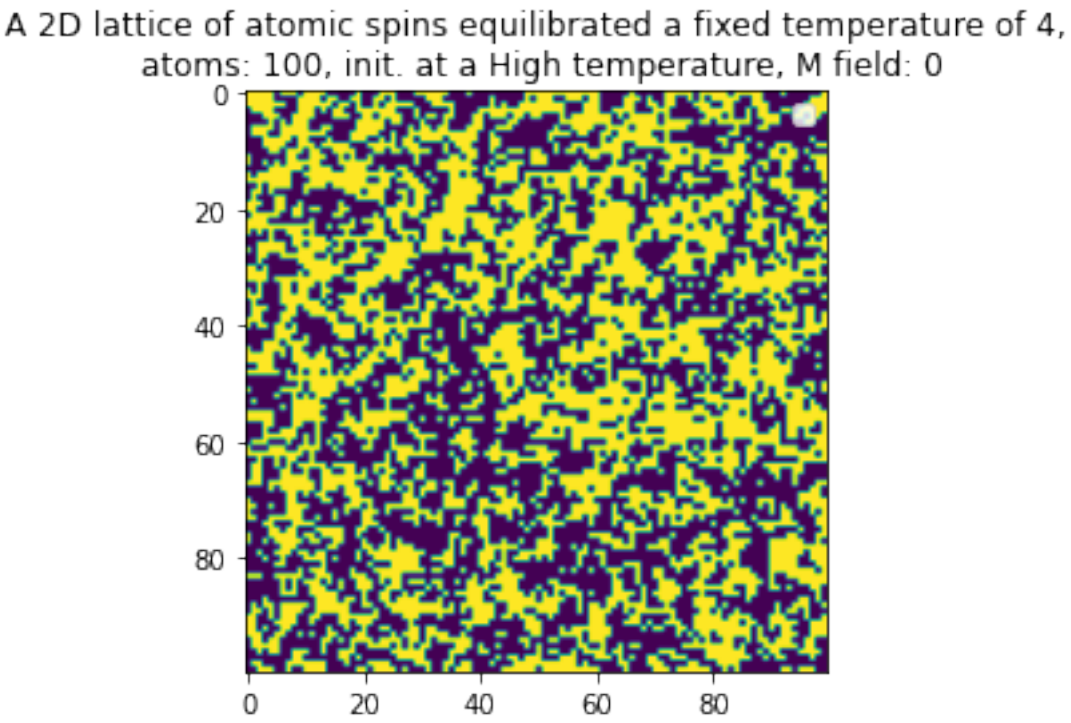
[25]:
```
exp3_hot_3p5=model.plots(N=100,start='High',inc=0.1,T=3.5)
exp3_hot_3p5.lattice()
exp3_hot_3p5.show()
```

```
No handles with labels found to put in legend.
```



[26]:
```
exp3_hot_4=model.plots(N=100,start='High',inc=0.1,T=4)
exp3_hot_4.lattice()
exp3_hot_4.show()
```

```
No handles with labels found to put in legend.
```



At $T = 1.5$ it is clear that the metropolis algorithm infers a state of quasi-equilibrium where domains are established. Similarly to the cold case, as the temperature increases the chaotic thermal effects dominate and break up these established domains.

This accounts for the magnetisation vs temperature plot for the hot start in Experiment 1, whereby the magnetisation approaches zero and the spins are largely random.

In both starts, one can observe an approximate transition phase between ordered domains and chaotic spin distributions. This transition phase occurs at T_C and exhibits maximum magnetic susceptibility.

2.4 External Magnetic Field

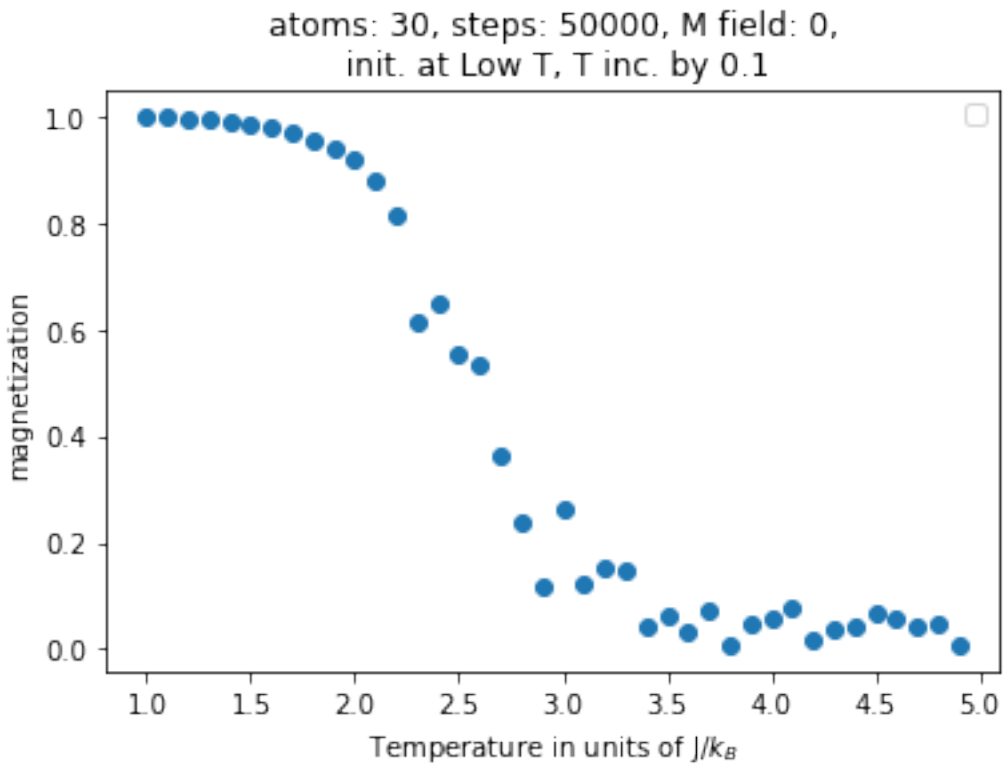
Next I explore the effect of an external magnetic field for a cold start model on the magnetism, susceptibility, and energy, comparing to that with no external field.

First I shall look at magnetic susceptibility.

[70]:
```
exp4_noB=model.plots(N=30,B=0,start='Low',inc=0.1,x0=1,x1=5,T=1)
exp4_withB=model.plots(N=30,B=1,start='Low',inc=0.05,x0=1,x1=5,T=1)
```

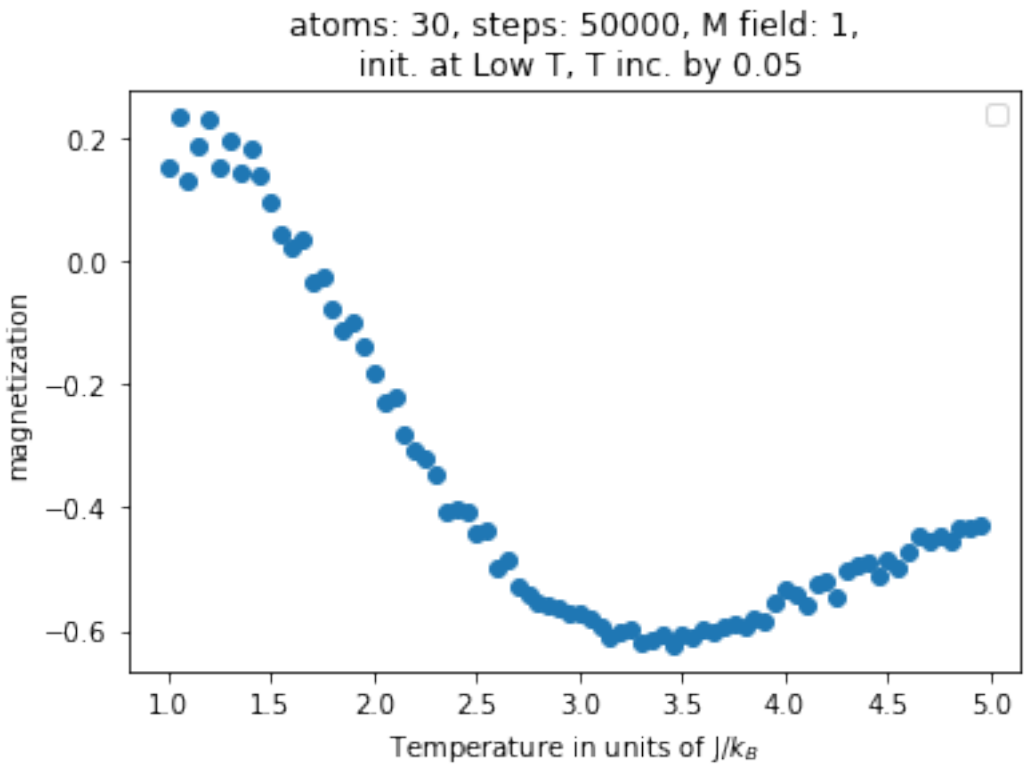
[71]:
```
exp4_noB.mag()
exp4_noB.show()
```

```
No handles with labels found to put in legend.
```



[72]:
```
exp4_withB.mag()
exp4_withB.show()
```

```
No handles with labels found to put in legend.
```

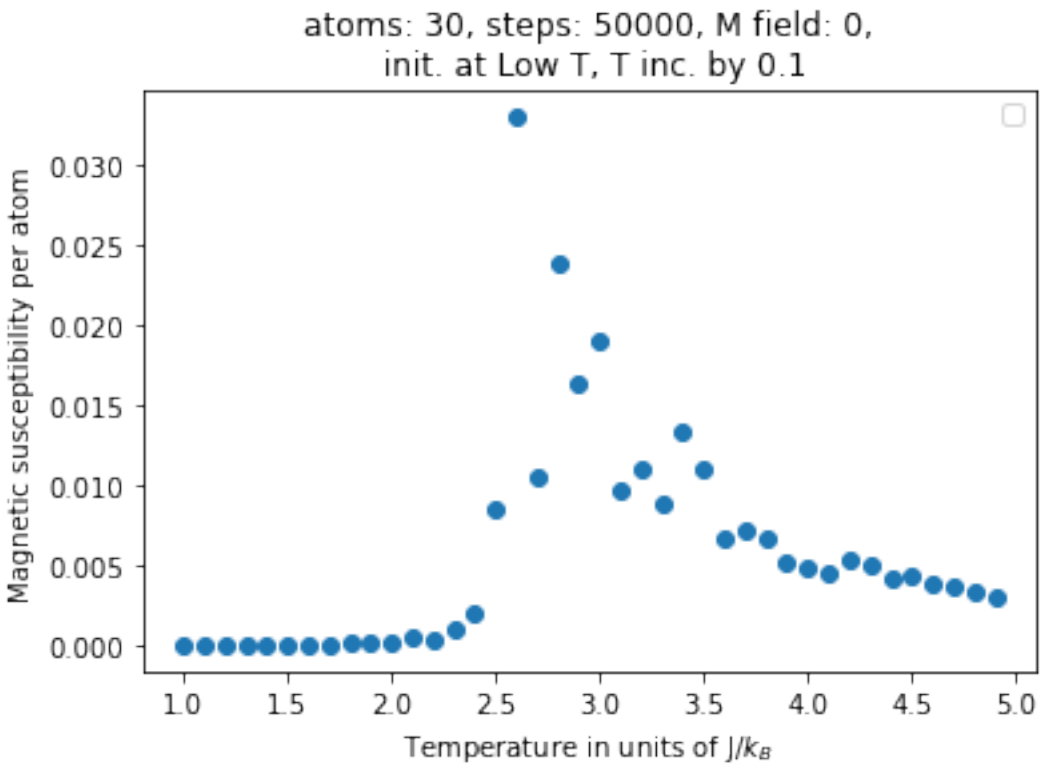


What can be observed is initially the magnetisation is lower than that without an external field. It continues to become more negative reaching a maximum negative magnetisation slightly past the critical temperature, where it has the greatest magnetic susceptibility. Further on of course chaotic thermal effects dominate and magnetisation approaches zero.

Even more interesting is the effect on magnetic susceptibility:

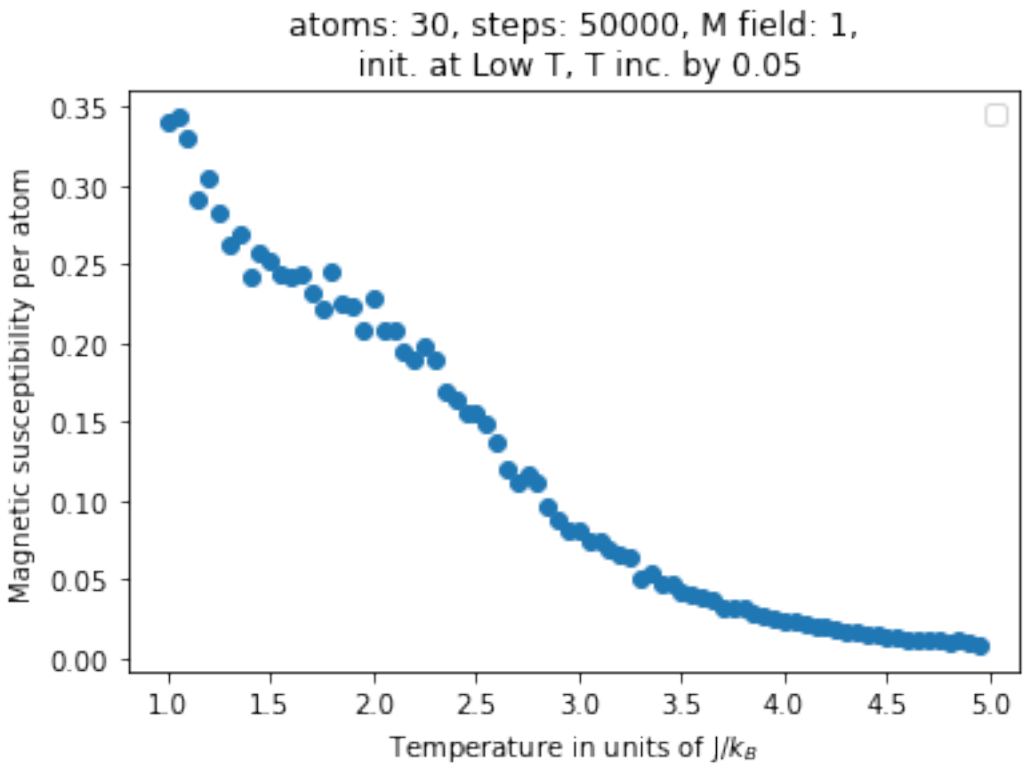
[73]:
```
exp4_noB.mag_sus()
exp4_noB.show()
```

```
No handles with labels found to put in legend.
```



[74]:
```
exp4_withB.mag_sus()
exp4_withB.show()
```

```
No handles with labels found to put in legend.
```

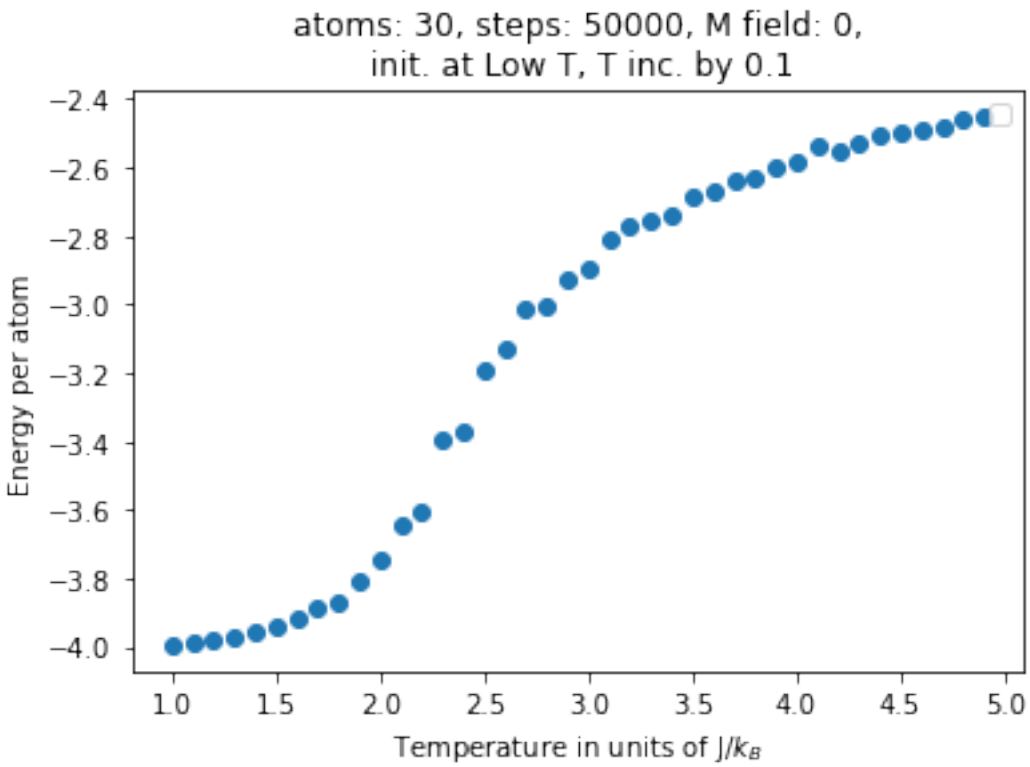


Magnetic susceptibility is seen to be a maximum at low temperatures with an applied magnetic field, as opposed to that without. As expected it soon approaches zero when $T > T_C$.

Next looking at energy per atom:

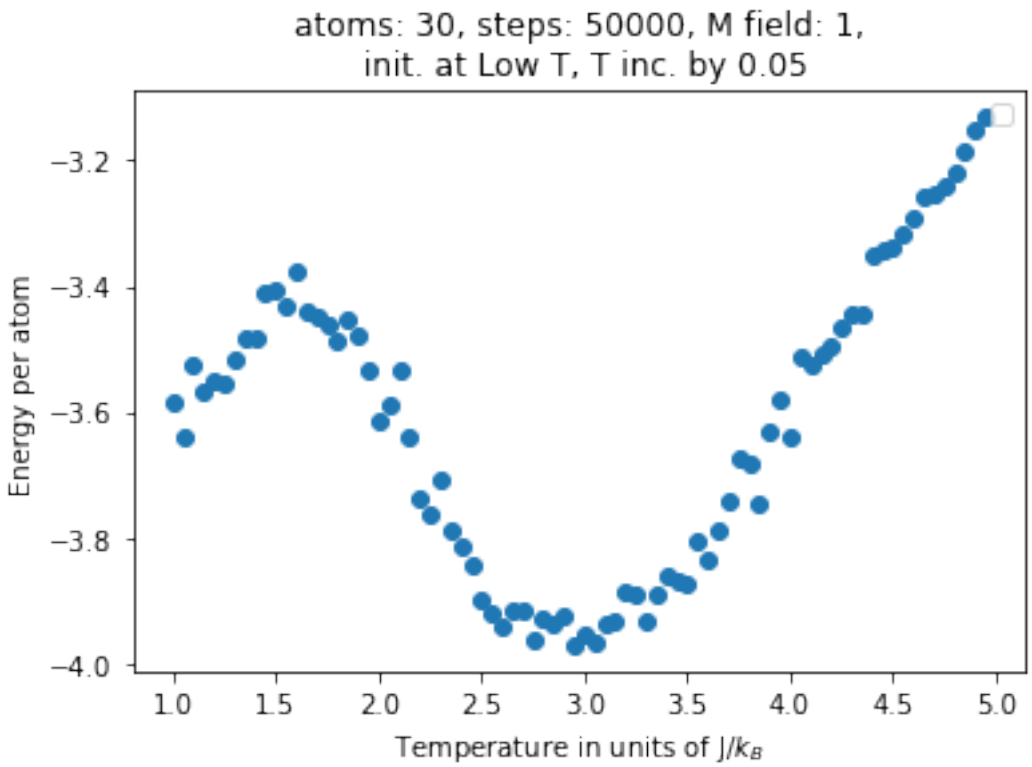
[75]:
```
exp4_noB.E()
exp4_noB.show()
```

```
No handles with labels found to put in legend.
```



[76]:
```
exp4_withB.E()
exp4_withB.show()
```

```
No handles with labels found to put in legend.
```



For both cases of course energy increases as thermal energy (temperature) increases. Aside from this, energy per atom is greater initially with an applied magnetic field and reaches a minimum where approximately where the magnetisation was seen to be most significant.

3 Further Experiments

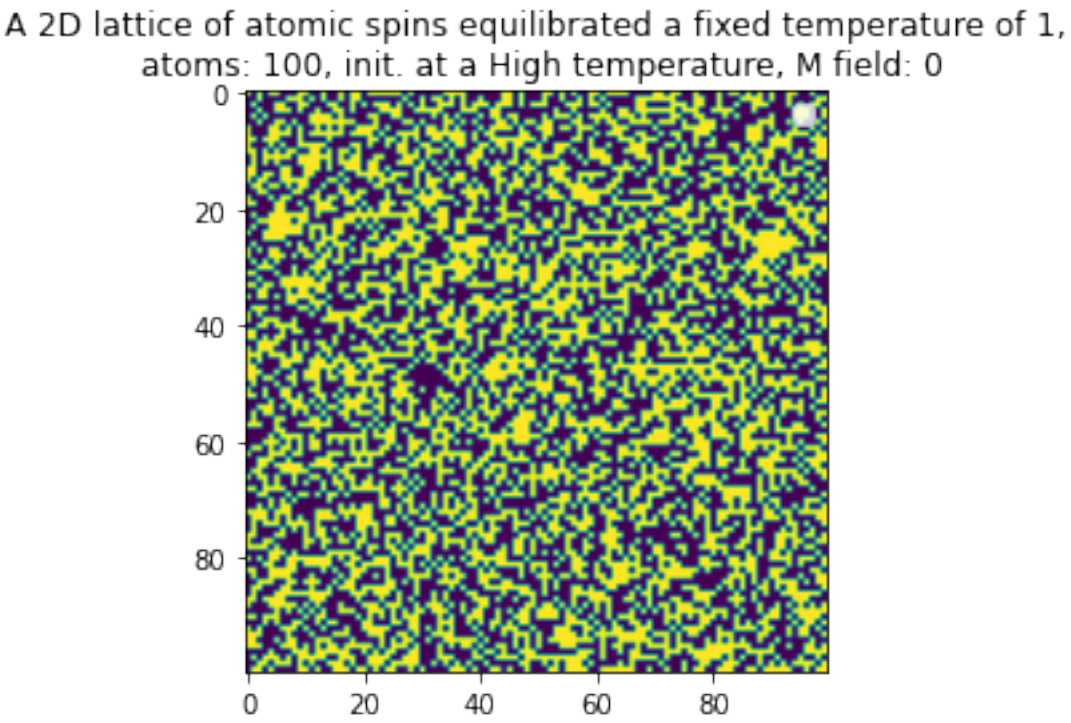
3.1 Is the initial state truly random?

It is accepted that no random number is *truly* random when obtained from a deterministic machine such as the laptop I ran this Jupyter Notebook on. One must assume (or hope) however that the random numbers supplied are 'as random as required'.

So it is interesting to investigate the two following spin distribution maps for hot starts, no metropolis steps, and at two different sizes, 100x100 and 200x200.

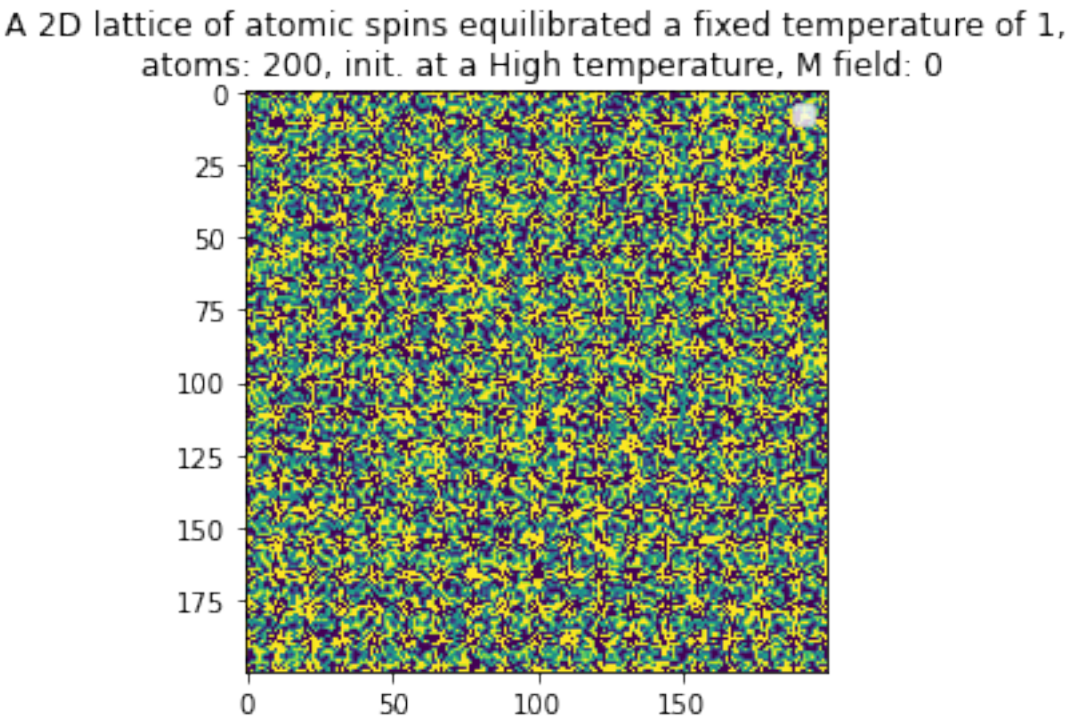
[36]:
```
ext1_100 = model.plots(N=100, start='High', steps=0)
ext1_100.lattice()
ext1_100.show()
```

```
No handles with labels found to put in legend.
```



[42]:
```
ext1_200 = model.plots(N=200, start='High', steps=0)
ext1_200.lattice()
ext1_200.show()
```

```
No handles with labels found to put in legend.
```



While the 100x100 case looks to be largely random, a distinct grid-like pattern emerges for the 200x200 case. This is strongly suggests that some sort of pattern is arising in the initial spin distributions for the hot start case (obtained using Python's `random.choice()` function). Even if you run this cell over and over again, the same pattern emerges.

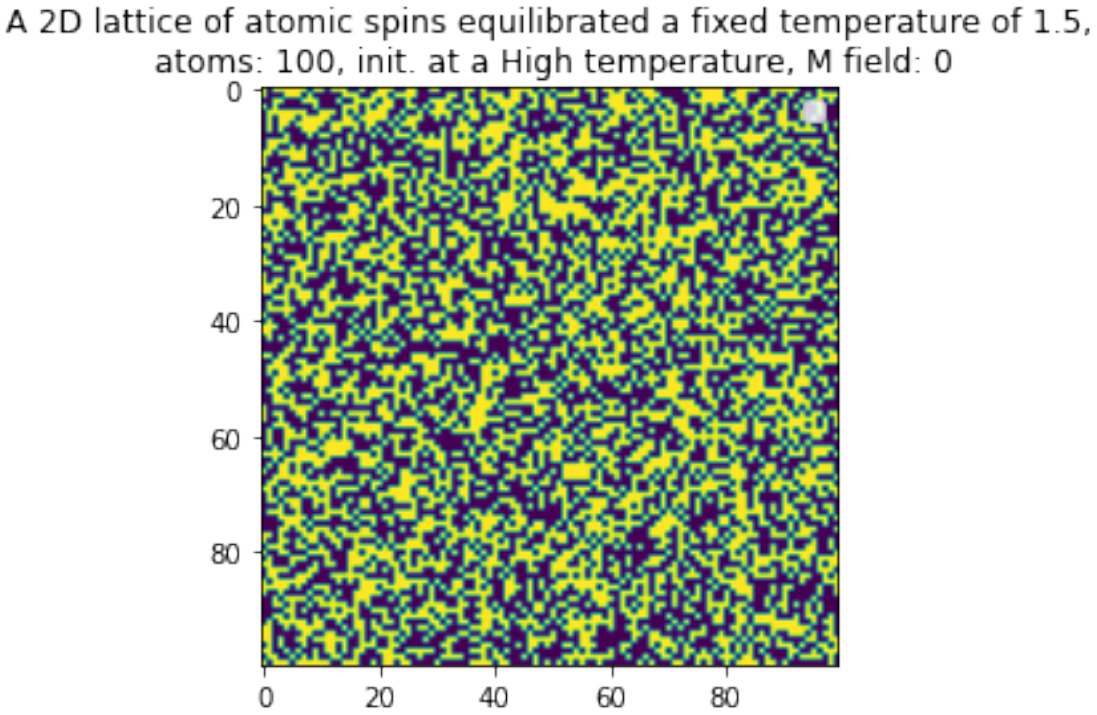
This is interesting to consider as though the initial conditions for a hot start have an obvious pattern emerging, the further randomness associated with the metropolis algorithm would essentially resolve all unintended consequences of this somewhat predictable initial conditions.

3.2 Effect of increasing metropolis steps on spin distribution

What is also interesting is observing the effect increasing the number of metropolis steps performed has on spin distribution for a hot start at low temperature. Here I plot the spin distribution for `steps = 0, 10000,` and `1000000`.

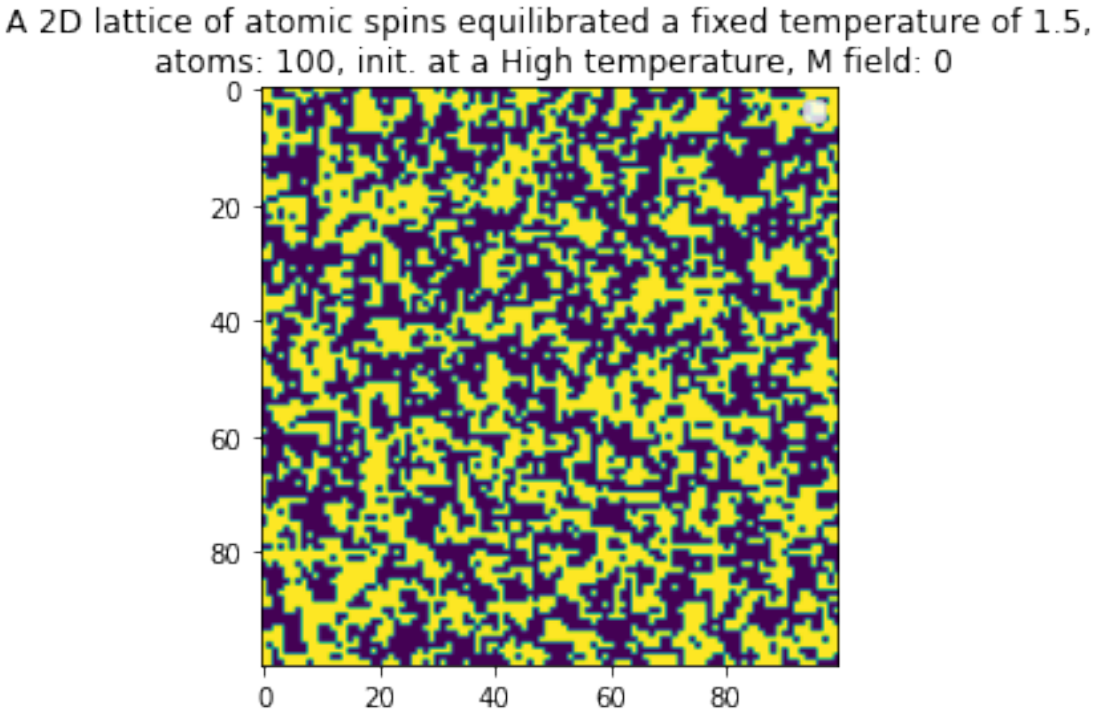
[79]:
```
ext2_a=model.plots(N=100,start='High',inc=0.1,steps=0,T=1.5)
ext2_a.lattice()
ext2_a.show()
```

```
No handles with labels found to put in legend.
```



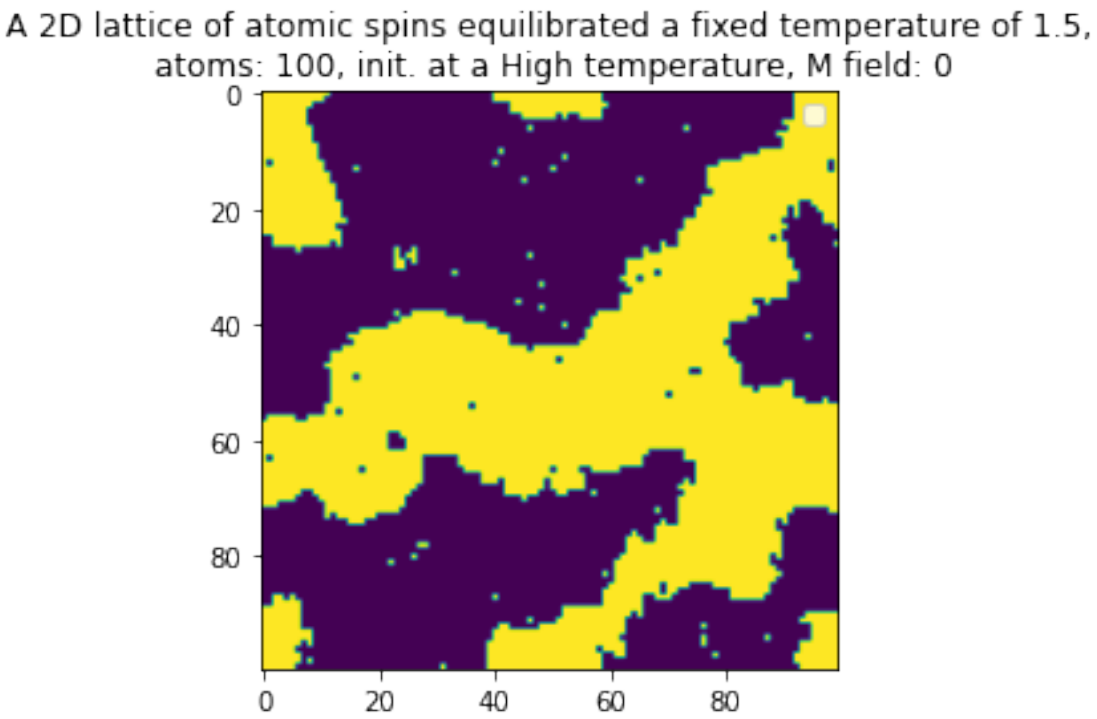
[80]:
```
ext2_b=model.plots(N=100,start='High',inc=0.1,steps=10000,T=1.5)
ext2_b.lattice()
ext2_b.show()
```

```
No handles with labels found to put in legend.
```



[81]:
```
ext2_c=model.plots(N=100,start='High',inc=0.1,steps=1000000,T=1.5)
ext2_c.lattice()
ext2_c.show()
```

```
No handles with labels found to put in legend.
```



It is observed that, as expected, the longer the model performs the Metropolis, the more the magnetic domains form. Ultimately if enough steps were to be performed, the entire lattice would have spin either $+1$ or -1, dependent on the inital conditions.

4 Conclusion

In conclusion, the Ising Model offers a particularly interesting perspective on the case of atomic lattices and their magnetic behaviours. Particularly the critical temperature T_C which I suggest a powerful way to obtain through fitting with the Curie-Weiss Law.

The discrepency between the Cure-Weiss Law T_C and maximum magnetic susceptibility T_C may be due to the idealisation of the model, but would benefit from further investigation.

I also investigated the effects of Metropolis steps, temperature, and starting conditions, have on the measurables of magnetisation, magnetic susceptibility, energy, and spin distribution.