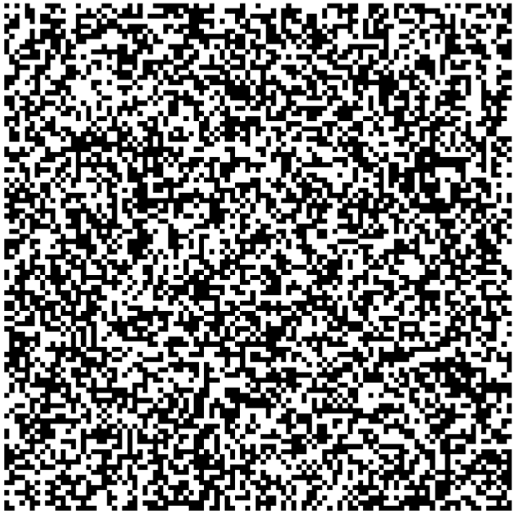
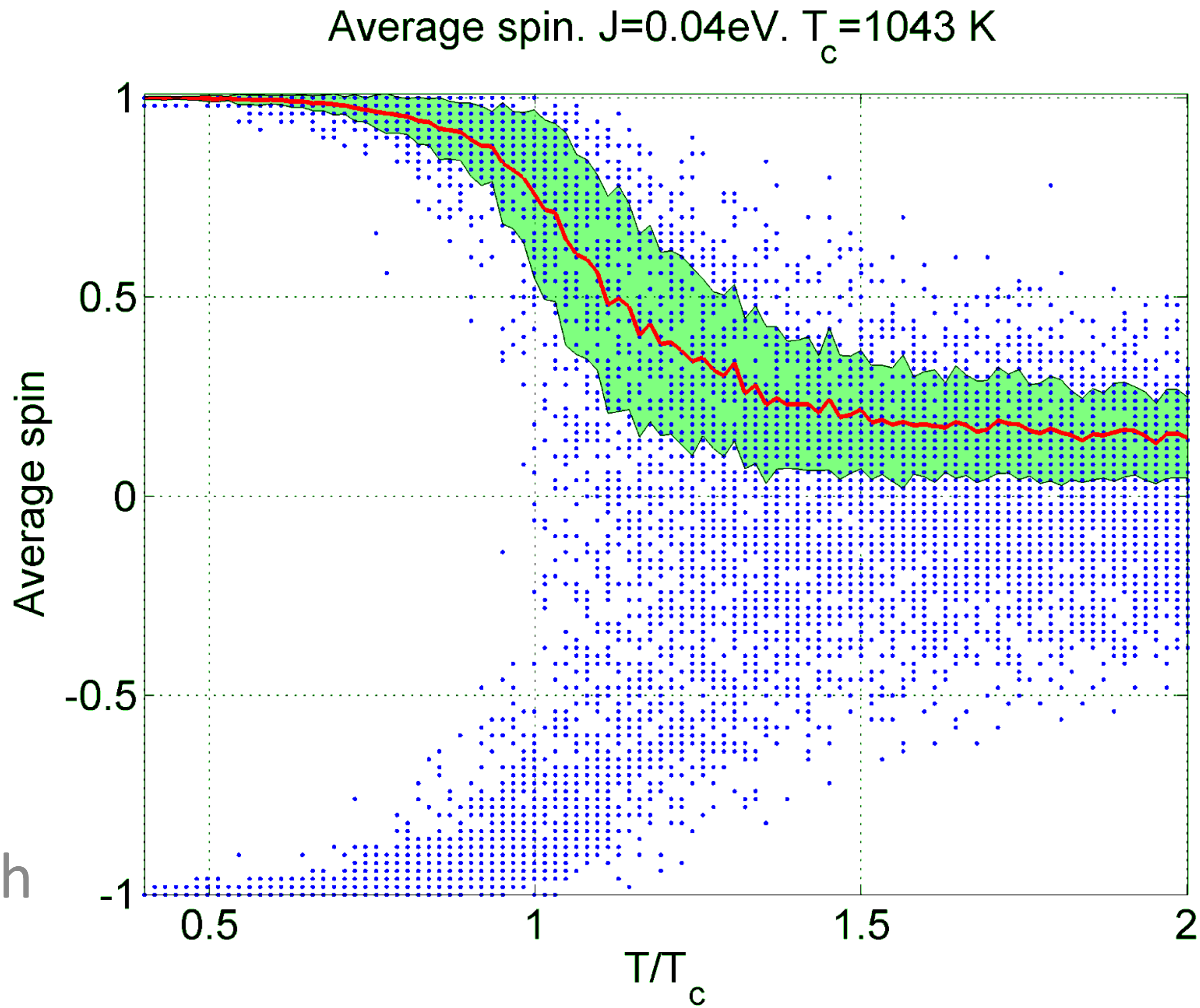
The Ising model of Ferromagnetism





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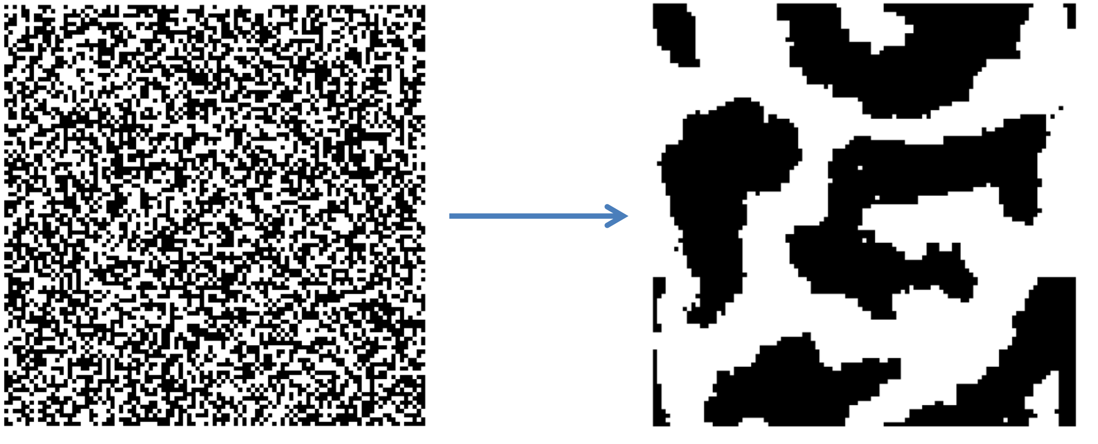
The Ising Model of Ferromagnetism

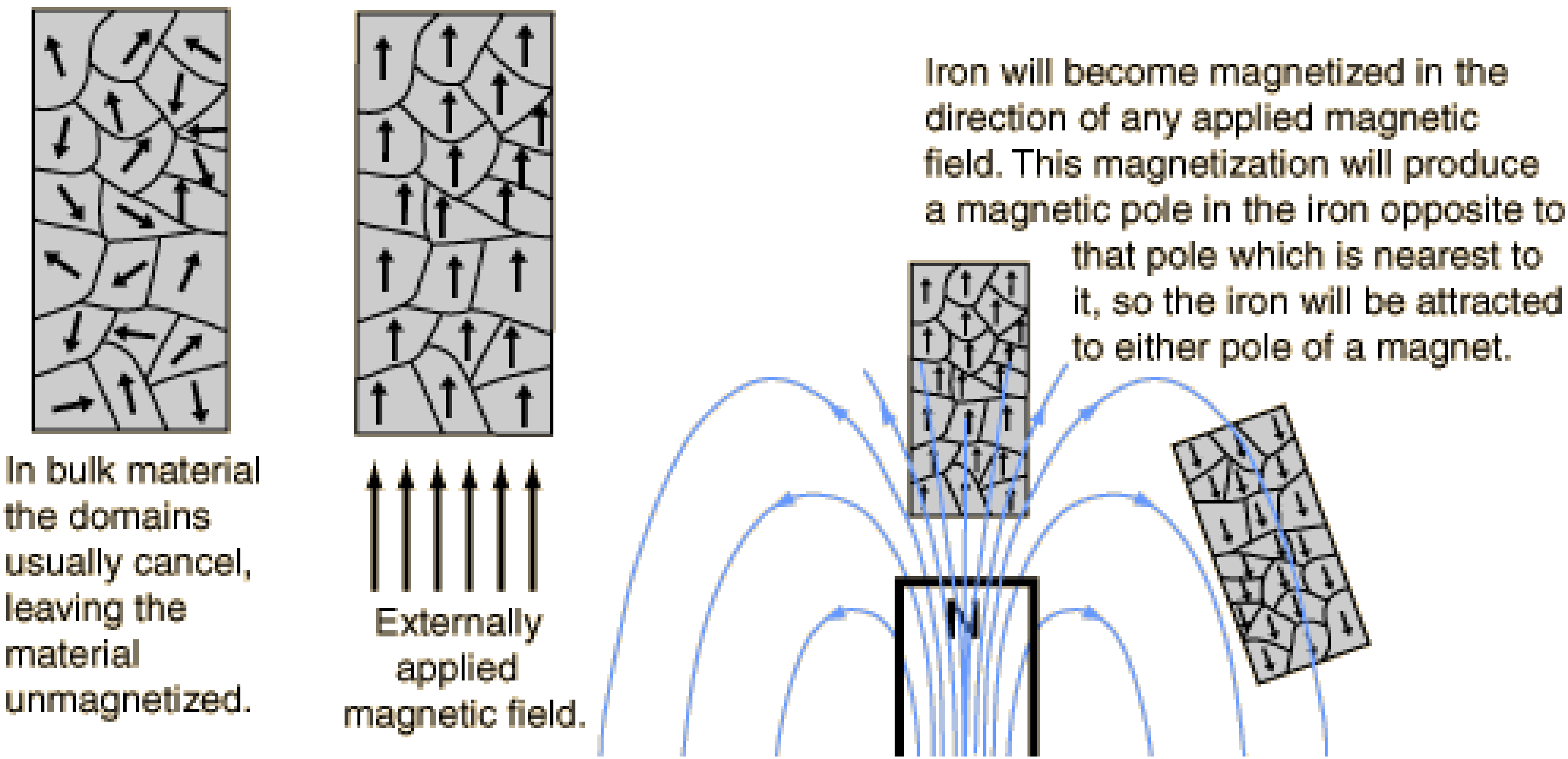
All atoms will respond in some fashion to **magnetic fields.** The angular momentum (and spin) properties of electrons imply a circulating charge, which means they will be subject to a Lorentz force in a magnetic field. **However the effects of *diamagnetism, paramagnetism* and *anti-ferromagnetism* are typically very small. Ferromagnetic materials** (iron, cobalt, nickel, some rare earth metal compounds) respond strongly to magnetic fields and can intensify them by orders of magnitude. i.e. the *relative permeability* can be tens or hundreds, or possibly thousands.

The Ising model is a simplified model of a **ferromagnet** which exhibits a **phase transition** above the **Curie temperature**. Below this, magnetic dipole alignment will tend to cluster into **domains**, and its is these micro-scale groupings which give rise to ferromagnetic behaviour.

Ernst Ising (1900-1998)

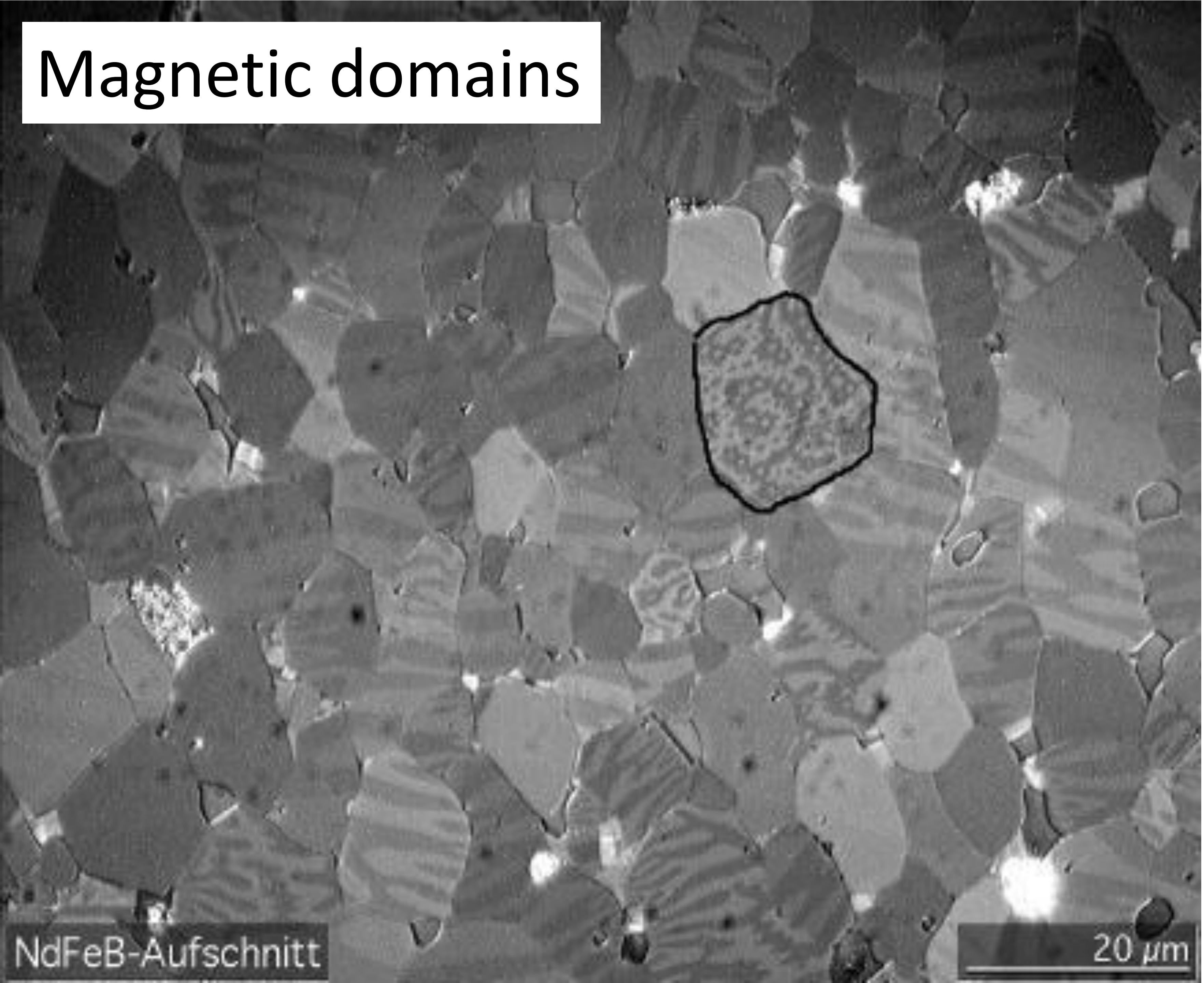


“Soft” magnetism - Ferromagnets



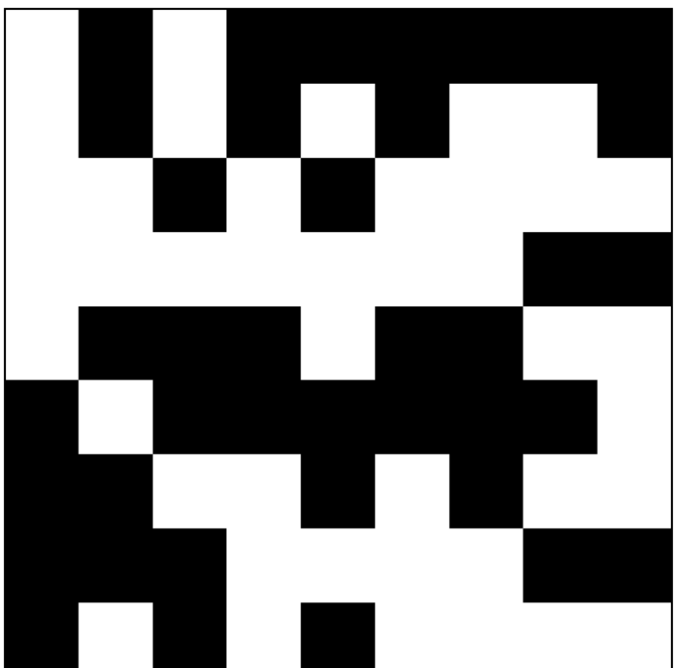
Unlike permanent “hard” magnets, once the applied field is removed, the domain alignment will randomize again, effectively zeroing the net magnetism.

Magnetic domains



The **Ising model** can be used to demonstrate spontaneous mass alignment of magnetic dipoles, and possibly a mechanism for domain formation.

Perhaps the simplest model which yields characteristic behaviour is an *N* x *N* square grid, where each square is initially randomly assigned a +1 or -1 value, with equal probability. The +/-1 values correspond to a single direction of magnetic dipole moment in a rectangular lattice of ferromagnetic atoms, or in the case of individual electrons, *spin*.



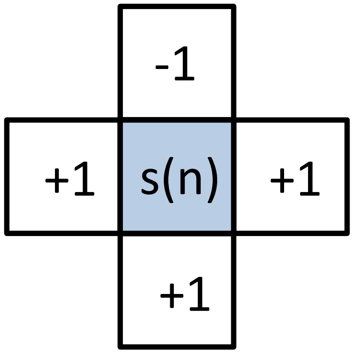
10 x 10 grid

White squares represent +1
Black squares represent -1

100 x 100 grid

Original Metropolis algorithm

1. Choose one square at random from the N x N grid. Let its spin be s(n) = +1 or -1.
2. Find the spins of the nearest neighbours. Use *circular boundary conditions* e.g. if s(n) is at the edge of the grid, use the nearest neighbour to be that of the other end.



3. Compute a sum of **spin-coupling energies** for s(n) and its neighbours, and work out the energy change if s(n) were to **change sign**

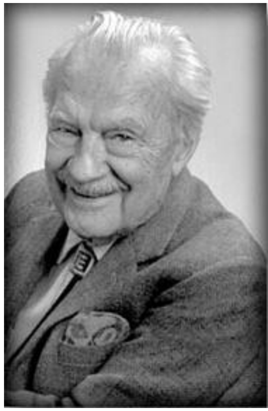
$$\Delta E = 2 \times \left(F + J \sum_{k=1}^{4} s_n(k) \right) s(n)$$

J is the spin coupling energy in eV and F is the energy in eV associated with the alignment of spin s(n) with an applied external magnetic field. Let us ignore any energy contributions from non-nearest neighbours.

$$r \sim \mathrm{U}(0,1)$$

Now change the sign of spin s(n) according to the following rule:

$$s(n) \to -s(n) \quad \text{if} \quad e^{-\frac{\Delta E}{k_B T}} \geq r \quad \text{or} \quad \Delta E < 0$$



Nicholas Metropolis 1915-1999

Apply the Metropolis method for I x N x N iterations, and then compute from the N x N grid the following parameters

$$\langle s \rangle = \frac{1}{N^2} \sum_{n=1}^{N^2} s(n)$$

Mean spin

$$\langle E \rangle = -\tfrac{1}{2} \frac{1}{N^2} \sum_{n=1}^{N^2} \left(J \sum_{k=1}^{4} s_n(k) + F \right) s(n)$$

Mean energy per spin

$$k_B T^2 \langle C \rangle = \tfrac{1}{4} \frac{1}{N^2} \sum_{n=1}^{N^2} \left(J s(n) \sum_{k=1}^{4} s_n(k) + F s(n) \right)^2 - \langle E \rangle^2$$

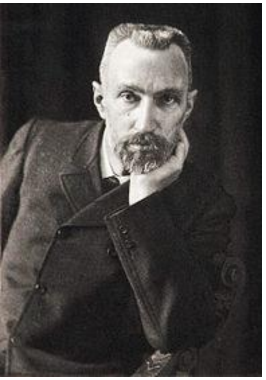
Heat capacity in eV per K

This is a well known result in Statistical Thermodynamics

$$\boxed{k_B T^2 \langle C \rangle = \mathrm{Var}\left[E \right]}$$

For a 2D Ising model, Lars Onsager determined in 1944 the relationship between the phase transition Curie temperature and coupling energy J

$$\boxed{\frac{2J}{\ln\left(1+\sqrt{2}\right)} = k_B T_C}$$

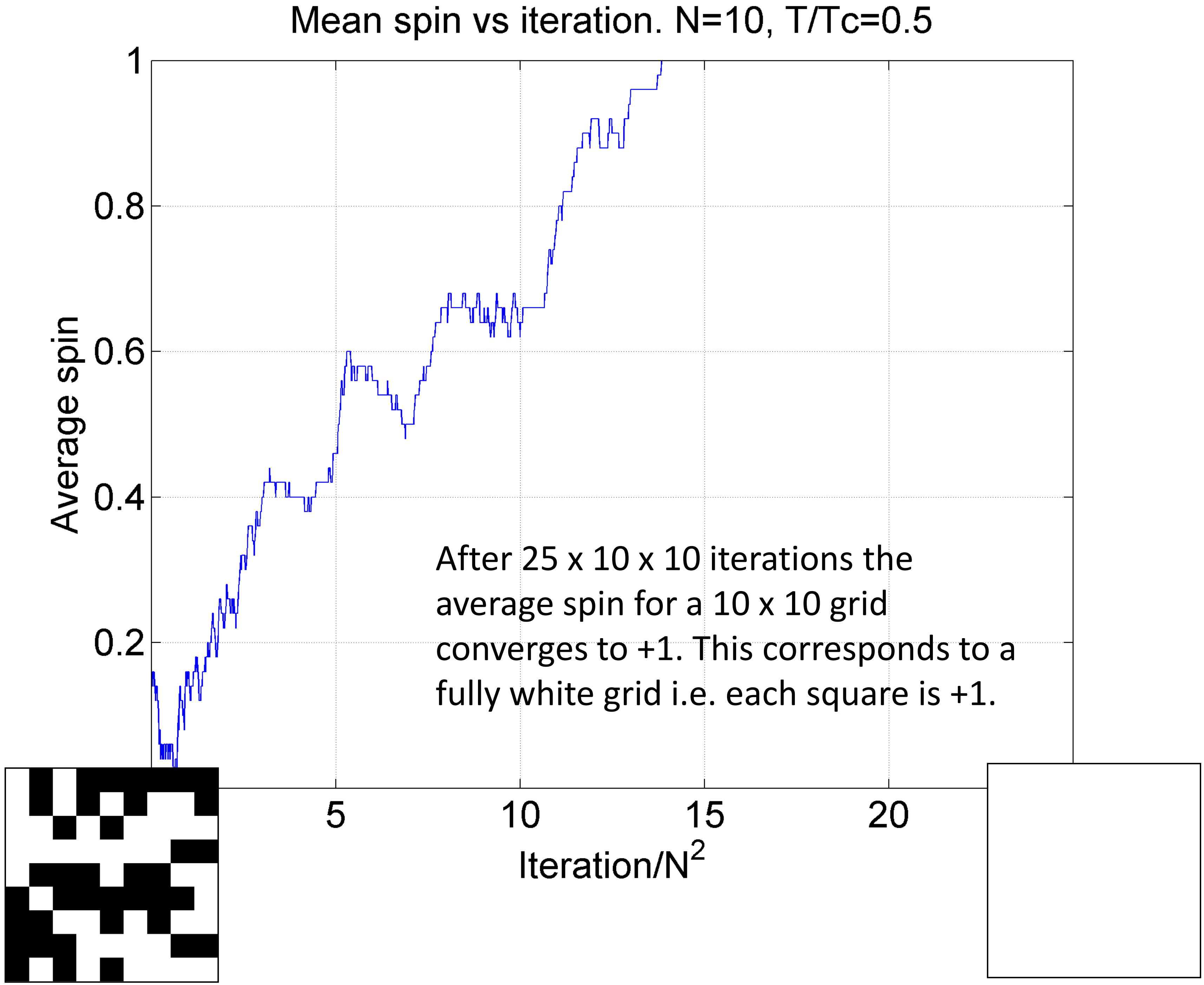


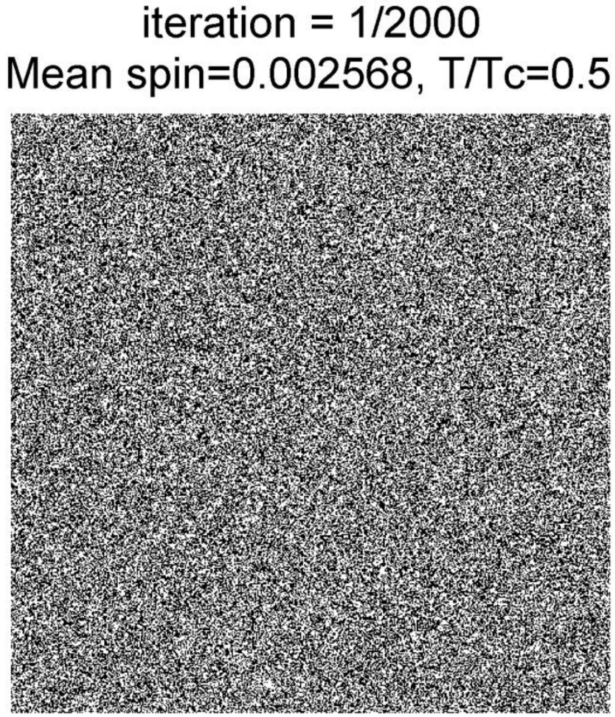
Peter Curie
(1859-1906)

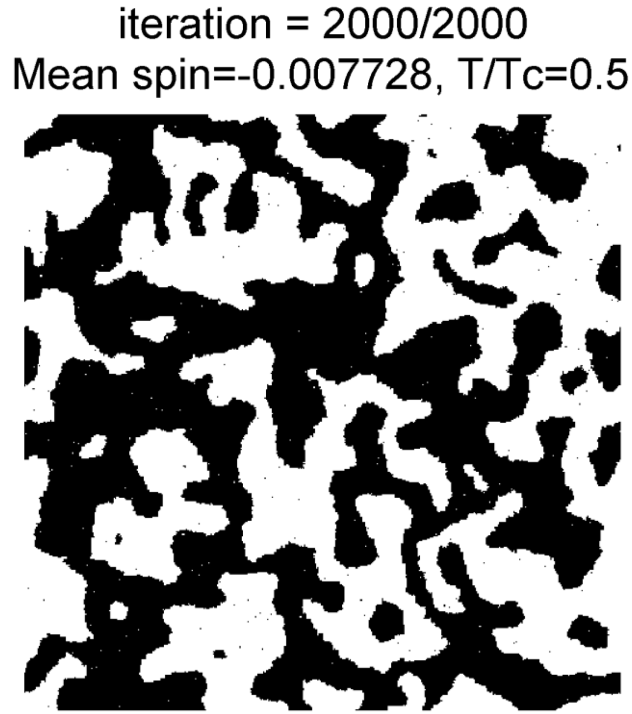
(Note this expression assumes coupling energy J is in joules)

Boltzmann's constant
$k_B = 1.38 \times 10^{-23}\ \mathrm{JK}^{-1}$

Lars Onsager
(1903-1976)

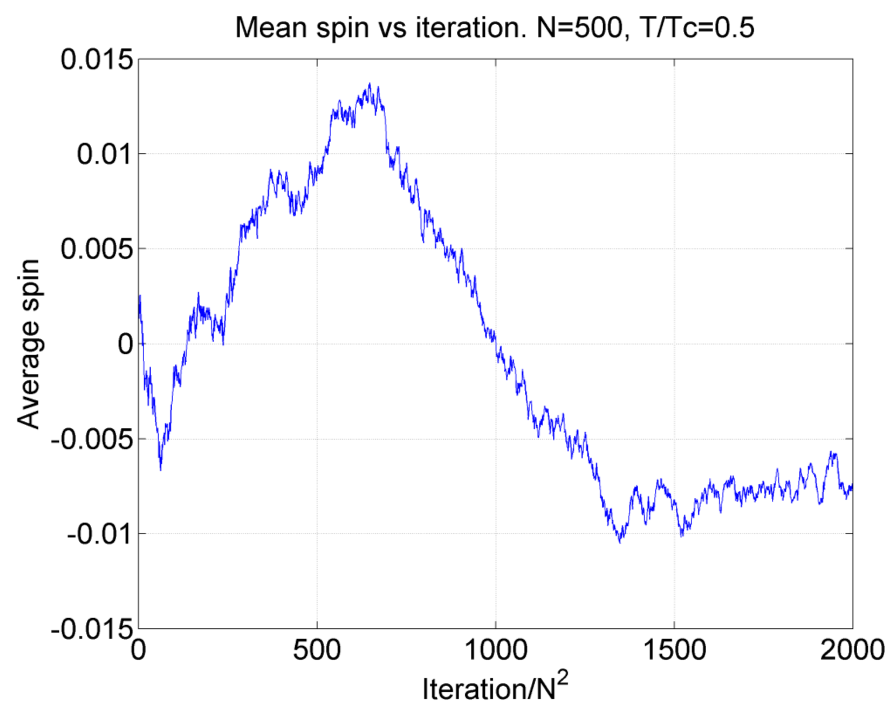

Mean spin vs iteration. N=10, T/Tc=0.5
Average spin
Iteration/N^2
0.2
0.4
0.6
0.8
1
5
10
15
20
After 25 x 10 x 10 iterations the average spin for a 10 x 10 grid converges to +1. This corresponds to a fully white grid i.e. each square is +1.





For a 500 x 500 grid, a similar equilibrium is not yet reached, even after I = 2000 x 500 x 500 iterations.

However, domain-like structures are clearly visible in this intermediate state.

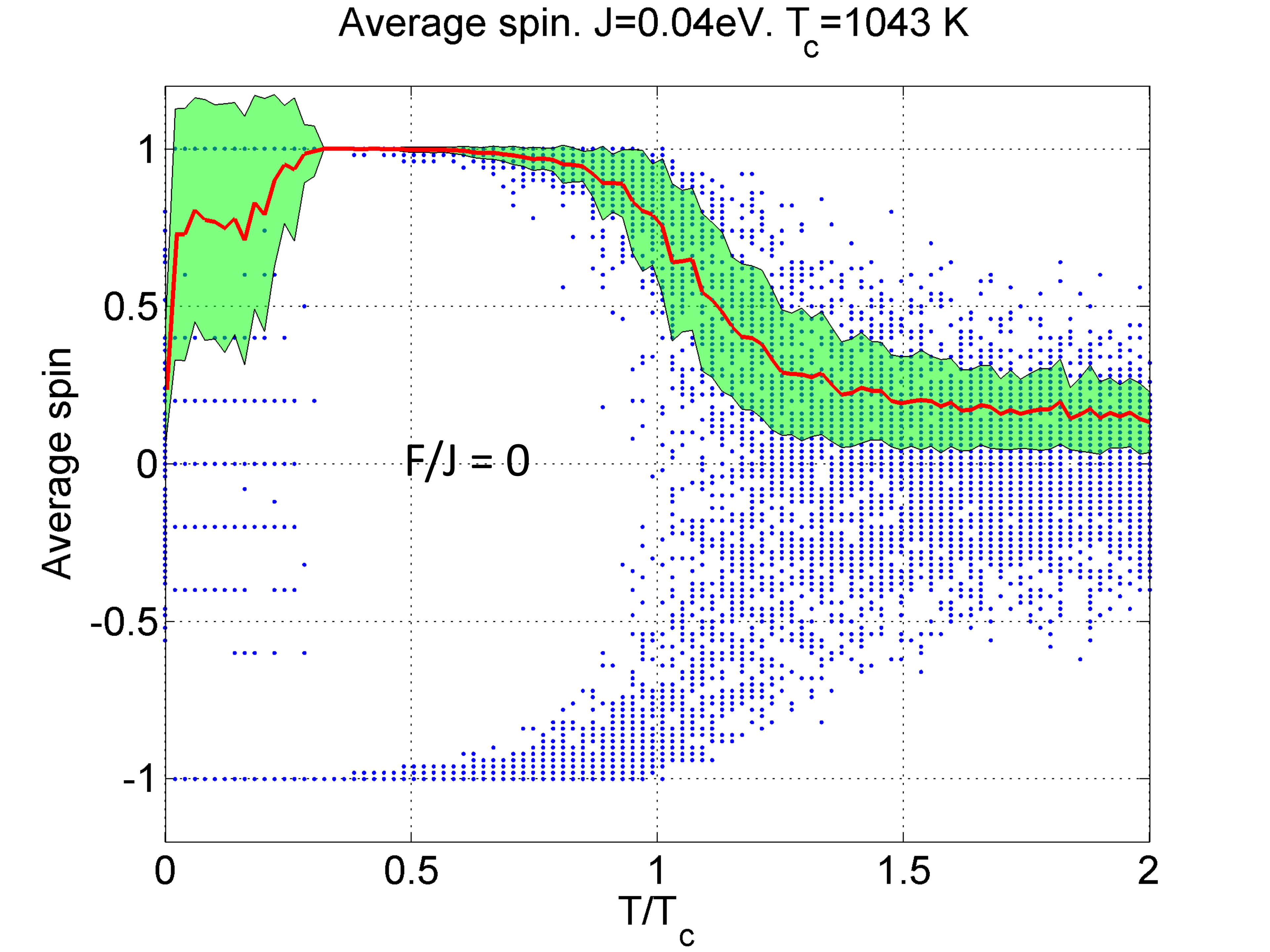


Results of a MATLAB simulation:

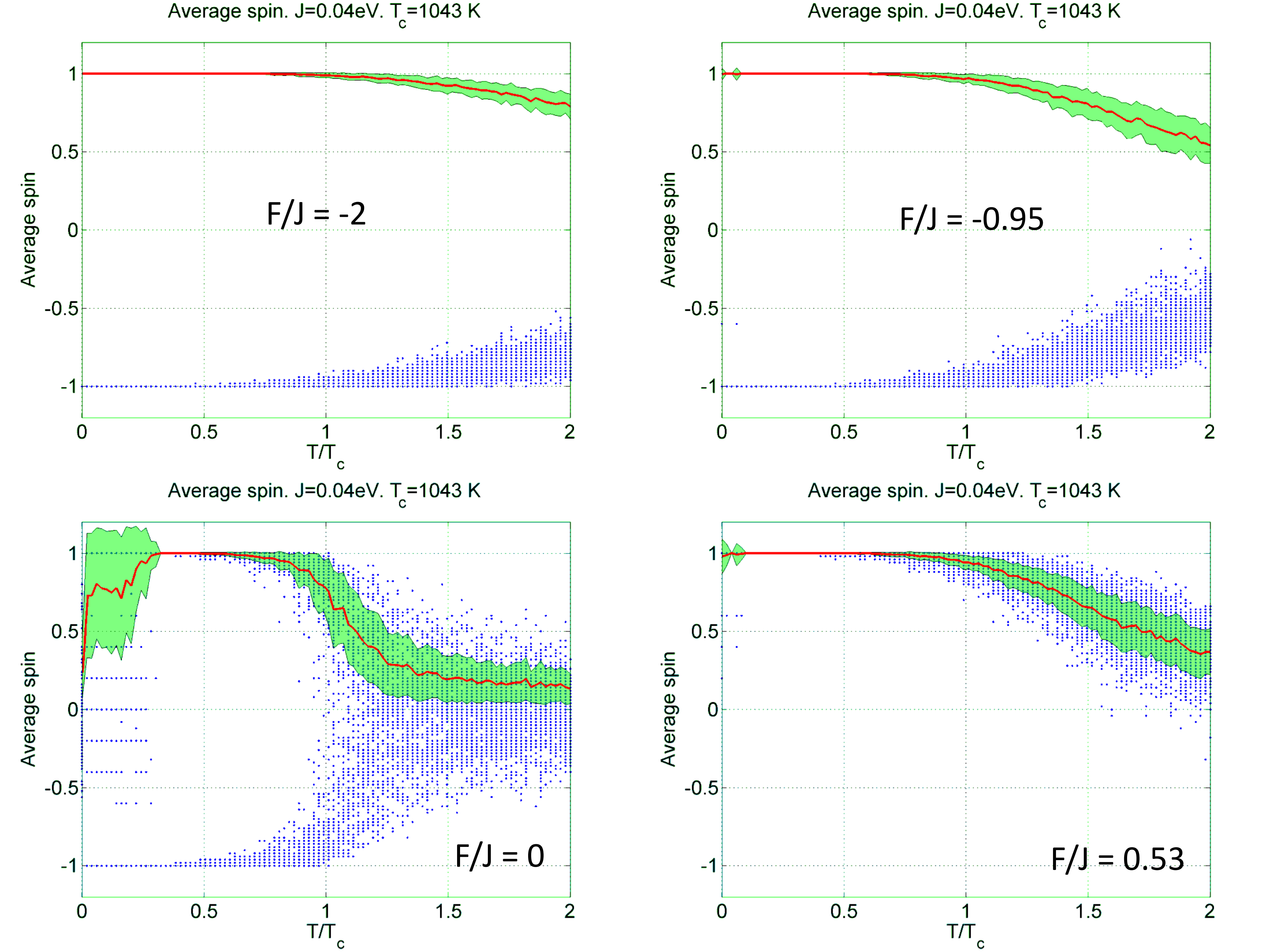
10 x 10 grid
I = 2000 (x 10 x 10) iterations of Metropolis algorithm
R = 100 repeats for each temperature
100 different temperatures from T/Tc = 0.0 ... 2.0
21 different F/J values from -2 to 2

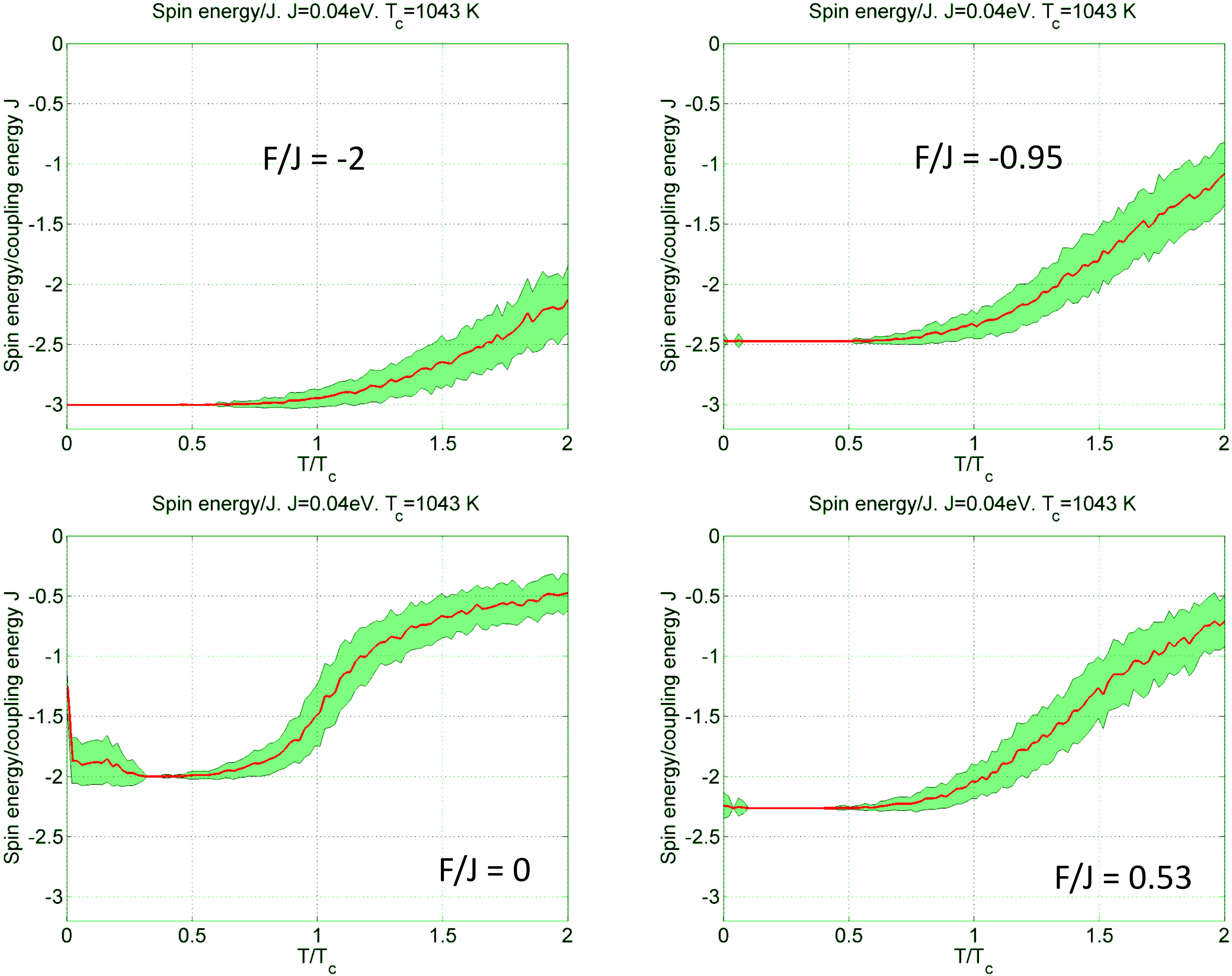
i.e. 2000 x 10 x 10 x 100 x 100 x 21 =
42 billion iterations of the Metropolis algorithm

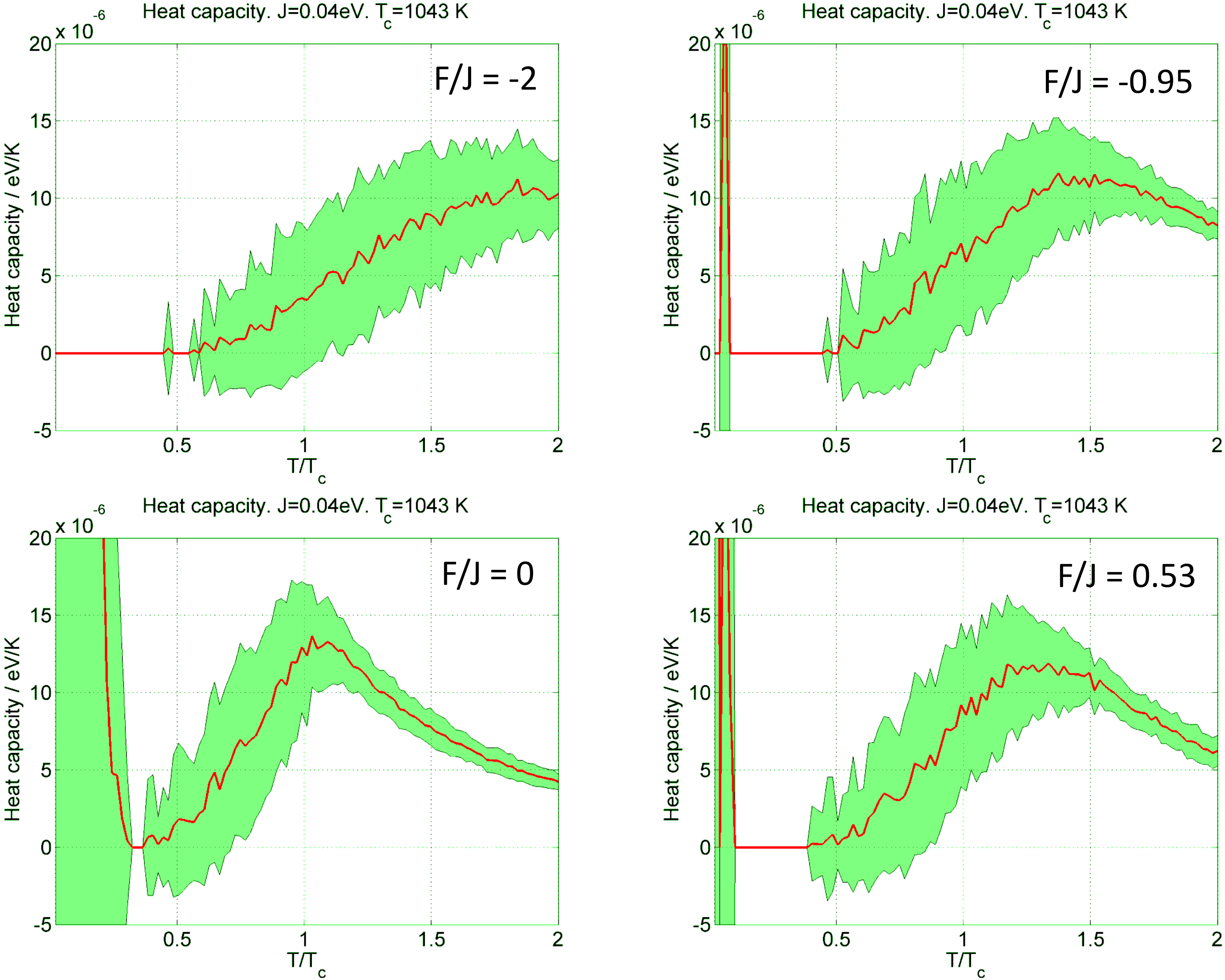
Running time on an i5 PC was about five days! Opportunity for *parallel processing.*

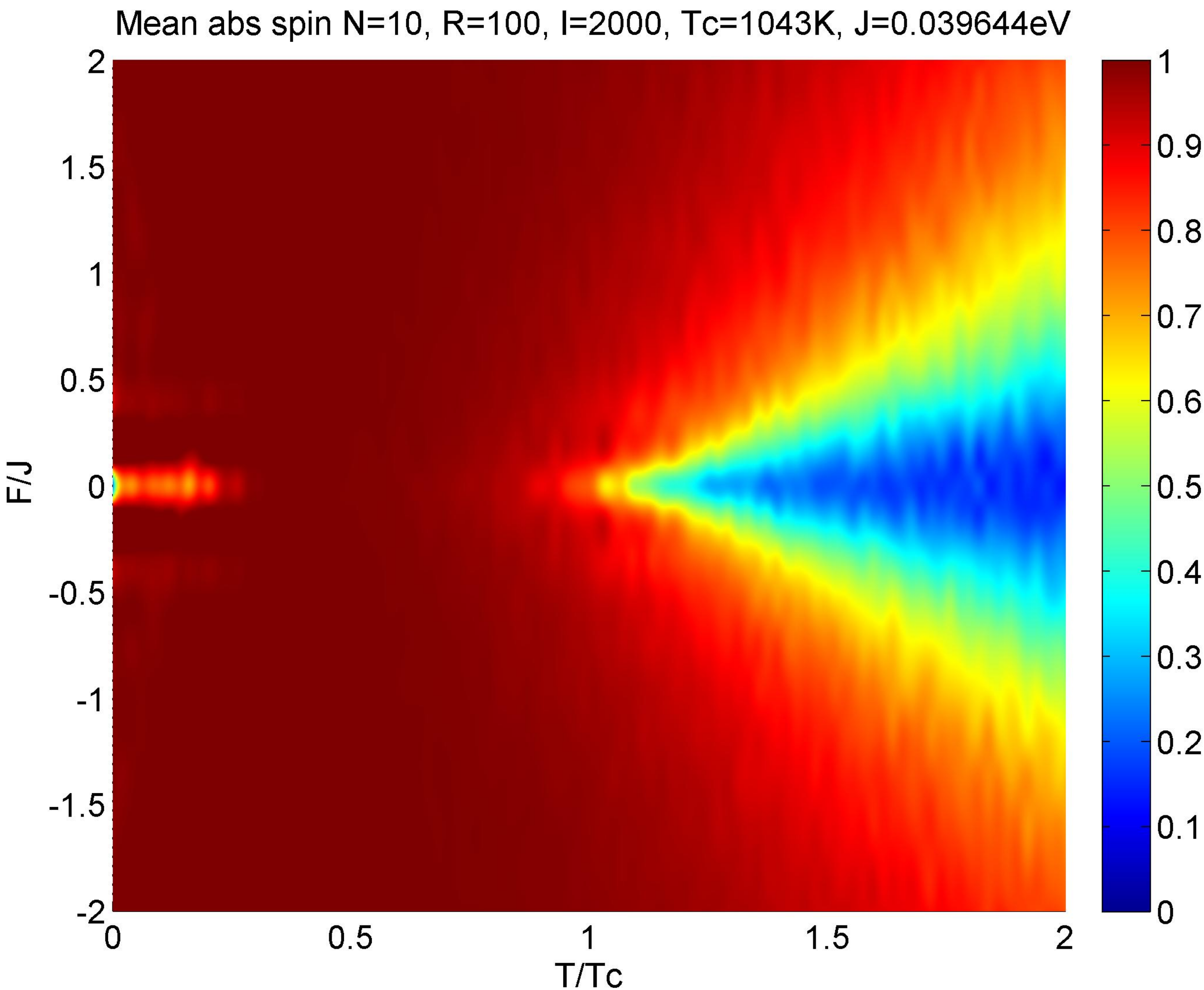


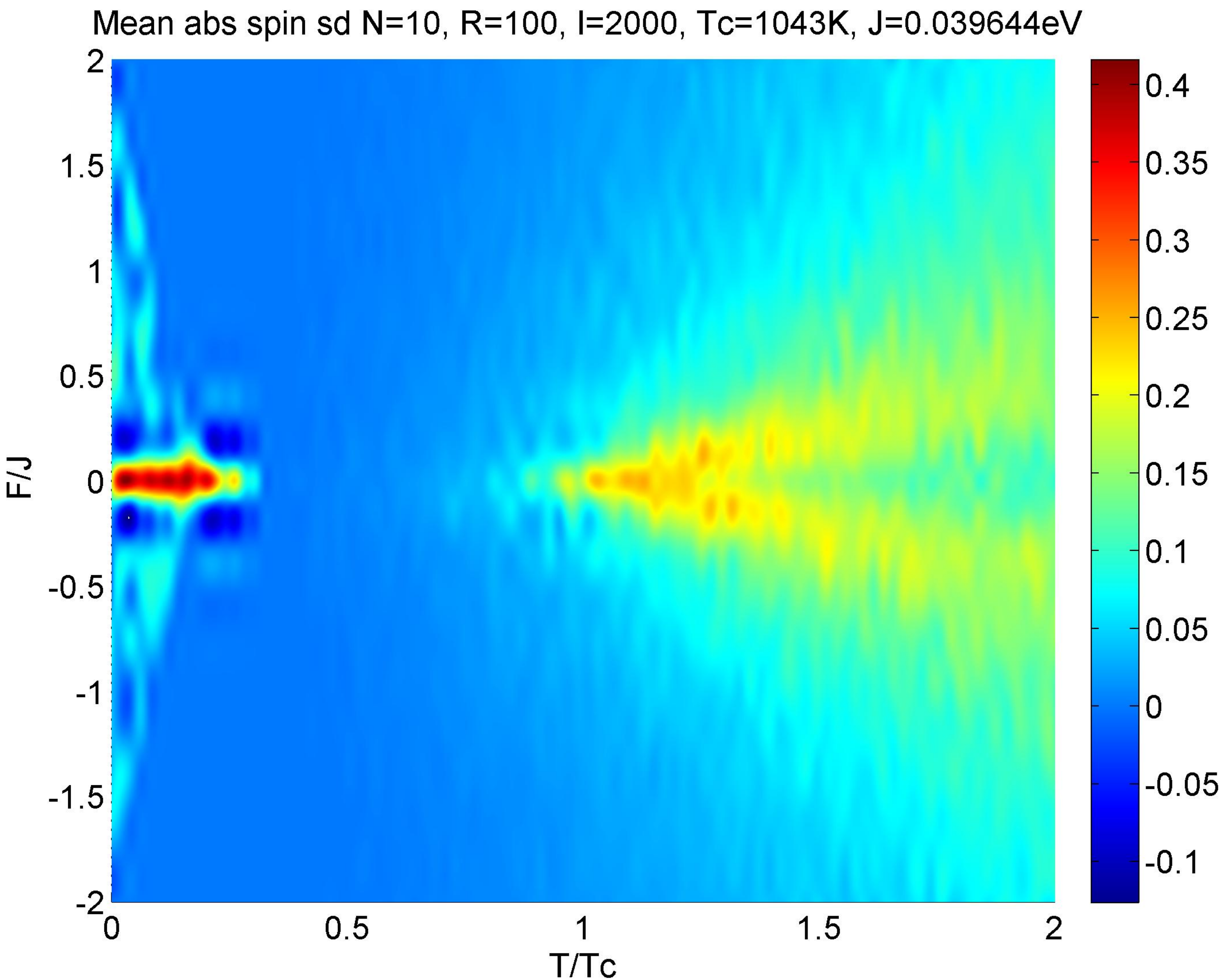
Average spin. J=0.04eV. T
c
=1043 K
Average spin
F/J = 0
T/T
c
1
0.5
0
-0.5
-1
0
0.5
1
1.5
2


Average spin. J=0.04eV. T_c=1043 K
F/J = -2
Average spin
T/T_c
Average spin. J=0.04eV. T_c=1043 K
F/J = -0.95
Average spin
T/T_c
Average spin. J=0.04eV. T_c=1043 K
F/J = 0
Average spin
T/T_c
Average spin. J=0.04eV. T_c=1043 K
F/J = 0.53
Average spin
T/T_c

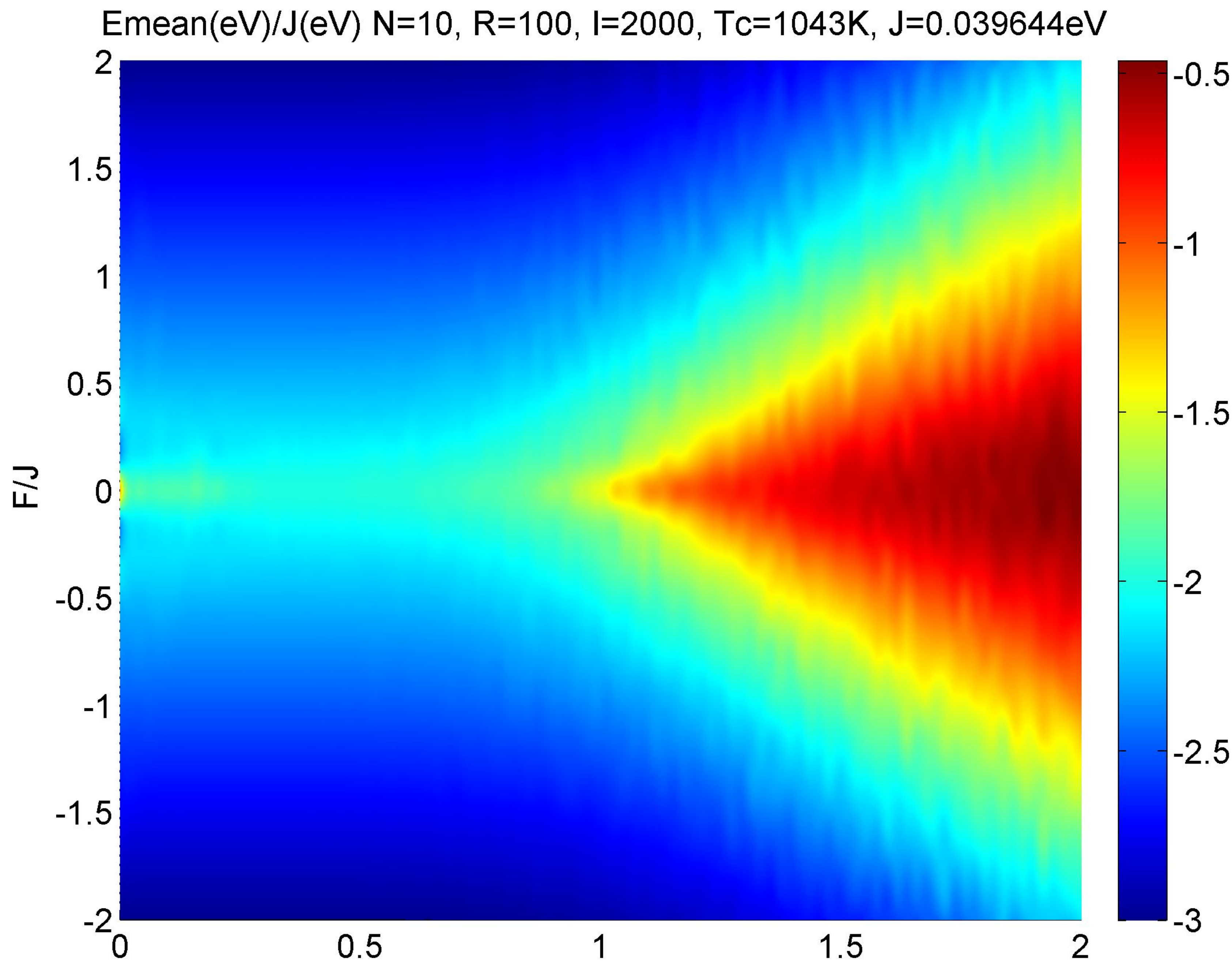

Spin energy/J. J=0.04eV. T_c=1043 K
Spin energy/coupling energy J
T/T_c
F/J = -2
Spin energy/J. J=0.04eV. T_c=1043 K
Spin energy/coupling energy J
T/T_c
F/J = -0.95
Spin energy/J. J=0.04eV. T_c=1043 K
Spin energy/coupling energy J
T/T_c
F/J = 0
Spin energy/J. J=0.04eV. T_c=1043 K
Spin energy/coupling energy J
T/T_c
F/J = 0.53


Heat capacity. J=0.04eV. T_c=1043 K
F/J = -2
Heat capacity. J=0.04eV. T_c=1043 K
F/J = -0.95
Heat capacity. J=0.04eV. T_c=1043 K
F/J = 0
Heat capacity. J=0.04eV. T_c=1043 K
F/J = 0.53
Heat capacity / eV/K
x 10^{-6}
T/T_c
20
15
10
5
0
-5
0.5
1
1.5
2

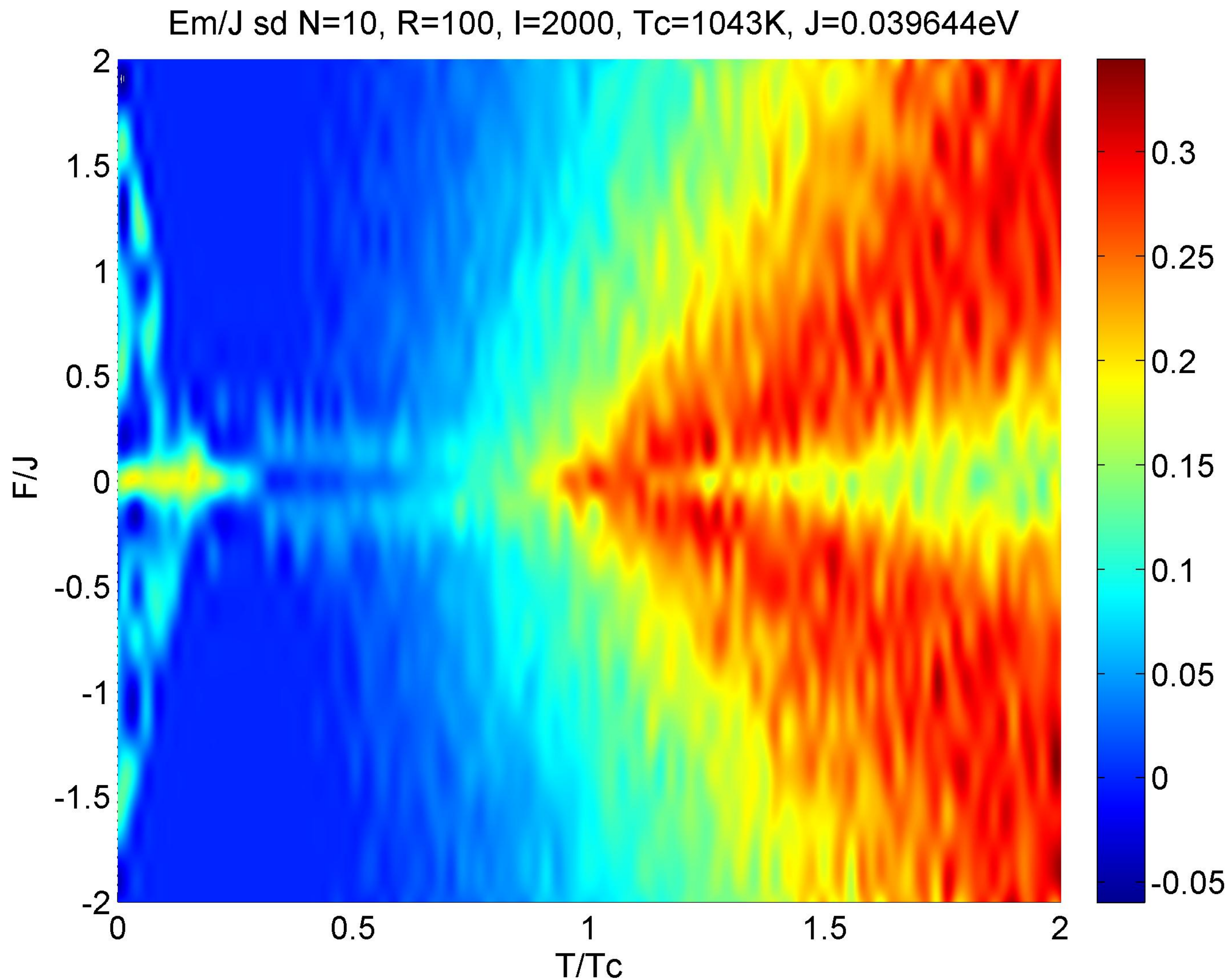

Mean abs spin N=10, R=100, I=2000, Tc=1043K, J=0.039644eV
F/J
T/Tc
2
1.5
1
0.5
0
-0.5
-1
-1.5
-2
0
0.5
1
1.5
2
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0

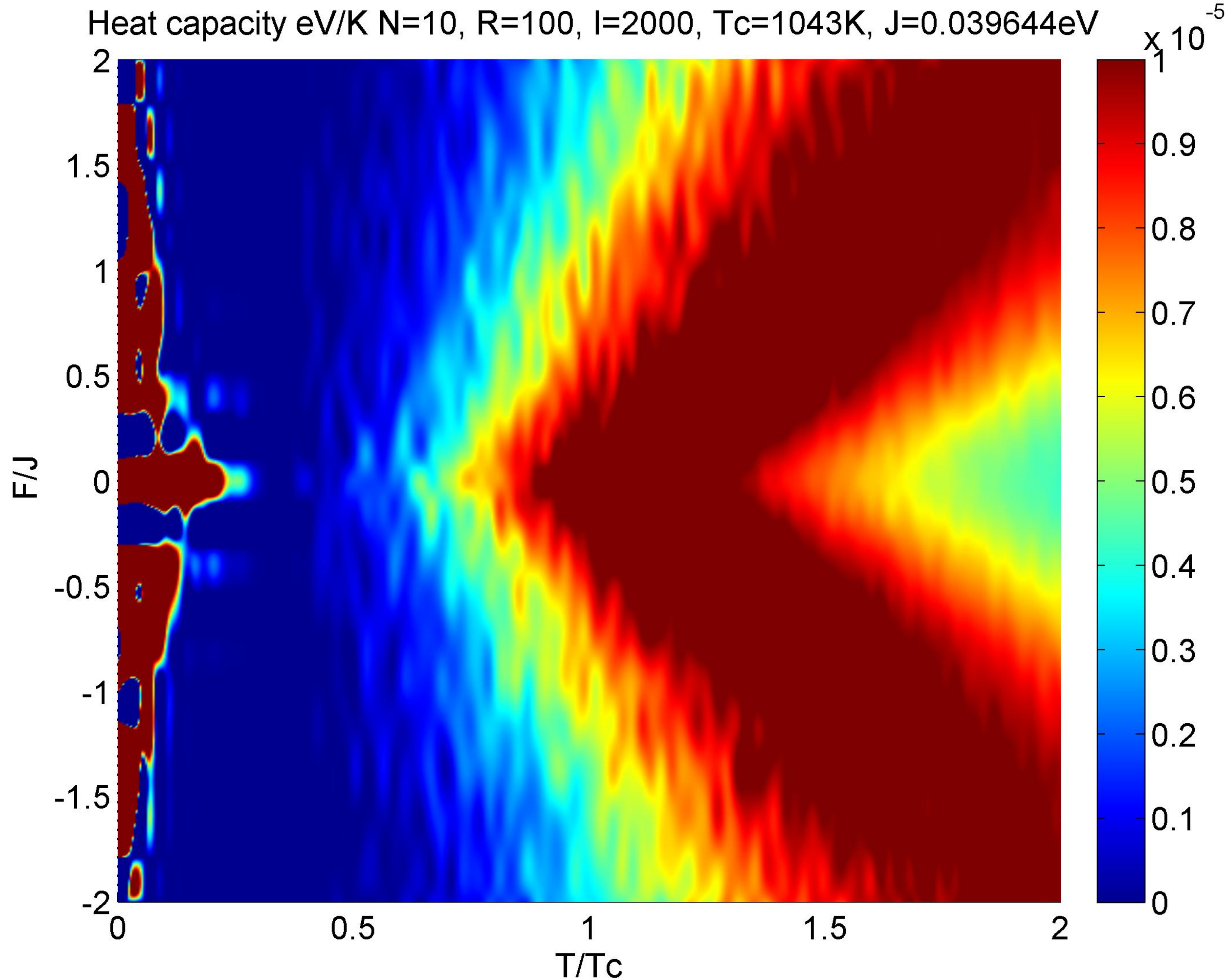


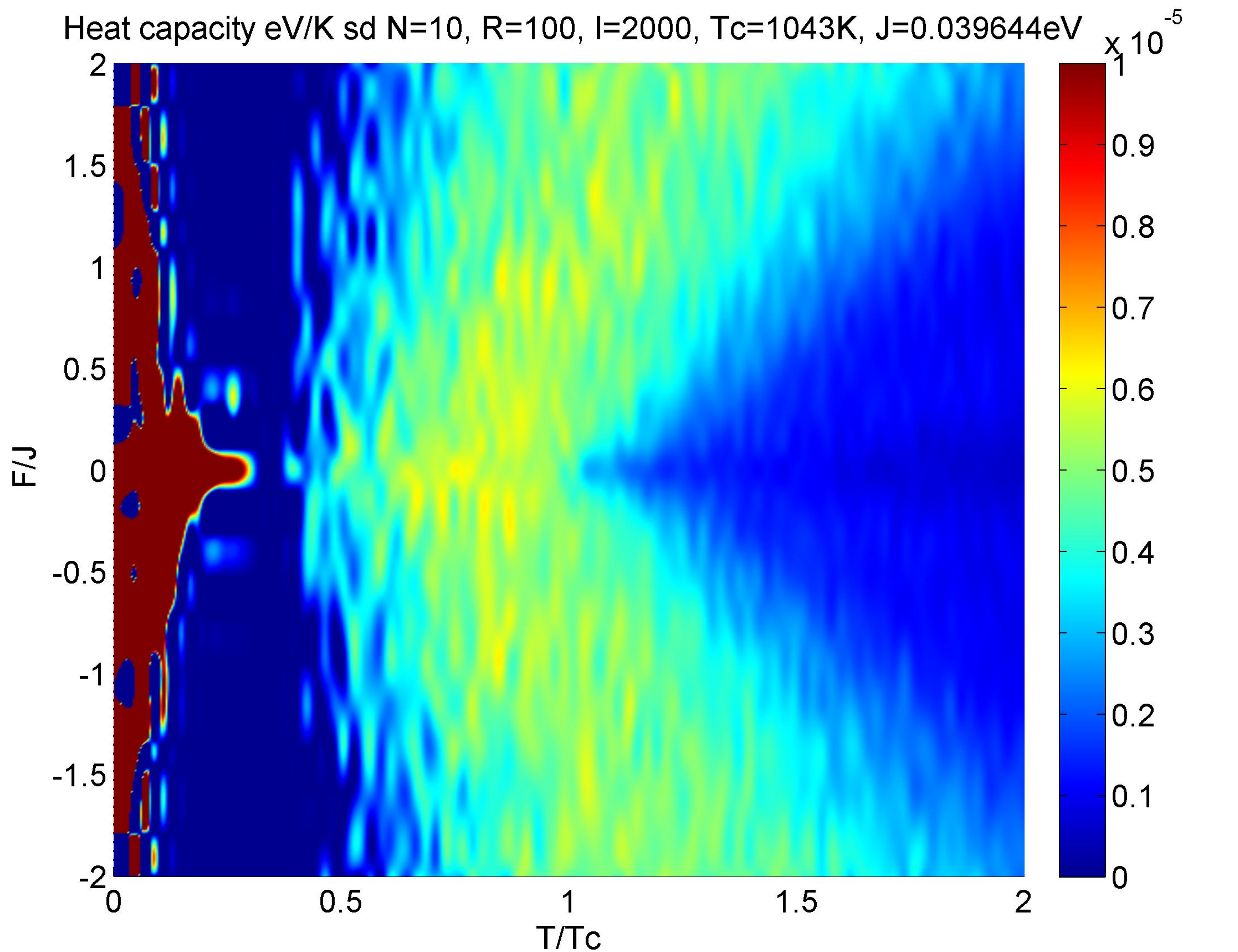
Mean abs spin sd N=10, R=100, I=2000, Tc=1043K, J=0.039644eV
F/J
T/Tc
2
1.5
1
0.5
0
-0.5
-1
-1.5
-2
0
0.5
1
1.5
2
0.4
0.35
0.3
0.25
0.2
0.15
0.1
0.05
0
-0.05
-0.1



Emean(eV)/J(eV) N=10, R=100, I=2000, Tc=1043K, J=0.039644eV
F/J
T/Tc
2
1.5
1
0.5
0
-0.5
-1
-1.5
-2
0
0.5
1
1.5
2
-0.5
-1
-1.5
-2
-2.5
-3


Em/J sd N=10, R=100, I=2000, Tc=1043K, J=0.039644eV
F/J
T/Tc
2
1.5
1
0.5
0
-0.5
-1
-1.5
-2
0
0.5
1
1.5
2
0.3
0.25
0.2
0.15
0.1
0.05
0
-0.05


Heat capacity eV/K N=10, R=100, I=2000, Tc=1043K, J=0.039644eV
x 10^-5
F/J
T/Tc
2
1.5
1
0.5
0
-0.5
-1
-1.5
-2
0
0.5
1
1.5
2
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0



Heat capacity eV/K sd N=10, R=100, I=2000, Tc=1043K, J=0.039644eV
x 10^-5
F/J
T/Tc
2
1.5
1
0.5
0
-0.5
-1
-1.5
-2
0
0.5
1
1.5
2
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0

References

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