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Computing the Magnetic Critical Temperature from Experimental Data

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Abstract

This project investigated how the magnetic critical temperature (Tc) of a bcc Iron lattice changed as fluctuations in spin orientation, spin length, and atomic position were introduced. The system studied had 512 atomic sites and a periodic boundary condition.

Methods

Energy Workflow

- The Heisenberg Hamiltonian was used to calculate the temperature - dependent magnetization up to the second nearest neighbour with the Landau Hamiltonian capturing fluctuations in spin length.

Vary Spin Orientation
- Use Heisenberg Hamiltonian
- $H_H = \sum_{i,j} J_{ij} \vec{S_i} \cdot \vec{S_j}$

J_1 = 22.52 meV, J_2 = 17.99 meV [1]

T_{C1}

Vary Spin Length
- Use Landau Hamiltonian
- $H_L = \sum_i (AS_i^2 + BS_i^4 + CS_i^6)$

A = - 440.987 meV, B = 150.546 meV, C = 50.6794 meV [1]

T_{C2}

Vary Atomic Position
- Extend Heisenberg Hamiltonian
- $H_H = \sum_{i,j} J_n (1 - \Delta r_{ij}/r_n)^3 \vec{S_i} \cdot \vec{S_j}$

where $\Delta r_{ij} = |(r_{ij} - r_n)|$

T_{C3}

Test Landau Sensitivity
- $H_L = \sum_i (0.8 * AS_i^2 + BS_i^4 + CS_i^6)$

T_{C4}

RESULTS

FIG. 1. Workflow for the calculation of the lattice energy per site using the Heisenberg and Landau Hamiltonians.

Metropolis Monte Carlo Algorithm

- Two Metropolis Algorithms ran simultaneously to update the spin and atomic position configurations such that the system moved towards a lower energy state with decreasing temperature.

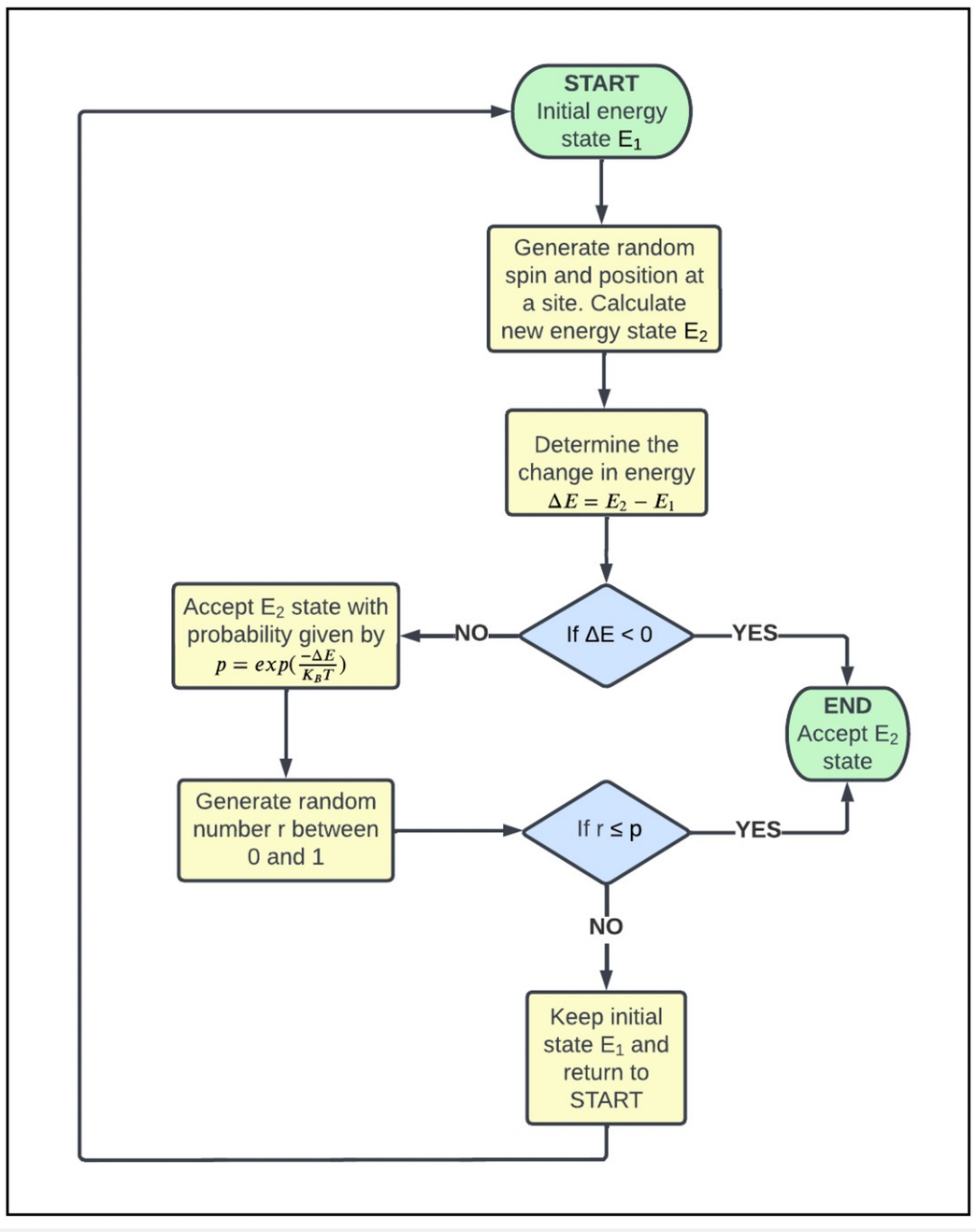

FIG. 2. The implementation of the Metropolis Algorithm in the simulations [2].

- Specific heat computed by $C_V = \frac{1}{K_B T^2} (\langle E^2 \rangle - \langle E \rangle^2)$ [2]
- Susceptibility computed by $\chi = \frac{1}{K_B T} (\langle M^2 \rangle - \langle M \rangle^2)$ [2]

Full Report

Results

- Uniform sampling a spherical volume to create random spin length and orientation in 3D.

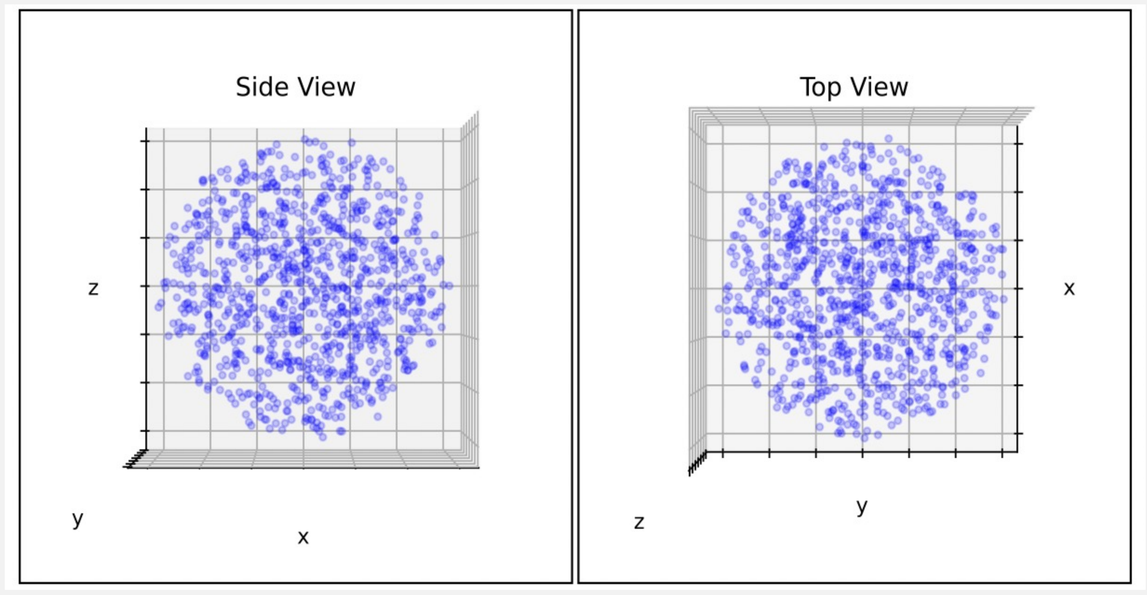

FIG. 3. Random points generated from the uniform sampling of the spherical volume. No clustering of sample points observed.

- The action of local potential wells resulted in sites sitting closer to equilibrium positions.

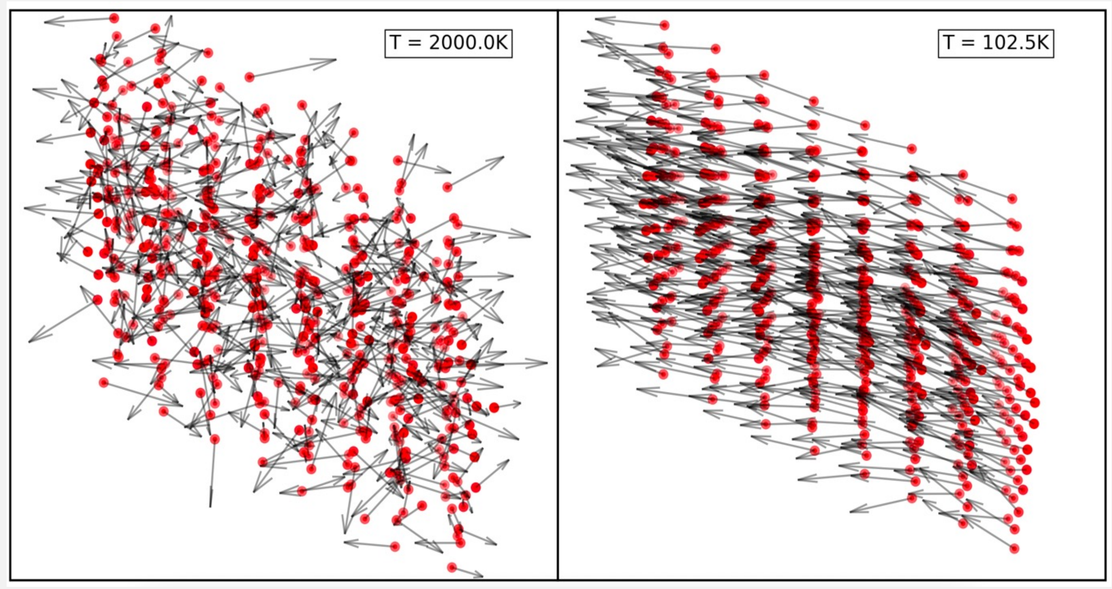

FIG 4. Snapshots of the Iron lattice in the α – Potential simulation taken at a temperature well above (*Left*) and well below (*Right*) the Tc of 771K.

Estimation of the Critical Temperature (Tc)

- Sudden change in lattice properties at Tc.
- Magnetization saturated towards expected 2.2μ_B per site at 0K [3]. → $S_i \approx \frac{M_i}{2\mu_B}$
- Tc estimated from the position of peaks in the specific heat curves.

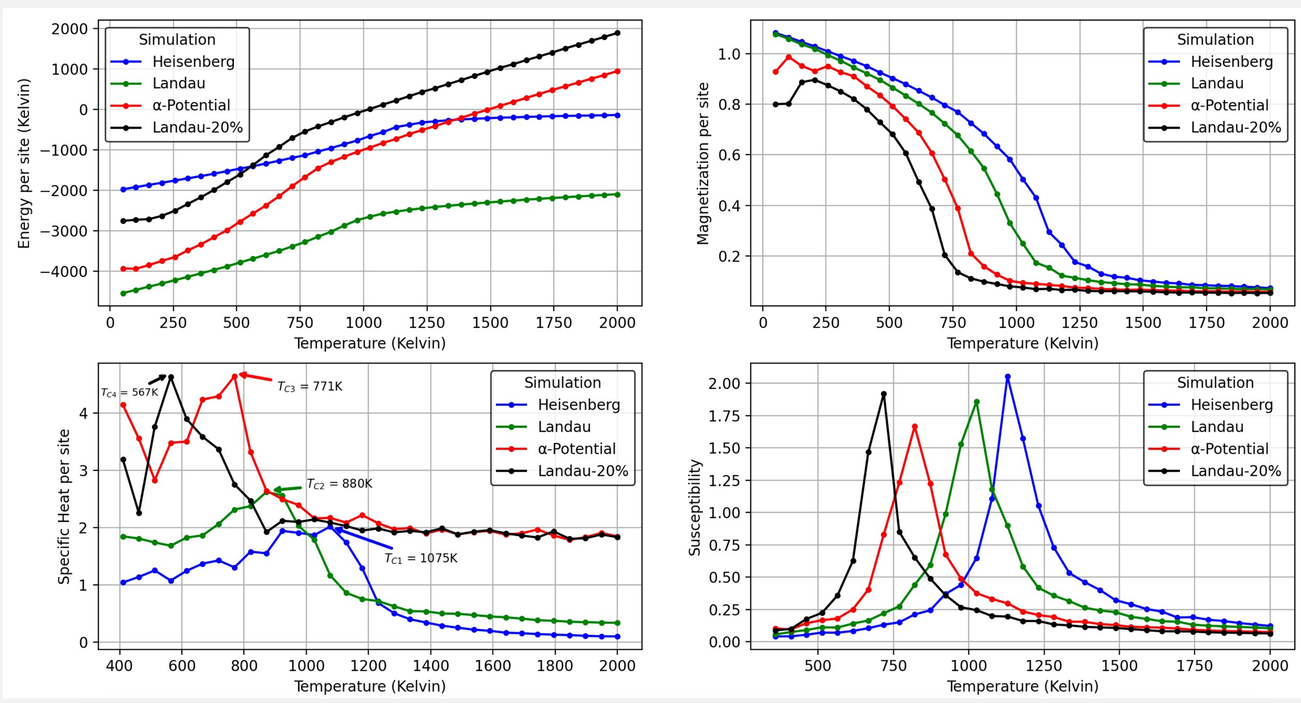

FIG 5. Results from each simulation per site for Energy vs Temperature (*Top Left*), Magnetization vs Temperature (*Top Right*), Specific Heat vs Temperature (*Bottom Left)* and Susceptibility vs Temperature (*Bottom Right*).

- Simulations performed to find how Tc changed as more fluctuations added into lattice.

	Simulation	Tc
1	Heisenberg	1075K
2	Landau	880K
3	α – Potential	771K
4	Landau–20%	567K

Tc decreased

TABLE 1. Critical temperature estimations taken from the peak positions of the specific heat curves for each simulation in FIG. 5.

Conclusions

- The 8x8x8 cell size was found to have a good balance between accuracy and computational effort.
- The critical temperature of the lattice decreased as more fluctuations were added into the system.

REFERENCES
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[2] H. Gould, J. Tobochnik, and W. Christian, 'Monte Carlo Simulations of Thermal Systems', in *An introduction to computer simulation methods: applications to physical systems*, 3rd ed. San Francisco: Pearson Addison Wesley, 2007, ch. 15, pp. 590-672.
[3] M. Domina, M. Cobelli, and S. Sanvito, 'Spectral neighbor representation for vector fields: Machine learning potentials including spin', *Phys. Rev. B*, vol. 105, no. 21, p. 214439, Jun. 2022, doi: 10.1103/PhysRevB.105.214439.

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