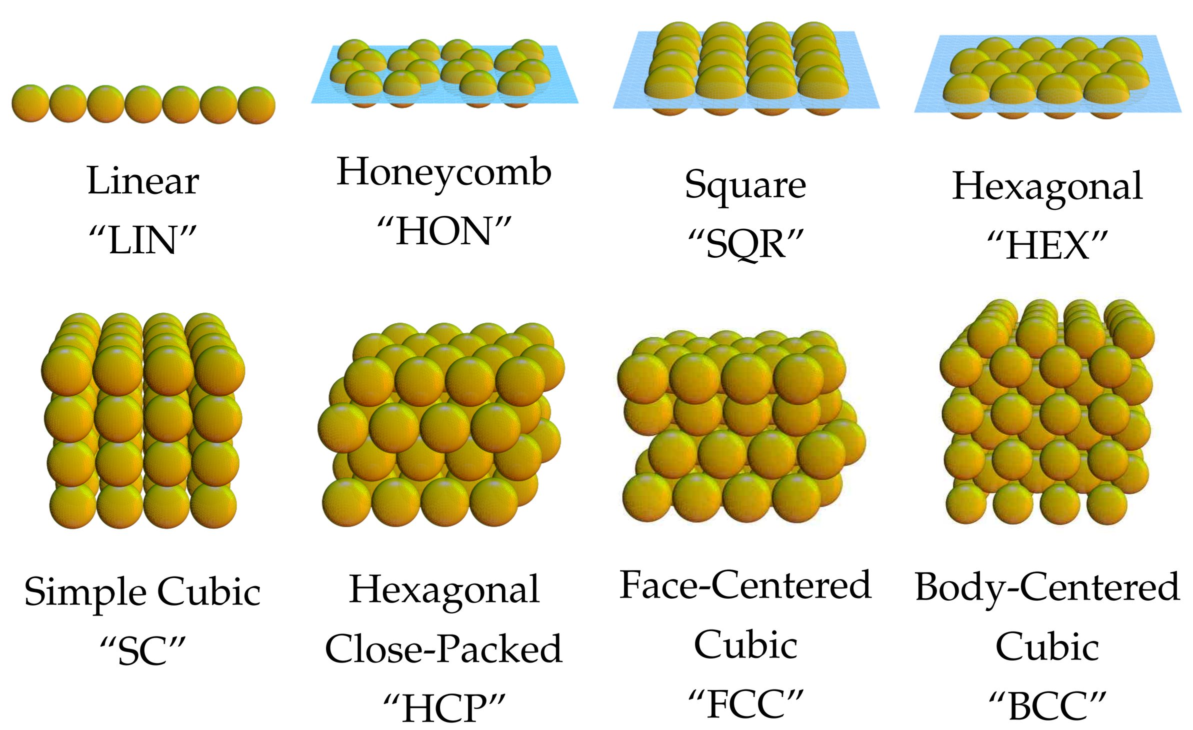
Monte Carlo Studies of the Globally-Coupled Ising Model

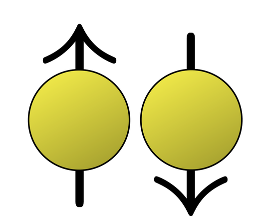
Daniel E. Shai, John F. Lindner, Virginia B. Pett, and Sarah J. Schmidtke,
Departments of Chemistry and Physics, The College of Wooster, Wooster, OH 44691

Model of Ferromagnetism:

- Atoms arranged in various lattice types:

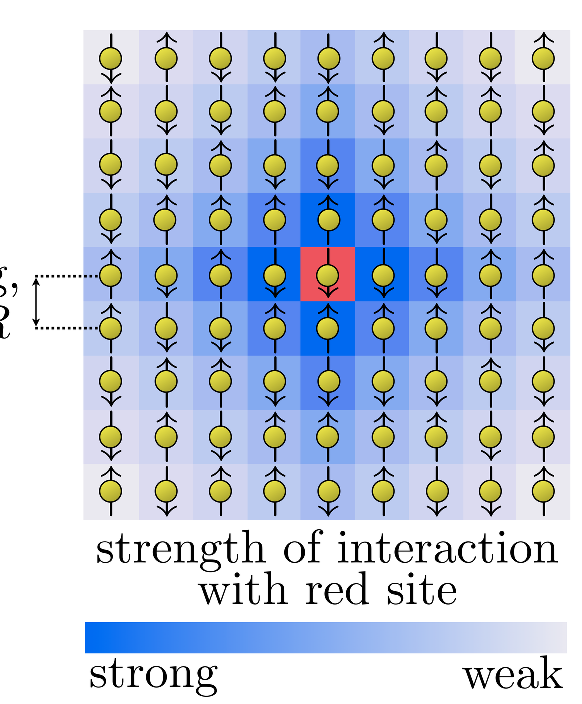


- Classical vector represents atom's magnetic moment:



$\vec{s} = \pm 1\hat{z}$

- "Global Coupling" $\Rightarrow$ Every atom interacts with every other atom:



- Global coupling decays exponentially with distance:

$$J\left[\vec{d}\right] = J\exp\left[-\frac{d \cdot R}{\rho}\right],$$

where ρ/R is the characteristic length scale.

- The system energy depends on the coupling:

$$E = -\sum_{i>j} J\left[\vec{d}\right]\vec{s}_i \cdot \vec{s}_j,$$

where atoms are indexed by i and j.

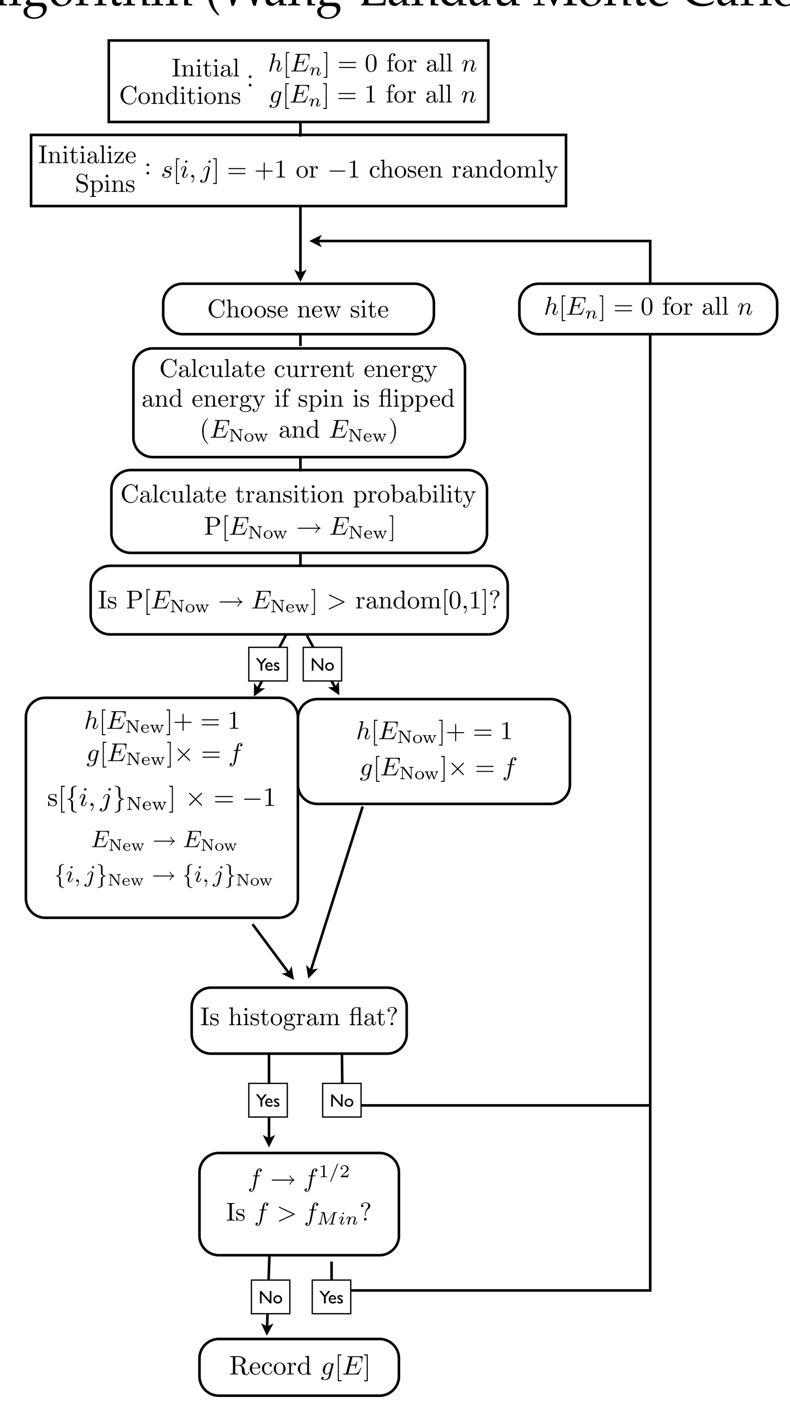
- Ferromagnetic interactions ($\uparrow\uparrow$) are more stable than nonmagnetic ($\uparrow\downarrow$).

Computer Simulation:

- Goal: determine the *density of states* ($g[E]$): the number of spin configurations producing an energy, E.
- In an unbiased random walk in energy space, realized by randomly flipping spins, the histogram of the energy distribution ($h[E]$) converges to the density of states ($g[E]$), but too slowly to be practical.
- When the random walk is biased inversely to $g[E]$ so that $h[E]$ becomes flat, $g[E]$ is constructed to within an error $\propto \ln[f]$ if at each energy visited, $g[E]$ is redefined as $g[E] \times f$. If f is incrementally reduced to $= 1$, $g[E]$ becomes exact.
- Random walk acceptance bias:

$$P[E_1 \to E_2] = \min\left[\frac{g[E_1]}{g[E_2]}, 1\right]$$

- Schematic of algorithm (Wang-Landau Monte Carlo):



- Given $g[E]$, the partition function is readily evaluated:

$$Z = \sum_n g[E_n]\exp[-E_n/(k_B T)],$$

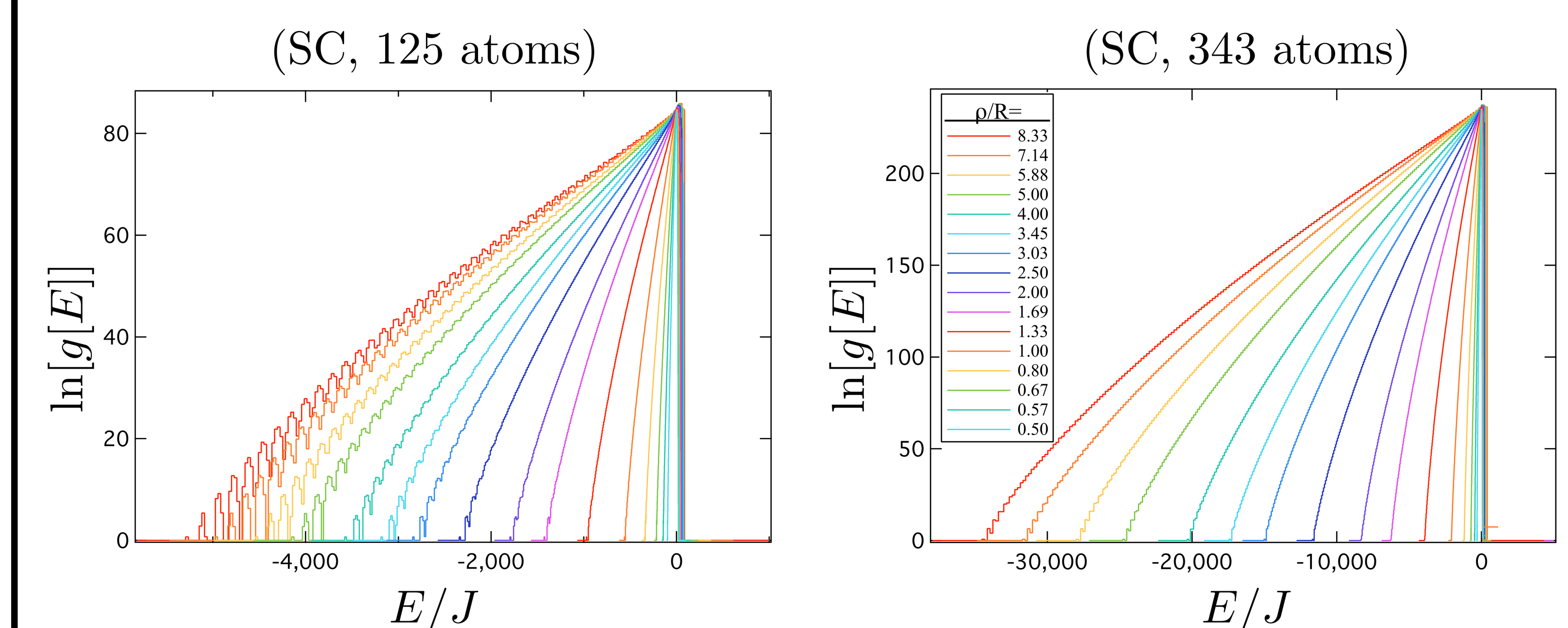
from which, thermodynamic observables are derived.

Project Goals:

1. Reproduce the experimentally-observed ferromagnetic $\to$ nonmagnetic phase transition, occurring as the temperature increases.
2. Determine the effect of lattice structure and coupling length (ρ/R) on the stability of the ferromagnetic phase.

Density of States: generated by computer simulation.

- Example data:



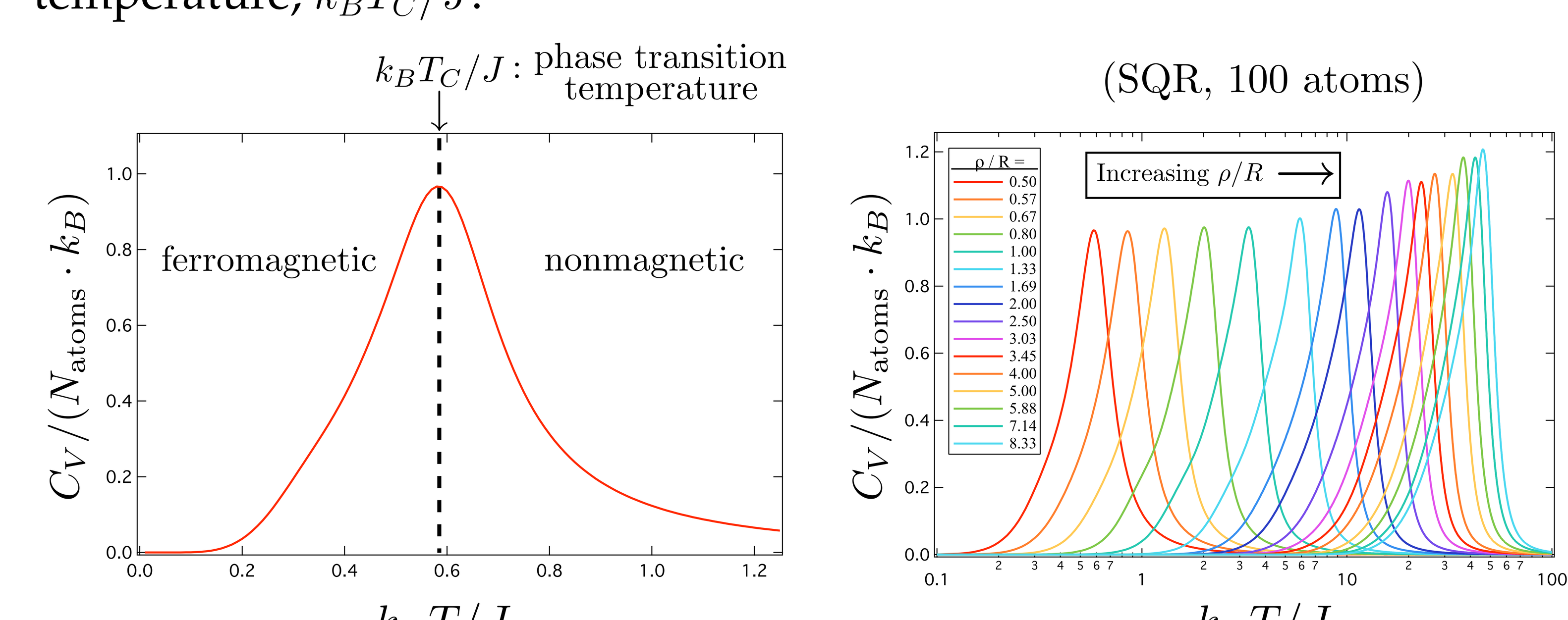
- Conclusion: When ρ/R is large, the coupling is global and the density of states includes more negative (more stable) energy levels.

Heat Capacity: elucidates the phase transition.

- Heat capacity is derived from the density of states:

$$C_V = \frac{\langle E^2\rangle - \langle E\rangle^2}{k_B T^2}, \text{ where } \langle E\rangle = \frac{\sum_n E_n \cdot g[E_n] \cdot \exp[-E_n/(k_B T)]}{\sum_n g[E_n] \cdot \exp[-E_n/(k_B T)]}$$

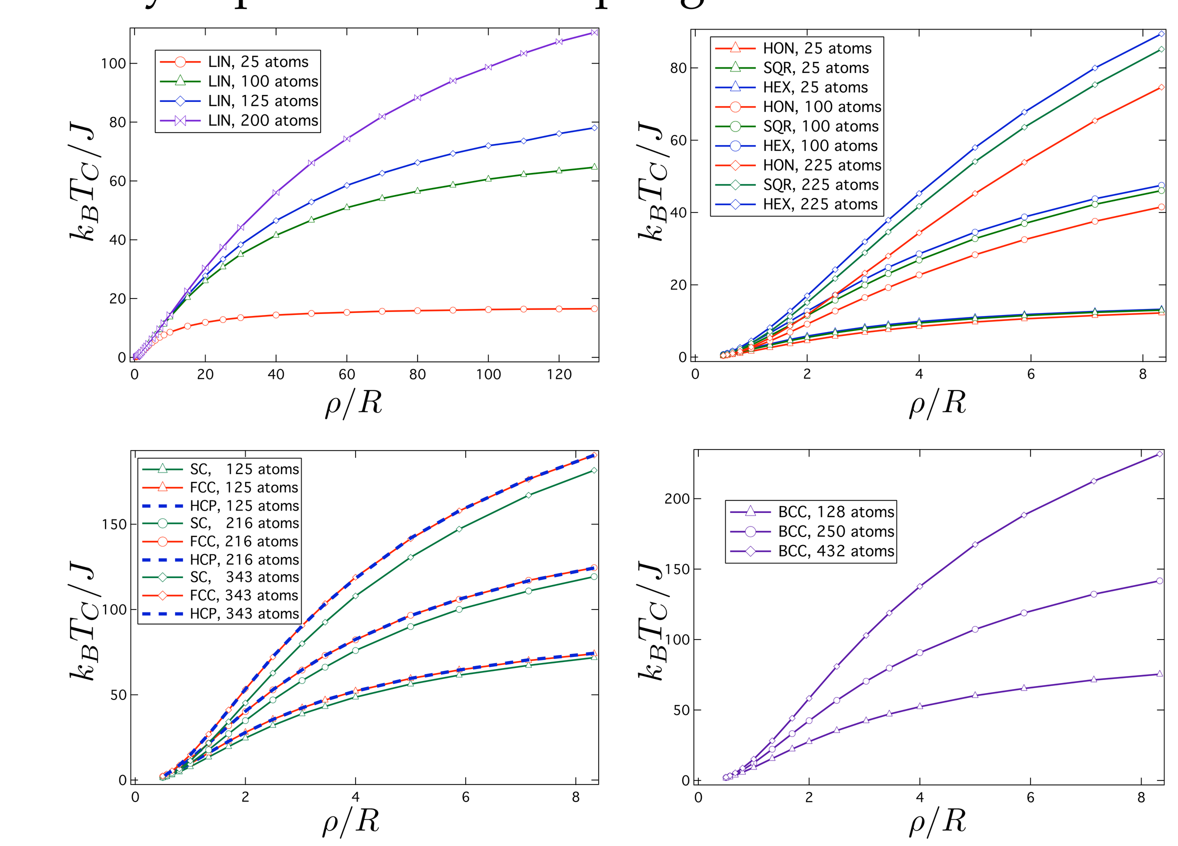
- Peak in the heat capacity provides a clear indicator of the phase transition temperature, $k_B T_C/J$:



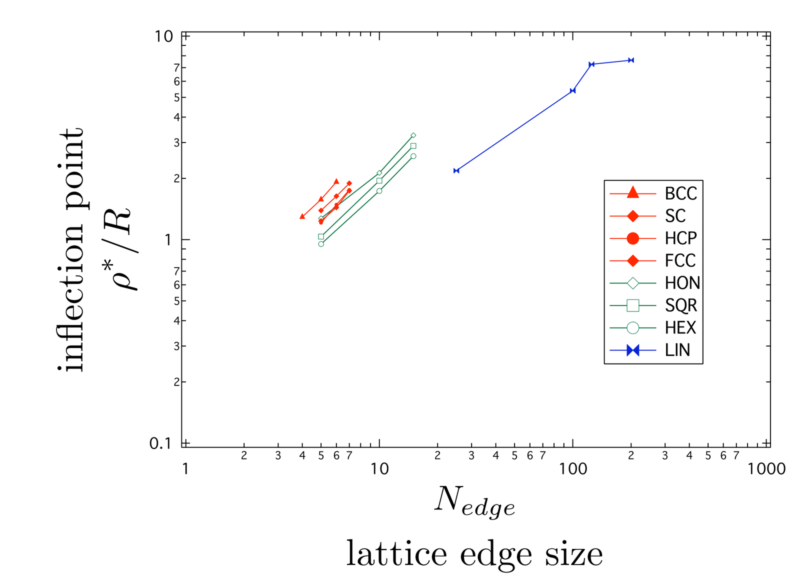
- Conclusion: As ρ/R increases, the phase transition temperature increases, thereby stabilizing the ferromagnetic phase.

Ferromagnetic Stability:

- $k_B T_C/J$ gives a direct indication of how the ferromagnetic stability depends on the coupling:



- Conclusion: $k_B T_C/J$ increases predictably as ρ/R increases for all lattices. Increased ρ/R implies ferromagnetic stability.
- Plots of $k_B T_C/J$ versus ρ/R (above) show an inflection point ($\equiv \rho^*/R$), which increases linearly with the lattice edge size:



- Conclusion: Inflection point occurs when the coupling length is of the same order as the system size. These edge effects are destabilizing.

Future Work:

1. Improve quality of $g[E]$ calculation (stricter convergence rules) to eliminate noise in inflection point data.
2. Study larger systems to further explore asymptotic limits of inflection points.
3. Explore more complicated coupling potentials (non-monotonic), that may better approximate real magnets.