Investigating Critical Phenomena through Monte Carlo Simulation of 2D Lattice Gas Model

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1 Isomorphism of the lattice gas and Ising model

Part 1. $$\mathcal{H}_{LG} = -\epsilon \sum_{<i,j>} c_i c_j - \mu \sum_i c_i$$

Substitute in $c_i = \frac{s_i+1}{2}$

$$\sum_{<i,j>} c_i c_j = \frac{1}{4}\sum_{<i,j>} s_i s_j + \frac{1}{4}\sum_{<i,j>}(s_i + s_j) + \frac{1}{4}\sum_{<i,j>} 1$$

s_i appreas in N bonds with total number of bonds being $\frac{Nq}{2}$

$$\sum_{<i,j>} c_i c_j = \frac{1}{4}\sum_{<i,j>} s_i s_j + \frac{q}{4}\sum_i s_i + \frac{1}{8}Nq$$

similarly

$$\sum_i c_i = \sum_i \frac{s_i+1}{2} = \frac{1}{2}\sum_i s_i + \frac{1}{2}N$$

By substituting $\sum_{<i,j>} c_i c_j$ and $\sum_i c_i$ back into $\mathcal{H}_{LG}$

$$\mathcal{H}_{LG} = -\epsilon(\frac{1}{4}\sum_{<i,j>} s_i s_j + \frac{q}{4}\sum_i s_i + \frac{1}{8}Nq) - \mu(\frac{1}{2}\sum_i s_i + \frac{1}{2}N)$$

Now reassign variables:

$$\epsilon = 4J, \quad \mu = \frac{4h - \epsilon q}{2}$$

$$\mathcal{H}_{LG} = -J(\sum_{<i,j>} s_i s_j + q\sum_i s_i + \frac{1}{2}Nq) - (h - Jq)(\sum_i s_i + N)$$

$$= -J\sum_{<i,j>} s_i s_j - Jq\sum_i s_i - J\tfrac{1}{2}Nq - (h - Jq)\sum_i s_i - (h - Jq)N$$

$$\mathcal{H}_{\mathbf{LG}} = \underbrace{-J\sum_{<i,j>} s_i s_j}_{\text{Interaction term}} \underbrace{-(2Jq - h)\sum_i s_i}_{\text{Field term}} + \underbrace{\left(\frac{JNq}{2} - hN\right)}_{\text{Constant}}$$

Part 2.

$$T_c \approx 2.269\frac{J}{k_B} = 2.269\frac{1}{4}\frac{\epsilon}{k_B}$$

$$T_{ising} \approx 0.567\frac{\epsilon}{k_B}$$

2 Code modifications

2.1 Calculating radially averaged structure factor

By using the average form of the 2d structure factor $S(K)$ the 1D, radially averaged structure factor $S(|K|)$ could be calculated and plotted. To do this a function called `compute_structure_factor` was defined. The function makes use of the preexistent `compute_structure_factor` whos output was parsed in as `S_2D`. The 2D structure factor was normalised by dividing by N. A 2D k-space grid was then created by calculating the distance between points (`R`), dividing them by `L` and multiplying by 2π. The center point was excluded to avoid division by zero errors later in the program and flattens the 2D arrays into a 1D list. The k values were then put into 100 bins, and a weighted sum was produced along with the number of counter per bin. The average number of points in each bin was then found as `S_k`.

```
def compute_radial_structure_factor(S_2D):
    """
    Computes the 1D radially averaged
    structure factor S_k from the 2D S_2D.
    """

    # Define system shape
    L = S_2D.shape[0]
    center = L // 2

    # Normalize (compute_structure_factor
    doesn't do this)
    S_2D = S_2D / (L * L)

    # Create k-space grid
    Y, X = np.indices((L, L))
    R = np.sqrt((X - center)**2 + (Y - center)
    **2)
    k = 2 * np.pi * R / L

    # Exclude k=0 to prevent div0 errs
    mask = R > 0.5
    k_flat = k[mask]
    S_flat = S_2D[mask]

    # Radial binning
    k_edges = np.linspace(k_flat.min(), k_flat
    .max(), 101)
    S_sum, _ = np.histogram(k_flat, bins=
    k_edges, weights=S_flat)
```

```
    counts, _ = np.histogram(k_flat, bins=
    k_edges)

    # Average and return bins
    S_k = S_sum / counts
    k_centers = 0.5 * (k_edges[:-1] + k_edges
    [1:])

    return k_centers, S_k
```

2.2 Calculating Cv and E

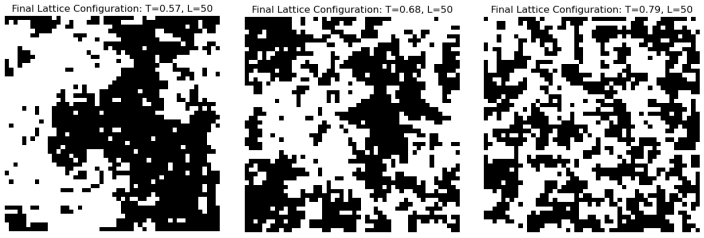
Next, the total dimensionless energy and specific heat of the energy was calculated using a function called `compute_whole_system_thermo`. This function parses `accum_H , accum_H_sq , n_meas , L , T` as variables; `N`, the total number of sites is calculated as L^2, the average energy and average energy squared is simply found by taking their cumulative energies from the simulation and dividing by the number of sites. C_V is then calculated through the equation $C_V = (\langle H^2 \rangle - \langle H \rangle^2)/T^2$ as in equation 2.3 in the assignment, however in unit-less form.

```
def compute_whole_system_thermo(accum_H,
    accum_H_sq, n_meas, L, T):
    """
    Computes the whole system energy (E_system
    ) and whole system specific heat (C_V).

    """

    # Average H and H^2 over all measurements
    avg_H = accum_H / n_meas
    avg_H_sq = accum_H_sq / n_meas

    E_system = avg_H

    # C_V = ( <H^2> - <H>^2 ) / T^2
    C_V = (avg_H_sq - avg_H**2) / (T**2)

    return E_system, C_V
```

3 Computational investigations of correlations on the approach to criticality

3.1 Investigating supercritical configurations temperature dependence

The configurations of 6 systems at side length 50 with temperatures varying from T_c to $2T_C$ were simulated and their final configurations are bellow: (AR = acceptance rate)



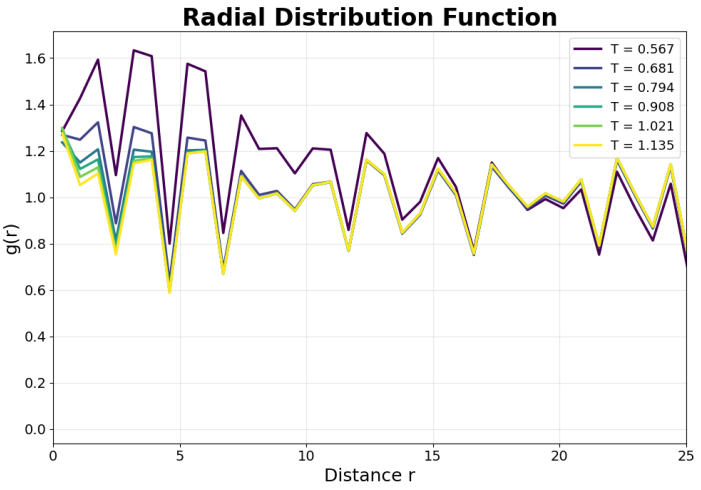
T = 0.57 ≈ $\frac{T_c}{2}$, AR: 0.5510 | T = 0.68, AR: 0.6151 | T = 0.79, AR: 0.6660

T = 0.91, AR: 0.7050 | T = 1.02, AR: 0.7363 | T = 1.13 ≈ $2T_c$, AR: 0.7617.

The plots show an increase in disorder as the temperature increases (less clustering as $\uparrow T$). For $T \approx T_C$ there is a clear moderate phase separation with rough domain boundaries indicating fluctuations. As the temperature increases in subsequent configurations, these phases become fractured and eventually a randomized structure is present for high T. In order to check for equilibrium, the simulation was run over a variety of numbers of sweeps (1000 to 5000). There was no significant change in behavior of acceptance rate or final configuration from changing the number of sweeps. This illustrates that the system is sufficiently equilibrated.

3.2 Investigating supercritical radial distribution functions and radially averaged structure factors temperature dependence.

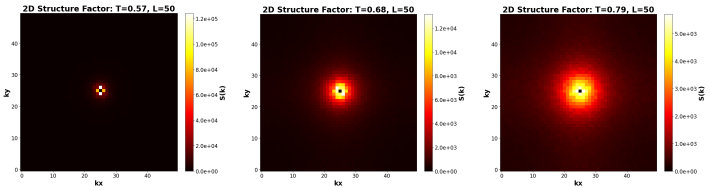
The radial distribution function $g(r)$, structure factor $S(K)$, and its radially averaged form ($S(|k|)$) were also calculated for these temperatures:



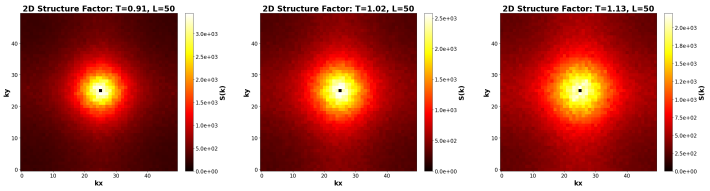
Radial Distribution Function For Supercritical Temps.

The radial distribution function varies around approximately $g(r) \approx 1$ with characteristic peaks between

neighboring particles and troughs in the voids between them. The heights of these peaks reflects the order of the system, for low T (close to T_c) the peaks are enhanced due to greater clustering effects. As temperature decreases, so do the values of the peaks, disrupting the ordering and approaching the random limit of $g(r) = 1$. The gradual damping of the peaks over distance (r) reflects the finite correlation length (ξ) of the lattice.

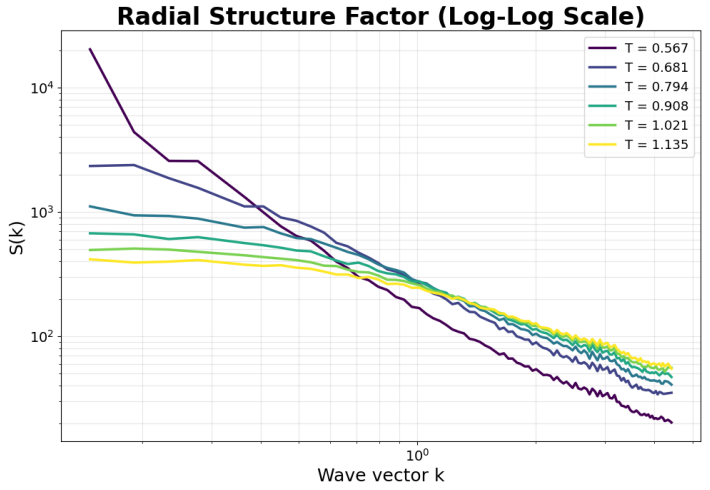


$T = 0.57 \approx \frac{T_c}{2}$ $T = 0.68$ $T = 0.79$



$T = 0.91$ $T = 1.02$ $T = 1.13 \approx 2T_c$

The 2D structure factors also demonstrate the progressive loss of correlations with increasing T. At $T \approx T_c$ there is an intense peak at $k_x, k_y = 0$, this peak then broadens and reduces in intensity as temperature increases. This again represents depreciation of ξ with $\uparrow T$, approaching a uniform distribution as $T \to \infty$. The circular symmetry confirms the absence of directional ordering, as expected in a gas model.



Log Radial Structure Factor Supercritical Temps

In order to better illustrate the power law decay of the 1D structure factor, it was plotted with a logarithmic scale. All temperatures exhibit a decay from a maximum at $k = 0$, with a greater initial $S(k)$ for $T \approx T_c$ and lower for higher T. The rate of decay also increases as $T \to T_c$ indicating the same temperature - correlation length behavior.

3.3 Investigating supercritical clustering behavior

Both $g(r)$ and $S(|k|)$ exhibit a peak at $r = 0$ and $k = 0$, which with distance or wavenumber. As $T \to T_c$ peaks are more pronounced, this reflects corelation lengths in the lattice. The oscillating behavior in $g(r)$ corresponds to nearest neighbor interactions and separations, this is not exhibited in $S(|k|)$ due to the fourier transform relationship between real and reciprocal space. $S(|k|)$ instead captures the dominant length scale ξ as a smooth decay.

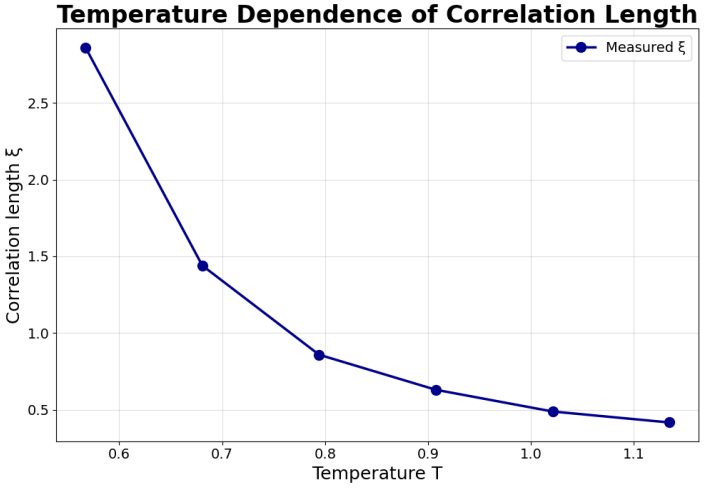
3.4 Investigating supercritical correlation lengths ξ

In order to calculate find corelation length (ξ) for each temperature, the full width at half maximum (FWHM) needed to be calculated. The FWHM is distance between the x values corresponding to the y values of the maximum peak half of the maximum peak in $S(|k|)$. From the FWHM, ξ can be calculated as $\xi = 1/FWHM$. The FWHM was calculated for each of the supercritical temperatures, and converted to a correlation length:

Temperature	FWHM	ξ
$0.5673 \approx T_c$	0.34957	2.861
0.6807	0.69437	1.440
0.7942	1.16361	0.859
0.9076	1.58486	0.631
1.0211	2.04311	0.489
1.1345	2.39199	0.418

Correlation Length ξ Analysis Of Supercritical Temperatures.

The correlation lengths were then plotted against each temperature:

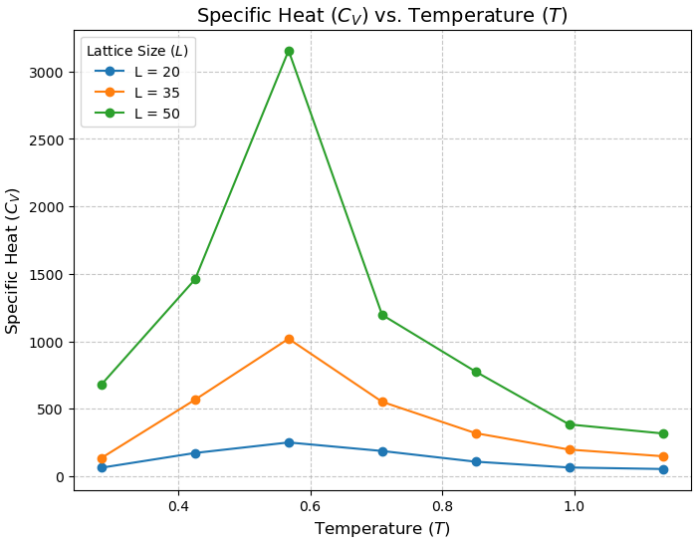


Correlation length (ξ) Vs Supercritical Temperatures.

The behavior exhibited is expected, decaying exponentially with temperature, again demonstrating the effect of increased disorder on correlation length and clustering.

4 Temperature and system size dependence of the specific heat

Next, the specific heat was calculated for 7 values of T and L values of 20, 35 and 50. As expected, there is a peak around the critical temperature of 0.56725. The size of this peak decreased with system size this is due to finite size scaling - as the system is smaller and smaller, it less accurately portrays the true critical behavior expected.



C_V vs T for varying L

I have not made use of Artificial Intelligence tools in completing this assessment beyond those of category 2 in the University's categorisation scheme.