Physics 129L: Classical Simulation (part1)

2D Classical Ising model (lattice Ising model)

The classical Ising model is a mathematical model used in statistical mechanics to study phase transitions in ferromagnetic materials. It was first proposed by the physicist Ernst Ising in 1925 as a simplified representation of the magnetic behavior of certain materials, such as iron. The Ising model has since become a fundamental tool in statistical mechanics and condensed matter physics.

The Ising model is typically defined on a lattice (or grid), which is a regular arrangement of discrete points in space. In this demonstration, we will be focusing on the 2D model. The structure is given below:

In [1]:
```
import numpy as np
import matplotlib.pyplot as plt
from IPython.display import display, clear_output
import time
```

2D Lattice generation

We can treat spins lattice as random variables, denoted as $\{S_{x,y}\}$. Let's define a function to initialize a random spin configuration. When working with a numpy array, we can naturally assign its dimensional index to be its special location, with value -1 or 1.

In [2]:
```
def initialize_spins(shape):
    spins = np.random.choice([-1, 1], size=shape)
    return spins
```

Ising Hamiltonian

Depending on the arrangement of spins, the Hamiltonian for the classical Ising model is often given by the following expression:

$$H = -J \sum_{\langle i,j \rangle} S_i S_j - B \sum_i S_i$$

where J is the coupling constant, representing the strength of the interaction between neighboring spins. $\langle i, j \rangle$ denotes a sum over pairs of nearest-neighbor spins, S_i represents the spins, and B represents an external magnetic field.

In [30]:
```
# Variables
J_value = 2  # coupling constant
B_value = 0 # external magnetic field
L_size =10    # lattice size
beta_value=0.05 # Temperature
```

In [4]:
```python
# Function to calculate the energy of the system
def net_energy(spins, J, B,print_val=False):
    energy = 0  # initial

    for i in range(spins.shape[0]):
        for j in range(spins.shape[1]):
            # Two neighboring spin coupling
            # Calculate indices of neighboring spins using modulo for periodic boundary conditions
            neighbor_down = spins[(i + 1) % spins.shape[0], j]
            neighbor_right = spins[i, (j + 1) % spins.shape[1]]

            # Interaction terms should be added to the energy
            energy -= J * spins[i, j] * (neighbor_down + neighbor_right)
            # External magnetic field
            energy -= B * spins[i, j]
            if print_val==True:


                print('*Index**********')
                print(i,j)
                print('*****Energy******')
                print(energy)
                print('**neighbor Index*********')
                print((i + 1) % spins.shape[0], j)
                print(i, (j + 1) % spins.shape[1])



    return energy

# Function to generate a random spin configuration of size L
def generate_random_spin_configuration(L):
    return np.random.choice([-1, 1], size=(L, L))
```

Example:

In [ ]:
```
spins = generate_random_spin_configuration(L_size)
print(spins)
energy = net_energy(spins,J=J_value,B=B_value)
print(energy)
fig, ax = plt.subplots()
im = ax.imshow(spins, cmap='binary', interpolation='none')
display(fig)
```

Statistical description of the Ising model

Let's look at various thermodynamic properties and statistical measures. The fundamential quatity is the partition function,

$$Z = \sum_{i,j} e^{-\beta H}$$

where $\beta = 1/k_B T$. For Ising model, we have,

$$Z = e^{-\beta\left(-J \sum_{\langle i,j \rangle} S_i S_j - B \sum_i S_i\right)}.$$

In particular, the joint distribution is a probability mass function (since we are working on a finite system), and it has a form,

$$P(S) = \frac{1}{Z} e^{-\beta H},$$

where $S = \{S_1, S_2, \cdots, S_L\}$, and each S defines a unique energy. As one can see, it is very hard to draw sample from this multi-variable distribution. It is easy to see that the total number of unique spin configurations exponentially grows with the system's dimension, 2^{L^2}, , making computations difficult for large system size $L > 20$.

In [5]:
```python
import numpy as np
from itertools import product


def generate_all_configurations(grid_size):
    # Generate all possible spin configurations
    spins = np.array(list(product([-1, 1], repeat=grid_size**2)))

    # Reshape spins to a 2D array for easier manipulation
    configurations = spins.reshape((-1, grid_size, grid_size))

    # Find unique configurations
    unique_configurations = np.unique(configurations, axis=0)

    return unique_configurations



def ising_boltzmann_weight(beta,J, B, spins):
    # J: coupling constant, B: external magnetic field, spins: 2D array representing spin configurati

    # Calculate the energy for the given spin configuration
    energy = net_energy(spins,J,B)

    # Calculate the Boltzmann weight
    weight = np.exp(-beta * energy)
#     print(energy)
#     print(weight)
    return weight,energy




def calculate_partition_function(beta, J, B, grid_size):
    # energy array
    energy_arry=np.zeros(int(2**(grid_size**2)))
    # probability array
    prob_arry=np.zeros(int(2**(grid_size**2)))
    # Generate all unique spin configurations
    unique_configurations = generate_all_configurations(grid_size)

    # Calculate Boltzmann weights for each unique configuration
    for i,config in enumerate(unique_configurations):
```

```
#           if i==6: # Example grid plot
#               fig, ax = plt.subplots()
#               im = ax.imshow(config, cmap='binary', interpolation='none')
#               display(fig)
#               print(f"The energy is:\n{energy}")

        weights,energy = ising_boltzmann_weight(beta, J, B, config)
        energy_arry[i]=energy
        prob_arry[i]=weights


    # Calculate the partition function as the sum of Boltzmann weights
    partition_function = np.sum(prob_arry)


    unique_values, index,counts = np.unique(prob_arry,return_index=True, return_counts=True)
    unique_energy=energy_arry[index]

    pdf=counts*unique_values/(partition_function)

    return partition_function,unique_energy,pdf
```

Example:

In [51]:
```
# Record the start time
start_time = time.time()
Z, energy_arry,pdf= calculate_partition_function(beta_value, J_value, B_value, L_size)
# Record the end time
end_time = time.time()

print(f"The partition function Z for the Ising model is: {Z}")
print(pdf)
print(energy_arry)


# Calculate the elapsed time
elapsed_time = end_time - start_time

# Print the elapsed time
print(f"Elapsed Time: {elapsed_time:.4f} seconds")

# fig, ax = plt.subplots(figsize=(8, 6))
# # Generate a list of colors using a colormap
# colors = plt.cm.viridis(np.linspace(0, 1, num_bars))

# # Create a bar plot
# ax.bar(energy_arry, pdf,color= colors)

# # Adding labels and title

# ax.grid(True)
# ax.set_title('Exact Boltzmann Distribution of Configurations for Ising Model')

# plt.show()
```

```
The partition function Z for the Ising model is: 43180521.331920676
[2.84790584e-06 2.54570562e-05 2.12340219e-04 1.20316844e-03
 5.84875478e-03 2.25405651e-02 6.70627521e-02 1.40572363e-01
 2.10215642e-01 2.20706644e-01 1.69722482e-01 9.53120138e-02
 4.36835874e-02 1.55709909e-02 5.08235943e-03 1.46057954e-03
 5.89837368e-04 1.03521642e-04 7.72180708e-05 6.87407908e-06]
[  60.   52.   44.   36.   28.   20.   12.    4.   -4.  -12.  -20.  -28.
  -36.  -44.  -52.  -60.  -68.  -76.  -84. -100.]
Elapsed Time: 701.4607 seconds
```

Gibbs Sampler on Ising model

Calculating the exact partition function and obtaining the exact boltzmann weight for a spin configuration becomes hard as we increase the system size. Let's consider a conditional distribution function: a variable S_i given the rest spins,

$$P(S_i|S_{\text{rest}}) = \frac{e^{\beta\left(-2JS_i\sum_{\langle j\rangle}S_j - B\sum_j S_j - BS_i\right)}}{1 + e^{\beta\left(-2JS_i\sum_{\langle j\rangle}S_j - B\sum_j S_j - BS_i\right)}}$$

A Gibbs sampling process involves drawing a sample from the distribution of that variable while fixing the values of all other variables.

In [6]:

```python
# Gibbs Update
import numpy as np

def Gibbs_sampler(spins, spin_index_x, spin_index_y, beta, J, B, grid_size):
    # Initialize energy to zero
    energy = 0

    # Two neighboring spin coupling
    # Calculate indices of neighboring spins using modulo for periodic boundary conditions
    neighbor_down = spins[(spin_index_x + 1) % grid_size, spin_index_y]
    neighbor_right = spins[spin_index_x, (spin_index_y + 1) % grid_size]

    neighbor_up = spins[(spin_index_x - 1) % grid_size, spin_index_y]
    neighbor_left = spins[spin_index_x, (spin_index_y - 1) % grid_size]


    # Interaction terms should be added to the energy
    energy -= J * spins[spin_index_x, spin_index_y] * (neighbor_down + neighbor_right+neighbor_up+nei
    # External magnetic field
    energy -= B * spins[spin_index_x, spin_index_y]

    # Calculate the weight factor using the Boltzmann factor
    weight_factor = np.exp(-2*beta * energy)

    # Calculate the conditional probability
    prob = weight_factor / (1 + weight_factor)

    # Generate a uniform random number between 0 and 1
    uniform_num = np.random.rand()

    # Update the spin value based on the conditional probability
    if uniform_num <= prob:
        new_spin_val = spins[spin_index_x, spin_index_y]
    else:
        new_spin_val = -spins[spin_index_x, spin_index_y]

    # Return the calculated energy, conditional probability, and the new spin value
    return energy, prob, new_spin_val

# spin_index_x=0
# spin_index_y=0

# # Example Spin
```

```
# spins = generate_random_spin_configuration(L_size)
# print(spins)

# energy_c,prob_c,new_spin_val_c=Gibbs_sampler(spins,spin_index_x,spin_index_y, beta=beta_value,J=J_v
# print(new_spin_val_c)
# print(prob_c)
```

Sampler Stepping

For each variable in the distribution, sample a new value from its conditional distribution given the current values of all other variables (e.g. in our case, for each spin site).

In [7]:

```
# Function to perform a Gibbs stepping
def Gibbs_step(spins_init, beta, J, B, grid_size,burnin_=13000,sample_size=5000):
    spins=spins_init
    burnin_step=0
    s=0
    sample_gibbs_energy=[]
    while burnin_step<=burnin_:
        for i in range(grid_size):
            for j in range(grid_size):
                energy_c,prob_c,new_spin_val_c=Gibbs_sampler(spins,spin_index_x=i,spin_index_y=j, bet
                spins[i,j]=new_spin_val_c
        burnin_step+=1

    while s<sample_size:
        for i in range(grid_size):
            for j in range(grid_size):
                energy_c,prob_c,new_spin_val_c=Gibbs_sampler(spins,spin_index_x=i,spin_index_y=j, bet
                spins[i,j]=new_spin_val_c

        weights,energy = ising_boltzmann_weight(beta, J, B, spins)
        sample_gibbs_energy.append(energy)
                #spins[i,j]=new_spin_val_c
        s+=1
    return sample_gibbs_energy
```

Example:

In [ ]:

```
# Record the start time
start_time = time.time()


spins = generate_random_spin_configuration(L_size)
print(spins)

energy_arry_MC=Gibbs_step(spins_init=spins,beta=beta_value,J=J_value, B=B_value,grid_size=L_size,burn

net_size=len(energy_arry_MC)
energy_arry_MC, count_MC = np.unique(energy_arry_MC, return_counts=True)

pdf_MC=count_MC/net_size

pdf_MC_full=np.zeros(len(pdf))
for i in range(0,len(energy_arry_MC)):
    indices = np.where(energy_arry_MC[i]==energy_arry)[0]
    pdf_MC_full[indices]=pdf_MC[i]

# Record the end time
end_time = time.time()


# Calculate the elapsed time
elapsed_time = end_time - start_time

# Print the elapsed time
print(f"Elapsed Time: {elapsed_time:.4f} seconds")



# Create a subplot with 1 row and 3 columns, specifying the width ratios
fig = plt.figure(figsize=(10, 10))
gs = fig.add_gridspec(2, 2, height_ratios=[1, 1])

num_bars = len(pdf_MC_full)

# Generate a list of colors using a colormap
colors = plt.cm.viridis(np.linspace(0, 1, num_bars))


# First subplot (1 row, 3 columns, first plot)
```

```python
ax1 = fig.add_subplot(gs[0])
ax1.bar(energy_arry, pdf_MC_full,color= colors)

ax1.set_xlabel('Energy')
ax1.set_ylabel('Probability')
ax1.grid(True)
ax1.set_title('Simulated Boltzmann Distribution for Ising Model')


# Second subplot (1 row, 3 columns, second plot)
ax2 = fig.add_subplot(gs[1])
ax2.bar(energy_arry, pdf ,color= colors)
ax2.set_xlabel('Energy')
ax2.set_ylabel('Probability')
ax2.grid(True)
ax2.set_title('Exact Boltzmann Distribution for Ising Model')

# Third subplot (1 row, 3 columns, third plot - elongated)
ax3 = fig.add_subplot(gs[1, :])
ax3.bar(energy_arry, np.abs(pdf_MC_full-pdf),color= colors )
ax3.set_xlabel('Energy')
ax3.set_ylabel('Probability (percent difference)')
ax3.grid(True)
ax3.set_title(' Simulated v.s. Exact')
```

magnetization, Landau theory, and phase transition of the Ising model

Magnetization is a measure of the average magnetic moment per spin in a given direction. In the context of the Ising model, the magnetic moment is represented by the sum of the spins. The **magnetization** M is defined as:

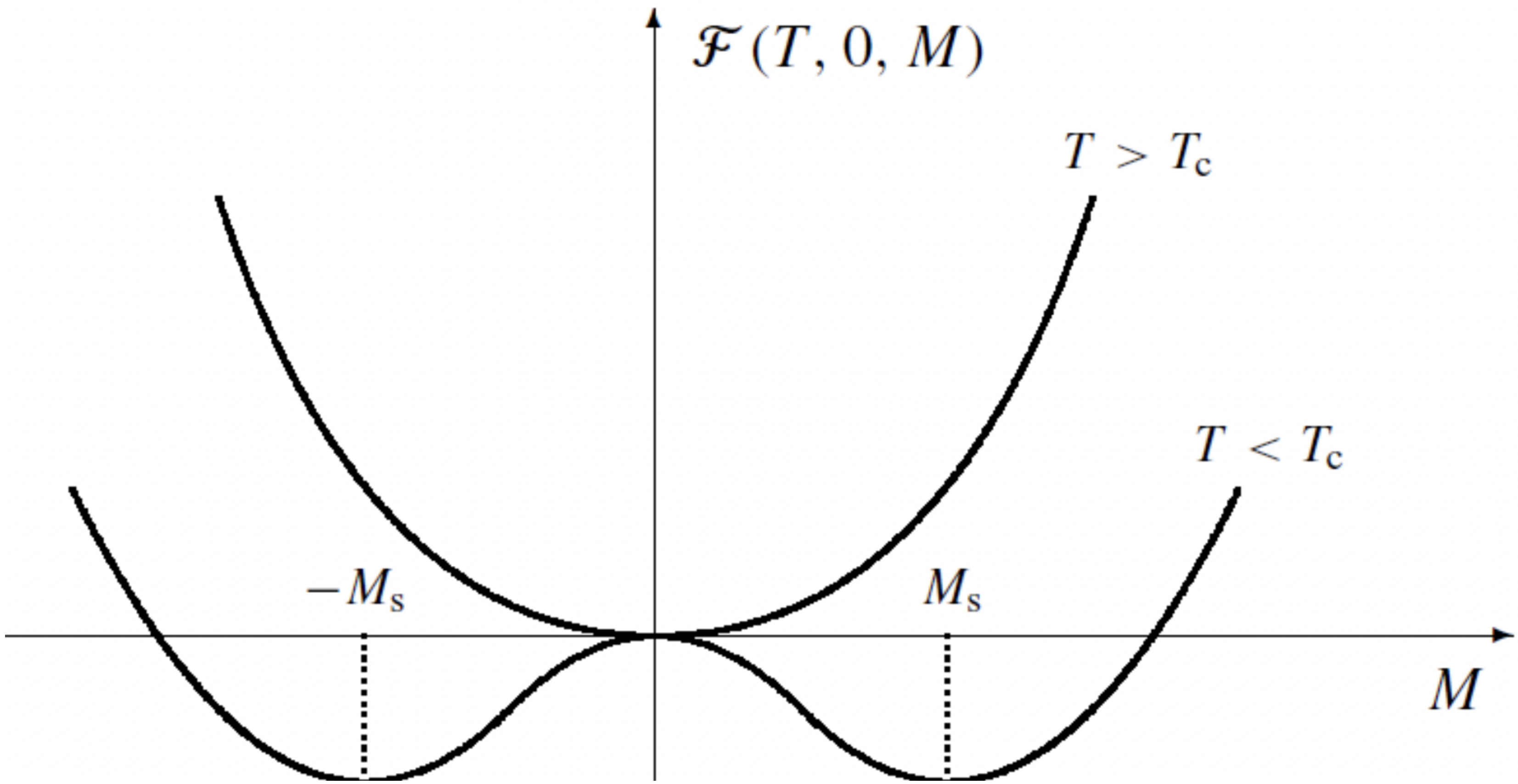
$$M = \frac{1}{N} \sum_i S_i$$

where $N = L^2$ is the total number of spins. In the absence of an external magnetic field (B=0), the Ising model exhibits a spontaneous magnetization at low temperatures, where most spins tend to align in the same direction. In the Ising model, the magnetization serves as an order parameter that indicates the presence of a magnetic order in the system. The order parameter is often used to characterize the different phases of the model, especially in the study of phase transitions.

Landau theory, in the context of phase transitions, is a phenomenological approach that describes the free energy of a system near a critical point. It provides a framework for understanding the symmetry-breaking mechanisms and the emergence of order parameters. When near a second-order phase transition, the **Landau free energy** can often be written as a Taylor expansion in terms of an order parameter, typically the magnetization

$$F = F_0 + a(T - T_c)M^2 + bM^4 + \ldots$$

where F_0 is the free energy at the critical temperature (T_c), a and b are phenomenological coefficients, T is the temperature.



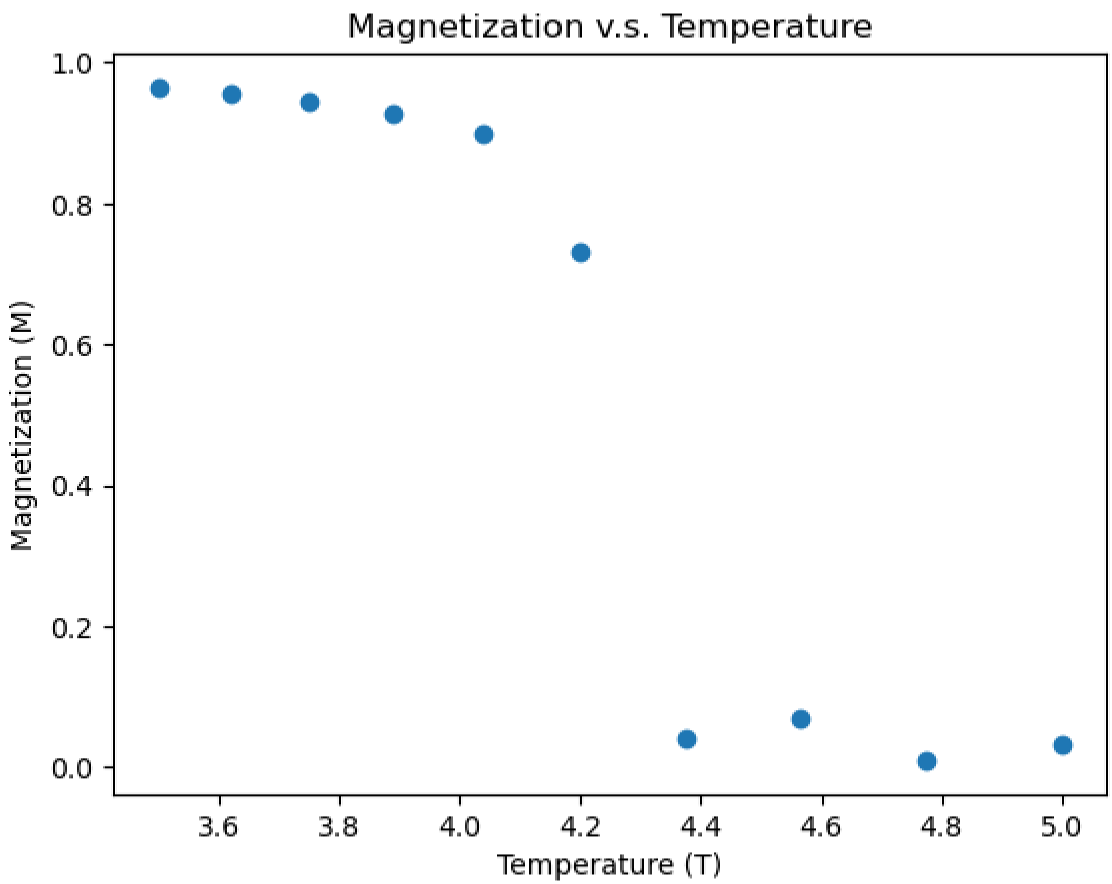
Example: magnetization at different temperature

In [20]:

```python
# Function to perform a Gibbs stepping with magnetization
def Gibbs_step_with_M(spins_init, beta_arry, J, B, grid_size,burnin_=13000,sample_size=5000):
    sample_M=[]
    for f in range(0,len(beta_arry)):
        beta=beta_arry[f]
        spins=spins_init
        burnin_step=0
        s=0
        M=0

        while burnin_step<=burnin_:
            for i in range(grid_size):
                for j in range(grid_size):
                    energy_c,prob_c,new_spin_val_c=Gibbs_sampler(spins,spin_index_x=i,spin_index_y=j,
                    spins[i,j]=new_spin_val_c
            burnin_step+=1

        while s<sample_size:
            for i in range(grid_size):
                for j in range(grid_size):
                    energy_c,prob_c,new_spin_val_c=Gibbs_sampler(spins,spin_index_x=i,spin_index_y=j,
                    spins[i,j]=new_spin_val_c

            M+=np.sum(spins)/(grid_size**2)

            s+=1
        print(M)
        sample_M.append(M/sample_size)

    return sample_M

beta_arry=np.linspace(0.2,1/3.5,10)

T_array=1/beta_arry

spins = generate_random_spin_configuration(L_size)
sample_M=energy_arry_MC=Gibbs_step_with_M(spins_init=spins,beta_arry=beta_arry,J=J_value, B=B_value,g
# Create scatter plot
plt.scatter(T_array, np.abs(sample_M), color='tab:blue', marker='o' )

# Add labels and title
plt.xlabel('Temperature (T)')
plt.ylabel('Magnetization (M)')
```

```python
plt.title('Magnetization v.s. Temperature')


# Show the plot
plt.show()
```

```
-279.5400000000005
86.38000000000038
631.9400000000003
365.2599999999956
6575.319999999883
8080.59999999959
8338.83999999944
8487.959999999355
8597.719999999284
8680.81999999924
```



In [ ]:

MC convergence and lattice size

Let's look at the MC convergence at different lattice size.

In [40]:

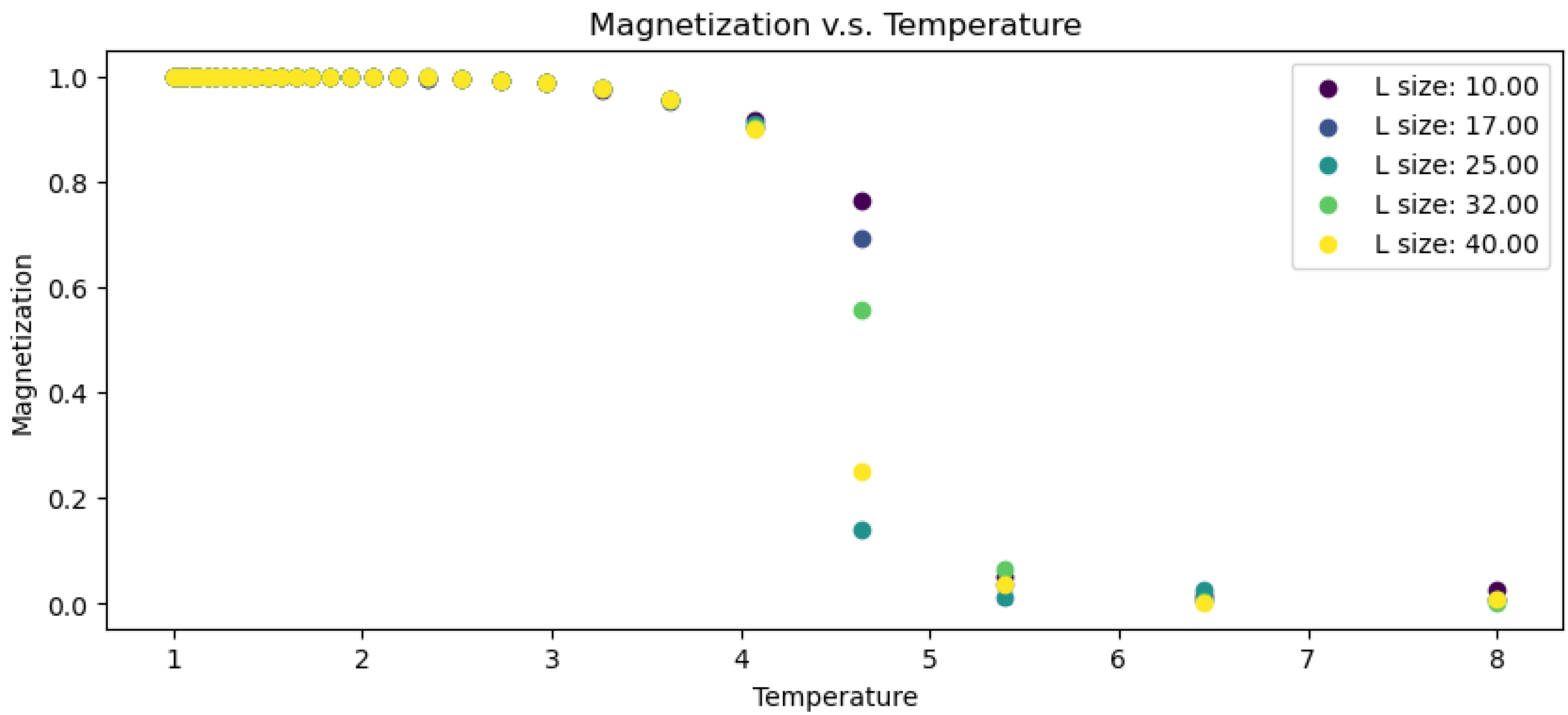
```python
# Create a figure and axis objects
fig, axs = plt.subplots(1, 1, figsize=(10, 4))

L_arry=np.linspace(10,40,5)
# Generate a list of colors using a colormap
colors = plt.cm.viridis(np.linspace(0, 1, len(L_arry)))

for g in range(0,len(L_arry)):
    L_size =int(L_arry[g])    # lattice size

    beta_arry=np.linspace(1/8,1/1,30)

    T_array=1/beta_arry

    spins = generate_random_spin_configuration(L_size)
    sample_M=Gibbs_step_with_M(spins_init=spins,beta_arry=beta_arry,J=J_value, B=B_value,grid_size=L_
    # Create scatter plot
    axs.scatter(T_array, np.abs(sample_M), color=colors[g], marker='o', label=f'L size: {L_size:.2f}'
axs.axvline(x=Tc, color='tab:red', linestyle='--', label=f'Critical Temperature (Tc): {Tc:.2f}')


# Add labels and title
axs.set_xlabel('Temperature')
axs.set_ylabel('Magnetization')
axs.set_title('Magnetization v.s. Temperature')
axs.legend()

# Show the plot
plt.show()
```

-12.900000000000013
7.999999999999996
-26.42000000000002
382.0199999999998
459.35999999999916
478.79999999999984
486.6800000000002
493.56000000000057
496.74000000000063
497.6800000000004
498.5000000000003
499.18000000000023
499.42000000000024
499.72000000000014
499.7800000000001
499.8
499.94000000000005
499.90000000000003
499.98
500.0
500.0
500.0
500.0
500.0
500.0
500.0
500.0
500.0
500.0
500.0
3.9307958477508644
4.2006920415225055
-17.757785467127984
-345.51557093425635
-450.9826989619379
-476.98961937716325
-488.844290657439
-493.70242214532846
-496.29757785467075
-497.9792387543253
-498.60207612456776
-499.3910034602079
-499.6055363321802

-499.70242214532885
-499.8339100346022
-499.86159169550183
-499.96539792387546
-500.0
-499.99307958477505
-499.99307958477505
-500.0
-499.9792387543253
-499.9861591695502
-500.0
-499.99307958477505
-500.0
-500.0
-500.0
-500.0
-500.0
3.801600000000002
12.870399999999986
6.022399999999997
-70.29120000000003
-455.0464
-479.0143999999999
-488.31999999999897
-493.5071999999991
-496.7104000000008
-498.00000000000136
-498.7072000000015
-499.2800000000007
-499.4752000000006
-499.71200000000044
-499.8144000000003
-499.92640000000017
-499.9040000000001
-499.9680000000001
-499.97440000000006
-499.9904
-499.9936
-499.9936
-500.0
-499.9936
-499.9968
-499.9968

-500.0
-500.0
-500.0
-500.0
1.21484375
2.853515625
-32.841796875
279.17578125
450.685546875
477.369140625
488.658203125
493.8203125
496.349609375
497.96484375
498.671875
499.17578125
499.517578125
499.708984375
499.818359375
499.9140625
499.9296875
499.9609375
499.974609375
499.98046875
499.982421875
499.9921875
499.998046875
500.0
499.998046875
499.99609375
500.0
500.0
500.0
499.998046875
4.111250000000003
-1.5899999999999987
-18.83000000000001
124.77125
450.11999999999944
477.3887500000002
488.28625000000056
493.5237499999997
496.4687499999988

497.93749999999784
498.75124999999764
499.2637499999973
499.56749999999784
499.7299999999985
499.8162499999985
499.891249999999
499.9487499999996
499.96874999999966
499.98249999999985
499.9774999999998
499.99249999999995
499.99875
499.99749999999995
499.995
499.99875
500.0
500.0
500.0
500.0
500.0



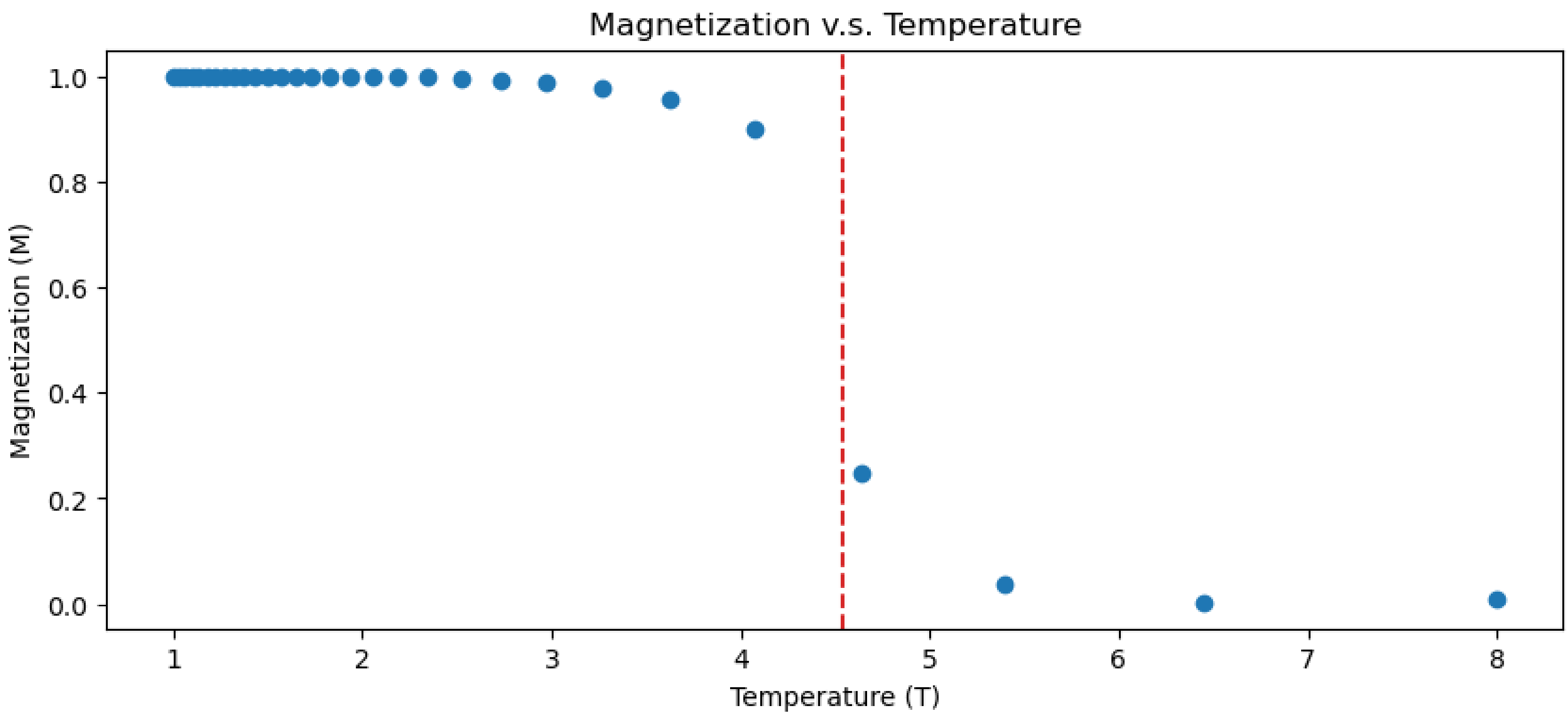
The critical temperature

In 2D Ising model, the critical temperature can be calculated via the following,

$$T_C = \frac{2J}{\log(1+\sqrt{2})}.$$

In [42]:

```python
# Define the power-law function
Tc=2*J_value/(np.log(1+np.sqrt(2)))

fig, axs = plt.subplots(1, 1, figsize=(10, 4))

plt.scatter(T_array, np.abs(sample_M), color='tab:blue', marker='o' )

# Add labels and title
plt.xlabel('Temperature (T)')
plt.ylabel('Magnetization (M)')
plt.title('Magnetization v.s. Temperature')

# Show the plot
plt.show()
```



Magnetic Field dependence: magnetization of the 2D Ising model

Let's look at the MC convergence at different lattice size.

In [13]:

```
# Function to perform a Gibbs stepping with magnetization
def Gibbs_step_with_M_vary_B(spins_init, beta, J, B_array, grid_size,burnin_=13000,sample_size=5000):
    sample_M=[]
    for f in range(0,len(B_array)):
        B=B_array[f]
        spins=spins_init
        burnin_step=0
        s=0
        M=0

        while burnin_step<=burnin_:
            for i in range(grid_size):
                for j in range(grid_size):
                    energy_c,prob_c,new_spin_val_c=Gibbs_sampler(spins,spin_index_x=i,spin_index_y=j,
                    spins[i,j]=new_spin_val_c
            burnin_step+=1

        while s<sample_size:
            for i in range(grid_size):
                for j in range(grid_size):
                    energy_c,prob_c,new_spin_val_c=Gibbs_sampler(spins,spin_index_x=i,spin_index_y=j,
                    spins[i,j]=new_spin_val_c

            M+=np.sum(spins)/(grid_size**2)

            s+=1
        print(M)
        sample_M.append(M/sample_size)

    return sample_M
```

Example

In [ ]:

```
B_arry=np.linspace(-50,50,100)

beta_value=0.05 # Temperature
L_size =5

spins = generate_random_spin_configuration(L_size)
sample_M=energy_arry_MC=Gibbs_step_with_M_vary_B(spins_init=spins,beta=beta_value,J=J_value, B_array=
# Create scatter plot
plt.scatter(B_arry, np.sign(B_arry)*np.abs(sample_M), color='tab:blue', marker='o' )

# Add labels and title
plt.xlabel('Temperature (T)')
plt.ylabel('Magnetization (M)')
plt.title('Magnetization v.s. Temperature')


# Show the plot
plt.show()
```

MC convergence and lattice size

Let's look at the MC convergence at different lattice size.

In [54]:
```python
# Create a figure and axis objects
fig, axs = plt.subplots(1, 1, figsize=(10, 4))

L_arry=np.linspace(10,40,5)
# Generate a list of colors using a colormap
colors = plt.cm.viridis(np.linspace(0, 1, len(L_arry)))

for g in range(0,len(L_arry)):
    L_size =int(L_arry[g])    # lattice size

    B_arry=np.linspace(-50,50,100)

    spins = generate_random_spin_configuration(L_size)
    # Create scatter plot

    sample_M=Gibbs_step_with_M_vary_B(spins_init=spins,beta=beta_value,J=J_value, B_array=B_arry,grid
    axs.scatter(B_arry, np.sign(B_arry)*np.abs(sample_M), color=colors[g], marker='o', label=f'L size

# Add labels and title
axs.set_xlabel('Magnetic Field')
axs.set_ylabel('Magnetization')
axs.set_title('Magnetization v.s. Magnetic Field')
axs.legend()

# Show the plot
plt.show()
```

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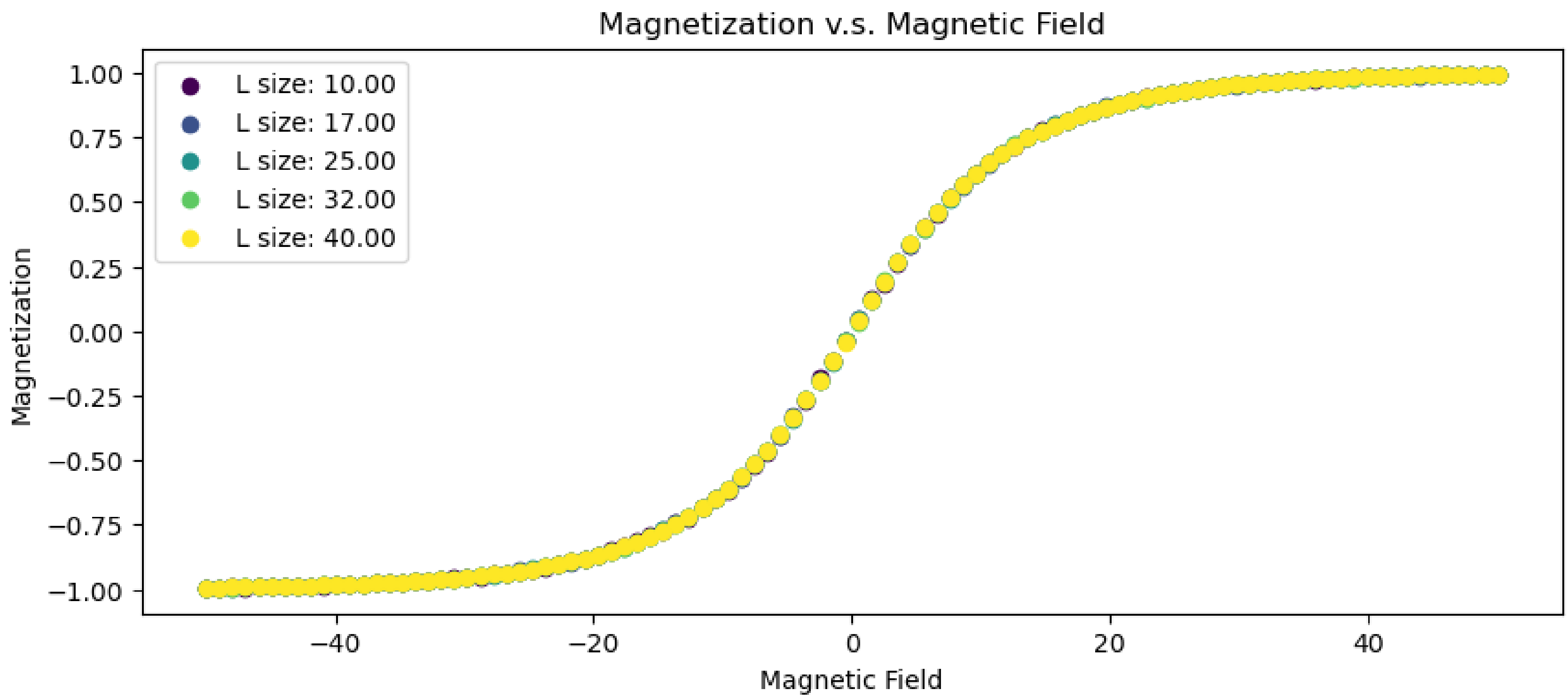

Specific Heat of the 2D Ising model

The specific heat (C_v) measures the amount of heat energy required to change the temperature of a substance by a unit temperature. It can be related to the variance of the energy in the 2D Ising model, e.g.,

$$C_v = \frac{\beta^2}{N}\left(\langle E^2 \rangle - \langle E \rangle^2\right),$$

where N is the total number of spins.

In [15]:

```
# Function to perform a Gibbs stepping with magnetization
def Gibbs_step_with_E(spins_init, beta_arry, J, B, grid_size,burnin_=13000,sample_size=5000):
    sample_M=[]
    sample_C=[]
    for f in range(0,len(beta_arry)):
        beta=beta_arry[f]
        spins=spins_init
        burnin_step=0
        s=0
        M=0
        E=0 #define average energy
        E_square=0
        while burnin_step<=burnin_:
            for i in range(grid_size):
                for j in range(grid_size):
                    energy_c,prob_c,new_spin_val_c=Gibbs_sampler(spins,spin_index_x=i,spin_index_y=j,
                    spins[i,j]=new_spin_val_c
            burnin_step+=1

        while s<sample_size:
            for i in range(grid_size):
                for j in range(grid_size):
                    energy_c,prob_c,new_spin_val_c=Gibbs_sampler(spins,spin_index_x=i,spin_index_y=j,
                    spins[i,j]=new_spin_val_c

            M+=np.sum(spins)/(grid_size**2)

            s+=1
            current_delta_E=net_energy(spins, J, B,print_val=False)
            E+=np.abs(current_delta_E)
            E_square+=current_delta_E**2
        print(M)
        sample_M.append(M/sample_size)

        E_2=(E/sample_size)**2
        E2=E_square/sample_size

        C=(1/grid_size**2)*beta**2*(E2-E_2)
        sample_C.append(C)
        print(C)
        print('---------')
```

```
    return sample_C
```

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---------
-23.759999999999994
0.14307988171660715
---------
21.600000000000005
0.12418177927139604
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-5.439999999999996
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0.0710889439159676
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-1.6800000000000144
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6.160000000000001
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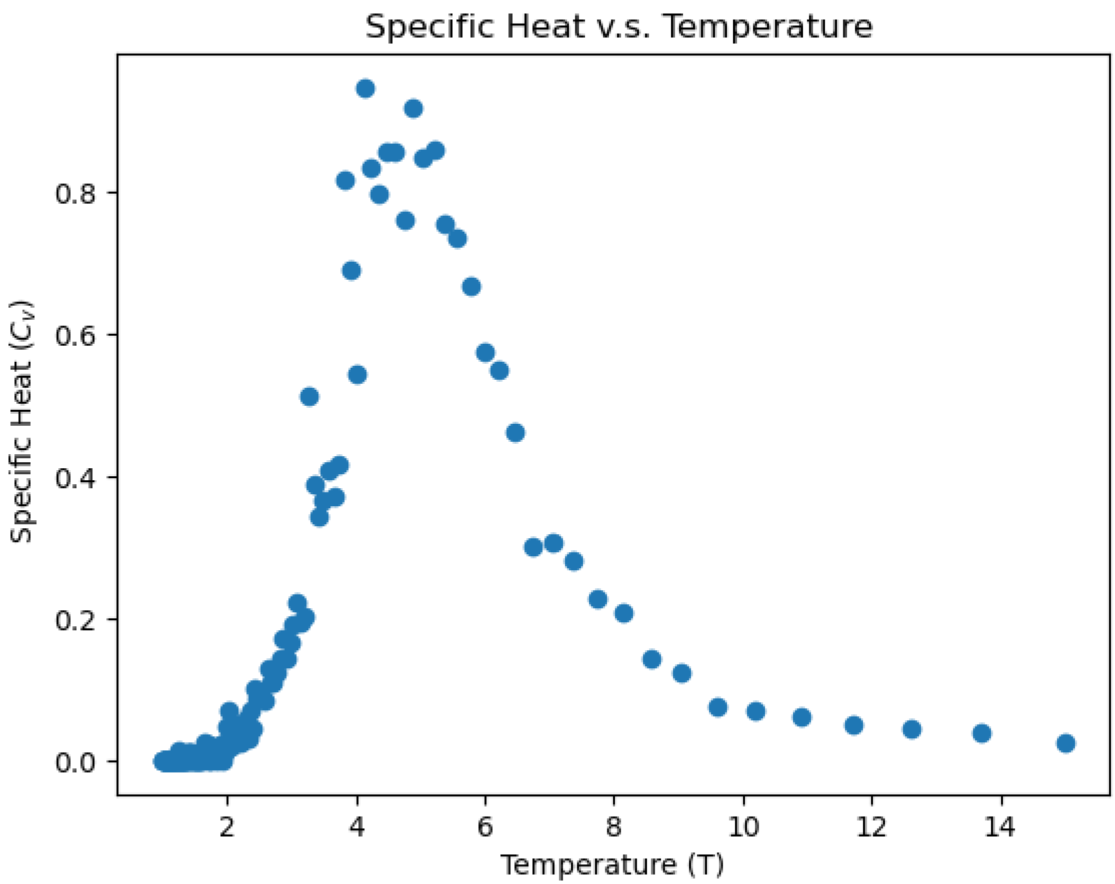
---------
```



Specific Heat v.s. Temperature
Specific Heat (C_v)
Temperature (T)
0.0
0.2
0.4
0.6
0.8
2
4
6
8
10
12
14

Example

In [ ]:

```
beta_arry=np.linspace(1/1,1/15,150)

T_array=1/beta_arry
L_size =5

spins = generate_random_spin_configuration(L_size)
sample_C=Gibbs_step_with_E(spins_init=spins,beta_arry=beta_arry,J=J_value, B=B_value,grid_size=L_size
# Create scatter plot
plt.scatter(T_array, (sample_C), color='tab:blue', marker='o' )

# Add labels and title
plt.xlabel('Temperature (T)')
plt.ylabel(' Specific Heat ($C_v$)')
plt.title(' Specific Heat v.s. Temperature')


# Show the plot
plt.show()
```

Magnetic Susceptibility of the 2D Ising model

Similarly, the magnetic susceptibility quantifies the material's ability to become magnetized per unit change in the external magnetic field strength,

$$\chi = \frac{\beta}{N}\left(\langle M^2\rangle - \langle M\rangle^2\right).$$

In [48]:

```python
# Function to perform a Gibbs stepping with magnetization
def Gibbs_step_with_MS(spins_init, beta_arry, J, B, grid_size,burnin_=13000,sample_size=5000):
    sample_M=[]
    sample_Chi=[]
    for f in range(0,len(beta_arry)):
        beta=beta_arry[f]
        spins=spins_init
        burnin_step=0
        s=0
        M=0
        MS=0 #define average energy
        MS_square=0
        while burnin_step<=burnin_:
            for i in range(grid_size):
                for j in range(grid_size):
                    energy_c,prob_c,new_spin_val_c=Gibbs_sampler(spins,spin_index_x=i,spin_index_y=j,
                    spins[i,j]=new_spin_val_c
            burnin_step+=1

        while s<sample_size:
            for i in range(grid_size):
                for j in range(grid_size):
                    energy_c,prob_c,new_spin_val_c=Gibbs_sampler(spins,spin_index_x=i,spin_index_y=j,
                    spins[i,j]=new_spin_val_c

            M+=np.sum(spins)/(grid_size**2)

            s+=1

            MS+=np.abs(np.sum(spins) )
            MS_square+=((np.sum(spins))**2)
        print(M)
        print(MS)
        print(MS_square)
        sample_M.append(M/sample_size)

        MS_2=(MS/sample_size)**2
        MS2=MS_square/sample_size

        Chi=1/(grid_size**2)*beta*(MS2-MS_2)
        print(Chi)
        sample_Chi.append(Chi)
```

```
        print('---------')

    return sample_Chi
```

Example

In [50]:

```
beta_arry=np.linspace(1/1,1/15,150)

T_array=1/beta_arry
L_size =5

spins = generate_random_spin_configuration(L_size)
sample_Chi=Gibbs_step_with_MS(spins_init=spins,beta_arry=beta_arry,J=J_value, B=B_value,grid_size=L_s
# Create scatter plot
plt.scatter(T_array, (sample_Chi), color='tab:red', marker='o' )

# Add labels and title
plt.xlabel('Temperature (T)')
plt.ylabel(' Magnetic Susceptibility ($\chi$)')
plt.title('Magnetic Susceptibility v.s. Temperature')


# Show the plot
plt.show()
```

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500.0
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499.92
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312404
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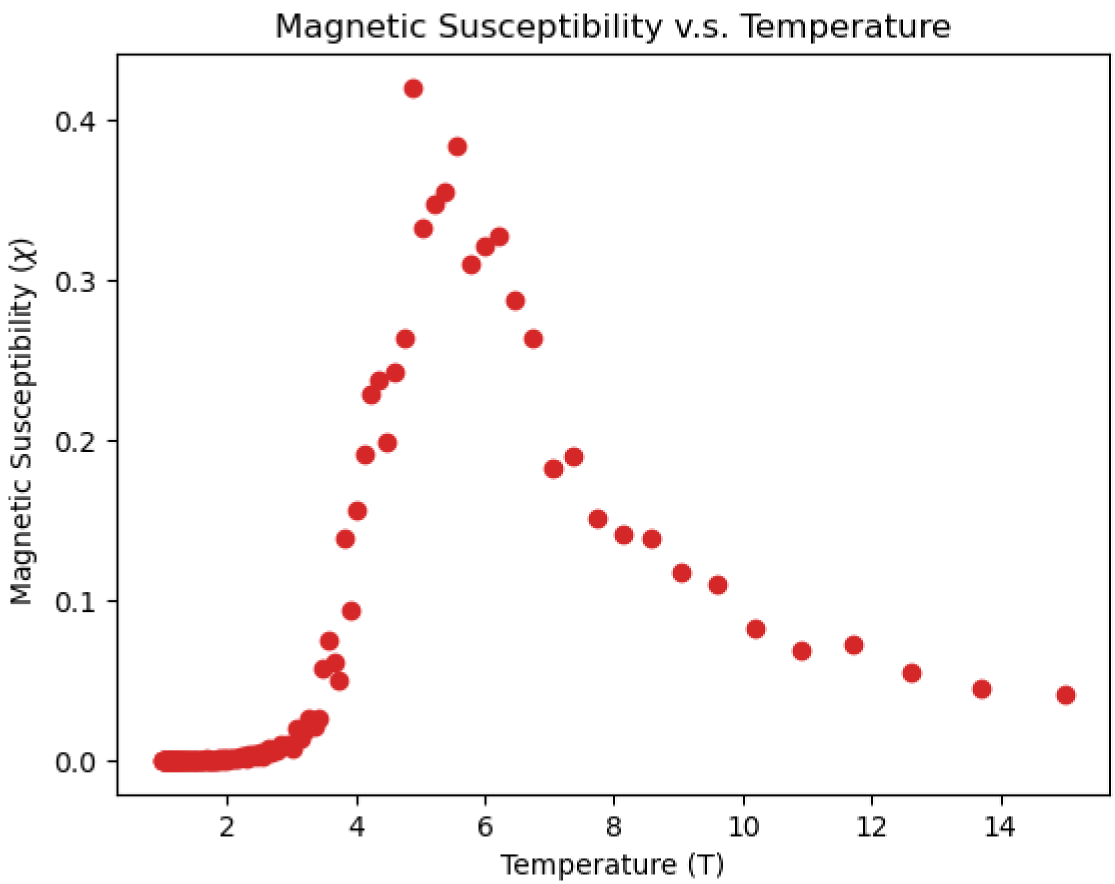
Magnetic Susceptibility v.s. Temperature
Magnetic Susceptibility (χ)
0.4
0.3
0.2
0.1
0.0
2
4
6
8
10
12
14
Temperature (T)

```
In [ ]:
```