Blog

Ising Model

Model of phase transition in Statistical Physics

May 22, 2014 • 10 min read

Statistical Physics

View On GitHub launch binder Open in Colab

Ising model

The Ising Hamiltonian can be written as,

$$\mathcal{H} = -J \sum_{\langle ij \rangle} S_i S_j.$$

- The spins S_i can take values ± 1,
- $\langle ij \rangle$ implies nearest-neighbor interaction only,
- $J > 0$ is the strength of exchange interaction.

The system undergoes a 2nd order phase transition at the critical temperature T_c. For temperatures less than T_c, the system magnetizes, and the state is called the ferromagnetic or the ordered state. This amounts to a globally ordered state due to the presence of local interactions between the spin. For temperatures greater than T_c, the system is in the disordered or the paramagnetic state. In

this case, there are no long-range correlations between the spins.

The order parameter

$$m = \frac{\langle S \rangle}{N},$$

for this system is the average magnetization. The order parameter distinguishes the two phases realized by the systems. It is zero in the disordered state, while non-zero in the ordered, ferromagnetic, state.

The one dimensional (1D) Ising model does not exhibit the phenomenon of phase transition while higher dimensions do. This can be argued based on arguments, due to Peierls, related to the net change in free energy, $F = E - TS$. Here E and S are, respectively, the energy and entropy of the system. We estimate the net change in free energy for introducing a disorder in an otherwise ordered system. The ordered state can only be stable if the net change in free energy is positive, $\Delta F > 0$, for any non-zero temperature.

1D Ising model: Introducing a domain wall (defect) in an ordered state increases the energy by $4J$, while the entropy change is $k_B \ln N$, due to N choices to introduce the domain. So net change in the free energy, $\Delta F = 4J - k_B T \ln N$, is always negative for $N \to \infty$. Thus, the system prefers a disordered state. So, there is no spontaneous symmetry breaking in 1D for an infinite Ising chain. This argument can be generalized for any domain of length L and higher dimensions.

2D Ising model: For two and higher dimensions, we can introduce islands of defects, which cost only at the boundaries, and are thus, proportional to the perimeter $L = \varepsilon N^2$, where $0 < \varepsilon < 1$. In 2D, the number of islands scale as $3^{\varepsilon N^2}$, while $\Delta E = \varepsilon 4 J N^2$. ΔF is then $\varepsilon 4 J N^2 - k_B T \ln(N^2 3^{\varepsilon N^2})$. This gives a rough estimate of the critical temperature $T_c \sim J/k_B$.

Monte-Carlo simulation of 2D Ising model

The following code simulates the Ising model in 2D using the Metropolis algorithm. The main steps of Metropolis algorithm are:

1. Prepare an initial configuration of N spins
2. Flip the spin of a randomly chosen lattice site.
3. Calculate the change in energy dE.
4. If dE < 0, accept the move. Otherwise accept the move with probability exp^{-dE/T}. This satisfies the detailed balance condition, ensuring a final equilibrium state.
5. Repeat 2-4.

In the code below, we have estimated and plotted energy, magnetization, specific heat and susceptibility of the system.

```
%matplotlib inline
import numpy as np
from numpy.random import rand
import matplotlib.pyplot as plt
```

```
#---------------------------------------------------------------------
##  BLOCK OF FUNCTIONS USED IN THE MAIN CODE
#---------------------------------------------------------------------
def initialstate(N):
    ''' generates a random spin configuration for initial condition'''
    state = 2*np.random.randint(2, size=(N,N))-1
    return state


def mcmove(config, beta):
    '''Monte Carlo move using Metropolis algorithm '''
    for i in range(N):
        for j in range(N):
                a = np.random.randint(0, N)
                b = np.random.randint(0, N)
                s =  config[a, b]
                nb = config[(a+1)%N,b] + config[a,(b+1)%N] + config[(a-1)%N,b] + config[a,(b-1)%N]
                cost = 2*s*nb
                if cost < 0:
                    s *= -1
                elif rand() < np.exp(-cost*beta):
                    s *= -1
                config[a, b] = s
```

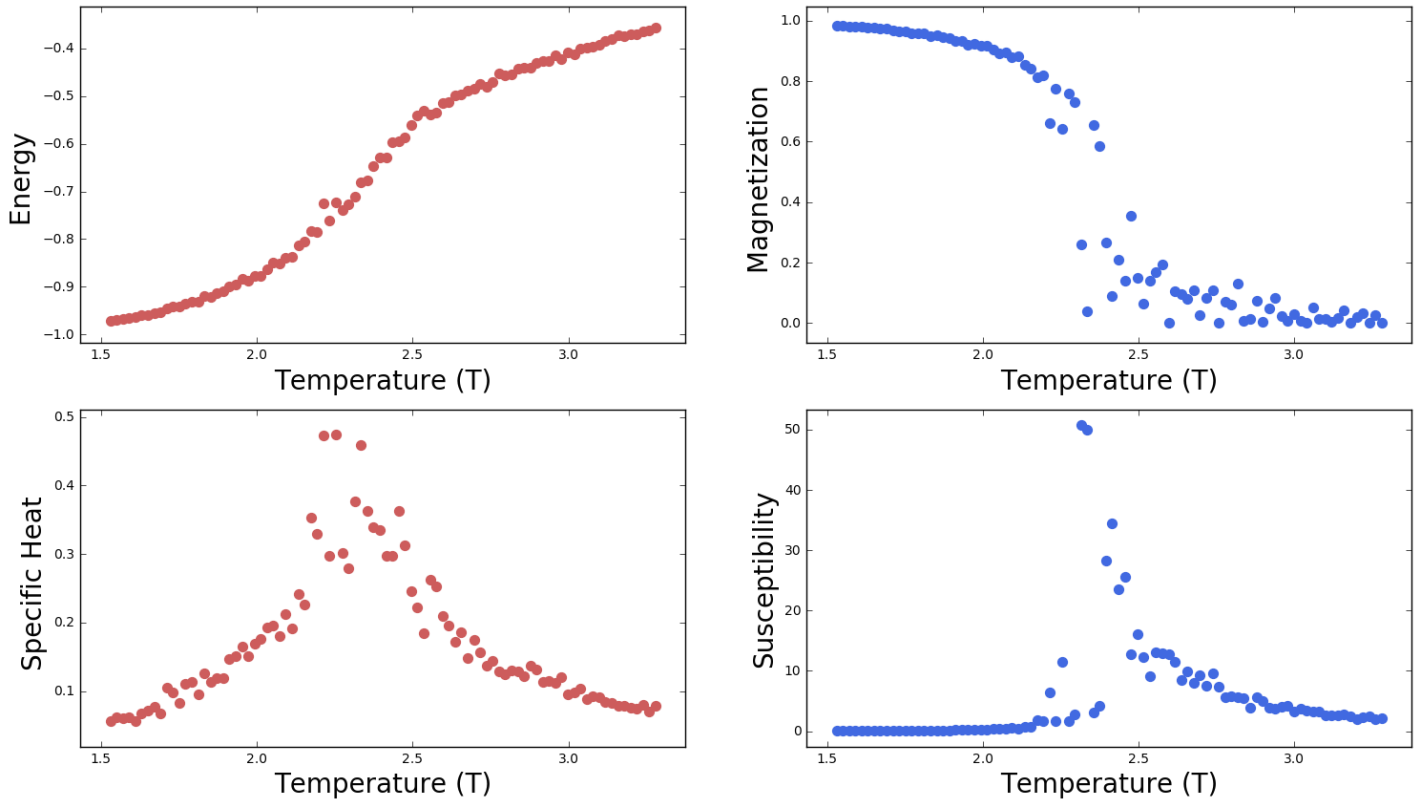
```
    return config


def calcEnergy(config):
    '''Energy of a given configuration'''
    energy = 0
    for i in range(len(config)):
        for j in range(len(config)):
            S = config[i,j]
            nb = config[(i+1)%N, j] + config[i,(j+1)%N] + config[(i-1)%N, j] + config[i,(j-1)%N]
            energy += -nb*S
    return energy/4.


def calcMag(config):
    '''Magnetization of a given configuration'''
    mag = np.sum(config)
    return mag
```

```
## change these parameters for a smaller (faster) simulation
nt      = 32         #  number of temperature points
N       = 10         #  size of the lattice, N x N
eqSteps = 1024       #  number of MC sweeps for equilibration
mcSteps = 1024       #  number of MC sweeps for calculation

T       = np.linspace(1.53, 3.28, nt);
E,M,C,X = np.zeros(nt), np.zeros(nt), np.zeros(nt), np.zeros(nt)
n1, n2  = 1.0/(mcSteps*N*N), 1.0/(mcSteps*mcSteps*N*N)
# divide by number of samples, and by system size to get intensive values
```

```
#---------------------------------------------------------------------
#  MAIN PART OF THE CODE
#---------------------------------------------------------------------
for tt in range(nt):
    E1 = M1 = E2 = M2 = 0
    config = initialstate(N)
    iT=1.0/T[tt]; iT2=iT*iT;

    for i in range(eqSteps):         # equilibrate
        mcmove(config, iT)           # Monte Carlo moves

    for i in range(mcSteps):
        mcmove(config, iT)
        Ene = calcEnergy(config)     # calculate the energy
        Mag = calcMag(config)        # calculate the magnetisation

        E1 = E1 + Ene
        M1 = M1 + Mag
        M2 = M2 + Mag*Mag
        E2 = E2 + Ene*Ene

    E[tt] = n1*E1
```

```
    E[tt] = n1*E1
    M[tt] = n1*M1


    C[tt] = (n1*E2 - n2*E1*E1)*iT2
    X[tt] = (n1*M2 - n2*M1*M1)*iT
```

```
f = plt.figure(figsize=(18, 10)); # plot the calculated values

sp =  f.add_subplot(2, 2, 1 );
plt.scatter(T, E, s=50, marker='o', color='IndianRed')
plt.xlabel("Temperature (T)", fontsize=20);
plt.ylabel("Energy ", fontsize=20);         plt.axis('tight');

sp =  f.add_subplot(2, 2, 2 );
plt.scatter(T, abs(M), s=50, marker='o', color='RoyalBlue')
plt.xlabel("Temperature (T)", fontsize=20);
plt.ylabel("Magnetization ", fontsize=20);   plt.axis('tight');

sp =  f.add_subplot(2, 2, 3 );
plt.scatter(T, C, s=50, marker='o', color='IndianRed')
plt.xlabel("Temperature (T)", fontsize=20);
plt.ylabel("Specific Heat ", fontsize=20);   plt.axis('tight');

sp =  f.add_subplot(2, 2, 4 );
plt.scatter(T, X, s=50, marker='o', color='RoyalBlue')
plt.xlabel("Temperature (T)", fontsize=20);
plt.ylabel("Susceptibility", fontsize=20);   plt.axis('tight');
```



Note: A better optimized version of the above code can be found here. One of the difference being that we do not calculate the exponential in the loop in the optimized cython version. Thus, avoiding N^2 calls to a special function. We can do thisas the spins only take values 1 and -1. Thus, there are only two possibilities for an energy increasing move. They are:

```
# change in energy is 8J
#    d          d               u          u
# d  d  d => d  u  d   or    u  u  u => u  d  u
#    d          d               u          u
#
# change in energy is 4J
#    d          d               u          u
# d  d  u => d  u  u   or    u  u  d => u  d  d
#    d          d               u          u
#
# Here u and d are used for up and down configuration of the spins
```

Snapshots of the configurations

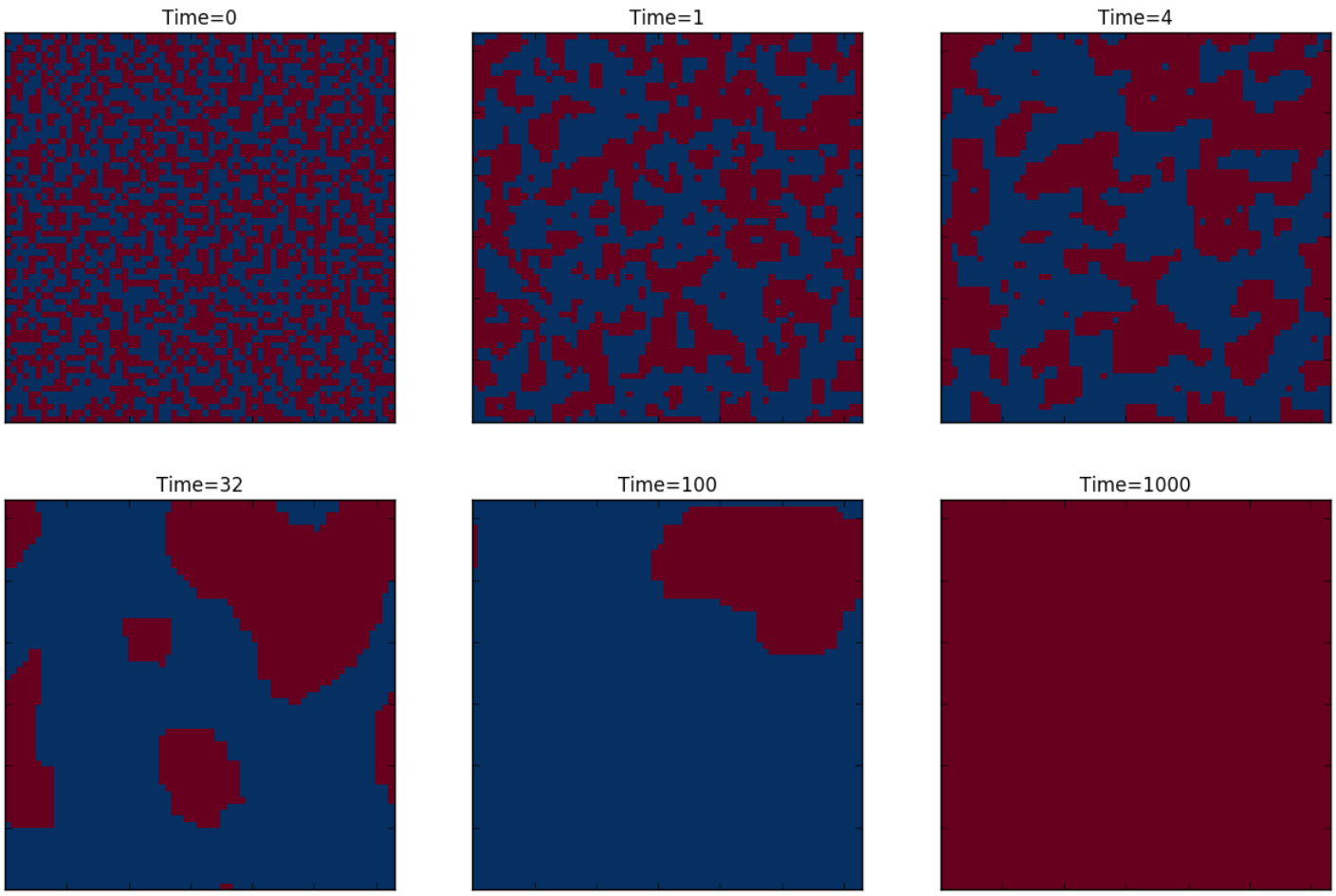
We start with a random initial condition and then plot the instantaneous configurations, as the system coarsens to its equilibrium state.

```
%matplotlib inline
# Simulating the Ising model
from __future__ import division
import numpy as np
from numpy.random import rand
import matplotlib.pyplot as plt

class Ising():
    ''' Simulating the Ising model '''
    ## monte carlo moves
    def mcmove(self, config, N, beta):
        ''' This is to execute the monte carlo moves using
        Metropolis algorithm such that detailed
        balance condition is satisified'''
        for i in range(N):
            for j in range(N):
                    a = np.random.randint(0, N)
                    b = np.random.randint(0, N)
                    s =  config[a, b]
                    nb = config[(a+1)%N,b] + config[a,(b+1)%N] + config[(a-1)%N,b] + config[a,(b-1)%N]
                    cost = 2*s*nb
                    if cost < 0:
                        s *= -1
```

```
                    s *= -1
                elif rand() < np.exp(-cost*beta):
                    s *= -1

                config[a, b] = s
        return config

    def simulate(self):
        ''' This module simulates the Ising model'''
        N, temp     = 64, .4        # Initialse the lattice
        config = 2*np.random.randint(2, size=(N,N))-1
        f = plt.figure(figsize=(15, 15), dpi=80);
        self.configPlot(f, config, 0, N, 1);

        msrmnt = 1001
        for i in range(msrmnt):
            self.mcmove(config, N, 1.0/temp)
            if i == 1:       self.configPlot(f, config, i, N, 2);
            if i == 4:       self.configPlot(f, config, i, N, 3);
            if i == 32:      self.configPlot(f, config, i, N, 4);
            if i == 100:     self.configPlot(f, config, i, N, 5);
            if i == 1000:    self.configPlot(f, config, i, N, 6);


    def configPlot(self, f, config, i, N, n_):
        ''' This modules plts the configuration once passed to it along with time etc '''
        X, Y = np.meshgrid(range(N), range(N))
        sp =  f.add_subplot(3, 3, n_ )
        plt.setp(sp.get_yticklabels(), visible=False)
        plt.setp(sp.get_xticklabels(), visible=False)
        plt.pcolormesh(X, Y, config, cmap=plt.cm.RdBu);
        plt.title('Time=%d'%i); plt.axis('tight')
    plt.show()
```

```
rm = Ising()
```

```
rm.simulate()
```



Field theoretic description

- Ising model has no Hamiltonian given dynamics. For kinetics we assume that an associated heat bath generates spin flip $(S_i \rightarrow -S_i)$.
- The kinetics can be
  - The spin system, which have a non-conserved kinetics. At the microscopic level, spin-flip Glauber model is used to describe the non-conserved kinetics of the paramagnetic to ferromagnetic transition
  - The binary (AB) mixture or Lattice Gas. The spin-exchange Kawasaki model is used to describe the conserved kinetics of binary mixtures at the microscopic level
- Purely dissipative and stochastic models are ofter referred to as Kinetic Ising models.
- At the coarse-grained level the respective order parameters, $\phi(\vec{r}, t)$ are used

to describe the dynamics.

Domain Growth with non-conserved kinetics

- At $t = 0$, a paramagnetic phase is quenched below the critical temperature T_c.
- The paramagnetic state is no longer the preferred equilibrium state.
- The far-from-equilibrium, homogeneous, state evolves towards its new equilibrium state by separating in domains.
- These domains coarsen with time and are characterized by length scale $L(t)$.
- A finite system becomes ordered in either of two equivalent states as $t \to \infty$.
- The simplest kinetics Ising model for non-conserved scalar field $\phi(\vec{r})$ is the time dependent Ginzburg-Landau (TDGL) model.

TDGL equation

The equation of motion for ϕ can be written as:

$$\frac{\partial \phi}{\partial t} = -\Gamma \frac{\delta \mathcal{F}}{\delta \phi} + \theta(\vec{r}, t)$$

where $\frac{\delta \mathcal{F}}{\delta \phi}$ denotes functional derivative of free-energy functional

$$\mathcal{F}(\phi) = \int \left[a\phi^2 + b\phi^4 + \frac{1}{2} K (\nabla \phi)^2 \right]$$

For $T < T_c$ we can write TDGL in terms of rescaled variables as

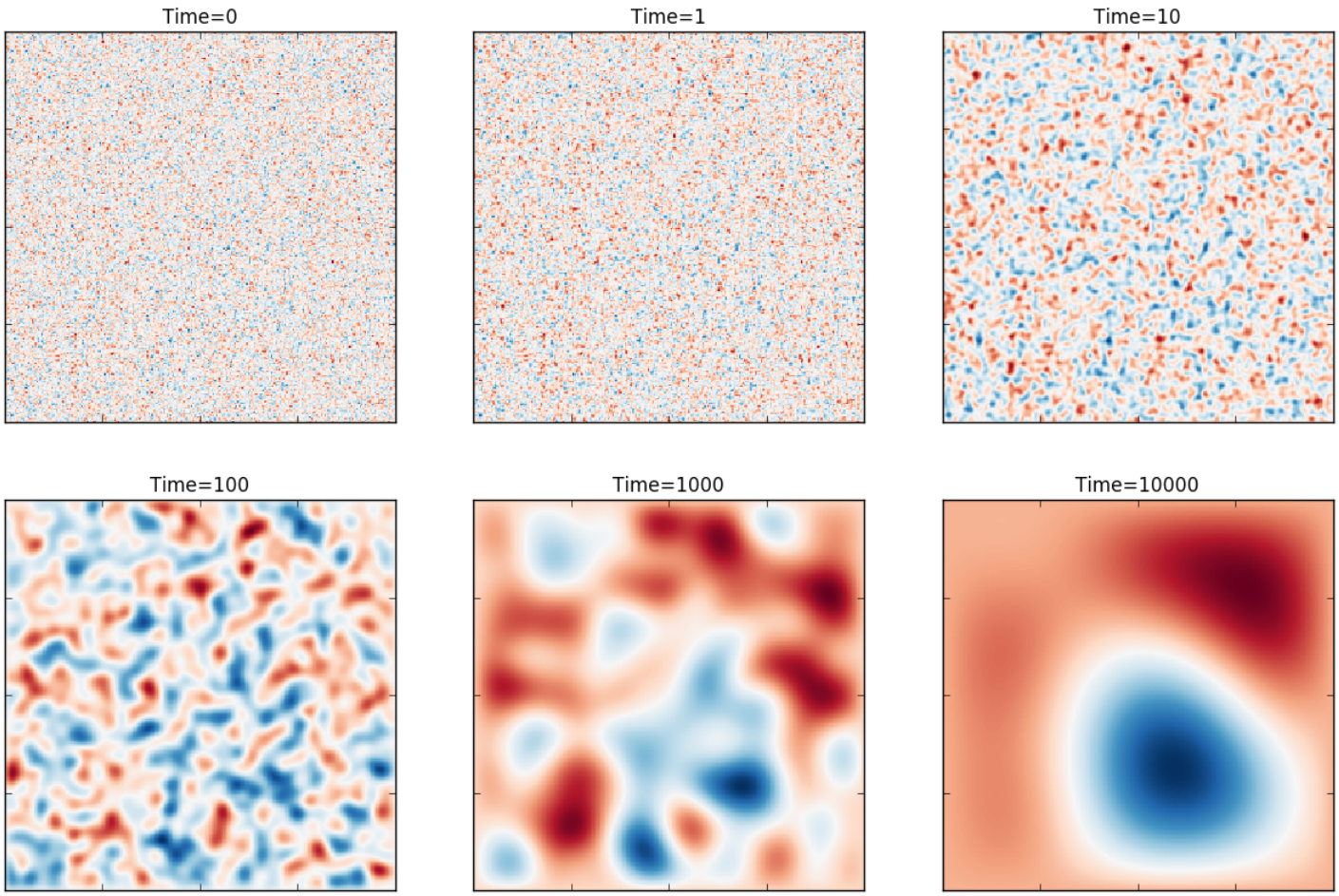
$$\frac{\partial \phi}{\partial t} = \phi - \phi^3 + \nabla^2 \phi$$

In the next section we will simulate the TDGL equation.

```
# Simulating the TDGL equation
# This example uses the 5-point Laplacian discretization from
# [here](https://github.com/ketch/finite-difference-course)
```

```
#
%matplotlib inline
import numpy as np
from __future__ import division
from scipy.sparse import spdiags,linalg,eye
import matplotlib.pyplot as plt


a,b, k = 0, 1.0, 100.0
dh, dt = 1.0, 1e-3
Ng, Tf = 256, 10001

class TDGL():
    '''
    Class to solve a PDE
    '''
    def mu(self, u):
        return a*u + b*u*u*u

    def laplacian(self, Ng):
        '''Construct a sparse matrix that applies the 5-point Laplacian discretization'''
        e=np.ones(Ng**2)
        e2=([1]*(Ng-1)+[0])*Ng
        e3=([0]+[1]*(Ng-1))*Ng
        h=dh
        A=spdiags([-4*e,e2,e3,e,e],[0,-1,1,-Ng,Ng],Ng**2,Ng**2)
        A/=h**2
        return A

    def integrate(self, L, x, y, u):
        '''  simulates the equation and plots it at different instants '''

        f = plt.figure(figsize=(15, 15), dpi=80);

        for i in range(Tf):
            u = u - dt*(self.mu(u) - k*L.dot(u))

            if (i==0):      self.configPlot(x, y, u, f, 1, i);
            if (i==1):      self.configPlot(x, y, u, f, 2, i);
            if (i==10):     self.configPlot(x, y, u, f, 3, i);
            if (i==100):    self.configPlot(x, y, u, f, 4, i);
            if (i==1000):   self.configPlot(x, y, u, f, 5, i);
            if (i==10000):  self.configPlot(x, y, u, f, 6, i);

    def configPlot(self, x, y, u,f, n_, i):
        U= u.reshape((Ng, Ng))
        sp =  f.add_subplot(3, 3, n_ )
        plt.setp(sp.get_yticklabels(), visible=False)
        plt.setp(sp.get_xticklabels(), visible=False)
        plt.pcolormesh(x,y,U, cmap=plt.cm.RdBu);
        plt.title('Time=%d'%i)
    plt.show()
```

```
rm = TDGL()   # instantiate the class

# generate the grid and initialise the field
x = np.linspace(-1,1,Ng)
y = np.linspace(-1,1,Ng)
X, Y = np.meshgrid(x, y)

u=np.random.randn(Ng*Ng, 1);  # Initial data
L = rm.laplacian(Ng)          # construct the laplacian
rm.integrate(L, x, y, u)    # simulate

#simulation completed!!
```



Thus we see that time evolution of the Monte carlo simulation of the Ising model and that of the TDGL equation are similar. The TDGL equation is a hydrodynamic model while the simulation of the Ising model was done at the molecular level. We still see a similarity in the time evolution, as expected!

Write Preview

Sign in to comment

Styling with Markdown is supported Sign in with GitHub

Subscribe