Xch2

June 23, 2024

[29]:

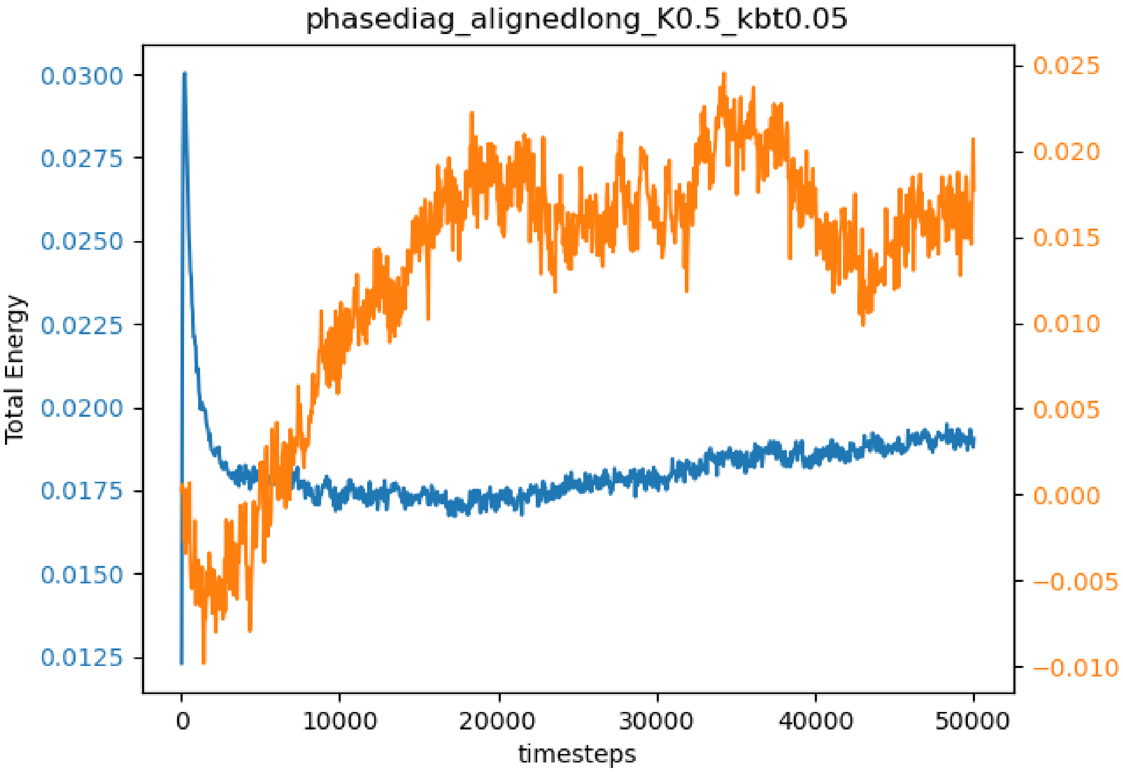
```python
import numpy as np
import matplotlib.pyplot as plt
from mpl_toolkits.mplot3d import axes3d
import os
# loading all of the csv's from all of the simulations with the macro measured␣
 ↪data (total energy, ent. excess, Paccept....)
simlist = []
datafiles = []
csvfiles = []
for root, dirs, files in os.walk("../data/50000"):
    for file in files:
        if file.endswith(".npz"):
            datafiles.append(os.path.join(root,file))
        if file.endswith(".csv"):
            csvfiles.append(os.path.join(root,file))
    for name in dirs:
        simlist.append(name)
simlist = sorted(simlist)
datafiles = sorted(datafiles)
csvfiles = sorted(csvfiles)
assert len(simlist) == len(datafiles) == len(csvfiles)


def load_csv(fname,verbose=True):
    if verbose:
        with open(fname) as f:
            print(f.readline().strip('\n'))
    return np.loadtxt(fname,skiprows=1,delimiter=",")

def plot_energy(fpath,csv1,save=False):
    fig,ax1 = plt.subplots()
    ax1.set_title(fpath.split("/")[-2])
    ax1.plot(csv1[:,0],csv1[:,1],label="TotalEnergy")
    ax1.set_xlabel("timesteps")
    ax1.set_ylabel("Total Energy")
    ax1.tick_params(axis ='y', labelcolor="tab:blue")
    ax2  = ax1.twinx()
    ax2.plot(csv1[:,0],csv1[:,2],label="Eexcess",color="tab:orange")
    ax2.set_ylabel("Ent. Excess")
    ax2.tick_params(axis ='y', labelcolor = "tab:orange")
    #plt.show()
    if save:
        fname = fpath[:-4]+"_energy.png"
        print(fname)
        fig.savefig(fname)

%matplotlib ipympl
```

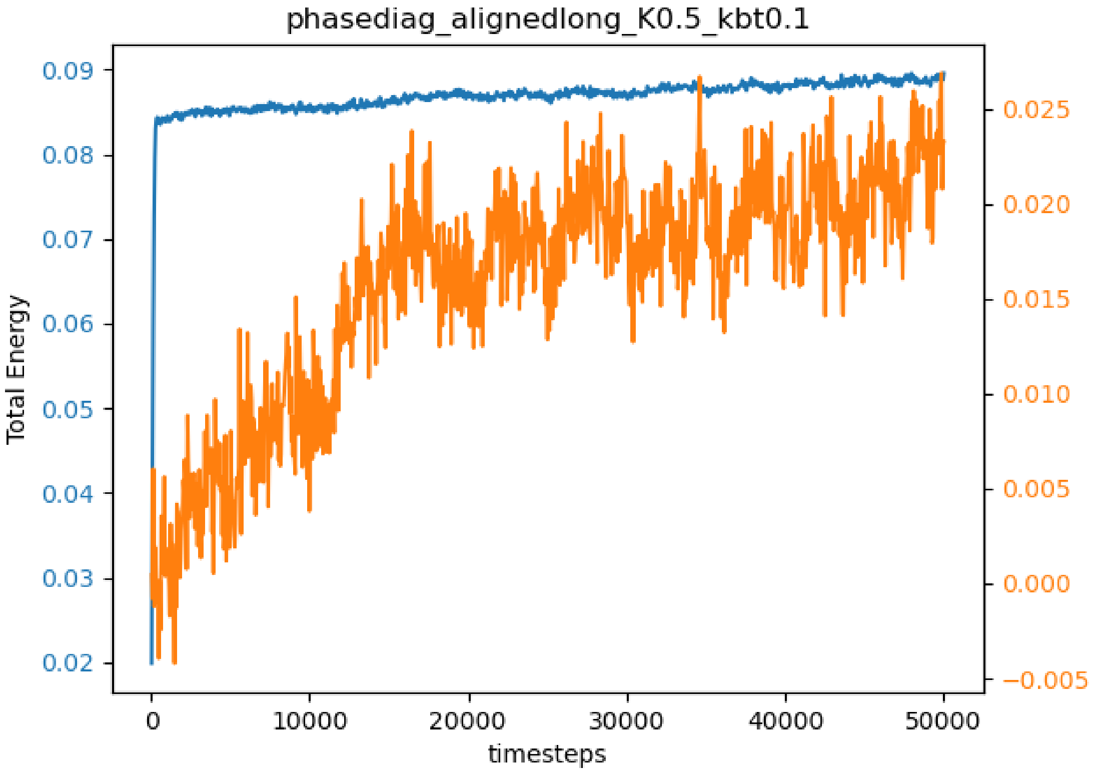
[30]:

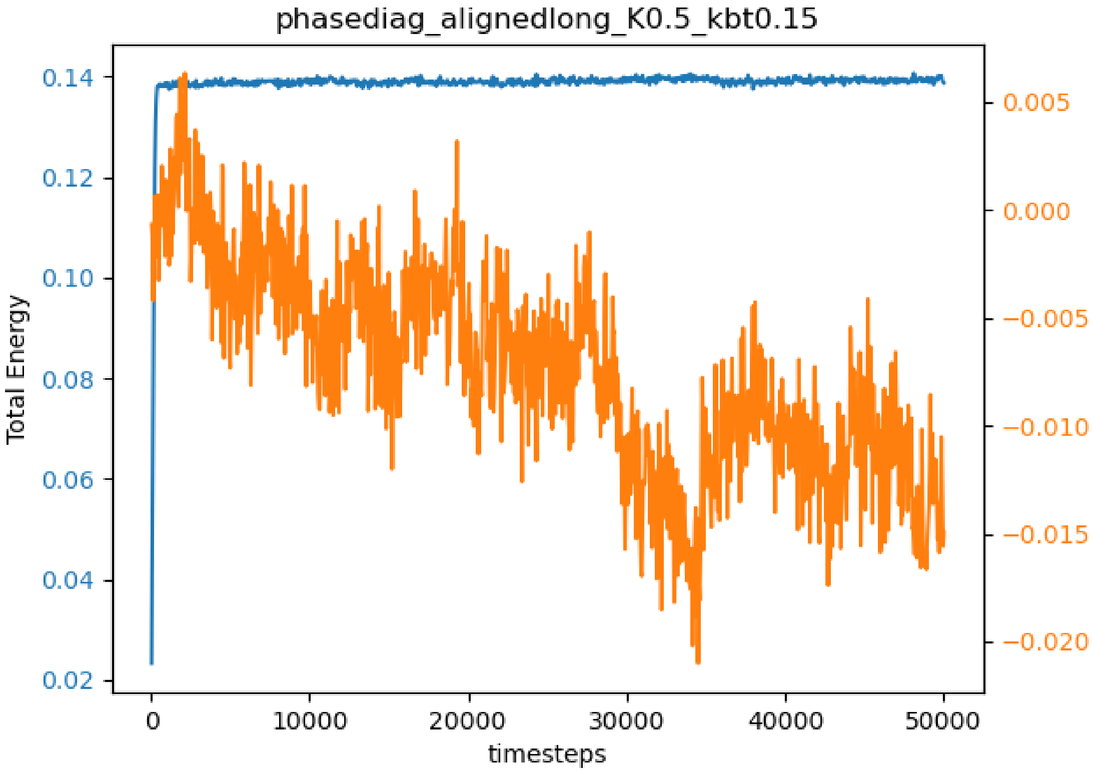
```
# saving a plot of total energy vs. time and entatiomeric excess vs time
for csvfile  in csvfiles:
    csvdata = load_csv(csvfile,verbose=False)
    plot_energy(csvfile,csvdata,save=True)
```

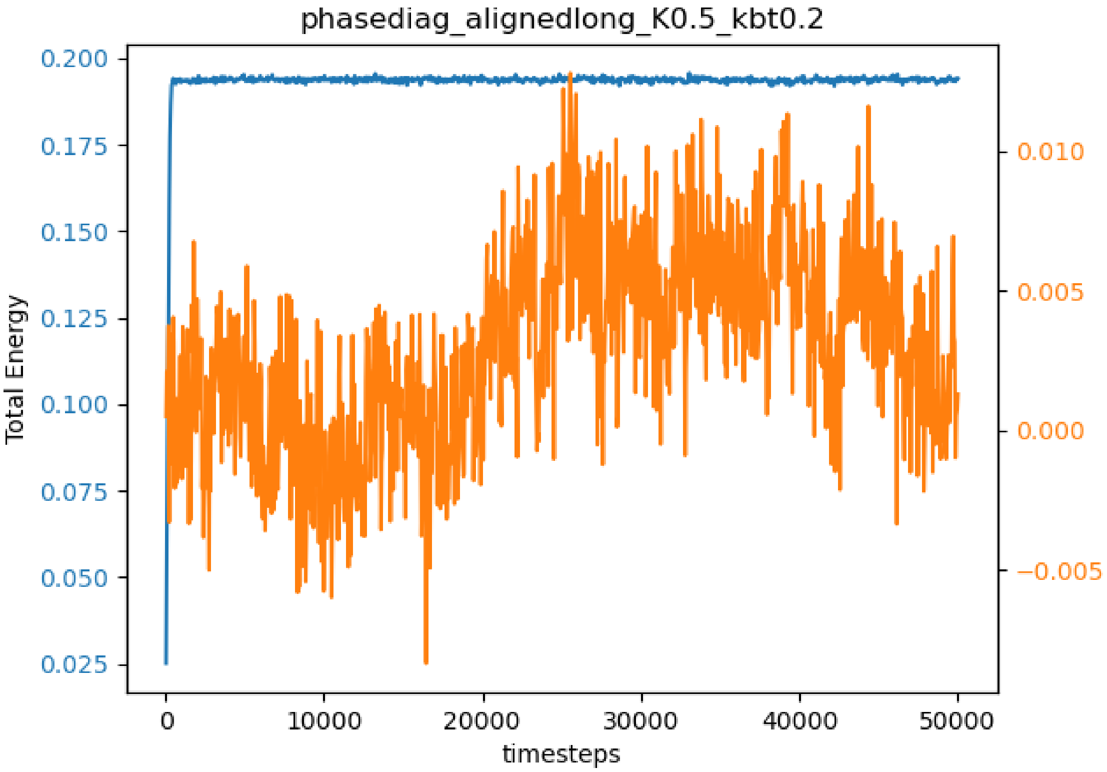
```
../data/50000/phasediag_alignedlong_K0.5_kbt0.05/phasediag_alignedlong_K0.5_kbt0
.05_energy.png
../data/50000/phasediag_alignedlong_K0.5_kbt0.1/phasediag_alignedlong_K0.5_kbt0.
1_energy.png
../data/50000/phasediag_alignedlong_K0.5_kbt0.15/phasediag_alignedlong_K0.5_kbt0
.15_energy.png
../data/50000/phasediag_alignedlong_K0.5_kbt0.2/phasediag_alignedlong_K0.5_kbt0.
2_energy.png
../data/50000/phasediag_alignedlong_K0.5_kbt0.25/phasediag_alignedlong_K0.5_kbt0
.25_energy.png
../data/50000/phasediag_alignedlong_K0.5_kbt0.3/phasediag_alignedlong_K0.5_kbt0.
3_energy.png
../data/50000/phasediag_alignedlong_K0.5_kbt0.35/phasediag_alignedlong_K0.5_kbt0
.35_energy.png
../data/50000/phasediag_alignedlong_K0.5_kbt0.4/phasediag_alignedlong_K0.5_kbt0.
4_energy.png
../data/50000/phasediag_alignedlong_K0.5_kbt0.45/phasediag_alignedlong_K0.5_kbt0
.45_energy.png
../data/50000/phasediag_alignedlong_K0.5_kbt0.5/phasediag_alignedlong_K0.5_kbt0.
5_energy.png
../data/50000/phasediag_alignedlong_K0.5_kbt0.55/phasediag_alignedlong_K0.5_kbt0
.55_energy.png
../data/50000/phasediag_alignedlong_K0.5_kbt0.6/phasediag_alignedlong_K0.5_kbt0.
6_energy.png
../data/50000/phasediag_alignedlong_K0.5_kbt0.65/phasediag_alignedlong_K0.5_kbt0
.65_energy.png
../data/50000/phasediag_alignedlong_K0.5_kbt0.7/phasediag_alignedlong_K0.5_kbt0.
7_energy.png
../data/50000/phasediag_alignedlong_K0.5_kbt0.75/phasediag_alignedlong_K0.5_kbt0
.75_energy.png
../data/50000/phasediag_alignedlong_K0.5_kbt0.8/phasediag_alignedlong_K0.5_kbt0.
8_energy.png
```

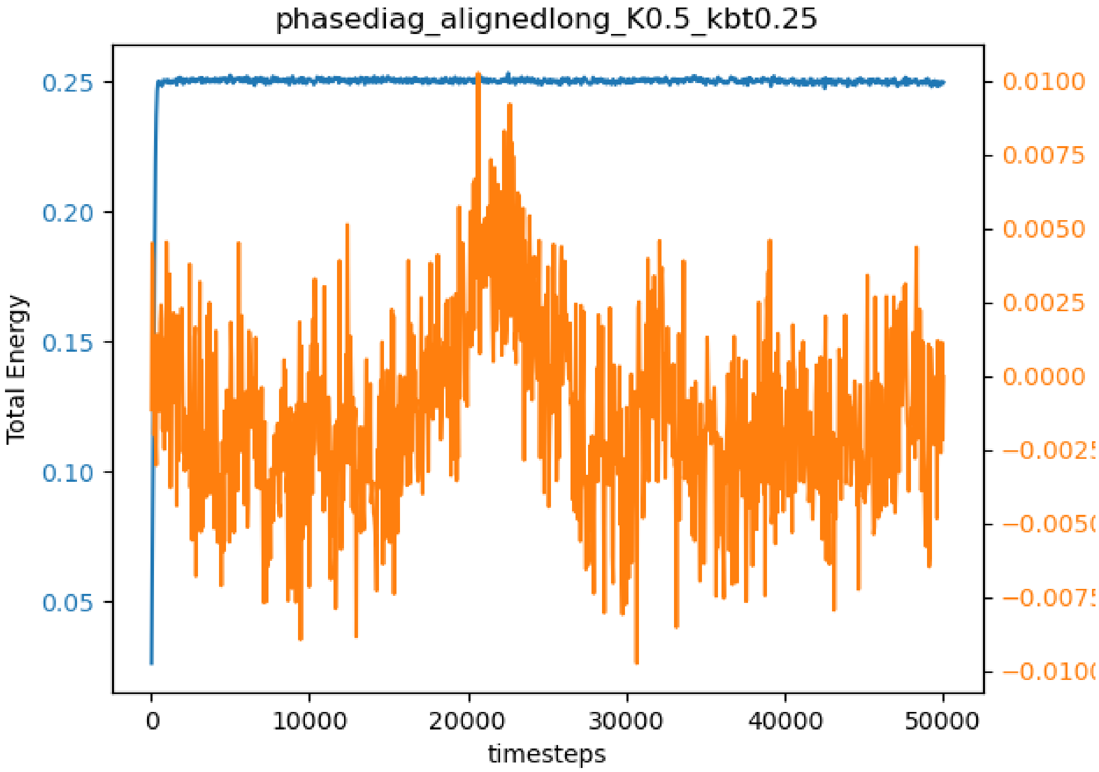
```
../data/50000/phasediag_alignedlong_K0.5_kbt0.85/phasediag_alignedlong_K0.5_kbt0
.85_energy.png
../data/50000/phasediag_alignedlong_K0.5_kbt0.9/phasediag_alignedlong_K0.5_kbt0.
9_energy.png
../data/50000/phasediag_alignedlong_K0.5_kbt0.95/phasediag_alignedlong_K0.5_kbt0
.95_energy.png
../data/50000/phasediag_alignedlong_K0.5_kbt1.0/phasediag_alignedlong_K0.5_kbt1.
0_energy.png
../data/50000/phasediag_alignedlong_K0.5_kbt1.05/phasediag_alignedlong_K0.5_kbt1
.05_energy.png
../data/50000/phasediag_alignedlong_K0.5_kbt1.1/phasediag_alignedlong_K0.5_kbt1.
1_energy.png
../data/50000/phasediag_alignedlong_K0.5_kbt1.15/phasediag_alignedlong_K0.5_kbt1
.15_energy.png
../data/50000/phasediag_alignedlong_K0.5_kbt1.2/phasediag_alignedlong_K0.5_kbt1.
2_energy.png
../data/50000/phasediag_alignedlong_K0.5_kbt1.25/phasediag_alignedlong_K0.5_kbt1
.25_energy.png
../data/50000/phasediag_alignedlong_K0.5_kbt1.3/phasediag_alignedlong_K0.5_kbt1.
3_energy.png
../data/50000/phasediag_alignedlong_K0.5_kbt1.35/phasediag_alignedlong_K0.5_kbt1
.35_energy.png
../data/50000/phasediag_alignedlong_K0.5_kbt1.4/phasediag_alignedlong_K0.5_kbt1.
4_energy.png
../data/50000/phasediag_alignedlong_K0.5_kbt1.45/phasediag_alignedlong_K0.5_kbt1
.45_energy.png
../data/50000/phasediag_alignedlong_K0.5_kbt1.5/phasediag_alignedlong_K0.5_kbt1.
5_energy.png
```

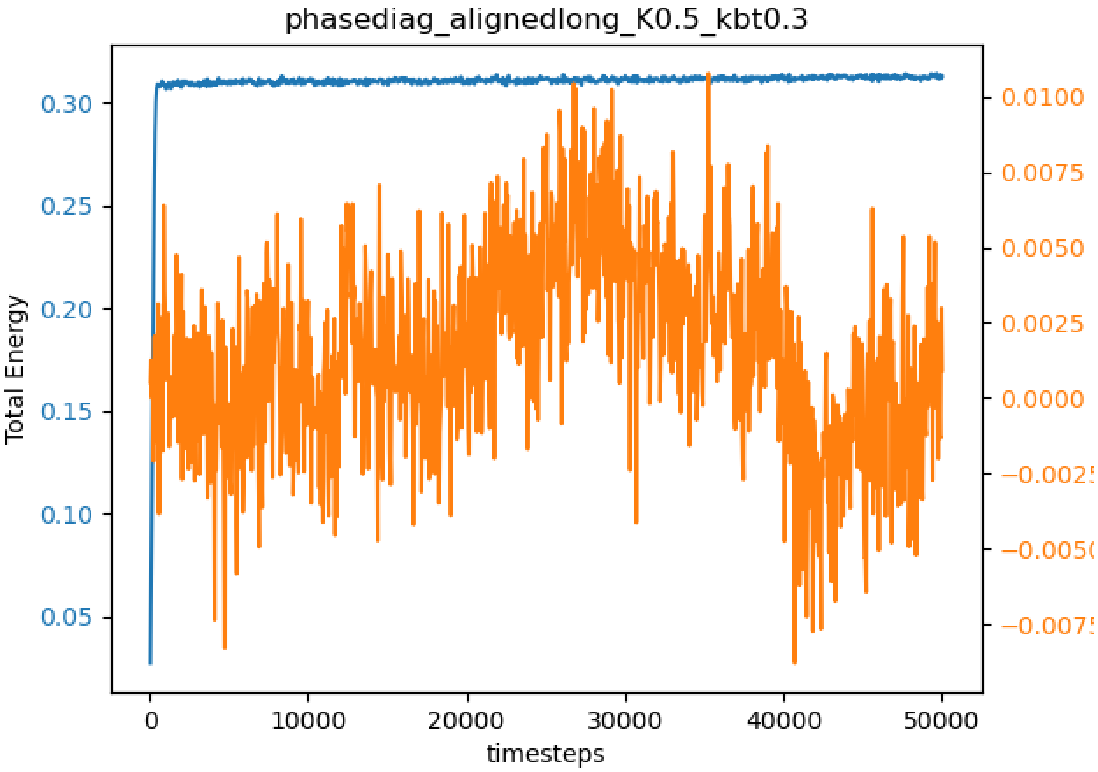

phasediag_alignedlong_K0.5_kbt0.05
Total Energy
0.0125
0.0150
0.0175
0.0200
0.0225
0.0250
0.0275
0.0300
−0.010
−0.005
0.000
0.005
0.010
0.015
0.020
0.025
0
10000
20000
30000
40000
50000
timesteps

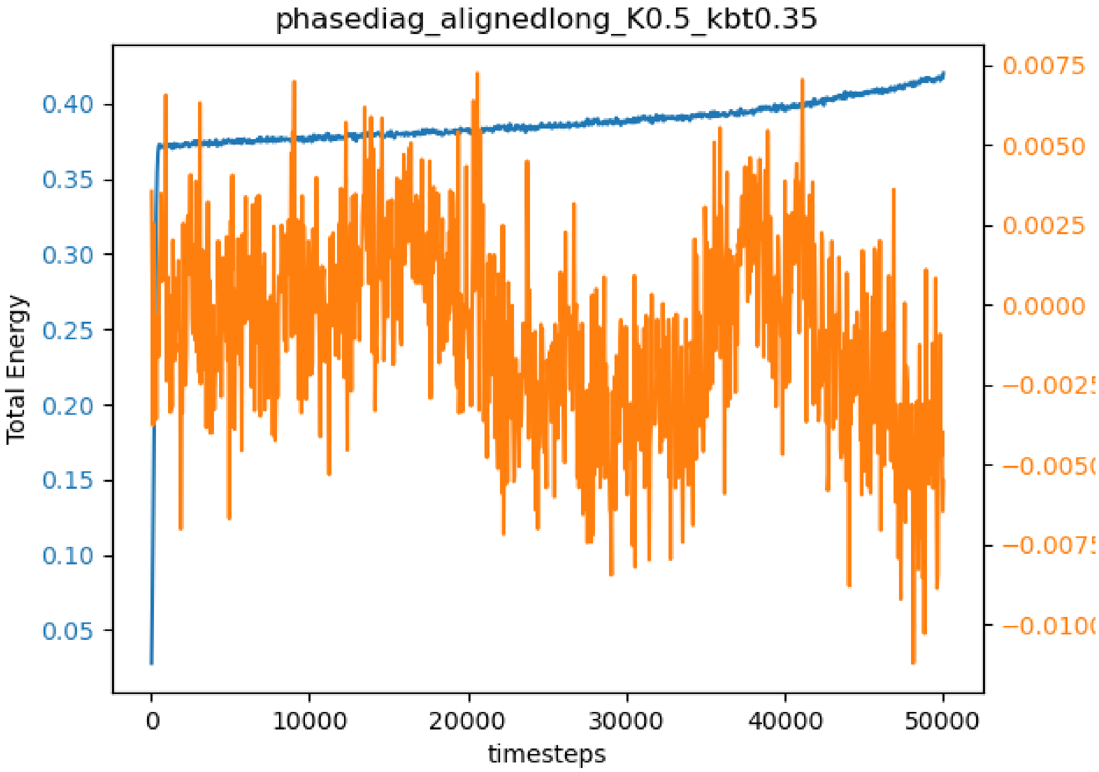

phasediag_alignedlong_K0.5_kbt0.1
Total Energy
0.02
0.03
0.04
0.05
0.06
0.07
0.08
0.09
−0.005
0.000
0.005
0.010
0.015
0.020
0.025
0
10000
20000
30000
40000
50000
timesteps

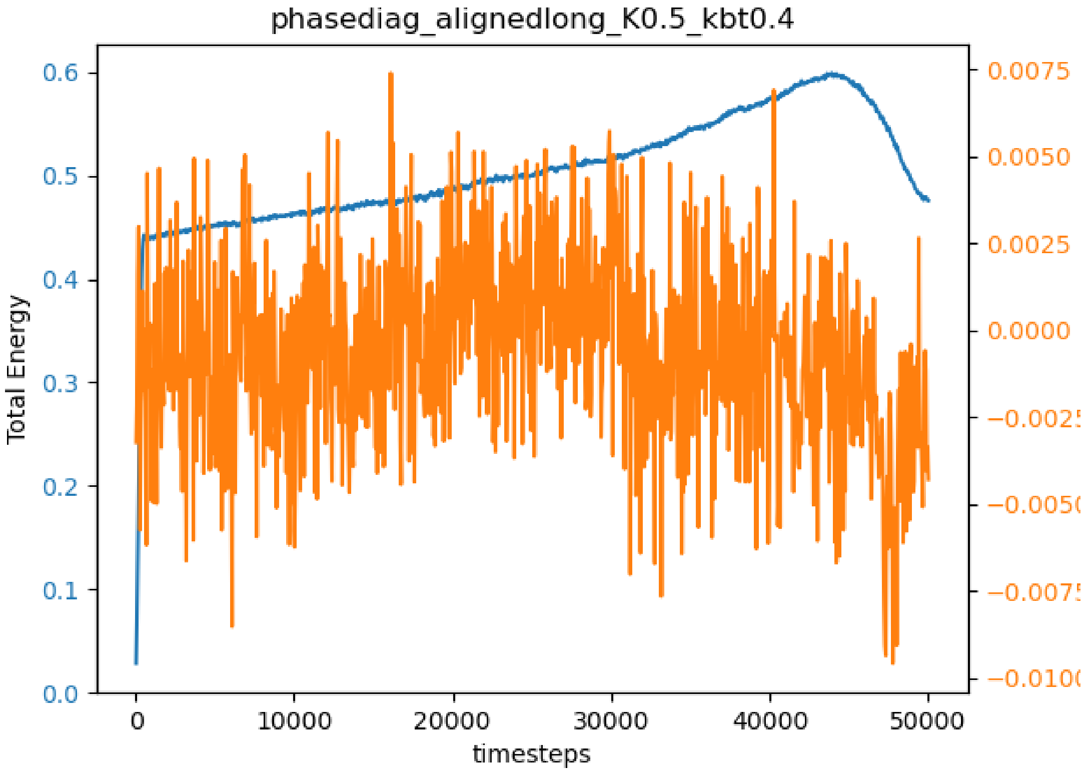

phasediag_alignedlong_K0.5_kbt0.15
Total Energy
0.14
0.12
0.10
0.08
0.06
0.04
0.02
0.005
0.000
−0.005
−0.010
−0.015
−0.020
0
10000
20000
30000
40000
50000
timesteps

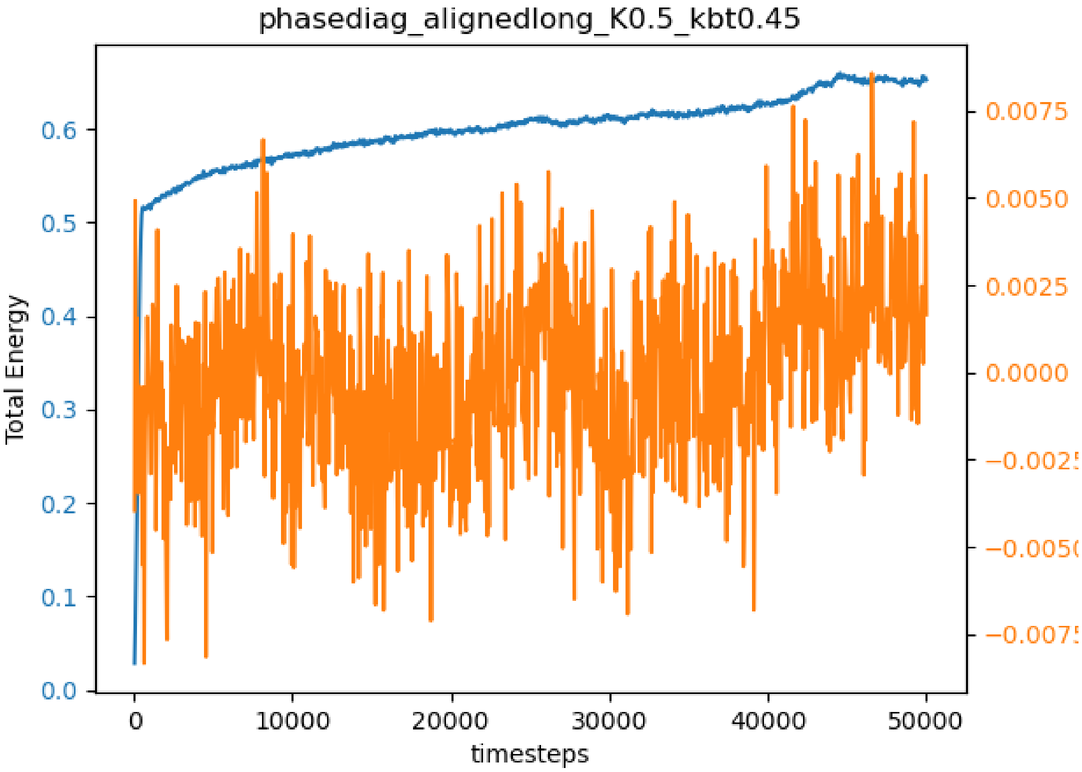

phasediag_alignedlong_K0.5_kbt0.2
Total Energy
0.200
0.175
0.150
0.125
0.100
0.075
0.050
0.025
0.010
0.005
0.000
−0.005
0
10000
20000
30000
40000
50000
timesteps

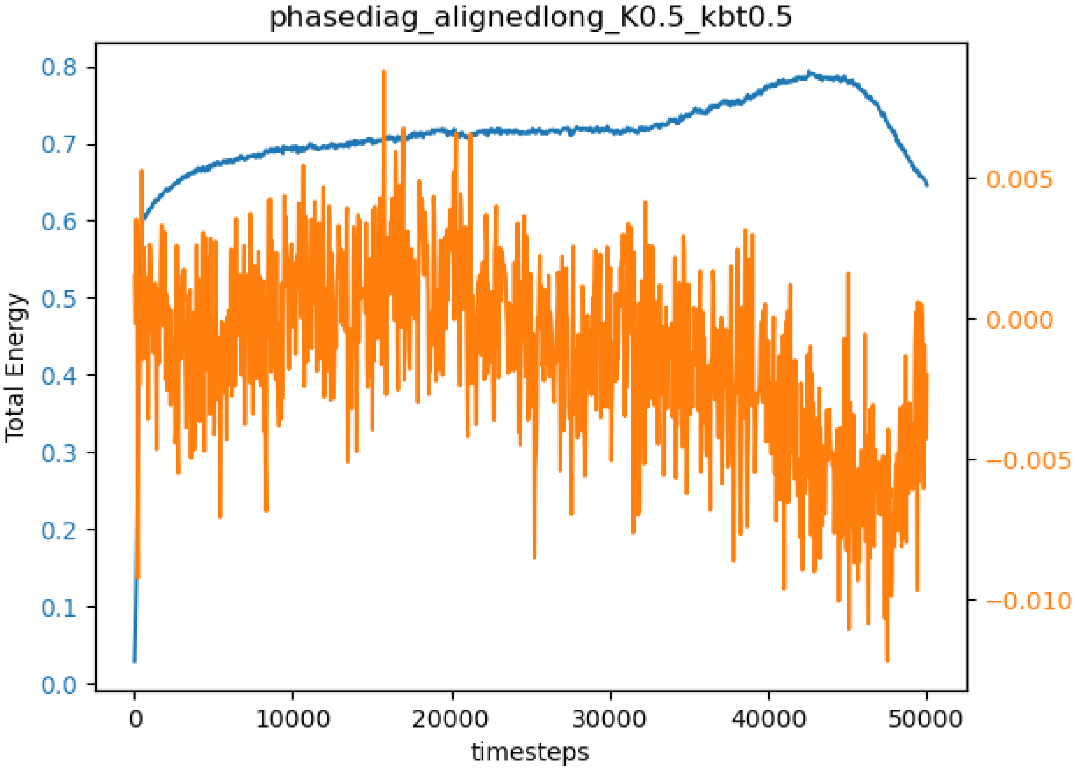

phasediag_alignedlong_K0.5_kbt0.25
Total Energy
0.25
0.20
0.15
0.10
0.05
0
10000
20000
30000
40000
50000
timesteps
0.0100
0.0075
0.0050
0.0025
0.0000
−0.0025
−0.0050
−0.0075
−0.0100

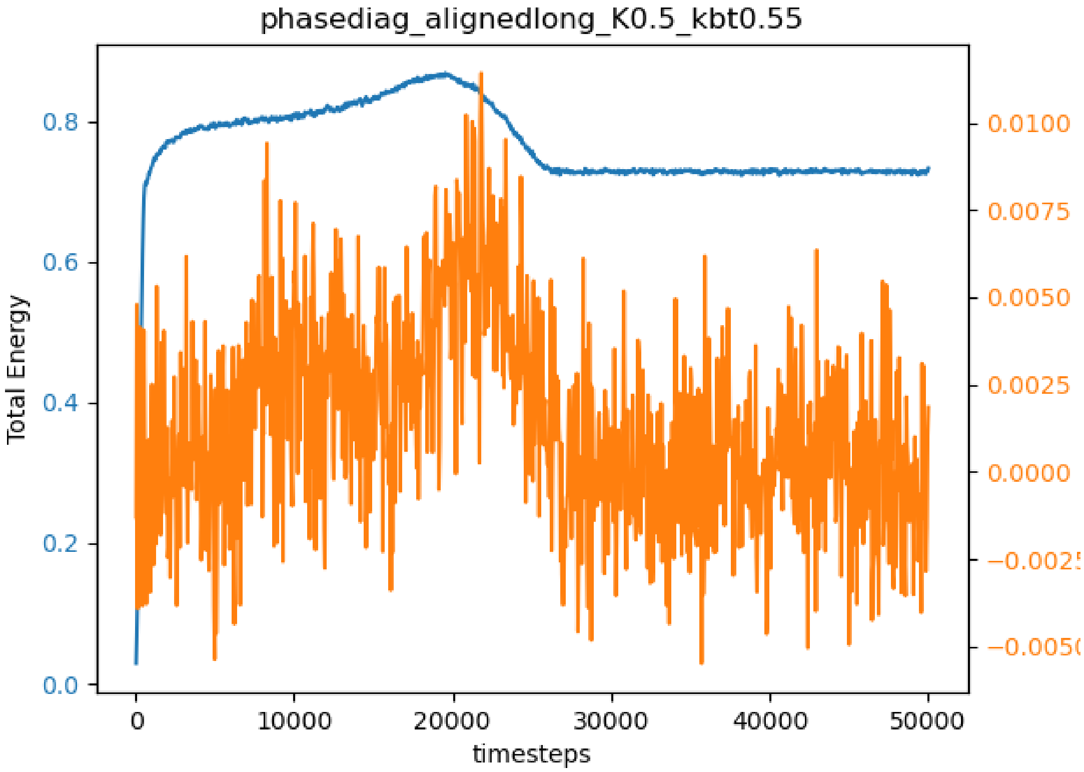

phasediag_alignedlong_K0.5_kbt0.3
Total Energy
0.30
0.25
0.20
0.15
0.10
0.05
0.0100
0.0075
0.0050
0.0025
0.0000
−0.0025
−0.0050
−0.0075
0
10000
20000
30000
40000
50000
timesteps

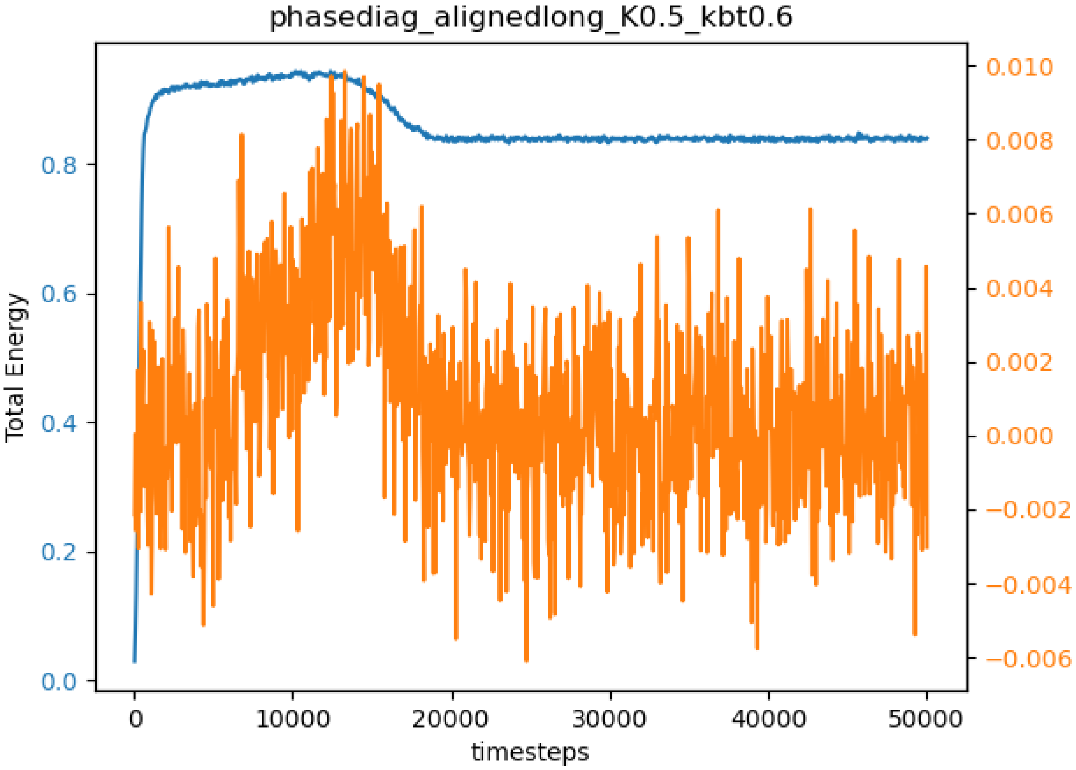

phasediag_alignedlong_K0.5_kbt0.35
Total Energy
0.40
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.0075
0.0050
0.0025
0.0000
−0.0025
−0.0050
−0.0075
−0.0100
0
10000
20000
30000
40000
50000
timesteps

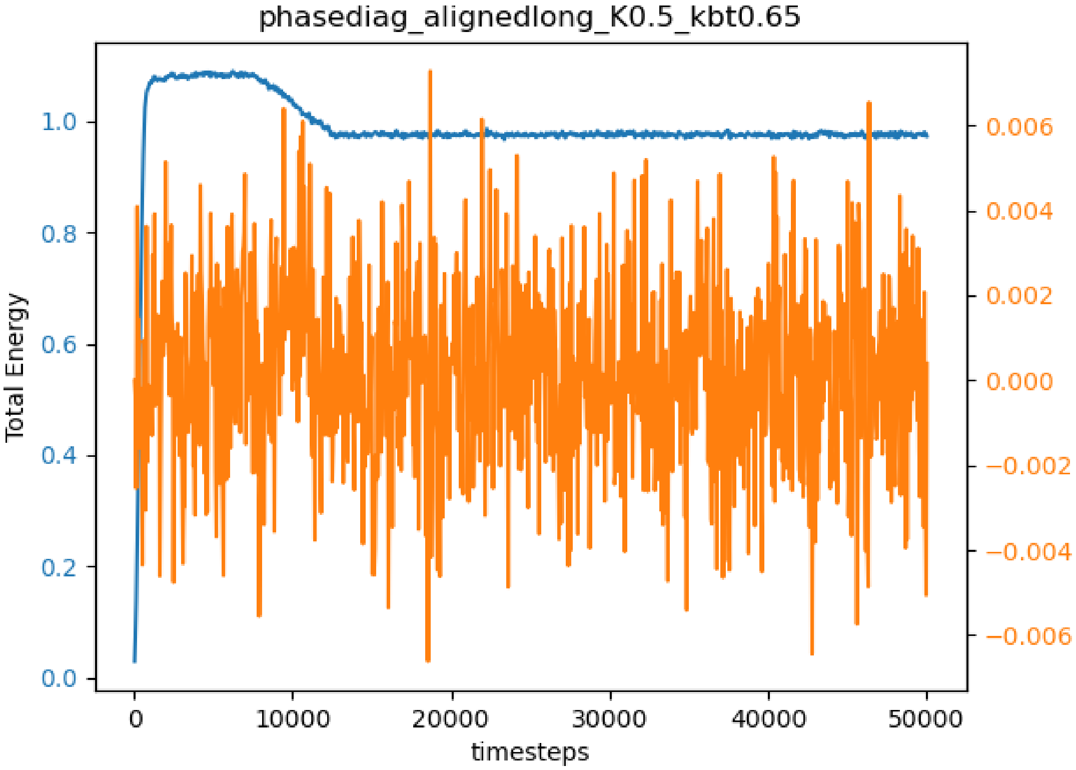

phasediag_alignedlong_K0.5_kbt0.4
Total Energy
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.0075
0.0050
0.0025
0.0000
−0.0025
−0.0050
−0.0075
−0.0100
0
10000
20000
30000
40000
50000
timesteps

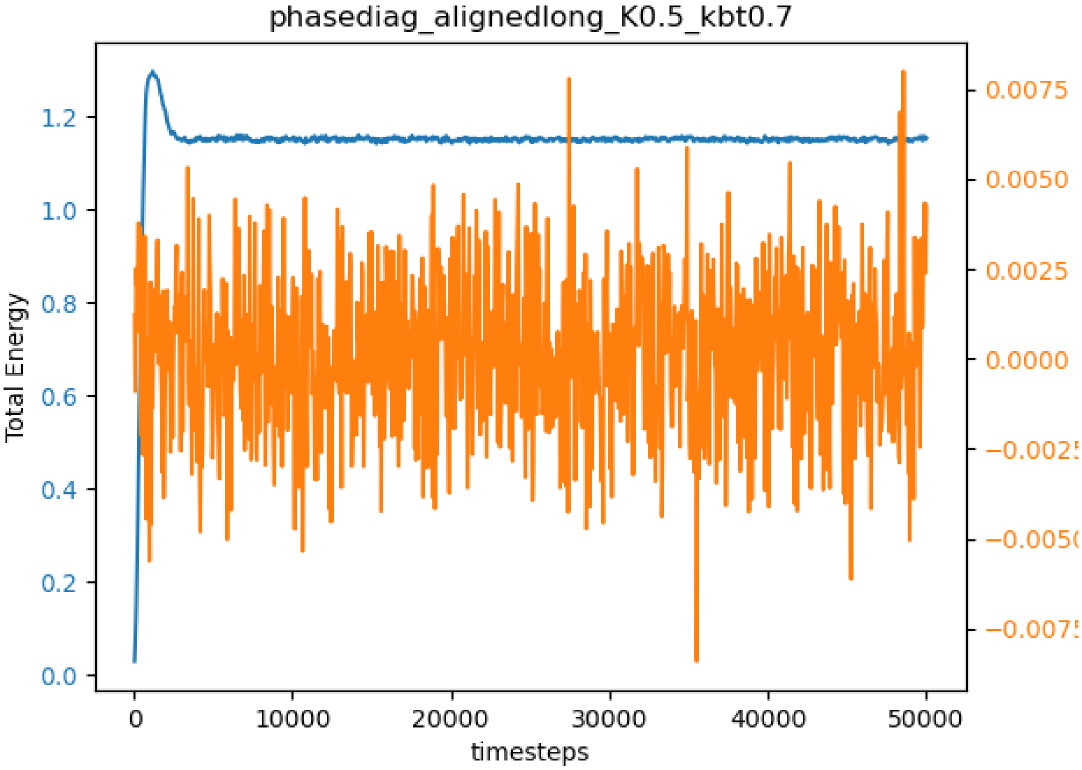

phasediag_alignedlong_K0.5_kbt0.45
Total Energy
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0
10000
20000
30000
40000
50000
timesteps
0.0075
0.0050
0.0025
0.0000
−0.0025
−0.0050
−0.0075

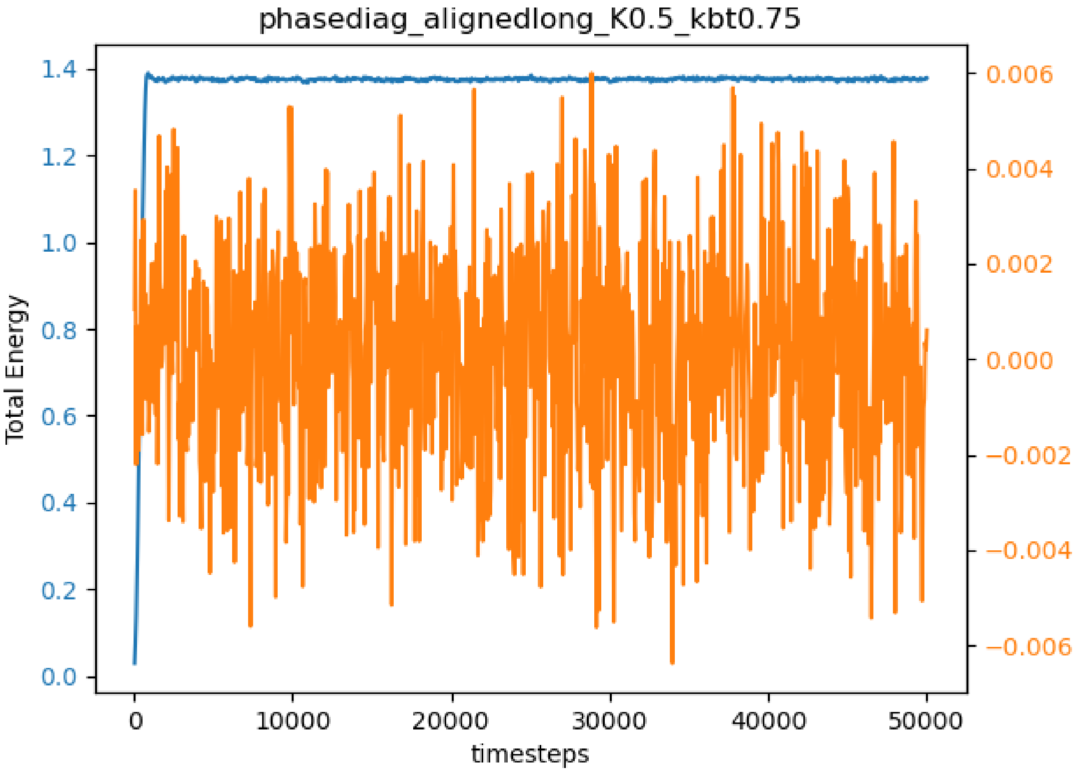

phasediag_alignedlong_K0.5_kbt0.5
Total Energy
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.005
0.000
−0.005
−0.010
0
10000
20000
30000
40000
50000
timesteps

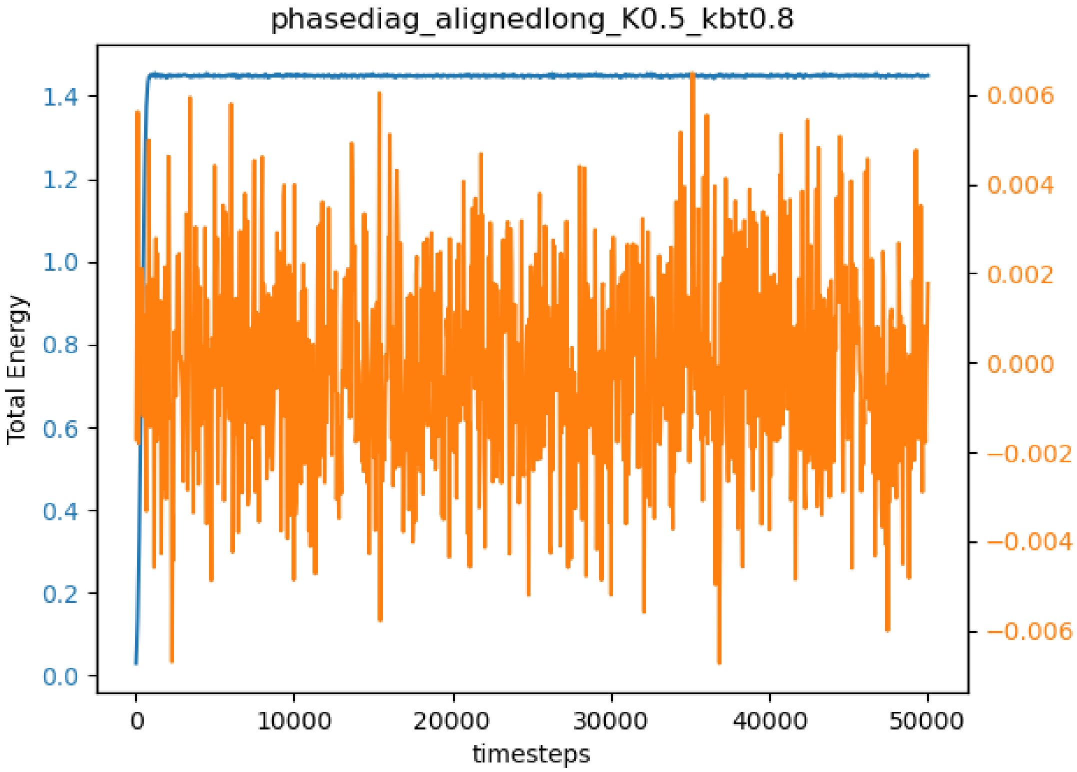

phasediag_alignedlong_K0.5_kbt0.55
Total Energy
0.0
0.2
0.4
0.6
0.8
0
10000
20000
30000
40000
50000
timesteps
0.0100
0.0075
0.0050
0.0025
0.0000
−0.0025
−0.0050

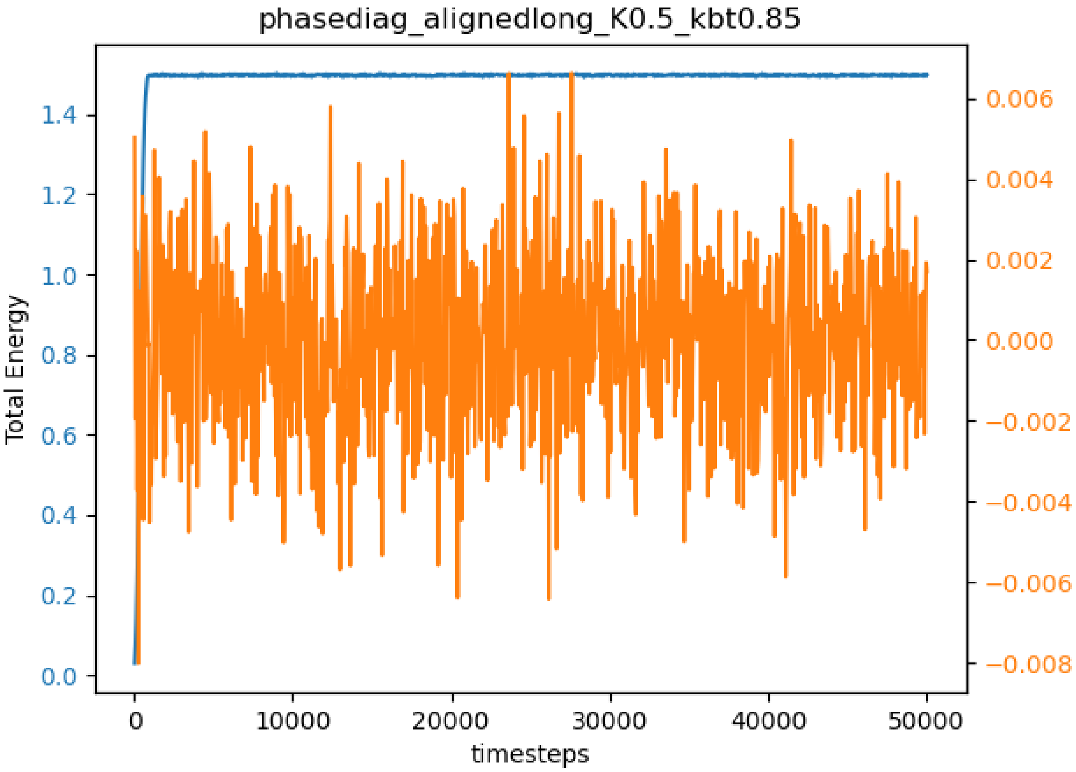

phasediag_alignedlong_K0.5_kbt0.6
Total Energy
0.0
0.2
0.4
0.6
0.8
0
10000
20000
30000
40000
50000
timesteps
0.010
0.008
0.006
0.004
0.002
0.000
−0.002
−0.004
−0.006

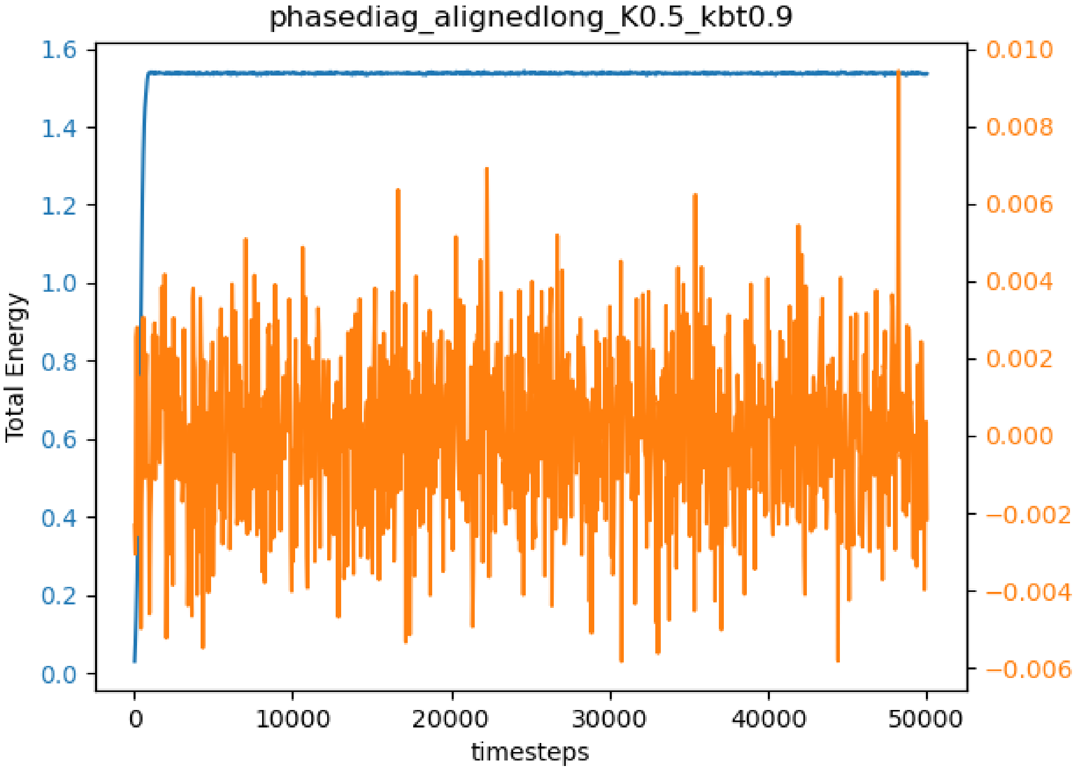

phasediag_alignedlong_K0.5_kbt0.65
Total Energy
0.0
0.2
0.4
0.6
0.8
1.0
0.006
0.004
0.002
0.000
−0.002
−0.004
−0.006
0
10000
20000
30000
40000
50000
timesteps

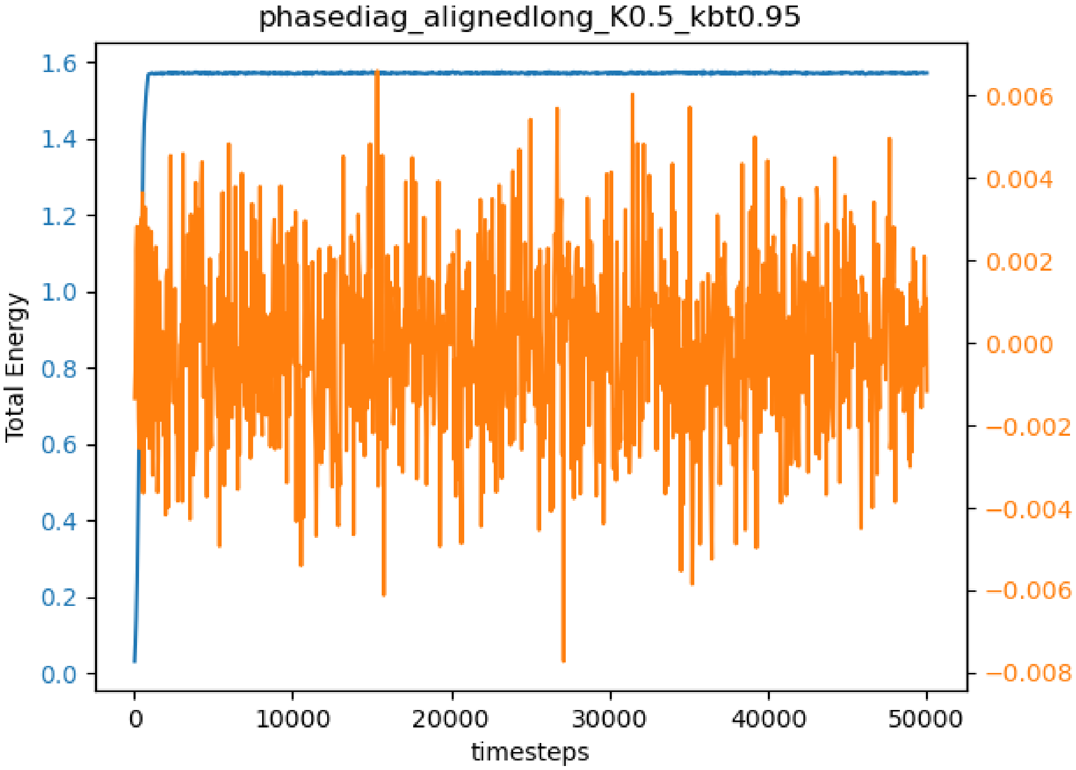

phasediag_alignedlong_K0.5_kbt0.7
Total Energy
timesteps
0.0
0.2
0.4
0.6
0.8
1.0
1.2
0
10000
20000
30000
40000
50000
0.0075
0.0050
0.0025
0.0000
−0.0025
−0.0050
−0.0075

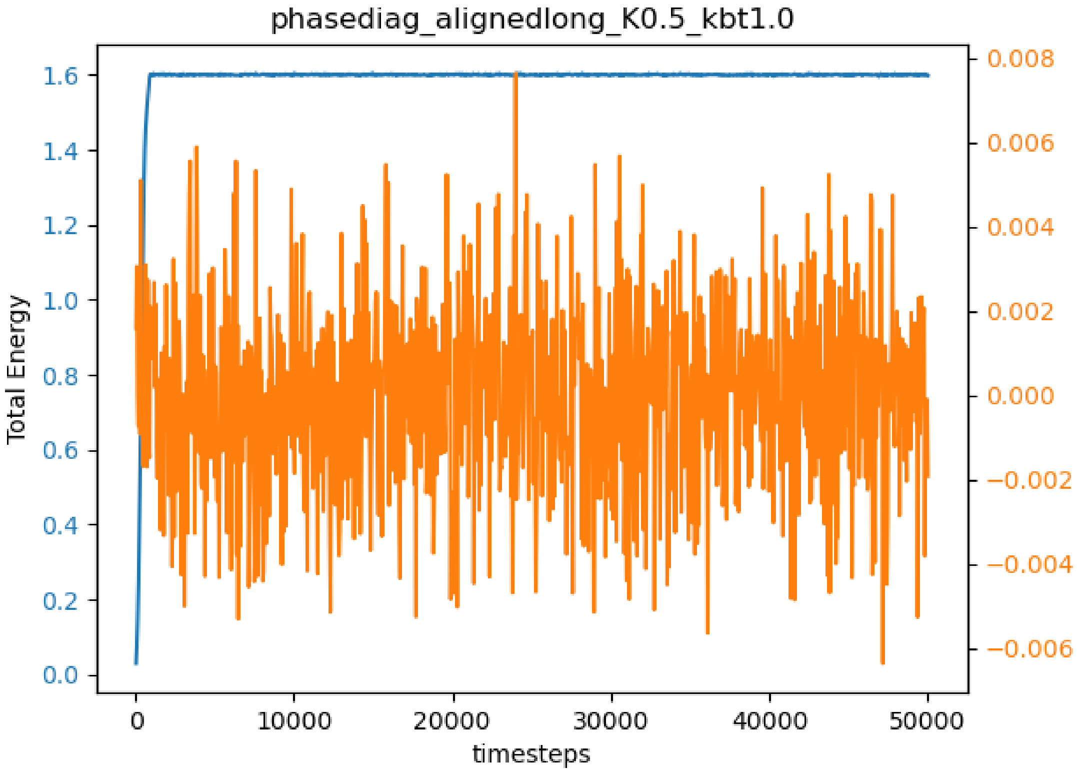

phasediag_alignedlong_K0.5_kbt0.75
Total Energy
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
0.006
0.004
0.002
0.000
−0.002
−0.004
−0.006
0
10000
20000
30000
40000
50000
timesteps

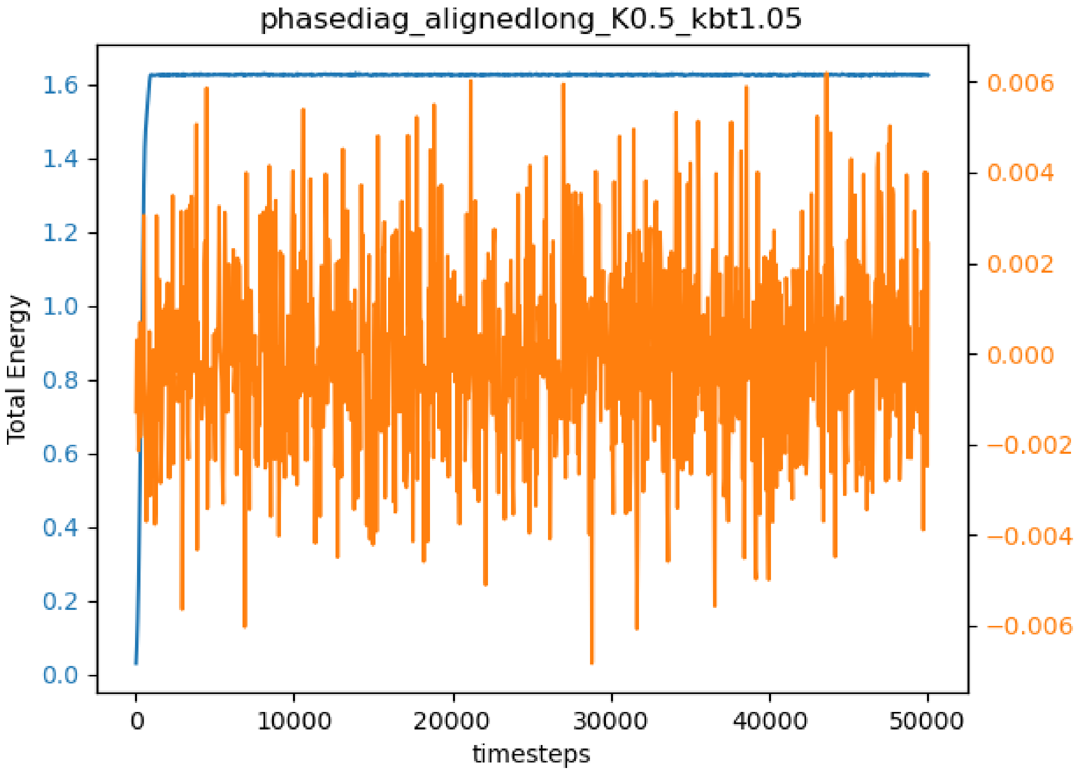

phasediag_alignedlong_K0.5_kbt0.8
Total Energy
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
0.006
0.004
0.002
0.000
−0.002
−0.004
−0.006
0
10000
20000
30000
40000
50000
timesteps

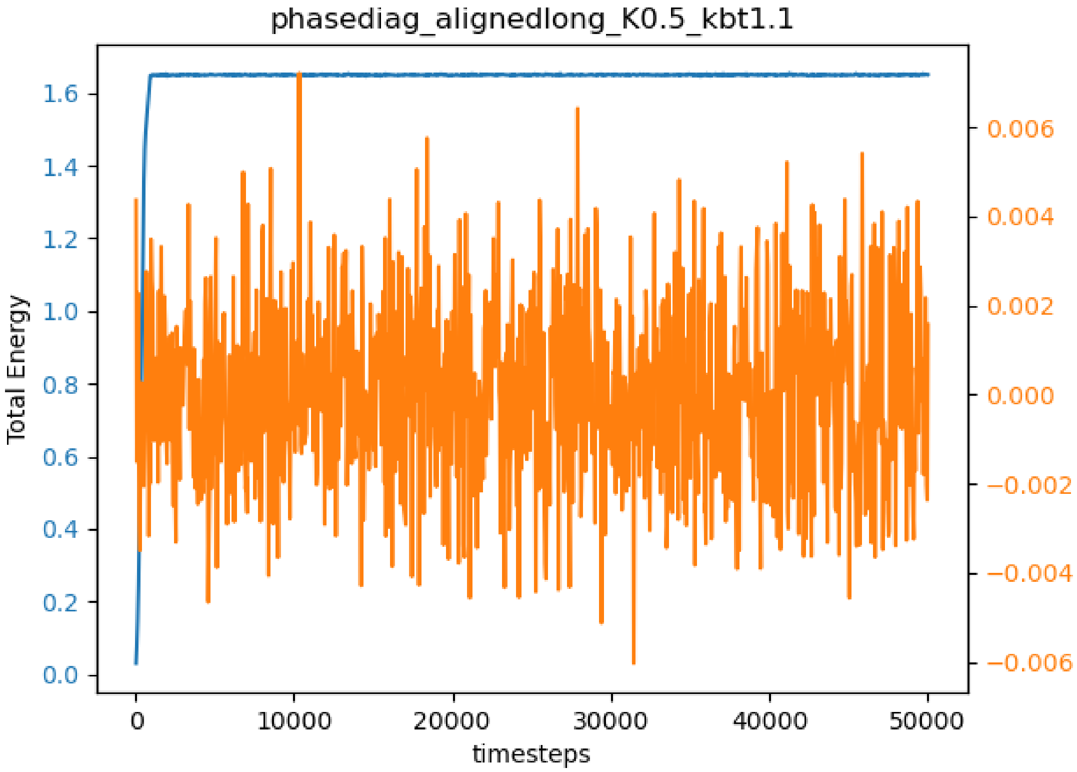

phasediag_alignedlong_K0.5_kbt0.85
Total Energy
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
0.006
0.004
0.002
0.000
−0.002
−0.004
−0.006
−0.008
0
10000
20000
30000
40000
50000
timesteps

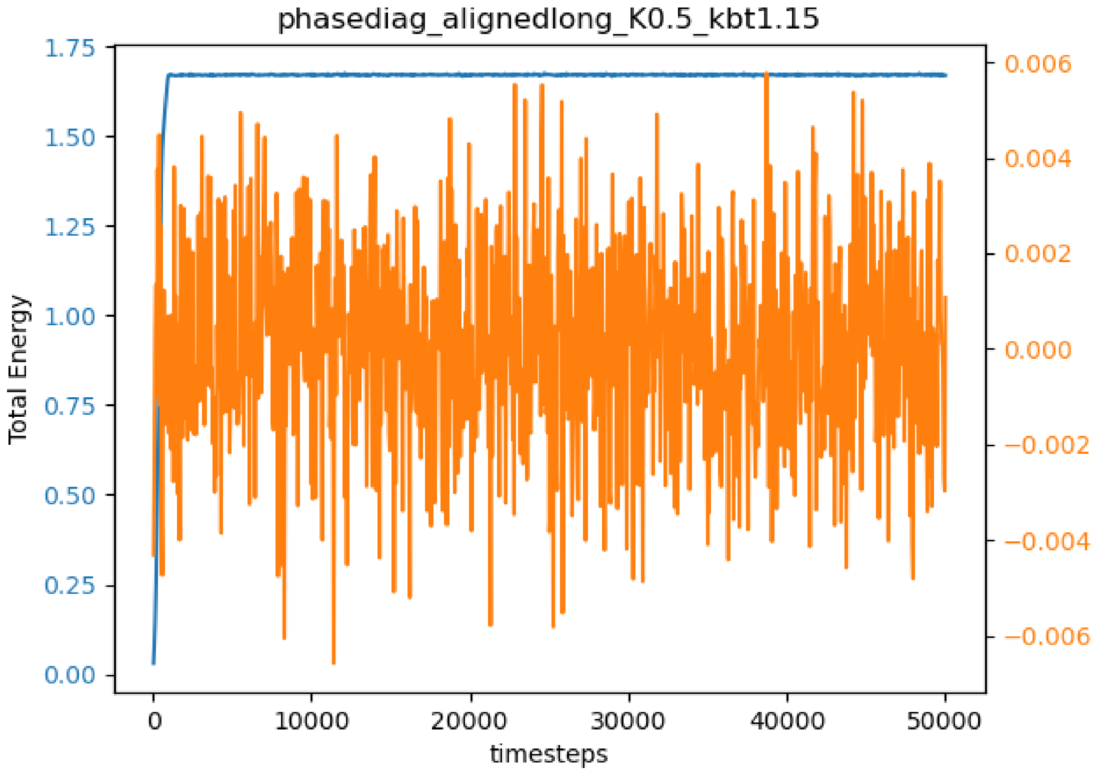

phasediag_alignedlong_K0.5_kbt0.9
Total Energy
timesteps
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
0
10000
20000
30000
40000
50000
−0.006
−0.004
−0.002
0.000
0.002
0.004
0.006
0.008
0.010

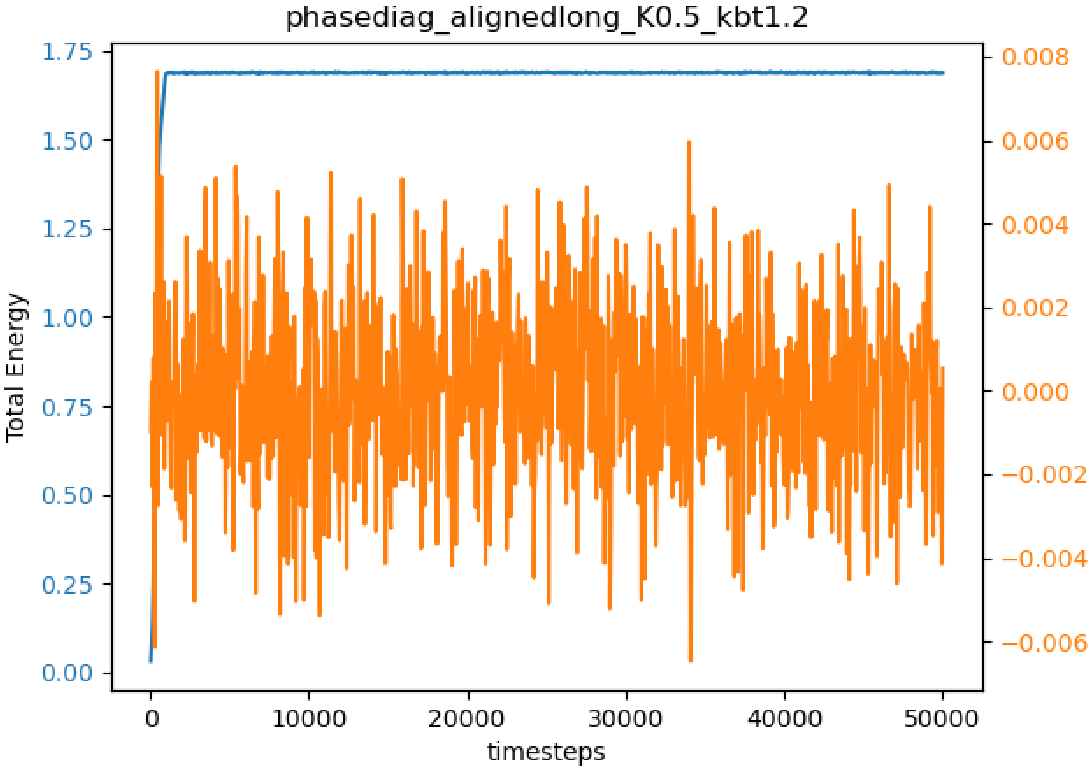

phasediag_alignedlong_K0.5_kbt0.95
Total Energy
1.6
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
0.006
0.004
0.002
0.000
−0.002
−0.004
−0.006
−0.008
0
10000
20000
30000
40000
50000
timesteps

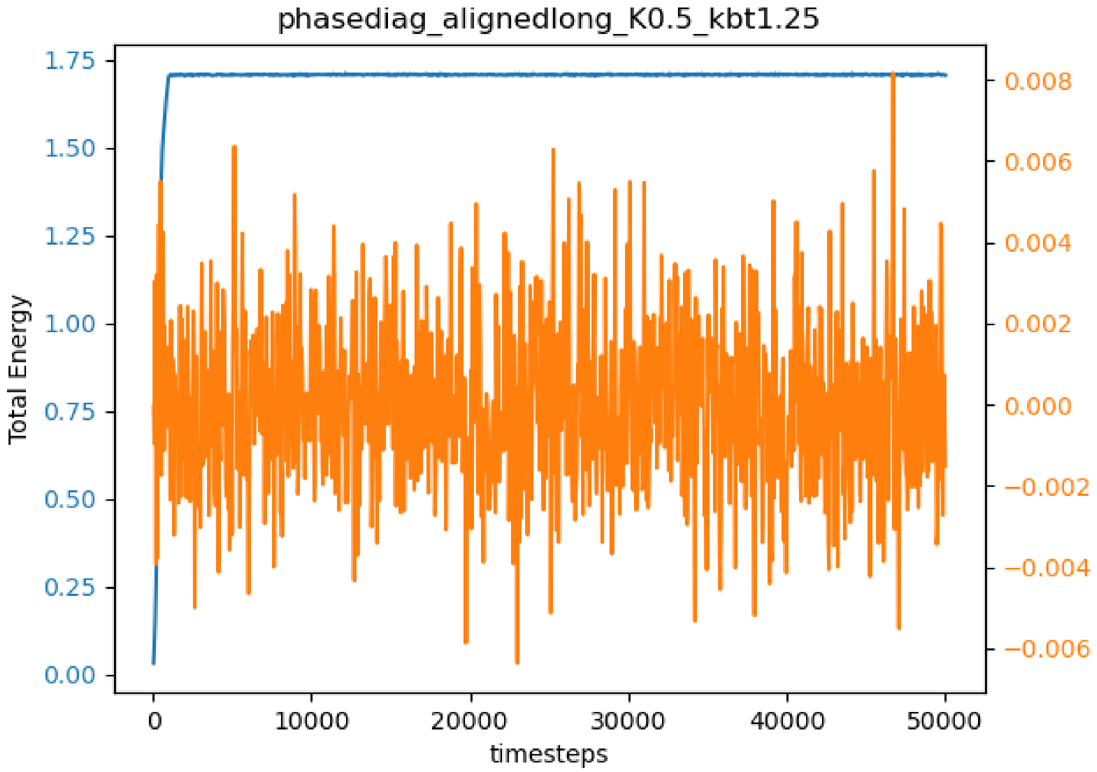

phasediag_alignedlong_K0.5_kbt1.0
Total Energy
1.6
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
0.008
0.006
0.004
0.002
0.000
−0.002
−0.004
−0.006
0
10000
20000
30000
40000
50000
timesteps

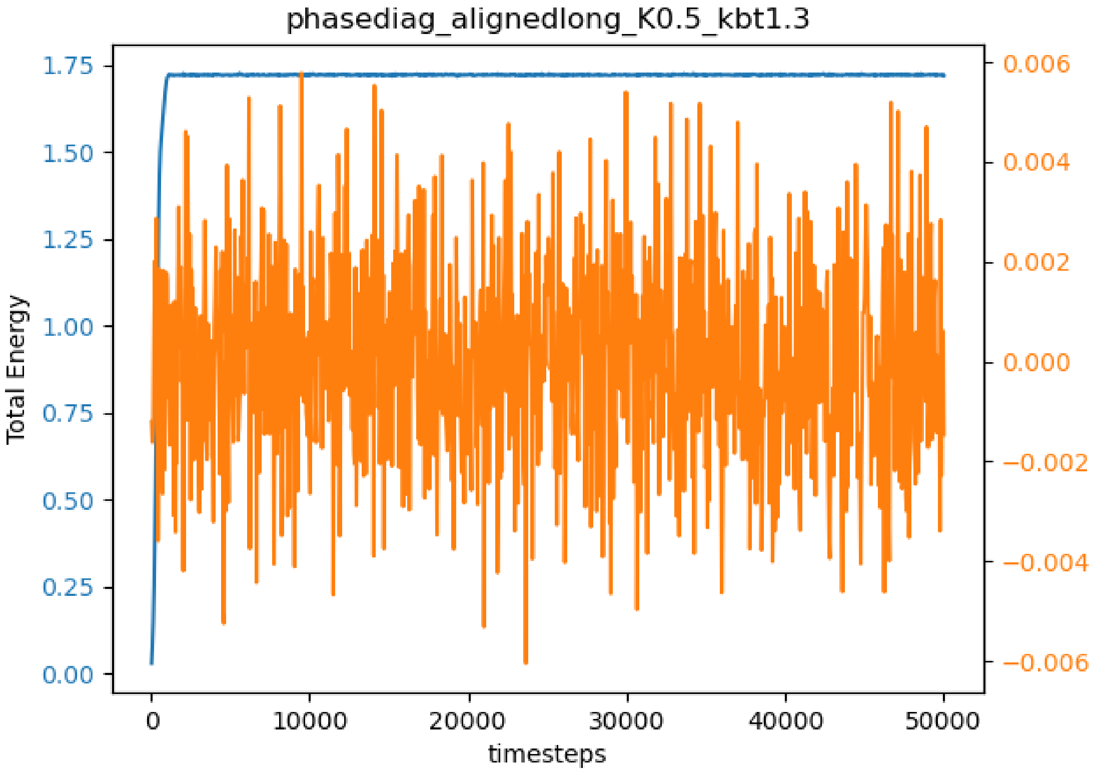

phasediag_alignedlong_K0.5_kbt1.05
Total Energy
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
0.006
0.004
0.002
0.000
−0.002
−0.004
−0.006
0
10000
20000
30000
40000
50000
timesteps

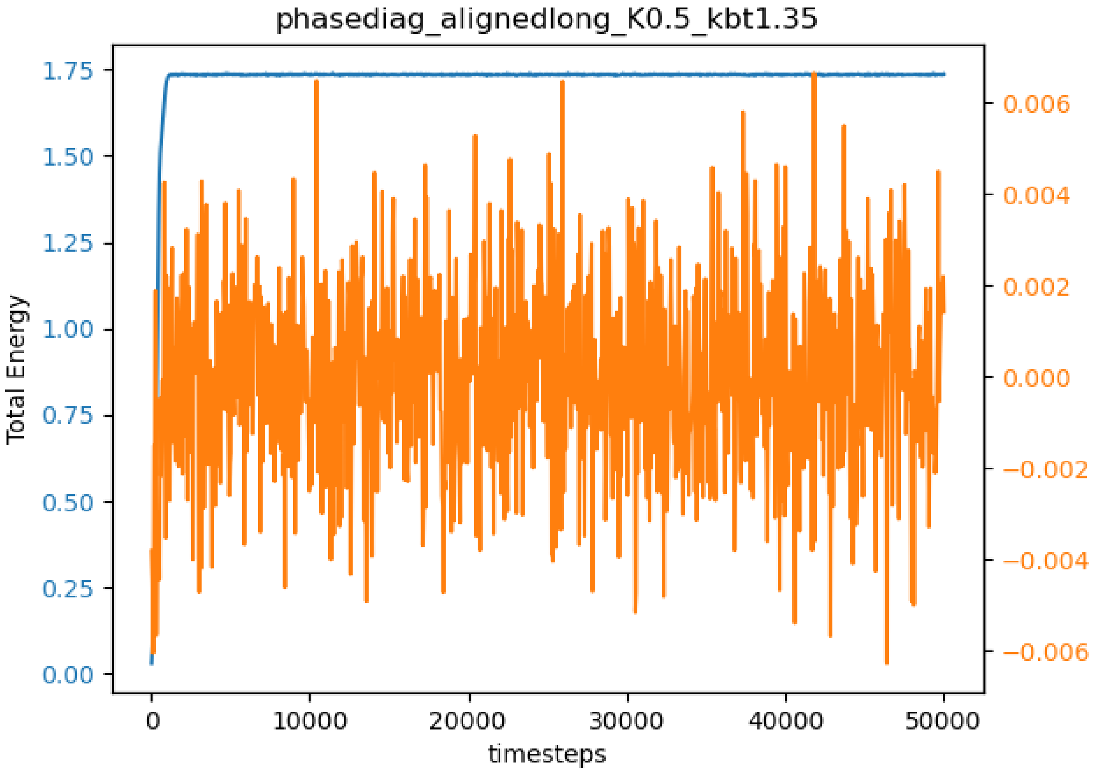

phasediag_alignedlong_K0.5_kbt1.1
Total Energy
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
0.006
0.004
0.002
0.000
−0.002
−0.004
−0.006
0
10000
20000
30000
40000
50000
timesteps

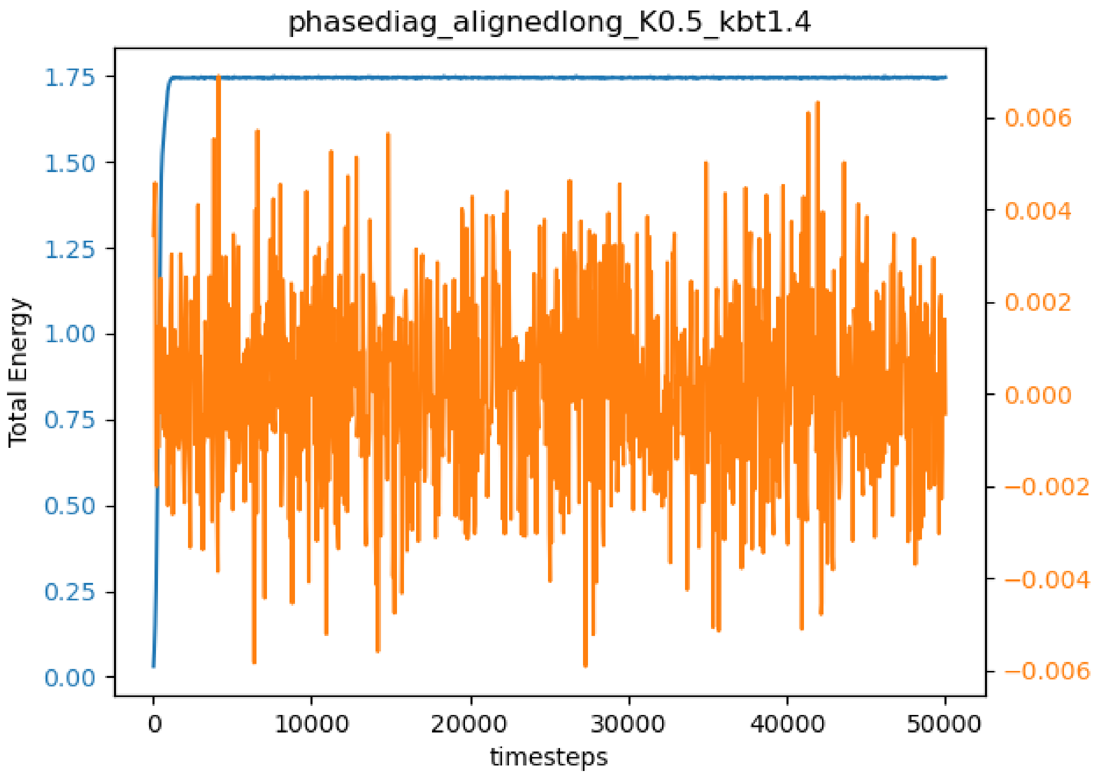

phasediag_alignedlong_K0.5_kbt1.15
Total Energy
1.75
1.50
1.25
1.00
0.75
0.50
0.25
0.00
0.006
0.004
0.002
0.000
−0.002
−0.004
−0.006
0
10000
20000
30000
40000
50000
timesteps

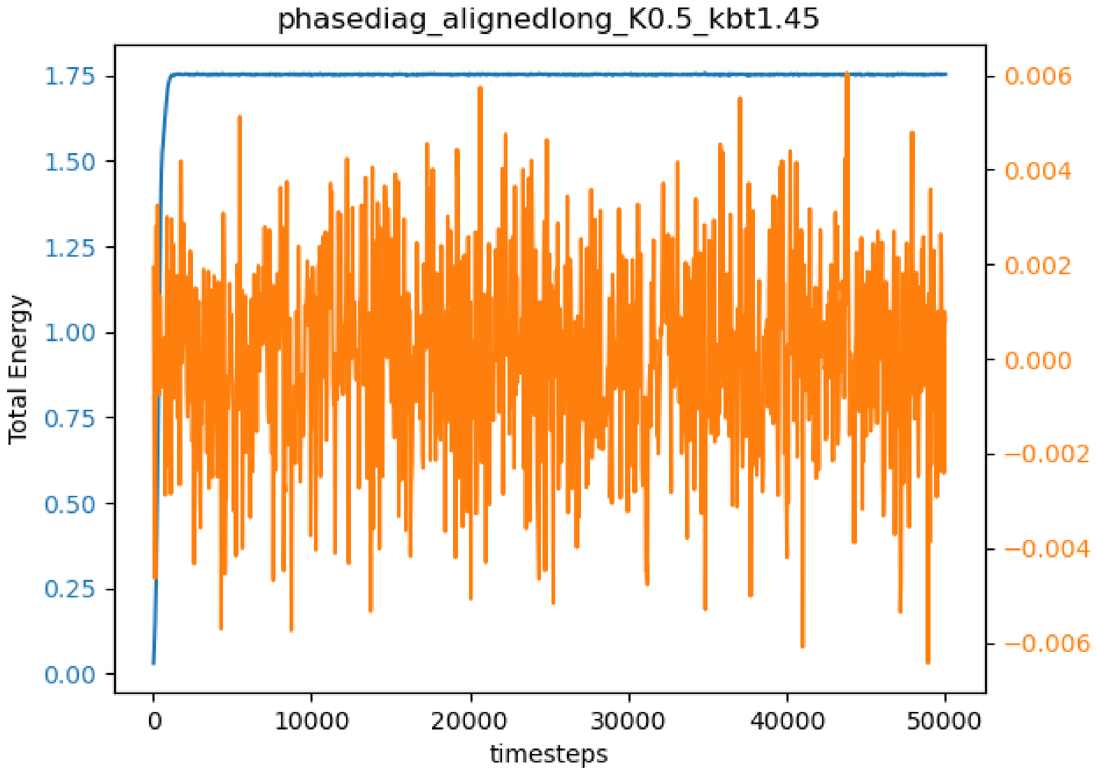

phasediag_alignedlong_K0.5_kbt1.2
Total Energy
1.75
1.50
1.25
1.00
0.75
0.50
0.25
0.00
0.008
0.006
0.004
0.002
0.000
−0.002
−0.004
−0.006
0
10000
20000
30000
40000
50000
timesteps

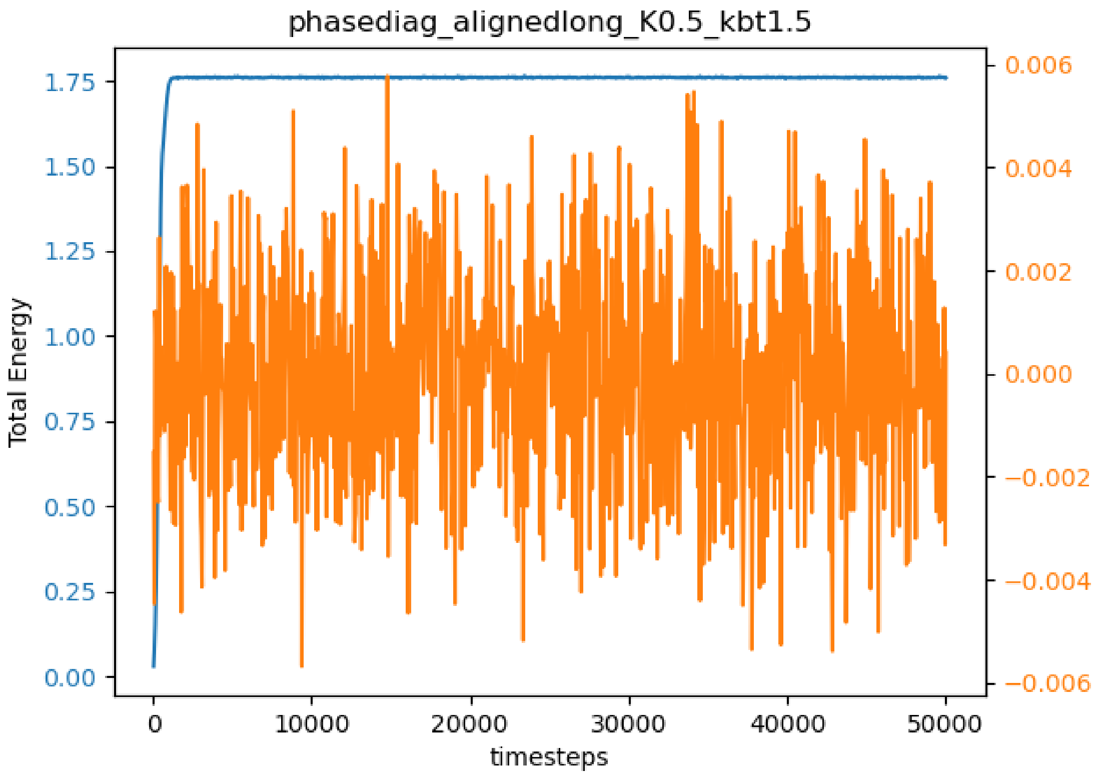

phasediag_alignedlong_K0.5_kbt1.25
Total Energy
1.75
1.50
1.25
1.00
0.75
0.50
0.25
0.00
0.008
0.006
0.004
0.002
0.000
−0.002
−0.004
−0.006
0
10000
20000
30000
40000
50000
timesteps


phasediag_alignedlong_K0.5_kbt1.3
Total Energy
timesteps
0.00
0.25
0.50
0.75
1.00
1.25
1.50
1.75
0.006
0.004
0.002
0.000
−0.002
−0.004
−0.006
0
10000
20000
30000
40000
50000


phasediag_alignedlong_K0.5_kbt1.35
Total Energy
1.75
1.50
1.25
1.00
0.75
0.50
0.25
0.00
0.006
0.004
0.002
0.000
−0.002
−0.004
−0.006
0
10000
20000
30000
40000
50000
timesteps

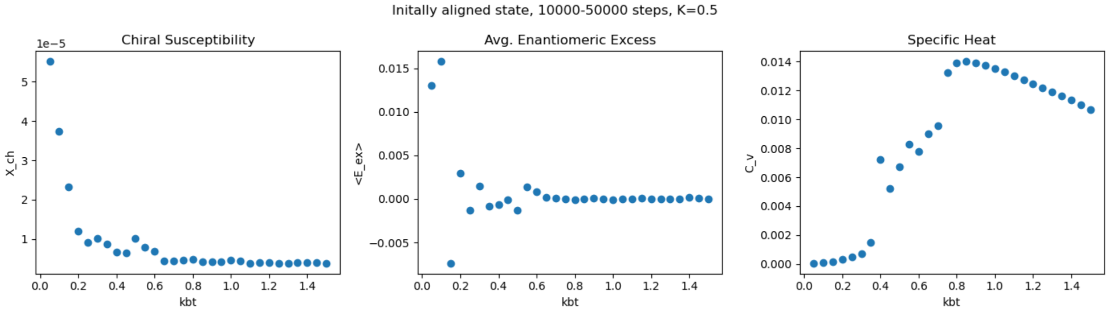

phasediag_alignedlong_K0.5_kbt1.4
Total Energy
timesteps
0.00
0.25
0.50
0.75
1.00
1.25
1.50
1.75
0
10000
20000
30000
40000
50000
0.006
0.004
0.002
0.000
−0.002
−0.004
−0.006


phasediag_alignedlong_K0.5_kbt1.45
Total Energy
1.75
1.50
1.25
1.00
0.75
0.50
0.25
0.00
0.006
0.004
0.002
0.000
−0.002
−0.004
−0.006
0
10000
20000
30000
40000
50000
timesteps

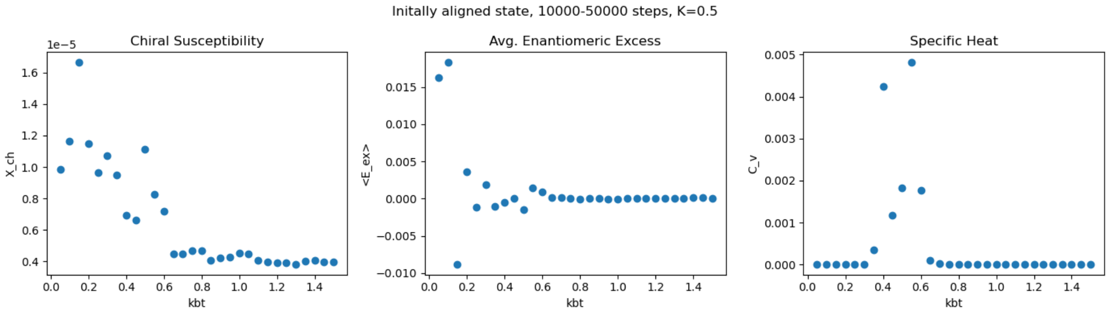


[33]:

```
# measuring chiral susceptibility mean(enantionmeric excess^2) -␣
↪mean(enantiomeric excess^2)
def measure_chi(Kin,init_type="alignedlong"):
    ch_sus = []
    kbts = []
    avg_ent = []
    c_v = []
    for csvfile in csvfiles:
        csv1 = load_csv(csvfile,verbose=False)
        K = float(csvfile.split("/")[3].split("_")[-2][1:])
        if K == Kin and init_type in csvfile:
            kbt = float(csvfile.split("/")[3].split("_")[-1][3:])
            kbts.append(kbt)
            # chiral susceptibility
            excess = csv1[:,2]
            ch_sus.append(np.mean(excess**2) - np.mean(excess)**2)
            # average enantiomeric excess
            avg_ent.append(np.mean(excess))
            #specific heat
            E = csv1[:,1]
            c_v.append((np.mean(E**2) - np.mean(E)**2)/kbt)

    fig,(ax1,ax2,ax3) = plt.subplots(1,3,figsize=(14,4))
    fig.suptitle("Initally aligned state, all50000 steps, K="+str(Kin))
    ax1.set_title("Chiral Susceptibility")
    ax1.set_ylabel("X_ch")
    ax1.set_xlabel("kbt")
    ax1.scatter(kbts,ch_sus)

    ax2.set_title("Avg. Enantiomeric Excess")
    ax2.set_ylabel("<E_ex>")
    ax2.set_xlabel("kbt")
    ax2.scatter(kbts,avg_ent)

    ax3.set_title("Specific Heat")
    ax3.set_ylabel("C_v")
    ax3.set_xlabel("kbt")
    ax3.scatter(kbts,c_v)
    fig.tight_layout()
    plt.show()

measure_chi(0.5)
```



[34]:
```
# measuring chiral susceptibility mean(enantionmeric excess^2) -␣
 ↪mean(enantiomeric excess^2)
def measure_chi(Kin,init_type="alignedlong"):
    ch_sus = []
    kbts = []
    avg_ent = []
    c_v = []
    for csvfile in csvfiles:
        csv1 = load_csv(csvfile,verbose=False)
        K = float(csvfile.split("/")[3].split("_")[-2][1:])
        if K == Kin and init_type in csvfile:
            kbt = float(csvfile.split("/")[3].split("_")[-1][3:])
            kbts.append(kbt)
            # chiral susceptibility
            excess = csv1[200:,2]
            ch_sus.append(np.mean(excess**2) - np.mean(excess)**2)
            # average enantiomeric excess
            avg_ent.append(np.mean(excess))
            #specific heat
            E = csv1[200:,1]
            c_v.append((np.mean(E**2) - np.mean(E)**2)/kbt)

    fig,(ax1,ax2,ax3) = plt.subplots(1,3,figsize=(14,4))
    fig.suptitle("Initally aligned state, 10000-50000 steps, K="+str(Kin))
    ax1.set_title("Chiral Susceptibility")
    ax1.set_ylabel("X_ch")
    ax1.set_xlabel("kbt")
    ax1.scatter(kbts,ch_sus)

    ax2.set_title("Avg. Enantiomeric Excess")
    ax2.set_ylabel("<E_ex>")
    ax2.set_xlabel("kbt")
    ax2.scatter(kbts,avg_ent)

    ax3.set_title("Specific Heat")
    ax3.set_ylabel("C_v")
    ax3.set_xlabel("kbt")
    ax3.scatter(kbts,c_v)
    fig.tight_layout()
    plt.show()

measure_chi(0.5)
```



[ ]: