Methods of Computational Physics

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Problem Sheet 3
Quantum Monte Carlo Simulations

Diffusion Monte Carlo for Ground state wavefunction

1. Rescaling diffusion propagator and weight change

$$V = \frac{1}{2}m\omega^2 x^2; x_o^2 = \frac{\hbar}{m\omega}; \tilde{x} = \frac{x}{x_o}$$

$$P(x_j, x_{j-1}) = \sqrt{\frac{m}{2\pi\hbar^2\Delta\tau}} \exp\left(-\frac{m}{2\hbar^2\Delta\tau}(x_j - x_{j-1})^2\right)$$

$$P(\tilde{x_j}, \tilde{x_{j-1}}) \sim \exp\left(-\frac{m}{2\hbar^2\Delta\tau}x_o^2(\tilde{x_j} - \tilde{x_{j-1}})^2\right)$$

$$P(\tilde{x_j}, \tilde{x_{j-1}}) \sim \exp\left(-\frac{(\tilde{x_j} - \tilde{x_{j-1}})^2}{2\hbar\omega\Delta\tau}\right)$$

$$W(\tilde{x}) = \exp\left(-\hbar\omega\Delta\tau(\frac{\tilde{x}^2}{2} - \frac{E_T}{\hbar\omega})\right)$$

For simulation the following parameters were chosen -
$i\hbar\Delta\tau = 0.01$, Number of replicas -10^6, Starting point $x(t=0) = 0$, Simulation Time = 1000

The DQMC process was carried out in 3 steps -
1. The Initial State - Describing an initial position of replicas. Started from $x(t=0) = 0$.
2. Diffusive Displacement of Replicas - Per time step, positions of all the replicas are updated simultaneously. Update: $x(t=1) = x(t=0) + \sqrt{\Delta\tau} \times \rho$, where ρ is a random number sampled from a Gaussian distribution with mean 0 and variance 1.
3. Birth and Death Process - Depending on the value of m, described as m= $min(int(W+u), 3)$, where u is uniformly distributed random number between [0,1].

- if m=0, Kill the Replica

- if m=1, No change
- if m=2, Add one more replica to that point x(t)
- if m=3, Add two more replicas to that point x(t)

E_T is adjusted in such a way that W($\tilde{x}$) $\approx$ 1, using -
$E_T =< V > (t) + (1 - \frac{N(t}{N(t-1}$), where N(t) is population of replicas at time t.

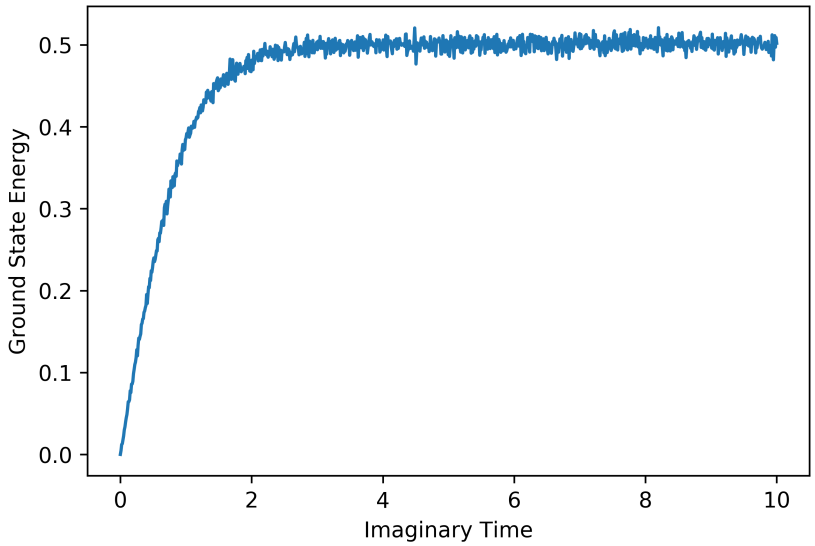

Figure 1: Ground state energy plot

Ground state energy was found to be converging at a value ~0.5, which matches appropriately with analytically known equation $H = (n + \frac{1}{2})\hbar\omega$. For n=0, it stands a value of $0.5\hbar\omega$ which matches our result in the dimensionless units.

Analytically known wave for the ground state reads - $\psi(x) = \frac{1}{\pi^{\frac{1}{4}}} e^{-\tilde{x}^2/2}$ in our dimensionless units. The blue curve in figure 2 shows it. The final distribution of replica points in x-space, provides us our ground state wave function; shown in figure 2 with + points.

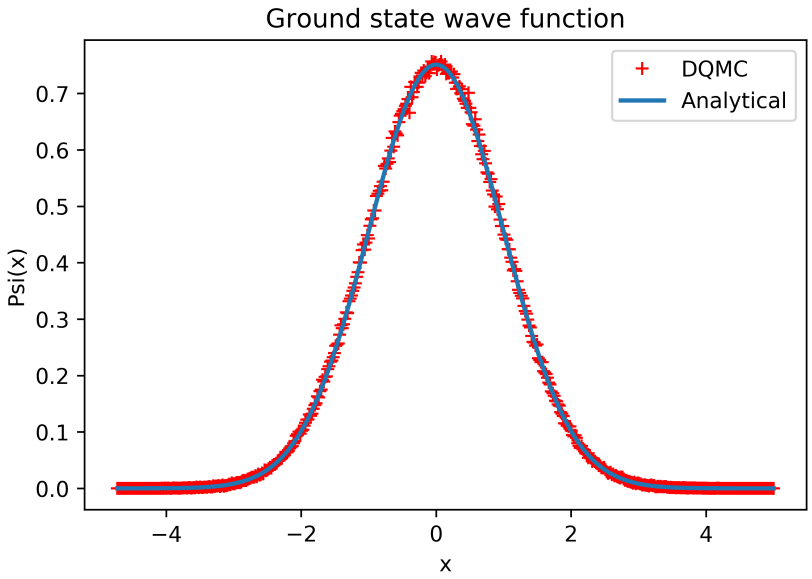

Figure 2:

2. Estimate for the ground state energy for different time slices.

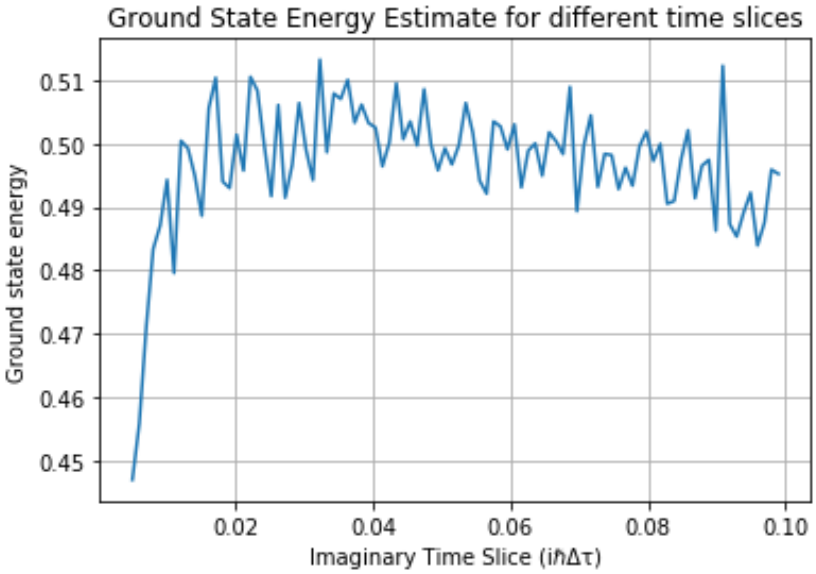

Figure 3:

3. Condition where all the replicas start from $x_o = 0$. Required propagation time to reach the ground state ~ 1.75 (in units of $i\hbar\tau$)

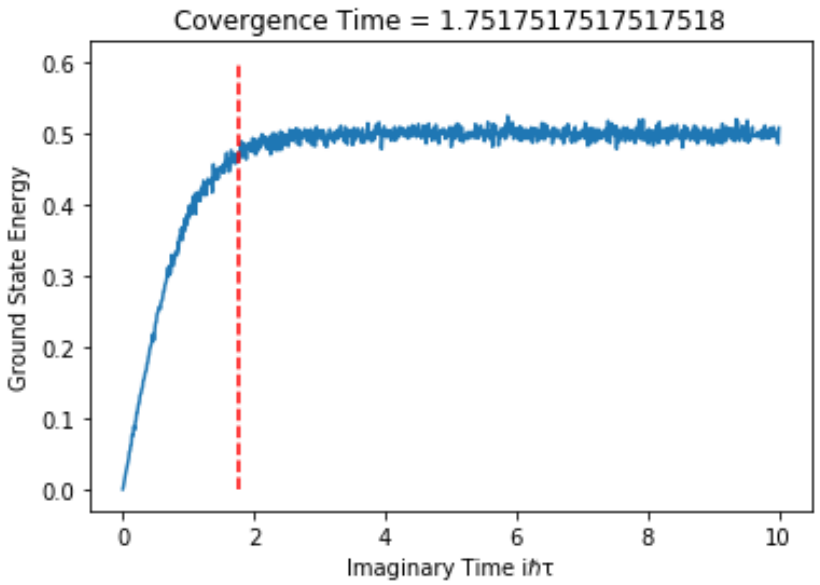

Figure 4:

4. Double Potential

Figure 4 shows the variation of double potential $V(x) = \frac{((\frac{x}{x_o})^2 - d^2)^2}{8d^2}$ with various values of d. For small values of d$\leq$1, this potential behaves like a single potential well. For bigger values d, two valleys start to emerge.
Figure 5 depicts, the the ground state energies for different values of d.

- d=0.1, E_{ground} =1.50665
- d=2, E_{ground} =0.355452
- d=8 E_{ground} =0.498487

For larger values of d, the ground state energy decreases, plus the time taken to reach the ground state also increases. The reason for this increased time requirement to converge to the ground state can be understood by looking at figure 8 and 9. Starting from x=0 signifies to starting from highest potential. The replicas have to traverse down the peak at x=0 to x=4 which is the ground state. For small values of d between [0,1], the peak height is almost negligible, and starting nearing x=0, is like starting in the ground state. Figure 9, compares time taken to reach the ground state with starting points as x=0 and x=4 for d=4. Starting from x=4 takes less time to reach the ground state energy value in comparison to starting from x=0.

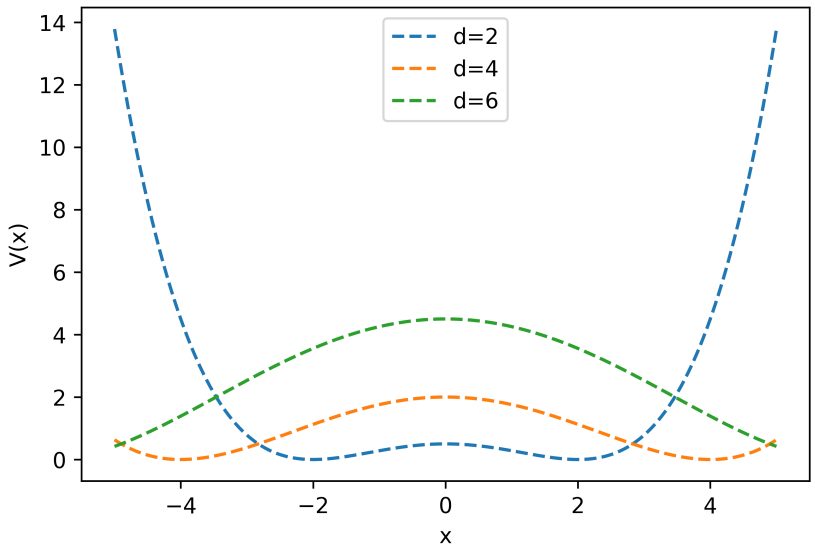

Figure 5: Variation of double potential V(x) with different values of d

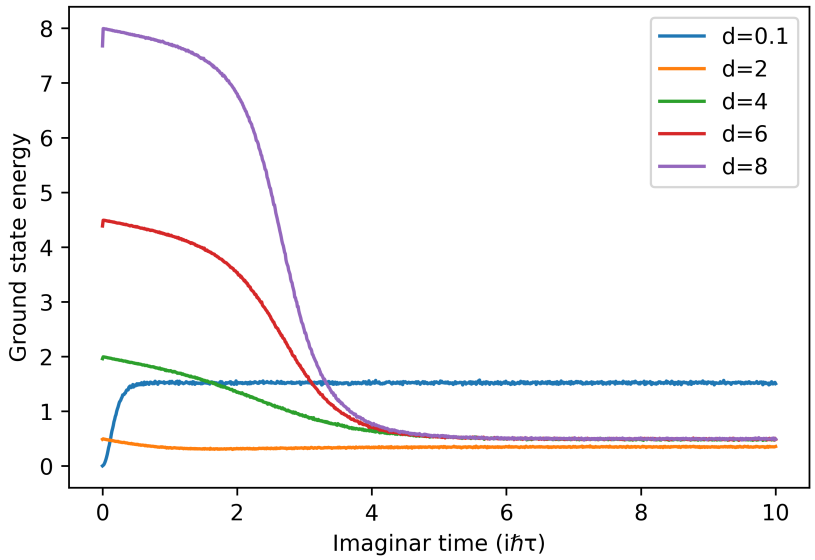

Figure 6: Ground state energy convergence in imaginary time propagation for various values of d

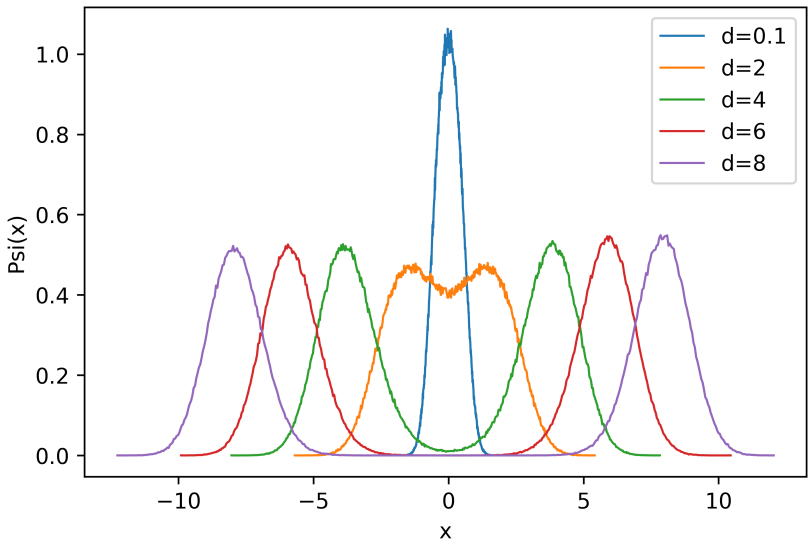

Figure 7: Ground state wave function for different values of d

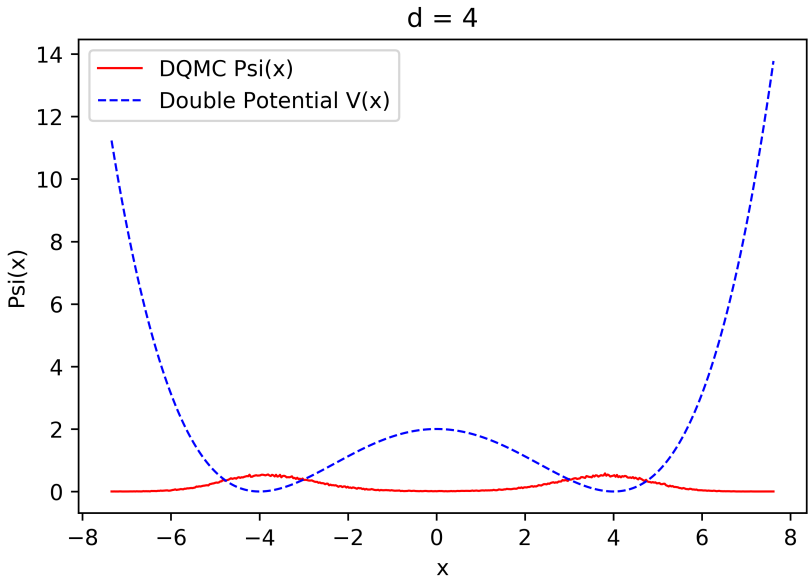

Figure 8: For d=4, the ground state wave function and the double potential

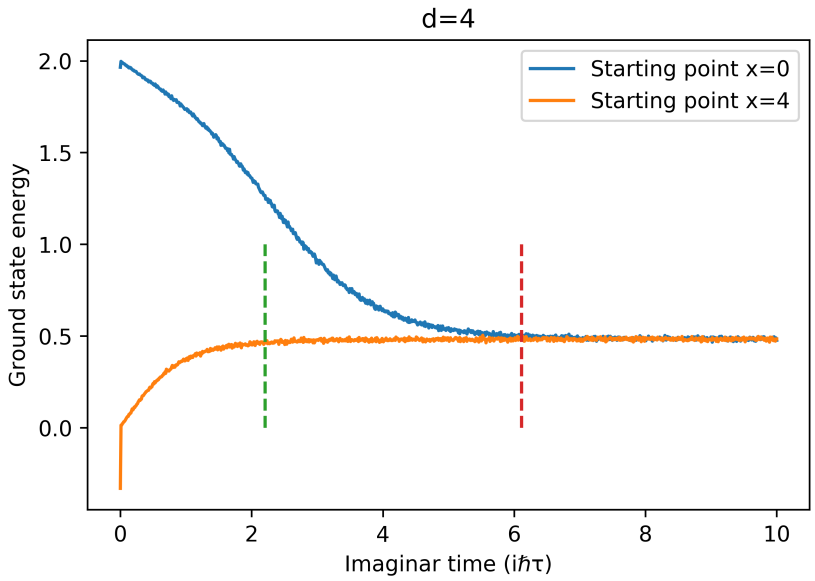

Figure 9:

- Starting point x=4.
  Time to reach ground state energy - 2.2044088176352705
- Starting point x=0.
  Time to reach ground state energy - 6.112224448897796

Path Integral Monte Carlo $T > 0$

1. Density matrix in position representation - $< x_n|\rho|x_o >=< x_n|e^{-\beta H}|x_o >$, insterting closure relations -

$< x_n|\rho|x_o >= \int dx_1...d_{n-1} \prod_{j=1}^{n} < x_j|e^{-\beta H}|x_{j-1} >$

$< x_n|\rho|x_o >= \int dx_1...d_{n-1} e^{-\sum_{j=1}^{n} S_j}$,

where $S_j = \frac{dN}{2} \log(\frac{2\pi\hbar^2\Delta\tau}{m}) + \frac{m}{2}(\frac{x_j - x_{j-1}}{\hbar\sqrt{\Delta\tau}})^2 + \frac{\Delta\tau}{2}(V(x_j) + V(x_{j-1}))$

In units where - $\tilde{x} = \frac{x}{x_o}$ and $x_o^2 = \frac{\hbar}{m\omega}$

$S = Const. + \frac{n}{2\beta\hbar\omega} \sum_{j=1}^{n} (\tilde{x_j} - \tilde{x_{j-1}})^2 + \frac{\beta\hbar\omega}{n} \sum_{j=1}^{n} \frac{\tilde{x}^2}{2}, \beta = \frac{1}{KT}$

It can be seen from the equation for action (S) that the only relevant parameters are n and $\beta\hbar\omega$.

2. For simulation, the following parameters were used -
a) Number of beads n - 100
b) $\Delta\tau$=0.1, or say $\beta = 10$
c) Total simulation time = 10^6
d) Number of MCS steps = 10^4
e) dN =1 (dN dimensional quantum system)

To perform PIMC -

- A starting configuration was chosen randomly, giving each bead a point in spacetime (x,t).
- For the first time step in a MC cycle, a bead is chosen at random and displaced according to - $x_{new} = x_{old} + \sqrt{\Delta\tau} \times \rho$, where ρ is a random number between [0,1].
- Compare the action (S) of the displaced config. to the old config. and accept the displaced config. according to metrop(1,exp(ΔS)).
- Repeat the above steps for 10^4 MCS steps. Calculate autocorrelation C(t,0)=$< x(t)x(0) >$, Kinetic Energy = $\frac{n}{2\Delta\tau} - \frac{1}{n}\sum_{j=1}^{n} < \frac{1}{2}(\frac{x_j - x_{j-1}}{\Delta\tau})^2 >$, Potential Energy = $\frac{1}{n}\sum_{j=1}^{n} < \frac{x_j^2}{2} >$ and Total Energy.

Figure 10 displays the final configuration obtained after 10^4 MCS steps.

Figure 11 marks the required number of MCS steps (21 steps) in order to obtain independent configurations.

Figure 12 is a plot for kinetic energy and potential energy.

For the given parameters, the following quantities were obtained -

- Kinetic energy = 0.25518079045216413
- Potential energy = 0.24057351642110575,
- Total energy = 0.4957543068732699.

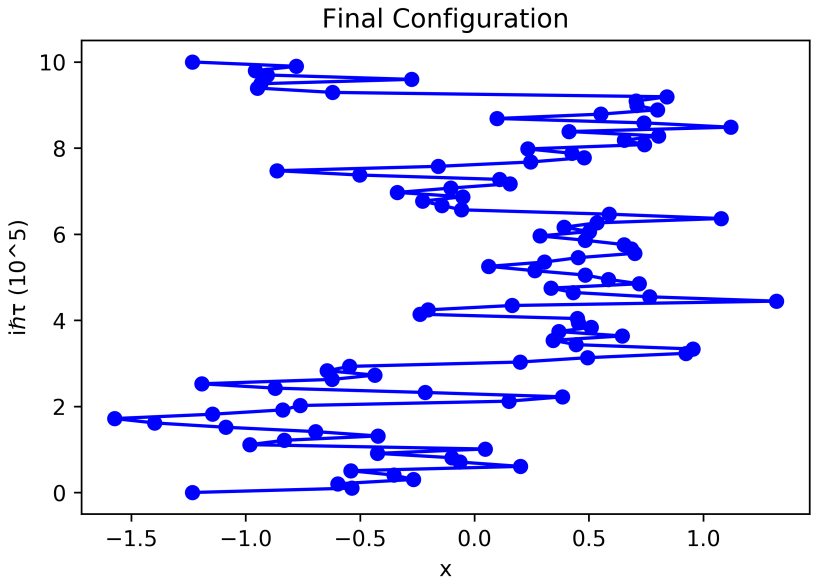

Figure 10:

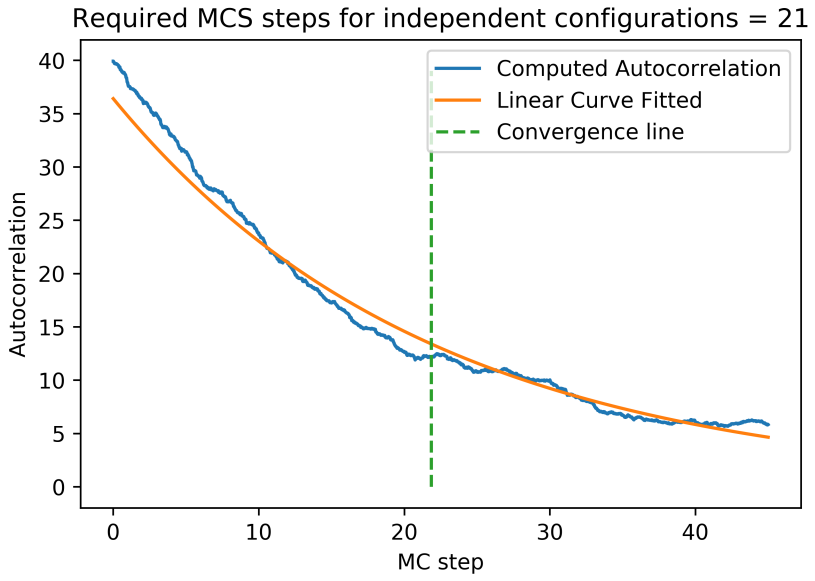

Figure 11: Convergence plot for independent configurations

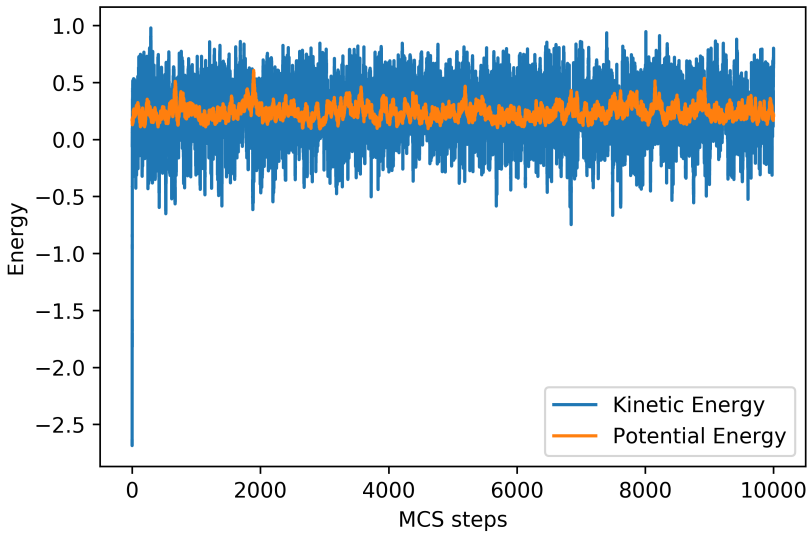

Figure 12: Variation in Kinetic and Potential energy along MC steps

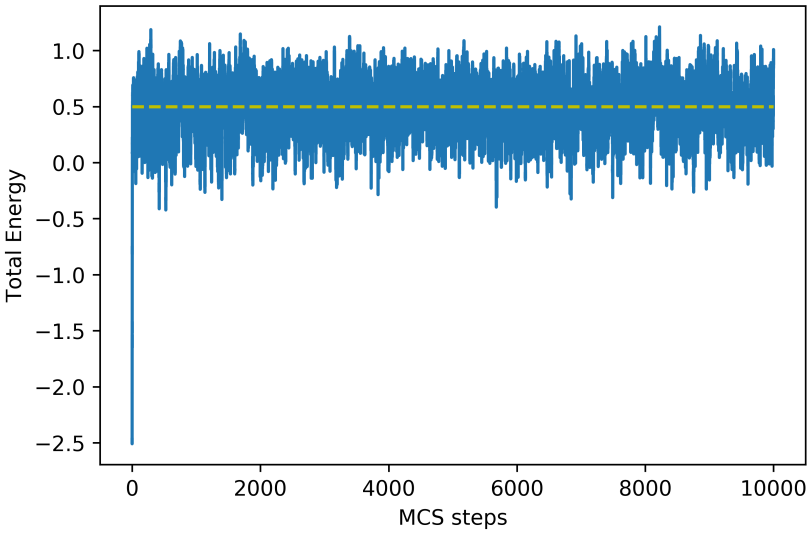

Figure 13: Total Energy = Kinetic Energy + Potential Energy, Total energy's variation with time