
PHYSICS 142: ASSIGNMENT 3

JESSICA BIRKY (A13002163)

Preliminary Notes:

(a) Error calculation: Error in average energy for energy samples χ_i is computed as

$$\langle E \rangle_T = \frac{1}{N} \sum_{i=1}^N \chi_i \pm \frac{\sigma}{\sqrt{N}}$$

$$\sigma^2 = \langle \chi_i^2 \rangle - \langle \chi_i \rangle^2$$

(b) Simulation setup parameters:

Nstep	Total number of steps computed per walker
Nburn	Number of samples removed from beginning
Nskip	Number of steps skipped between data point collection

Nburn and Nskip are implemented to remove the effect of autocorrelation and draw independent samples. So the total number of samples used to compute average and the error for E is $N = (\text{Nstep} - \text{Nburn})/\text{Nskip}$. These parameters and other physical constants are defined in setup.cpp.

(c) Step size choices: For the classical harmonic oscillator I sample (x_1, x_2, p_1, p_2) using a gaussian distribution with mean 0 and standard deviation 1, using a Box-Muller transformation to draw a gaussian random numbers (X,Y) using uniform distributions U_1, U_2 on the interval [0,1]:

$$\Theta = 2\pi U_1 \quad R = \sqrt{-2\ln(U_2)}$$

$$X = R \cos \Theta \quad Y = R \sin \Theta$$

For the quantum oscillators I select the step to be -1, 0, or 1, each with equal probability, except when the current value of $n=0$, then the proposed value will be 0 with 2/3 probability and 1 with 1/3 probability.

(d) Numerically determining $\bar{E}(T)$: For determining the relationship between T and $\langle E \rangle$ I use linear regression, for $x = T$, $y = \langle E \rangle$, and σ as the error computed as above. Letting $Y = [y_i]$, $A = [1, x_i]$, and C a diagonal matrix with $C_{ii} = \sigma_i^2$, then solving $Y = AX$ for X gives the slope and intercept:

$$\begin{bmatrix} b \\ m \end{bmatrix} = X = [A^T C^{-1} A]^{-1} [A^T C^{-1} Y]$$

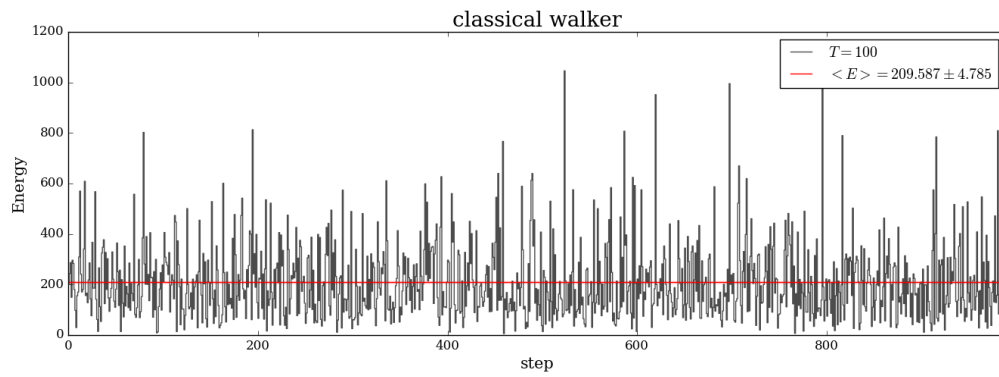
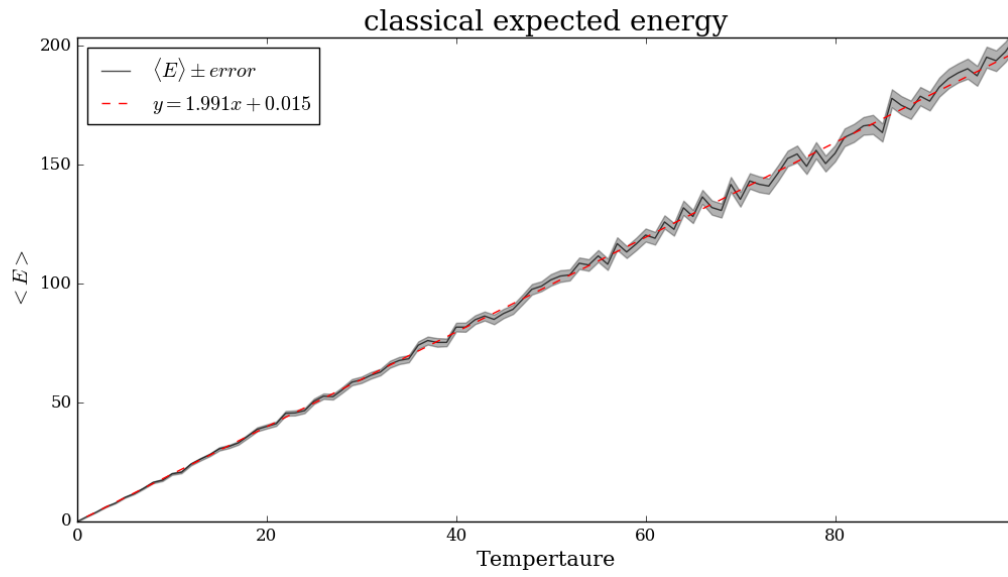
Question 1: Electron in a 2D classical harmonic oscillator.

$$E = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 r^2$$

(a) Determine $\bar{E}(T)$ the thermal average of the energy at temperature T.

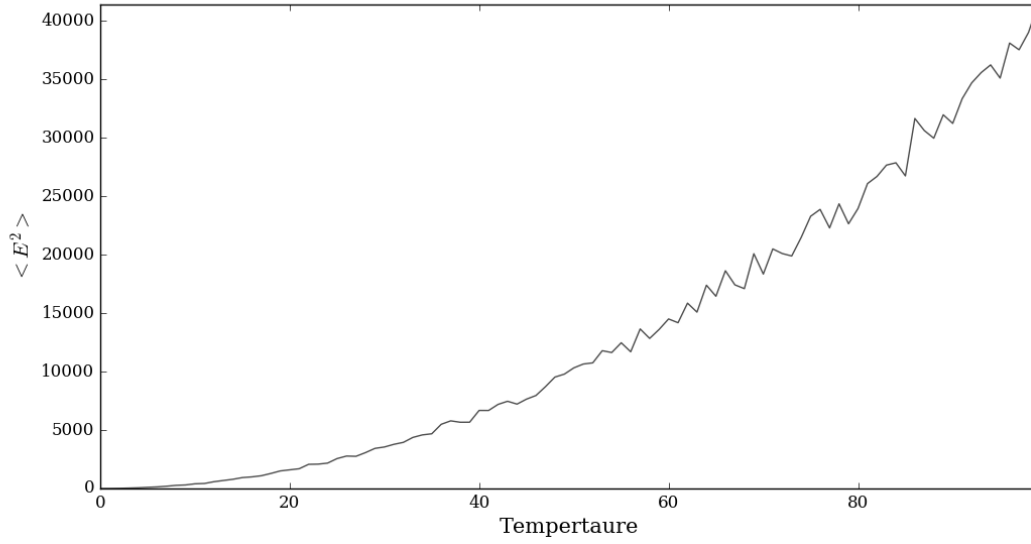
(b) Design and run a Monte Carlo simulation to numerically determine $\bar{E}(T)$.

Nstep	10^6
Nburn	10^4
Nskip	10^3
Run time	205.521 sec



Note that the simulaiton yields $\langle E \rangle_T \approx 2T$ as expected.

(c) Determine $\bar{E}_2(T)$.



Question 2: Electron in a 1D quantum harmonic oscillator.

$$E_n = \left(n + \frac{1}{2}\right) \hbar\omega$$

(a) Determine $\bar{E}(T)$ the thermal average of the energy at temperature T .

Let $\beta = \frac{\hbar\omega}{kT}$.

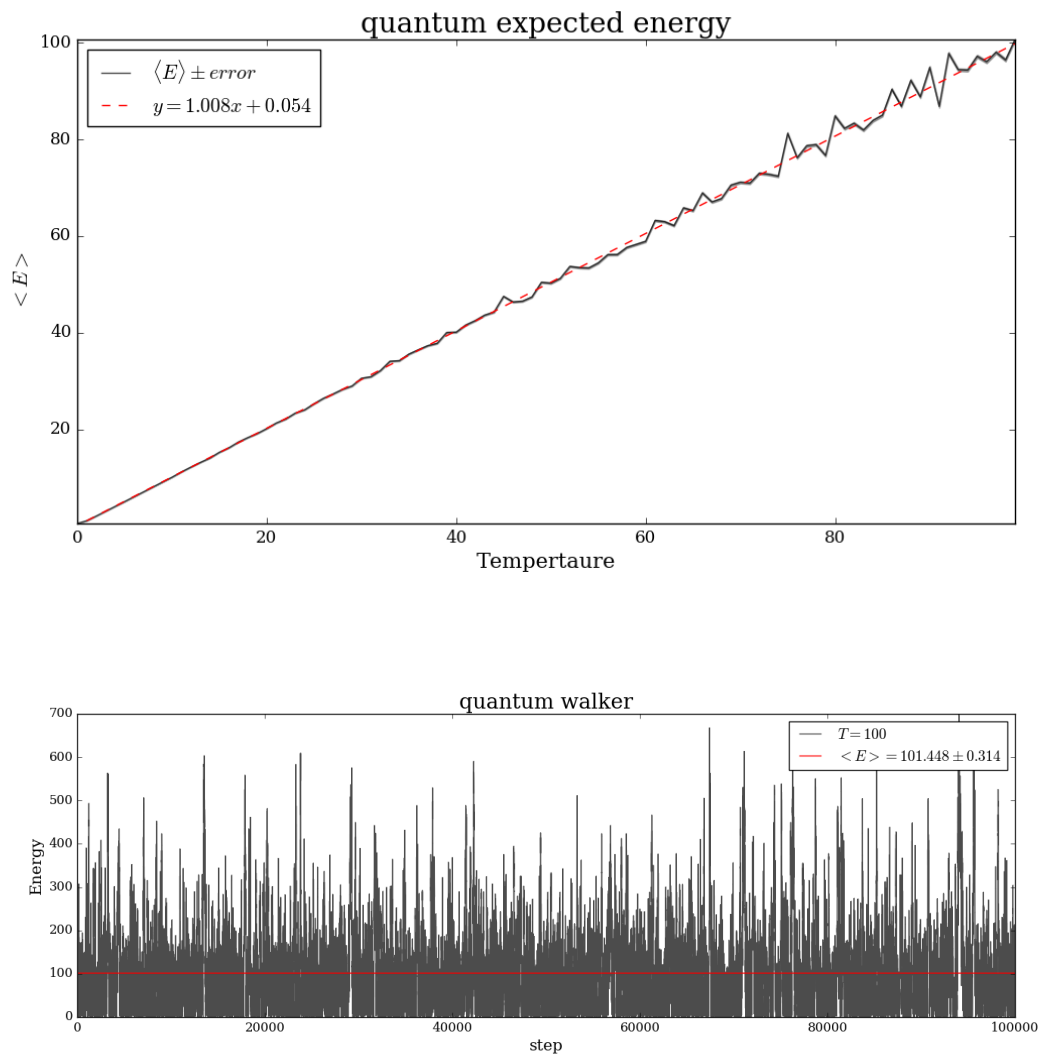
$$\begin{aligned} \langle E \rangle &= \frac{\sum_{n=0}^{\infty} E_n e^{E_n/kT}}{\sum_{n=0}^{\infty} e^{E_n/kT}} = \frac{\sum (n + \frac{1}{2}) \hbar\omega e^{(n+\frac{1}{2})\hbar\omega/kT}}{\sum e^{(n+\frac{1}{2})\hbar\omega/kT}} \\ &= \hbar\omega \left[\frac{\sum n e^{-\beta(n+\frac{1}{2})}}{\sum e^{-\beta(n+\frac{1}{2})}} + \frac{\frac{1}{2} \sum e^{-\beta(n+\frac{1}{2})}}{\sum e^{-\beta(n+\frac{1}{2})}} \right] \\ &= \hbar\omega \left[\frac{e^{-\beta/2}}{(e^{\beta} - 1)^2} \cdot \frac{(e^{\beta} - 1)}{e^{-\beta/2}} + \frac{1}{2} \right] = \hbar\omega \left[\frac{1}{e^{\beta} - 1} + \frac{1}{2} \right] \end{aligned}$$

Since $\hbar\omega \ll kT$, then $\beta \ll 1$ and we can Taylor expand $\frac{1}{e^{\beta}-1} = \frac{1}{\beta} - \frac{1}{2} + O(\beta)$ and get

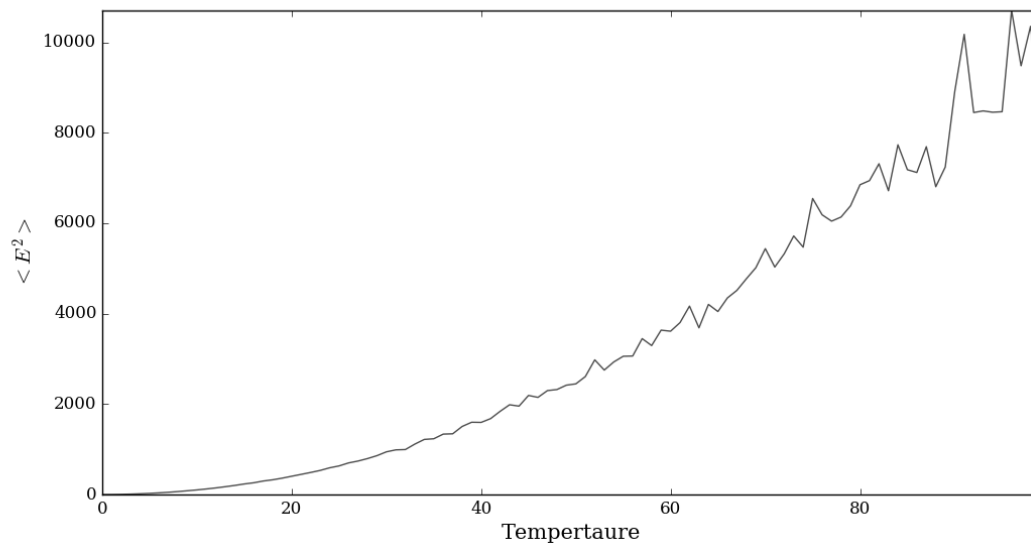
$$\langle E \rangle \approx \hbar\omega \left[\frac{1}{\beta} - \frac{1}{2} + \frac{1}{2} \right] = \frac{\hbar\omega}{\beta} = \hbar\omega \left(\frac{kT}{\hbar\omega} \right) = kT$$

(b) Design and run a Monte Carlo simulation to numerically determine $\bar{E}(T)$.

Nstep	10^8
Nburn	10^4
Nskip	10^3
Run time	625.997 sec



(c) Determine $\bar{E}_2(T)$.

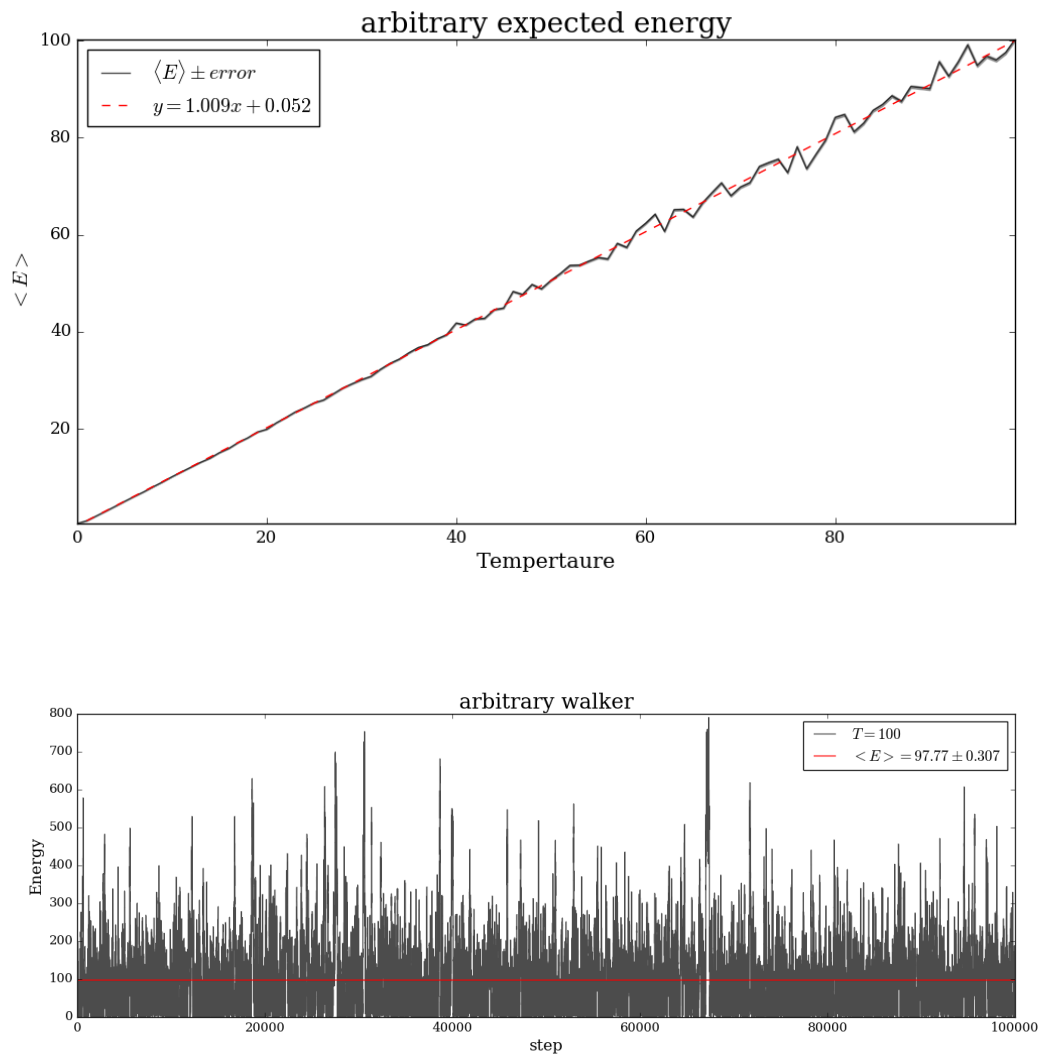


Question 3: An arbitrary harmonic energy.

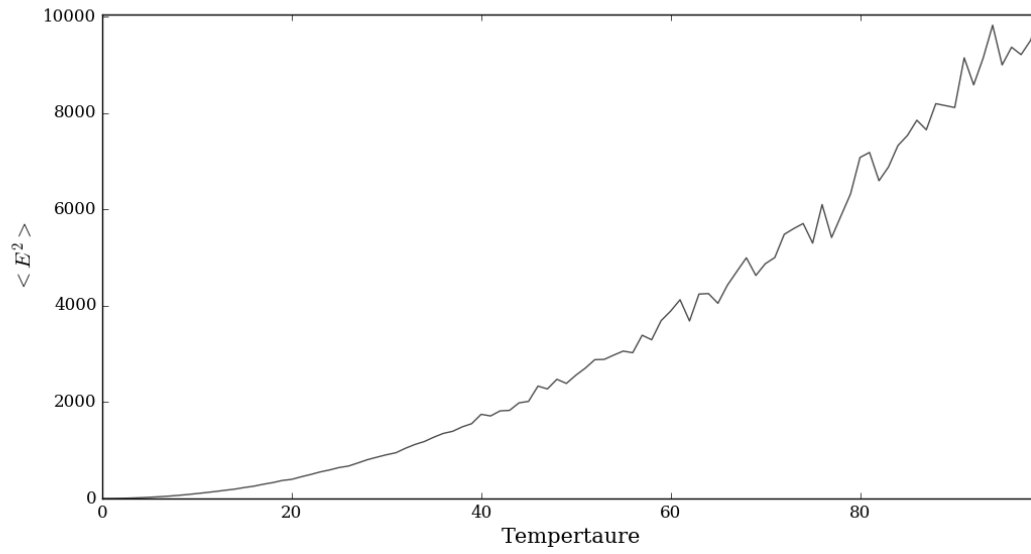
$$E_n = \left(n^2 + \frac{1}{2} \right) \hbar \omega$$

- (a) Determine $\bar{E}(T)$ the thermal average of the energy at temperature T.
- (b) Design and run a Monte Carlo simulation to numerically determine $\bar{E}(T)$.

Nstep	10^8
Nburn	10^4
Nskip	10^3
Run time	650.525 sec



(c) Determine $\bar{E}_2(T)$.

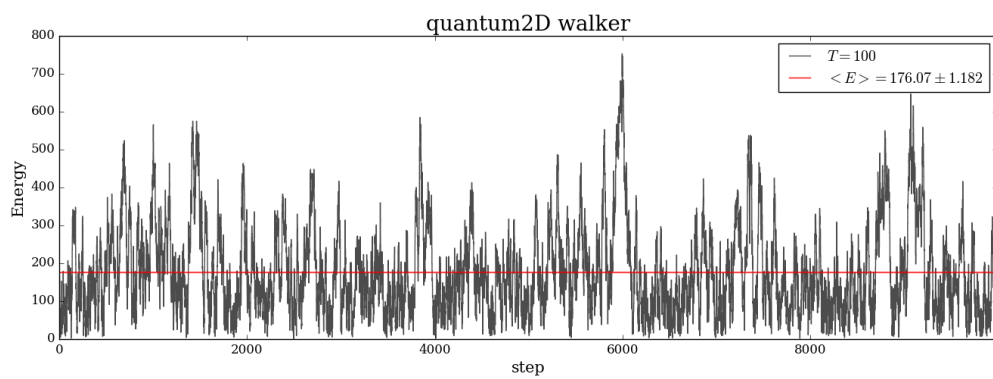
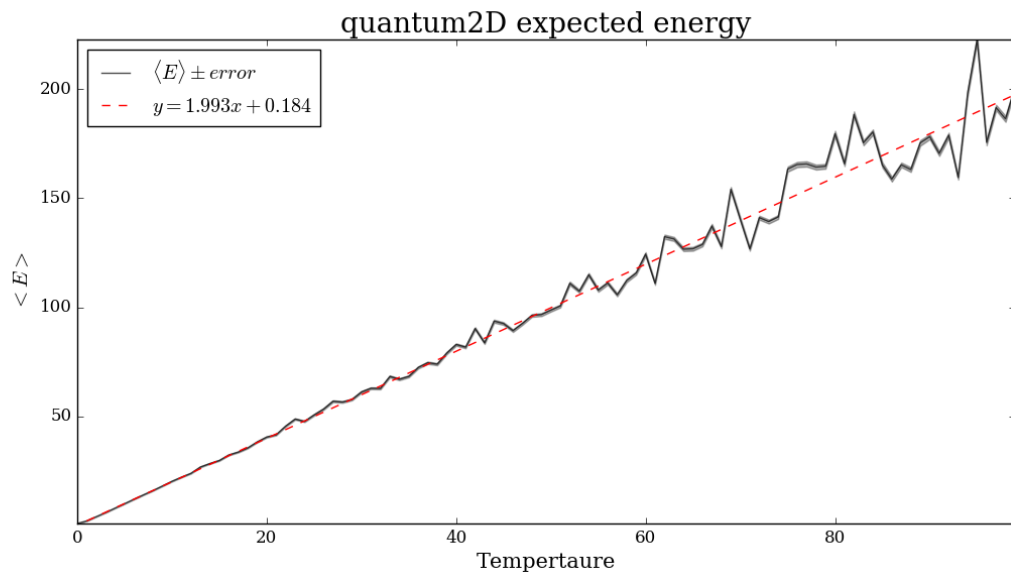


Question 4: Electron in a 2D quantum harmonic oscillator.

$$E_{n_1, n_2} = \left(n_1 + \frac{1}{2}\right) \hbar\omega + \left(n_2 + \frac{1}{2}\right) \hbar\omega$$

- (a) Determine $\bar{E}(T)$ the thermal average of the energy at temperature T.
- (b) Design and run a Monte Carlo simulation to numerically determine $\bar{E}(T)$.

Nstep	10^7
Nburn	10^4
Nskip	10^3
Run time	296.068 sec



(c) Determine $\bar{E}_2(T)$.

