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 = (Nstep - Nburn)/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]:

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

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

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.

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

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

Notice E can be split up into x and y components:

$$E = \frac{\vec{p}^2}{2m} + \frac{1}{2} m\omega^2 \vec{r}^2 = \frac{1}{2m}(p_x^2 + p_y^2) + \frac{1}{2} m\omega^2 (x^2 + y^2)$$

$$= \underbrace{\frac{1}{2m} p_x^2 + \frac{1}{2} m\omega^2 x^2}_{E_x} + \underbrace{\frac{1}{2m} p_y^2 + \frac{1}{2} m\omega^2 y^2}_{E_y}$$

So $\langle E \rangle = \langle E_x \rangle + \langle E_y \rangle$. Let's compute for the x direction:

$$\langle E_x \rangle = \frac{\int\limits_{-\infty}^{\infty}\int\limits_{-\infty}^{\infty} E_x e^{-E_x/kT}\, dx\, dp_x}{\int\limits_{-\infty}^{\infty}\int\limits_{-\infty}^{\infty} e^{-E_x/kT}\, dx\, dp_x} = \frac{\int\int (\frac{p_x^2}{2m} + \frac{1}{2}m\omega^2 x^2) e^{-(\frac{p_x^2}{2m} + \frac{1}{2}m\omega^2 x^2)/kT}\, dx\, dp_x}{\int\int e^{-(\frac{p_x^2}{2m} + \frac{1}{2}m\omega^2 x^2)/kT}\, dx\, dp_x}$$

For the top integral, the two parts in the sum are:

$$\int\limits_{-\infty}^{\infty}\int\limits_{-\infty}^{\infty} \frac{p_x^2}{2m} e^{-(\frac{p_x^2}{2m} + \frac{1}{2}m\omega^2 x^2)/kT}\, dx\, dp_x = \frac{1}{2m}\int\limits_{-\infty}^{\infty} e^{-m\omega^2 x^2/2kT}\, dx \int\limits_{-\infty}^{\infty} p_x^2 e^{-\frac{p_x^2}{2m}}\, dp_x$$

$$= \frac{1}{2m}\left[\sqrt{\frac{2\pi}{m\omega^2 kT}}\right]\left[\sqrt{2\pi}(mkT)^{3/2}\right] = \frac{\pi(kT)^2}{\omega}$$

$$\int\limits_{-\infty}^{\infty}\int\limits_{-\infty}^{\infty} \frac{1}{2}m\omega^2 x^2\, e^{-(\frac{p_x^2}{2m} + \frac{1}{2}m\omega^2 x^2)/kT}\, dx\, dp_x = \frac{1}{2}m\omega^2 \int\limits_{-\infty}^{\infty} x^2\, e^{-m\omega^2 x^2/2kT}\, dx \int\limits_{-\infty}^{\infty} e^{-\frac{p_x^2}{2m}}\, dp_x$$

$$= \frac{1}{2}m\omega^2 \left[\sqrt{2\pi mkT}\right]\left[\sqrt{2\pi}\left(\frac{kT}{m\omega^2}\right)^{3/2}\right] = \frac{\pi(kT)^2}{\omega}$$

The top integral is the sum of these two parts, so:

$$top = \frac{\pi(kT)^2}{\omega} + \frac{\pi(kT)^2}{\omega} = \frac{2\pi(kT)^2}{\omega}$$

And the bottom integral is:

$$\int\limits_{-\infty}^{\infty}\int\limits_{-\infty}^{\infty} e^{-(\frac{p_x^2}{2m} + \frac{1}{2}m\omega^2 x^2)/kT}\, dx\, dp_x = \int\limits_{-\infty}^{\infty} e^{-m\omega^2 x^2/2kT}\, dx \int\limits_{-\infty}^{\infty} e^{-\frac{p_x^2}{2mkT}}\, dp_x$$

$$= \left[\sqrt{2\pi mkT}\right]\left[\sqrt{\frac{2\pi}{m\omega^2/kT}}\right] = \frac{2\pi kT}{\omega}$$

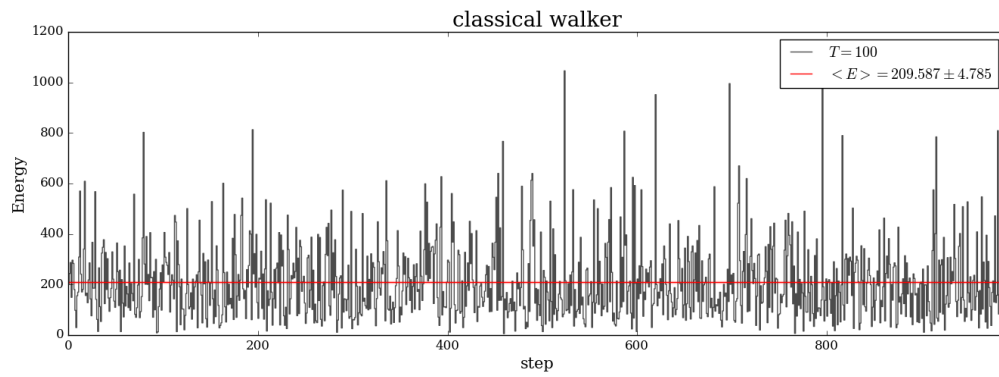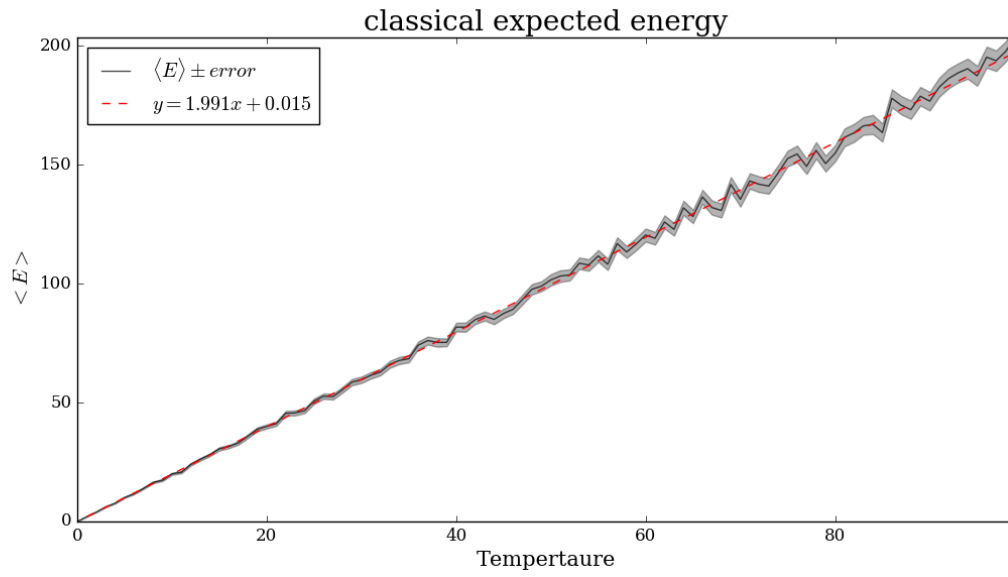Finally dividing the top and bottom we get $\langle E_x \rangle$:

$$\langle E_x \rangle = \left(\frac{2\pi(kT)^2}{\omega}\right)\left(\frac{\omega}{2\pi kT}\right) = kT$$

Because of symmetry $\langle E_x \rangle = \langle E_y \rangle = kT$, thus the total energy for a partical in a classical harmonic oscillator is

$$\langle E \rangle = \langle E_x \rangle + \langle E_y \rangle = 2kT$$
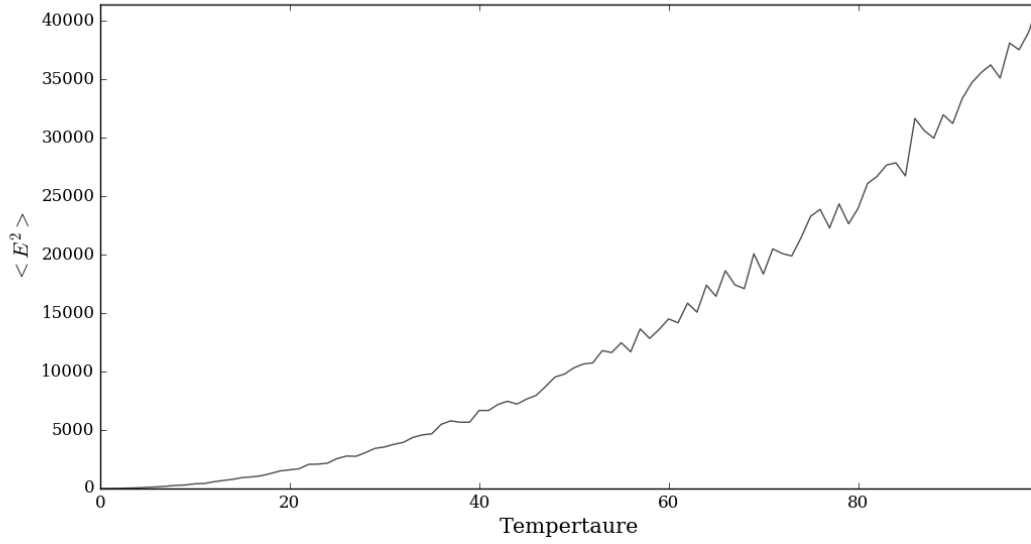
(b) Design and run a Monte Carlo simulation to numerically determine $\bar{E}(T)$.

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

classical expected energy

classical walker

Note that the simulaiton yields $\langle E \rangle_T \approx 2T$ as expected for $k = 1$.

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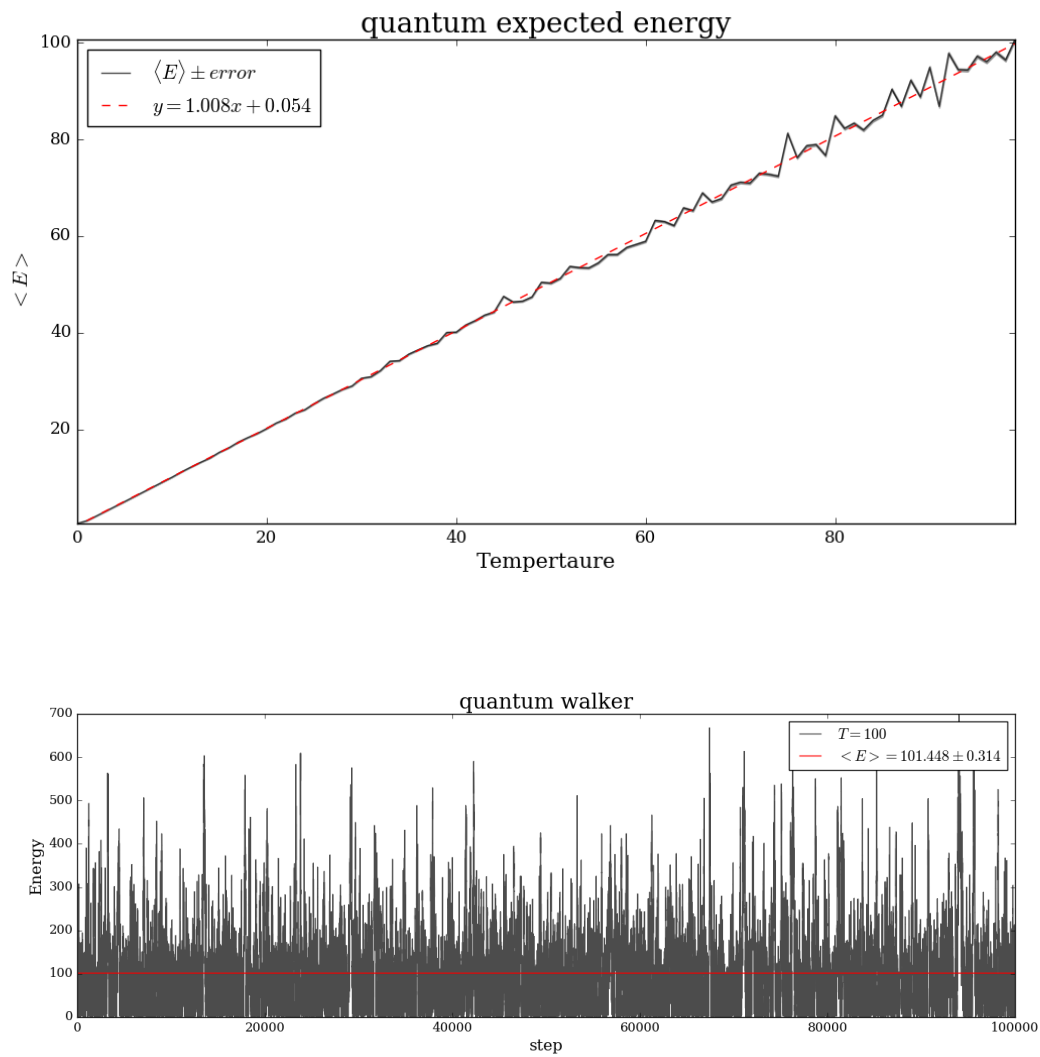
Let $\beta = \frac{\hbar\omega}{kT}$.

$$\langle E \rangle = \frac{\sum\limits_{n=0}^{\infty} E_n e^{E_n/kT}}{\sum\limits_{n=0}^{\infty} e^{E_n/kT}} = \frac{\sum (n+\frac{1}{2})\hbar\omega\, e^{(n+\frac{1}{2})\hbar\omega/kT}}{\sum e^{(n+\frac{1}{2})\hbar\omega/kT}}$$

$$= \hbar\omega \left[\frac{\sum n e^{-\beta(n+\frac{1}{2})}}{\sum e^{-\beta(n+\frac{1}{2})}} + \frac{\frac{1}{2}\sum e^{-\beta(n+\frac{1}{2})}}{\sum e^{-\beta(n+\frac{1}{2})}} \right]$$

$$= \hbar\omega \left[\frac{e^{-\beta/2}}{(e^\beta - 1)^2} \cdot \frac{(e^\beta - 1)}{e^{-\beta/2}} + \frac{1}{2} \right] = \hbar\omega \left[\frac{1}{e^\beta - 1} + \frac{1}{2} \right]$$

Since $\hbar\omega << kT$, then $\beta << 1$ and we can Taylor series expand $\frac{1}{e^\beta - 1} = \frac{1}{\beta} - \frac{1}{2} + O(\beta)$ and get
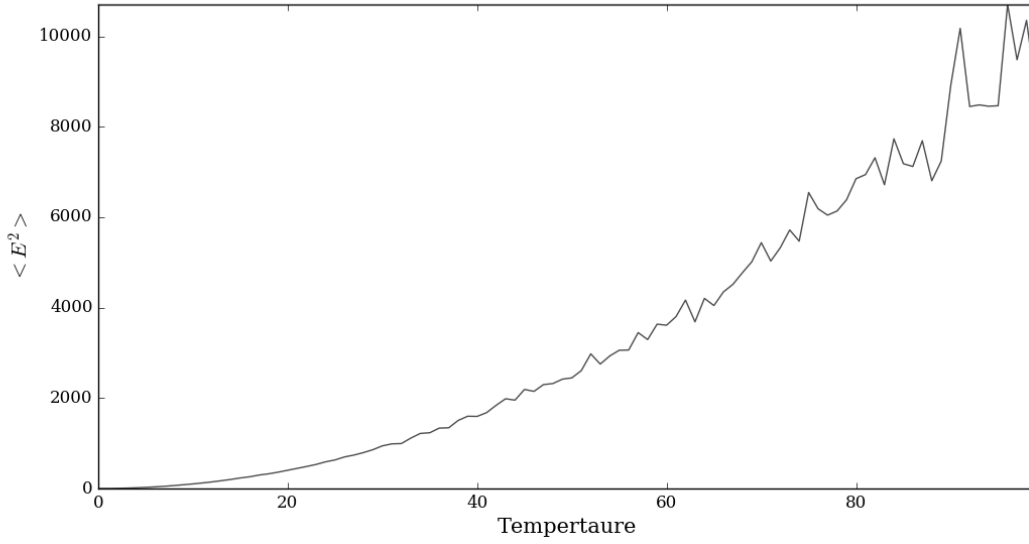
$$\langle E \rangle \approx \hbar\omega \left[\frac{1}{\beta} - \frac{1}{2} + \frac{1}{2} \right] = \frac{\hbar\omega}{\beta} = \hbar\omega \left(\frac{kT}{\hbar\omega} \right) = kT$$

(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

4

quantum expected energy

quantum walker

(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.

$$\langle E \rangle = \frac{\sum_{n=0}^{\infty} E_n e^{E_n/kT}}{\sum_{n=0}^{\infty} e^{E_n/kT}} = \frac{\sum (n+\frac{1}{2})\hbar\omega\, e^{(n+\frac{1}{2})\hbar\omega/kT}}{\sum e^{(n+\frac{1}{2})\hbar\omega/kT}}$$

$$= \hbar\omega \left[\frac{\sum n^2 e^{-\beta(n^2+\frac{1}{2})}}{\sum e^{-\beta(n^2+\frac{1}{2})}} + \frac{\frac{1}{2}\sum e^{-\beta(n^2+\frac{1}{2})}}{\sum e^{-\beta(n^2+\frac{1}{2})}} \right]$$

$$= \hbar\omega \left[\frac{\sum n^2 e^{-\beta(n^2+\frac{1}{2})}}{\sum e^{-\beta(n^2+\frac{1}{2})}} + \frac{1}{2} \right]$$

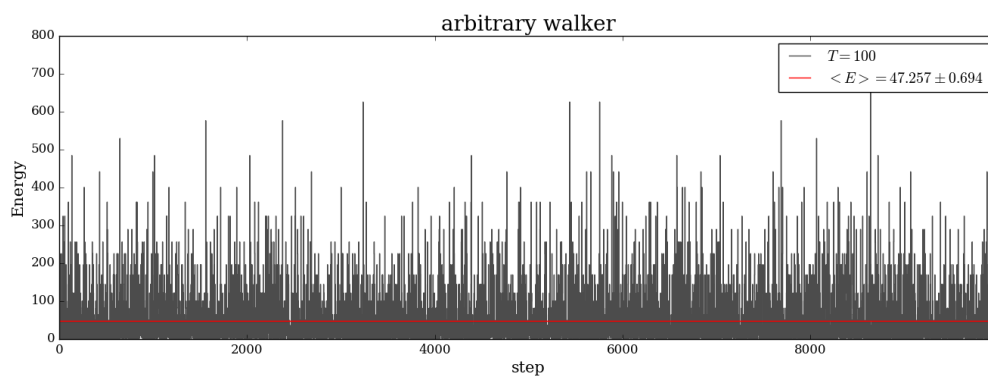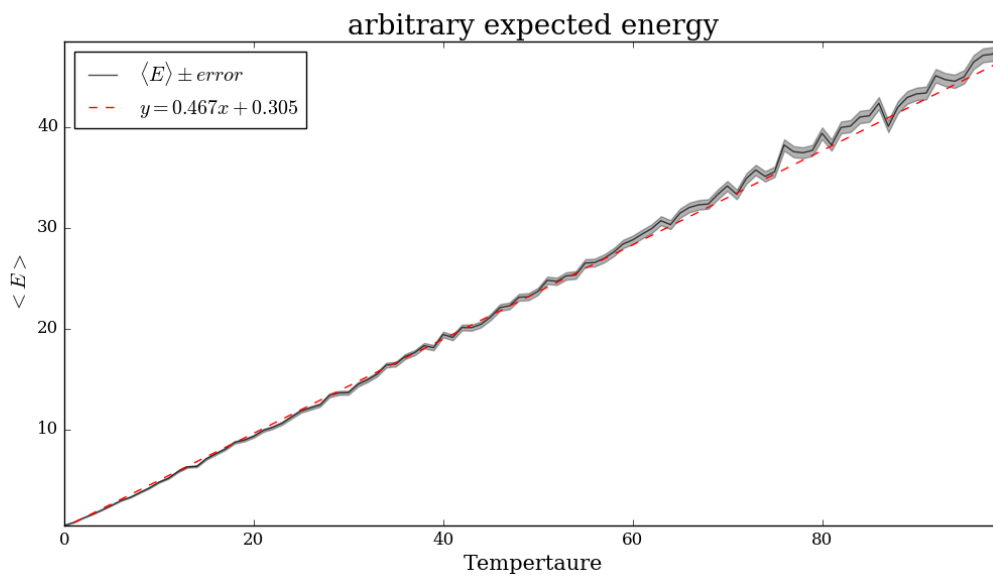Since it is very difficult to evaluate this sum, we can look at the approximation by replacing the sum with an integral:

$$\langle E \rangle \approx \hbar\omega \left[\frac{\int_0^\infty n^2 e^{-\beta(n^2+\frac{1}{2})}}{\int_0^\infty e^{-\beta(n^2+\frac{1}{2})}} + \frac{1}{2} \right] = \hbar\omega \left[\frac{1}{2\beta} + \frac{1}{2} \right] = \frac{\hbar\omega}{2}\left(\frac{kT}{\hbar\omega}\right) + \frac{\hbar\omega}{2} = \frac{kT}{2} + \frac{\hbar\omega}{2}$$
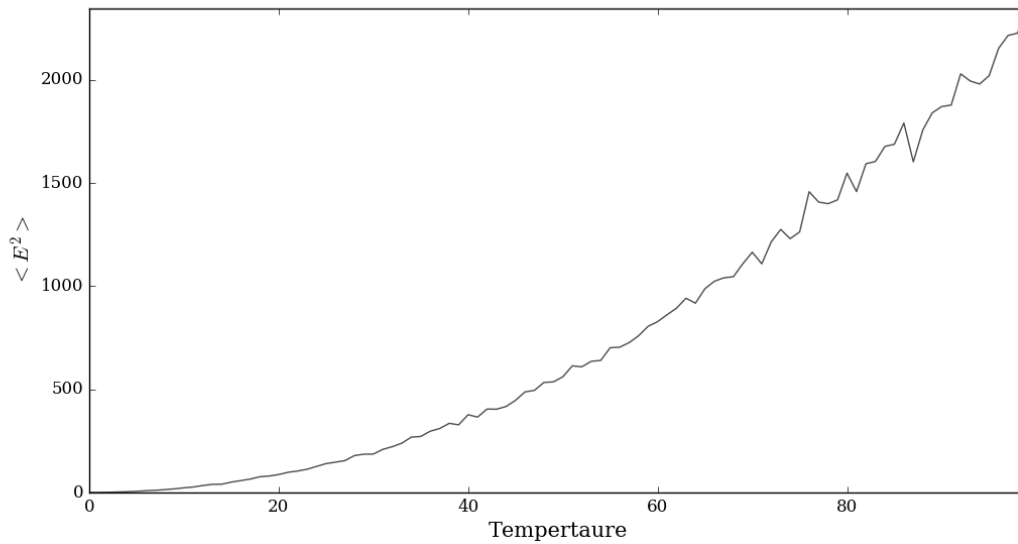
Now since $kT >> \hbar\omega$, we get

$$\langle E \rangle \approx \frac{kT}{2}$$

(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	84.1588 sec

6

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

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

$$E_{n_1,n_2} = \left(n_1 + \frac{1}{2} \right) \hbar\omega + \left(n_2 + \frac{1}{2} \right) \hbar\omega$$
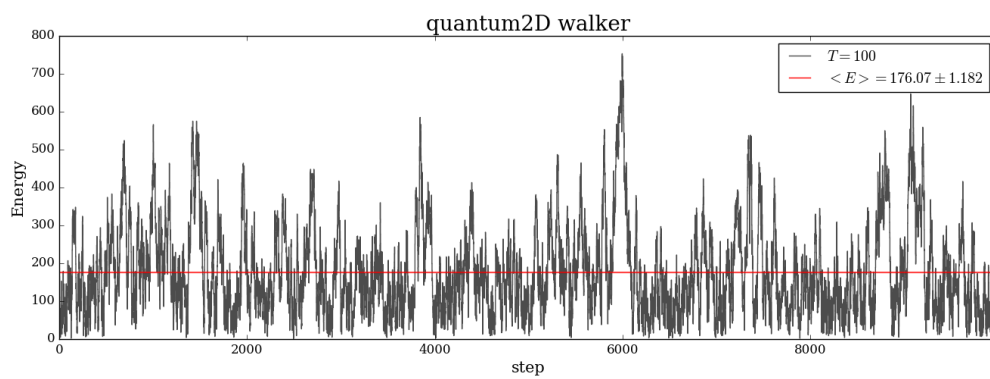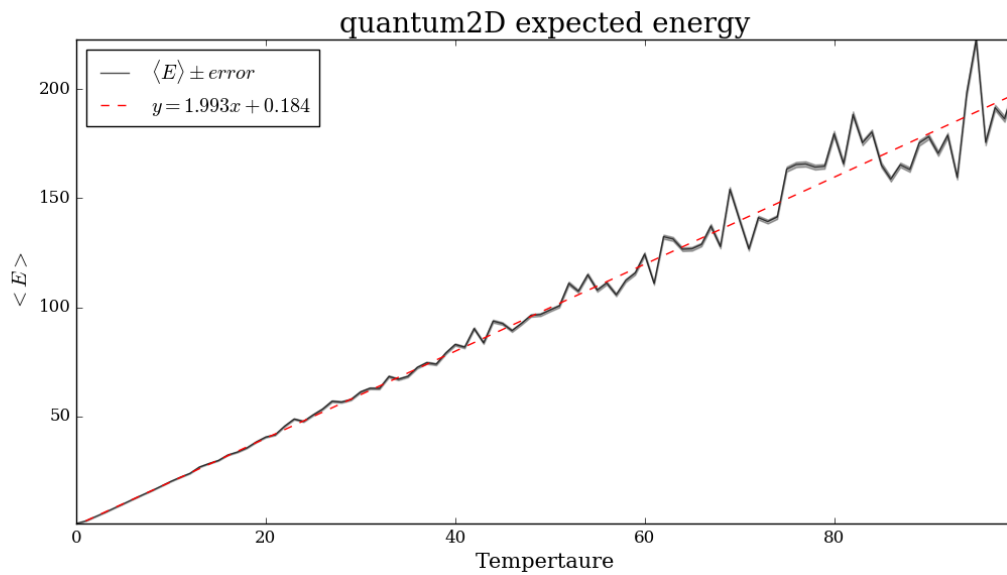
(a) Determine $\bar{E}(T)$ the thermal average of the energy at temperature T.

Since n_1 and n_2 are sampled independently of each other, the total average energy is the sum of the average energy of n_1 plus the average energy of n_2, where $\langle E \rangle_{n_1} = \langle E \rangle_{n_1} = kT$ as calculated for the 1D QHO. Thus the average energy for a 2D QHO is:

$$\langle E \rangle_T = \langle E \rangle_{n_1} + \langle E \rangle_{n_2} = kT + kT = 2kT$$

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