# Physics 142: Assignment 3

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**Preliminary Notes:**

**(a)** Error calculation: Error in average energy for energy samples $\chi_i$ 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 $\sigma$ 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:

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

**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:

$$\begin{aligned} E &= \frac{\vec{p}^2}{2m} + \frac{1}{2}m\omega^2\vec{r}^2 = \frac{1}{2m}(p_x^2 + p_y^2) + \frac{1}{2}m\omega^2(x^2+y^2) \\ &= \underbrace{\frac{1}{2m}p_x^2 + \frac{1}{2}m\omega^2x^2}_{E_x} + \underbrace{\frac{1}{2m}p_y^2 + \frac{1}{2}m\omega^2y^2}_{E_y} \end{aligned}$$

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

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

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

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

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

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

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

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:

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

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

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

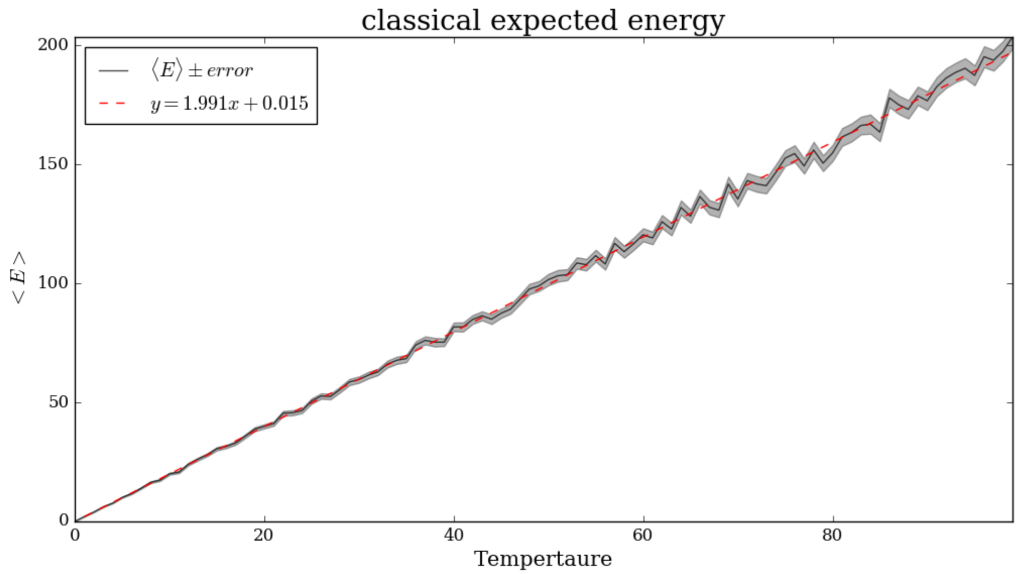
$$\langle E_x\rangle = \left(\frac{2\pi(kT)^2}{\omega}\right)\left(\frac{\omega}{2\pi kT}\right) = kT$$

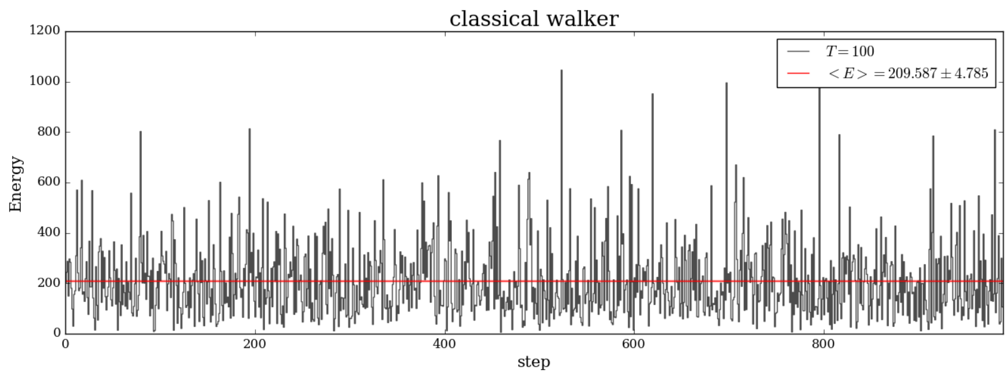
Because of symmetry $\langle E_x\rangle = \langle E_y\rangle = kT$, thus the total energy for a partical in a classical harmonic oscillator is

$$\langle E\rangle = \langle E_x\rangle + \langle E_y\rangle = 2kT$$

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

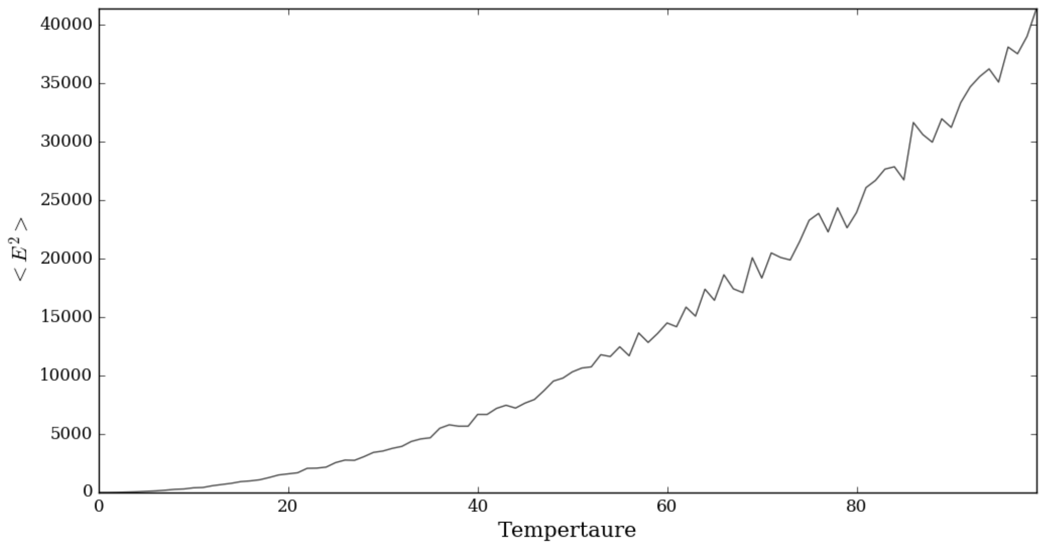
| | |
|---|---|
| Nstep | $10^6$ |
| Nburn | $10^4$ |
| Nskip | $10^3$ |
| Run time | 205.521 sec |




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

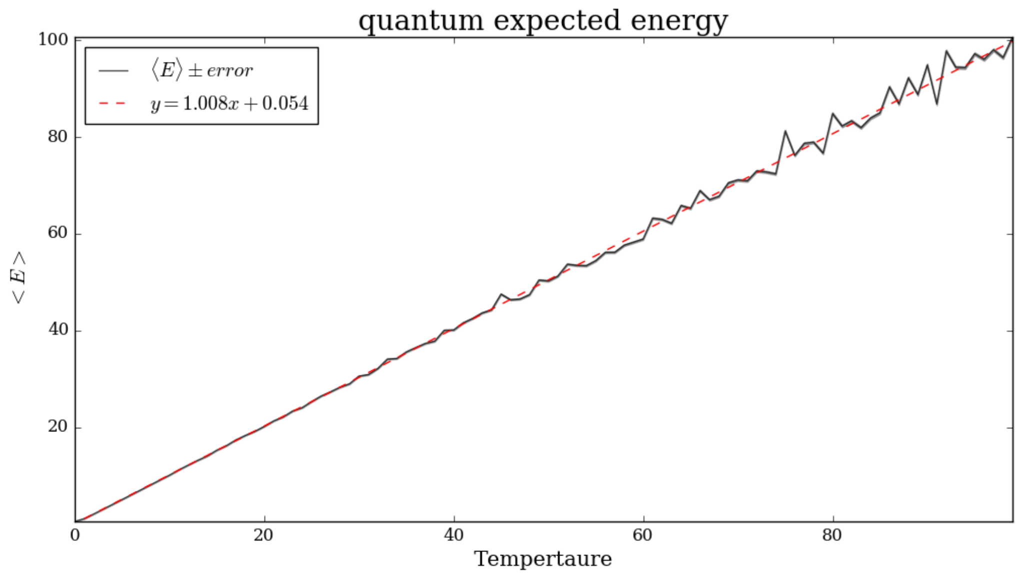
$$\begin{aligned}
\langle E \rangle = \frac{\sum\limits_{n=0}^{\infty} E_n e^{E_n/kT}}{\sum\limits_{n=0}^{\infty} e^{E_n/kT}} &= \frac{\sum (n+\frac{1}{2})\hbar\omega\, e^{(n+\frac{1}{2})\hbar\omega/kT}}{\sum e^{(n+\frac{1}{2})\hbar\omega/kT}} \\
&= \hbar\omega \left[ \frac{\sum n e^{-\beta(n+\frac{1}{2})}}{\sum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

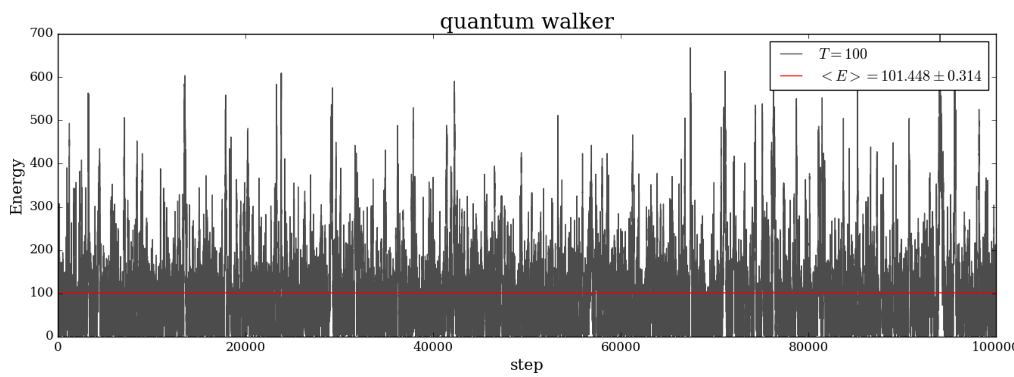
Since $\hbar\omega << kT$, then $\beta << 1$ and we can Taylor series expand $\frac{1}{e^{\beta}-1} = \frac{1}{\beta} - \frac{1}{2} + O(\beta)$ and get

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

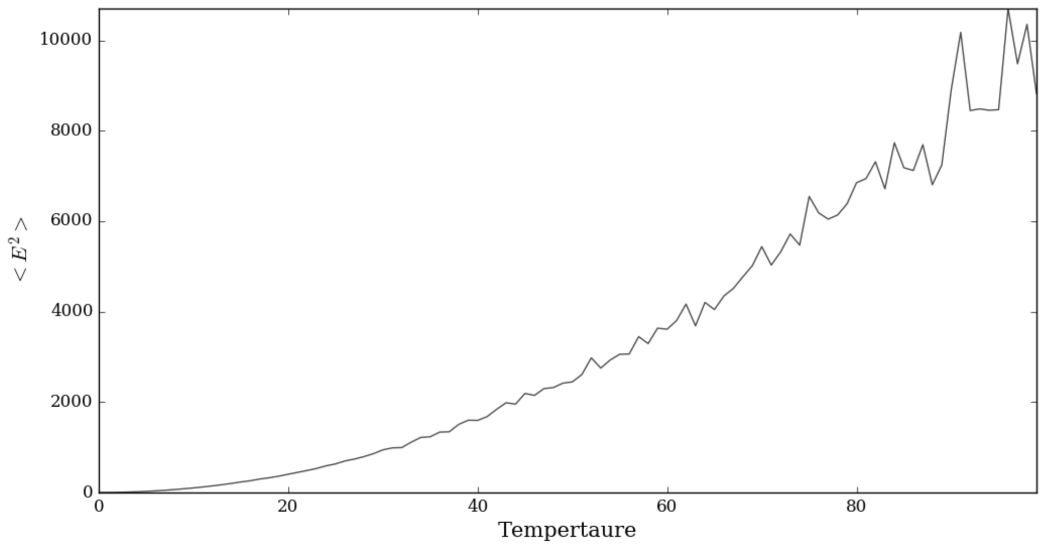
**(b)** Design and run a Monte Carlo simulation to numerically determine $\bar{E}(T)$.

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




**(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.

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

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

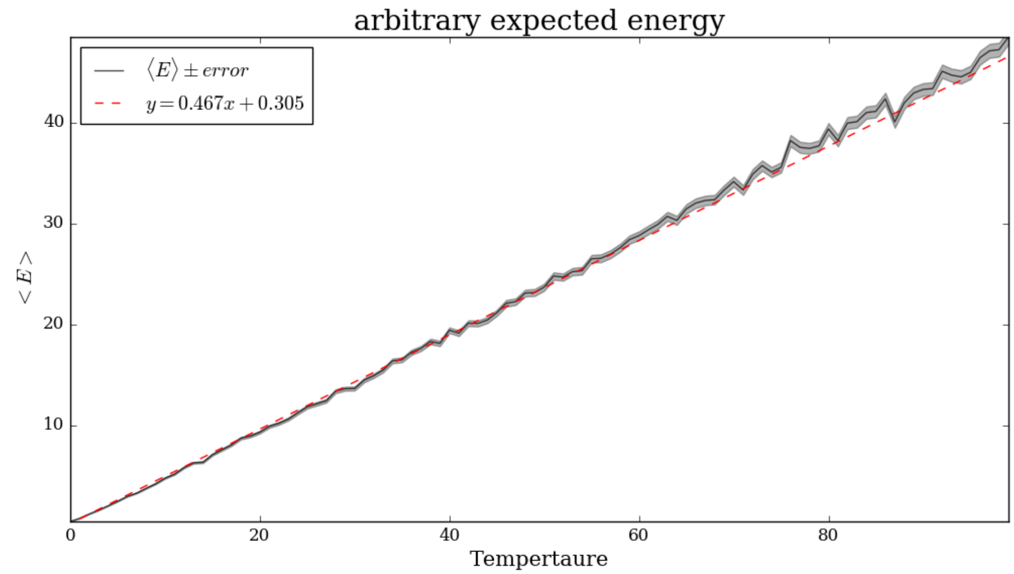
$$\langle E \rangle \approx \hbar\omega \left[ \frac{\int\limits_0^{\infty} n^2 e^{-\beta(n^2+\frac{1}{2})}}{\int\limits_0^{\infty} e^{-\beta(n^2+\frac{1}{2})}} + \frac{1}{2} \right] = \hbar\omega \left[ \frac{1}{2\beta} + \frac{1}{2} \right] = \frac{\hbar\omega}{2}\left(\frac{kT}{\hbar\omega}\right) + \frac{\hbar\omega}{2} = \frac{kT}{2} + \frac{\hbar\omega}{2}$$

Now since $kT >> \hbar\omega$, we get

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

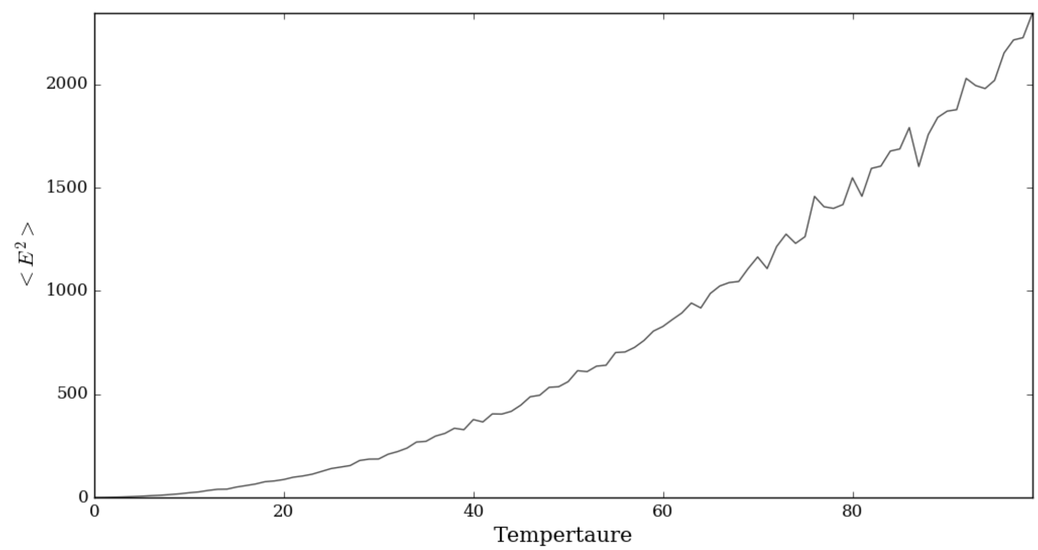
**(b)** Design and run a Monte Carlo simulation to numerically determine $\bar{E}(T)$.

| | |
|---|---|
| Nstep | $10^8$ |
| 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.

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

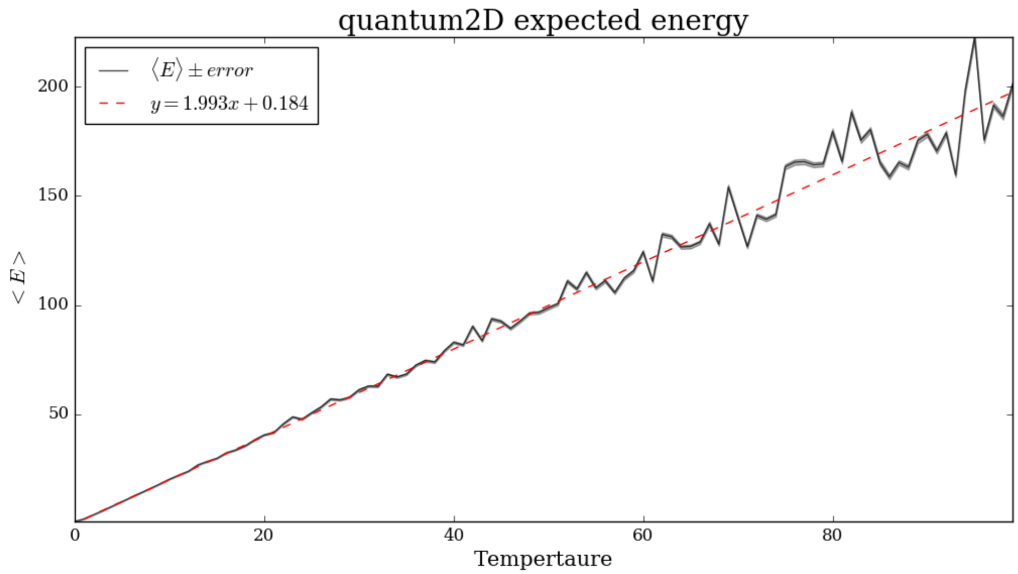
**(a)** Determine $\bar{E}(T)$ the thermal average of the energy at temperature T.

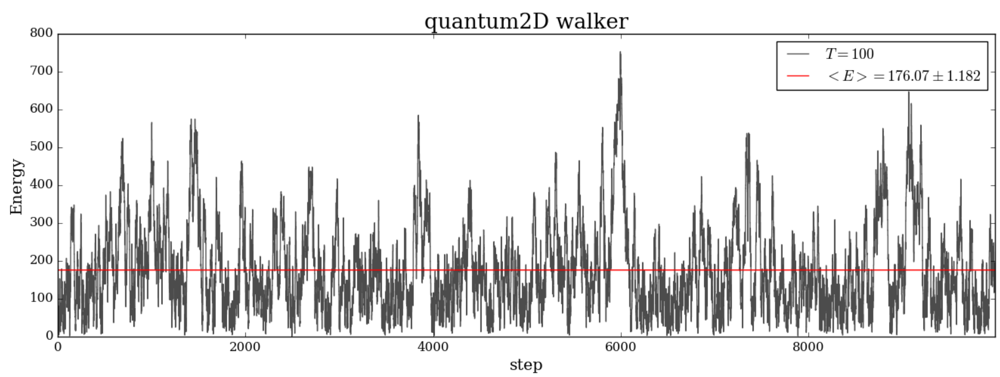
Since $n_1$ and $n_2$ are sampled independently of each other, the total average energy is the sum of the average energy of $n_1$ plus the average energy of $n_2$, where $\langle E \rangle_{n_1} = \langle E \rangle_{n_1} = kT$ as calculated for the 1D QHO. Thus the average energy for a 2D QHO is:

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

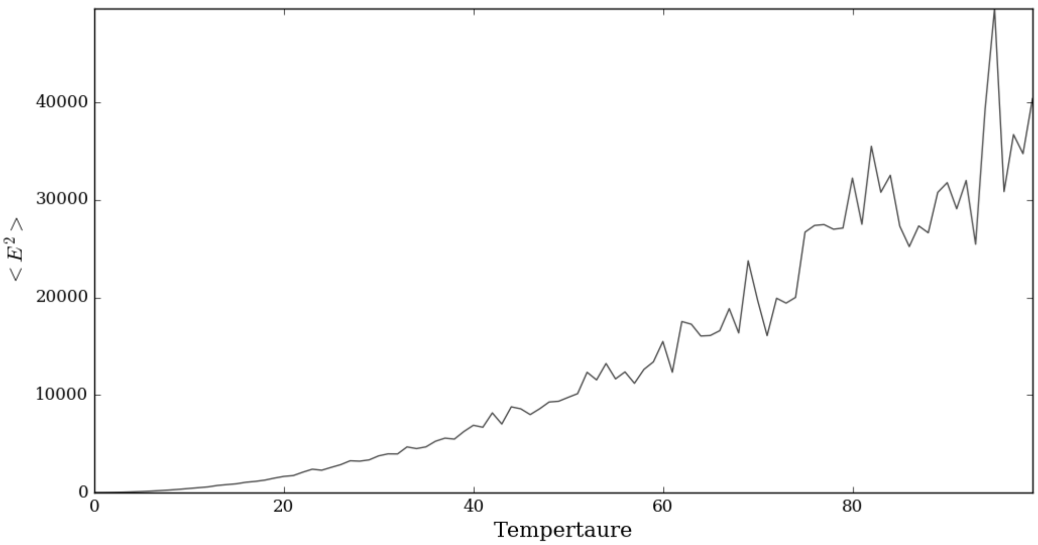
**(b)** Design and run a Monte Carlo simulation to numerically determine $\bar{E}(T)$.

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




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