(1) Consider a classical electron in a two-dimensional harmonic oscillator and in thermal equilibrium with a heat bath at temperature $T$.

(a) calculate analytically the thermal average of the energy, $E(T)$, as a function of $T$.

(b) design and run a Monte Carlo simulation to determine $E(T)$.

(c) If $E_2(T)$ designates the thermal average of $E^2$, calculate this function with your Monte Carlo simulation.

Notation and hints:

$$E = \frac{\vec{p}^2}{2m} + V(r)$$

$$\vec{p} = (p_1, p_2)$$

$$V = \frac{1}{2} m \omega^2 r^2$$

$$\vec{r} = (x_1, x_2)$$
\[ p(E(p, r)) = \frac{e^{\frac{-E(p, r)}{k_B T}}}{Z} \]

*probability Boltzmann factor*

partition function \( Z = \int e^{\frac{-1}{k_B T} E(p, r)} \, d^2p \, d^2r \)

\[ E(T) = \frac{\int E(p, r) e^{\frac{-1}{k_B T} E(p, r)} \, d^2p \, d^2r}{Z} \]

(a) *Theoretical calculation only needs Gaussian type integrals*

(b) *Use your convenient units \( k_B, m, a \) for the MC simulation*

(c) *When you calculate \( E_2(T) \) replace \( E \) being averaged by \( E^2 \)*
(y) Consider a quantum electron in a one-dimensional harmonic oscillator and in thermal equilibrium with a heat bath at temperature T.

(a) calculate analytically the thermal average of the energy, $\mathcal{E}(T)$, as a function of T.

(b) design and run a Monte Carlo simulation to determine $\mathcal{E}(T)$

(c) If $E_2(T)$ designates the thermal average of $E^2$, calculate this function with your Monte Carlo simulation.

Notation and hints:

$E_n = (n + \frac{1}{2}) \hbar \omega$  \( n = 0, 1, 2, \ldots \)

Energy levels from Schrödinger eq.

is accepted
\[ p_n = \frac{e^{-\frac{E_n}{k_B T}}}{Z} \quad \text{Boltzmann probabilities} \]

\[ Z = \sum_{n=0}^{\infty} e^{-\frac{E_n}{k_B T}} \]

\[ E(T) = \sum_n E_n \cdot p_n \]

(a) The theoretical calculation only needs geometric summation

(b) Use your convenient units for the MC simulation

(c) When you calculate \( E_2(T) \) replace \( E \) being averaged by \( E^2 \)
(3) repeat \( E(T) \) of problem (2) with anharmonic

\[ E_n = (n^2 + \frac{1}{2})\hbar \omega \]

\( n=0,1,2,... \)

(4) Generalize problem (2) to the 2-dim quantum oscillator with harmonic potential \( V(r) = \frac{1}{2}m\omega^2 r^2 \).

Calculate \( E(T) \) again assuming

\[ E_{n_1, n_2} = (n_1 + \frac{1}{2})\hbar \omega + (n_2 + \frac{1}{2})\hbar \omega \]

\( n_1, n_2 \) run from 0 to \( \infty \).