Assignment 3

due May 30

(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, $\mathcal{E}(T)$, as a function of T.

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

(c) If $\mathcal{E}_2(T)$ designates the thermal average of E^2, calculate this function with your Monte Carlo simulation

Notation and hints:

$$E = \frac{\vec{p}^{\,2}}{2m} + \underbrace{V(r)}_{\frac{1}{2} m \omega^2 r^2}$$

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

$\vec{r}\ (x_1, x_2)$

$$p\left(E(\vec{p},\vec{r})\right) = \frac{e^{-E(\vec{p},\vec{r})}}{Z}$$

probability $\qquad$ Boltzman factor

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

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

(a) the theoretical calculation only needs Gaussian type integrals

(b) use your convenient units k_B, m, ω for the MC simulation

(c) When you calculate $\mathcal{E}_2(T)$ replace E being averaged by E^2

(2) 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 $\mathcal{E}_2(T)$ designates the thermal average of E^2, calculate this function with your Monte Carlo simulation

Notation and hints:

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega \qquad n = 0, 1, 2, \dots$$

energy levels from Schrödinger eq. is accepted

$$P_n = \frac{e^{-\frac{1}{k_B T} E_n}}{Z}$$ Boltzman probabilities

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

$$\mathcal{E}(T) = \sum_n E_n \cdot P_n$$

(a) the theoretical calculation only needs geometric summation

(b) use your convenient units for the MC simulation

(c) When you calculate $\mathcal{E}_2(T)$ replace E being averaged by E^2

(3) repeat $\mathcal{E}(T)$ of problem (2) with anharmonic $E_n = (n^2 + \frac{1}{2})\hbar\omega$

$n = 0, 1, 2, \ldots$

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

Calculate $\mathcal{E}(T)$ 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 ∞