

Assignment 3

due May 28

(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:

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

$\uparrow \quad \frac{1}{2} m \omega^2 r^2$

$\vec{p} (p_1, p_2)$
 $\vec{r} (x_1, x_2)$

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

probability Boltzmann factor

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

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

- (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 $E_2(T)$ replace E being averaged by E^2

(1) 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 :

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

energy levels from Schrödinger eq. is accepted

$$P_n = \frac{e^{-\frac{1}{k_B T} E_n}}{Z} \quad \text{Boltzmann probabilities}$$
$$Z = \sum_{n=0}^{\infty} e^{-\frac{E_n}{k_B T}}$$

$$E(T) = \sum_n E_n \cdot P_n$$

- (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

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

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

(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

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

n_1, n_2 run from 0 to ∞