HOMEWORK 4, THERMAL PHYSICS (PHY306)

1.A particle is in the potential $V(x) = A|x|$ (modulus x, $A > 0$). Find the mean energy $\langle E\rangle$ and r.m.s. deviation $\sqrt{\langle x^2\rangle}$ when it is in contact with the heat bath with energy T, assuming that the temperature T is high enough to use classical Boltzmann factor (ignoring quantization of the energy levels).

2.Interaction potential between neutral atoms is often modeled by the Lennard-Jones potential

$$V(r) = 4\epsilon\left[\left[\frac{\sigma}{r}\right]^{12} - \left[\frac{\sigma}{r}\right]^{6}\right]$$

where r is (one-dimensional) distance between the atoms. (a) Find the location of its minimum r_{min} and the coefficient α of the quadratic term $V \approx V(r_{min}) + \alpha(r - r_{min})^2/2$;
(b) Assume the temperature T is low enough to use this quadratic approximation and equipartition theorem, and high enough to use classical Boltzmann factor, ignoring quantization of energy levels. What is the distribution over the coordinate r, and root-mean-square deviation (r.m.s.) $\sqrt{\langle(r - r_{min})^2\rangle}$?

3.Quantum vibrational partition function in harmonic oscillator approximation is

$$R(T) = \sum_{n=0}^{\infty} exp\left[-\frac{\hbar\omega(n+1/2)}{k_B T}\right]$$

(a) Find its analytic form (hint: use geometric series).
(b) Using it show that at high T it agrees with the result from classical equipartition theorem
(c) For $\hbar\omega/k_B = 100K$ and room temperature $T = 300K$ calculate the exact $R(T)$ found in (a) and compare it to the classical value found in (b).

4.Quantum rotational partition function in "solid rotator" approximation is

$$R(T) = \sum_{L=0}^{\infty} (2L+1) exp\left[-\frac{\hbar^2 L(L+1)}{2Ik_B T}\right]$$

where integer L is the angular momentum of the energy level and I is the momentum of inertia. For a molecule of HCl the combination of parameters entering here is numerically

$$\Theta \equiv \frac{\hbar^2}{2Ik_B} = 15K$$

(a) At $T \gg \Theta$, when L are large, the sum over levels can be approximated by the integral. Find the resulting classical expression for this partition function $R_{classical}(T)$
(b) Calculate a table of values for the ratio $R(T, L \leq L_{max})/R_{classical}$ in the approximation in which $L_{max} = 0, 1, 2, 3, 4$ (include up to 5 terms in the sum) at room temperature $T = 300K$.