Physical Chemistry Cume
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In this cume you can show how you understand the principles of statistical mechanics. (try to answer as many problems as possible – partial answers are welcome too)

1. Describe briefly how you can understand relaxation and equilibration of a quantum system initially described by some wave function.

2. How would you describe a quantum system in equilibrium when it is at a fixed temperature and it has a fixed average number of particles? Is the energy of the system fixed? Which states are populated?

3. How would you obtain from statistical mechanics thermodynamical properties of a NH_3 gas at room temperature and at P=1 atm? Explain in full details.

4. Explain what happens to He gas that is cooled down. Consider various possible effects at different temperatures.

Possibly useful formulas:

$$\hat{\rho} = \sum_{n} \frac{\exp(-\beta E_n)}{Z} \left| E_n \right\rangle \left\langle E_n \right|, \qquad U = \left\langle E \right\rangle = \sum_{\alpha=1}^{n^D} P_\alpha \, E_\alpha, \qquad S = k \ln Z + \frac{U}{T},$$

$$z_{vib} = \sum_{n=0}^{\infty} e^{-(n+1/2)x} = \frac{e^{-x/2}}{1-e^{-x}}, \quad x = \frac{h\nu_0}{kT}, \qquad Z(T,V,N) = \frac{z(T,V,N)^N}{N!}, \quad \varepsilon = \varepsilon_{tr} + \varepsilon_{int},$$

$$z_{rot} = \sum_{J=0}^{\infty} (2J+1) \exp\left[-\frac{J(J+1)\frac{\hbar^2}{2I}}{kT} \right], \qquad p(v) = \frac{n(v)}{N} = 4\pi \left[\frac{m}{2\pi kT} \right]^{3/2} \exp\left[-\frac{mv^2}{2kT} \right] v^2.$$