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※請在答案卷內作答

1. If we consider a canonical ensemble with fixed variables temperature (T), volume (V), and number of particles (N), and all particles are indistinguishable, derive briefly the canonical partition function Q using the dominant configuration concept. The dominant configuration has overwhelming probability, one will observe a macroscopic state of the system characterized by the dominant configuration. Starting with the definition of canonical ensemble and write down the weighting of a configuration and just describe how you attain $Q = \sum_n e^{-\beta E_n}$, in which $\beta = (k_B T)^{-1}$, k_B is Boltzmann constant, and E represents energy of state n. (12%)

2. The canonical partition function related to the molecular partition function q is given by $Q = \frac{q^N}{N!}$ for indistinguishable particles. Derive the internal energy U_{trans} of one dimensional translational motion for the canonical system with number of particles N, volume V and temperature T. The molecular partition function for translation of one dimension particle-in a-box is $q_{trans} = (\frac{2\pi m k_B T}{h^2})^{1/2} a$, where a is the length of box, k_B is Boltzmann constant, m is mass of particle, and h is Planck constant. Write down the derivation. What is the heat capacity at constant volume $C_{v,\,trans}$ for this one-dimensional translational motion system? (16%)

3. In a consecutive reaction $A_1 \xrightarrow{k_1} A_2 \xrightarrow{k_2} A_3$, when $k_1 \neq k_2$, you can use the trial function $a_1 e^{-k_1 t} + a_2 e^{-k_2 t} + a_3$ to derive the integrated rate law. Given the initial conditions $[A_1](t = 0) = A_0$ and $[A_2](t = 0) = [A_2](t = 0) = 0$, derive the integrated rate equation, the concentrations $[A_1]$, $[A_2]$, and $[A_3]$ as a function of time. Plot the concentrations of them as a function of time when (a) $k_1 \cong 10\ k_2$ and (b) $k_1 \cong 0.1\ k_2$. You will find out some variations in these two plots. Describe the differences in these two plots and explain why. (14%)

注意：背面有試題

4. If a gas is represented by the truncated virial equation of state $\frac{PV_m}{RT} = 1 + B_2 / V_m$ where the virial coefficient B_2 depends on temperature and V_m denotes molar volume, find an expression for the molar entropy change for an isothermal volume change of the gas. (8%)

5. Write down a general form of the time-dependent Schrodinger equation in both the compact operator and explicit presentations. Define all of the operators and parameters used in your answer. (10%)

6. Given the matrix representation for the operator $S_y = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$. Find the eigenvalues and eigenvectors of the operator S_y. (20%)

7. Write down a time-independent Schrodinger equation for a particle of mass m constrained to move on a circle of radius a. Solve the equation for the corresponding normalized wave function. Discuss what boundary condition is appropriate for the system and use the condition to determine the system energy. (Note: Use the moment of inertia $I=ma^2$.) (20%)