淡江大學 105 學年度日間部轉學生招生考試試題

系別：化學工程與材料工程學系三年級　　科目：物理化學　　46

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1. For a particle in a one-dimensional box of length L, the solution from Schrödinger equation, in case of potential energy $V = 0$, is

$$\psi_n = \left(\frac{2}{L}\right)^{1/2} \sin\left(\frac{n\pi x}{L}\right), for\ 0 \le x \le L$$

Knowing that the momentum operator is

$$\hat{p}_x = \frac{\hbar}{i}\frac{d}{dx}$$

a. Derive the expression for energy E_n.

Given that

$$\int \sin^2 axdx = \frac{x}{2} - \frac{\sin 2ax}{4a}$$

b. Estimate the expectation value of momentum $\langle \hat{p}_x \rangle$.

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2. The definition of partition function is

$$q = \sum_{i=1}^{\infty} e^{-\varepsilon_i/kT}$$

where ε_i is the energy of i-level relative to the level of $i = 1$, i.e. by defining $\varepsilon_1 = 0$.
Using the expression of E_n derived in the previous problem, and given that

$$\int_0^{\infty} e^{-ax^2} dx = \frac{1}{2}\left(\frac{\pi}{a}\right)^{1/2}$$

prove that for a particle in a one-dimensional box with $L = X$, the translational partition function q_X^T is approximated as

$$q_X^T = \frac{X}{\Lambda}, where\ \Lambda = \frac{h}{(2\pi mkT)^{1/2}}\ is\ termed\ "Thermal\ wavelength"$$

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3. In a gas-phase reaction

$$A + B \rightleftarrows C + 2D$$

it was found that, when 2.00 mol A, 1.00 mol B and 3.00 mol D were mixed and allowed to come to equilibrium at 25 °C, the resulting mixture contained 0.79 mol C at a total pressure of 1.00 bar. Calculate
a. equilibrium constant K,
b. $\Delta_r G^{\ominus}$.

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4. The osmotic pressure of solutions of polystyrene in toluene were measured at 25°C and the pressure was expressed in terms of the height of the solvent of density 1.004g cm^{-3}:

c/(g dm^{-3})	2.042	6.613	9.521	12.602
h/cm	0.592	1.910	2.750	3.600

Calculate the molar mass of the polymer.

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5. Calculate q, w, ΔU, ΔS the change in entropies of the system, and $\Delta S_{surrounding}$ the change in entropies of the surrounding, and the total change in entropy ΔS_{total}, when 28 g nitrogen gas, taken as perfect gas with constant C_p = 29.1 J mol^{-1}, at 300 K and 6.0 bar expands to three times its initial volume in an adiabatic irreversible expansion against p_{ex} = 1.0 bar.

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