

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

考試日期：7月22日(星期五) 第3節

本試題共

大題，

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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

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

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

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

- 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

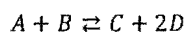
$$\int_0^{\infty} e^{-ax^2} dx = \frac{1}{2} \left(\frac{\pi}{a}\right)^{1/2}$$

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

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

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3. In a gas-phase reaction



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 1.004 g cm⁻³:

$c/(\text{g dm}^{-3})$	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 $\Delta S_{\text{surrounding}}$ 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 $C_p = 29.1 \text{ J mol}^{-1}$, at 300 K and 6.0 bar expands to three times its initial volume in an adiabatic irreversible expansion against $p_{\text{ex}} = 1.0 \text{ bar}$.

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