

國立中央大學八十四學年度碩士班研究生入學試題卷

所別：化學研究所

組

科目：物理化學

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參考用

- (1). 20% As we understand the Hamiltonian expressed in Cartesian frame can be written as

$$\hat{H} = \frac{-\hbar^2}{2m} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) + V(x, y, z) = \frac{-\hat{p}^2}{2m} + V(x, y, z)$$

we have used the relationship $\hat{p}_x = -i\hbar \frac{\partial}{\partial x}$ in the above equation. Please

evaluate the commutators (a). $[x, p_x]$, (b). $[x, p_x^2]$ (c). $[x, p_y]$, (d). $[x, V(x, y, z)]$ and (e). $[x, H]$.

- (2). 10% From the above results we have $[x, H] = \frac{\hbar^2}{m} \frac{\partial}{\partial x} = \frac{i\hbar}{m} \hat{p}_x$. please show that

$$\langle \psi_1 | \frac{\partial}{\partial x} | \psi_2 \rangle = \frac{m}{\hbar} (E_2 - E_1) \langle \psi_1 | x | \psi_2 \rangle$$

where ψ_1 and ψ_2 are eigen functions of Hamiltonian with eigenvalues E_1 and E_2 .

- (3) 20% As we understand, there existed a common complete sets of eigenfunctions for commuting operators.:

(a). Explain what does it mean by commuting operators.

(b). Define $L_- = L_x - iL_y$ and $L_+ = L_x + iL_y$. Please evaluate the commutators $[L_-, L_x]$ and $[L_+, L_y]$.

(c). Using the above result, show that

$$L_+ L_- = L^2 - L_z + \hbar L_z \quad \text{and} \quad L_- L_+ = L^2 - L_z - \hbar L_z$$

(d). Are the spherical harmonics $Y_{l,m}(\theta, \phi)$ also eigenfunctions of the operators $L_+ L_-$ and $L_- L_+$?

(e). What are the eigenfunctions expressed in terms of $Y_{l,m}(\theta, \phi)$ for operators $L_+ L_-$ and $L_- L_+$ with eigenvalues equal to zero?

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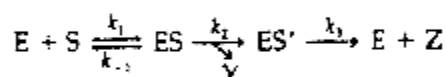
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參閱

- (4) 7% (a) State the postulates of the kinetic molecular theory of gases.
8%(b) Modify ideal gas equation $PV=RT$ to account for the violation of the postulates for real gas (Van der Waals equation) and explain.
- (5) 10% Explain why Li^+ has lower ionic conductivity than Na^+ in aqueous solution and why the value for H^+ is so much higher than the values for both of these ions.
- (6) 10% Obtain the rate equation corresponding to the mechanism



assuming ES and ES' to be in the steady state and the substrate concentration to be much higher than the enzyme concentration. Express the catalytic constant k_c and the Michaelis constant K_m in terms of k_1 , k_{-1} , k_2 , and k_3 . The rate can be expressed as $\text{rate} = k_c[E]_0[S]/(K_m + [S])$

- (7) 15% A pressure-volume diagram for the Carnot cycle is shown below: AB and CD are isotherms and BC , DA are adiabatics. Calculate ΔU , q , and w for the four reversible steps and the net change for the whole cycle.

