

# 化學數學期末考

(2012/1/9)

## 一、單選題 (30 pts)

1. The wavefunction:  $\frac{1}{4\sqrt{2\pi}} \left(\frac{Z}{a}\right)^{3/2} \frac{Zr}{a} e^{-Zr/2a} \cos \theta$  is usually named as the hydrogen orbital of

(A)  $2s$  (B)  $2p_z$  (C)  $3d_{z^2}$  (D)  $3p_z$  (E)  $4s$

Ans :B

2. Which of the following is an allowed energy value of a quantum mechanical harmonic oscillator?

(A)  $1.50 h\nu$  (B)  $0.0 h\nu$  (C)  $2.0 h\nu$  (D)  $0.25 h\nu$  (E)  $0.75 h\nu$

Ans :A

3. If the transposition of A gives the inverse of A, then must be what kind of matrix?

(A) symmetric (B) diagonal (C) hermitian (D) orthogonal (E) skew-symmetric

Ans :D

4. If the reactant of a first-order irreversible reaction becomes 50% of its initial concentration in 10 minutes, how long does it take for the reaction to >90% completion?

(A) 15 min. (B) 20 min. (C) 25 min. (D) 30 min. (E) 40 min.

Ans :E

5. The ellipse of the form  $17x^2 - 30xy + 17y^2 = 128$  has a semi-long axis of ?

(A) 8 (B) 6 (C) 4 (D) 2 (E) 12

Ans :A

6. Which of the following is *not* a linear ODE?

(A)  $y'' - e^x y = 0$  (B)  $xy''' - 2x^2 y'' = \cos x$  (C)  $y'' - yy' = y$  (D)  $y' + 3y = 3x^2$  (E)  $y'' - y = e^x y$

Ans :C

## 二、計算題 (105 pts)

1. Please solve the following ordinary differential equations. (10%)

(i)  $y'' + 4y = 16 \cos 2x$ ,  $y(0) = 0$ ,  $y'(0) = 0$       (ii)  $y'' - 6y' + 9y = 0$

(i)

$$\text{令 } y = e^{\lambda t} \quad \lambda^2 + 4 = 0 \quad \lambda = \pm 2i$$

$$\text{令 } y_h = A \cos 2x + B \sin 2x$$

$$y_p = ax \cos 2x + b \sin 2x$$

$$y_p' = a \cos 2x - 2ax \sin 2x + b \sin 2x + 2bx \cos 2x$$

$$y_p'' = -2a \sin 2x - 2a \sin 2x - 4ax \cos 2x + 2b \cos 2x + 2b \cos 2x - 4bx \sin 2x$$

$$\Rightarrow a = 0, b = 4$$

$$y = A \cos 2x + B \sin 2x + 4x \sin x$$

$$y' = -2A \sin 2x + B \cos 2x + 4x \sin 2x + 8x \cos 2x$$

$$y(0) = A$$

$$y'(0) = 0 = 2B$$

$$B = 0$$

$$y = 4x \sin 2x$$

(ii)

$$\Leftrightarrow y = e^\lambda$$

$$\Rightarrow \lambda^2 - 6\lambda + 9 = 0 , \quad \lambda = 3 \quad \Rightarrow y = c_1 e^{3x} + c_2 x e^{3x}$$

$$2. \quad A = \begin{bmatrix} -1 & 1 & 2 \\ 3 & -1 & 1 \\ -1 & 3 & 4 \end{bmatrix} \quad B = \begin{bmatrix} 1 & 2 & 5 \\ 0 & -1 & 2 \\ 2 & 4 & 1 \end{bmatrix}$$

Please find (i)  $A \times B^T$  (ii)  $A^{-1}$  (iii)  $\det(AB)$  (15%)

(i)

$$A = \begin{bmatrix} -1 & 1 & 2 \\ 3 & -1 & 1 \\ -1 & 3 & 4 \end{bmatrix} \quad B^T = \begin{bmatrix} 1 & 0 & 2 \\ 2 & -1 & 4 \\ 5 & 2 & 1 \end{bmatrix}$$

$$A \times B^T = \begin{bmatrix} 11 & 3 & 4 \\ 6 & 3 & 3 \\ 25 & 5 & 14 \end{bmatrix}$$

(ii)

$$\det(A) = 10$$

$$C_{11} = \begin{vmatrix} -1 & 1 \\ 3 & 4 \end{vmatrix} = -7 \quad C_{12} = \begin{vmatrix} 1 & 3 \\ 4 & -1 \end{vmatrix} = -13 \quad C_{13} = \begin{vmatrix} 3 & -1 \\ -1 & 3 \end{vmatrix} = 8$$

$$C_{21} = \begin{vmatrix} 3 & 4 \\ 1 & 2 \end{vmatrix} = 2 \quad C_{22} = \begin{vmatrix} 4 & -1 \\ 2 & -1 \end{vmatrix} = -2 \quad C_{23} = \begin{vmatrix} -1 & 3 \\ -1 & -1 \end{vmatrix} = 2$$

$$C_{31} = \begin{vmatrix} 1 & 2 \\ -1 & 1 \end{vmatrix} = 3 \quad C_{32} = \begin{vmatrix} 2 & -1 \\ 1 & 3 \end{vmatrix} = 7 \quad C_{33} = \begin{vmatrix} -1 & 1 \\ 3 & -1 \end{vmatrix} = -2$$

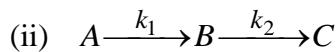
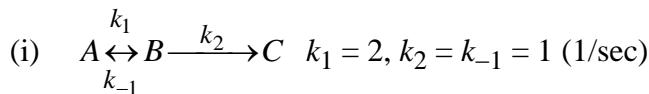
$$A^{-1} = \frac{1}{10} \begin{bmatrix} -7 & 2 & 3 \\ -13 & -2 & 7 \\ 8 & 2 & -2 \end{bmatrix}$$

(iii)

$$\det(A) = 10 \quad \det(B) = 9$$

$$\det(AB) = 10 \times 9 = 90$$

3. Please derive and solve the integrated rate laws for the reactions and plot the concentrations of all the species as function of times. (initially  $[A] = 1.0 \text{ M}$ ,  $[B] = [C] = 0.0 \text{ M}$ ) (20%)



(i)

$$y_1' = \frac{d[A]}{dt} = -k_1[A] + k_{-1}[B] = -2[A] + [B] = -2y_1 + y_2$$

$$y_2' = \frac{d[B]}{dt} = k_1[A] - k_2[B] - k_{-1}[B] = 2[A] - 2[B] = 2y_1 - 2y_2$$

$$A = \begin{bmatrix} -2 & 1 \\ 2 & -2 \end{bmatrix}$$

$$\begin{bmatrix} -2 - \lambda & 1 \\ 2 & -2 - \lambda \end{bmatrix} \Rightarrow \lambda = -2 \pm \sqrt{2}$$

$$\text{If } \lambda = -2 + \sqrt{2}$$

$$\begin{cases} -\sqrt{2}y_1 + y_2 = 0 \\ 2y_1 - \sqrt{2}y_2 = 0 \end{cases}$$

$$2y_1 = \sqrt{2}y_2$$

$$y_1 = \frac{\sqrt{2}}{2}y_2$$

$$X_1 = \begin{bmatrix} 1 \\ \sqrt{2} \end{bmatrix}$$

If  $\lambda = -2 - \sqrt{2}$

$$\begin{cases} \sqrt{2}y_1 + y_2 = 0 \\ 2y_1 + \sqrt{2}y_2 = 0 \end{cases}$$

$$2y_1 = -\sqrt{2}y_2$$

$$y_1 = -\frac{\sqrt{2}}{2}y_2$$

$$X_2 = \begin{bmatrix} 1 \\ -\sqrt{2} \end{bmatrix}$$

$$\begin{bmatrix} y_1 \\ y_2 \end{bmatrix} = c_1 \begin{bmatrix} 1 \\ \sqrt{2} \end{bmatrix} e^{(-2+\sqrt{2})t} + c_2 \begin{bmatrix} 1 \\ -\sqrt{2} \end{bmatrix} e^{(-2-\sqrt{2})t}$$

由起始條件:  $A(t=0) = A_0$ ,  $B(t=0) = 0$ ,  $c_1 = c_2 = 1/2 A_0$

$$\therefore A = \frac{1}{2}A_0 e^{(-2+\sqrt{2})t} + \frac{1}{2}A_0 e^{(-2-\sqrt{2})t}$$

$$B = \frac{\sqrt{2}}{2}A_0 e^{(-2+\sqrt{2})t} - \frac{\sqrt{2}}{2}A_0 e^{(-2-\sqrt{2})t}$$

$$\frac{d[A]}{dt} = -k_1[A]$$

$$\frac{d[B]}{dt} = k_1[A] - k_2[B]$$

$$[A] = A_0 e^{-k_1 t}$$

$$\frac{d[B]}{dt} = k_1 A_0 e^{-k_1 t} - k_2 [B]$$

$$[B] = \frac{k_1}{k_2 - k_1} A_0 (e^{-k_1 t} - e^{-k_2 t})$$

$$[C] = A_0 - [B] - [A]$$

$$= A_0 \left[ 1 - \frac{k_1}{k_2 - k_1} (e^{-k_1 t} - e^{-k_2 t}) - e^{-k_1 t} \right]$$

4.  $A = \begin{bmatrix} 3 & 5 & 3 \\ 0 & 4 & 6 \\ 0 & 0 & 1 \end{bmatrix}$ , find the eigenvalues and eigenvectors of A. (15%)

$$(3-\lambda)(4-\lambda)(1-\lambda) = 0 \quad \lambda = 1, 3, 4$$

If  $\lambda = 1$

$$\begin{cases} 2x_1 + 5x_2 + 3x_3 = 0 \\ 3x_2 + 6x_3 = 0 \\ 0x_3 = 0 \end{cases}$$

$$x_3 = a$$

$$3x_2 = -6a$$

$$2x_1 - 10a + 3a = 0$$

$$2x_1 = 7a$$

$$x_1 = \frac{7}{2}a$$

$$X_1 = a \begin{bmatrix} \frac{7}{2} \\ 2 \\ -2 \\ 1 \end{bmatrix}$$

If  $\lambda = 3$

$$\begin{cases} 0x_1 + 5x_2 + 3x_3 = 0 \\ x_2 + 6x_3 = 0 \\ -2x_3 = 0 \end{cases}$$

$$5x_2 + 3x_3 = 0$$

$$2x_2 = -6x_3$$

$$x_1 = a$$

$$x_3 = 0$$

$$x_2 = 0$$

$$X_2 = a \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}$$

If  $\lambda = 4$

$$\begin{cases} -x_1 + 5x_2 + 3x_3 = 0 \\ 0x_2 + 6x_3 = 0 \\ -x_3 = 0 \end{cases}$$

$$0x_3 = 0$$

$$x_2 = a$$

$$-x_1 = -5a$$

$$x_1 = 5a$$

$$X_3 = a \begin{bmatrix} 5 \\ 1 \\ 0 \end{bmatrix}$$

5. Please prove (a) if B is similar to A, then B has the same eigenvalues as A (b) An orthogonal transformation preserves the value of the inner product of vectors  $\mathbf{a} \bullet \mathbf{b}$ . (10%)
6. Find the positive solution of  $x^3 + 2x - 1 = 0$  using fixed-point iteration and Newton's methods (4D) (10%)

### Newton's methods:

$$f(x) = x^3 + 2x - 1$$

$$f'(x) = 3x^2 + 2$$

$$\Rightarrow x_{n+1} = x_n - \frac{x_n^3 + 2x_n - 1}{3x_n^2 + 2}$$

$$x_0 = 1$$

$$x_1 = 0.6$$

$$x_2 = 0.464935$$

$$x_3 = 0.453467$$

$$x_4 = 0.453397$$

$$x_5 = 0.453397 \#$$


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### Fixed-point iteration

$$x^3 + 2x - 1 \Rightarrow 2x = -x^3 + 1$$

$$x = 1/2(-x^3 + 1)$$

$$\Rightarrow x_{n+1} = 1/2(-x_n^3 + 1)$$

$x_0 = 1$   
 $x_1 = 0.5$   
 $x_2 = 0.4375$   
 $x_3 = 0.458129$   
 $x_4 = 0.451923$   
 $x_5 = 0.453850$   
 $x_6 = 0.453258$   
 $x_7 = 0.453440$   
 $x_8 = 0.453384$   
 $x_9 = 0.453401$   
 $x_{10} = 0.453396$   
 $\underline{x_{11} = 0.453398 \#}$

7. A function  $f$  such that  $f(1.0) = 1.00$ ,  $f(2.0) = 1.4142$ ,  $f(3.0) = 1.7321$ , and  $f(5.0) = 2.2361$ . (i) Can you recognize what type of function  $f$  is? (5%) (ii) Find a third-order polynomial function that passes the four points. Find  $f(4.0)$  and compare the value with the correct values if you can answer (i) (10%) (iii) Calculate the integral  $\int f(x) dx$  numerically from  $x = 1$  to  $x = 5$  using the Trapezoidal and Simpson's rules ( $h = 1.0$ ), and compare your result with the correct one (10%).

(i)

$$f(x) = \sqrt{x}$$

(ii)

$$\begin{array}{ll}
 x_0 = 1 & f(x_0) = 1 \\
 x_1 = 2 & f(x_1) = 1.4142 \\
 x_2 = 3 & f(x_2) = 1.7321 \\
 x_3 = 5 & f(x_3) = 2.2361
 \end{array}$$

$$P_3(x) = L_0 f_0 + L_1 f_1 + L_2 f_2 + L_3 f_3$$

$$L_0 = \frac{(x - x_1)(x - x_2)(x - x_3)}{(x_0 - x_1)(x_0 - x_2)(x_0 - x_3)} = \frac{(x - 2)(x - 3)(x - 5)}{(1 - 2)(1 - 3)(1 - 5)} = -\frac{1}{8}(x - 2)(x - 3)(x - 5) \Rightarrow L(4) = 0.25$$

$$L_1 = \frac{(x - x_0)(x - x_2)(x - x_3)}{(x_1 - x_0)(x_1 - x_2)(x_1 - x_3)} = \frac{(x - 1)(x - 3)(x - 5)}{(2 - 1)(2 - 3)(2 - 5)} = \frac{1}{3}(x - 1)(x - 3)(x - 5) \Rightarrow L(4) = -1$$

$$L_2 = \frac{(x - x_0)(x - x_1)(x - x_3)}{(x_2 - x_0)(x_2 - x_1)(x_2 - x_3)} = \frac{(x - 1)(x - 2)(x - 5)}{(3 - 1)(3 - 2)(3 - 5)} = -\frac{1}{4}(x - 1)(x - 2)(x - 5) \Rightarrow L(4) = 1.5$$

$$L_3 = \frac{(x - x_0)(x - x_1)(x - x_2)}{(x_3 - x_0)(x_3 - x_1)(x_3 - x_2)} = \frac{(x - 1)(x - 2)(x - 3)}{(5 - 1)(5 - 2)(5 - 3)} = -\frac{1}{24}(x - 1)(x - 2)(x - 5) \Rightarrow L(4) = 0.25$$

$$P(4) = 0.25 \times 1 + (-1) \times 1.4142 + 1.5 \times 1.7321 + 0.25 \times 2.2361 = 1.992975$$

$$\sqrt{4} = 2$$

誤差 :  $2 - 1.992975 = 0.007025$

(iii)

**Simpson:**

$$\int_a^b f(x)dx = \frac{1}{3}(f_0 + 4f_1 + 2f_2 + 4f_3 + \dots + f_m)$$

$$S_0 = f_0 + f_m = 1 + 2.2361 = 3.2361$$

$$S_1 = f_1 + f_3 = \sqrt{2} + \sqrt{4} = 3.4142$$

$$S_2 = f_2 = \sqrt{3} = 1.7321$$

$$\therefore \int_1^5 \sqrt{x} dx = \frac{1}{3}[3.2361 + 4 \times (3.4142) + 2 \times (1.7321)] = 6.7857$$

**Trapezoidal:**

$$\int_a^b f(x)dx = h\left(\frac{1}{2}f(x) + f(2) + f(3) + f(4) + \frac{1}{2}f(5)\right)$$

$$\therefore \int_1^5 \sqrt{x} dx = 1 \times \left(\frac{1}{2} + 1.4142 + 1.7321 + 2 + \frac{1}{2} \times 2.2361\right) = 6.76435$$