Solutions Problem Set #3 2007

① $$\tilde{A}\tilde{B} = \begin{pmatrix} 1 & 2 & -1 \\ 3 & 0 & 2 \\ 4 & 5 & 0 \end{pmatrix}\begin{pmatrix} 1 & 0 & 0 \\ 2 & 1 & 0 \\ 0 & 1 & 3 \end{pmatrix} = \begin{pmatrix} 1+4+0 & 0+2-1 & 0+0-3 \\ 3+0+0 & 0+0+2 & 0+0+6 \\ 4+10+0 & 0+5+0 & 0+0+0 \end{pmatrix}$$

$$= \begin{pmatrix} 5 & 1 & -3 \\ 3 & 2 & 6 \\ 14 & 5 & 0 \end{pmatrix}$$

$$\tilde{B}\tilde{A} = \begin{pmatrix} 1 & 0 & 0 \\ 2 & 1 & 0 \\ 0 & 1 & 3 \end{pmatrix}\begin{pmatrix} 1 & 2 & -1 \\ 3 & 0 & 2 \\ 4 & 5 & 0 \end{pmatrix} = \begin{pmatrix} 1+0+0 & 2+0+0 & -1+0+0 \\ 2+3+0 & 4+0+0 & -2+2+0 \\ 0+3+12 & 0+0+15 & 0+2+0 \end{pmatrix}$$

$$= \begin{pmatrix} 1 & 2 & -1 \\ 5 & 4 & 0 \\ 15 & 15 & 2 \end{pmatrix}$$

$\tilde{A}\tilde{B} \neq \tilde{B}\tilde{A}$ $\therefore$ 2 matrices do not commute.

② $$\begin{vmatrix} 1 & -1 & 1 & -1 \\ 0 & 1 & -1 & 1 \\ 0 & 0 & 1 & -1 \\ 0 & 0 & 0 & 1 \end{vmatrix}$$

Can expand along any row or coloumn $\therefore$ here, the determinant is expanded along coloumn 1 $\because$ it has a lot of zeros.

$$= +(1)\begin{vmatrix} 1 & -1 & 1 \\ 0 & 1 & -1 \\ 0 & 0 & 1 \end{vmatrix}$$ expand again along column 1.

$$\Rightarrow +(1)(1)\begin{vmatrix} 1 & -1 \\ 0 & 1 \end{vmatrix} = (1)(1)(1) = \boxed{1}$$

③ a) $\tilde{A}$ is Hermitian if $\tilde{A}^\dagger = \tilde{A} \Rightarrow (\tilde{A}^T)^* = \tilde{A}$

$$\tilde{A} = \begin{pmatrix} 1 & i & 1 \\ -i & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix} \quad \therefore \hat{A}^T = \begin{pmatrix} 1 & -i & 1 \\ i & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix} \Rightarrow (\tilde{A}^T)^* = \begin{pmatrix} 1 & i & 1 \\ -i & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix} = \tilde{A}$$

$\therefore$ yes; $\tilde{A}$ is Hermitian.

b) solve secular determinant $|\tilde{A} - \lambda \tilde{I}| = 0$ for eigenvalues $\{\lambda\}$.

$$\Rightarrow \begin{vmatrix} 1-\lambda & i & 1 \\ -i & -\lambda & 0 \\ 1 & 0 & -\lambda \end{vmatrix} = 0 \Rightarrow (1-\lambda)\begin{vmatrix} -\lambda & 0 \\ 0 & -\lambda \end{vmatrix} - i\begin{vmatrix} -i & 0 \\ 1 & -\lambda \end{vmatrix} + (1)\begin{vmatrix} -i & -\lambda \\ 1 & 0 \end{vmatrix} = 0$$

$$\Rightarrow (1-\lambda)\lambda^2 - ii\lambda + \lambda = 0 \Rightarrow (1-\lambda)\lambda^2 + \lambda + \lambda = 0 \quad \because ii = +1$$

$$\therefore \lambda^2 - \lambda^3 + 2\lambda = 0 \quad \text{or} \quad \lambda^3 - \lambda^2 - 2\lambda = 0$$

$$\Rightarrow \lambda(\lambda^2 - \lambda - 2) = 0 \Rightarrow \boxed{\lambda = 0} \text{ and } \lambda^2 - \lambda - 2 = 0$$

solve quadratic $\Rightarrow \lambda = \dfrac{+1 \pm \sqrt{(-1)^2 - 4(1)(-2)}}{2} = \dfrac{1 \pm \sqrt{9}}{2} = \dfrac{1 \pm 3}{2} \Rightarrow \boxed{\lambda = -1, +2}$

note: $\tilde{A}$ is Hermitian $\Rightarrow$ eigenvalues are real. $\tilde{A}$ would be a suitable operator in quantum mechanics.

④ a) to find exact eigenvalues of $\hat{H}$ consider

$$\hat{H} = \begin{pmatrix} 1 & c & 0 \\ c & 3 & 0 \\ 0 & 0 & -2+c \end{pmatrix}$$

$\therefore$ secular determinant for eigenvalues, λ, is

$$\left| \begin{pmatrix} 1 & c & 0 \\ c & 3 & 0 \\ 0 & 0 & -2+c \end{pmatrix} - \lambda \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \right| = 0$$

$$\therefore \begin{vmatrix} 1-\lambda & c & 0 \\ c & 3-\lambda & 0 \\ 0 & 0 & c-2-\lambda \end{vmatrix} = 0$$

$$\Rightarrow \quad (1-\lambda)\begin{vmatrix} 3-\lambda & 0 \\ 0 & c-2-\lambda \end{vmatrix} - c\begin{vmatrix} c & 0 \\ 0 & c-2-\lambda \end{vmatrix} = 0$$

$$= \quad (1-\lambda)(3-\lambda)(c-2-\lambda) - c^2(c-2-\lambda) = 0$$

$$= \quad (c-2-\lambda)\left[1+\lambda^2-3\lambda-\lambda-c^2+3\right] = 0$$

$$= \quad (c-2-\lambda)\left[\lambda^2-4\lambda+3-c^2\right] = 0$$

$$\therefore \boxed{\lambda = c-2} \quad \text{and} \quad \lambda^2-4\lambda+3-c^2=0$$

$$\therefore \lambda = \frac{4 \pm \sqrt{16-4(3-c^2)}}{2} = \frac{4 \pm \sqrt{4+4c^2}}{2}$$

$$\therefore \boxed{\lambda = 2 \pm \sqrt{1+c^2}}$$

b) $E_1^{(1)} = \langle \psi_1 | \hat{H}^{(1)} | \psi_1 \rangle = H_{11}^{(1)} = 0$

$E_2^{(1)} = H_{22}^{(1)} = 0$

$E_3^{(1)} = H_{33}^{(1)} = c$

2nd order correction $\quad E_q^{(2)} = -\sum_{k\neq q} \frac{|H_{qk}^{(1)}|^2}{E_k^{(0)}-E_q^{(0)}}$

$$E_1^{(2)} = -\frac{|H_{12}^{(1)}|^2}{E_2^{(0)}-E_1^{(0)}} - \frac{|H_{13}^{(1)}|^2}{E_3^{(0)}-E_1^{(0)}} = \frac{-c^2}{3-1} - 0 = \frac{-c^2}{2}$$

$$E_2^{(2)} = -\frac{|H_{21}^{(1)}|^2}{E_1^{(0)}-E_2^{(0)}} - \frac{|H_{23}|^2}{E_3^{(0)}-E_2^{(0)}} = \frac{-c^2}{1-3} - 0 = +\frac{c^2}{2}$$

$$E_3^{(2)} = -\frac{|H_{31}^{(1)}|^2}{E_1^{(0)}-E_3^{(0)}} - \frac{|H_{32}^{(1)}|^2}{E_2^{(0)}-E_3^{(0)}} = -0-0 = 0$$

$$\therefore\ E_1 = E_1^{(0)} + E_1^{(1)} + E_1^{(2)} = \boxed{1 - \frac{c^2}{2}}$$

$$E_2 = E_2^{(0)} + E_2^{(1)} + E_2^{(2)} = \boxed{3 + \frac{c^2}{2}}$$

$$E_3 = E_3^{(0)} + E_3^{(1)} + E_3^{(2)} = \boxed{-2 + c}$$

c) Compare a) and b) results.

$\lambda_{exact} = c-2$ $\quad\quad$ $\lambda_{pert} = c-2$

$\lambda_{exact} = 2 \pm \sqrt{1+c^2}$; if $c \ll 1 \Rightarrow \lambda \sim 2 \pm \left(1 + \frac{c^2}{2}\right)$ binomial expansion $n = \frac{1}{2}$

$\therefore\ \lambda_{pert} = 3 + \frac{c^2}{2}$ and $\lambda_{pert} = 1 - \frac{c^2}{2}$ $\equiv$ results of part b).