QM I
Phys 651

Solution of HW #3

Problem #1

(a) $\mathrm{Tr}\, A = \sum_n \langle \varphi_n | A | \varphi_n \rangle \Rightarrow$ similarly,

$$\underline{\mathrm{Tr}\,(ABC)} = \sum_n \langle \varphi_n | ABC | \varphi_n \rangle =$$

$$= \sum_{n,m,k} \langle \varphi_n | A | \varphi_m \rangle \langle \varphi_m | B | \varphi_k \rangle \langle \varphi_k | C | \varphi_n \rangle =$$

$$= \sum_{n,m,k} \langle \varphi_k | C | \underbrace{\varphi_n \rangle \langle \varphi_n}| A | \underbrace{\varphi_m \rangle \langle \varphi_m} | B | \varphi_k \rangle =$$

$$= \sum_k \langle \varphi_k | CAB | \varphi_k \rangle = \underline{\mathrm{Tr}\,(CAB)} =$$

$$= \sum_{n,m,k} \langle \varphi_m | B | \underbrace{\varphi_k \rangle \langle \varphi_k} | C | \underbrace{\varphi_n \rangle \langle \varphi_n} | A | \varphi_m \rangle =$$

$$= \sum_m \langle \varphi_m | BCA | \varphi_m \rangle = \underline{\mathrm{Tr}\,(BCA)}$$

(b) $\mathrm{Tr}\left(|\psi\rangle\langle\varphi|\right) = \sum_n \underbrace{\langle\varphi_n|\psi\rangle}_{\text{scalars}}\underbrace{\langle\varphi|\varphi_n\rangle}_{} =$

$= \sum_n \langle\varphi|\varphi_n\rangle\langle\varphi_n|\psi\rangle = \langle\varphi|\psi\rangle$

Problem #2

$$A \doteq \begin{pmatrix} 7 & 0 & 0 \\ 0 & 1 & -i \\ 0 & i & -1 \end{pmatrix} \; ; \; B \doteq \begin{pmatrix} 1 & 0 & 3 \\ 0 & 2i & 0 \\ i & 0 & -5i \end{pmatrix}$$

(a)

$$A^{+} \doteq \begin{pmatrix} 7 & 0 & 0 \\ 0 & 1 & -i \\ 0 & i & -1 \end{pmatrix} = A \Rightarrow \text{Hermitian}$$

$$B^{+} \doteq \begin{pmatrix} 1 & 0 & -i \\ 0 & -2i & 0 \\ 3 & 0 & 5i \end{pmatrix} \neq B \Rightarrow \text{not Hermitian}$$

(b)

$$\det \begin{pmatrix} 7-\lambda & 0 & 0 \\ 0 & 1-\lambda & -i \\ 0 & i & -1-\lambda \end{pmatrix} = 0 \Rightarrow \underline{\lambda_1 = 7}$$

$$-(1-\lambda)(\lambda+1) - 1 = 0$$

$$\underline{\lambda_{2,3} = \pm\sqrt{2}}$$

$|\lambda=7\rangle$:

$$\begin{pmatrix} 0 & 0 & 0 \\ 0 & -6 & -i \\ 0 & i & -7 \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix} = 0 \Rightarrow c_1 \text{ - arbitrary}$$

$$c_2 = 0,\ c_3 = 0 \Rightarrow \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$$

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$$|\lambda = \sqrt{2}\rangle : \quad \begin{pmatrix} 7-\sqrt{2} & 0 & 0 \\ 0 & 1-\sqrt{2} & -i \\ 0 & i & -1-\sqrt{2} \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix} = 0$$

$$\Downarrow$$

$$c_1 = 0$$
$$(1-\sqrt{2})\, c_2 = i c_3 \quad \Rightarrow \quad \begin{pmatrix} 0 \\ 1 \\ -i(1-\sqrt{2}) \end{pmatrix}$$

<u>Normalize</u>: $1 + |-i(1-\sqrt{2})|^2 = 1 + 1 - 2\sqrt{2} + 2 =$
$= 4 - 2\sqrt{2}$

$$\Downarrow$$

$$|\lambda = \sqrt{2}\rangle \doteq \begin{pmatrix} 0 \\ 1 \\ i(\sqrt{2}-1) \end{pmatrix} \cdot \frac{1}{\sqrt{4-2\sqrt{2}}}$$

$$|\lambda = -\sqrt{2}\rangle : \quad \begin{pmatrix} 7+\sqrt{2} & 0 & 0 \\ 0 & 1+\sqrt{2} & -i \\ 0 & i & -1+\sqrt{2} \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix} = 0$$

$$\Downarrow$$

$$c_1 = 0$$
$$(1+\sqrt{2})\, c_2 = i c_3 \quad \Rightarrow \quad \begin{pmatrix} 0 \\ 1 \\ -i(1+\sqrt{2}) \end{pmatrix}$$

<u>Normalize</u>: $1 + |-i(1+\sqrt{2})|^2 = 1 + 1 + 2\sqrt{2} + 2 = 4 + 2\sqrt{2}$

$$|\lambda = -\sqrt{2}\rangle \doteq \begin{pmatrix} 0 \\ 1 \\ -i(1+\sqrt{2}) \end{pmatrix} \cdot \frac{1}{\sqrt{4+2\sqrt{2}}}$$

$$\mathrm{Tr}(A) = 7+1-1 = 7 = \underbrace{\lambda_1}_{7} + \underbrace{\lambda_2}_{\sqrt{2}} + \underbrace{\lambda_3}_{-\sqrt{2}}$$

This is expected since Tr is invariant under such transformations (including diagonalization of the original matrix A, which is the eigenvalue problem)

(c) Check orthogonality:

$$\langle \lambda=7 | \lambda=\sqrt{2}\rangle \doteq \begin{bmatrix}1 & 0 & 0\end{bmatrix}\begin{bmatrix}0\\1\\i(\sqrt{2}-1)\end{bmatrix}\cdot\frac{1}{\sqrt{4-2\sqrt{2}}} =$$

$$= 0 \underset{\substack{\uparrow\\ \text{clearly!}}}{=} \langle \lambda=7 | \lambda=-\sqrt{2}\rangle$$

$$|\lambda=7\rangle\langle\lambda=7| + |\lambda=\sqrt{2}\rangle\langle\lambda=\sqrt{2}| +$$

$$+ |\lambda=-\sqrt{2}\rangle\langle\lambda=-\sqrt{2}| \doteq \begin{bmatrix}1\\0\\0\end{bmatrix}\begin{bmatrix}1 & 0 & 0\end{bmatrix} +$$

$$+ \frac{1}{4-2\sqrt{2}}\begin{bmatrix}0\\1\\i(\sqrt{2}-1)\end{bmatrix}\begin{bmatrix}0 & 1 & -i(\sqrt{2}-1)\end{bmatrix} + \frac{1}{4+2\sqrt{2}}\begin{bmatrix}0\\1\\-i(\sqrt{2}+1)\end{bmatrix}\cdot$$

$$\cdot\begin{bmatrix}0 & 1 & i(\sqrt{2}+1)\end{bmatrix} = \begin{bmatrix}1&0&0\\0&0&0\\0&0&0\end{bmatrix} + \begin{bmatrix}0&0&0\\0&1&-i(\sqrt{2}-1)\\0&i(\sqrt{2}-1)&(\sqrt{2}-1)^2\end{bmatrix}\cdot$$

$$\cdot\frac{1}{4-2\sqrt{2}} + \frac{1}{4+2\sqrt{2}}\begin{bmatrix}0&0&0\\0&1&i(\sqrt{2}+1)\\0&-i(\sqrt{2}+1)&(\sqrt{2}+1)^2\end{bmatrix} = \begin{bmatrix}1&0&0\\0&1&0\\0&0&1\end{bmatrix} = I$$

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(d)
$$AB = \begin{pmatrix} 7 & 0 & 0 \\ 0 & 1 & -i \\ 0 & i & -1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 3 \\ 0 & 2i & 0 \\ i & 0 & -5i \end{pmatrix} = \underbrace{\begin{pmatrix} 7 & 0 & 21 \\ 1 & 2i & -5 \\ -i & -2 & 5i \end{pmatrix}}$$

$$BA = \begin{pmatrix} 1 & 0 & 3 \\ 0 & 2i & 0 \\ i & 0 & -5i \end{pmatrix} \begin{pmatrix} 7 & 0 & 0 \\ 0 & 1 & -i \\ 0 & i & -1 \end{pmatrix} = \underbrace{\begin{pmatrix} 7 & 3i & -3 \\ 0 & 2i & 2 \\ 7i & 5 & 5i \end{pmatrix}}$$

$$\mathrm{Tr}(AB) = 7 + 2i + 5i = 7 + 7i = \mathrm{Tr}(BA),$$

as expected with cyclic permutation

$$\det \underbrace{\begin{pmatrix} 7 & 0 & 21 \\ 1 & 2i & -5 \\ -i & -2 & 5i \end{pmatrix}}_{AB} = 7(-10-10) + 21(-2-2) = -140 - 84 = \underline{-224}$$

$$\det(A) = 7(-1-1) = \underline{-14}$$

$$\det(B) = 10 + 3 \cdot 2 = \underline{16}$$

$$\Rightarrow -14 \cdot 16 = \underline{-224}$$

$$\underline{\det(AB) = \det(A)\det(B)}$$, as expected

$$\det(B^+) = 10 - i \cdot 6i = 16 = \det(B)$$ in this case

(e)
$$[A,B] \doteq \underbrace{\begin{pmatrix} 7 & 0 & 21 \\ 1 & 2i & -5 \\ -i & -2 & 5i \end{pmatrix}}_{AB} - \underbrace{\begin{pmatrix} 7 & 3i & -3 \\ 0 & 2i & 2 \\ 7i & 5 & 5i \end{pmatrix}}_{BA} = \underline{\begin{pmatrix} 0 & -3i & 24 \\ 1 & 0 & -7 \\ -8i & -7 & 0 \end{pmatrix}}$$

$\underline{Tr([A,B]) = 0}$, once again as expected (since $Tr(AB) = Tr(BA)$)

(f)

$$A^{-1} = -\frac{1}{14}\begin{pmatrix} -2 & 0 & 0 \\ 0 & -7 & 7i \\ 0 & -7i & 7 \end{pmatrix} = \underline{\begin{pmatrix} \frac{1}{7} & 0 & 0 \\ 0 & \frac{1}{2} & -\frac{i}{2} \\ 0 & \frac{i}{2} & -\frac{1}{2} \end{pmatrix}}$$

$$A_{11} = \frac{-1-i(-i)}{\underbrace{\det(A)}_{-14}} = \frac{-2}{-14}$$

$$A_{22} = \frac{-7}{-14}\ ; \quad A_{33} = \frac{7}{-14}$$

$$A_{12} = \frac{\text{cofactor of } A_{21}}{-14}\cdot(-1) = 0 = A_{13} = A_{21} = A_{31}$$

$$A_{23} = \frac{\text{cofactor of } A_{32}}{-14}\cdot(-1) = \frac{7i}{-14} = -A_{32}$$

Check:

$$\underbrace{\begin{pmatrix} \frac{1}{7} & 0 & 0 \\ 0 & \frac{1}{2} & -\frac{i}{2} \\ 0 & \frac{i}{2} & -\frac{1}{2} \end{pmatrix}}_{A^{-1}} \underbrace{\begin{pmatrix} 7 & 0 & 0 \\ 0 & 1 & -i \\ 0 & i & -1 \end{pmatrix}}_{A} = \underbrace{\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}}_{I}$$

$$\det(A^{-1} - \lambda I) \Rightarrow \det\begin{pmatrix} \frac{1}{7}-\lambda & 0 & 0 \\ 0 & \frac{1}{2}-\lambda & -\frac{i}{2} \\ 0 & \frac{i}{2} & -\frac{1}{2}-\lambda \end{pmatrix} = 0 \Rightarrow \underline{\lambda_1 = \frac{1}{7}}$$

$$\underline{\lambda_{2,3} = \pm\frac{1}{\sqrt{2}}}$$

As expected, eigenvalues of A^{-1} are

$$\frac{1}{\text{eigenvalues of } A} \; !$$

Problem #3

$$\hat{H} = \alpha\left(|\varphi_1\rangle\langle\varphi_2| + |\varphi_2\rangle\langle\varphi_1|\right)$$

(a) $$\hat{H}^2 = \alpha^2\left(|\varphi_1\rangle\langle\varphi_2| + |\varphi_2\rangle\langle\varphi_1|\right)\left(|\varphi_1\rangle\langle\varphi_2| + |\varphi_2\rangle\langle\varphi_1|\right) = \alpha^2\left(|\varphi_1\rangle\langle\varphi_1| + |\varphi_2\rangle\langle\varphi_2|\right) =$$

assume $\langle\varphi_1|\varphi_1\rangle = \langle\varphi_2|\varphi_2\rangle = 1$

$= \alpha^2 I$ ← assuming that $\{|\varphi_i\rangle\}$ $(i=1,2)$ form complete orthonormal basis

Then $\hat{H}^2 \neq \hat{H} \Rightarrow \hat{H}$ is <u>not</u> a projector

$$\left(\alpha^{-2}\hat{H}^2\right)^2 = \alpha^{-4}\cdot\alpha^4 I = I = \alpha^{-2}\underbrace{(\alpha^2 I)}_{\hat{H}^2}$$

obviously Hermitian (real α) $\Rightarrow$ $\alpha^{-2}\hat{H}^2$ is a projector

(b) $\hat{H}|\varphi_1\rangle = \alpha\left(|\varphi_1\rangle\langle\varphi_2| + |\varphi_2\rangle\langle\varphi_1|\right)|\varphi_1\rangle$

$= \alpha|\varphi_2\rangle$; $\hat{H}|\varphi_2\rangle = \alpha|\varphi_1\rangle$

$\Downarrow$

Obviously, $|\varphi_1\rangle$, $|\varphi_2\rangle$ are <u>not</u> eigenstates of H

(e) $H_{11} = \langle \varphi_1 | \hat{H} | \varphi_1 \rangle = 0 = H_{22}$

$H_{12} = \langle \varphi_1 | \hat{H} | \varphi_2 \rangle = \alpha = H_{21}$

Then, $\hat{H} \doteq \alpha \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ (in $\{|\varphi_i\rangle\}$ basis)

Eigenvalues: $\det \begin{pmatrix} -\lambda & 1 \\ 1 & -\lambda \end{pmatrix} = \lambda^2 - 1 = 0$

$\lambda = \pm 1 \Rightarrow \pm\alpha$

Eigenvectors: $|\alpha\rangle$: $\begin{pmatrix} -\alpha & \alpha \\ \alpha & -\alpha \end{pmatrix} \begin{pmatrix} C_1 \\ C_2 \end{pmatrix} = 0 \Rightarrow$

$C_1 = C_2 \Rightarrow$

$|\alpha\rangle \doteq \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$

$|-\alpha\rangle$: $\begin{pmatrix} \alpha & \alpha \\ \alpha & \alpha \end{pmatrix} \begin{pmatrix} C_1 \\ C_2 \end{pmatrix} = 0 \Rightarrow C_1 = -C_2 \Rightarrow |-\alpha\rangle \doteq \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}$

Same as in (d)!

Problem #4

~~While~~ One could imagine showing the identity

$$e^{B} A e^{-B} = A + [B, A] + \frac{1}{2!}[B,[B,A]] + \dots$$

to be true using $e^{\alpha B} = \sum_n \frac{(\alpha B)^n}{n!}$ and collecting the appropriate terms (and that's fine!)

However, more elegant way of doing this is the following:

Consider the operator $C(\alpha) = e^{\alpha B} A e^{-\alpha B}$, where α is a parameter.

Then, $$\frac{d\,C(\alpha)}{d\alpha} = B\underbrace{e^{\alpha B} A e^{-\alpha B}}_{''C(\alpha)} - \underbrace{e^{\alpha B} A e^{-\alpha B}}_{C''(\alpha)} B =$$

$$= [B, C(\alpha)]$$

$$\frac{d^2 C(\alpha)}{d\alpha^2} = \left[B, \frac{dC(\alpha)}{d\alpha}\right] = [B, [B, C(\alpha)]],$$

$$\frac{d^3 C(\alpha)}{d\alpha^3} = \left[B, \frac{d^2C(\alpha)}{d\alpha^2}\right] = \left[B, \left[B, \frac{dC(\alpha)}{d\alpha}\right]\right] =$$

$$= [B, [B, [B, C(\alpha)]]]$$

and so on . . .

Now combine all these derivatives:

$$C(\alpha=1) = C(\alpha=0) + \left.\frac{dC}{d\alpha}\right|_{\alpha=0} + \frac{1}{2!}\left.\frac{d^2C}{d\alpha^2}\right|_{\alpha=0} +$$

Taylor expansion around $\alpha = 0$

$$+ \frac{1}{3!}\left.\frac{d^3C}{d\alpha^3}\right|_{\alpha=0} + \ldots = A + [B, A] + \frac{1}{2!}[B, [B, A]] +$$

$$+ \frac{1}{3!}[B, [B, [B, A]]] + \ldots$$