Quantum Mechanics : : Homework 04

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Problem 01

a

I do the matrix multiplication by hand.

$$
\begin{aligned}
\hat{\sigma}_1\hat{\sigma}_2 &= \begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\begin{pmatrix}0 & -i\\ i & 0\end{pmatrix} = \begin{pmatrix}i & 0\\ 0 & -i\end{pmatrix} = i\hat{\sigma}_3\\
\hat{\sigma}_2\hat{\sigma}_1 &= \begin{pmatrix}0 & -i\\ i & 0\end{pmatrix}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix} = \begin{pmatrix}-i & 0\\ 0 & i\end{pmatrix} = -i\hat{\sigma}_3\\
\hat{\sigma}_2\hat{\sigma}_3 &= \begin{pmatrix}0 & -i\\ i & 0\end{pmatrix}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix} = \begin{pmatrix}0 & i\\ i & 0\end{pmatrix} = i\hat{\sigma}_1\\
\hat{\sigma}_3\hat{\sigma}_2 &= \begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}\begin{pmatrix}0 & -i\\ i & 0\end{pmatrix} = \begin{pmatrix}0 & -i\\ -i & 0\end{pmatrix} = -i\hat{\sigma}_1\\
\hat{\sigma}_3\hat{\sigma}_1 &= \begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix} = \begin{pmatrix}0 & 1\\ -1 & 0\end{pmatrix} = i\hat{\sigma}_2\\
\hat{\sigma}_1\hat{\sigma}_3 &= \begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix} = \begin{pmatrix}0 & -1\\ 1 & 0\end{pmatrix} = -i\hat{\sigma}_2
\end{aligned}
$$

The cross product

$$
\begin{aligned}
\hat{\vec{\sigma}} \times \hat{\vec{\sigma}} &= \begin{vmatrix}\vec{n}_x & \vec{n}_y & \vec{n}_z\\ \sigma_1 & \sigma_2 & \sigma_3\\ \sigma_1 & \sigma_2 & \sigma_3\end{vmatrix}\\
&= \vec{n}_x\left(\sigma_2\sigma_3 - \sigma_3\sigma_2\right) + \vec{n}_y\left(\sigma_3\sigma_1 - \sigma_1\sigma_3\right) + \vec{n}_z\left(\sigma_1\sigma_2 - \sigma_2\sigma_1\right)\\
&= \vec{n}_x(2i\sigma_1) + \vec{n}_y\left(2i\sigma_2\right) + \vec{n}_z\left(2i\sigma_3\right)\\
&= 2i\left(\sigma_1\vec{n}_x + \sigma_2\vec{n}_y + \sigma_3\vec{n}_z\right)\\
&= 2i\hat{\vec{\sigma}}
\end{aligned}
$$

Note this also is alluring to the Levi-Civita Symbol because

$$
\text{cyclic } i \to j \to k \to i \to j \to k \implies \quad \sigma_i\sigma_j = i\epsilon_{ij}\sigma_k \qquad\qquad (\text{where } \{i,j,k\} \in \{1,2,3\})
$$

a

$$
\left(\vec{U}\cdot\hat{\vec{\sigma}}\right)\left(\vec{V}\cdot\hat{\vec{\sigma}}\right) = \left(U_1\sigma_1 + U_2\sigma_2 + U_3\sigma_3\right)\left(V_1\sigma_1 + V_2\sigma_2 + V_3\sigma_3\right)
$$

$$
\begin{aligned}
\left(\vec{U}\cdot\hat{\vec{\sigma}}\right)\left(\vec{V}\cdot\hat{\vec{\sigma}}\right) &= \left(\sum_{i=1}^{3} U_i\sigma_i\right)\left(\sum_{j=1}^{3} V_j\sigma_j\right)\\
&= \sum_{i,j=1}^{3} U_iV_j\sigma_i\sigma_j\\
&= \sum_{i,j=1,i\neq j}^{3} U_iV_j\sigma_i\sigma_j + \sum_{n=1}^{3} U_nV_n\sigma_n\sigma_n\\
&= \sum_{i,j=1,i\neq j}^{3} iU_iV_j\epsilon_{ij}\sigma_k + \sum_{n=1}^{3} U_nV_n\sigma_n\sigma_n\\
&= [i(U_1V_2-U_2V_1)\sigma_3 + i(U_2U_3-U_3U_2)\sigma_1 + i(U_3U_1-U_1U_3)\sigma_2] + (U_1V_1+U_2V_2+U_3V_3)\hat{I}\\
&= [\vec{U}\times\vec{V}]_3 i\sigma_3 + [\vec{U}\times\vec{V}]_1 i\sigma_1 + [\vec{U}\times\vec{V}]_2 i\sigma_2 + (\vec{U}\cdot\vec{V})\hat{I}\\
&= i\left[\vec{U}\times\vec{V}\right]\cdot\hat{\vec{\sigma}} + \left(\vec{U}\cdot\vec{V}\right)\hat{I}
\end{aligned}
$$

Problem 02

a

Considering the simplest basis in column vector forms

$$|1\rangle = \begin{pmatrix}1\\0\\0\end{pmatrix} \quad |2\rangle = \begin{pmatrix}0\\1\\0\end{pmatrix} \quad |3\rangle = \begin{pmatrix}0\\0\\1\end{pmatrix}$$

We want to compute the following operator $\hat{H}$

$$\hat{H} = E_0\left(|1\rangle\langle 1| + |2\rangle\langle 2| + |3\rangle\langle 3|\right) - J\left(|1\rangle\langle 2| + |2\rangle\langle 1| + |2\rangle\langle 3| + |3\rangle\langle 2| + |3\rangle\langle 1| + |1\rangle\langle 3|\right)$$

Matrices for the first term

$$\begin{aligned}
|1\rangle\langle 1| + |2\rangle\langle 2| + |3\rangle\langle 3| &= \begin{bmatrix}1\\0\\0\end{bmatrix}\begin{bmatrix}1 & 0 & 0\end{bmatrix} + \begin{bmatrix}0\\1\\0\end{bmatrix}\begin{bmatrix}0 & 1 & 0\end{bmatrix} + \begin{bmatrix}0\\0\\1\end{bmatrix}\begin{bmatrix}0 & 0 & 1\end{bmatrix} \\
&= \begin{pmatrix}1 & 0 & 0\\0 & 0 & 0\\0 & 0 & 0\end{pmatrix} + \begin{pmatrix}0 & 0 & 0\\0 & 1 & 0\\0 & 0 & 0\end{pmatrix} + \begin{pmatrix}0 & 0 & 0\\0 & 0 & 0\\0 & 0 & 1\end{pmatrix} \\
&= \begin{pmatrix}1 & 0 & 0\\0 & 1 & 0\\0 & 0 & 1\end{pmatrix} = \hat{I}
\end{aligned}$$

Matrices for the second term

$$\begin{aligned}
&|1\rangle\langle 2| + |2\rangle\langle 1| + |2\rangle\langle 3| + |3\rangle\langle 2| + |3\rangle\langle 1| + |1\rangle\langle 3| \\
&= \begin{pmatrix}1\\0\\0\end{pmatrix}\begin{pmatrix}0 & 1 & 0\end{pmatrix} + \begin{pmatrix}0\\1\\0\end{pmatrix}\begin{pmatrix}1 & 0 & 0\end{pmatrix} + \begin{pmatrix}0\\1\\0\end{pmatrix}\begin{pmatrix}0 & 0 & 1\end{pmatrix} + \begin{pmatrix}0\\0\\1\end{pmatrix}\begin{pmatrix}0 & 1 & 0\end{pmatrix} + \begin{pmatrix}0\\0\\1\end{pmatrix}\begin{pmatrix}1 & 0 & 0\end{pmatrix} + \begin{pmatrix}1\\0\\0\end{pmatrix}\begin{pmatrix}0 & 0 & 1\end{pmatrix} \\
&= \begin{bmatrix}0 & 1 & 0\\0 & 0 & 0\\0 & 0 & 0\end{bmatrix} + \begin{bmatrix}0 & 0 & 0\\1 & 0 & 0\\0 & 0 & 0\end{bmatrix} + \begin{bmatrix}0 & 0 & 0\\0 & 0 & 1\\0 & 0 & 0\end{bmatrix} + \begin{bmatrix}0 & 0 & 0\\0 & 0 & 0\\0 & 1 & 0\end{bmatrix} + \begin{bmatrix}0 & 0 & 0\\0 & 0 & 0\\1 & 0 & 0\end{bmatrix} + \begin{bmatrix}0 & 0 & 1\\0 & 0 & 0\\0 & 0 & 0\end{bmatrix} \\
&= \begin{bmatrix}0 & 1 & 1\\1 & 0 & 1\\1 & 1 & 0\end{bmatrix}
\end{aligned}$$

Put them all together

$$\begin{aligned}
\hat{H} &= E_0\left(|1\rangle\langle 1| + |2\rangle\langle 2| + |3\rangle\langle 3|\right) - J\left(|1\rangle\langle 2| + |2\rangle\langle 1| + |2\rangle\langle 3| + |3\rangle\langle 2| + |3\rangle\langle 1| + |1\rangle\langle 3|\right) \\
&= \begin{bmatrix}E_0 & -J & -J\\-J & E_0 & -J\\-J & -J & E_0\end{bmatrix}
\end{aligned}$$

b (i)

The $|E_1\rangle$ in column vector representation

$$|E_1\rangle = \frac{1}{\sqrt{3}}\left(|1\rangle + |2\rangle + |3\rangle\right) = \frac{1}{\sqrt{3}}\begin{bmatrix}1\\1\\1\end{bmatrix}$$

Computing $\hat{H}|E_1\rangle$

$$
\begin{aligned}
\hat{H}|E_1\rangle &= \begin{bmatrix} E_0 & -J & -J \\ -J & E_0 & -J \\ -J & -J & E_0 \end{bmatrix} \left(\frac{1}{\sqrt{3}} \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix} \right) \\
&= \frac{1}{\sqrt{3}} \begin{bmatrix} E_0 - J - J \\ -J + E_0 - J \\ -J - J + E_0 \end{bmatrix} \\
&= \frac{1}{\sqrt{3}} \begin{bmatrix} E_0 - 2J \\ E_0 - 2J \\ E_0 - 2J \end{bmatrix} \\
&= \frac{E_0 - 2J}{\sqrt{3}} \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix} \\
&= (E_0 - 2J)\,|E_1\rangle
\end{aligned}
$$

We see the eigen-equation for the Hamiltonian

$$\hat{H}|E_1\rangle = E_1|E_1\rangle \implies E_1 = E_0 - 2J$$

b (ii) and (iii)

We algebraically initialize the elements of the matrix to minimize the computational effort by hand. Keep in mind that $\hat{H} - E\hat{I} = \hat{0} = \frac{1}{J}\hat{H} - \frac{1}{J}E\hat{I}$ hence

$$
\begin{aligned}
\frac{1}{J}\hat{H} &= \begin{bmatrix} \frac{E_0}{J} & -1 & -1 \\ -1 & \frac{E_0}{J} & -1 \\ -1 & -1 & \frac{E_0}{J} \end{bmatrix} \\
\left(\frac{1}{J}\hat{H}\right) - \frac{E}{J}\hat{I} &= \begin{bmatrix} \frac{E_0 - E}{J} & -1 & -1 \\ -1 & \frac{E_0 - E}{J} & -1 \\ -1 & -1 & \frac{E_0 - E}{J} \end{bmatrix} \\
&= (-1) \begin{bmatrix} \lambda & 1 & 1 \\ 1 & \lambda & 1 \\ 1 & 1 & \lambda \end{bmatrix} = 0 \qquad (\lambda = (E - E_0)/J) \\
&\implies \det \begin{bmatrix} \lambda & 1 & 1 \\ 1 & \lambda & 1 \\ 1 & 1 & \lambda \end{bmatrix} = 0 \\
&\implies \lambda^3 + 3\lambda + 2 = 0 \\
&\implies (\lambda - 1)^2(\lambda + 2) = 0 \\
&\implies (\lambda^2 - 2\lambda + 1)(\lambda + 2) \\
&\implies \lambda = 1, 1, -2
\end{aligned}
$$

As stated in the problem statement, $0 = (\lambda - \lambda_1)(\lambda^2 + b\lambda + c) \implies 0 = (\lambda - (-2))(\lambda^2 + (-2)\lambda + 1)$ giving us $(b, c) = (-2, 1)$

$$\text{For } \lambda = -2 \text{ the eigen-energy is } \frac{E - E_0}{J} = -2 \implies E = E_0 - 2J$$

$$\text{For } \lambda = 1 \text{ the eigen-energy is } \frac{E - E_0}{J} = 1 \implies E = E_0 + J$$

The eigenvalues are

$$\lambda_1 = -2, \quad \lambda_2 = 1, \quad \lambda_3 = 1$$

And corresponding eigen-energy

$$E_1 = E_0 - 2J, \quad E_2 = E_0 + J, \quad E_3 = E_0 + J$$

Problem 03

a

$$\hat{T}|n\rangle = |n+1\rangle \implies \langle n|T^\dagger = \langle n+1|$$
$$\text{now, } \langle n|T^\dagger|n+1\rangle = \langle n+1||n+1\rangle = 1$$
$$\text{or, } \langle n|T^\dagger T|n\rangle = 1$$
$$\text{and, } \langle n|T^\dagger|k+1\rangle = \langle n+1||k+1\rangle = 0 \qquad (n \neq k)$$
$$\implies T^\dagger T = \hat{I}$$

b

To compute $\left[\hat{H}, \hat{T}\right]$ we compute the two operator terms individually

$$\hat{H}\hat{T} = \left(\sum_{n=-\infty}^{\infty} \left[E_0|n\rangle\langle n| + J\left(|n+1\rangle\langle n| + |n\rangle\langle n+1|\right)\right]\right)\hat{T}$$

$$\hat{H}\hat{T}|n\rangle = \left(\sum_{n=-\infty}^{\infty} \left[E_0|n\rangle\langle n| + J\left(|n+1\rangle\langle n| + |n\rangle\langle n+1|\right)\right]\right)|n+1\rangle$$
$$= \Big[E_0|n\rangle\langle n| + J\Big(|n+1\rangle\langle n| + |n\rangle\langle n+1|\Big)\Big]|n+1\rangle + \Big[E_0|n+1\rangle\langle n+1| + J\Big(|n+2\rangle\langle n+1| + |n+1\rangle\langle n+2|\Big)\Big]|n+1\rangle$$
$$= J|n\rangle + E_0|n+1\rangle + J\left(|n+2\rangle\right)$$

$$\hat{T}\hat{H}|n\rangle = \hat{T}\Bigg(\Big[E_0|n\rangle\langle n| + J\Big(|n+1\rangle\langle n| + |n\rangle\langle n+1|\Big)\Big]|n\rangle + \Big[E_0|n-1\rangle\langle n-1| + J\Big(|n\rangle\langle n-1| + |n-1\rangle\langle n|\Big)\Big]|n\rangle\Bigg)$$
$$= \hat{T}\big(E_0|n\rangle + J|n+1\rangle + J|n-1\rangle\big)$$
$$= E_0|n+1\rangle + J|n+2\rangle + J|n\rangle = \hat{H}\hat{T}|n\rangle$$

$$\therefore \left(\hat{H}\hat{T} - \hat{T}\hat{H}\right)|n\rangle = |0\rangle \implies \left[\hat{H}, \hat{T}\right] = 0$$

c

Using the form given for the energy, and the eigen-equation for $\hat{T}$, we determine the general formula for $\psi_{E,n}$ in terms of $\psi_{E,0}$

$$\begin{aligned}
|E\rangle &= \sum_{n=-\infty}^{\infty} |n\rangle \psi_{E,n} \\
T|E\rangle &= \sum_{n=-\infty}^{\infty} T|n\rangle \psi_{E,n} \\
e^{-i\phi}|E\rangle &= \sum_{n=-\infty}^{\infty} |n+1\rangle \psi_{E,n} \\
\sum_{n=-\infty}^{\infty} e^{-i\phi}|n\rangle \psi_{E,n} &= \sum_{n=-\infty}^{\infty} |n+1\rangle \psi_{E,n} \\
\implies e^{-i\phi}|n+1\rangle \psi_{E,n+1} &= |n+1\rangle \psi_{E,n} \\
\therefore\ e^{-i\phi} &= \frac{\psi_{E,n}}{\psi_{E,n+1}}
\end{aligned}$$

The inductive relation between two coefficient is

$$\psi_{E,n+1} = e^{i\phi}\psi_{E,n} \implies \psi_{E,1} = e^{i\phi}\psi_{E,0} \implies \psi_{E,2} = e^{i\phi}\psi_{E,1} = e^{2i\phi}\psi_{E,0}$$

$$\implies \psi_{E,n} = e^{in\phi}\psi_{E,0}$$

The general form of energy is then

$$|E\rangle = \psi_{E,0} \sum_{n=-\infty}^{\infty} e^{in\phi}|n\rangle$$

$$\begin{aligned}
\hat{H}|E_n\rangle &= \psi_{E,n}\hat{H}|n\rangle = \psi_{E,n}\Big(E_0|n\rangle + J|n+1\rangle + J|n-1\rangle\Big) \\
\hat{H}|E\rangle = \hat{H}\left(\sum_{n=-\infty}^{\infty} \psi_{E,n}|n\rangle\right) &= \sum_{n=-\infty}^{\infty} \psi_{E,n}\Big(E_0|n\rangle + J|n+1\rangle + J|n-1\rangle\Big) \\
\langle n'|\hat{H}|E\rangle &= \sum_{n=-\infty}^{\infty} \psi_{E,n}\Big(E_0\langle n'|n\rangle + J\langle n'|n+1\rangle + J\langle n'|n-1\rangle\Big) \\
&= \psi_{E,n'} + \psi_{E,n'-1} + \psi_{E,n'+1} \\
&= \psi_{E,n'} + \frac{\psi_{E,n'}}{e^{i\phi}} + e^{i\phi}\psi_{E,n'} \\
&= \psi_{E,n'}(1 + e^{-i\phi} + e^{i\phi}) \\
&= \psi_{E,n'}(1 + 2\cos(\phi))
\end{aligned}$$

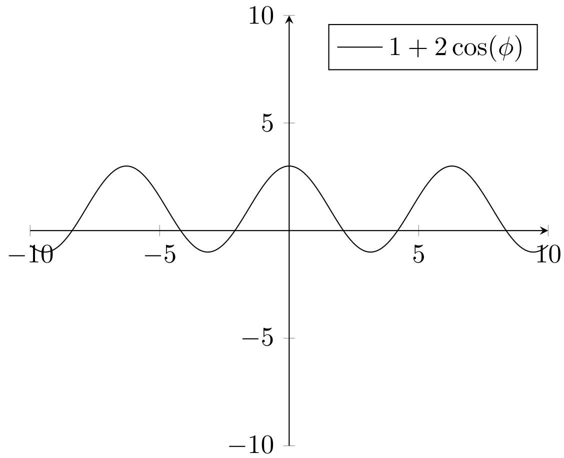

Figure 1: Simple pgfplot for aesthetic purposes

$$[1 + 2\cos(\phi)]_{\text{max}} = 3$$
$$[1 + 2\cos(\phi)]_{\text{min}} = -1$$