Physics 711: Assignment 2 Solutions

1. Three states have energy ϵ, 2ϵ, and 3ϵ. Small hopping amplitudes of strength $-t$ connect states 1 and 2 and states 2 and 3.
$$H = \begin{pmatrix} \epsilon & -t & 0 \\ -t & 2\epsilon & -t \\ 0 & -t & 3\epsilon \end{pmatrix}$$

   (a) Show that the energy eigenvalues are $E_1 = 2\epsilon$, $E_2 = 2\epsilon - \sqrt{2t^2+\epsilon^2}$, and $E_3 = 2\epsilon + \sqrt{2t^2+\epsilon^2}$. Try doing this by hand and then verifying with the `Eigenvalues` command.
   The characteristic polynomial of H is
$$\begin{aligned}\mathcal{P}_H(E) = \det(H - EI) &= \begin{vmatrix} \epsilon - E & -t & 0 \\ -t & 2\epsilon - E & -t \\ 0 & -t & 3\epsilon - E \end{vmatrix} \\ &= (\epsilon - E)\begin{vmatrix} 2\epsilon - E & -t \\ -t & 3\epsilon - E \end{vmatrix} - (-t)\begin{vmatrix} -t & -t \\ 0 & 3\epsilon - E \end{vmatrix} + 0 \\ &= (\epsilon - E)\big[(2\epsilon - E)(3\epsilon - E) - (-t)^2\big] + t\big[(-t)(3\epsilon - E)\big] \\ &= (\epsilon - E)(6\epsilon^2 - 5\epsilon E + E^2 + t^2) - t^2(3\epsilon - E) \\ &= -E^3 + 2t^2E + 6\epsilon E^2 - 4t^2\epsilon - 11\epsilon^2 E + 6\epsilon^3 \\ &= -(E - 2\epsilon)(E^2 - 4\epsilon E - 2t^2 + 3\epsilon^2),\end{aligned}$$
   which vanishes at the roots $E_1 = 2\epsilon$ and
$$E_{2,3} = \frac{4\epsilon \mp \sqrt{(-4\epsilon)^2 - 4(-2t^2 + 3\epsilon^2)}}{2} = 2\epsilon \mp \sqrt{4\epsilon^2 + 2t^2 - 3\epsilon^2} = 2\epsilon \mp \sqrt{2t^2 + \epsilon^2}.$$

   (b) Find the matrix V with normalized columns such that
$$HV = V\begin{pmatrix} 2\epsilon & 0 & 0 \\ 0 & 2\epsilon - \sqrt{2t^2+\epsilon^2} & 0 \\ 0 & 0 & 2\epsilon + \sqrt{2t^2+\epsilon^2} \end{pmatrix}.$$
   Here, $V = \big(v_1|v_2|v_3\big)$ is the matrix formed by stitching together as columns the three eigenvectors that satisfy $Hv_n = E_n v_n$ (for $n = 1, 2, 3$). That is to say, $\sum_j H_{i,j}(v_n)_j = E_n(v_n)_i$ or
$$\sum_j H_{i,j}V_{j,n} = (v_n)_i E_n = \sum_j V_{i,j}E_n\delta_{j,n},$$
   where $V_{j,n} = (v_n)_j$ is the jth component of the nth eigenvector. Don't attempt this by hand. Make use of the `Eigenvectors` or `Eigensystem` commands.

(c) Prove that $\operatorname{tr} H = 6\epsilon$ and $\operatorname{tr} H^2 = 4t^2 + 14\epsilon^2$.

$$H = V\begin{pmatrix} 2\epsilon & 0 & 0 \\ 0 & 2\epsilon - \sqrt{2t^2+\epsilon^2} & 0 \\ 0 & 0 & 2\epsilon + \sqrt{2t^2+\epsilon^2} \end{pmatrix} V^{-1}$$

$$\begin{aligned}
\operatorname{tr} H &= \operatorname{tr} V\begin{pmatrix} 2\epsilon & 0 & 0 \\ 0 & 2\epsilon - \sqrt{2t^2+\epsilon^2} & 0 \\ 0 & 0 & 2\epsilon + \sqrt{2t^2+\epsilon^2} \end{pmatrix} V^{-1} = \operatorname{tr} V^{-1}V\begin{pmatrix} 2\epsilon & 0 & 0 \\ 0 & 2\epsilon - \sqrt{2t^2+\epsilon^2} & 0 \\ 0 & 0 & 2\epsilon + \sqrt{2t^2+\epsilon^2} \end{pmatrix} \\
&= \operatorname{tr}\begin{pmatrix} 2\epsilon & 0 & 0 \\ 0 & 2\epsilon - \sqrt{2t^2+\epsilon^2} & 0 \\ 0 & 0 & 2\epsilon + \sqrt{2t^2+\epsilon^2} \end{pmatrix} = 2\epsilon + 2\epsilon - \sqrt{2t^2+\epsilon^2} + 2\epsilon + \sqrt{2t^2+\epsilon^2} = 6\epsilon
\end{aligned}$$

$$\begin{aligned}
\operatorname{tr} H^2 &= \operatorname{tr} V\begin{pmatrix} 2\epsilon & 0 & 0 \\ 0 & 2\epsilon - \sqrt{2t^2+\epsilon^2} & 0 \\ 0 & 0 & 2\epsilon + \sqrt{2t^2+\epsilon^2} \end{pmatrix} V^{-1}V\begin{pmatrix} 2\epsilon & 0 & 0 \\ 0 & 2\epsilon - \sqrt{2t^2+\epsilon^2} & 0 \\ 0 & 0 & 2\epsilon + \sqrt{2t^2+\epsilon^2} \end{pmatrix} V^{-1} \\
&= \operatorname{tr}\begin{pmatrix} (2\epsilon)^2 & 0 & 0 \\ 0 & (2\epsilon - \sqrt{2t^2+\epsilon^2})^2 & 0 \\ 0 & 0 & (2\epsilon + \sqrt{2t^2+\epsilon^2})^2 \end{pmatrix} \\
&= \operatorname{tr}\begin{pmatrix} 4\epsilon^2 & 0 & 0 \\ 0 & 4\epsilon^2 - 2\epsilon\sqrt{2t^2+\epsilon^2} + 2t^2 + \epsilon^2 & 0 \\ 0 & 0 & 4\epsilon^2 + 2\epsilon\sqrt{2t^2+\epsilon^2} + 2t^2 + \epsilon^2 \end{pmatrix} \\
&= 4\epsilon^2 + 4\epsilon^2 - \cancel{2\epsilon\sqrt{2t^2+\epsilon^2}} + 2t^2 + \epsilon^2 + 4\epsilon^2 + \cancel{2\epsilon\sqrt{2t^2+\epsilon^2}} + 2t^2 + \epsilon^2 \\
&= 4t^2 + 14\epsilon^2
\end{aligned}$$

(d) Find a closed-form expression for $\operatorname{tr} H^k$, where $k = 1, 2, 3, \ldots$ is a positive integer. You should be able to apply the binomial theorem to show that

$$\operatorname{tr} H^k = (2\epsilon)^k \left[1 + \sum_{j=0}^{\lfloor k/2 \rfloor} \frac{2(k!)}{4^j (2j)!(k-2j)!} \left(1 + \frac{2t^2}{\epsilon^2} \right)^j \right].$$

$$\begin{aligned}
\operatorname{tr} H^k &= (2\epsilon)^k + \left(2\epsilon - \sqrt{2t^2+\epsilon^2}\right)^k + \left(2\epsilon + \sqrt{2t^2+\epsilon^2}\right)^k \\
&= (2\epsilon)^k + \sum_{j=0}^{k} \binom{k}{j} (2\epsilon)^{k-j} [(-1)^j + (+1)^j](2t^2+\epsilon^2)^{j/2} \\
&= \epsilon^k + \sum_{j=0,2,4,\ldots}^{k} \binom{k}{j} (2\epsilon)^{k-j} (2)(2t^2+\epsilon^2)^{j/2} \\
&= (2\epsilon)^k + \sum_{j=0}^{\lfloor k/2 \rfloor} \binom{k}{2j} (2\epsilon)^{k-2j} (2)(2t^2+\epsilon^2)^j \\
&= (2\epsilon)^k \left(1 + \sum_{j=0}^{\lfloor k/2 \rfloor} \binom{k}{2j} 2(2\epsilon)^{-2j} (2t^2+\epsilon^2)^j \right) \\
&= (2\epsilon)^k \left(1 + \sum_{j=0}^{\lfloor k/2 \rfloor} \binom{k}{2j} 2^{1-2j} (\epsilon^2)^{-j} (2t^2+\epsilon^2)^j \right) \\
&= (2\epsilon)^k \left(1 + \sum_{j=0}^{\lfloor k/2 \rfloor} \binom{k}{2j} 2^{1-2j} (1 + 2t^2/\epsilon^2)^j \right) \\
&= (2\epsilon)^k \left[1 + \sum_{j=0}^{\lfloor k/2 \rfloor} \frac{2(k!)}{4^j (2j)!(k-2j)!} \left(1 + \frac{2t^2}{\epsilon^2} \right)^j \right]
\end{aligned}$$

(e) Prove these two closely related identities:

$$\operatorname{tr} e^{iHt/\hbar} = e^{i2\epsilon t/\hbar} \left(1 + 2\cos\left[(2t^2+\epsilon^2)^{1/2} t/\hbar \right] \right),$$

$$\operatorname{tr} e^{-\beta H} = e^{-2\beta\epsilon} \left(1 + 2\cosh\left[\beta (2t^2+\epsilon^2)^{1/2} \right] \right).$$

The diagonalized form

$$H = V \begin{pmatrix} 2\epsilon & 0 & 0 \\ 0 & 2\epsilon - \sqrt{2t^2+\epsilon^2} & 0 \\ 0 & 0 & 2\epsilon + \sqrt{2t^2+\epsilon^2} \end{pmatrix} V^{-1}$$

implies that

$$\begin{aligned}
\operatorname{tr} e^{-\beta H} &= \operatorname{tr} \begin{pmatrix} e^{-\beta 2\epsilon} & 0 & 0 \\ 0 & e^{-\beta(2\epsilon - \sqrt{2t^2+\epsilon^2})} & 0 \\ 0 & 0 & e^{-\beta(2\epsilon - \sqrt{2t^2+\epsilon^2})} \end{pmatrix} \\
&= e^{-\beta 2\epsilon} + e^{-\beta(2\epsilon - \sqrt{2t^2+\epsilon^2})} + e^{-\beta(2\epsilon + \sqrt{2t^2+\epsilon^2})} \\
&= e^{-2\beta\epsilon} \left(1 + e^{\beta\sqrt{2t^2+\epsilon^2}} + e^{-\beta\sqrt{2t^2+\epsilon^2}} \right) \\
&= e^{-2\beta\epsilon} \left[1 + 2\cosh\left(\beta\sqrt{2t^2+\epsilon^2} \right) \right].
\end{aligned}$$

2. The operators

$$\hat{P} = \sum_{i,j=1,2} |i\rangle P_{i,j} \langle j| = \big(|1\rangle\ |2\rangle\big)\, P \begin{pmatrix} \langle 1| \\ \langle 2| \end{pmatrix}$$

$$\text{and}\ \ \hat{Q} = \sum_{i,j=1,2} |i\rangle Q_{i,j} \langle j| = \big(|1\rangle\ |2\rangle\big)\, Q \begin{pmatrix} \langle 1| \\ \langle 2| \end{pmatrix}$$

are defined by the matrix kernels $P = \vec{p} \cdot \vec{\sigma}$ and $Q = \vec{q} \cdot \vec{\sigma}$, which have elements $P_{i,j} = p^a \sigma^a_{i,j}$ and $Q_{i,j} = q^a \sigma^a_{i,j}$. (Because of the repeated index, there is an implied summation over $a = x, y, z$.)

Show that

$$[P, Q] = 2i(\vec{p} \times \vec{q}) \cdot \vec{\sigma} \ \ \text{and} \ \ [\hat{P}, \hat{Q}] = 2i\epsilon^{abc} p^a q^b \sigma^c_{i,j} |i\rangle\langle j|.$$

Furthermore, argue that $\hat{P}$ and $\hat{Q}$ commute iff $\vec{p}$ and $\vec{q}$ are colinear.

$$\begin{aligned}
[P,Q]_{ij} = P_{ik}Qkj - Q_{ik}P_{kj} &= p^a \sigma^a_{i,k} q^b \sigma^b_{k,j} - q^a \sigma^a_{i,k} p^b \sigma^b_{k,j} = p^a \sigma^a_{i,k} q^b \sigma^b_{k,j} - q^b \sigma^b_{i,k} p^a \sigma^a_{k,j} \\
&= p^a q^b (\sigma^a_{i,k} \sigma^b_{k,j} - \sigma^b_{i,k} \sigma^a_{k,j}) = p^a q^b [\sigma^a, \sigma^b]_{i,j} \\
&= p^a q^b \left(2i\epsilon^{abc} \sigma^c\right)_{i,j} = 2i\epsilon^{abc} p^a q^b \sigma^c_{i,j} \\
&= 2i(\vec{p} \times \vec{q}) \cdot \vec{\sigma}_{i,j} \\
\implies \quad [P,Q] &= 2i(\vec{p} \times \vec{q}) \cdot \vec{\sigma}
\end{aligned}$$

3. Let's prove the the operator $e^{i\hat{p}\xi/\hbar}$ is a *generator of translations* in real space. In particular show that

$$\langle x | e^{i\hat{p}\xi/\hbar} | \psi \rangle = \psi(x + \xi),$$

where $\langle x|\psi\rangle = \psi(x)$ is the real-space representation (i.e., the wave function) of the state $|\psi\rangle$. You may find it helpful to expand the exponentiated operator as a powerseries in ξ and then to re-sum the series. You can make use of the result $\langle x|\hat{p}|\psi\rangle = -i\hbar(d/dx)\langle x|\psi\rangle = -i\hbar\psi'(x)$.

$$\begin{aligned}
\langle x | e^{i\hat{p}\xi/\hbar} | \psi \rangle &= \sum_{n=0}^{\infty} \frac{(i\xi/\hbar)^n}{n!} \langle x | \hat{p}^n | \psi \rangle \\
&= \sum_{n=0}^{\infty} \frac{(i\xi/\hbar)^n}{n!} (-i\hbar)^n \frac{d^n \psi(x)}{dx^n} \\
&= \sum_{n=0}^{\infty} \frac{\xi^n}{n!} \frac{d^n \psi(x)}{dx^n} = \psi(x + \xi)
\end{aligned}$$