Physics 711: Assignment 1 Solutions

1. A linear vector space is spanned by three orthonomal vectors, denoted by the kets $|a\rangle$, $|b\rangle$, and $|c\rangle$. A state $|\psi\rangle$ is constructed as the linear combination $|\psi\rangle = \alpha|a\rangle + \beta|b\rangle + \gamma|c\rangle$, where $\alpha, \beta, \gamma \in \mathbb{C}$. The corresponding state in the dual space is $\langle\psi| = \alpha^*\langle a| + \beta^*\langle b| + \gamma^*\langle c|$.

   (a) Show that the inner product (or "overlap") is

   $$\langle\psi|\psi\rangle = |\alpha|^2 + |\beta|^2 + |\gamma|^2$$

   and that

   $$|\tilde{\psi}\rangle = \frac{|\psi\rangle}{\sqrt{\langle\psi|\psi\rangle}} = \frac{\alpha|a\rangle + \beta|b\rangle + \gamma|c\rangle}{\sqrt{|\alpha|^2 + |\beta|^2 + |\gamma|^2}}.$$

   is a properly normalized state.

   By orthonormality,

   $$\begin{aligned}\langle\psi|\psi\rangle &= \big(\alpha^*\langle a| + \beta^*\langle b| + \gamma^*\langle c|\big)\big(\alpha|a\rangle + \beta|b\rangle + \gamma|c\rangle\big) \\ &= \alpha^*\alpha\,\cancelto{1}{\langle a|a\rangle} + \alpha^*\beta\,\cancelto{0}{\langle a|b\rangle} + \alpha^*\gamma\,\cancelto{0}{\langle a|c\rangle} \\ &\quad \beta^*\alpha\,\cancelto{0}{\langle b|a\rangle} + \beta^*\beta\,\cancelto{1}{\langle b|b\rangle} + \beta^*\gamma\,\cancelto{0}{\langle b|c\rangle} \\ &\quad \gamma^*\alpha\,\cancelto{0}{\langle c|a\rangle} + \gamma^*\beta\,\cancelto{0}{\langle c|b\rangle} + \gamma^*\gamma\,\cancelto{1}{\langle c|c\rangle} = |\alpha|^2 + |\beta|^2 + |\gamma|^2.\end{aligned}$$

   The square root of this factor can be used to normalize the state:

   $$\langle\tilde{\psi}|\tilde{\psi}\rangle = \frac{\langle\psi|}{\sqrt{\langle\psi|\psi\rangle}}\frac{|\psi\rangle}{\sqrt{\langle\psi|\psi\rangle}} = \frac{\langle\psi|\psi\rangle}{\langle\psi|\psi\rangle} = 1.$$

   (b) Suppose that the system is prepared in the state $|\psi\rangle$ and we perform an experiment to determine if the system is found in microstate a, b, or c (mutually exclusive after a measurement). What is the classical probability of finding the system in microstate b? *Hint:* You can understand this as the expectation value of the filtering operator $\hat{P}_b = |b\rangle\langle b|$ with respect to $|\psi\rangle$.

   Note that an *expectation value* must always be properly normalized; this is necessary for it to be interpreted as a classical probability or a weighted average over measurement outcomes:

   $$\begin{aligned}\text{Prob(b)} &= \frac{\langle\psi|\hat{P}_b|\psi\rangle}{\langle\psi|\psi\rangle} = \langle\tilde{\psi}|\hat{P}_b|\tilde{\psi}\rangle \\ &= \frac{\big(\alpha^*\langle a| + \beta^*\langle b| + \gamma^*\langle c|\big)|b\rangle\langle b|\big(\alpha|a\rangle + \beta|b\rangle + \gamma|c\rangle\big)}{|\alpha|^2 + |\beta|^2 + |\gamma|^2} \\ &= \frac{\big(\alpha^*\cancelto{0}{\langle a|b\rangle} + \beta^*\cancelto{1}{\langle b|b\rangle} + \gamma^*\cancelto{0}{\langle c|b\rangle}\big)\big(\alpha\cancelto{0}{\langle b|a\rangle} + \beta\cancelto{1}{\langle b|b\rangle} + \gamma\cancelto{0}{\langle b|c\rangle}\big)}{|\alpha|^2 + |\beta|^2 + |\gamma|^2} \\ &= \frac{\beta^*\beta}{|\alpha|^2 + |\beta|^2 + |\gamma|^2} = \frac{|\beta|^2}{|\alpha|^2 + |\beta|^2 + |\gamma|^2}.\end{aligned}$$

   (c) Prove that $\hat{\mathbb{1}} = |a\rangle\langle a| + |b\rangle\langle b| + |c\rangle\langle c|$ is the identity operator for the vector space.

   Since $\{|a\rangle, |b\rangle, |c\rangle\}$ serves as a complete, orthonormal basis, it suffices to show that $\hat{\mathbb{1}}|a\rangle = |a\rangle$, $\hat{\mathbb{1}}|b\rangle = |b\rangle$, and $\hat{\mathbb{1}}|c\rangle = |c\rangle$. For instance,

   $$\hat{\mathbb{1}}|a\rangle = \big(|a\rangle\langle a| + |b\rangle\langle b| + |c\rangle\langle c|\big)|a\rangle = \cancelto{1}{\langle a|a\rangle}|a\rangle + \cancelto{0}{\langle b|a\rangle}|b\rangle + \cancelto{0}{\langle c|a\rangle}|c\rangle = |a\rangle.$$

(d) For the cyclic permutation operator $\hat{T} = |b\rangle\langle a| + |c\rangle\langle b| + |a\rangle\langle c|$, compute the expectation value $\langle\tilde{\psi}|\hat{T}|\tilde{\psi}\rangle = \langle\psi|\hat{T}|\psi\rangle/\langle\psi|\psi\rangle$. You should be able to show that

$$\langle\tilde{\psi}|\hat{T}|\tilde{\psi}\rangle = \frac{\alpha^*\gamma + \beta^*\alpha + \gamma^*\beta}{|\alpha|^2 + |\beta|^2 + |\gamma|^2}.$$

Since, $\langle i|j\rangle = \delta_{i,j}$, most terms vanish. The terms that survive are marked with a contraction:

$$\frac{(\alpha^*\langle a| + \beta^*\langle b| + \gamma^*\langle c|)(|b\rangle\langle a| + |c\rangle\langle b| + |a\rangle\langle c|)(\alpha|a\rangle + \beta|b\rangle + \gamma|c\rangle)}{|\alpha|^2 + |\beta|^2 + |\gamma|^2} = \frac{\alpha^*\gamma + \beta^*\alpha + \gamma^*\beta}{|\alpha|^2 + |\beta|^2 + |\gamma|^2}.$$

(e) Find the eigenstates and corresponding eigenvalues of $\hat{T}$. Proceed by computing the matrix elements in the *abc* basis:

$$T = \begin{pmatrix} \langle a|\hat{T}|a\rangle & \langle a|\hat{T}|b\rangle & \langle a|\hat{T}|c\rangle \\ \langle b|\hat{T}|a\rangle & \langle b|\hat{T}|b\rangle & \langle b|\hat{T}|c\rangle \\ \langle c|\hat{T}|a\rangle & \langle c|\hat{T}|b\rangle & \langle c|\hat{T}|c\rangle \end{pmatrix}$$

$$T = \begin{pmatrix} \langle a|(|b\rangle\langle a| + |c\rangle\langle b| + |a\rangle\langle c|)|a\rangle & \langle a|(|b\rangle\langle a| + |c\rangle\langle b| + |a\rangle\langle c|)|b\rangle & \langle a|(|b\rangle\langle a| + |c\rangle\langle b| + |a\rangle\langle c|)|c\rangle \\ \langle b|(|b\rangle\langle a| + |c\rangle\langle b| + |a\rangle\langle c|)|a\rangle & \langle b|(|b\rangle\langle a| + |c\rangle\langle b| + |a\rangle\langle c|)|b\rangle & \langle b|(|b\rangle\langle a| + |c\rangle\langle b| + |a\rangle\langle c|)|c\rangle \\ \langle c|(|b\rangle\langle a| + |c\rangle\langle b| + |a\rangle\langle c|)|a\rangle & \langle c|(|b\rangle\langle a| + |c\rangle\langle b| + |a\rangle\langle c|)|b\rangle & \langle c|(|b\rangle\langle a| + |c\rangle\langle b| + |a\rangle\langle c|)|c\rangle \end{pmatrix}$$

$$= \begin{pmatrix} \langle a|b\rangle\langle a|a\rangle + \langle a|c\rangle\langle b|a\rangle + \langle a|a\rangle\langle c|a\rangle & \langle a|b\rangle\langle a|b\rangle + \langle a|c\rangle\langle b|b\rangle + \langle a|a\rangle\langle c|b\rangle & \cdots \\ \cancelto{1}{\langle b|b\rangle\langle a|a\rangle} + \cancelto{0}{\langle b|c\rangle\langle b|a\rangle} + \cancelto{0}{\langle b|a\rangle\langle c|a\rangle} & \ddots & \\ \vdots & & \end{pmatrix}$$

$$= \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$$

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T = {{0, 0, 1}, {1, 0, 0}, {0, 1, 0}}
{Evals, Evecs} = Eigensystem[T]
Evecs = Normalize /@ Evecs
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There are three eigensolutions of the form $Tv = \lambda v$ with

$$\lambda_1 = 1, \lambda_2 = \frac{1}{2}(-1 + I\sqrt{3}), \lambda_3 = \frac{1}{2}(-1 - i\sqrt{3})$$

and

$$v_1 = \begin{pmatrix} 1/\sqrt{3} \\ 1/\sqrt{3} \\ 1/\sqrt{3} \end{pmatrix}, \quad v_2 = \begin{pmatrix} (-1 + i\sqrt{3})/(2\sqrt{3}) \\ (-1 - i\sqrt{3})/(2\sqrt{3}) \\ i/\sqrt{3} \end{pmatrix}, \quad v_3 = \begin{pmatrix} (-1 - i\sqrt{3})/(2\sqrt{3}) \\ (-1 + i\sqrt{3})/(2\sqrt{3}) \\ i/\sqrt{3} \end{pmatrix}$$

(f) Find the unitary transformation matrix V such that

$$V^\dagger T V = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1/2 + i\sqrt{3}/2 & 0 \\ 0 & 0 & -1/2 - i\sqrt{3}/2 \end{pmatrix}$$

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V = Transpose[Evecs]
Expand[Transpose[Conjugate[V]].T.V]
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(g) Prove that $\hat{T}^{-1} = \hat{T}^\dagger$ is unitary and that $\hat{T}^3 = \hat{\mathbb{1}}$.

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Inverse[T] == Transpose[Conjugate[T]]
T.T.T == IdentityMatrix[3]
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2. Consider the 4×4 matrix

$$h = \begin{pmatrix} 1 & 2 & 3 & 4 \\ 5 & 6 & 7 & 8 \\ 9 & 10 & 11 & 12 \\ 13 & 14 & 15 & 16 \end{pmatrix}.$$

Suppose that a quantum system has the Hamiltonian matrix $H = h + h^\dagger$.

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h = ArrayReshape[Range[16], {4, 4}]
H = h + Transpose[h]
H // MatrixForm
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(a) Express the matrix elements $h_{i,j}$ as a function of the rows $i = 1, 2, 3, 4$ and columns $j = 1, 2, 3, 4$. Find an analogous index-notation expression for $H_{i,j}$.

The matrix elements of h increase by one from column to column, moving left to right along each row. They increase by four from row to row, moving top to bottom along each column. This can be accommodated with a linear combination of i and j, the former having stride 4 and offset by 1: $h_{i,j} = 4(i-1) + j$. This implies that

$$H_{i,j} = h_{i,j} + h^*_{j,i} = 4(i-1) + j + 4(j-1) + i = 4(i+j-2) + i + j = 5(i+j) - 8.$$

In tableau form, this is

$$H = \begin{pmatrix} 2 & 7 & 12 & 17 \\ 7 & 12 & 17 & 22 \\ 12 & 17 & 22 & 27 \\ 17 & 22 & 27 & 32 \end{pmatrix}.$$

(b) Consider the operator

$$\hat{H} = \sum_{i=1}^{4} \sum_{j=1}^{4} |i\rangle H_{i,j} \langle j|$$

that acts on vectors in the linear vector space of kets. First verify that $H_{i,j} = \langle i|\hat{H}|j\rangle$. Then prove that two applications of the operator are equivalent to

$$\hat{H}^2 = \sum_{i=1}^{4} \sum_{j=1}^{4} |i\rangle \left(\sum_{k=1}^{4} H_{i,k} H_{k,j} \right) \langle j|.$$

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H.H == Table[Sum[H[[i,k]]*H[[k,j]],{k,1,4}],{i,1,4},{j,1,4}]
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First we confirm the matrix elements. Be careful to choose internal dummy indices for the summations that are distinct from the i and j labels in the outer bra and ket of the matrix element:

$$\langle i|\hat{H}|j\rangle = \langle i| \left(\sum_{k=1}^{4} \sum_{l=1}^{4} |k\rangle H_{k,l} \langle l| \right) |j\rangle = \sum_{k=1}^{4} \sum_{l=1}^{4} \langle i|k\rangle H_{k,l} \langle l|j\rangle = \sum_{k=1}^{4} \sum_{l=1}^{4} \delta_{i,k} H_{k,l} \delta_{l,j} = H_{i,j}.$$

Then we compute the square of the Hamiltonian:

$$\hat{H}^2 = \sum_{i=1}^{4}\sum_{j=1}^{4}|i\rangle H_{i,j}\langle j|\sum_{k=1}^{4}\sum_{l=1}^{4}|k\rangle H_{k,l}\langle l| = \sum_{i=1}^{4}\sum_{j=1}^{4}\sum_{k=1}^{4}\sum_{l=1}^{4}|i\rangle H_{i,j}\langle j|k\rangle H_{k,l}\langle l|$$
$$= \sum_{i=1}^{4}\sum_{j=1}^{4}\sum_{k=1}^{4}\sum_{l=1}^{4}|i\rangle H_{i,j}\delta_{j,k}H_{k,l}\langle l| = \sum_{i=1}^{4}\sum_{j=1}^{4}\sum_{l=1}^{4}|i\rangle H_{i,j}H_{j,l}\langle l|$$
$$= \sum_{i=1}^{4}\sum_{j=1}^{4}\sum_{l=1}^{4}|i\rangle H_{i,j}H_{j,l}\langle l| = \sum_{i=1}^{4}\sum_{j=1}^{4}|i\rangle\left(\sum_{k=1}^{4} H_{i,k}H_{k,j}\right)\langle j|.$$

(c) Solve for the energy eigenstates and corresponding energy eigenvalues.

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{Evals, Evecs} = Eigensystem[H]
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Argue that $|\phi_0\rangle = 2|1\rangle - 3|2\rangle + |4\rangle$ and $|\phi_0'\rangle = |1\rangle - 2|2\rangle + |3\rangle$ are states of zero energy. Show explicitly that $\hat{H}$ annihilates both kets.

Here is the calculation is the matrix style:

$$H\phi_0 = \begin{pmatrix} 2 & 7 & 12 & 17 \\ 7 & 12 & 17 & 22 \\ 12 & 17 & 22 & 27 \\ 17 & 22 & 27 & 32 \end{pmatrix}\begin{pmatrix} 2 \\ -3 \\ 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 2(2)+7(-3)+12(0)+17(1) \\ 7(2)+12(-3)+17(0)+22(1) \\ 12(2)+17(-3)+22(0)+27(1) \\ 17(2)+22(-3)+27(0)+32(1) \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} = (0)\phi_0,$$
$$H\phi_0' = \begin{pmatrix} 2 & 7 & 12 & 17 \\ 7 & 12 & 17 & 22 \\ 12 & 17 & 22 & 27 \\ 17 & 22 & 27 & 32 \end{pmatrix}\begin{pmatrix} 1 \\ -2 \\ 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 2(1)+7(-2)+12(1)+17(0) \\ 7(1)+12(-2)+17(1)+22(0) \\ 12(1)+17(-2)+22(1)+27(0) \\ 17(1)+22(-2)+27(1)+32(0) \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} = (0)\phi_0'.$$

In Dirac notation, we might write

$$\hat{H}|\phi_0\rangle = \sum_{i=1}^{4}\sum_{j=1}^{4}|i\rangle H_{i,j}\langle j|\psi\rangle = \sum_{i=1}^{4}\sum_{j=1}^{4}|i\rangle[5(i+j)-8]\langle j|\psi\rangle$$
$$= \sum_{i=1}^{4}\sum_{j=1}^{4}[5(i+j)-8](2\delta_{j,1} - 3\delta_{j,2} + \delta_{j,4})|i\rangle$$
$$= \sum_{i=1}^{4}(2[5(i+1)-8] - 3[5(i+2)-8] + [5(i+4)-8])|i\rangle$$
$$= \sum_{i=1}^{4}[(10-15+5)i - 16 + 24 - 8]|i\rangle = 0.$$

(d) For the operator $\hat{N}$ obeying $\hat{N}|n\rangle = n|n\rangle$, compute the expectation values of $\hat{N}$ with respect to $|\phi_0\rangle$ and $|\phi_0'\rangle$. As a check, note that these have to take on a value between 1 and 4.

$$\frac{\langle\phi_0|\hat{N}|\phi_0\rangle}{\langle\phi_0|\phi_0\rangle} = \frac{(2)(2)\langle 1|\hat{N}|1\rangle + (-3)(-3)\langle 2|\hat{N}|2\rangle + \langle 4|\hat{N}|4\rangle}{4+9+1}$$
$$= \frac{(4)(1)+(9)(2)+(4)(1)}{4+9+1} = \frac{26}{14} = \frac{13}{7} \doteq 1.86$$
$$\frac{\langle\phi_0'|\hat{N}|\phi_0'\rangle}{\langle\phi_0'|\phi_0'\rangle} = \frac{(1)(1)\langle 1|\hat{N}|1\rangle + (-2)(-2)\langle 2|\hat{N}|2\rangle + (1)(1)\langle 3|\hat{N}|3\rangle}{1+4+1}$$
$$= \frac{(1)(1)+(4)(2)+(1)(3)}{1+4+1} = \frac{12}{6} = 2$$