

HOMEWORK ASSIGNMENT 1

PHYS851 Quantum Mechanics I, Fall 2009

- [10 pts] What is the relationship between $\langle\psi|\phi\rangle$ and $\langle\phi|\psi\rangle$? What is the relationship between the matrix elements of \hat{M}^\dagger and the matrix elements of \hat{M} . Assume that $H^\dagger = H$ what is $\langle n|H^\dagger|m\rangle$ in terms of $\langle m|H|n\rangle$?

$$\langle\psi|\phi\rangle = \langle\phi|\psi\rangle^*$$

$$\langle m|\hat{M}^\dagger|n\rangle = \langle n|\hat{M}|m\rangle^*$$

$$\langle n|\hat{H}^\dagger|m\rangle = \langle n|\hat{H}|m\rangle^\dagger$$

Also, because $H^\dagger = H$, we have $\langle n|H^\dagger|m\rangle = \langle n|H|m\rangle$.

Putting these together gives $\langle n|H|m\rangle = \langle m|H|n\rangle$, which is an equivalent definition of Hermiticity

This says firstly, the diagonal elements of a hermitian operator must be real in every possible basis, and secondly, the off-diagonal elements come in complex-conjugate pairs, such that $H_{nm} = H_{mn}^*$.

Thus we can tell just by looking at it whether a matrix is Hermitian or not.

- Use the matrix representation and summation notation to prove that $(AB)^\dagger = B^\dagger A^\dagger$, where A and B are both operators. Use summation notation to expand $\langle\phi|AB|\psi\rangle^\dagger$ in terms of the constituent matrix elements and vector components?

step 1: by definition, we have $(\hat{A}\hat{B})^\dagger = (\hat{A}^*\hat{B}^*)^T$

step 2: by the standard rules of matrix algebra, we have $(A^*B^*)_{mn}^T = (A^*B^*)_{nm} = \sum_k A_{nk}^* B_{km}^* = \sum_k (B^*)_{mk}^T (A^*)_{kn}^T = \sum_k B_{mk}^\dagger A_{kn}^\dagger = (B^\dagger A^\dagger)_{mn}$

- Consider the discrete orthonormal basis $\{|m\rangle\}$, $m = 1, 2, 3, \dots, M$ that spans an M -dimensional Hilbert space, \mathcal{H}_M .

- Show that the identity operator, $I = \sum_m |m\rangle\langle m|$, satisfies $I^2 = I$.

$$I^2 = (\sum_m |m\rangle\langle m|)(\sum_n |n\rangle\langle n|) = \sum_{mn} |m\rangle\langle m|n\rangle\langle n| = \sum_{mn} mn|m\rangle\delta_{m,n}\langle n| = \sum_m |m\rangle\langle m| = I$$

- Form a new projector, I_{13} , by removing the state $|3\rangle$, i.e. $I_{13} := \sum_{m \neq 3} |m\rangle\langle m|$. Does $I_{13}^2 = I_{13}$? Is I_{13} also the identity operator?

$I_{13}^2 = \sum_{m,n \neq 3} |m\rangle\langle m|n\rangle\langle n| = \sum_{m,n \neq 3} |m\rangle\delta_{m,n}\langle n| = \sum_{m \neq 3} |m\rangle\langle m| = I_{13}$, so **yes** to first question. Based on their definitions, I_{13} is clearly not equivalent to I , so **no** on second question?

- Compute the trace of I_{13} and compare it to the trace of I .

$$\text{Tr}\{I_{13}\} = \sum_{\substack{m=1 \\ m \neq 3}}^M \langle m|m\rangle = \sum_{\substack{m=1 \\ m \neq 3}}^M 1 = M - 1$$

$$\text{Tr}\{I\} = \sum_{m=1}^M \langle m|m\rangle = \sum_{m=1}^M 1 = M$$

- Based on the previous results, formulate the two necessary and sufficient conditions for an operator to be the identity operator in the space \mathcal{H}_M .

We should have both $I^2 = I$, and $\text{Tr}\{I\} = M$, where M is the dimensionality of the Hilbert space.

An equivalent definition (more standard) is $I|\psi\rangle = |\psi\rangle$, $\forall |\psi\rangle \in \mathcal{H}$

- Now consider the continuous basis $\{|x\rangle\}$, whose elements are orthogonal, but delta-normalized, i.e. $\langle x|x'\rangle = \delta(x-x')$. Show that in this case, the projector $I = \int dx |x\rangle\langle x|$ also satisfies $I^2 = I$. $I^2 = \int dx dx' |x\rangle\langle x|x'\rangle\langle x'| = \int dx dx' |x\rangle\delta(x-x')\langle x'| = \int dx |x\rangle\langle x| = I$.

4. Start from the equation $\frac{d}{dt}|\psi\rangle = H|\psi\rangle$. Hit it from the left with $\langle n|$ and insert the projector $\hat{I} = \sum_n |n\rangle\langle n|$ to derive the equation of motion for $c_n = \langle n|\psi(t)\rangle$? (Hint: be careful not to use the same symbol for two different things)

$$\frac{d}{dt}|\psi\rangle = H|\psi\rangle$$

$$\frac{d}{dt}\langle n|\psi\rangle = \langle n|H|\psi\rangle$$

$$\frac{d}{dt}\langle n|\psi\rangle = \sum_m \langle n|H|m\rangle\langle m|\psi\rangle$$

$$\frac{d}{dt}c_n(t) = \sum_m H_{n,m}c_m(t).$$

5. Suppose you have a set of d linearly independent vectors; $|e_1\rangle, |e_2\rangle, \dots, |e_d\rangle$; in a d -dimensional space, but they are not orthonormal. The **Gram-Schmidt procedure** is a systematic algorithm for generating from it an orthonormal basis: $|e'_1\rangle, |e'_2\rangle, \dots, |e'_d\rangle$. The procedure is as follows:

i Normalize the first vector by dividing by its norm: $|e'_1\rangle = \frac{|e_1\rangle}{\|e_1\|}$

ii Find the projection of the second operator along the first and subtract it off: $|e''_2\rangle = |e_2\rangle - |e'_1\rangle\langle e'_1|e_2\rangle$ then normalize the resulting vector: $|e'_2\rangle = \frac{|e''_2\rangle}{\|e''_2\|}$

iii Then subtract from $|e_3\rangle$ its projections along $|e'_1\rangle$ and $|e'_2\rangle$ and form $|e'_3\rangle$ by normalizing this vector, and so on for the remaining vectors

- (a) For the case $d = 3$ explicitly verify that the new unit vectors are orthogonal

In addition to the above expressions we need $|e'_3\rangle = \frac{|e_3\rangle}{\|e_3\|}$, where $|e''_3\rangle = |e_3\rangle - |e'_1\rangle\langle e'_1|e_3\rangle - |e'_2\rangle\langle e'_2|e_3\rangle$.

$$\langle e'_1|e'_2\rangle \propto \langle e_1|e_2\rangle = \langle e_1|e_2\rangle - \frac{\langle e_1|e_1\rangle\langle e_1|e_2\rangle}{\|e_1\|^2} = \langle e_1|e_2\rangle - \frac{\langle e_1|e_1\rangle\langle e_1|e_2\rangle}{\langle e_1|e_1\rangle} = 0.$$

$$\langle e'_1|e'_3\rangle \propto \langle e_1|e_3\rangle = \langle e_1|e_3\rangle - \langle e_1|e'_1\rangle\langle e'_1|e_3\rangle - \langle e_1|e'_2\rangle\langle e'_2|e_3\rangle = -\langle e_1|e'_2\rangle\langle e'_2|e_3\rangle \propto \langle e'_1|e'_2\rangle = 0.$$

$$\begin{aligned} \langle e'_2|e'_3\rangle &\propto \langle e''_2|e''_3\rangle = (\langle e_2| - \langle e_2|e'_1\rangle\langle e'_1|)(\langle e_3| - \langle e_3|e'_1\rangle\langle e'_1| - \langle e_3|e'_2\rangle\langle e'_2|) \\ &= \langle e_2|e_3\rangle - \langle e_2|e'_1\rangle\langle e'_1|e_3\rangle - \langle e_2|e'_2\rangle\langle e'_2|e_3\rangle - \langle e_2|e'_1\rangle\langle e'_1|e_3\rangle + \langle e_2|e'_1\rangle\langle e'_1|e'_1\rangle\langle e'_1|e_3\rangle + \langle e_2|e'_1\rangle\langle e'_1|e'_2\rangle\langle e'_2|e_3\rangle \\ &= -\langle e_2|e'_2\rangle\langle e'_2|e_3\rangle \propto \langle e_2|e''_2\rangle\langle e''_2|e_3\rangle = \langle e_2|e''_2\rangle(\langle e_2|e_3\rangle - \langle e_2|e'_1\rangle\langle e'_1|e_3\rangle) = 0. \end{aligned}$$

- (b) Use the Gram-Schmidt procedure to generate an orthonormal basis from the vectors $|e_1\rangle = (1+i)|1\rangle + |2\rangle + i|3\rangle$, $|e_2\rangle = i|1\rangle + 3|2\rangle + |3\rangle$, and $|e_3\rangle = 28|2\rangle$. Please follow the procedure exactly as described above, i.e. first compute $|e'_1\rangle$ using $|e_1\rangle$ and so on.

$$|e'_1\rangle = \frac{1+i}{2}\hat{x} + \frac{1}{2}\hat{y} + \frac{i}{2}\hat{z}.$$

$$|e'_2\rangle = -\frac{1}{\sqrt{7}}\hat{x} + \frac{2}{\sqrt{7}}\hat{y} + \frac{1-i}{\sqrt{7}}\hat{z}.$$

$$|e'_3\rangle = \frac{1-7i}{2\sqrt{35}}\hat{x} + \frac{\sqrt{5}}{2\sqrt{7}}\hat{y} - \frac{8-i}{2\sqrt{35}}\hat{z}.$$

- (c) Use the Gram-Schmidt procedure to generate an orthonormal basis from the vectors $|f_1\rangle, |f_2\rangle$, and $|f_3\rangle$, defined via $\langle x|f_1\rangle = e^{-x^2/2}$, $\langle x|f_2\rangle = xe^{-x^2/2}$, and $\langle x|f_3\rangle = x^2e^{-x^2/2}$. As your answer, give expressions for $\langle x|f'_1\rangle$, $\langle x|f'_2\rangle$, and $\langle x|f'_3\rangle$.

$$|f'_1\rangle = \frac{|f_1\rangle}{\sqrt{\langle f_1|f_1\rangle}}$$

$$\langle f_1|f_1\rangle = \int_{-\infty}^{\infty} dx \langle f_1|x\rangle\langle x|f_1\rangle = \int_{-\infty}^{\infty} dx e^{-x^2} = \sqrt{\pi} \text{ so that } |f'_1\rangle = \pi^{-1/4}|f_1\rangle.$$

$$|f''_2\rangle = |f_2\rangle - |f'_1\rangle\langle f'_1|f_2\rangle$$

$$\langle f'_1|f_2\rangle = \pi^{-1/4} \int dx \langle f_1|x\rangle\langle x|f_2\rangle = \pi^{-1/4} \int dx xe^{-x^2} = 0, \text{ so that } |f''_2\rangle = |f_2\rangle.$$

$$|f'_2\rangle = \frac{|f''_2\rangle}{\sqrt{\langle f''_2|f''_2\rangle}}$$

$$\langle f''_2|f''_2\rangle = \int dx \langle f_2|x\rangle\langle x|f_2\rangle = \int dx x^2e^{-x^2} = \frac{\sqrt{\pi}}{2}, \text{ so that } |f'_2\rangle = \sqrt{2}\pi^{-1/4}|f_2\rangle$$

$$|f''_3\rangle = |f_3\rangle - |f'_1\rangle\langle f'_1|f_3\rangle - |f'_2\rangle\langle f'_2|f_3\rangle$$

$$\langle f'_1 | f_3 \rangle = \pi^{-1/4} \int dx x^2 e^{-x^2} = \frac{\pi^{1/4}}{2}$$

$$\langle f'_2 | f_3 \rangle = 0 \text{ by parity.}$$

$$|f_3''\rangle = |f_3\rangle - \frac{1}{2}|f_1\rangle$$

$$\langle f_3'' | f_3'' \rangle = \langle f_3 | f_3 \rangle - \frac{1}{2}\langle f_1 | f_3 \rangle - \frac{1}{2}\langle f_3 | f_1 \rangle + \frac{1}{4}\langle f_1 | f_1 \rangle = \frac{\pi^{1/2}}{2}, \text{ so that } |f_3'\rangle = \frac{1}{\sqrt{2\pi^{1/2}}}(2|f_3\rangle - |f_1\rangle)$$

$$\langle x | f_1' \rangle = \pi^{-1/4} e^{-x^2/2}$$

$$\langle x | f_2' \rangle = \sqrt{2}\pi^{-1/4} x e^{-x^2/2}$$

$$\langle x | f_3' \rangle = \frac{1}{\sqrt{2\pi^{1/2}}}(2x^2 - 1)e^{-x^2/2}$$

6. Two operators, A and B , can be represented by the matrices $A = \begin{pmatrix} -1 & i \\ 2i & 2 \end{pmatrix}$ and $B = \begin{pmatrix} 2 & -i \\ i & 2 \end{pmatrix}$.

Use matrix algebra to compute the elements of (a) $C = A + B$, (b) $C = AB$, (c) $C = [A, B] := AB - BA$, (d) A^\dagger and B^\dagger , (e) B^{-1} . Verify that $BB^{-1} = 1$. (f) Does A have an inverse?

$$(a) C = A + B = \begin{pmatrix} 1 & 0 \\ 3i & 4 \end{pmatrix}.$$

$$(b) C = AB = \begin{pmatrix} -3 & 3i \\ 6i & 6 \end{pmatrix}.$$

$$(c) C = [A, B] = \begin{pmatrix} -3 & 3i \\ 3i & 3 \end{pmatrix}.$$

$$(d) A^\dagger = \begin{pmatrix} -1 & -2i \\ -i & 2 \end{pmatrix} \quad B^\dagger = B$$

$$(e) B^{-1} = \frac{1}{3} \begin{pmatrix} 2 & i \\ -i & 2 \end{pmatrix} \quad B^{-1}B = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}.$$

$$(f) \text{ no because } \det[A] = -1 \cdot 2 - 2i \cdot i = -2 + 2 = 0$$

7. [20 pts] Let the set of states $|k\rangle$ be an alternate basis for the space spanned by the states $|x\rangle$ where x and k are continuous variables on the intervals $-\infty < k < +\infty$ and $-\infty < x < +\infty$. The inner product is defined as $\langle x | k \rangle = \frac{1}{\sqrt{2\pi}} e^{ikx}$.

- (a) What is $\langle k | x \rangle$?

$$\langle k | x \rangle = \langle x | k \rangle^* = \frac{1}{\sqrt{2\pi}} e^{-ikx}.$$

- (b) Use the relation $\langle x | x' \rangle = \delta(x - x')$ to compute the integral $\int_{-\infty}^{\infty} dx e^{ikx}$.

$$\int_{-\infty}^{\infty} dx e^{i(k-k')x} = 2\pi \int dx \langle k' | x \rangle \langle x | k \rangle = 2\pi \langle k' | k \rangle = 2\pi \delta(k' - k).$$

- (c) Consider the vector $|f\rangle$, defined via $\langle x | f \rangle = \frac{1}{\sqrt{\pi\sigma^2}} e^{-(x-x_0)^2/2\sigma^2}$. What is the norm $\|f\|$?

$$\|f\|^2 = \langle f | f \rangle = \int dx \langle f | x \rangle \langle x | f \rangle = \frac{1}{\sqrt{\pi\sigma^2}} \int_{-\infty}^{\infty} dx e^{-(x-x_0)^2/\sigma^2} = 1$$

- (d) What is the representation of $|f\rangle$ in the k -basis, i.e. $\langle k | f \rangle$? Hint: start with the thing you want, in this case $\langle k | f \rangle$, and insert the projector onto the basis in which $|f\rangle$ is known.

$$\langle k | f \rangle = \int dx \langle k | x \rangle \langle x | f \rangle = \frac{1}{\sqrt{4\pi^3\sigma^2}} \int_{-\infty}^{\infty} dx e^{-ikx} e^{-(x-x_0)^2/2\sigma^2} = \sqrt{\frac{\sigma^2}{\pi}} e^{-ikx_0} e^{-k^2\sigma^2/2}$$