HOMEWORK ASSIGNMENT 1

PHYS851 Quantum Mechanics I, Fall 2009

1. [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.

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

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

   (a) Show that the identity operator, $I = \sum_m |m\rangle\langle m|$, satisfies $I^2 = I$.
   $I^2 = (\sum_m |m\rangle\langle m|)(\sum_n |n\rangle\langle n|) = \sum_{mn} |m\rangle\langle m|n\rangle\langle n| = \sum mn|m\rangle\delta_{m,n}\langle n| = \sum_m |m\rangle\langle m| = I$

   (b) Form a new projector, $I_{!3}$, by removing the state $|3\rangle$, i.e. $I_{!3} := \sum_{m\neq 3} |m\rangle\langle m|$. Does ${I_{!3}}^2 = I_{!3}$? Is $I_{!3}$ also the identity operator?
   $I_{!3}^2 = \sum_{m,n\neq 3} |m\rangle\langle m|n\rangle\langle n| = \sum_{m,n\neq 3} |m\rangle\delta_{m,n}\langle n| = \sum_{m\neq 3} |m\rangle\langle m| = I_{!3}$, so **yes** to first question. Based on their definitions, $I_{!3}$ is clearly not equivalent to I, so **no** on second question?

   (c) Compute the trace of $I_{!3}$ and compare it to the trace of I.
   $$\mathrm{Tr}\{I_{!3}\} = \sum_{\substack{m=1\\ m\neq 3}}^{M} \langle m|m\rangle = \sum_{\substack{m=1\\ m\neq 3}}^{M} 1 = M-1$$
   $$\mathrm{Tr}\{I\} = \sum_{m=1}^{M} \langle m|m\rangle = \sum_{m=1}^{M} 1 = M$$

   (d) 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 $\mathrm{Tr}\{I\} = M$, where M is the dimensionality of the Hilbert space.
   An equivalent definition (more standard) is $I|\psi\rangle = |\psi\rangle$, $\forall\ |\psi\rangle \in \mathcal{H}$

   (e) 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 $I^2 = I$.
   $I^2 = \int dxdx'\, |x\rangle\langle x|x'\rangle\langle x'| = \int dxdx'\, |x\rangle\delta(x - x')\langle x'| = \int dx\, |x\rangle\langle x| = I$.

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; $|e_1\rangle, |e_2\rangle, \ldots, |e_d\rangle$; 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: $|e_1'\rangle, |e_2'\rangle \ldots, |e_d'\rangle$. 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 $|e_3''\rangle = |e_3\rangle - |e_1'\rangle\langle e_1'|e_3\rangle - |e_2'\rangle\langle e_2'|e_3\rangle$.
   $\langle e_1'|e_2'\rangle \propto \langle e_1|e_2''\rangle = \langle e_1|e_2\rangle - \langle e_1|e_1'\rangle\langle e_1'|e_2\rangle = \langle e_1|e_2\rangle - \frac{\langle e_1|e_1\rangle\langle e_1|e_2\rangle}{||e_1||^2} = \langle e_1|e_2\rangle - \frac{\langle e_1|e_1\rangle\langle e_1|e_2\rangle}{\langle e_1|e_1\rangle} = 0.$
   $\langle e_1'|e_3'\rangle \propto \langle e_1|e_3''\rangle = \langle e_1|e_3\rangle - \langle e_1|e_1'\rangle\langle e_1'|e_3\rangle - \langle e_1|e_2'\rangle\langle e_2'|e_3\rangle = -\langle e_1|e_2'\rangle\langle e_2'|e_3\rangle \propto \langle e_1'|e_2'\rangle = 0.$
   $\langle e_2'|e_3'\rangle \propto \langle e_2''|e_3''\rangle = (\langle e_2| - \langle e_2|e_1'\rangle\langle e_1'|)(|e_3\rangle - |e_1'\rangle\langle e_1'|e_3\rangle - |e_2'\rangle\langle e_2'|e_3\rangle)$
   $= \langle e_2|e_3\rangle - \langle e_2|e_1'\rangle\langle e_1'|e_3\rangle - \langle e_2|e_2'\rangle\langle e_2'|e_3\rangle - \langle e_2|e_1'\rangle\langle e_1'|e_3\rangle + \langle e_2|e_1'\rangle\langle e_1'|e_1'\rangle\langle e_1'|e_3\rangle + \langle e_2|e_1'\rangle\langle e_1'|e_2'\rangle\langle e_2'|e_3\rangle$
   $= -\langle e_2|e_2'\rangle\langle e_2'|e_3\rangle \propto \langle e_2|e_2''\rangle\langle e_2''|e_3\rangle = \langle e_2|e_2''\rangle(\langle e_2|e_3\rangle - \langle e_2|e_1'\rangle\langle e_1'|e_3\rangle) = 0.$

   (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 $\langle x|f_,'\rangle$, $\langle x|f_2'\rangle$, and $\langle x|f_3'\rangle$.
   $|f_1'\rangle = \frac{|f_1\rangle}{\sqrt{\langle f_1|f_1\rangle}}$
   $\langle f_1|f_1\rangle = \int_{-\infty}^{\infty} dx\, \langle f_1|x\rangle\langle x|f_1\rangle = \int_{-\infty}^{\infty} dx\, e^{-x^2} = \sqrt{\pi}$ so that $|f_1'\rangle = \pi^{-1/4}|f_1\rangle$.
   $|f_2''\rangle = |f_2\rangle - |f_1'\rangle\langle f_1'|f_2\rangle$
   $\langle f_1'|f_2\rangle = \pi^{-1/4}\int dx\, \langle f_1|x\rangle\langle x|f_2\rangle = \pi^{-1/4}\int dx x e^{-x^2} = 0$, so that $|f_2''\rangle = |f_2\rangle$.
   $|f_2'\rangle = \frac{|f_2''\rangle}{\sqrt{\langle f_2''|f_2''\rangle}}$
   $\langle f_2''|f_2''\rangle = \int dx\, \langle f_2|x\rangle\langle x|f_2\rangle = \int dx\, x^2e^{-x^2} = \frac{\sqrt{\pi}}{2}$, so that $|f_2'\rangle = \sqrt{2}\pi^{-1/4}|f_2\rangle$
   $|f_3''\rangle = |f_3\rangle - |f_1'\rangle\langle f_1'|f_3\rangle - |f_2'\rangle\langle f_2'|f_3\rangle$

$\langle f_1'|f_3\rangle = \pi^{-1/4}\int dx\, x^2 e^{-x^2} = \frac{\pi^{1/4}}{2}$
$\langle f_2'|f_3\rangle = 0$ by parity.
$|f_3''\rangle = |f_3\rangle - \frac{1}{2}|f_1\rangle$
$\langle f_3''|f_3''\rangle = \langle f_3|f_3\rangle - \frac{1}{2}\langle f_1|f_3\rangle - \frac{1}{2}\langle f_3|f_1\rangle + \frac{1}{4}\langle f_1|f_1\rangle = \frac{\pi^{1/2}}{2}$, so that $|f_3'\rangle = \frac{1}{\sqrt{2\pi^{1/2}}}(2|f_3\rangle - |f_1\rangle)$
$\langle x|f_1'\rangle = \pi^{-1/4}e^{-x^2/2}$
$\langle x|f_2'\rangle = \sqrt{2}\pi^{-1/4}xe^{-x^2/2}$
$\langle x|f_3'\rangle = \frac{1}{\sqrt{2\pi^{1/2}}}(2x^2-1)e^{-x^2/2}$

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) $A^\dagger = \begin{pmatrix} -1 & -2i \\ -i & 2 \end{pmatrix}$ $\qquad B^\dagger = B$
(e) $B^{-1} = \frac{1}{3}\begin{pmatrix} 2 & i \\ -i & 2 \end{pmatrix}$ $\qquad B^{-1}B = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$.
(f) 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 $\langle x|f\rangle = \frac{1}{\sqrt[4]{\pi\sigma^2}}e^{-(x-x_0)^2/2\sigma^2}$. 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.
   $\langle k|f\rangle = \int dx\, \langle k|x\rangle\langle x|f\rangle = \frac{1}{\sqrt[4]{4\pi^3\sigma^2}}\int_{-\infty}^{\infty} dx\, e^{-ikx}e^{-(x-x_0)^2/2\sigma^2} = \sqrt[4]{\frac{\sigma^2}{\pi}}e^{-ikx_0}e^{-k^2\sigma^2/2}$