Chem 442: Homework for lecture L21

(only turn in **BOLD** assignment first lecture next week of classes; do <u>all</u> assignments)

1. In the previous lecture, Hilbert spaces were introduced with an example where you define the axes as $\varphi_1(x) = \cos x$ and $\varphi_2(x) = \sin x$. Then, according to the bracket (Dirac) notation for basis functions, what are $\frac{\partial}{\partial x}|1\rangle =$ and $\frac{\partial}{\partial x}|2\rangle =$?

2. By using the analogy between Dirac and conventional integral notation, prove that $\langle n|\psi\rangle = (\langle\psi|n\rangle)^*$. [Hint: write down the analogous integral expression, and then remember that $a^*b = (ab^*)^*$.]

3. **Turn in** Postulate 4 states that $P(A = a_n) = \left|\int_{-\infty}^{\infty} dx\ \varphi_n{}^*\psi\right|^2 = |\langle n|\psi\rangle|^2$, where the states $|n\rangle$ are the eigenfunctions of the operator A with eigenvalues a_n. Use the identity operator expressed in bracket notation and your result from problem (2) to prove that the average value of A, written as $\langle A\rangle$, is equal to $\langle\psi|A|\psi\rangle$. [Hint: remember $\langle A\rangle = \Sigma\ a_n\ P(A=a_n)$.]
   The average value is also called the "expectation value" in quantum mechanics.

Note: in the next problem, a tilde "~" denotes a matrix.

4. The technique of finding the eigenvalues and eigenvectors of an operator in matrix form is called "diagonalization". In this problem, you will diagonalize the matrix
   $$\widetilde{M} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}.$$
   The starting point is the equation $(\widetilde{M} - \tilde{\Lambda}) \cdot \mathbf{v} = 0$, where $\widetilde{M}$ is your non-diagonal matrix, $\tilde{\Lambda}$ is the corresponding diagonal eigenvalue matrix, obtained by $\tilde{\Lambda} = \lambda \tilde{I}$, with λ being any of the eigenvalues, and $\mathbf{v}$ is one of the eigenvectors, a column vector. In order to obtain a non-trivial solution, we need the condition $\det\left\|\widetilde{M} - \tilde{\Lambda}\right\| = 0$.

   a. Multiply out the determinant equation of the matrix $\widetilde{M} - \tilde{\Lambda}$, to get a quadratic equation for the two eigenvalues λ. Solve for λ. This gives you the 2 eigenvalues of the 2x2 matrix. [Hint: yes, eigenvalues can be complex numbers.]
   b. Plug each of these eigenvalues (one at a time) into the equation $(\widetilde{M} - \tilde{\Lambda}) \cdot \mathbf{v} = 0$, writing the vector $\mathbf{v}$ as a column vector
   $$\mathbf{v} = \begin{pmatrix} c_1 \\ c_2 \end{pmatrix},$$
   Note that you can solve for c_1 in terms of c_2 or *vice versa*, but not both, so you know the eigenvector only within a constant factor. The reason is that if **v** is an eigenvector, then any multiple of **v** is also an eigenvector. Show this is true in general. [Hint: easy.] Then determine both eigenvectors up to an unknown constant.
   c. Normalize the eigenvectors. Remember, $\mathbf{v}^{\dagger}\cdot\mathbf{v}=c$, then divide by $\sqrt{c}$ to normalize, just like for wavefunctions. The analogy between vectors and functions works both ways.
   d. Check that the eigenvectors satisfy $\widetilde{M}\mathbf{v} = \lambda\mathbf{v}$ and prove that they are orthogonal (i.e. that $\mathbf{v}_1{}^{\dagger}\cdot\mathbf{v}_2=0$).