Vector spaces and matrices; two-state systems

Assignment 1
Quantum Mechanics 1, 2008

These assignments will be graded, and the grades will count towards the final consolidated performance in the course. The assignment is due on September 4. Every day's delay after that will cause a 10% loss in marks.

1. Consider the matrix

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

   (a) Is this matrix Hermitean?
   (b) What are the eigenvalues and eigenvectors of this matrix?
   (c) Are there linear combinations of eigenvectors which are also eigenvectors?
   (d) Is the unitary transformation that diagonalizes M unique?

2. Consider the set of all 2×2 unitary matrices.
   (a) How many real parameters are needed to construct the most general 2×2 unitary matrix?
   (b) Provide an explicit parametrization of such a matrix using only angles as parameters.
   (c) When the parameters that you have chosen are infinitesimal, what is the form of the unitary matrix?
   (d) Given an arbitrary 2×2 Hermitean matrix, H, $\exp(iH)$ is an unitary matrix. Are all unitary matrices of this form?
   (e) Prove that all such matrices form a group. This group is called U(2), *i.e.*, the unitary group of order 2.

3. Take the set of all 2×2 unitary matrices with unit determinant.
   (a) How many real parameters are needed to specify such a matrix?
   (b) Show that they form a group. This group is called SU(2), *i.e.*, the special unitary group of order 2.
   (c) From the parametrization of U(2), what special values must one of the parameters have, in order for the matrix to belong to SU(2)?
   (d) What is the form of an SU(2) matrix when all the parameters are infinitesimal?
   (e) Since $\exp(iH)$ is unitary when H is Hermitean, what special property must H have for the exponential to be special unitary?

4. Read up the physics of the ammonia molecule in order to answer these questions—
   (a) What is the energy of the lowest electronic excitation of the molecule? State this in units of eV, joules, Hz (where the conversion to Hz is performed using $\hbar$) and nm (nanometers).
   (b) There could be vibrational states of the molecule in which the distance between the N nucleus and the centroid of the 3H nuclei change. What is the lowest excitation energy for these vibrations? State the results in eV, joules, Hz and nm.
   (c) What is the energy splitting between the two states of the N nucleus (symmetric on the two sides of the plane of 3H and antisymmetric)? State the result in eV, joules, Hz and nm.
   (d) What source did you use to find the above data (if it is a book or journal give the full reference; if it is a web site give the url)? How did you locate these sources? Why do you consider the source to be reliable?
   (e) Create a Mathematica function which takes an energy in eV and converts it to a three component array with its values in joules, Hz and nm respectively. (Test the function before submitting your answer)
   (f) Present a model Hamiltonian for the two states of N (discussed in part c) in the basis in which it is on one side of the plane or the other. What are the values of the parameters in the model you have written down.

5. Consider real matrices such as

$$M = \begin{pmatrix} a & b & b \\ b & a & b \\ b & b & a \end{pmatrix}.$$

This matrix is invariant under permutations or its rows and column. Equivalently, it is invariant under permutations of the basis vectors.

(a) Construct a vector which is invariant under permutations, and check that it is an eigenvector of M. What is the eigenvalue?

(b) Since M is symmetric, its eigenvectors are orthogonal. Construct two vectors which are orthogonal to the symmetric vector above, and to each other, using the Gram-Schmidt procedure. Check that these are eigenvectors of M. What are the corresponding eigenvalues?

(c) Since M is invariant under permutation of its basis, one can take unitary representations of permutation operators such as

$$P_{12} = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \qquad C_+ = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix},$$

and check that M commutes with them. Generate all possible permutation operators of three things, and check that the corresponding unitary matrices form a group. This group is called S_3, the permutation group of order 3. Write down the group multiplication table. Show that the powers of C_+ form an Abelian subgroup.

(d) How many of the permutation operators can be diagonalized simultaneously? Represent the permutation group elements in the basis where the maximum number of mutually commuting elements are diagonalized.

(e) Represent the matrix M as a linear combination of elements of the elements of S_3 and hence diagonalize it.

6. Extend the method of problem 3 to diagonalize $N \times N$ real matrices of the form

$$M = \begin{pmatrix} a & b & b & \cdots \\ b & a & b & \cdots \\ b & b & a & \cdots \\ \vdots & \vdots & \vdots & \cdots \end{pmatrix}.$$

7. Consider a molecule which is a ring of N identical atoms. The valence electrons of the isolated atoms have energy E_0, *i.e.*, $\langle n|H|n\rangle$, where H is the Hamiltonian and $|n\rangle$ is the state in which a valence electron sits at the n-th atom. Consider a model in which the molecular binding is due to a Hamiltonian which allows electrons to hop between neighbouring atoms, *i.e.*, $\langle n\pm 1|H|n\rangle$. Find the binding energies of the molecule. Could this be used as a model for Benzene (considering each CH unit together)? If yes, how should a more detailed computation be done? If no, then what prevents such a model from being written down?

8. In the space of all three-state Hamiltonians find all the Hamiltonians with at least two degenerate eigenstates. What special symmetries do these Hamiltonians have? What is the symmetry of the Hamiltonian with all three states degenerate?