Physics 251b
PROBLEM SET 1

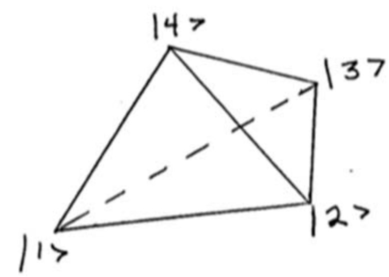
Spring 2016 Due: Wednesday, Feb. 10

Reading: Sakurai/Napolitano (S/N), 3.1-3.3, 3.5-3.8, 3.11 (some of this was covered last semester)

1. Consider a tight binding Hamiltonian

$$H = \varepsilon_0 \sum_{i=1}^{4} |i><i| - t \sum_{<i,j>} \left(|i><j| + |j><i| \right) \qquad (1)$$

defined on the vertices of a regular tetrahedron, where $\langle i, j \rangle$ means a neighboring pair of sites i and j.



(a) List the 12 symmetry operations of the tetrahedron which are continuously connected to the identity, i.e. exclude reflections and inversions.

(b) Which of these 12 is the symmetry operation

$$g_{234} g_{123} , \qquad (2)$$

where g_{123} is a counter-clockwise 120° rotation about the axis perpendicular to the face 123 and g_{243} is the same rotation about the face 243? Show explicitly that

$$g' = g_{123} g_{234} \neq g_{234} g_{123} = g , \qquad (3)$$

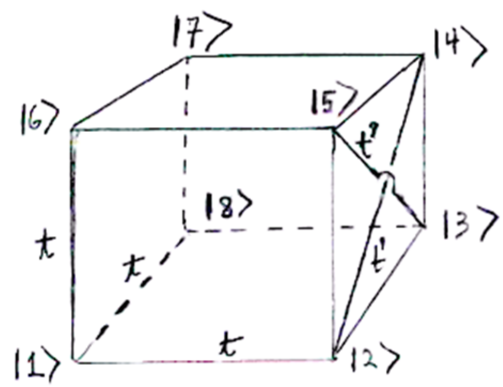
which shows that this group is non-Abelian, thus suggesting that the above Hamiltonian has degenerate eigenvalues. State the symmetry operation correspond to g'.

(c) Construct the 4×4 representation matrices corresponding to g_{123} and g_{234}.

(d) It is known that the tetrahedral point group discussed above has only 1- and 3-dimensional irreducible representations. These should be the degeneracies of the eigenvalues for <u>any</u> Hamiltonian with a tetrahedral symmetry. Verify this fact for the Hamiltonian H by finding its eigenvalues and an orthonormal set of eigenfunctions explicitly.

[You might try <u>guessing</u> eigenvectors by trial and error. One energy level is like the s-state of a hydrogen atom. The other is a three-fold degenerate.]

2. (a.) Using any technique you choose (MatLab, guesswork, Mathematica, brute force),



find the eigenvectors and eigenvalues the above eight-dimensional Hamiltonian connecting the vertices of a cube (it's functional form is similar to Eq. (1), problem 1) and identical nearest neighbor hopping matrix elements $-t$ on each of the 12 cube edges. Assume for now that all next nearest neighbor <u>diagonal</u> hopping matrix elements $-t'$ vanish.

(b.) Discuss the eigenvalue degeneracies in light of the dimensionalities of irreducible representations A_1, A_2, E, T_1 and T_2 of the 24 element cubic point group T_d.

(c.) Now allow in addition nonzero next-nearest neighbor hoppings $-t'$ on the two diagonals of each of the six cube faces, where $0 < t' < t$. Using Mathematica, MatLab or a similar program, plot the 8 eigenvalues $\lambda_j(\varepsilon_0, t, t')$ after first arguing that these must be expressible in the form $\lambda_j = \varepsilon_0 + t\, f_j(t'/t)$, i.e. determine numerically the eight functions $f_j(x)$, $j = 1,...,8$. Comment on any similarities or differences compared to the case $t' = 0$.

3. Because the angular momentum operators L_z and L^2 acting on the angular momentum $Y_{lm}(\theta,\phi)$ basis states satisfy (with $\ell = 0,1,2,....; \quad -\ell < m < \ell,$)

$$L_z Y_{lm}(\theta,\phi) = \frac{\hbar}{i}\frac{\partial Y_{lm}}{\partial\phi} = \hbar m Y_{lm}(\theta,\phi), \quad L^2 Y_{lm}(\theta,\phi) = \hbar^2 \ell(\ell+1) Y_{lm}(\theta,\phi),$$

the squared eigenvalue of L_z must always be less than the eigenvalue of L^2, except in the special case $l = m = 0$. Comment on how this result constrains the "direction"of $\vec{L}$, if we regard $\vec{L}$ as a classical vector. Show that this inequality is a consequence the uncertainty principle (S/N, Eq. (1.4.53) applied to angular momentum operators, and explain why the case $l = m = 0$ is special.

4. (Rotation operators; reviewing S/N would be helpful)
(a) For any well-behaved periodic function $f(\phi)$ with period 2π, show that

$$f(\phi - \phi_0) = e^{-iL_z\phi_0/\hbar} f(\phi) \tag{4}$$

where ϕ_0 is any constant angle. For this reason, $L_z/\hbar$ is called the generator of rotations about the *z*-axis. More generally, $L\cdot\hat{n}/\hbar$ is the generator of rotations about the direction $\hat{n}$, in the sense that $\exp(-iL\cdot\hat{n}\psi/\hbar)$ effects a rotation through angle ψ (in the counterclockwise sense) about the axis $\hat{n}$. In the case of spin, the generator of rotations is $\vec{S}\cdot\hat{n}/\hbar$. In particular, for spin 1/2, the transformation

$$\chi' = e^{i(\sigma\cdot\hat{n})\varphi/2}\chi \ , \tag{5}$$

where $\vec{S} = (1/2)\hbar\vec{\sigma}$, tells us how at two-component *spinor* changes under a rotation.

(b) Using a Taylor series expansion and the properties of the Pauli matrices $\vec{\sigma}$, demonstrate that

$$e^{-i(\sigma\cdot\hat{n})\varphi/2} = \cos(\varphi/2) - i(\hat{n}\cdot\sigma)\sin(\varphi/2) \ . \tag{6}$$

(c) Construct the 2×2 matrix representing a counterclockwise rotation of 180° about the *x*-axis, and show that it converts "spin up" $(\chi = \chi^+ \equiv (1,0))$ into "spin down" $(\chi = \chi^- \equiv (0,1))$, as one might would expect. What happens if you instead rotate by 180° about the y-axis?

(d) Now construct the matrix representing a counterclockwise rotation by 90° about the *y*-axis and determine what it does to $\chi+$.

(e) Construct the matrix representing rotation by 360° about the *z*-axis. If the answer is not quite what one might expect from classical physics, are there observable consequences.

5. (a) If the operators A and B both commute with $[A,B]$, prove that

$$[A,B^n] = nB^{n-1}[A,B]; \quad [A^n,B] = nA^{n-1}[A,B]. \tag{7}$$

Assume that the function $f(x)$ has a power series expansion about the origin, and use this result to derive a compact expression for $[p_x, f(x)]$ of the form $[p_x, f(x)] = g(x)$. Determine the function $g(x)$.

(b) Prove that for a particle in a potential $V(\vec{r})$ the rate of change of the expectation value of the orbital angular momentum operator $\vec{L}_{op}$ is equal to the expectation value of the torque:

$$\frac{d}{dt} < \vec{L}_{op} > = < \vec{N}_{op} > \tag{7}$$

where the quantum operator corresponding to torque is

$$\vec{N}_{op} = \vec{r} \times (-\vec{\nabla} V(\vec{r})). \tag{8}$$

(This is the rotational analog to Ehrenfest's theorem*.)

(c) Use the quantum equation of motion for a possibly time-dependent operator $\hat{A}(t)$, $i\hbar \frac{d\hat{A}(t)}{dt} = i\hbar \frac{\partial \hat{A}(t)}{\partial t} + [\hat{A}(t), H]$, to show that $d < \vec{L}_{op} > / dt = 0$ for any spherically symmetric potential. (This is quantum statement of the conservation of angular momentum).

Hint: The result of part (a) might be useful.

*Ehrenfest's theorem states that $m \frac{d}{dt} \langle \vec{r} \rangle = \langle \vec{p}_{op} \rangle$ and $\frac{d < \vec{p}_{op} >}{dt} = -\langle \vec{\nabla} V(\vec{r}) \rangle$ where $\vec{p}_{op}$ is the momentum operator. The expectation values of these operators thus obey Newton's classical equations of motion.