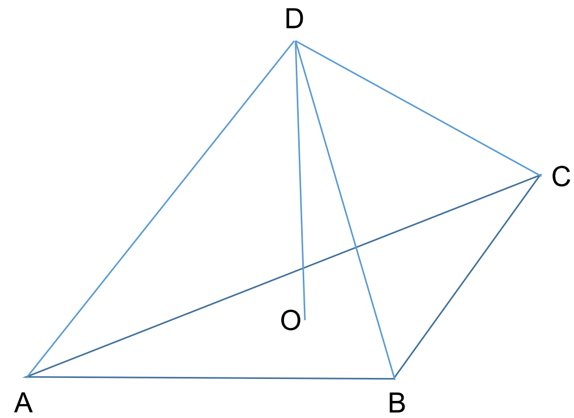
Physics 129a **Homework 7** **Due 11/17/22**

1. The point group C_{3v} is, among other things, the symmetry group of the ammonia molecule NH_3, which forms a right pyramid on an equilateral triangle base, as shown below. $AB = BC = CA$. O is the center of the triangle and OD is perpendicular to ΔABC.



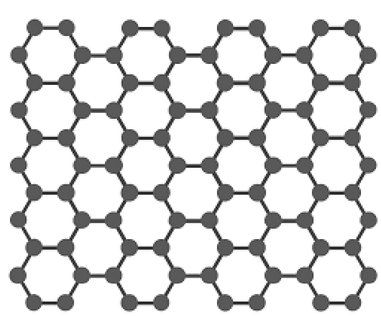
The symmetry group is generated by a 3-fold rotation c around the axis OD and a reflection σ_v with respect to plane OAD.

(a) Show that $C_{3v} \simeq$ (is isomorphic to)D_3.

(b) Show that the molecule can possess a permanent electric dipole moment $\vec{P}$. What is the direction of this electric dipole moment?

(c) A magnetic dipole moment, like a magnetic field, is an *axial* vector. Under reflection symmetry, it gets an extra minus sign compared to a regular vector (such as electric dipole). For example, under reflection with respect to the xy plane, the magnetic field (M_x, M_y, M_z) goes to $(-M_x, -M_y, M_z)$. Its transformation under rotation is the same as a regular vector. Show that the NH_3 molecule cannot possess a permanent magnetic moment.

(d) Now put this NH_3 molecule onto the lattice site of a two dimensional honeycomb lattice, such that it sees some lattice potential (which perturbs the original Hamiltonian of the molecule). The molecule can be oriented in different directions with respect to the lattice. In what orientation does the energy spectrum degeneracy structure remain the same? Explain your reason.



2. Conjugacy classes of $SO(3)$

In this problem we are going to show that the conjugacy classes of $SO(3)$ consist of rotations around different axes but with the same angle. That is we are going to demonstrate the relation

$$e^{-i\phi\vec{n}_2\cdot\vec{J}}e^{i\theta\vec{n}_1\cdot\vec{J}}e^{i\phi\vec{n}_2\cdot\vec{J}} = e^{i\theta\vec{n}_3\cdot\vec{J}} \tag{1}$$

where $\vec{n}_3 = R_{\vec{n}_2}(\phi)\vec{n}_1$. $R_{\vec{n}_2}(\phi)$ is the three dimensional real orthogonal representation of rotation around $\vec{n}_2$ through angle ϕ and it acts on the three dimensional real vector space of $\vec{n}$.

(1) Define $S^x_y(\phi) = e^{-i\phi J_x}J_y e^{i\phi J_x}$, $S^x_z(\phi) = e^{-i\phi J_x}J_z e^{i\phi J_x}$. Take the derivative of $S^x_y(\phi)$ with respect to ϕ and show that $\frac{\partial}{\partial\phi}S^x_y(\phi) = S^x_z(\phi)$. (hint: $\frac{\partial}{\partial\phi}e^{i\phi J_x} = e^{i\phi J_x}iJ_x$).

(2) Similarly show that $\frac{\partial}{\partial\phi}S^x_z(\phi) = -S^x_y(\phi)$

(3) Combining these two equations and use the boundary condition that $S^x_y(0) = J_y$, $S^x_z(0) = J_z$ to obtain solutions $S^x_y(\phi) = \cos\phi J_y + \sin\phi J_z$, $S^x_z(\phi) = \cos\phi J_z - \sin\phi J_y$. That is, J_y and J_z rotate into each other under the conjugation of $e^{-i\phi J_x}$ as if they are the y and z component of a three dimensional vector transforming under rotation around x axis through angle ϕ.

(4) Taking into account the fact that $S^x_x(\phi) = e^{-i\phi J_x}J_x e^{i\phi J_x} = J_x$, show that $S^x_{\vec{n}}(\phi) = e^{-i\phi J_x}\left(\vec{n}\cdot\vec{J}\right)e^{i\phi J_x} = (R_x(\phi)\vec{n})\cdot\vec{J}$, where $R_x(\phi)$ is the three dimensional orthogonal matrix representing rotation around x axis through angle ϕ and it acts on the three dimensional vector $\vec{n}$.

Now convince yourself that this relation works not only for x axis rotation but for rotation around arbitrary axis as well. That is, $e^{-i\phi\vec{n}_2\cdot\vec{J}}\left(\vec{n}_1\cdot\vec{J}\right)e^{i\phi\vec{n}_2\cdot\vec{J}} = (R_{\vec{n}_2}(\phi)\vec{n}_1)\cdot\vec{J}$. You don't need to show work for this part, but if you want to work everything out, it is helpful to choose three vectors $\vec{n}_2$, $\vec{n}^a_2$, $\vec{n}^b_2$ which are orthogonal to each other and build up the relation from there.

(5) Now use the above relation and show that

$$e^{-i\phi\vec{n}_2\cdot\vec{J}}e^{i\theta\vec{n}_1\cdot\vec{J}}e^{i\phi\vec{n}_2\cdot\vec{J}} = e^{i\theta\vec{n}_3\cdot\vec{J}} \tag{2}$$

where $\vec{n}_3 = R_{\vec{n}_2}(\phi)\vec{n}_1$. (hint: decompose $e^{i\theta\vec{n}_1\cdot\vec{J}}$ as a polynomial series.)

3. P orbital

The p orbital of an electron has three components p_x, p_y, p_z. The angular part of the wave function in these orbitals are given by

$$\psi_x(\theta,\phi) = \mathcal{N}\sin\theta\cos\phi, \quad \psi_y(\theta,\phi) = \mathcal{N}\sin\theta\sin\phi, \quad \psi_z(\theta,\phi) = \mathcal{N}\cos\theta \tag{3}$$

where θ and ϕ are the usual polar coordinates and $\mathcal{N}$ is some pre-factor independent of θ and ϕ.

(1) Show that the three wave functions are orthogonal to each other. Hint: inner product of wave functions in polar coordinates is given by $\int_{\theta=0}^{\pi}\int_{\phi=0}^{2\pi}\psi^*(\theta,\phi)\tilde{\psi}(\theta,\phi)\sin\theta d\theta d\phi$

(2) The angular momentum operator in z direction is given by $J_z = -i\frac{\partial}{\partial\phi}$. How is it represented as a three dimensional matrix in the Hilbert space spanned by ψ_x, ψ_y and ψ_z?

(3) The angular momentum operator in x direction is given by $J_x = i\left(\sin\phi\frac{\partial}{\partial\theta} + \cot\theta\cos\phi\frac{\partial}{\partial\phi}\right)$. How is it represented as a three dimensional matrix in the Hilbert space spanned by ψ_x, ψ_y and ψ_z?

(4) The angular momentum operator in y direction is given by $J_y = i\left(-\cos\phi\frac{\partial}{\partial\theta} + \cot\theta\sin\phi\frac{\partial}{\partial\phi}\right)$. How is it represented as a three dimensional matrix in the Hilbert space spanned by ψ_x, ψ_y and ψ_z?

(5) Show that if the electron moves on a spherical shell of radius r, then ψ_x, ψ_y and ψ_z are proportional to the x, y, z coordinates of the electron respectively.

(6) Which irreducible representation do p_x, p_y and p_z orbitals form under $SO(3)$ rotation?