Theoretical Physics 2019/20 — Problem QT2.5

The ammonia molecule (NH_3) can be thought of as a tetrahedron (a triangular pyramid) in which the three hydrogen atoms form an equilateral triangle and the nitrogen atom is, roughly speaking, either above or below the plane of the hydrogen atoms. Amongst the many energy levels of this system are some corresponding to different states of rotation of the molecule as a whole or to various states of vibration of the atoms about their equilibrium position. Many of these energy levels are split by a tiny amount, about 1×10^{-4} eV in the ground vibrational state. The origin of this splitting can be understood within a simple two-state model in which the Hamiltonian is given by the following equation:

$$\hat{H} = E_0|A\rangle\langle A| + \Delta|A\rangle\langle B| + \Delta|B\rangle\langle A| + E_0|B\rangle\langle B|.$$

In this equation, E_0 and Δ are two energies and $|A\rangle$ and $|B\rangle$ represent states in which the nitrogen atom is, respectively, above or below the plane of the hydrogen atoms. These two ket vectors form a basis for the relevant Hilbert space and are orthonormal ($\langle A|A\rangle = \langle B|B\rangle = 1$ and $\langle A|B\rangle = \langle B|A\rangle = 0$).

(a) (i) Verify that the vectors $|+\rangle = (|A\rangle + |B\rangle)/\sqrt{2}$ and $|-\rangle = (|A\rangle - |B\rangle)/\sqrt{2}$ are eigenvectors of $\hat{H}$, corresponding, respectively, to the eigenenergies $E_0 + \Delta$ and $E_0 - \Delta$.

(ii) Show that $|A\rangle$ and $|B\rangle$ are eigenvectors of $\hat{H}$ if $\Delta = 0$ but not if $\Delta \neq 0$.

Note: The difference 2Δ between $E_0 + \Delta$ and $E_0 - \Delta$ is the splitting of about 1×10^{-4} eV found in the ground vibrational state of that molecule. The physical origin of this splitting is explained in the model solution of this question.

(b) Why can one say that the vectors $|+\rangle$ and $|-\rangle$ form an orthonormal basis of the Hilbert space spanned by $|A\rangle$ and $|B\rangle$?

(c) Show that the Hamiltonian is represented by the matrix H in the $\{|A\rangle, |B\rangle\}$ basis and by the matrix H' in the $\{|+\rangle, |-\rangle\}$ basis, where

$$\mathsf{H} = \begin{pmatrix} E_0 & \Delta \\ \Delta & E_0 \end{pmatrix}, \qquad \mathsf{H}' = \begin{pmatrix} E_0 + \Delta & 0 \\ 0 & E_0 - \Delta \end{pmatrix}.$$

(d) Find the eigenvalues and the corresponding eigenvectors of H and of H', assuming that $\Delta \neq 0$. Are your results consistent with the results of Part (a)?