

M05Q.3 - Nitrogen and Explosives

Problem

The nitrogen nucleus, ^{14}N is in a chemical environment (an explosive) where the nuclear spin Hamiltonian H can be described by

$$H/\hbar = Q_x I_x^2 + Q_y I_y^2 + Q_z I_z^2 + \boldsymbol{\omega} \cdot \mathbf{I}.$$

The nuclear spin operators are I_x, I_y and I_z and the nuclear spin quantum number is $I = 1$.

The interaction of the nuclear electric quadrupole moment with the electric-field gradient at the site of the nucleus is characterized by the parameters Q_x, Q_y and Q_z . The coordinate system is chosen so that the gradient tensor is diagonal. The energy scale is chosen so that $Q_x + Q_y + Q_z = 0$.

The Larmor frequency due to the earth's magnetic field is ω , with components ω_x, ω_y and ω_z along the principal axes of the field-gradient tensor. You can assume that $\omega_x^2 + \omega_y^2 + \omega_z^2 \ll Q_x^2 + Q_y^2 + Q_z^2$.

- a) For $\omega = 0$, find the energy eigenvalues and eigenfunctions for the nucleus.
- b) For sufficiently symmetric environments, for example, for the anion NO^{3-} , the field gradient is axially symmetric and can be characterized by a single frequency parameter Q , with $Q_x = Q_y = -Q$ and $Q_z = 2Q$. To lowest nonvanishing order in $\omega \neq 0$, find the energy perturbations for this symmetric situation.