Phys 402: Applications of Quantum Mechanics

Homework II (due 930am, Thursday, Jan 21, 2016)

Ammonia molecules

Two states for ammonia molecules: |u>, one with Nitrogen atom above the hydrogen plane and |d>, one with Nitrogen atom below the plane (see handouts on ammonia molecules). These two states have opposite permanent dipole moments (plus-minus \mu) so that when an electric field E is applied along the z-direction, state |u> will be shifted upward by an amount \mu E and state |d> will be shifted downward by an amount -\mu E. |u> state is coupled with |d> via quantum tunneling.

In this problem, you need to construct a Hamiltonian matrix for these molecules. What basis would you like to work with? how does the matrix look like?

\mu = μ – dipole moment; E ~ external electric field

1) When there is no external field, what is the ground state and excited state? Is there a dipole moment in either of the states?

What is the operator for dipole moment in the matrix form?

2) Assume the field is weak and can be treated as a perturbation. Calculate the polarizability of the ammonia molecules for both the ground state and the excited state using the non-degenerate second order perturbation. Discuss qualitatively the difference between the polarizability here and the polarizability of a hydrogen atom that you worked on in HW set I.

Here, the second order correction can be written as $E_n^{(2)} = -\frac{1}{2}\alpha_n E^2$, α_n — polarizability for state $|n\rangle^0$. For the ground state, $\alpha_n > 0$.

One can also show the induced dipole moment

$d_n = \alpha_n E$.

3) When the field is very strong, find the approximate ground state and excited state.

4) Using the degenerate perturbation theory to find the eigen values and eigen states for ammonia molecues as a function of external field E. Plot schematically two eigen values as a function of electric field.

5) Assume an ammonia molecule is prepared in state |u> at t=0. Find out the probability of find the molecule in state |d> at an arbitrary later time t=T. At what T, the probability of finding molecules in state |u> is zero. No external field for this part.