

SYMMETRIES IN QUANTUM MECHANICS

(14/01/2013 (13u30-20u45))

1 A carbon dioxide molecule can be modeled as three interacting point particles (two of mass m_O , one of mass m_C), with position vectors \vec{r}_{O_1} , \vec{r}_C , \vec{r}_{O_2} , which in static equilibrium are lying on a line, arranged as O – C – O. In (x, y, z) coordinates such an equilibrium configuration is given e.g. by $\vec{R}_{O_1} = (0, 0, -a)$, $\vec{R}_C = (0, 0, 0)$, $\vec{R}_{O_2} = (0, 0, +a)$. The nontrivial vibrational normal modes of the molecule around this static equilibrium configuration are given by two transversal modes T_x and T_y , a symmetric longitudinal mode L_s and an antisymmetric longitudinal mode L_a .

- (a) What is the spatial symmetry group G of the equilibrium configuration?
- (b) Write out the four normal modes explicitly, i.e. as $\vec{r}_C = T_x(t) \vec{v}_{x,C} + T_y(t) \vec{v}_{y,C} + L_s(t) \vec{v}_{s,C} + L_a(t) \vec{v}_{a,C}$ etc for suitable constant vectors $\vec{v}_{x,C}$, \vec{v}_{x,O_1} , etc, with $T_x(t) = \sin(\omega_x t + c_x)$ etc. No need to relate the mode frequencies to merge fundamental quantities, but do show that these modes are indeed decoupled.
- (c) Discuss how the normal modes transform under the symmetry group G of the equilibrium configuration.
- (d) Find the quantum normal mode energy eigenfunction $\psi(T_x, T_y, L_s, L_a)$, which will be characterized by four quantum numbers (n_1, n_2, n_3, n_4) , and discuss how the symmetry group G is represented on the energy levels.
- (e) Discuss the selection rules for matrix elements of the form

$$\langle n_1, n_2, n_3, n_4 | \vec{E} \cdot (\vec{r}_{O_1} + \vec{r}_C + \vec{r}_{O_2}) | n'_1, n'_2, n'_3, n'_4 \rangle.$$

Here \vec{E} is some constant vector. (Such matrix elements appear e.g. in radiative dipole transition rates.)

2 Come up with an original (not just copied from the book) exam-type problem relevant to the material covered in this course and solve it.