CTC2, exercises week 1, NWI-MOL176

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Question 1: Chapter 1

The harmonic oscillator Hamiltonian for a particle with mass m and a harmonic potential with force constant k is

$$\hat{H}_0 = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2}kx^2. \tag{1}$$

1a. Find a coordinate transformation, $x = \alpha y$, to rewrite the Hamiltonian as

$$\hat{H}_0 = A\left(-\frac{1}{2}\frac{\partial^2}{\partial y^2} + \frac{1}{2}y^2\right) \tag{2}$$

and determine A as a function of m and k. Note that y must be dimensionless (why?).

1b. Show that Hamilton's classical equations of motion for one particle in one dimension is equivalent to Newton's equation.

Question 2: Chapter 4

2a. Use first order perturbation theory to show that the energy levels of a diatomic molecule can be written as

$$E_{vl} = \epsilon_v + B_v l(l+1), \tag{3}$$

where $v = 0, 1, 2, \ldots$ is the vibrational quantum number and $l = 0, 1, 2, \ldots$ is the rotational quantum number. Take the vibrational Schrödinger equation with $l = 0$ as the zeroth order problem, and treat the centrifugal term as a perturbation. Assume that the solutions $\chi_v(r)/r$ of the zeroth-order problem are known and give the expression for B_v.

Reminder first order perturbation theory: Assume the Hamiltonian can be written as

$$\hat{H} = \hat{H}_0 + \hat{H}_1 \tag{4}$$

and we want to find approximate solutions of

$$\hat{H}\Psi_n = E_n\Psi_n. \tag{5}$$

We assume that the zeroth-order problem has been solved

$$\hat{H}_0\phi_n = \epsilon_n\phi_n \tag{6}$$

In first order perturbation theory, the energies E_n are given by

$$E_n = \epsilon_n + \frac{\langle\phi_n|\hat{H}_1|\phi_n\rangle}{\langle\phi_n|\phi_n\rangle}. \tag{7}$$

A Morse potential has the functional form

$$V(r) = D_e[1 - e^{-\alpha(r-r_e)}]^2. \tag{8}$$

2b. Derive an expression for the vibrational energies ϵ_v, for given parameters D_e, r_e, and α, and assuming the reduced mass of the diatom is μ. To simplify the problem, make an harmonic approximation of the Morse potential, i.e., make a Taylor expansion up to second order around the minimum, and use that as the potential.

2c. Give the expression for B_v in terms of the Morse parameters and the reduced mass.

2d. Show that the wave functions in Eq. (4.66) of the lecture notes are solutions to the Schrödinger equation (4.54).

Question 3: Chapter 4: "left as an exercise" in lecture notes

When studying chapter 4 you will find some of the math "left as an exercise". These exercises are collected here. The answers will be put online, use this question if you want to give it a try yourself.

3a. Show that

$$\epsilon_{ijk}\epsilon_{ij'k'} = \delta_{jj'}\delta_{kk'} - \delta_{jk'}\delta_{kj'}. \tag{9}$$

3b. Show that

$$p_r \equiv \hat{\boldsymbol{r}} \cdot \boldsymbol{p} \tag{10}$$

is the moment conjugate to the coordinate $r = |\boldsymbol{r}|$.

3c. Derive this commutation relation

$$[\hat{A}, \hat{B}\hat{C}] = \hat{B}[\hat{A}, \hat{C}] + [\hat{A}, \hat{B}]\hat{C}. \tag{11}$$

3d. Using Levi-Civita tensors, show that

$$[\hat{l}_i, \hat{l}_{i'}] = i\hbar\epsilon_{ii'j}\hat{l}_j. \tag{12}$$

3e. Show that

$$\hat{l}^2 = r^2\hat{p}^2 + \hbar^2(\boldsymbol{r} \cdot \boldsymbol{\nabla})^2 + \hbar^2\boldsymbol{r} \cdot \boldsymbol{\nabla}. \tag{13}$$

Use the Levi-Civita tensor relation

$$\epsilon_{ijk}\epsilon_{ij'k'} = \delta_{jj}\delta_{kk} - \delta_{jk'}\delta_{j'k}. \tag{14}$$

3f. For the vector $\boldsymbol{r}$, defined by spherical polar angles θ, ϕ, and length r, calculate the Jacobian,

$$\boldsymbol{J} = \left[\frac{\partial \boldsymbol{r}}{\partial r}\,\frac{\partial \boldsymbol{r}}{\partial \theta}\,\frac{\partial \boldsymbol{r}}{\partial \phi}\right], \tag{15}$$

show that the columns of $\boldsymbol{J}$ are orthogonal, and calculate their lengths.