Quantum Dynamics, NWI-SM295, exercises week 4

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Question 1: Kinetic energy operator in 3D

In this exercise we derive

$$-\frac{\hbar^2}{2\mu}\nabla^2 = -\frac{\hbar^2}{2\mu}\frac{1}{r}\frac{\partial^2}{\partial r^2}r + \frac{\hat{l}^2}{2\mu r^2}. \tag{1}$$

The angular momentum operator is defined by

$$\hat{\boldsymbol{l}} = \boldsymbol{r} \times \hat{\boldsymbol{p}}, \tag{2}$$

where the linear momentum operator is

$$\hat{\boldsymbol{p}} = -i\hbar\boldsymbol{\nabla}. \tag{3}$$

The first step is to work out the $\hat{l}^2$ operator and to show that

$$\hat{l}^2 = -\hbar^2(\boldsymbol{r}\times\boldsymbol{\nabla})\cdot(\boldsymbol{r}\times\boldsymbol{\nabla}) = \hbar^2[-r^2\nabla^2 + \boldsymbol{r}\cdot\boldsymbol{\nabla} + (\boldsymbol{r}\cdot\boldsymbol{\nabla})^2]. \tag{4}$$

A convenient way to work with cross products,

$$\boldsymbol{a} = \boldsymbol{b}\times\boldsymbol{c}, \tag{5}$$

is to write the components using the Levi-Civita tensor ϵ_{ijk},

$$a_i = \epsilon_{ijk}b_jc_k \equiv \sum_{j=1}^{3}\sum_{k=1}^{3}\epsilon_{ijk}b_jc_k, \tag{6}$$

where we introduced the Einstein summation convention: whenever an index appears twice one assumes there is a sum over this index.

1a. Write the cross product in components and show that

$$\epsilon_{1,2,3} = \epsilon_{2,3,1} = \epsilon_{3,1,2} = 1, \tag{7}$$

$$\epsilon_{3,2,1} = \epsilon_{2,1,3} = \epsilon_{1,3,2} = -1, \tag{8}$$

and all other component of the tensor are zero. Note: the tensor is +1 for $\epsilon_{1,2,3}$, it changes sign whenever two indices are permuted, and as a result it is zero whenever two indices are equal.

1b. Check this relation

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

(Remember the implicit summation over index i).

1c. Use Eq. (9) to derive Eq. (4).

1d. Show that

$$r\frac{\partial}{\partial r} = \boldsymbol{r}\cdot\boldsymbol{\nabla} \tag{10}$$

1e. Show that

$$\frac{1}{r}\frac{\partial^2}{\partial r^2}r = \frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} \tag{11}$$

1f. Combine the results to derive Eq. (1).

Question 2: Coupled channels equation for collinear $A + BC$

Three particles move along a line. Their coordinates are x_A, x_B, and x_C, and their masses m_A, m_B, and m_C. The kinetic energy operator is given by

$$\hat{T} = -\frac{\hbar^2}{2m_A}\frac{\partial^2}{\partial x_A^2} - \frac{\hbar^2}{2m_B}\frac{\partial^2}{\partial x_B^2} - \frac{\hbar^2}{2m_C}\frac{\partial^2}{\partial x_C^2}. \tag{12}$$

The center of mass coordinate is

$$X \equiv \frac{m_A x_A + m_B x_B + m_C x_C}{m_A + m_B + m_C} \tag{13}$$

and the Jacobi-coordinates for the $A + BC$ arrangement are

$$r \equiv x_B - x_C. \tag{14}$$

$$R \equiv x_A - \frac{m_B x_B + m_C x_C}{m_B + m_C}. \tag{15}$$

2a. Rewrite the kinetic energy in Jacobi/center-of-mass coordinates (X, R, r).

The potential V is assumed to be independent of X, so the Hamiltonian can be written as

$$\hat{H} = \hat{T} + V(R, r). \tag{16}$$

For large R we find the potential for molecule BC:

$$V_{BC}(r) = \lim_{R\to\infty} V(R, r). \tag{17}$$

2b. Derive the Schrödinger equation for the vibrational wave functions $\phi_v(r)$ of molecule BC.

The multichannel expansion is given by

$$\Psi(R, r) = \sum_v \phi_v(r) u_v(R). \tag{18}$$

2c. Derive the coupled channels equation

$$\boldsymbol{u}''(R) = \boldsymbol{W}(R)\boldsymbol{u}(R) \tag{19}$$

and find an expression for the $\boldsymbol{W}$ matrix.