# QTC, NWI-MOL112, exercises week 5

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## Question 1: Coupled basis for atom-diatom system

**1a**. Show that for coupled angular momentum states, with $|j-l| \leq J \leq j+l$, we have this orthonormality relation:

$$\langle (jl)JM|(j'l')JM\rangle = \delta_{jj'}\delta_{ll'}.$$

Hint: start by expanding the coupled basis in the uncoupled one:

$$|(jl)JM\rangle = \sum_{m_j=-j}^{j} \sum_{m_l=-l}^{l} |jm_j\rangle|lm_l\rangle\langle jm_j lm_l|JM\rangle.$$

For the atom-diatom system, the angular part of the kinetic energy is given by [Eq. (7.27) of lecture notes]

$$\hat{T} = \frac{\hat{j}^2}{2\mu_{\rm AB}r^2} + \frac{\hat{l}^2}{2\mu R^2}.$$

**1b**. Evaluate the matrix elements of $\hat{T}$ in the coupled basis.

The angular part of the potential can be expanded in Legendre polynomials [Eq. (8.2)] of the lecture notes.

**1c**. Evaluate the matrix element of $P_L(\cos\theta)$ in the coupled basis:

$$\langle (j_1 l_1)JM|P_L(\cos\theta)|(j_2 l_2)JM\rangle.$$

Hint: use the spherical harmonics addition theorem and Eq. (8.7) from the lecture notes.

## Question 2: Questions chapter 8

## Legendre polynomials

**2a**. Use the recursion relation to find the expression for $P_2(z)$.

**2b**. Check the normalization and orthogonality relations for $P_0(z)$, $P_1(z)$, and $P_2(z)$.

**2c**. *(Keep this exercise for last)* Still for $n = 2$, show that the eigenvalues of the $\hat{z}$ operator expressed in a basis of normalized Legendre polynomials are indeed the zeros of $P_2(z)$.

## Gauss-Legendre quadrature

A $n$-point Gauss-Legendre quadrature is exact for polynomials of degree $2n-1$. The abscissae are the zeros of $P_n(z)$.

**2d**. Derive the points and weights for the 2-point Gauss-Legendre quadrature, and show that it exact for Legendre polynomials up to $P_3(z)$.

## Clebsch-Gordan series

**2e**. Show that the orthonormality of spherical harmonics follows from the orthogonality relation for Wigner D-matrices.

**2f**. Use the orthonormality relations of Clebsch-Gordan coefficients to derive Eq. (8.49) from Eq. (8.48).

**2g**. Derive the matrix elements of spherical harmonics [Eq. (8.7)] as a special case of Eq. (8.49).

**2h**. Using the definition of $C_{lm}$ from the lecture notes, show that

$$D^{(l),*}_{m,0}(\boldsymbol{R}) = C_{lm}(\hat{\boldsymbol{r}})$$

when

$$\hat{\boldsymbol{r}} = \boldsymbol{R}\boldsymbol{e}_z.$$