CTC2, NWI-MOL176, exercises week 3

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Question 1: Questions chapter 5 (II)

1a. In the derivation in Chapter 5.8 we used

$$(\boldsymbol{n} \times \boldsymbol{r}) \cdot \boldsymbol{\nabla} = \boldsymbol{n} \cdot (\boldsymbol{r} \times \boldsymbol{\nabla})$$

Derive this equation using the Levi-Civita tensor.

Answer: *On the lhs we have*

$$(\boldsymbol{n} \times \boldsymbol{r}) \cdot \boldsymbol{\nabla} = \epsilon_{ijk} n_j r_k \nabla_i. \tag{1}$$

On the rhs we havve

$$\boldsymbol{n} \cdot (\boldsymbol{r} \times \boldsymbol{\nabla}) = \epsilon_{ijk} n_i r_j \nabla_k \tag{2}$$

The Levi-Civita tensor is invariant under cyclic permutations, so $\epsilon_{ijk} = \epsilon_{kij}$, *and we have*

$$\boldsymbol{n} \cdot (\boldsymbol{r} \times \boldsymbol{\nabla}) = \epsilon_{kji} n_i r_j \nabla_k = \epsilon_{ijk} n_j r_k \nabla_i = (\boldsymbol{n} \times \boldsymbol{r}) \cdot \boldsymbol{\nabla}. \tag{3}$$

where we swapped the summation indices k and i in the second step.

1b. Compute the matrix elements of the rotation operator

$$\langle lm|\hat{R}(\boldsymbol{e}_z, \alpha)|lm'\rangle.$$

Answer:

$$\langle lm|\hat{R}(\boldsymbol{e}_z, \alpha)|lm'\rangle = \langle lm|e^{-\frac{i}{\hbar}\alpha \hat{l}_z}|lm'\rangle = e^{-im\alpha}\delta_{mm'}. \tag{4}$$

1c. Compute the Wigner D-matrix elements

$$d^{(l)}_{mk}(\beta) = \langle lm|e^{-\frac{i}{\hbar}\beta \hat{l}_y}|lk\rangle$$

for $l = 1/2$.

Answer: *If we keep the order of the basis functions in the same order as in the previous question, we need to compute*

$$e^{-\frac{i}{\hbar}\beta \boldsymbol{L}_y} = e^{\frac{1}{2}\beta \boldsymbol{A}} \tag{5}$$

with

$$\boldsymbol{A} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}. \tag{6}$$

First, we calculate the eigenvalues of the matrix from

$$\det(\boldsymbol{A} - \lambda \boldsymbol{I}) = \det \begin{pmatrix} -\lambda & 1 \\ -1 & -\lambda \end{pmatrix} = \lambda^2 + 1 = 0, \tag{7}$$

so $\lambda_\pm = \pm i$. Note that the eigenvalues are imaginary, since the matrix $\boldsymbol{A}$ is anti-*Hermitian. For $\lambda_+ = i$, we find the eigenvector from*

$$(\boldsymbol{A} - i\boldsymbol{I})\boldsymbol{c} = 0 \tag{8}$$

i.e.

$$\begin{pmatrix} -i & 1 \\ -1 & -i \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}. \tag{9}$$

so

$$\begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = \begin{pmatrix} 1 \\ i \end{pmatrix}. \tag{10}$$

For the eigenvalue $\lambda_- = -i$ we find the eigenvector from

$$\begin{pmatrix} i & 1 \\ -1 & i \end{pmatrix} \begin{pmatrix} d_1 \\ d_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}. \tag{11}$$

so

$$\begin{pmatrix} d_1 \\ d_2 \end{pmatrix} = \begin{pmatrix} i \\ 1 \end{pmatrix}. \tag{12}$$

Note that the eigenvectors are orthogonal, since

$$\boldsymbol{c}^\dagger \boldsymbol{d} = (1 - i) \begin{pmatrix} i \\ 1 \end{pmatrix} = i - i = 0. \tag{13}$$

We now construct a unitary matrix $\boldsymbol{U}$ *from the normalized eigenvectors*

$$\boldsymbol{U} = \frac{1}{\sqrt{2}}[\boldsymbol{c}\ \boldsymbol{d}] = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & i \\ i & 1 \end{pmatrix} \tag{14}$$

so we can write the spectral decomposion of $\boldsymbol{A}$ *as*

$$\boldsymbol{A} = \boldsymbol{U}\boldsymbol{\Lambda}\boldsymbol{U}^\dagger \tag{15}$$

where

$$\boldsymbol{\Lambda} = \begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix}. \tag{16}$$

We can now compute the $l = 1/2$ *Wigner d-matrix from*

$$\boldsymbol{U} e^{\frac{1}{2}\beta\boldsymbol{\Lambda}} \boldsymbol{U}^\dagger = \frac{1}{2} \begin{pmatrix} 1 & i \\ i & 1 \end{pmatrix} \begin{pmatrix} e^{\frac{1}{2}\beta i} & 0 \\ 0 & e^{-\frac{1}{2}\beta i} \end{pmatrix} \begin{pmatrix} 1 & -i \\ -i & 1 \end{pmatrix} \tag{17}$$

$$= \frac{1}{2} \begin{pmatrix} 1 & i \\ i & 1 \end{pmatrix} \begin{pmatrix} e^{\frac{1}{2}\beta i} & -ie^{\frac{1}{2}\beta i} \\ -ie^{-\frac{1}{2}\beta i} & e^{-\frac{1}{2}\beta i} \end{pmatrix} = \frac{1}{2} \begin{pmatrix} e^{i\frac{\beta}{2}} + e^{-i\frac{\beta}{2}} & -ie^{i\frac{\beta}{2}} + ie^{-i\frac{\beta}{2}} \\ ie^{i\frac{\beta}{2}} - ie^{-i\frac{\beta}{2}} & e^{i\frac{\beta}{2}} + e^{-i\frac{\beta}{2}} \end{pmatrix} \tag{18}$$

$$= \begin{pmatrix} \cos\frac{\beta}{2} & \sin\frac{\beta}{2} \\ -\sin\frac{\beta}{2} & \cos\frac{\beta}{2} \end{pmatrix}. \tag{19}$$

Note that since the matrix representations of the ladder operators are real, so the $\boldsymbol{L}_y$*-matrix is purely imaginary, the Wigner-d matrix is always real.*

1d. Show that the Wigner-D matrices satisfy the matrix representation property

$$\boldsymbol{D}^{(l)}(\hat{R}_1\hat{R}_2) = \boldsymbol{D}^{(l)}(\hat{R}_1)\boldsymbol{D}^{(l)}(\hat{R}_2), \tag{20}$$

starting from the defining equation of the $\boldsymbol{D}$-matrices.

Answer: *The defining equation is*

$$\hat{R}_i|lm\rangle = \sum_k |lk\rangle D^{(l)}_{km}(\hat{R}_i) \tag{21}$$

so

$$(\hat{R}_1\hat{R}_2)|lm\rangle = \sum_k |lk\rangle D^{(l)}_{km}(\hat{R}_1\hat{R}_2). \tag{22}$$

but also

$$\hat{R}_1\hat{R}_2|lm\rangle = \hat{R}_1 \sum_{k'} |lk'\rangle D^{(l)}_{k'm}(\hat{R}_2) \tag{23}$$

$$= \sum_k \sum_{k'} |lk\rangle D^{(l)}_{kk'}(\hat{R}_1) D^{(l)}_{k'm}(\hat{R}_2) \tag{24}$$

$$= \sum_k |lk\rangle [\boldsymbol{D}^{(l)}(\hat{R}_1)\boldsymbol{D}^{(l)}(\hat{R}_2)]_{km}. \tag{25}$$

Comparing Eqs. (22) and (25) we find

$$D^{(l)}_{km}(\hat{R}_1\hat{R}_2) = [\boldsymbol{D}^{(l)}(\hat{R}_1)\boldsymbol{D}^{(l)}(\hat{R}_2)]_{km}, \tag{26}$$

for $k, m = -l, -l+1, \ldots, l$, which proves Eq. (20).

Question 2: Questions chapter 7

For Jacobi vectors $\boldsymbol{r}$ and $\boldsymbol{R}$ the corresponding angular momentum operators are defined by

$$\hat{\boldsymbol{j}} = \boldsymbol{r} \times \hat{\boldsymbol{p}}_r \tag{27}$$

$$\hat{\boldsymbol{l}} = \boldsymbol{R} \times \hat{\boldsymbol{p}}_R \tag{28}$$

where $\hat{\boldsymbol{p}}_r$ and $\hat{\boldsymbol{p}}_R$ are the momentum operators for $\boldsymbol{r}$ and $\boldsymbol{R}$, respectively. The total angular momentum operator is defined by

$$\hat{\boldsymbol{J}} = \hat{\boldsymbol{j}} + \hat{\boldsymbol{l}}. \tag{29}$$

2a. Derive the following commutation relations, for $i = x, y, z$,

$$[\hat{\boldsymbol{J}}_i, r^2] = 0 \tag{30}$$

$$[\hat{\boldsymbol{J}}_i, R^2] = 0 \tag{31}$$

$$[\hat{\boldsymbol{J}}_i, \boldsymbol{r} \cdot \boldsymbol{R}] = 0 \tag{32}$$

2b. For two Hermitian matrices $\boldsymbol{A}$ and $\boldsymbol{B}$ that commute, $[\boldsymbol{A}, \boldsymbol{B}] = \boldsymbol{0}$, show that

$$e^{\boldsymbol{A}+\boldsymbol{B}} = e^{\boldsymbol{A}} e^{\boldsymbol{B}}$$

2c. Show that the previous result also holds if the matrices are not Hermitian (but still commute).

2d. Use the method described in chapter 7.5 to find the coupled angular momentum state $|(jl)JM\rangle$ with $j = 2$, $l = 3$, $J = 5$, $M = 4$.

2e. Use the method described in chapter 7.5 to find the coupled angular momentum state $|(jl)JM\rangle$ with $j = 2$, $l = 3$, $J = 4$, $M = 4$.