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

$$(\boldsymbol{n} \times \boldsymbol{r}) \cdot \boldsymbol{\nabla} = \boldsymbol{n} \cdot (\boldsymbol{r} \times \boldsymbol{\nabla}). \tag{1}$$

Derive this equation using the Levi-Civita tensor.

Answer: *On the lhs we have*

$$(\boldsymbol{n} \times \boldsymbol{r}) \cdot \boldsymbol{\nabla} = \epsilon_{ijk} n_j r_k \nabla_i. \tag{2}$$

On the rhs we havve

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

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

$$\boldsymbol{n} \cdot (\boldsymbol{r} \times \boldsymbol{\nabla}) = \epsilon_{kji} n_i r_j \nabla_k = \epsilon_{ijk} n_j r_k \nabla_i = (\boldsymbol{n} \times \boldsymbol{r}) \cdot \boldsymbol{\nabla}. \tag{4}$$

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

1b. Show that the Wigner $\boldsymbol{D}$-matrix for rotation around the y-axis is real (see Section 5.11, Eq. (5.119) of the lecture notes).

Answer: *The ladder operators are*

$$\hat{l}_\pm = \hat{l}_x \pm i\hat{l}_y \tag{5}$$

so

$$\hat{l}_y = \frac{\hat{l}_+ - \hat{l}_-}{2i} = -\frac{i}{2}(\hat{l}_+ - \hat{l}_-) \tag{6}$$

The rotation operator is

$$\hat{R}_y(\phi) = e^{-\frac{i}{\hbar}\phi \hat{l}_y} = e^{-\phi\frac{\hat{l}_+ - \hat{l}_-}{2\hbar}} \tag{7}$$

the matrix representation of the ladder operators is real, so $\hat{R}_y(\phi)$ *is real.*

1c. Compute the matrix elements of the rotation operator

$$\langle lm|\hat{R}(\boldsymbol{e}_z, \alpha)|lm'\rangle. \tag{8}$$

Answer:

$$\langle lm|\hat{R}(\boldsymbol{e}_z, \alpha)|lm'\rangle = \langle lm|e^{-\frac{i}{\hbar}\alpha \hat{l}_z}|lm'\rangle = e^{-im\alpha}\delta_{mm'}. \tag{9}$$

1d. 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*

$$e^{-\frac{i}{\hbar}\beta \boldsymbol{L}_y} = e^{\frac{1}{2}\beta \boldsymbol{A}} \tag{10}$$

with

$$\boldsymbol{A} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}. \tag{11}$$

First, we calculate the eigenvalues of the matrix from

$$\det(\boldsymbol{A} - \lambda \boldsymbol{I}) = \det \begin{pmatrix} -\lambda & 1 \\ -1 & -\lambda \end{pmatrix} = \lambda^2 + 1 = 0, \tag{12}$$

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

$$(\boldsymbol{A} - i\boldsymbol{I})\boldsymbol{c} = 0 \tag{13}$$

i.e.

$$\begin{pmatrix} -i & 1 \\ -1 & -i \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}. \tag{14}$$

so

$$\begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = \begin{pmatrix} 1 \\ i \end{pmatrix}. \tag{15}$$

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

$$\begin{pmatrix} i & 1 \\ -1 & i \end{pmatrix} \begin{pmatrix} d_1 \\ d_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}. \tag{16}$$

so

$$\begin{pmatrix} d_1 \\ d_2 \end{pmatrix} = \begin{pmatrix} i \\ 1 \end{pmatrix}. \tag{17}$$

Note that the eigenvectors are orthogonal, since

$$\boldsymbol{c}^\dagger \boldsymbol{d} = (1 \; -i) \begin{pmatrix} i \\ 1 \end{pmatrix} = i - i = 0. \tag{18}$$

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

$$\boldsymbol{U} = \frac{1}{\sqrt{2}}[\boldsymbol{c} \; \boldsymbol{d}] = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & i \\ i & 1 \end{pmatrix} \tag{19}$$

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

$$\boldsymbol{A} = \boldsymbol{U}\boldsymbol{\Lambda}\boldsymbol{U}^\dagger \tag{20}$$

where

$$\boldsymbol{\Lambda} = \begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix}. \tag{21}$$

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

$$\boldsymbol{U} e^{\frac{1}{2}\beta\boldsymbol{\Lambda}} \boldsymbol{U}^\dagger = \frac{1}{2} \begin{pmatrix} 1 & i \\ i & 1 \end{pmatrix} \begin{pmatrix} e^{\frac{1}{2}\beta i} & 0 \\ 0 & e^{-\frac{1}{2}\beta i} \end{pmatrix} \begin{pmatrix} 1 & -i \\ -i & 1 \end{pmatrix} \tag{22}$$

$$= \frac{1}{2} \begin{pmatrix} 1 & i \\ i & 1 \end{pmatrix} \begin{pmatrix} e^{\frac{1}{2}\beta i} & -ie^{\frac{1}{2}\beta i} \\ -ie^{-\frac{1}{2}\beta i} & e^{-\frac{1}{2}\beta i} \end{pmatrix} = \frac{1}{2} \begin{pmatrix} e^{i\frac{\beta}{2}} + e^{-i\frac{\beta}{2}} & -ie^{i\frac{\beta}{2}} + ie^{-i\frac{\beta}{2}} \\ ie^{i\frac{\beta}{2}} - ie^{-i\frac{\beta}{2}} & e^{i\frac{\beta}{2}} + e^{-i\frac{\beta}{2}} \end{pmatrix} \tag{23}$$

$$= \begin{pmatrix} \cos\frac{\beta}{2} & \sin\frac{\beta}{2} \\ -\sin\frac{\beta}{2} & \cos\frac{\beta}{2} \end{pmatrix}. \tag{24}$$

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.

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

$$\boldsymbol{D}^{(l)}(\hat{R}_1\hat{R}_2) = \boldsymbol{D}^{(l)}(\hat{R}_1)\boldsymbol{D}^{(l)}(\hat{R}_2), \tag{25}$$

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

Answer: *The defining equation is*

$$\hat{R}_i|lm\rangle = \sum_k |lk\rangle D^{(l)}_{km}(\hat{R}_i) \tag{26}$$

so

$$(\hat{R}_1\hat{R}_2)|lm\rangle = \sum_k |lk\rangle D^{(l)}_{km}(\hat{R}_1\hat{R}_2). \tag{27}$$

but also

$$\hat{R}_1\hat{R}_2|lm\rangle = \hat{R}_1 \sum_{k'} |lk'\rangle D^{(l)}_{k'm}(\hat{R}_2) \tag{28}$$

$$= \sum_{k}\sum_{k'} |lk\rangle D^{(l)}_{kk'}(\hat{R}_1) D^{(l)}_{k'm}(\hat{R}_2) \tag{29}$$

$$= \sum_{k} |lk\rangle [\boldsymbol{D}^{(l)}(\hat{R}_1)\boldsymbol{D}^{(l)}(\hat{R}_2)]_{km}. \tag{30}$$

Comparing Eqs. (27) and (30) we find

$$D^{(l)}_{km}(\hat{R}_1\hat{R}_2) = [\boldsymbol{D}^{(l)}(\hat{R}_1)\boldsymbol{D}^{(l)}(\hat{R}_2)]_{km}, \tag{31}$$

for $k, m = -l, -l+1, \ldots, l$, *which proves Eq. (25).*

Question 2: Questions chapter 7

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

$$\hat{\boldsymbol{j}} = \boldsymbol{r} \times \hat{\boldsymbol{p}}_r \tag{32}$$

$$\hat{\boldsymbol{l}} = \boldsymbol{R} \times \hat{\boldsymbol{p}}_R, \tag{33}$$

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

$$\hat{\boldsymbol{J}} = \hat{\boldsymbol{j}} + \hat{\boldsymbol{l}}. \tag{34}$$

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

$$[\hat{J}_i, r^2] = 0 \tag{35}$$

$$[\hat{J}_i, R^2] = 0 \tag{36}$$

$$[\hat{J}_i, \boldsymbol{r}\cdot\boldsymbol{R}] = 0. \tag{37}$$

Answer:

$$[\hat{J}_i, r^2] = [\hat{j}_i + \hat{l}_i, r^2] = [\hat{j}_i, r^2] + [\hat{l}_i, r^2]. \tag{38}$$

Since $\hat{l}_i$ *is not acting of* $\boldsymbol{r}$ *we have*

$$[\hat{l}_i, r^2] = 0. \tag{39}$$

For the first term

$$[\hat{j}_i, r^2] = [\epsilon_{ijk} r_j \hat{p}_k, r^2] = \epsilon_{ijk}(r_j[\hat{p}_k, r^2] + [r_j, r^2]\hat{p}_k) = \epsilon_{ijk} r_j [\hat{p}_k, r^2] \tag{40}$$

Remember that $k = x, y,$ *or* z, *so*

$$[\hat{p}_k, r^2] = [\hat{p}_k, r_k^2] = r_k[\hat{p}_k, r_k] + [\hat{p}_k, r_k]r_k = \frac{\hbar}{i} 2r_k \tag{41}$$

Thus,

$$\epsilon_{ijk} r_j [\hat{p}_k, r^2] = \frac{\hbar}{i}\epsilon_{ijk} r_j r_k = 0. \tag{42}$$

In the last step we use that the Levi-Cevita tensor changes sign if we interchange j *and* k, *but the product* $r_j r_k$ *does not, for for each* i *you get two terms that cancel.*

The derivation for $[\hat{J}_i, R^2] = 0$ *is completely analogous.*

For the third

$$[\hat{J}_i, \boldsymbol{r}\cdot\boldsymbol{R}] = [\hat{J}_i, r_j R_j] = r_j[\hat{J}_i, R_j] + [\hat{J}_i, r_j]R_j = r_j[\hat{l}_i, R_j] + [\hat{j}_i, r_j]R_j \tag{43}$$

Furthermore

$$[\hat{j}_i, r_j] = \epsilon_{ikl}[r_k\hat{p}_l, r_j] = \epsilon_{ikl}r_k[\hat{p}_l, r_j] = \frac{\hbar}{i}\epsilon_{ikl}r_k\delta_{lj} = \frac{\hbar}{i}\epsilon_{ikj}r_k \tag{44}$$

so

$$[\hat{j}, r_j]R_j = \frac{\hbar}{i}\epsilon_{ikj}r_kR_j \tag{45}$$

and similarly

$$r_j[\hat{l}, R_j] = \frac{\hbar}{i}\epsilon_{ikj}r_jR_k \tag{46}$$

so

$$r_j[\hat{l}, R_j] + [\hat{j}, r_j]R_j\frac{\hbar}{i} = \epsilon_{ikj}(r_kR_j + r_jR_k) = \epsilon_{ikj}r_kR_j + \epsilon_{ikj}r_jR_k = (\epsilon_{ikj} + \epsilon_{ijk})r_kR_j = 0, \tag{47}$$

where we used $\epsilon_{ijk} = -\epsilon_{ikj}$.

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

$$e^{\boldsymbol{A}+\boldsymbol{B}} = e^{\boldsymbol{A}}e^{\boldsymbol{B}}. \tag{48}$$

Answer: *Since the matrices commute and are Hermition, they have a common set of eigenvectors*

$$\boldsymbol{AU} = \boldsymbol{U\Lambda}_A \tag{49}$$

$$\boldsymbol{BU} = \boldsymbol{U\Lambda}_B \tag{50}$$

and so

$$e^{\boldsymbol{A}+\boldsymbol{B}} = \boldsymbol{U}e^{\boldsymbol{\Lambda}_A+\boldsymbol{\Lambda}_B}\boldsymbol{U}^\dagger \tag{51}$$

For diagonal matrices we have

$$e^{\boldsymbol{\Lambda}_A+\boldsymbol{\Lambda}_B} = e^{\boldsymbol{\Lambda}_A}e^{\boldsymbol{\Lambda}_B} \tag{52}$$

and by inserting the identity matrix $\boldsymbol{1} = \boldsymbol{U}^\dagger\boldsymbol{U}$ *we find*

$$\boldsymbol{U}e^{\boldsymbol{\Lambda}_A+\boldsymbol{\Lambda}_B}\boldsymbol{U}^\dagger = \boldsymbol{U}e^{\boldsymbol{\Lambda}_A}\boldsymbol{U}^\dagger\,\boldsymbol{U}e^{\boldsymbol{\Lambda}_B}\boldsymbol{U}^\dagger = e^{\boldsymbol{A}}e^{\boldsymbol{B}}. \tag{53}$$

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

Answer: *In this case we can use the Taylor expansion*

$$e^{\boldsymbol{A}} = \sum_{n=0}^{\infty}\frac{\boldsymbol{A}^n}{n!} \tag{54}$$

For the sum we have

$$e^{\boldsymbol{A}+\boldsymbol{B}} = \sum_{n=0}^{\infty}\frac{(\boldsymbol{A}+\boldsymbol{B})^n}{n!} = \sum_{n=0}^{\infty}\sum_{k=0}^{n}\left(\begin{array}{c} n \\ k \end{array}\right)\frac{1}{n!}\boldsymbol{A}^k\boldsymbol{B}^{n-k} = \sum_{n=0}^{\infty}\sum_{k=0}^{n}\frac{1}{k!(n-k)!}\boldsymbol{A}^k\boldsymbol{B}^{n-k}. \tag{55}$$

If we define $m = n - k$ *then we get*

$$e^{\boldsymbol{A}+\boldsymbol{B}} = \sum_{n=0}^{\infty}\sum_{\substack{k=0 \\ (m=n-k)}}^{n}\frac{\boldsymbol{A}^k}{k!}\frac{\boldsymbol{B}^m}{m!} \tag{56}$$

and we note that for every value of k, m takes the values from infinity to zero, so

$$e^{\boldsymbol{A}+\boldsymbol{B}} = \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} \frac{\boldsymbol{A}^k}{k!} \frac{\boldsymbol{B}^m}{m!} = e^{\boldsymbol{A}} e^{\boldsymbol{B}}. \tag{57}$$