11.13 & ROTATIONAL SYM.

OUR TASK IS TO APPLY EQ^N 11.63.

THE DIFFICULT PART IS THE CALCULATION OF $|\wp|^2$, THE DIPOLE MOMENT VECTOR SQUARED.

THERE IS REASON TO EXPECT OUR WORK TO SIMPLIFY. INDEED, THE $|\wp|^2$ QUANTITY WILL END UP BEING THE SAME FOR ALL STATES OF EQUAL l QUANTUM NUMBER [i.e. m - INDEPENDENT]! THE REASON IS THAT THE OBJECTS WE ARE WORKING W/ ARE ~~HIGHLY~~ SYMMETRIC:

- THE INITIAL & FINAL STATES ARE ONES OF DEFINITE ANGULAR MOMENTUM, i.e. DEF. ROT. SYMMETRY.

- THE PERTURBATION IS A VECTOR OPERATOR, SO IT TOO HAS DEF. ROT. SYM.

- FURTHER, THE INITIAL STATE ~~HAS~~ ZERO ANG. MOM., SO IT IS INVARIANT UNDER ALL ROTATIONS.

- THE $|\wp|^2$ QUANTITY IS AN EVEN SUM OVER THE SQUARES OF THE

COMPONENTS OF $\vec{r}$, WHICH ITSELF AS WE MENTIONED HAS DEF. ROT. SYM.

SO LET'S INSPECT $|r|^2$ FOR SOME INITIAL STATE l, m :

$$|r|^2 = \sum_i \left| \langle 100 | x_i | 2lm \rangle \right|^2$$

[I'VE DROPPED THE FACTOR OF $-e$ FOR CONVENIENCE]

(A) $$= \sum_i \langle 2lm | x_i | 100 \rangle \langle 100 | x_i | 2lm \rangle$$

OUR GOAL IS TO SHOW THAT THIS QUANTITY IS INDEPENDENT OF m FOR FIXED l.

TO THIS END WE WILL MAKE USE OF THE FACT THAT THE SPAN OF THE VECTORS $|2lm\rangle$, $m = -l, -l+1, \ldots, +l$ FORMS A LINEAR SPACE THAT IS WHAT IS CALLED AN "IRREDUCIBLE REPRESENTATION", A MORE GENERAL NOTION OF WHICH "STATES OF DEFINITE n & l" IS A SPECIFIC EXAMPLE.

ANY TWO VECTORS IN AN IRREDUCIBLE REP. ARE EQUIVALENT IN THE SENSE THAT ONE CAN BE OBTAINED FROM THE OTHER BY SOME [WEIGHTED] COMBINATION OF

SYMMETRY OPERATIONS. FOR STATES OF DEF ℓ, THE RELEVANT SYMMETRY OPERATIONS ARE ROTATION OPERATORS [SEE SEC 6.5.2]. IN FACT, GIVEN ANY TWO VECTORS ~~in an~~ $|\psi\rangle$ + $|\phi\rangle$ IN AN IRRED. REP., WE CAN CONSTRUCT AN OPERATOR $|\psi\rangle\langle\phi|$ THAT CAN BE WRITTEN AS A WEIGHTED SUM OF ROT. OPERATORS O_R, i.e.

$$|\psi\rangle\langle\phi| = \sum_R c_R O_R$$

WHERE THE c_R ARE SOME COEFFICIENTS. [ACTUALLY, THE SUM SHOULD BE AN INTEGRAL BUT THE DISTINCTION DOES NOT CONCERN US HERE].

THE ABOVE SUGGESTS THAT WE $\langle 2\ell m|$ IN THE EQ^{n} ABOVE MARKED (A) AND MULTIPLY IT BY $1 = \langle 2\ell m'|2\ell m'\rangle$ FOR SOME OTHER $m' \neq m$, i.e.

$$\begin{aligned}\langle 2\ell m| &= \langle 2\ell m'|2\ell m'\rangle\langle 2\ell m| \\ &= \langle 2\ell m'|\left[|2\ell m'\rangle\langle 2\ell m|\right]\end{aligned}$$

Q1: SHOW THAT IF $|2\ell m'\rangle\langle 2\ell m|$ COMMUTES W/ $\sum_i x_i |100\rangle\langle 100| x_i$, THEN $|\gamma|^2$ IS INDEPENDENT OF m [FOR FIXED ℓ].

Q2: SHOW THAT IF $\sum_i X_i |100\rangle\langle 100| X_i$ COMMUTES W/ ARBITRARY ROTATIONS OR [i.e. IF IT IS A ROTATIONAL SCALAR], THEN $|2\ell m'\rangle\langle 2\ell m|$ COMMUTES W/ $\sum_i X_i |100\rangle\langle 100| X_i$.

SO IF WE CAN SHOW THAT $\sum_i X_i |100\rangle\langle 100| X_i$ IS A ROTATIONAL SCALAR, THEN OUR WORK IS DONE.

Q3: PROVE THAT $\sum_i X_i |100\rangle\langle 100| X_i$ IS A ROTATIONAL SCALAR, i.e. THAT IT COMMUTES W/ ANY ROTATION OPERATOR.

MAKE USE OF THE FACTS GIVEN IN THE BULLET POINTS ON THE FIRST PAGE, ESPECIALLY THE LAST THREE.

SO THERE YOU HAVE IT. IT SUFFICES TO COMPUTE ~~TWO~~ $|\vec{r}|^2$ FOR JUST TWO STATES, ONE FROM $n=2$, $\ell=1$ AND ONE FROM $n=2$, $\ell=0$. ~~FOR $|\vec{r}|^2$ W/ $\ell=0$~~ FOR $\ell=0$ $|\vec{r}|^2$ IS ZERO BY SELECTION RULES [WHICH ONE?!] AND FOR $\ell=1$ YOU ONLY NEED TO COMPUTE

ONE MATRIX ELEMENT, AGAIN BECAUSE OF SELECTION RULES.

KEEPING ~~WITH~~ YOUR SYMMETRY RESULTS IN MIND, HOW CAN WE ANSWER THEN Q 11.16 a) AND b) WITHOUT ANY CALCULATIONS? FOR c) IT SHOULD ONLY BE NECESSARY TO EVALUATE ONE RADIAL INTEGRAL.

ANSWERS

A1: $\sum_i \langle 2\ell m | x_i | 100\rangle\langle 100 | x_i | 2\ell m\rangle$

$$= \sum_i \langle 2\ell m' | \left[|2\ell m'\rangle\langle 2\ell m| \right] \cdot x_i |100\rangle\langle 100| x_i \; |2\ell m\rangle$$

$$(!) = \sum_i \langle 2\ell m' | x_i |100\rangle\langle 100| x_i \cdot |2\ell m'\rangle \cancelto{1}{\langle 2\ell m | 2\ell m\rangle}$$

$$= \sum_i \langle 2\ell m' | x_i |100\rangle\langle 100| x_i |2\ell m'\rangle$$

WHERE IN THE (!) STEP WE USE THE ASSUMPTION GIVEN IN THE QUESTION.

A2: $|2\ell m\rangle$ STATES ARE IN THE SAME IRRED. REP. SO THE OPERATOR ~~CAN~~ $|2\ell m'\rangle\langle 2\ell m|$ CAN BE WRITTEN AS A SUM $\sum_R c_R O_R$. A SUM OF OPERATORS COMMUTES W/ SOME OTHER OPERATOR IF EACH TERM INDIVIDUALLY COMMUTES.

A3 : $O_R \sum_i x_i |100\rangle\langle 100| x_i$

$= \sum_i O_R x_i |100\rangle\langle 100| x_i$

(α) $= \sum_i O^{+}_{R^{-1}} x_i |100\rangle\langle 100| x_i$

(β) $= \sum_i O^{+}_{R^{-1}} x_i O_{R^{-1}} |100\rangle\langle 100| x_i$

(γ) $= \sum_i \underbrace{\left[R^{-1} \vec{r} \cdot \hat{x}_i \right]}_{=[R^{-1}\vec{x}]_i} |100\rangle\langle 100| x_i$

$= \sum_i [R^{-1}\vec{x}]_i |100\rangle\langle 100| O^{+}_{R^{-1}} x_i O_{R^{-1}} O^{+}_{R^{-1}}$

$= \sum_i [R^{-1}\vec{x}]_i |100\rangle\langle 100| [R^{-1}\vec{x}]_i \, O^{+}_{R^{-1}}$

$= \sum_i [R^{-1}\vec{x}]_i |100\rangle\langle 100| [R^{-1}\vec{x}]_i \, O_R$

(δ) $= \sum_{\substack{i \\ \cancel{jk}}} \left[\sum_{j=1}^{3} R^{-1}_{ij} x_j \right] |100\rangle\langle 100|$

$\left[\sum_{k=1}^{3} R^{-1}_{ik} x_k \right] O_R$

(ε) $= \sum_{jk} \left(\sum_i R^{T-1}_{ji} R^{-1}_{ik} \right) x_j |100\rangle\langle 100| x_k O_R$

(ζ) $= \sum_{jk} \delta_{jk} x_j |100\rangle\langle 100| x_k O_R$

$= \sum_j x_j |100\rangle\langle 100| x_j O_R$

~~WHERE WE~~ DISCUSSION POINTS

(α) : O_R IS A UNITARY OPERATOR SO

$$O_R^{\dagger} = O_R^{-1}$$

ALSO O_R^{-1} IS ~~THE~~ EQUAL TO $O_{R^{-1}}$ WHERE R^{-1} IS THE INVERSE ROTATION.

(β) : $|100\rangle$ IS A ROTATIONAL SCALAR

SO $O_R|100\rangle = |100\rangle$

(γ) : X_i IS A COMPONENT OF A VECTOR OPERATOR SO UNDER ROTATION IT ROTATES LIKE A VECTOR:

$$O_R^{\dagger} X_i O_R = [R\vec{x}]_i$$

WHERE $\vec{x} = (x, y, z)$ AND R IS THE 3×3 ORTHOGONAL MATRIX ASSOCIATED W/ THE ROTATION.

(δ) : EXPAND THE EXPRESSION IN TERMS OF THE MATRIX ELEMENTS OF R^{-1}

($\cancel{\zeta}$ φ) : R IS BY DEFINITION ORTHOGONAL

SO $R^T = R^{-1}$

(ε) : GROUPING TERMS AND TAKING TRANSPOSE SO ~~SOME~~ BRACKETED EXPRESSION TAKES FORM OF MATRIX PRODUCT.