

The 9 matrix elements of \vec{T} .

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Matrix Elements of \vec{T} -Vectors

refs. Sakurai, Sec. 3.10;
Landau & Lifshitz "QM", § 29.

- 1) We know that for any \vec{T} -vector: $\langle \alpha j m | \vec{T} | \alpha' j' m' \rangle = 0$, unless $j' = j, j \pm 1$ and $m' = m, m \pm 1$. So only 9 non-zero matrix elements are possible. These can be inter-related, and their m -dependence specified, by exploiting various commutation relations between \vec{T} and its companion \vec{J} .

Our first reduction of the problem is to write \vec{T} in the form...

$$\begin{aligned} \vec{T} &= \hat{x} T_x + \hat{y} T_y + \hat{z} T_z \dots (\hat{x}, \hat{y}, \hat{z}) = \text{coordinate unit vectors,} \\ \vec{T} &= \frac{1}{2} (\hat{x} - i\hat{y}) T^+ + \frac{1}{2} (\hat{x} + i\hat{y}) T^- + \hat{z} T_z, \quad T^\pm = T_x \pm i T_y. \end{aligned} \quad (1)$$

We do this in order to use the selection rules...

$$T^\pm = 0 \text{ unless } m' = m \mp 1, \quad T_z = 0 \text{ unless } m' = m;$$

$$\begin{aligned} \text{So // } \langle \alpha j m | \vec{T} | \alpha' j' m' \rangle &= \frac{1}{2} (\hat{x} - i\hat{y}) \delta_{m', m-1} \langle \alpha j m | T^+ | \alpha' j' m' \rangle + \\ &\quad \boxed{\text{G.M.E.'s}} \left\{ \begin{aligned} &+ \frac{1}{2} (\hat{x} + i\hat{y}) \delta_{m', m+1} \langle \alpha j m | T^- | \alpha' j' m' \rangle + \\ &+ \hat{z} \delta_{m', m} \langle \alpha j m | T_z | \alpha' j' m' \rangle, \end{aligned} \right\} \text{ and } j' = j, j \pm 1. \end{aligned} \quad (2)$$

Furthermore, we can get the T^+ matrix elements from the T^- . Since \vec{T} is Hermitian, then $(T^+)^\dagger = T^-$, and we can write...

$$\rightarrow \langle \alpha j m | T^+ | \alpha' j' m' \rangle = (\langle \alpha' j' m' | T^- | \alpha j m \rangle)^* \quad (3)$$

The problem is reduced to calculating appropriate matrix elements of T^\pm & T_z . Then we will have all possible matrix elements of \vec{T} , as desired.

Vector Matrix Elements : non-zero M.E.'s of T^- .

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2) Certain T^- matrix elements follow from the commutator identity...

→ $[J^-, T^-] = 0$ ← proof is straightforward,

$$\langle \alpha j m-1 | \widehat{J^- T^-} | \alpha' j' m' \rangle = \langle \alpha j m-1 | T^- \widehat{J^-} | \alpha' j' m' \rangle,$$

$$\langle J^+ (\alpha j m-1) | T^- | \alpha' j' m' \rangle = \langle \alpha j m-1 | T^- | J^- (\alpha' j' m') \rangle.$$

→ But : $J^\pm | \alpha j \mu \rangle = \sqrt{(j \mp \mu)(j \pm \mu + 1)} | \alpha j \mu \pm 1 \rangle,$

$$\begin{aligned} \Rightarrow \sqrt{(j-m+1)(j+m)} \langle \alpha j m | T^- | \alpha' j' m' \rangle &= \\ &= \sqrt{(j'+m')(j'-m'+1)} \langle \alpha j m-1 | T^- | \alpha' j' m'-1 \rangle. \end{aligned} \quad (4)$$

By the T^- selection rule, both matrix elements here are $\equiv 0$, unless $m' = m+1$. Impose this, and rewrite Eq. (4) in the form...

$$\rightarrow \frac{\langle \alpha j m | T^- | \alpha' j' m+1 \rangle}{\sqrt{(j'+m+1)(j'-m)}} = \frac{\langle \alpha j m-1 | T^- | \alpha' j' m \rangle}{\sqrt{(j+m)(j-m+1)}}. \quad (5)$$

This must hold for all j & j' , and in particular $j' = j$. Impose this, and also define : $\mu = m-1$, on the RHS of the eqn. Then...

$$\rightarrow \frac{\langle \alpha j m | T^- | \alpha' j m+1 \rangle}{\sqrt{(j+m+1)(j-m)}} = \frac{\langle \alpha j \mu | T^- | \alpha' j \mu+1 \rangle}{\sqrt{(j+\mu+1)(j-\mu)}}, \quad \mu = m-1. \quad (6)$$

3) A semi-amazing fact now emerges : this ratio must be independent of the m -value involved, because it retains its form and remains the same as we step m through all its values : $m \rightarrow \mu = m-1 \rightarrow \mu' = \mu-1 = m-2 \rightarrow$ etc. We therefore define this m -independent ratio as

Vector Matrix Elements : reduced M.E. $\langle \alpha_j \| T \| \alpha'_j \rangle$.

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a new entity $\langle \alpha_j \| T \| \alpha'_j \rangle$, called a "reduced matrix element" and write

$$\langle \alpha_j m | T^- | \alpha'_j m+1 \rangle = \sqrt{(j-m)(j+m+1)} \langle \alpha_j \| T \| \alpha'_j \rangle. \quad (7)$$

Remarks

1. $\langle \alpha_j \| T \| \alpha'_j \rangle$ is called "reduced" because its m -dependence has been extracted.
2. Nothing more can be done about calculating $\langle \alpha_j \| T \| \alpha'_j \rangle$ until an explicit form for \vec{T} is given. However, we do know that $\langle \alpha_j \| T \| \alpha'_j \rangle$ is independent of m , and may calculate it from Eq. (7) for any convenient m -value ... e.g. for $m=0$: $\langle \alpha_j \| T \| \alpha'_j \rangle = \langle \alpha_j 0 | T^- | \alpha'_j 1 \rangle / \sqrt{j(j+1)}$.
3. T is a Hermitian operator if \vec{T} is -- we shall show this shortly.

Assuming T is Hermitian, and knowing that $T^+ = (T^-)^\dagger$, we can use Eq. (7) to write ...

$$\langle \alpha_j m | T^\mp | \alpha'_j m \pm 1 \rangle = \sqrt{(j \mp m)(j \pm m + 1)} \langle \alpha_j \| T \| \alpha'_j \rangle,$$

$$\Delta m = \pm 1 \quad \text{so} \quad \boxed{\langle \alpha_j m | \vec{T} | \alpha'_j m \pm 1 \rangle = \frac{1}{2} (\hat{x} \pm i \hat{y}) \sqrt{(j \mp m)(j \pm m + 1)} \langle \alpha_j \| T \| \alpha'_j \rangle.} \quad (8)$$

This gives 2 of the 9 matrix elements we are looking for.

4) Next, we relate T_z (for $j'=j, m'=m$) to $\langle \alpha_j \| T \| \alpha'_j \rangle$. We use ...

$$\rightarrow [J^+, T^-] = 2T_z \leftarrow \text{by straightforward arithmetic,}$$

$$\begin{aligned} \text{so} \quad 2 \langle \alpha_j m | T_z | \alpha'_j m \rangle &= \langle J^-(\alpha_j m) | T^- | \alpha'_j m \rangle - \langle \alpha_j m | T^- | J^+(\alpha'_j m) \rangle \\ &= \sqrt{(j+m)(j-m+1)} \langle \alpha_j m-1 | T^- | \alpha'_j m \rangle - \sqrt{(j-m)(j+m+1)} \langle \alpha_j m | T^- | \alpha'_j m+1 \rangle \end{aligned}$$

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Vector Matrix Elements: 3rd M.E. of \vec{T} for $\Delta j = 0$.

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These result from plugging in T^- matrix elements of Eq. (7) above.

$$2 \langle \alpha j m | T_z | \alpha' j m \rangle = \underbrace{\left[(\sqrt{j+m}(j-m+1))^2 - (\sqrt{j-m}(j+m+1))^2 \right]}_{= 2m} \langle \alpha j || \mathcal{T} || \alpha' j \rangle$$

$\Delta m = 0$ and //

$$\begin{aligned} \langle \alpha j m | T_z | \alpha' j m \rangle &= m \langle \alpha j || \mathcal{T} || \alpha' j \rangle, \\ \Rightarrow \langle \alpha j m | \vec{T} | \alpha' j m \rangle &= \hat{z} m \langle \alpha j || \mathcal{T} || \alpha' j \rangle \end{aligned}$$

(9)

Again, we can calculate $\langle \alpha j || \mathcal{T} || \alpha' j \rangle$ from T_z for any convenient m -value (except $m=0$, which gives an indeterminate expression). Eqs. (8) & (9) together give all 3 non-zero \vec{T} -vector matrix elements for $j' = j$.

Eq. (9) allows an easy demonstration that \mathcal{T} is Hermitian if T_z is -- as was assumed in Eq. (8). Start from...

$$\rightarrow \langle \alpha j || \mathcal{T} || \alpha' j \rangle = \frac{1}{m} \langle \alpha j m | T_z | \alpha' j m \rangle, \quad m \neq 0$$

$$\begin{aligned} \langle \alpha j || \mathcal{T} || \alpha' j \rangle^* &= \frac{1}{m} \langle \alpha j m | T_z | \alpha' j m \rangle^* = \frac{1}{m} \langle \alpha' j m | \underbrace{T_z^\dagger}_{= T_z} | \alpha j m \rangle \\ &= \frac{1}{m} \langle \alpha' j m | T_z | \alpha j m \rangle = \langle \alpha' j || \mathcal{T} || \alpha j \rangle. \end{aligned}$$

(10)

So $\mathcal{T}_{AB}^* = \mathcal{T}_{BA}$, for matrix elements, and \mathcal{T} is Hermitian if T_z is.

- 5) The calculation of the remaining 6 matrix elements of \vec{T} , for $j' = j \pm 1$ and $m' = m, m \pm 1$, proceeds in a similar fashion -- using certain semi-clever commutation rules, plus the selection rules, to pick out the desired matrix elements of T^- & T_z . Details are in Condon & Shortley, pp. 59-64. There are no big surprises, just a great deal of algebra.

Vector Matrix Elements: Summary of all non-zero $\langle \alpha_j m | \vec{T} | \alpha' j' m' \rangle$. 4 17

Just as the 3 \vec{T} -vector matrix elements for $j' = j$ could all be related to a single reduced matrix element $\langle \alpha_j \| \mathcal{T} \| \alpha' j \rangle$, so too are the 3 elements for $j' = j+1$ related to $\langle \alpha_j \| \mathcal{T} \| \alpha' j+1 \rangle$, and the 3 for $j' = j-1$ related to $\langle \alpha_j \| \mathcal{T} \| \alpha' j-1 \rangle$. These three reduced matrix elements are in general different, and we shall denote them by...

$$P = \langle \alpha_j \| \mathcal{T} \| \alpha' j+1 \rangle, \quad Q = \langle \alpha_j \| \mathcal{T} \| \alpha' j \rangle, \quad R = \langle \alpha_j \| \mathcal{T} \| \alpha' j-1 \rangle. \quad (11)$$

With that, the final results for all possible non-zero \vec{T} -vector matrix elements may be reduced to the following table...

① $j' = j+1$

$$\langle \alpha_j m | \vec{T} | \alpha' j+1, m \pm 1 \rangle = \mp \frac{1}{2} (\hat{x} \pm i \hat{y}) \sqrt{(j \pm m + 1)(j \pm m + 2)} [P],$$

$$\langle \alpha_j m | \vec{T} | \alpha' j+1, m \rangle = \hat{z} \sqrt{(j+1)^2 - m^2} [P];$$

② $j' = j$

$$\langle \alpha_j m | \vec{T} | \alpha' j, m \pm 1 \rangle = \frac{1}{2} (\hat{x} \pm i \hat{y}) \sqrt{(j \mp m)(j \pm m + 1)} [Q],$$

$$\langle \alpha_j m | \vec{T} | \alpha' j, m \rangle = \hat{z} m [Q];$$

③ $j' = j-1$

$$\langle \alpha_j m | \vec{T} | \alpha' j-1, m \pm 1 \rangle = \pm \frac{1}{2} (\hat{x} \pm i \hat{y}) \sqrt{(j \mp m)(j \mp m - 1)} [R],$$

$$\langle \alpha_j m | \vec{T} | \alpha' j-1, m \rangle = \hat{z} \sqrt{j^2 - m^2} [R].$$

(12)

These relations hold in any QM system where \hat{L} momentum \vec{J} is well-defined.

Vector Matrix Elements : Reduction of vector-coupling to 3 M.E.'s. X 18

6) This table represents an enormous simplification for calculating matrix elements involving vector coupling between any two states of well-defined ℓ momenta. . . this is the usual case in atomic & molecular systems, where the states do have a well-defined \vec{J} , and the couplings go like $(e\vec{r}) \cdot \vec{E}$ [electric dipole] or $\vec{\mu} \cdot \vec{B}$ [magnetic dipole]. The table reduces the calculational task to finding just 3 reduced matrix elements: P, Q, R .

As an example of the use of the table, consider electric dipole transitions: $(\alpha' j m') \rightarrow (\alpha j+1, m)$, driven by a coupling: $V = \vec{E} \cdot \vec{r}$, with $\vec{E} \propto$ an applied electric field. Since \vec{E} will be const over the dimensions \vec{r} of the atom, the key matrix element of the coupling is...

$$M = \langle \alpha, j+1, m | V | \alpha' j m' \rangle = \vec{E} \cdot \langle \alpha, j+1, m | \vec{r} | \alpha' j m' \rangle \quad (13)$$

Now use ③ in the table (with j shifted up one unit) to write...

$$\left. \begin{aligned} M(m' = m \pm 1) &= \pm \frac{1}{2} (\epsilon_x \pm i \epsilon_y) \sqrt{(j \mp m)(j \mp m + 1)} [R], \\ M(m' = m) &= \epsilon_z \sqrt{(j+1)^2 - m^2} [R], \quad R = \langle \alpha, j+1 || r || \alpha' j \rangle. \end{aligned} \right\} \quad (14)$$

In this case, R is called the radial matrix element for the system. The transition rate (or line strength) for the coupling is $\Gamma \propto |M|^2$, so...

$$\left\{ \begin{aligned} \Gamma(m' = m \pm 1) &= \frac{1}{4} \epsilon_{\perp}^2 |R|^2 (j \mp m)(j \mp m + 1), \quad \Gamma(m' = m) = \epsilon_{\parallel}^2 |R|^2 [(j+1)^2 - m^2], \\ \text{where: } \epsilon_{\perp} &= (\epsilon_x^2 + \epsilon_y^2)^{\frac{1}{2}}, \quad \epsilon_{\parallel} = \epsilon_z, \text{ are components of } \vec{E} \perp \& \parallel \text{ z-axis.} \end{aligned} \right. \quad (15)$$

Notice that you can get the ratios of the transition rates without knowing R . For elementary particle decays, the "branching ratios" are sometimes gotten this way.