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Differential operators in graphical spin algebra

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Abstract. The graphical representation of the differential operators is given within the framework of graphical spin algebra. Application is made to the evaluation of their reduced matrix element exhibiting the great simplicity of the method.

1. Introduction

Graphical techniques are now extensively used in nuclear, particle and atomic physics since they have obvious value in conciseness, structural clarity and as a mnemonic and book-keeping aid (Stedman 1975, 1976, Harary 1969, Lehman and O'Connell 1973, Canning 1973, Briggs 1971, Judd 1962, Brink and Satchler 1968, Yutsis *et al* 1962, Guichon 1975, Lulek 1975, Kibler and Guichon 1976). The graphical technique in angular momentum theory is an adequate illustration and we shall refer to it as the graphical spin algebra (GSA) and use the notations and conventions defined in Elbaz and Castel (1972). It concerns a development of the notations employed in different earlier published papers (Elbaz *et al* 1966a, b, c, 1967). The main difference comes from the introduction of a graphical representation of a ket by a simple arrow (outgoing for a positive magnetic momentum) and of a bra by a double arrow (ingoing for a positive magnetic momentum). Such a representation greatly simplifies the phase determination and allows a direct representation of a Clebsch–Gordan coefficient by a triangle at a node (the orientation of which does not matter). A practical digest of the GSA can be found in Elbaz and Castel (1971). Our notation differs from that of Stone (1976) by the fact that the $(-1)^{j-m}$ phase is always contained in the second arrow of a bra while a simple node on a j-line brings the factor $(2j+1)^{-1/2}$. Moreover, in the GSA a triangle node is always attached to a Clebsch–Gordan coefficient. Recently Danos and Gillet (1971) have used the graphical technique previously proposed by Danos (1971) to evaluate some specific reduced matrix elements of differential operators. Thus it appeared that the GSA could be a powerful tool to solve such a problem and this paper gives the graphical representation of the usual differential operators, shows that indeed one can easily obtain some well known results concerning these operators and, moreover, allows a straightforward evaluation of the reduced matrix element of any differential operator. It will certainly be of great help in relativistic nuclear theory for instance. We recall in § 2 the standardization of the vector operators and give the graphical equivalent of a vector and of a tensor product constructed with two vector operators. In § 3 we define the diagrammatic equivalent of the usual differential operators grad, div, curl, etc. We then show how to apply the Wigner–Eckart theorem to these operators and finally we give some interesting applications in the evaluation of the reduced matrix elements of these operators.

2. The standardization of the vector operators

2.1. Definitions

It is well known (Edmonds 1957) that one can define the standard components of a vector operator A as the components A_μ of a rank-one irreducible tensor operator

$$
\begin{aligned}
A_{11} &= -\frac{1}{\sqrt{2}}(A_x + \mathrm{i}A_y) \\
A_{10} &= A_z \\
A_{1-1} &= \frac{1}{\sqrt{2}}(A_x - \mathrm{i}A_y).
\end{aligned}
\tag{2.1}
$$

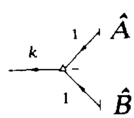
Graphically these components will be represented by

$$
A_\mu = \overset{\hat{A}}{\dashrightarrow}\overset{1\mu}{\longrightarrow} = \hat{A} \vdash\!\overset{1\mu}{\longrightarrow}. \tag{2.2}
$$

This representation is in fact a generalization of the graphical representation of the spherical harmonics and identical to the representation of any irreducible tensor operator (ITO) T_{kq} as proposed in the GSA. (Elbaz *et al* 1966a, b, c, 1967, Elbaz and Castel 1971, 1972).

One then obtains the Π_{kq} tensorial product of two vector operators with

$$
\Pi_{kq} = \sum_{\mu\nu} \langle 1\mu\, 1\nu | kq \rangle A_\mu B_\nu = \tag{2.3}
$$



with $k = 0, 1, 2$.

2.2. The scalar product

If one sets $k = 0$ in the previous diagram, one obtains the value

$$
\Pi_{00} = \frac{1}{\sqrt{3}} \sum_\mu A_\mu B_\mu^+ = \frac{1}{\sqrt{3}} \sum_\mu (-1)^{1-\mu} A_\mu B_{-\mu} = \frac{1}{\sqrt{3}}\, \hat{A} \vdash\!\overset{1}{\longrightarrow}\!\dashv \hat{B}
$$

$$
\Pi_{00} = \frac{1}{\sqrt{3}}(A_1 B_{-1} + A_{-1} B_1 - A_0 B_0).
$$

If one uses the definition (2.1) of the standard components one reads

$$
\Pi_{00} = \frac{1}{\sqrt{3}}(A_1 B_{-1} + A_{-1} B_1 - A_0 B_0) = -\frac{1}{\sqrt{3}} \boldsymbol{A} \cdot \boldsymbol{B} = \frac{1}{\sqrt{3}}\, \hat{A} \vdash\!\overset{1}{\longrightarrow}\!\dashv \hat{B}. \tag{2.4}
$$

We note here that if one uses Biedenharn's definition of the standard components of a tensor operator (Biedenharn and Rose 1953),

$$
\begin{aligned}
A_1 &= \frac{1}{\sqrt{2}}(-\mathrm{i}A_x + A_y) \\
A_0 &= \mathrm{i}A_z \\
A_{-1} &= \frac{1}{\sqrt{2}}(\mathrm{i}A_x + A_y),
\end{aligned}
\qquad (2.5)
$$

the minus sign goes out and one reads

$$\boldsymbol{A} \,.\, \boldsymbol{B} = \hat{A} \overset{1}{\longmapsto} \hat{B} \qquad (2.6)$$

but let us use, as is done commonly, Edmond's conventions.

2.3. The vector or cross product

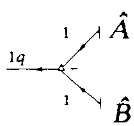
One sets the $k=1$ value in the Π_{kq} definition and gets, for instance,

$$\Pi_{11} = \frac{1}{\sqrt{2}}(A_1B_0 - A_0B_1) = \tfrac{1}{2}(A_zB_x - A_xB_z) + \tfrac{1}{2}\mathrm{i}(A_zB_y - A_yB_z)$$

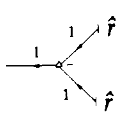
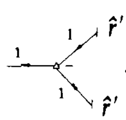
or, if one introduces the vector product $\boldsymbol{C} = \boldsymbol{A} \times \boldsymbol{B}$, one finds that

$$
\begin{aligned}
\Pi_{11} &= \frac{1}{2}(C_y - \mathrm{i}C_x) = \frac{\mathrm{i}}{\sqrt{2}}C_{11} \\
\Pi_{10} &= \frac{\mathrm{i}}{\sqrt{2}}C_z = \frac{\mathrm{i}}{\sqrt{2}}C_{10} \\
\Pi_{1-1} &= \frac{1}{2}(C_y + \mathrm{i}C_x) = \frac{\mathrm{i}}{\sqrt{2}}C_{1-1}.
\end{aligned}
\qquad (2.7)
$$

In other words

$$\Pi_{1q} = \frac{\mathrm{i}}{\sqrt{2}}(\boldsymbol{A} \times \boldsymbol{B})_{1q} =$$  . (2.8)

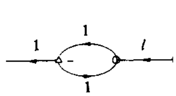
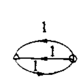
What happens with this representation if $\boldsymbol{A} = \boldsymbol{B} = \boldsymbol{r}$?

$$\frac{\mathrm{i}}{\sqrt{2}}(\boldsymbol{r} \times \boldsymbol{r})_{1q} =$$  $$= \int \mathrm{d}\hat{r}'\, \delta(\hat{r} - \hat{r}')$$  .

Since

$$\delta(\hat{r} - \hat{r}') = \sum_l \hat{r} \overset{l}{\longmapsto} \hat{r}'$$

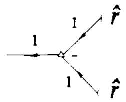
the closure relation of the spherical harmonics, one gets, after integration over the angular variable,

$$\frac{\mathrm{i}}{\sqrt{2}}(\boldsymbol{r} \times \boldsymbol{r})_{1q} =$$  $$\hat{r} = [l^{-1}]\delta_{l1}$$  $$\overset{1}{\longmapsto} \hat{r}. \qquad (2.9)$$

The circle symbol is the reduced matrix element of the $Y_{1\mu}$ spherical harmonic

$$\langle 1\|Y_1\|1\rangle = -\frac{[1\quad 1\quad 1]}{\sqrt{(4\pi)}}\begin{pmatrix}1 & 1 & 1\\ 0 & 0 & 0\end{pmatrix} = 0 \tag{2.10}$$

and one finds what we expected, namely

$$(\boldsymbol{r}\times\boldsymbol{r})_q =$$  $$= 0. \tag{2.11}$$

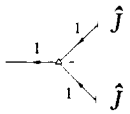
One other interesting application of the same technique concerns the cross product of the $\boldsymbol{J}$ kinetic momentum operator. In that case the closure relation reads

$$\delta(\hat{J}-\hat{J}') = \frac{1}{2}\sum_K \hat{J} \xrightarrow{K} \hat{J}' \tag{2.12}$$

and the reduced matrix element takes the value

$$\langle J\|J^{(1)}\|J\rangle = \sqrt{[J(J+1)(2J+1)]} = \sqrt{6} \qquad \text{when } J=1. \tag{2.13}$$

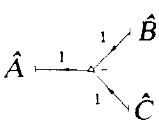
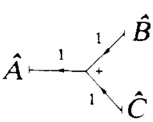
Collecting these results leads immediately to the well known relation

$$(\boldsymbol{J}\times\boldsymbol{J})_q = -\mathrm{i}\sqrt{2}$$  $$= \mathrm{i} \xrightarrow{1} \hat{J} = \mathrm{i}\, J_q. \tag{2.14}$$

More generally we can assert that the commutator of two vector operators $\boldsymbol{A}$ and $\boldsymbol{B}$ is graphically represented by the diagram (2.8). If $\boldsymbol{A}$ and $\boldsymbol{B}$ commute, a change of the lecture order at the pole must not affect the results while the usual rule brings a minus sign. The diagram must thus have a zero value. Such a result will be used later on.

2.4. *The triple scalar product*

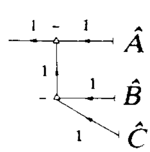
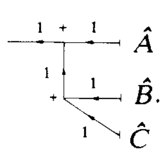
The definitions (2.4) and (2.8) of the scalar and cross products allow an easy graphical representation of a triple scalar product:

$$\boldsymbol{A}\,.\,(\boldsymbol{B}\times\boldsymbol{C}) = \mathrm{i}\sqrt{2}$$  $$= \mathrm{i}\sqrt{6}$$  $$. \tag{2.15}$$

It represents the volume of the parallelepiped having $\boldsymbol{A}$, $\boldsymbol{B}$ and $\boldsymbol{C}$ as three of its edges.

2.5. *The double cross product*

As previously done we obtain the diagrammatic representation of the double cross product by twice applying the definition (2.8):

$$(\boldsymbol{A}\times(\boldsymbol{B}\times\boldsymbol{C}))_q = -2$$  $$= -6$$  $$. \tag{2.16}$$

3. The differential operators

3.1. The symbolic vector gradient

The equation

$$\boldsymbol{\nabla} = \boldsymbol{i}\frac{\partial}{\partial x} + \boldsymbol{j}\frac{\partial}{\partial y} + \boldsymbol{k}\frac{\partial}{\partial z}$$

defines the vector differential operator $\boldsymbol{\nabla}$. Its standard components follow immediately:

$$\nabla_q = \hat{\nabla} \overset{1q}{\longrightarrow}. \tag{3.1}$$

The gradient of a scalar function $f(x, y, z)$ is

$$\boldsymbol{\nabla} f = \operatorname{grad} f = \boldsymbol{i}\frac{\partial f}{\partial x} + \boldsymbol{j}\frac{\partial f}{\partial y} + \boldsymbol{k}\frac{\partial f}{\partial z}$$

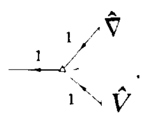
which reads graphically as

$$(\nabla f)_q = \hat{\nabla} f \overset{1}{\longrightarrow}. \tag{3.2}$$

3.2. The divergence

$$\operatorname{div} \boldsymbol{V} = \boldsymbol{\nabla} \,.\, \boldsymbol{V} = -\hat{\nabla} \overset{1}{\longleftrightarrow} \hat{V}. \tag{3.3}$$

3.3. The curl or rotation

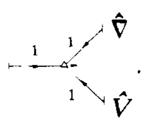
$$(\operatorname{curl} \boldsymbol{V})_q = (\boldsymbol{\nabla} \times \boldsymbol{V})_q = -\mathrm{i}\sqrt{2}$$  . (3.4)

3.4. The Laplacian operator

$$\Delta = \nabla^2 = \boldsymbol{\nabla} \,.\, \boldsymbol{\nabla} = -\hat{\nabla} \overset{1}{\longleftrightarrow} \hat{\nabla}. \tag{3.5}$$

3.5. The divergence of a curl and the curl of a grad

Let us first consider the divergence of a curl and set its diagrammatical representation:

$$\operatorname{div} \operatorname{curl} \boldsymbol{V} = \boldsymbol{\nabla} \,.\, \boldsymbol{\nabla} \wedge \boldsymbol{V} = -\hat{\nabla}$$  . (3.6)

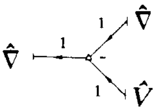
We expand this diagram and obtain easily

$$\operatorname{div} \operatorname{curl} \boldsymbol{V} = \sum_q (-1)^q \nabla_{1-q} \langle 1\mu\, 1\nu | 1q \rangle \nabla_{1\mu} V_{1\nu}.$$

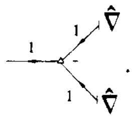
We note that the following Clebsch–Gordan (CG) coefficients vanish: $\langle 1\ -1\ 1\ 2|1\ 1\rangle$, $\langle 1\ 0\ 1\ 0|1\ 0\rangle$ and $\langle 1\ 1\ 1\ -2|1\ 1\rangle$. Thus we get

$$\begin{aligned}\operatorname{div} \operatorname{curl} \boldsymbol{V} = {} & \langle 1\ 1\ 1\ 0|1\ 1\rangle(\nabla_{-1}\nabla_1 V_0 - \nabla_{-1}\nabla_0 V_1) \\ & -\langle 1\ 1\ 1\ -1|1\ 0\rangle(\nabla_0\nabla_1 V_{-1} - \nabla_0\nabla_{-1} V_1) \\ & +\langle 1\ -1\ 1\ 0|1\ -1\rangle(\nabla_1\nabla_{-1} V_0 - \nabla_1\nabla_0 V_1).\end{aligned}$$

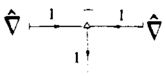
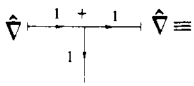
It turns out, after evaluation of the CG coefficients, that

div curl $\boldsymbol{V}=$  $\equiv 0$. (3.7)

The definition of the curl of a grad exhibits an analogous diagram:

$(\text{curl grad})_q = -\mathrm{i}\sqrt{2}$  . (3.8)

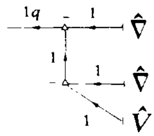
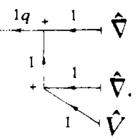
Since the previous diagram shown in (3.7) vanishes for any value of V we find that

 $\equiv \sqrt{3}$  $\equiv 0$. (3.9)

Such a result is effectively obtained by a direct evaluation of the diagram since a change of a lecture order must not affect the diagram while it appears that the sign is changed.

3.6. *The curl of a curl*

We use the graphical representation (2.16) of a double cross product to get

$(\text{curl curl } \boldsymbol{V})_q = -2$  $= -6$  (3.10)

One can evaluate explicitly the last diagram using the 3-*jm* coefficients:

$$(\text{curl curl } \boldsymbol{V})_q = -6 \sum_{\mu\nu\tau\sigma} (-1)^{\mu} \begin{pmatrix} 1 & 1 & 1 \\ q & -\nu & -\mu \end{pmatrix} \begin{pmatrix} 1 & 1 & 1 \\ \nu & -\tau & -\sigma \end{pmatrix} \nabla_\mu \nabla_\tau V_\sigma \tag{3.11}$$

with $q=\mu+\tau+\sigma$ and $\mu, \tau, \sigma = q$. We set, successively, μ or τ or σ equal to q and replace the remaining 3-*jm* coefficients by their values to get

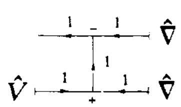
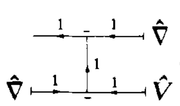
$$(\text{curl curl } \boldsymbol{V})_q = \nabla_q(-\nabla_1 V_{-1} - \nabla_{-1} V_1 + \nabla_0 V_0) - (-\nabla_1 \nabla_{-1} - \nabla_{-1}\nabla_1 + \nabla_0^2) V_q. \tag{3.12}$$

We recognize in the right-hand side of equation (3.12) the standard component of $\boldsymbol{\nabla}(\boldsymbol{\nabla} \cdot \boldsymbol{V}) - (\boldsymbol{\nabla} \cdot \boldsymbol{\nabla})\boldsymbol{V}$, thus we get the well known result

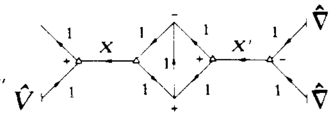
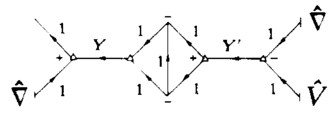
$$\text{curl curl } \boldsymbol{V} = \boldsymbol{\nabla}(\boldsymbol{\nabla} \cdot \boldsymbol{\nabla}) - (\boldsymbol{\nabla} \cdot \boldsymbol{\nabla})\boldsymbol{V}. \tag{3.13}$$

3.7. *An application of the* GSA

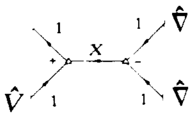
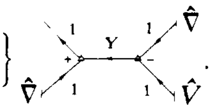
Let us now use the above result and the recoupling technique of the GSA to define two special new ITO of rank one:

$(\text{curl curl } \boldsymbol{V})_q = -6E = -6$  $= -6$  . (3.14)

We introduce intermediate momenta to get

$$E=\sum_{XX'}$$  $$=\sum_{YY'}$$  . (3.15)

A pinch on the XX' and YY' lines yields the result

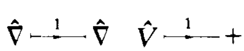
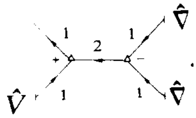
$$E=\sum_{X}(-1)^{X}\begin{Bmatrix}1 & 1 & 1\\ 1 & 1 & X\end{Bmatrix}$$  $$=\sum_{Y}(-1)^{1+Y}\begin{Bmatrix}1 & 1 & 1\\ 1 & 1 & Y\end{Bmatrix}$$  .

(3.16)

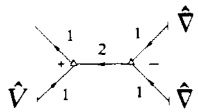
We note here that X can take the value zero, and the remaining diagram becomes

 $=(\nabla\,.\,\nabla)\,V_q.$

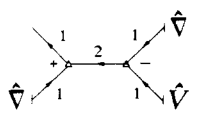
The X intermediate momentum cannot take the value one since the corresponding diagram is zero following (3.9). We are thus left with the following:

$$E=-\frac{1}{9}$$  $+\frac{1}{6}$  . (3.17)

It corresponds to the rank-one OTI:

 $=-(\text{curl curl } \boldsymbol{V})_q-\frac{2}{3}\nabla\,.\,\nabla V_q.$ (3.18)

The same procedure applied to the Y intermediate momentum gives

 $=\frac{1}{2}(\text{curl curl } \boldsymbol{V})_q-\frac{2}{3}\nabla_q(\nabla\,.\,\boldsymbol{V}).$ (3.19)

4. Application of the Wigner-Eckhart theorem

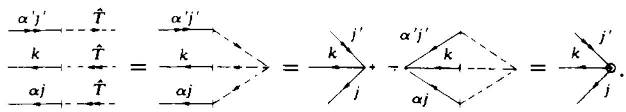
4.1. Definition

Let us first recall the Wigner-Eckhart theorem in its graphical form:

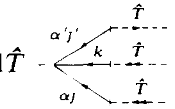
$$\langle\alpha'j'm'|T_{kq}|\alpha jm\rangle$$

$$=\int \mathrm{d}\hat{T}\langle\alpha'j'm'|\hat{T}\rangle T_{kq}(\hat{T})\langle\hat{T}|\alpha jm\rangle \tag{4.1}$$

$$=\begin{pmatrix}m' & k & j\\ j' & q & m\end{pmatrix}\langle\alpha'j'\|T_k\|\alpha j\rangle$$

$$=\int \mathrm{d}\hat{T}$$  . (4.2)

A comparison between the equations (4.1) and (4.2) defines the graphical symbol of the reduced matrix element of the T_{kq} tensor operator:

$$\langle\alpha' j'\|T_k\|\alpha j\rangle = \int \mathrm{d}\hat{T}$$  . (4.3)

We can thus recall some of the usual reduced matrix elements and especially those of the gradient:

$$\langle l_1\|Y_{l_2}\|l_3\rangle = \frac{1}{\sqrt{(4\pi)}}[l_1 l_2 l_3]\begin{pmatrix} 0 & l_2 & l_3 \\ l_1 & 0 & 0 \end{pmatrix} \tag{4.4}$$

$$\langle J'\|J^{(1)}\|J\rangle = \sqrt{[J(J+1)(2J+1)]}\delta_{JJ'} \tag{4.5}$$

$$\langle J'\|\mathbb{1}\|J\rangle = [J]\delta_{J'J} \tag{4.6}$$

$$\langle l'\|\nabla\|l\rangle = \frac{1}{[l'l]\left(\begin{smallmatrix} 0 & 1 & l \\ l' & 0 & 0 \end{smallmatrix}\right)}\left[(l+1)\delta_{l'l+1}\left(\frac{\mathrm{d}}{\mathrm{d}r}-\frac{l}{r}\right) - l\delta_{l'l-1}\left(\frac{\mathrm{d}}{\mathrm{d}r}+\frac{l+1}{r}\right)\right]. \tag{4.7}$$

If one defines the $\phi_p^{lm}(\boldsymbol{r})$ wavefunction as

$$\phi_p^{lm}(\boldsymbol{r}) = f_p^l(r)\,Y_{lm}(\hat{r}), \tag{4.8}$$

since

$$r_m^1 = \sqrt{(\tfrac{4}{3}\pi)}rY_{1m} \tag{4.9}$$

one obtains the following reduced matrix elements:

$$\langle\phi_{p'}^{l'}\|r^1\|\phi_p^l\rangle = [l\,l']\begin{pmatrix} 0 & 1 & l \\ l' & 0 & 0 \end{pmatrix}\langle f_{p'}^{l'}|r|f_p^l\rangle \tag{4.10}$$

while

$$\langle\phi_{p'}^{l'}\|\nabla^1\|\phi_p^l\rangle$$
$$= [l^{-1}l'^{-1}]\begin{pmatrix} 0 & 1 & l \\ l' & 0 & 0 \end{pmatrix}^{-1}\left((l+1)\delta_{l'l+1}\left\langle f_{p'}^{l'}\left|\frac{\mathrm{d}}{\mathrm{d}r}-\frac{l}{r}\right|f_p^l\right\rangle \right. \tag{4.11}$$
$$\left. -l\,\delta_{l'l-1}\left\langle f_{p'}^{l'}\left|\frac{\mathrm{d}}{\mathrm{d}r}+\frac{l+1}{r}\right|f_p^l\right\rangle\right).$$

4.2. Reduced matrix element of the kinetic momentum operator

One knows the matrix elements of the kinetic momentum operator considered as a rank-one irreducible tensor operator since

$$U_q = \langle\phi^{l'm'}|L_q^1|\phi^{lm}\rangle \tag{4.12}$$

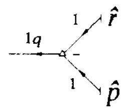
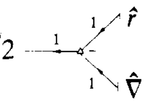
gives the standard components

$$U_1 = \langle\phi^{l'm'}|L_1^1|\phi^{lm}\rangle = -\frac{1}{\sqrt{2}}\langle\phi^{l'm'}|L_+|\phi^{lm}\rangle = -\frac{1}{\sqrt{2}}\delta_{ll'}\,\delta_{m'm+1}x_m$$
$$U_0 = \langle\phi^{l'm'}|L_0^1|\phi^{lm}\rangle = \langle\phi^{l'm'}|L_z|\phi^{lm}\rangle = m\,\delta_{ll'}\,\delta_{mm'} \tag{4.13}$$
$$U_{-1} = \langle\phi^{l'm'}|L_{-1}^1|\phi^{lm}\rangle = \frac{1}{\sqrt{2}}\langle\phi^{l'm'}|L_-|\phi^{lm}\rangle = \frac{1}{\sqrt{2}}\delta_{ll'}\,\delta_{m'm-1}x_{m-1}$$

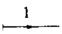
with

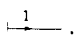
$$x_m = \sqrt{[(l-m)(l+m+1)]}.$$

Let us now use the graphical representation of the kinetic momentum operator to reach the matrix element

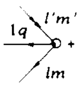
$$L_q = (\boldsymbol{r}\times\boldsymbol{p})_q = -\mathrm{i}\sqrt{2}$$

$$= -\hbar\sqrt{2}$$

(4.14)

since

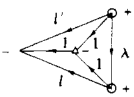
$$r^1_\mu = \sqrt{(\tfrac{4}{3}\pi)}\, rY_{1\mu}(\hat{r}) = \hat{r}$$


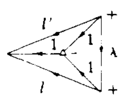
$$p^1_\nu = -\mathrm{i}\hbar\nabla^1_\nu = \hat{p}$$

(4.15)

The Wigner–Eckart theorem is applied to the L_q tensor operator and one easily obtains

$$U_q = \langle\phi^{l'm'}|L_q|\phi^{lm}\rangle =$$

(4.16)

with

$$\langle\phi^{l'}\|L^1\|\phi^l\rangle = -\hbar\sqrt{(\tfrac{8}{3}\pi)}$$

(4.17)

$$\langle\phi^{l'}\|L^1\|\phi^l\rangle = -\hbar\sqrt{(\tfrac{8}{3}\pi)}\langle f^{l'}\|r^1\|f^\lambda\rangle\langle f^\lambda\|\nabla^1\|f^l\rangle$$

(4.18)

The selection rules applied to the 6-j coefficient exhibit the only value $l' = l$ while $\lambda = l \pm 1$. One can then use the (4.10) and (4.11) values of the reduced matrix elements and the explicit values of the 3-j0 and 6-j symbols to get the reduced matrix element

$$\langle\phi^{l'}\|L^1\|\phi^l\rangle = \hbar\sqrt{[l(l+1)(2l+1)]}\,\delta_{ll'}. \tag{4.19}$$

As expected this reduced matrix element has been already obtained in (4.5). Bringing (4.19) into (4.16) leads to the matrix elements U_q as expressed in (4.13).

5. Particular cases with spherical Bessel functions

One can always expand a radial wavefunction on a spherical Bessel function basis (Glendenning and Nagarajan 1974, Nahabetian, private communication, Charlton 1973)

$$\phi^l(r) = \sum_n a_{nl} j_l(k_n r). \tag{5.1}$$

The reduced matrix elements of the differential operators between these functions must thus play a prominent role and it is essential to evaluate them.

5.1. *Reduced matrix element of the gradient*

When we use (4.11) with $f^l_p = j_l(pr)$ we easily get the value

$$\langle j_{l'}(p'r)\|\nabla^1\|j_l(pr)\rangle = \frac{\pi}{2p}\,\delta(p'-p)\alpha_{l'l} \tag{5.2}$$

with

$$\alpha_{l'l} = [l^{-1}l'^{-1}]\begin{pmatrix} 0 & 1 & l \\ l' & 0 & 0 \end{pmatrix}^{-1}[(l+1)\,\delta_{l'l+1} - l\,\delta_{l'l-1}] = \begin{cases} \sqrt{l'} & \text{if } l' = l+1 \\ 0 & \text{if } l' = l \\ -\sqrt{l} & \text{if } l' = l-1. \end{cases} \tag{5.3}$$

5.2. *Closure relation*

It is often necessary to introduce a closure relation with the spherical Bessel functions to handle the Wigner–Eckart theorem. Therefore we first recall the orthonormalization of these functions:

$$\int p^2\,\mathrm{d}p\,j_l(pr)j_l(pr') = \frac{\pi}{2r^2}\,\delta(r-r'). \tag{5.4}$$

If we combine it with the closure relation of the spherical harmonics we get

$$\delta(\boldsymbol{r}-\boldsymbol{r}') = \sum_{lm}\frac{2}{\pi}\int p^2\,\mathrm{d}p\,j_l(pr)\,Y_{lm}(\hat{r})j_l(pr')\,Y_{lm}(\hat{r}'). \tag{5.5}$$

We set

$$j_l(pr)\,Y_{lm}(\hat{r}) = \phi^{lm}_p(\boldsymbol{r}) = \boldsymbol{pr} \vdash\!\!\overset{lm}{\longrightarrow} \tag{5.6}$$

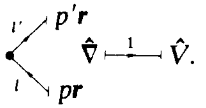
and the closure relation reads

$$\delta(\boldsymbol{r}-\boldsymbol{r}') = \sum_{l}\frac{2}{\pi}\int p^2\,\mathrm{d}p\ \ \boldsymbol{pr} \vdash\!\!\overset{l}{\longrightarrow}\!\!\dashv \boldsymbol{pr}'. \tag{5.7}$$

5.3. *Reduced matrix element of the divergence*

The definition (4.3) of a reduced matrix element and (3.3) of the divergence leads to the following:

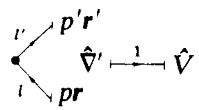
$$\langle\phi^{l'}_{p'}\|\,\mathrm{div}\ \boldsymbol{V}\|\phi^l_p\rangle = -\int \mathrm{d}\boldsymbol{r} \tag{5.8}$$



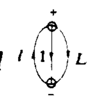
We introduce the closure relation (5.7) and integrate over $\boldsymbol{r}$ and $\boldsymbol{r}'$:

$\langle\phi^{l'}_{p'}\|\,\mathrm{div}\ \boldsymbol{V}\|\phi^l_p\rangle$

$$= -\int \mathrm{d}\boldsymbol{r}\,\mathrm{d}\boldsymbol{r}'\,\delta(\boldsymbol{r}-\boldsymbol{r}')$$



$$= -[l^{-1}]\,\delta_{ll'}\sum_L\frac{2}{\pi}\int q^2\,\mathrm{d}q$$



$$= -[l^{-1}]\,\delta_{ll'}\sum_L\frac{2}{\pi}\int q^2\,\mathrm{d}q\langle\phi^{l'}_{p'}\|\nabla\|j_L(qr)\rangle\langle j_L(qr)\|V^1\|\phi^l_p\rangle. \tag{5.9}$$

Using spherical Bessel functions and the reduced matrix element of the gradient operator we get finally,

$$\langle j_{l'}(p'r)\| \operatorname{div} \boldsymbol{V} \| j_l(pr)\rangle = -[l^{-1}]\, \delta_{ll'} p' \sum_L \alpha_{lL} \langle j_L(p'r)\| V^1 \| j_l(pr)\rangle. \tag{5.10}$$

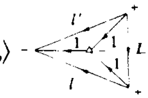
We can evaluate the α_{lL} coefficient from (5.3) and we find

$$\begin{aligned}\langle j_{l'}(p'r)\| \operatorname{div} \boldsymbol{V} \| j_l(pr)\rangle \\ &= \left(\frac{l+1}{2l+1}\right)^{1/2} p' \int r^2\, \mathrm{d}r\, j_{l+1}(p'r) V_z(r) j_l(pr) \\ &\quad - \left(\frac{l}{2l+1}\right)^{1/2} p' \int r^2\, \mathrm{d}r\, j_{l-1}(p'r) V_z(r) j_l(pr).\end{aligned} \tag{5.11}$$

5.4. *Reduced matrix element of the curl*

The same procedure gives the reduced matrix element of the curl in the form

$$\langle \phi_{p'}^{l'} \| \operatorname{curl} \boldsymbol{V} \| \phi_p^l \rangle = -\mathrm{i}\sqrt{2} \sum_L \frac{2}{\pi} \int q^2\, \mathrm{d}q \langle \phi_{p'}^{l'} \| \nabla^1 \| j_L(qr)\rangle \langle j_L(qr) \| V^1 \| \phi_p^l \rangle \cdot \tag{5.12}$$



After insertion of the explicit values of the reduced matrix element of the gradient and of the 6-j coefficient we are left with

$$\langle j_{l'}(p'r)\| \operatorname{curl} \boldsymbol{V} \| j_l(pr)\rangle = \mathrm{i}p'\sqrt{6} \sum_L \alpha_{lL} (-1)^{l+l'} \begin{Bmatrix} 1 & 1 & 1 \\ l & l' & L \end{Bmatrix} \int r^2\, \mathrm{d}r\, j_L(p'r) V_z(r) j_l(pr). \tag{5.13}$$

5.5. *Reduced matrix element of the Laplacian*

When we introduce the spherical form of the Laplacian operator

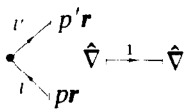
$$\nabla^2 = \frac{1}{r^2}\frac{\mathrm{d}}{\mathrm{d}r} r^2 \frac{\mathrm{d}}{\mathrm{d}r} - \frac{l(l+1)}{r^2} \tag{5.14}$$

its reduced matrix element reads

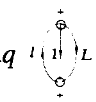
$$\langle \phi_{p'}^{l'} \| \nabla^2 \| \phi_p^l \rangle = \int_0^\infty r^2\, \mathrm{d}r\, \phi_{p'}^{l'*}(r) \nabla^2 \phi_p^l(r) \tag{5.15}$$

and its graphical determination follows the procedure previously described

$$\langle \phi_{p'}^{l'} \| \nabla^2 \| \phi_p^l \rangle = -\int \mathrm{d}r$$



$$= -[l^{-1}]\, \delta_{ll'} \sum_L \frac{2}{\pi} \int q^2\, \mathrm{d}q$$



$$= [l^{-1}]\, \delta_{ll'} \frac{2}{\pi} \sum_L (-1)^{l+L} \int_0^\infty q^2\, \mathrm{d}q \langle \phi_{p'}^{l'} \| \nabla \| j_L(qr)\rangle \langle j_L(qr) \| \nabla \| \phi_p^l \rangle.$$

When the $\phi_{p'}^{l'}$ and ϕ_p^l are spherical Bessel functions, the reduced matrix elements of the gradient are expressed by (5.2) and a great simplification follows:

$$\langle j_{l'}(p'r)\|\nabla^2\|j_l(pr)\rangle$$

$$=[l^{-1}]\,\delta_{ll'}\sum_L \frac{2}{\pi}(-1)^{l+L}\int \frac{\pi}{2q}\,\delta(p'-q)\alpha_{lL}\frac{\pi}{2q}\,\delta(q-p)\alpha_{Ll}q^2\,\mathrm{d}q$$

$$=[l^{-1}]\tfrac{1}{2}\pi\,\delta(p-p')(-1)^l\sum_L(-1)^L\alpha_{lL}\alpha_{Ll}.$$

The sum over L is easily evaluated as $(-1)^{l+1}[l^2]$ and one finds

$$\langle j_{l'}(p'r)\|\nabla^2\|j_l(pr)\rangle=-\tfrac{1}{2}\pi[l]\,\delta_{ll'}\delta(p-p'). \tag{5.16}$$

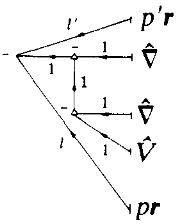
It is easy to get the same result by applying the Laplacian operator to a plane wave and thus evaluating

$$\int \mathrm{e}^{-\mathrm{i}\boldsymbol{p}'.\boldsymbol{r}}\nabla^2\,\mathrm{e}^{\mathrm{i}\boldsymbol{p}.\boldsymbol{r}}=-(2\pi)^3p^2\,\delta(\boldsymbol{p}-\boldsymbol{p}'). \tag{5.17}$$

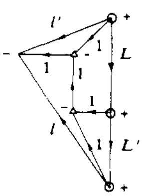
5.6. Reduced matrix element of the curl of a curl

$\langle\phi_{p'}^{l'}\|\mathrm{curl\ curl}\ \boldsymbol{V}\|\phi_p^l\rangle$

$$=-2\int \mathrm{d}\boldsymbol{r}$$



$$=-2\sum_{LL'}\left(\frac{2}{\pi}\right)^2\int q^2\,\mathrm{d}qs^2\,\mathrm{d}s \tag{5.18}$$



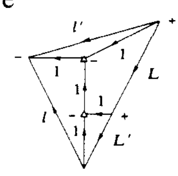
or

$\langle\phi_{p'}^{l'}\|\ \mathrm{curl\ curl}\ \boldsymbol{V}\|\phi_p^l\rangle$

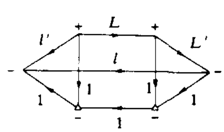
$$=-2\left(\frac{2}{\pi}\right)^2\sum_{LL'}\int q^2\,\mathrm{d}q\,s^2\,\mathrm{d}s\langle\phi_{p'}^{l'}\|\nabla\|j_L(qr)\rangle\langle j_L(qr)\|\nabla\|j_{L'}(sr)\rangle\langle j_{L'}(sr)\|V^1\|\phi_p^l\rangle D \tag{5.19}$$

where

$D=$



$=$



$$=3(-1)^{l+L+1}\begin{Bmatrix} l' & 1 & l\\ 1 & L & 1\end{Bmatrix}\begin{Bmatrix} L & 1 & l\\ 1 & L' & 1\end{Bmatrix}. \tag{5.20}$$

If one inserts the explicit value of the reduced matrix element of the gradient taken between the spherical Bessel functions one finds

$$\begin{aligned}\langle\phi_{p'}^{l'}\|\mathrm{curl\ curl}\ \boldsymbol{V}\|\phi_p^l\rangle &= \frac{12}{\pi}\sum_{LL'}\int q^3\,\mathrm{d}q\langle\phi_{p'}^{l'}\|\nabla\|j_L(qr)\rangle \\ &\quad\times\alpha_{LL'}\langle j_{L'}(qr)\|V^1\|\phi_p^l\rangle(-1)^{l+L}\begin{Bmatrix} l' & 1 & l \\ 1 & L & 1\end{Bmatrix}\begin{Bmatrix} L & 1 & l \\ 1 & L' & 1\end{Bmatrix}.\end{aligned} \tag{5.21}$$

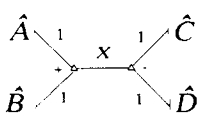
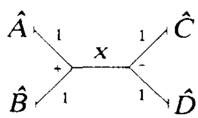
With spherical Bessel functions this result simplifies into

$$\begin{aligned}\langle j_{l'}(p'r)\|\ \mathrm{curl\ curl}\ \boldsymbol{V}\|j_l(pr)\rangle &= 6\sum_{LL'}(-1)^{l+L}\alpha_{l'L}\alpha_{LL'}\begin{Bmatrix} l' & 1 & l \\ 1 & L & 1\end{Bmatrix}\begin{Bmatrix} L & 1 & l \\ 1 & L' & 1\end{Bmatrix}p'^2\langle j_{L'}(p'r)\|V^1\|j_l(pr)\rangle.\end{aligned} \tag{5.22}$$

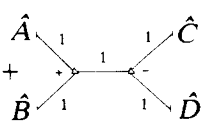
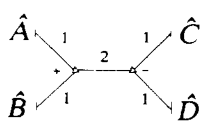
It can be noted that such a graphical representation of the differential operators within the GSA framework may be particularly useful when dealing with the electromagnetic field and the Maxwell equations.

Appendix

We use the GSA rules to obtain easily

$(\boldsymbol{A}\,.\,\boldsymbol{C})(\boldsymbol{B}\,.\,\boldsymbol{D}) = \begin{matrix}\hat{A} \overset{1}{\text{———}} \hat{C} \\ \hat{B} \overset{1}{\text{———}} \hat{D}\end{matrix} = \sum_X$  $= \sum_X [X^2]$  . (A.1)

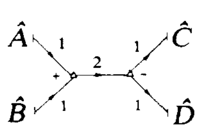
Since $X = 0$, 1 and 2 it follows that

$(\boldsymbol{A}\,.\,\boldsymbol{C})(\boldsymbol{B}\,.\,\boldsymbol{D}) = \frac{1}{3}\hat{A}\overset{1}{\text{———}}\hat{B}\ \ \hat{C}\overset{1}{\text{———}}\hat{D} +$  $+$  . (A.2)

When $[A, B] \neq 0$, $[C, D] \neq 0$ and $[A, C] = [B, D] = 0$ all the diagrams have a non-zero value and we get the analytical equivalent of (A.2):

$$(\boldsymbol{A}\,.\,\boldsymbol{C})(\boldsymbol{B}\,.\,\boldsymbol{D}) = \tfrac{1}{3}(\boldsymbol{A}\,.\,\boldsymbol{B})(\boldsymbol{C}\,.\,\boldsymbol{D}) + \tfrac{1}{2}(\boldsymbol{A}\times\boldsymbol{B})\,.\,(\boldsymbol{C}\times\boldsymbol{D}) + T_2(\boldsymbol{A}, \boldsymbol{B})\,.\,T_2(\boldsymbol{C}, \boldsymbol{D}). \tag{A.3}$$

The above equations define the graphical equivalent of the scalar product of two rank-two tensor operators:

$T_2(\boldsymbol{A}, \boldsymbol{B})\,.\,T_2(\boldsymbol{C}, \boldsymbol{D}) =$ 

$$= (\boldsymbol{A}\,.\,\boldsymbol{C})(\boldsymbol{B}\,.\,\boldsymbol{D}) - \tfrac{1}{3}(\boldsymbol{A}\,.\,\boldsymbol{B})(\boldsymbol{C}\,.\,\boldsymbol{D}) - \tfrac{1}{2}(\boldsymbol{A}\times\boldsymbol{B})\,.\,(\boldsymbol{C}\times\boldsymbol{D}) \tag{A.4}$$

(i) $\boldsymbol{A} = \boldsymbol{B} = \boldsymbol{J}_1$, $\boldsymbol{C} = \boldsymbol{D} = \boldsymbol{J}_2$

$$T_2(\boldsymbol{J}_1, \boldsymbol{J}_1)\,.\,T_2(\boldsymbol{J}_2, \boldsymbol{J}_2) = (\boldsymbol{J}_1\,.\,\boldsymbol{J}_2)^2 - \tfrac{1}{3}J_1^2J_2^2 + \tfrac{1}{2}\boldsymbol{J}_1\,.\,\boldsymbol{J}_2. \tag{A.5}$$

(ii) $\boldsymbol{C}=\boldsymbol{D}=\boldsymbol{\sigma}$, $T_2(\boldsymbol{\sigma},\boldsymbol{\sigma})=0$, as can be seen directly on the components of this rank-two tensor operator

$$0=(\boldsymbol{\sigma}\cdot\boldsymbol{A})(\boldsymbol{\sigma}\cdot\boldsymbol{B})-\tfrac{1}{3}(\boldsymbol{A}\cdot\boldsymbol{B})\boldsymbol{\sigma}^2-\tfrac{1}{2}(\boldsymbol{A}\times\boldsymbol{B})\cdot(\boldsymbol{\sigma}\times\boldsymbol{\sigma}).$$

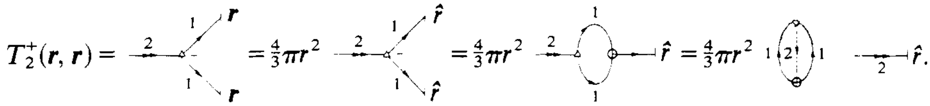
We use the fact that $\sigma^2=3$ and $\boldsymbol{\sigma}\times\boldsymbol{\sigma}=2\mathrm{i}\boldsymbol{\sigma}$ to reproduce the well known relation

$$(\boldsymbol{\sigma}\cdot\boldsymbol{A})(\boldsymbol{\sigma}\cdot\boldsymbol{B})=\boldsymbol{A}\cdot\boldsymbol{B}+\mathrm{i}\boldsymbol{\sigma}\cdot(\boldsymbol{A}\times\boldsymbol{B}). \tag{A.6}$$

(iii) $\boldsymbol{A}=\boldsymbol{S}_1, \boldsymbol{B}=\boldsymbol{S}_2, \boldsymbol{C}=\boldsymbol{D}=\boldsymbol{r}$

$$T_2(\boldsymbol{S}_1,\boldsymbol{S}_2)\cdot T_2(\boldsymbol{r},\boldsymbol{r})=(\boldsymbol{S}_1\cdot\boldsymbol{r})(\boldsymbol{S}_2\cdot\boldsymbol{r})-\tfrac{1}{3}(\boldsymbol{S}_1\cdot\boldsymbol{S}_2)r^2. \tag{A.7}$$

We can simplify the $T_2(\boldsymbol{r},\boldsymbol{r})$ tensor since $r_{1\mu}=\sqrt{(\frac{4}{3}\pi)}rY_{1\mu}(\hat{r})$:



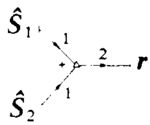
We express the triad with its reduced matrix element

$$T_2^+(\boldsymbol{r},\boldsymbol{r})=\sqrt{(\tfrac{4}{3}\pi)}r^2 3\sqrt{5}\begin{pmatrix}1 & 2 & 1\\ 0 & 0 & 0\end{pmatrix}Y_{2\mu}^*(\hat{r})=\sqrt{(\tfrac{4}{3}\pi)}\sqrt{(10)}r^2Y_{2\mu}^*(\hat{r}).$$

As usual we set

$$\xrightarrow{2}\boldsymbol{r}=\mathscr{Y}_{2\mu}^*(\boldsymbol{r})=r^2Y_{2\mu}^*(\hat{r}) \tag{A.8}$$

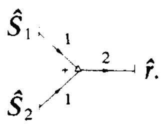
and then

$$T_2(\boldsymbol{S}_1,\boldsymbol{S}_2)\cdot T_2(\boldsymbol{r},\boldsymbol{r})=\sqrt{(\tfrac{4}{3}\pi)}\sqrt{(10)}$$  $$=(\boldsymbol{S}_1\cdot\boldsymbol{r})(\boldsymbol{S}_2\cdot\boldsymbol{r})-\tfrac{1}{3}(\boldsymbol{S}_1\cdot\boldsymbol{S}_2)r^2. \tag{A.9}$$

If we introduce the 'tensor force'

$$T_2(\boldsymbol{S}_1,\boldsymbol{S}_2)\cdot T_2(\boldsymbol{r},\boldsymbol{r})=r^2S_{12} \tag{A.10}$$

we easily see that

$$S_{12}=\frac{(\boldsymbol{S}_1\cdot\boldsymbol{r})(\boldsymbol{S}_2\cdot\boldsymbol{r})}{r^2}-\tfrac{1}{3}(\boldsymbol{S}_1\cdot\boldsymbol{S}_2)=\sqrt{(\tfrac{4}{3}\pi)}\sqrt{(10)}$$  (A.11)

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