As a last argument of the course we take the 9th chapter which fits more naturally into the discussion.

9. Transition between electronic states

In this section we deal with selection rules. Given an interaction Hamiltonian H' we ask the question whether

$$\langle \psi_\alpha | H' | \psi_\beta \rangle$$

vanishes or not, where ψ_α and ψ_β are eigenstates of the Hamiltonian H_0.
In principle the answer is easy: $\langle \psi_\alpha | H' | \psi_\beta \rangle$ is a number and if it does not transform as a number it must vanish.

9.1 Electromagnetic interaction as a perturbation.

The canonical way to insert electromagnetic fields into an Hamiltonian is

$$H = \frac{1}{2m}\left(p - \frac{e}{c}A\right)^2 + V$$

Expanding up to first order in $\frac{eA}{c}$

$$H = \frac{p^2}{2m} + V - \frac{e}{mc}\vec{p}\cdot\vec{A} = H_0 + H'_{em}$$

The symmetry (properties) of H'_{em} is in general lower than the one of H_0. This ensures that transitions between eigenstates of H_0 are possible due to perturbations.

9.2 Orthogonality of basis functions

H_0 defines a group: the group of the Hamiltonian of of the Schrödinger equation.

The first point is to determine selection rules for H_0, namely the orthogonality of basis functions

$$H_0 \longmapsto \text{Group of } H_0 \longmapsto \underset{\substack{\uparrow \\ \text{IR}}}{\Gamma^j} \longrightarrow \underset{\substack{\uparrow \\ \text{basis functions.}}}{\boxed{\varphi_\alpha^{(j)}}}$$

<u>Theorem</u> Two basis functions which belong either to different irreducible representations or to different columns (rows) of the same representation are orthogonal.

<u>proof</u> $\phi_\alpha^{(i)}$ and $\varphi_{\alpha'}^{(i')}$ two basis functions for IR (i) and (i') and associated to the columns α and α' of their representation

$$\hat{P}_R \phi_\alpha^{(i)} = \sum_{j=1}^{l_i} D^{(i)}(R)_{j\alpha} \phi_j^{(i)}$$

$$\hat{P}_R \varphi_{\alpha'}^{(i')} = \sum_{j'=1}^{l_{i'}} D^{(i')}(R)_{j'\alpha'} \varphi_{j'}^{(i')}$$

For the scalar product

$$\left(\phi_\alpha^{(i)}, \varphi_{\alpha'}^{(i')}\right) = \left(\hat{P}_R \phi_\alpha^{(i)}, \hat{P}_R \varphi_{\alpha'}^{(i')}\right) = \quad \longleftarrow$$

the scalar product is independent of the coordinate system!

$$= \sum_{jj'} D^{(i)}(R)^*_{j\alpha} D^{(i')}(R)_{j'\alpha'} \left(\phi_j^{(i)}, \varphi_{j'}^{(i')}\right)$$

$$= \frac{1}{h} \sum_R \sum_{jj'} D^{(i)}(R)^*_{j\alpha} D^{(i')}(R)_{j'\alpha'} \left(\phi_j^{(i)}, \varphi_{j'}^{(i')}\right) \quad \longleftarrow$$

The same argument is valid for all transformation R

$$\overset{\text{WOT}}{=} \frac{1}{l_i} \delta_{ii'} \delta_{\alpha\alpha'} \sum_{j=1}^{l_i} \left(\phi_j^{(i)}, \phi_j^{(i)}\right) = \delta_{ii'} \delta_{\alpha\alpha'}$$

if the basis functions are normalized.

$H_0 \psi^{(i')}_{\alpha'} = E^{(i')}_{\alpha'} \psi^{(i')}_{\alpha'}$ due to Schur's lemma $\Rightarrow$ the orthogonality relation is a selection rule for H_0. In general, though, $H'\psi$ does NOT transform like ψ.

9.3 Direct product of two groups

$$G_A = \{E, A_2, \ldots, A_{h_a}\} \qquad G_B = \{E, B_2, \ldots, B_{h_b}\}$$

are two groups of order h_a and h_b

$\Rightarrow$ Def: The direct product $G_A \otimes G_B$ is defined as

$$G_A \otimes G_B = E, A_2, \ldots, A_{h_a}, B_2, A_2B_2, \ldots, A_{h_a}B_2, \ldots, A_{h_a}B_{h_b}$$

and has $(h_a \times h_b)$ elements. It is easy to prove that $G_A \otimes G_B$ is also a group. Examples $D_{6h} = D_6 \otimes \{E, \sigma_h\} = D_6 \otimes \{E, i\}$.

9.4 Direct product of two irreducible representations

The solution to the problem comes from algebra. The direct product of matrices has the following definition

$$C = A \otimes B \qquad A_{ij} B_{kl} = C_{ik,jl}$$

C has simply double indices and if A is (2×2) and B (3×3) then C is (6×6).

Theorem: The direct product of the representations of the groups A and B forms a representation of the direct product group proof: We need to prove that

$$D^{(a)}_{ij}(A_i)\otimes D^{(b)}_{pq}(B_j) \stackrel{?}{=} \left(D^{(a\otimes b)}(A_iB_j)\right)_{ip,jq} \quad \text{is a good representation}$$

We know how to make the direct product of two matrices. But a representation is such if it respects the composition

$$D^{(a\otimes b)}(A_kB_\ell)\, D^{(a\otimes b)}(A_{k'}B_{\ell'}) = D^{(a\otimes b)}(A_iB_j)$$

where $A_kA_{k'} = A_i$ and $B_\ell B_{\ell'} = B_j$

$$D^{(a\otimes b)}(A_kB_\ell)\, D^{(a\otimes b)}(A_{k'}B_{\ell'}) = \left[D^{(a)}(A_k)\otimes D^{(b)}(B_\ell)\right]\left[D^{(a)}(A_{k'})\otimes D^{(b)}(B_{\ell'})\right]$$

now in elements

$$\left[D^{(a\otimes b)}(A_kB_\ell)\, D^{(a\otimes b)}(A_{k'}B_{\ell'})\right]_{ip,jq} =$$

$$= \sum_{sr}\left[D^{(a)}(A_k)\otimes D^{(b)}(B_\ell)\right]_{ip,sr}\left[D^{(a)}(A_{k'})\otimes D^{(b)}(B_{\ell'})\right]_{sr,jq}$$

$$= \sum_{sr} D^{(a)}(A_k)_{is}\, D^{(b)}(B_\ell)_{pr}\, D^{(a)}(A_{k'})_{sj}\, D^{(b)}(B_{\ell'})_{rq} =$$

$$= \sum_{s} D^{(a)}(A_k)_{is}\, D^{(a)}(A_{k'})_{sj} \sum_{r} D^{(b)}(B_\ell)_{pr}\, D^{(b)}(B_{\ell'})_{rq} =$$

$$= D^{(a)}(A_kA_{k'})_{ij}\, D^{(b)}(B_\ell B_{\ell'})_{pq} = D^{(a)}(A_i)_{ij}\, D^{(b)}(B_j)_{pq} = D^{(a\otimes b)}(A_iB_j)_{ip,jq}.$$

Further one can prove that: if A and B are different groups $\Rightarrow D^{(a\otimes b)}$ is irreducible if (a) and (b) have this property. Further notice that in the proof we never assumed that the product A_iB_j could not be performed.

If A and B belong to the <u>same</u> group

$$\left[D^{(\ell_1\otimes\ell_2)}(A)\right]_{ip,jq} := D^{(\ell_1)}(A)_{ij}\, D^{(\ell_2)}(A)_{pq}$$

$$\left[D^{(\ell_1\otimes\ell_2)}(B)\right]_{ip,jq} := D^{(\ell_1)}(B)_{ij}\, D^{(\ell_2)}(B)_{pq}$$

one has to prove that the composition is respected

$$D^{(\ell_1\otimes\ell_2)}(AB) = D^{(\ell_1\otimes\ell_2)}(A)\, D^{(\ell_1\otimes\ell_2)}(B).$$

In components

$$\left[D^{(\ell_1\otimes\ell_2)}(AB)\right]_{ip,jq} = D^{(\ell_1)}(AB)_{ij}\, D^{(\ell_2)}(AB)_{pq} =$$

$$= \sum_{rs} D^{(\ell_1)}(A)_{ir}\, D^{(\ell_1)}(B)_{rj}\, D^{(\ell_2)}(A)_{ps}\, D^{(\ell_2)}(B)_{sq} =$$

$$= \sum_{rs} D^{(\ell_1\otimes\ell_2)}(A)_{ip,rs}\, D^{(\ell_1\otimes\ell_2)}(B)_{rs,jq}$$

end of the proof ■

Nevertheless if ℓ_1 and ℓ_2 are irreducible $\ell_1\otimes\ell_2$ is, in general, REDUCIBLE.

9.5 <u>Characters for the direct product</u>

<u>Theorem</u>

- $\chi^{(a\otimes b)}(A_k B_\ell) = \chi^{(a)}(A_k)\,\chi^{(b)}(B_\ell)$

- $\chi^{(\ell_1\otimes\ell_2)}(R) = \chi^{(\ell_1)}(R)\,\chi^{(\ell_2)}(R)$

<u>proof</u> – $\chi^{(a\otimes b)}(A_k B_\ell) = \sum_{ip}\left[D^{(a\otimes b)}(A_k B_\ell)\right]_{ip,ip} = \sum_i D^{(a)}(A_k)_{ii} \sum_p D^{(b)}(B_\ell)_{pp} =$

$$= \chi^{(a)}(A_k)\,\chi^{(b)}(B_\ell)$$

$$- \quad \chi^{(\ell_1 \otimes \ell_2)}(R) = \sum_{ip} \left[D^{(\ell_1 \otimes \ell_2)}(R) \right]_{ip,ip} =$$

$$= \sum_i D^{(\ell_1)}(R)_{ii} \sum_p D^{(\ell_2)}(R)_{pp} = \chi^{(\ell_1)}(R)\, \chi^{(\ell_2)}(R)$$

Since for both (ℓ_1) and (ℓ_2) χ is a class function $\Rightarrow R \to \mathbb{C}$.

As we have already applied many times. We can check the reducibility of the character system for $(\ell_1 \otimes \ell_2)$ using the reduction formula

$$\chi^{(\lambda)}(R)\chi^{(\mu)}(R) = \sum_\nu n_{\lambda\mu}^{\nu}\, \chi^{(\nu)}(R) \quad \leftarrow$$ Clebsch-Gordan series

$$n_{\lambda\mu}^{\nu} = \frac{1}{h} \sum_{\mathcal{C}_\alpha} N_{\mathcal{C}_\alpha}\, \chi^{(\nu)}(\mathcal{C}_\alpha)^* \left[\chi^{(\lambda)}(\mathcal{C}_\alpha)\chi^{(\mu)}(\mathcal{C}_\alpha) \right]$$

for the simple examples like $D_{4h} = D_4 \otimes \{E, i\}$ we have already used this property for constructing character tables with associated gerade and ungerade representations.

9.6 Selection rules in group theoretical terms

$$\left(\psi_\alpha^{(i)} ,\ H' \phi_{\alpha'}^{(i')} \right)$$

$$\Gamma^i \otimes \left(\bigoplus_j \Gamma^j \right) \otimes \Gamma^{i'}$$

If this product of representations of the Schrödinger eq. group does NOT contain A_1 $\Rightarrow$ $(\ , \ ) = 0$!

Simpler $\left(\bigoplus_j \Gamma^j \right) \otimes \Gamma^{i'}$ should contain Γ^{i}.

9.7 Examples of selection rules

$$H'_{em} = -\frac{e}{mc}\,\vec{p}\cdot\vec{A}$$

$\vec{A}$ → invariant under the group of the Hamiltonian H_0.

$\vec{p}$ → transforms like a vector

Let us consider the cubic group O_h. The vector $\vec{p}$ transforms in O_h like T_{1u}. Now, if we assume a starting wave function of type T_{2g}

$$\begin{array}{cccccccccccc} & E & 8C_3 & 3C_2 & 6C_2 & 6C_4 & i & 8iC_3 & 3iC_2 & 6iC_2 & 6iC_4 \\ \chi(T_{1u}\otimes T_{2g}) = & [\,9 & 0 & 1 & -1 & -1 & -9 & 0 & -1 & 1 & 1\,] \end{array}$$

The reduction formula finally implies:

$$T_{1u}\otimes T_{2g} = A_{2u}\oplus E_u \oplus T_{1u}\oplus T_{2u}$$

which sets the selection rules. If the system symmetry is lowered to D_{4h}

$$z \to A_{2u}$$
$$(x,y) \to E_u$$

$\Rightarrow$ H_{em} transform like $A_{2u}\oplus E_u$ in D_{4h}. A state with symmetry T_{2g} goes to states with $E_g \oplus B_{2g}$ in D_{4h} (see chrystal field discussion)

$$E_g \otimes (A_{2u}\oplus E_u) = E_u \oplus (A_{1u}+A_{2u}+B_{1u}+B_{2u})$$

and analogously for the other term. In general one sees that the lower the symmetry the less restrictive the selection rules.

9.8 Wigner-Eckart theorem

Possibly it is the easiest to introduce the notion of Clebsch-Gordon coefficients and irreducible tensor operator for the case in which $\mathcal{G}$ is a group of coordinate transformations of $\mathbb{R}^3$. => to state the Wigner-Eckart theorem in this context. The theorem has though a much more general validity.

Given a generic group $\mathcal{G}$ with irreducible representations Γ^p and Γ^q of dimension d_p and d_q, we can identify in ψ_j^p $(j=1,2,\dots,d_p)$ and ψ_s^q $(s=1,\dots,d_q)$ the orthonormal bases associated to the two corresponding abstract inner product spaces V^p and V^q.

A $d_p d_q$-dimensional direct product space $V^p \otimes V^q$ is defined by the set of all quantities ϕ:

$$\phi = \sum_{j=1}^{d_p} \sum_{s=1}^{d_q} a_{js}\, \psi_j^p \otimes \psi_s^q$$

with $a_{js} \in \mathbb{C}$ and the inner product defined as:

$$(\phi, \psi) = \sum_{j=1}^{d_p} \sum_{s=1}^{d_q} a_{js}^* b_{js}$$

where $\psi = \sum_{j=1}^{d_p} \sum_{s=1}^{d_q} b_{js}\, \psi_j^p \otimes \psi_s^q$.

$\forall\, T \in \mathcal{G}$ one can construct the linear operators $\Phi^p(T)$ and $\Phi^q(T)$

$$\Phi^p(T)\, \psi_j^p = \sum_{k=1}^{d_p} \Gamma^p(T)_{kj}\, \psi_k^p$$

$$\Phi^q(T)\, \psi_s^q = \sum_{t=1}^{d_q} \Gamma^q(T)_{ts}\, \psi_t^q$$

A further linear operator acting on $V^p \otimes V^q$ may be defined

$$\Phi(T)\{\psi_j^p \otimes \psi_s^q\} = \sum_{k=1}^{d_p} \sum_{t=1}^{d_q} \left(\Gamma^p(T) \otimes \Gamma^q(T)\right)_{kt,js} \{\psi_k^p \otimes \psi_t^q\}$$

Thus the operators $\Phi(T)$ associated to the space $V^p \otimes V^q$ are the linear operators corresponding to the direct product representation $\Gamma^p \otimes \Gamma^q$ of $\mathcal{G}$.

Since $\Gamma^p \otimes \Gamma^q$ is in general reducible $\Gamma^p \otimes \Gamma^q \approx \bigoplus_r n_{pq}^r \Gamma^r$, there must be n_{pq}^r linearly independent sets of n_r basis vectors $\Theta_u^{r,\alpha}$ $\alpha = 1, \dots, n_{pq}^r$ $u = 1, \dots, n_r$ such that

$$\Phi(T)\, \Theta_\ell^{r,\alpha} = \sum_{u=1}^{d_r} \Gamma^r(T)_{u\ell}\, \Theta_u^{r,\alpha}$$

and

$$\Theta_\ell^{r,\alpha} = \sum_{j=1}^{d_p} \sum_{k=1}^{d_q} \underbrace{\begin{pmatrix} p & q \\ j & k \end{pmatrix}\begin{vmatrix} r, & \alpha \\ \ell & \end{pmatrix}}_{\text{Clebsch-Gordon coefficients.}} \psi_j^p \otimes \psi_k^q$$

In other terms, the Clebsch-Gordon coefficients give the appropriate linear combinations that form bases for the various irrep of $\Gamma^p \otimes \Gamma^q$.

In order to state the Wigner-Eckart theorem we have to introduce the concept of <u>irreducible tensor operator</u>.

Consider Q_1 and Q_2 linear mappings between V^p and V^r.

$Q_1 + Q_2$ and $a Q_i$ are also linear mappings between V^p and V^r

Moreover, all other properties defining a vector space are also satisfied $L(V^p, V^r)$

An homomorphism of $\mathcal{G}$ to $L(V^p, V^r)$ is given by the expression

$$\Phi'(T)\, Q = \Phi^r(T)\, Q\, \Phi^p(T)^{-1}$$

Theorem The (generalized) Wigner-Eckart Theorem

Let $\mathcal{G}$ be a finite group (or a compact Lie group). Let Γ^p, Γ^q and Γ^r be unitary irreducible representations of $\mathcal{G}$ of dimensions d_p, d_q, and d_r respectively and suppose that ϕ_j^p ($j = 1, 2, \dots, d_p$) and ψ_l^r ($l = 1, 2, \dots d_r$) are basis vectors of ortho-normal bases of the vector space V^p and V^r of Γ^p and Γ^r respectively. Finally, let Q_k^q ($k = 1, 2, \dots d_q$) be a set of irreducible tensor operators of Γ^q. Then

$$(\psi_l^r, Q_k^q \phi_j^p) = \sum_{\alpha=1}^{n_{pq}^r} \underbrace{\begin{pmatrix} p & q \\ j & k \end{pmatrix} \begin{vmatrix} r, & \alpha \\ l & \end{vmatrix}}\,^{*} (r | Q^q | p)_\alpha$$

for all $j = 1, 2, \dots, d_p$, $k = 1, 2, \dots, d_q$ and $l = 1, 2, \dots, d_r$ where $(r | Q^q | p)_\alpha$ are a set of n_{pq}^r "reduced matrix elements" that are independent of j, k and l.

$$(r | Q^q | p)_\alpha = \frac{1}{d_r} \sum_{j'=1}^{d_p} \sum_{k'=1}^{d_q} \sum_{l'=1}^{d_r} \left(\begin{matrix} p & q \\ s & t \end{matrix} \middle| \begin{matrix} r & \alpha \\ u & \end{matrix} \right) (\psi_{l'}^r, Q_{k'}^q \phi_{j'}^p)$$

proof: As the operators $\Phi^r(T)$ are unitary

$$(\psi_l^r, Q_k^q \phi_j^p) = (\Phi^r(T) \psi_l^r, \Phi^r(T) Q_k^q \phi_j^p)$$

$$= (\Phi^r(T) \psi_l^r, \{\Phi^r(T) Q_k^q \Phi^p(T)^{-1}\} \Phi^p(T) \phi_j^p)$$

$$= \sum_{j'=1}^{d_p} \sum_{k'=1}^{d_q} \sum_{l'=1}^{d_r} \Gamma^p(T)_{j'j} \Gamma^q(T)_{k'k} \Gamma^r(T)^*_{l'l} (\psi_{l'}^r, Q_{k'}^q \phi_{j'}^p)$$

In general we can only say that $\Gamma^p \otimes \Gamma^q$ is similar to the Clebsch-Gordan series $\bigoplus_r n_{pq}^r \Gamma^r$. Since, through all representations Γ^j can be chosen to be unitary, it follows that the Clebsch-Gordan coefficients may be chosen to be part of a unitary matrix =>

$$\left(\begin{matrix} r, & \alpha \\ l & \end{matrix} \middle| \begin{matrix} p & q \\ j & k \end{matrix} \right) = \left(\begin{matrix} p & q \\ j & k \end{matrix} \middle| \begin{matrix} r, & \alpha \\ l & \end{matrix} \right)^*$$

and we can write

$$\phi_j^p \otimes \psi_k^q = \sum_r \sum_{\alpha=1}^{n_{pq}^r} \sum_{l=1}^{d_r} \left({r \alpha \atop l} \middle| {p\, q \atop j\, k} \right) \theta_l^{r,\alpha}$$

$$= \sum_r \sum_{\alpha=1}^{n_{pq}^r} \sum_{l=1}^{d_r} \left({p\, q \atop j\, k} \middle| {r \alpha \atop l} \right)^* \theta_l^{r,\alpha}$$

Moreover, if we apply the projector $\mathcal{P}_{ll}^r$ to the tensor product $\psi_j^p \otimes \psi_k^q$

$$\mathcal{P}_{l'l}^r \left(\phi_j^p \otimes \psi_k^q \right) = \sum_{\alpha=1}^{n_{pq}^r} \left({p\, q \atop j\, k} \middle| {r \alpha \atop l} \right)^* \theta_{l'}^{r,\alpha}$$

$$= \sum_{\alpha=1}^{n_{pq}^r} \sum_{j'k'} \left({p\, q \atop j\, k} \middle| {r \alpha \atop l} \right)^* \left({p\, q \atop j'\, k'} \middle| {r \alpha \atop l'} \right) \phi_{j'}^p \otimes \psi_{k'}^q$$

On the other hand, thanks to WOT, $\mathcal{P}_{l'l}^r$ can also be written as

$$\mathcal{P}_{l'l}^r = \frac{d_r}{g} \sum_{T \in \mathcal{G}} \Gamma_{l'l}^r(T)^* \bar{\Phi}(T)$$

Thus:

$$\mathcal{P}_{l'l}^r \left(\phi_j^p \otimes \psi_k^q \right) = \frac{d_r}{g} \sum_{T \in \mathcal{G}} \Gamma_{l'l}^r(T)^* \sum_{j'=1}^{d_p} \sum_{k'=1}^{d_q} \Gamma_{j'j}^p(T) \Gamma_{k'k}^q(T) \phi_{j'}^p \otimes \psi_{k'}^q$$

By comparison we obtain:

$$\sum_{\alpha=1}^{n_{pq}^r} \left({p\, q \atop j\, k} \middle| {r \alpha \atop l} \right)^* \left({p\, q \atop j'\, k'} \middle| {r \alpha \atop l'} \right) = \frac{d_r}{g} \sum_{T \in \mathcal{G}} \Gamma_{l'l}^r(T)^* \Gamma_{j'j}^p(T) \Gamma_{k'k}^q(T)$$

Thus we can write:

$$\left(\psi_l^r, Q_k^q \phi_j^p \right) = \frac{1}{d_r} \sum_{\alpha=1}^{n_{qp}^r} \sum_{l'j'k'} \left({p\, q \atop j\, k} \middle| {r \alpha \atop l} \right)^* \left({p\, q \atop j'\, k'} \middle| {r \alpha \atop l'} \right) \left(\psi_{l'}^r, Q_{k'}^q \phi_{j'}^p \right)$$

which is the final result with the identification

$$(r \| Q^q \| p)_\alpha = \frac{1}{d_r} \sum_{j'l'k'} \left({p\, q \atop j'\, k'} \middle| {r \alpha \atop l'} \right) \left(\psi_{l'}^r, Q_{k'}^q \phi_{j'}^p \right).$$

■

Notice:

- The $j\,k\,l$ dependence of the matrix element $(\psi_l^r, Q_k^q \phi_j^p)$ is completely given by the Clebsch-Gordan coefficients

- The whole set of $d_p d_q d_r$ elements $(\psi_l^r, Q_k^q \phi_j^p)$ depends only on n_{pq}^r reduced matrix elements

- Although the explicit expression of the reduced matrix element is given, the most common praxis is to obtain it from direct calculation of a simple matrix element.

The calculation of the Clebsch-Gordan coefficients for finite order groups and $n_{pq}^r < 2$ is readily obtained. One starts from the equation (specialized to $\alpha = 1$)

$$\left(\begin{matrix} p & q \\ s & t \end{matrix}\middle|\begin{matrix} r & 1 \\ u & \end{matrix}\right)\left(\begin{matrix} r & 1 \\ l & \end{matrix}\middle|\begin{matrix} p & q \\ j & k \end{matrix}\right) = \frac{d_r}{g} \sum_{T \in \mathcal{G}} \Gamma^p(T)_{sj}\, \Gamma^q(T)_{tk}\, \Gamma^r(T)^*_{ul}$$

One looks for a set $j\,k\,l$ such that

$$A = \frac{d_r}{g} \sum_{T \in \mathcal{G}} \Gamma^p(T)_{jj}\, \Gamma^q(T)_{kk}\, \Gamma^r(T)^*_{ll} \neq 0$$

From the equation (*) and the unitarity of the Clebsch-Gordan "matrix", $A > 0$ and real. We can thus choose $\left(\begin{matrix} p & q \\ j & k \end{matrix}\middle|\begin{matrix} r & 1 \\ l & \end{matrix}\right)$ real and positive

$$\left(\begin{matrix} p & q \\ j & k \end{matrix}\middle|\begin{matrix} r & 1 \\ l & \end{matrix}\right) = \left\{ \frac{d_r}{g} \sum_{T \in \mathcal{G}} \Gamma^p(T)_{jj}\, \Gamma^q(T)_{kk}\, \Gamma^r(T)^*_{ll} \right\}^{1/2}$$

and finally deduce:

$$\begin{pmatrix} p & q & \bigg| & r, & 1 \\ s & t & \bigg| & u & \end{pmatrix} = \frac{\left(\frac{d_r}{g}\right)^{1/2} \sum_{T \in \mathcal{G}} \Gamma^p(T)_{sj}\, \Gamma^q(T)_{tk}\, \Gamma^r(T)^*_{ul}}{\left\{ \sum_{T \in \mathcal{G}} \Gamma^p(T)_{jj}\, \Gamma^q(T)_{kk}\, \Gamma^r(T)^*_{ll} \right\}^{1/2}}$$