Spin Multipole Graphical Techniques

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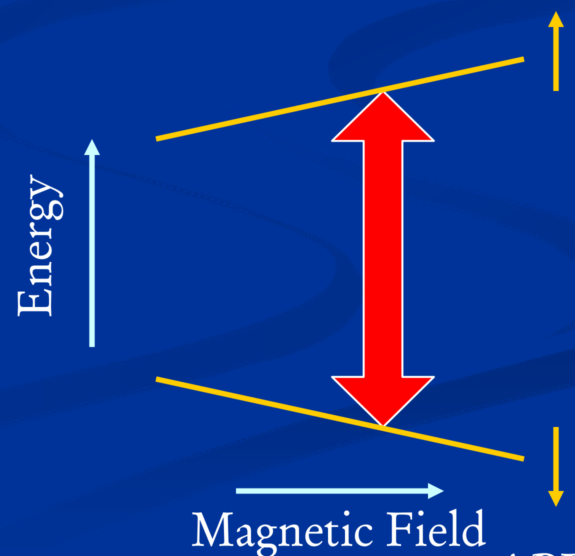
Levels, Transitions, Dynamics

- Interactions in nature give us energy levels
- Spectroscopists probe transitions between energy levels
- Generate torque terms

$$\hat{H} = -\beta \vec{H} \bullet \overleftrightarrow{g} \bullet \vec{S}$$

$$\frac{\partial \vec{S}}{\partial t} = \frac{i}{\hbar}\left[\hat{H}, \vec{S}\right]$$

$$\frac{\partial \vec{S}}{\partial t} \equiv i\hat{L}^{\times}\vec{S}$$



Statistical Operator

- Ensembles of spins
- Equation of motion
- Transitions as states
- Condition for non-vanishing trace

$$\frac{\partial \sigma}{\partial t} = -i\left[H, \sigma\right] \equiv -iL^{\times}\sigma$$

$$\left\langle S \right\rangle \equiv Tr\left\{\sigma S\right\} = \sum_{m,m'} \left\langle m \middle| \sigma \middle| m' \right\rangle \left\langle m' \middle| S \middle| m \right\rangle$$

Liouville Operator

- Maps Transitions
- $(2S+1)^2 \times (2S+1)^2$ matrix
- Spin S,I: $(2S+1)^2(2I+1)^2 \times (2S+1)^2(2I+1)^2$
- Automate computation for multiple spins

$$\frac{\partial \sigma(t)}{\partial t} = -iL^{\times}(t)\sigma(t)$$

$$\sigma(t+\Delta t) \approx \sigma(t) - iL^{\times}(t)\sigma(t)\Delta t$$

Example: Spin 1/2

$$\frac{\partial}{\partial t}\begin{bmatrix}\sigma_{++}\\ \sigma_{--}\\ \sigma_{+-}\\ \sigma_{-+}\end{bmatrix} = -i\begin{bmatrix} L_{++,++} & L_{++,--} & L_{++,+-} & L_{++,-+}\\ L_{--,++} & L_{--,--} & L_{--,+-} & L_{--,-+}\\ L_{+-,++} & L_{+-,--} & L_{+-,+-} & L_{+-,-+}\\ L_{-+,++} & L_{-+,--} & L_{-+,+-} & L_{-+,-+}\end{bmatrix}\begin{bmatrix}\sigma_{++}\\ \sigma_{--}\\ \sigma_{+-}\\ \sigma_{-+}\end{bmatrix}$$

Matrix Elements

- Compute matrix elements of the mapping
- Represent transitions as multipole operators
- Complete set of operators
- Can generalize to multiple spin systems

$$Q_{\sigma}^{[\Sigma]} \equiv (-i)^{\Sigma} \sum_{m,m'} \langle S,m;S,m' | \Sigma,\sigma \rangle \, | S,m \rangle \langle S,m' |$$

$$\left\langle Q_{\sigma_1}^{[\Sigma_1]} \middle| Q_{\lambda}^{[\Lambda]\times} \middle| Q_{\sigma_2}^{[\Sigma_2]} \right\rangle \equiv Tr\left\{ \left(Q_{\sigma_1}^{[\Sigma_1]} \right)^{\dagger} \left[Q_{\lambda}^{[\Lambda]}, Q_{\sigma_2}^{[\Sigma_2]} \right] \right\}$$

Adjoint

$$Q_0^{[0]} \equiv \sum_k \langle K, -k; K, k | 0, 0 \rangle Q_{-k}^{[K]} Q_k^{[K]}$$

$$\langle K, -k; K, k | 0, 0 \rangle = \frac{(-1)^{K+k}}{\sqrt{2K+1}} \equiv \frac{(-1)^{K+k}}{\hat{K}}$$

$$Q_0^{[0]} = \frac{1}{\hat{K}} \sum_k (-1)^{K+k} Q_{-k}^{[K]} Q_k^{[K]} \equiv \frac{1}{\hat{K}} \sum_k \left(Q_k^{[K]} \right)^\dagger Q_k^{[K]}$$

Mulitpole Operator Adjoint

- 0^{th} multipole defines scalar product
- Metric
- Invariants
- Tensorial sets

$$\left(Q_k^{[K]}\right)^\dagger \equiv (-1)^{K+k}\,\tilde{Q}_{-k}^{[K]}$$

$$\left(Y_m^{[l]}(\theta,\varphi)\right)^\dagger = (-1)^{l+m}\,Y_{-m}^{[l]}(\theta,\varphi)$$

$$Y_m^{[l]}(\theta,\varphi) \equiv (-i)^l\,Y_m^l(\theta,\varphi)$$

$$\left(Y_m^l(\theta,\varphi)\right)^* = (-1)^m\,Y_{-m}^l(\theta,\varphi)$$

Multipole Invariants

- Projection operators select a particular multipole
- Work only with invariant quantities

$$\left[\tilde{W}^{[K]} Q^{[K]}\right]^{[0]} \equiv \frac{1}{\hat{K}} \sum_k \left(W_k^{[K]}\right)^\dagger Q_k^{[K]}$$

$$\sum_k \left(W_k^{[K]}\right)^\dagger W_k^{[K]} = 1$$

$$Q_k^{[K]} = \hat{K}\left[W^{[K]} Q^{[K]}\right]^{[0]}$$

Orthonormal Multipoles

- Define orthonormal multipoles
- Express all quantities as invariants
- Need technology for recoupling multipoles

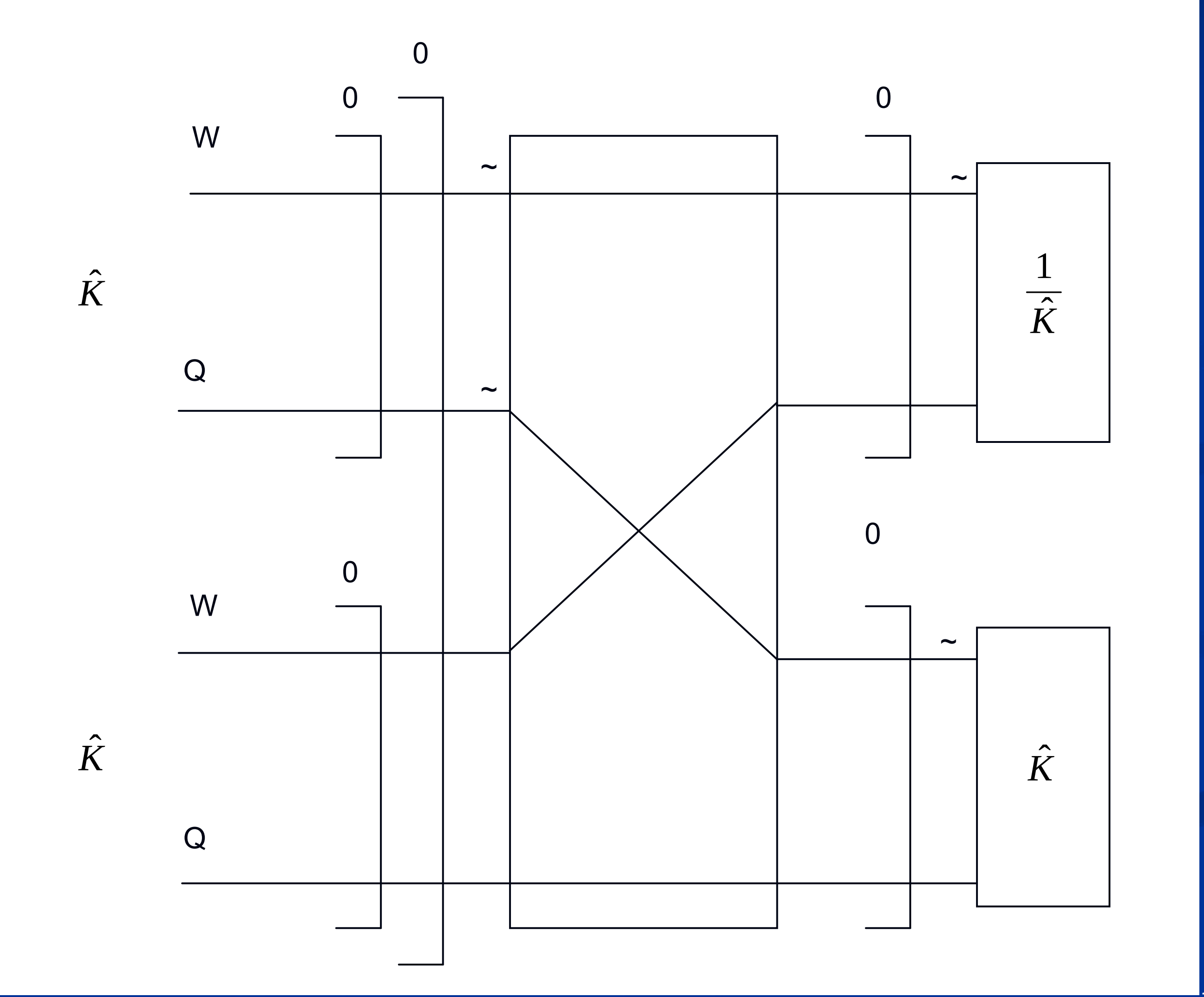
$$\left\langle Q_k^{[K]} \middle| Q_k^{[K]} \right\rangle = \int \hat{K} \left[\tilde{W}_k^{[K]} \tilde{Q}_k^{[K]} \right]^{[0]} \hat{K} \left[W_k^{[K]} Q_k^{[K]} \right]^{[0]}$$

$$\left\langle Q_k^{[K]} \middle| Q_k^{[K]} \right\rangle = \int \hat{K}^2 \begin{bmatrix} K & K & 0 \\ K & K & 0 \\ 0 & 0 & 0 \end{bmatrix} \left[\tilde{W}_k^{[K]} W_k^{[K]} \right]^{[0]} \left[\tilde{Q}_k^{[K]} Q_k^{[K]} \right]^{[0]}$$

$$\left\langle Q_k^{[K]} \middle| Q_k^{[K]} \right\rangle = \hat{K}^2 \frac{\hat{0}}{\hat{K}^2} \frac{1}{\hat{K}} \hat{K} = 1$$

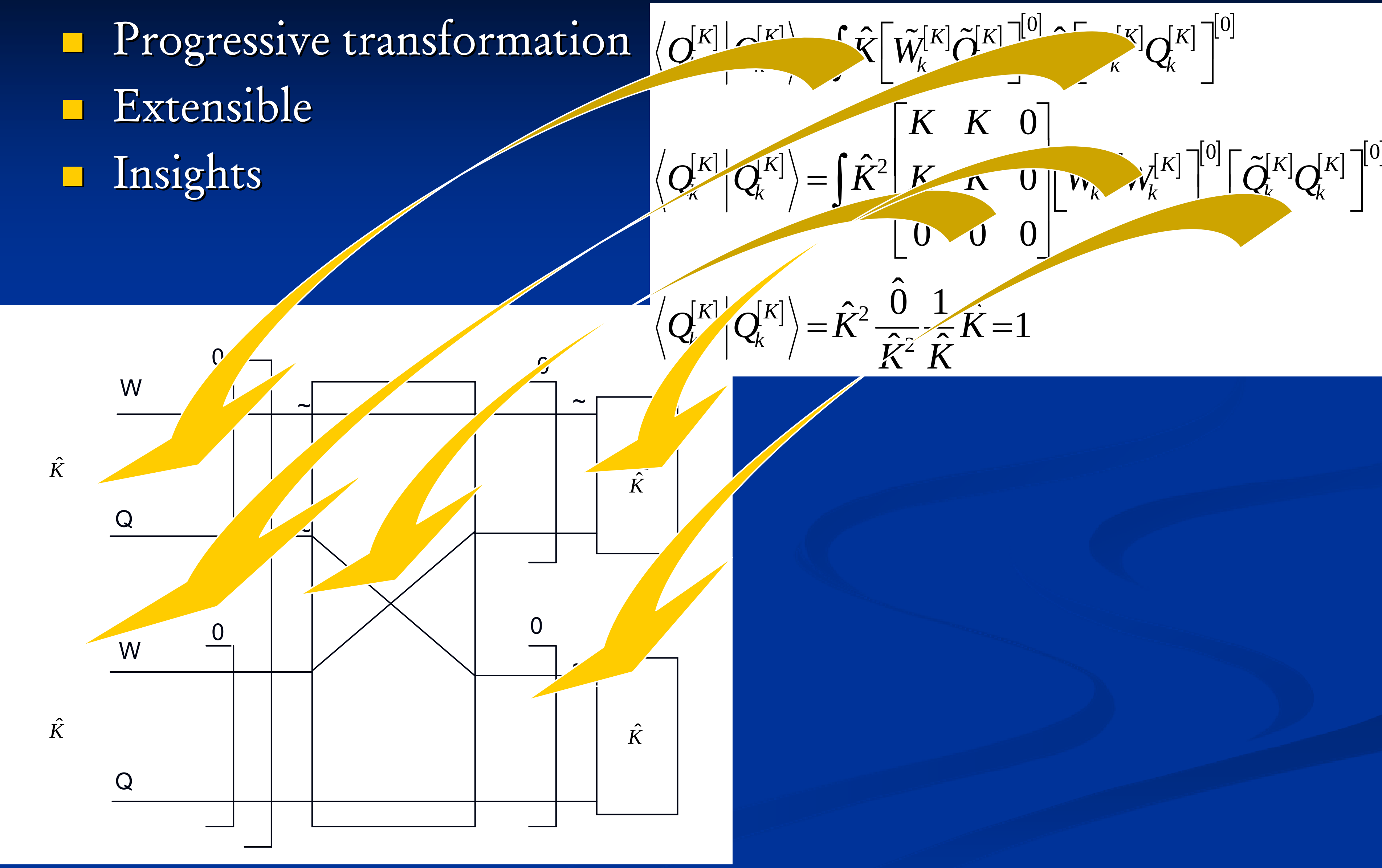
Graphical representation

- Graphs convey coupling information
- Details of coupling abstracted away.



Comparison

- Progressive transformation
- Extensible
- Insights



Matrix Elements II (or III)

- Difference between VCC and Wigner C
- Trace of products of 3 operators invariant
- Wigner Eckart Theorem

$$\left\langle Q_{k_1}^{[K_1]} \middle| Q_{k_2}^{[K_2]} \middle| Q_{k_3}^{[K_3]} \right\rangle \propto \left\langle K_1 - k_1; K_1 k_1 \middle| 00 \right\rangle \left\langle K_2 k_2; K_3 k_3 \middle| K_1 k_1 \right\rangle$$

$$\left\langle Q_{k_1}^{[K_1]} \middle| Q_{k_2}^{[K_2]} \middle| Q_{k_3}^{[K_3]} \right\rangle \propto \begin{pmatrix} K_1 & K_2 & K_3 \\ -k_1 & k_2 & k_3 \end{pmatrix}$$

$$\begin{pmatrix} K_1 & K_2 & K_3 \\ -k_1 & k_2 & k_3 \end{pmatrix} = (-1)^{K_2 - K_3 + k_1} \frac{1}{\hat{K}_1} \left\langle K_2 k_2; K_3 k_3 \middle| K_1 k_1 \right\rangle$$

Trace Invariant Form

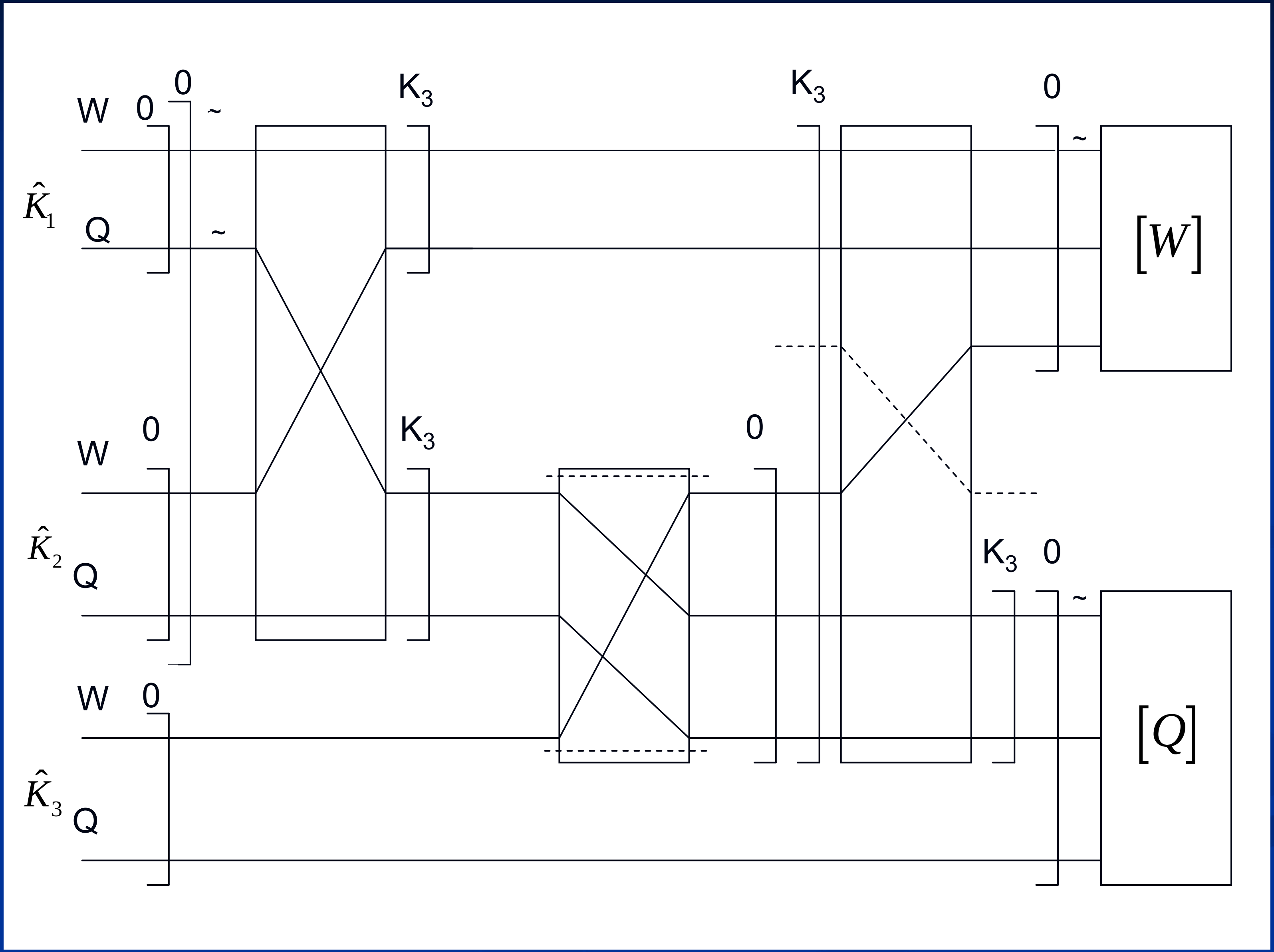
- Express trace in terms of invariants
- Recouple invariants
- Use prior results to simplify the expression
- Use graphs to represent the process

$$Tr\left\{\left(Q_{k_1}^{[K_1]}\right)^\dagger Q_{k_2}^{[K_2]} Q_{k_3}^{[K_3]}\right\} = \int \hat{K}_1\left[\tilde{W}^{[K_1]}\tilde{Q}^{[K_1]}\right]^{[0]} \hat{K}_2\left[W^{[K_2]}Q^{[K_2]}\right]^{[0]} \hat{K}_3\left[W^{[K_3]}Q^{[K_3]}\right]^{[0]}$$

$$Tr\left\{\left(Q_{k_1}^{[K_1]}\right)^\dagger Q_{k_2}^{[K_2]} Q_{k_3}^{[K_3]}\right\} = \int \left[\tilde{W}^{[K_1]}\left[W^{[K_2]}W^{[K_3]}\right]^{[K_1]}\right]^{[0]} \left[\tilde{Q}^{[K_1]}\left[Q^{[K_2]}Q^{[K_3]}\right]^{[K_1]}\right]^{[0]}$$

How did we get *this*!?

Graphical representation of Wigner Eckart Theorem

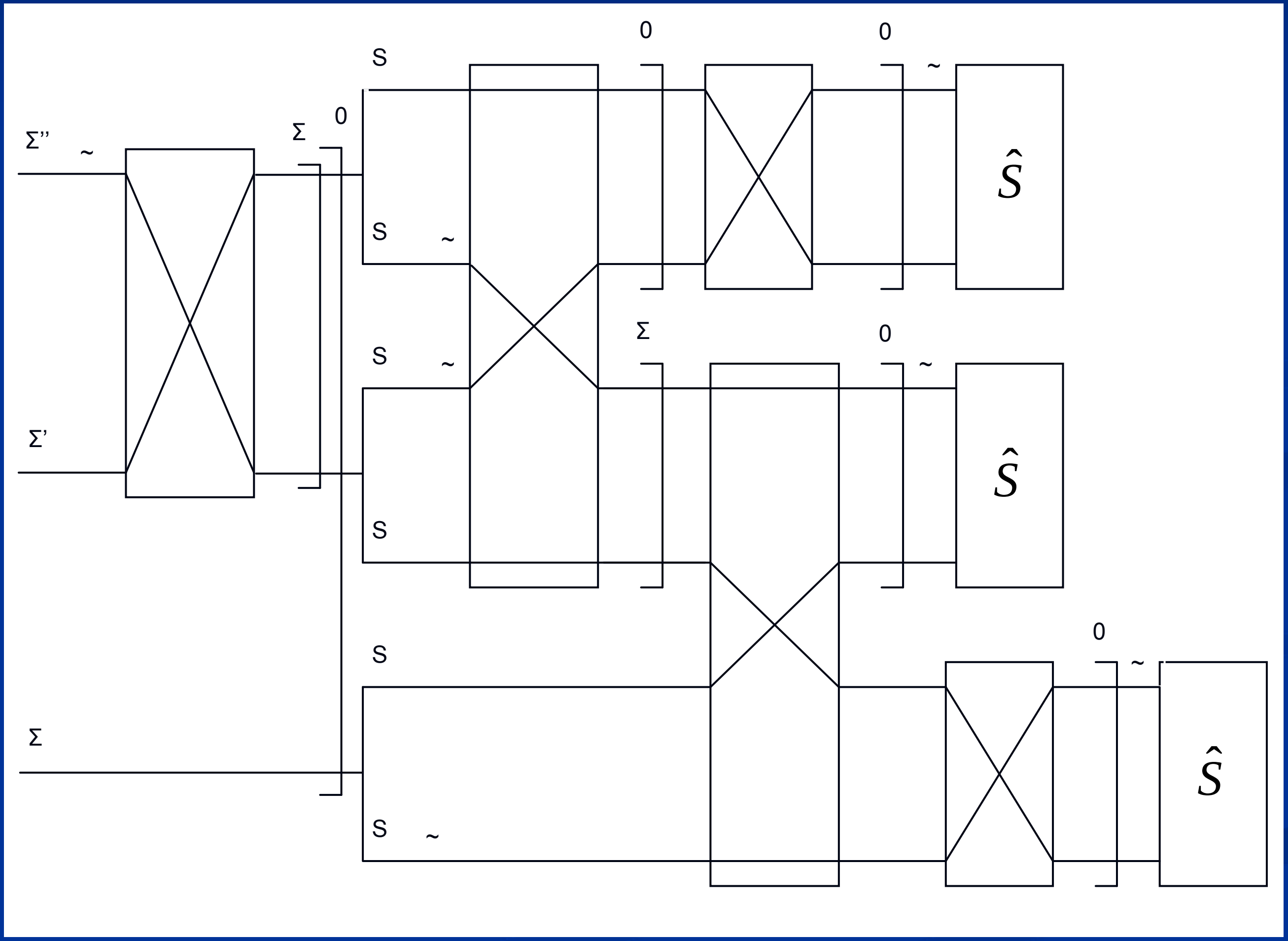


Interpretation

- [W] describes the geometry
  - Wigner 3j symbol
  - Polarizations
- [Q] describes the physics
  - Reduced matrix element
  - Contributions from different interactions
- Expression in invariant form
  - Independent of coordinates
  - Geometrical object

Reduced Matrix Element

- Use previous results to evaluate graphically
- Read off analytical expression



Analytical Expression

- Construct Analytical Expression
- Simplify phase
- Simplify amplitude

$$(-1)^{\Sigma''+\Sigma'-\Sigma}\,(-1)^{2S+\Sigma''+\Sigma'+\Sigma}\,(-i)^{\Sigma''+\Sigma'+\Sigma}\,\hat{\Sigma}''\hat{\Sigma}'\hat{\Sigma}\begin{Bmatrix}\Sigma'' & \Sigma' & \Sigma\\ S & S & S\end{Bmatrix}$$

Wigner-Eckart Result (one spin)

- Combine [W] and [Q] expressions
- Read off standard phase and amplitude

$$Tr\left\{\left(Q_{\sigma''}^{[\Sigma'']}\right)^{\dagger} Q_{\sigma'}^{[\Sigma']} Q_{\sigma}^{[\Sigma]}\right\} = (-1)^{\Sigma''-\sigma''} \begin{pmatrix} \Sigma'' & \Sigma' & \Sigma \\ -\sigma'' & \sigma' & \sigma \end{pmatrix} \left\langle \Sigma'' \middle\| \Sigma' \middle\| \Sigma \right\rangle$$

$$\left\langle \Sigma'' \middle\| \Sigma' \middle\| \Sigma \right\rangle = (-1)^{\Sigma''+\Sigma'+\Sigma+2S} (i)^{\Sigma''+\Sigma'+\Sigma} \hat{\Sigma}''\hat{\Sigma}'\hat{\Sigma} \begin{Bmatrix} \Sigma'' & \Sigma' & \Sigma \\ S & S & S \end{Bmatrix}$$

$$Tr\left\{\left(Q_{\sigma''}^{[\Sigma'']}\right)^{\dagger} \left[Q_{\sigma'}^{[\Sigma']}, Q_{\sigma}^{[\Sigma]}\right]\right\} = (-1)^{\Sigma''-\sigma''} \begin{pmatrix} \Sigma'' & \Sigma' & \Sigma \\ -\sigma'' & \sigma' & \sigma \end{pmatrix} \left\langle \Sigma'' \middle\| \Sigma' \middle\| \Sigma \right\rangle \left[1-(-1)^{\Sigma''+\Sigma'+\Sigma}\right]$$

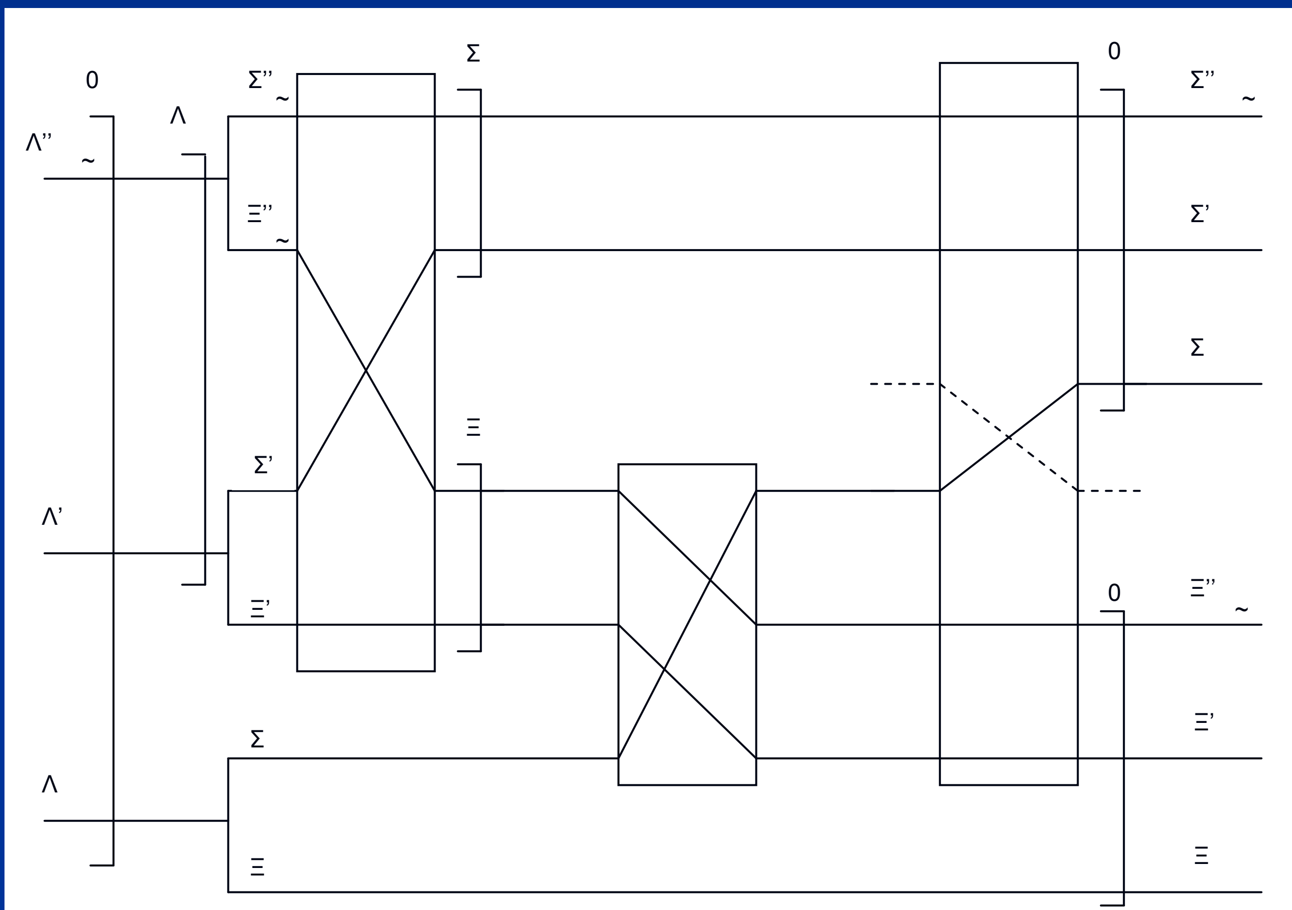
Coupled Spin Systems

- Coupled Basis Useful for Interacting Spins
- Generalizes to Multiple Coupled Spins
- Useful to define an adjoint operation

$$Q_{\ell}^{[L]}(S,I)=\sum_{j,k}\left\langle J,j;K,k\middle|L,\ell\right\rangle Q_{j}^{[J]}(S)\,Q_{k}^{[K]}(I)$$

Coupled Spin Systems

- Pair-wise couplings have recursive structure
- Generalized Wigner-Eckart Theorem
- Hamiltonian GUI



$$\hat{\Lambda}''\hat{\Lambda}'\hat{\Lambda}\begin{Bmatrix} \Lambda'' & \Lambda' & \Lambda \\ \Sigma'' & \Sigma' & \Sigma \\ \Xi'' & \Xi' & \Xi \end{Bmatrix}$$

Pair-wise Reduced Matrix Element

- Intermediate graph well-known result
- Apply recursively
- Many coupled spins

$$\langle \Lambda'' \| \Lambda' \| \Lambda \rangle = \hat{\Lambda}'' \hat{\Lambda}' \hat{\Lambda} \begin{Bmatrix} \Lambda'' & \Lambda' & \Lambda \\ \Sigma'' & \Sigma' & \Sigma \\ \Xi'' & \Xi' & \Xi \end{Bmatrix} \langle \Sigma'' \| \Sigma' \| \Sigma \rangle \langle \Xi'' \| \Xi' \| \Xi \rangle$$

Can apply to a tree of
pair-wise coupled spins.

Process terminates at
'leaf' or 'terminal' nodes

Example: Two Coupled Spins

- Very important practical case
- Zeeman and hyperfine interactions
- Fine structure and quadrupolar splittings

$$Tr\left\{\left(Q_{\lambda''}^{[\Lambda'']}\right)^{\dagger}\left[Q_{\lambda'}^{[\Lambda']},Q_{\lambda}^{[\Lambda]}\right]\right\}$$

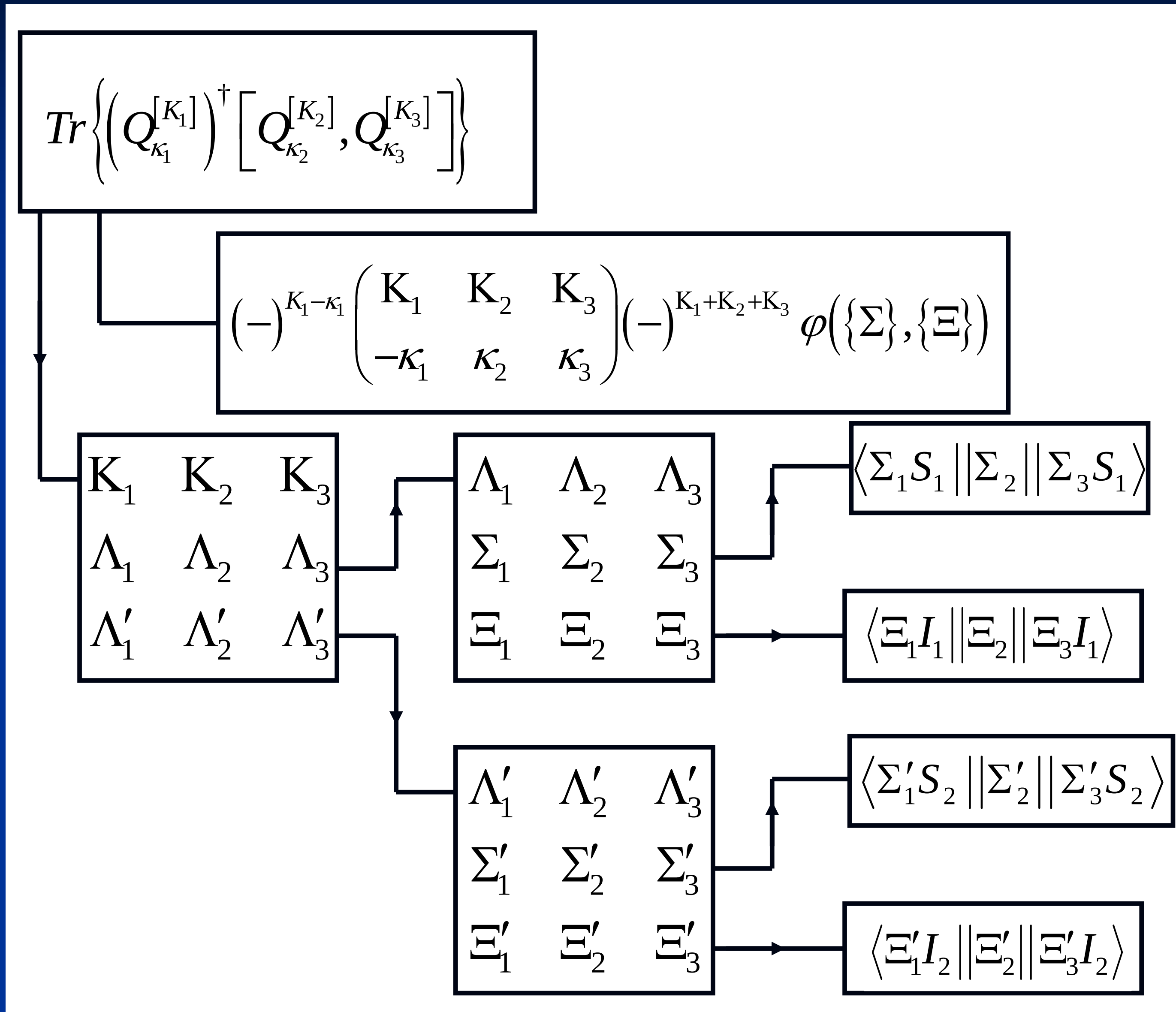
$$(-)^{\Lambda''-\lambda''}\begin{pmatrix}\Lambda'' & \Lambda' & \Lambda \\ -\lambda'' & \lambda' & \lambda\end{pmatrix}(-)^{\Lambda''+\Lambda'+\Lambda}\varphi\left(\{\Sigma\},\{\Xi\}\right)$$

$$\begin{Bmatrix}\Lambda'' & \Lambda' & \Lambda \\ \Sigma'' & \Sigma' & \Sigma \\ \Xi'' & \Xi' & \Xi\end{Bmatrix}$$

$$(-)^{2S}(i)^{\Sigma''+\Sigma'+\Sigma}\begin{Bmatrix}\Sigma'' & \Sigma' & \Sigma \\ S & S & S\end{Bmatrix}$$

$$(-)^{2I}(i)^{\Xi''+\Xi'+\Xi}\begin{Bmatrix}\Xi'' & \Xi' & \Xi \\ I & I & I\end{Bmatrix}$$

Example: Four Coupled Spins



Work in Progress

- Hamiltonian GUI based on Vision
- Python
- Object-oriented
- Free
- Example: Two spins
- Downloads: http://earlelab.rit.albany.edu
- Your comments Welcome
- Open source

Resources

- Documentation at earlelab.rit.albany.edu
- "Irreducible Tensorial Sets" Fano and Racah
- "Angular Momentum" Brink and Satchler
- "Angular Momentum" Zare
- "Density Matrix Theory and Applications" Blum
- "Angular Momentum Calculus in Quantum Physics" Danos and Gillet
- "Irreducible Tensor Methods" Silver
- "Graphical Methods of Spin Algebras" El Baz and Castel
- "Quantum Theory of Angular Momentum" Biedenharn and Louck
- "The Principles of Nuclear Magnetism" Abragam
- "EPR of Transition Metal Ions" Abragam and Bleaney
- "Gravitation" Misner, Thorne and Wheeler

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