

Interpreting Stone's model of Berry phases

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It provides a simple quantum-mechanical example in which the **Berry phase** gives rise to **Wess-Zumino** terms (Path-integral formulation). Indeed, for large μ , Stone's Hamiltonian describes the motion of a **constrained spin**, which is equivalent to **motion of a charged particle about a magnetic monopole** (Leinaas 1978).

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Magnetoelectricity is characterised by a local order parameter (to be identified), which is odd under both space inversion and time reversal, being thereby invariant under the combined action of these transformations.

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- **Magnetoelectricity of the (large- μ) ground state of Stone's model.**

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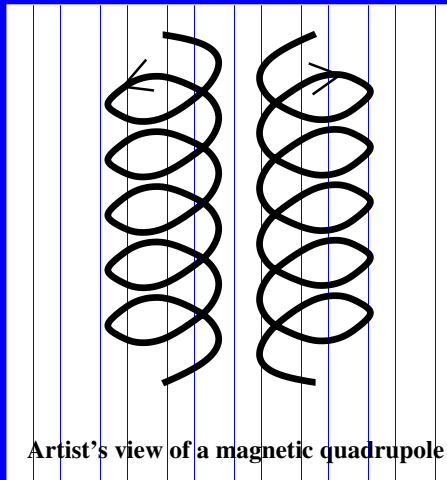
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as shown by recent theoretical work on **x-ray dichroism and resonant scattering in noncentrosymmetric crystals** (Carra *et al.* 2003, Marri and Carra 2004).

$([,]^{(k)}) \rightarrow$ Clebsch-Gordan coupling of irreducible tensors; $\mathbf{S} = \frac{1}{2}\boldsymbol{\sigma}$;

$\boldsymbol{\Omega}_L \equiv \frac{1}{2}(\mathbf{n} \times \mathbf{L} - \mathbf{L} \times \mathbf{n})$, orbital anapole; $\mathbf{Q}^{(2)} \equiv [\mathbf{L}, \mathbf{L}]^{(2)}$, orbital quadrupole.)



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[Order parameters: definition (2nd quant.)]

$$(\mathbf{O}_L^{(k)})_q = \sum_{\substack{l, l' = l \pm 1 \\ m, m', \sigma, \sigma'}} \frac{1}{2} \left[\langle \sigma' | \langle l' m' | (\mathbf{O}_L^{(k)})_q | l m \rangle | \sigma \rangle c_{l' m' \sigma'}^\dagger c_{l m \sigma} + \text{c.c.} \right],$$

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with $c_{lm\sigma}^\dagger$ and $c_{lm\sigma}$ fermionic operators.]

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The basis set $|j \pm \frac{1}{2}, jm\rangle$ provides a convenient framework for describing **parity-breaking electron hybridisation** (e.g. pd mixing in transition-metal oxides), in the jj coupling scheme. ($n \cdot \sigma/2 = n \cdot \mathbf{J}$, as $n \cdot \mathbf{L} = 0$.)

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- **Determine form of order parameters in jj coupling**

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- Determine form of order parameters in jj coupling
- LS \rightarrow jj transformations (Edmonds 1974)

Unit tensors

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Coupled double Tensors (Judd, 1967)

$$w_{\zeta}^{(xy)z}(l', l) = \sum_{\xi, \eta, \lambda, \lambda', \sigma, \sigma'} C_{x\xi; y\eta}^{z\zeta} C_{\frac{1}{2}\sigma'; \frac{1}{2}\sigma} C_{l'\lambda'; l\lambda}^{x\xi} c_{l'\lambda'\sigma'}^{\dagger} \tilde{c}_{l\lambda\sigma} + \text{h.c.}, \quad (LS)$$

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where $\tilde{c}_{l\lambda\sigma} = (-1)^{l-\lambda+\frac{1}{2}-\sigma} c_{l-\lambda-\sigma}$ and $\tilde{c}_{l, jm} = (-1)^{j-m} c_{l, j-m}$ (irreducibility).

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$$w^{(20)2}(l', l) = -\frac{\sqrt{2}}{\sqrt{l(l+1)} C_{l0;10}^{l'0} \left\{ \begin{matrix} 1 & 1 & 2 \\ l' & l & l \end{matrix} \right\}} \mathcal{M}_L^{(2)}(l', l).$$

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LS \rightarrow jj transformation

$$w^{(xy)z}(l', l) = \sum_{j, j'} (-1)^{x+y+z} [x, y, j, j']^{\frac{1}{2}} \left\{ \begin{matrix} l & l' & x \\ \frac{1}{2} & \frac{1}{2} & y \\ j & j' & z \end{matrix} \right\} v^{(j'j)z}(l', l),$$

Unit tensors (cont'd)

Importance of unit tensors: LS and jj order parameters can be expressed as multiples of them (Wigner-Eckart theorem); e.g.

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with $[a, \dots, b] = (2a+1) \cdots (2b+1)$.

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$$\begin{aligned}\widetilde{\mathcal{M}}_J^{(2)}(l', l) &= \frac{1}{5} \left(\frac{l+l'-1}{2} \right) \left(\frac{l+l'+3}{2} \right) \mathcal{M}_S^{(2)}(l', l) + \frac{2}{3} \mathcal{M}_T^{(2)}(l', l) \\ &+ \frac{1}{5} \mathcal{M}_F^{(2)}(l', l) - \frac{1}{2} \mathcal{M}_L^{(2)}(l', l) \\ &= -\frac{3}{2} (2l+1)(2l'+1) \left\{ [\mathbf{n}, \mathbf{J}]^{(l'+\frac{1}{2}, l-\frac{1}{2})^2} \delta_{l', l-1} + [\mathbf{n}, \mathbf{J}]^{(l'-\frac{1}{2}, l+\frac{1}{2})^2} \delta_{l', l+1} \right\} .\end{aligned}$$

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$$\begin{aligned}\tilde{\mathbf{P}}_J(l', l) &= \mathbf{n}(l', l) + \mathbf{P}_S(l', l) - 2\mathbf{P}_T(l', l) \\ &= -\frac{3(l + l' + 1)}{2} \left[\mathbf{n}_J^{l'+\frac{1}{2}, l-\frac{1}{2}} \delta_{l', l-1} + \mathbf{n}_J^{l'-\frac{1}{2}, l+\frac{1}{2}} \delta_{l', l+1} \right]\end{aligned}$$

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After some algebra, we find

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Our conclusion is further supported by what follows.

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[Reversing the sign of the coupling constant in Stone's model ($\mu \rightarrow -\mu$, large μ) would change the ground state to $|g\rangle_+ = \frac{1}{\sqrt{2}} (|j + \frac{1}{2}, jm\rangle + |j - \frac{1}{2}, jm\rangle)$, which is characterised by an **antiparallel alignment of the moments** and by a **magnetic quadrupole with opposite sign**.]

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Symmetry: Rotation group - SU(n)

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