GROUP PARAMETRIZED TUNNELING AND LOCAL SYMMETRY CONDITIONS

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Recently, Hougen[a] showed an ad hoc symmetry-based parameterization scheme for analyzing tunneling dynamics and high resolution spectra of fluxional molecular structure similar to S-parameter analysis of superfine structure in SF_6[b] or NH_3 maser inversion dynamics by Feynman *et.al.*[c] The problem is that ad hoc parametrization, like path integration in general, can lead to logjams of parameters or "paths" with no way to pick out the relevant ones.
We show a way to identify and use relevant parameters for a tunneling Hamiltonian H having global G-symmetry-defined bases by first expressing H as a linear combination $\bar{\gamma}^i\bar{\mathbf{g}}_\mathbf{i}$ of operators in dual symmetry group $\bar{G}$. The coefficients $\bar{\gamma}^i$ are parameters that define a complete set of allowed paths for any H with G-symmetry and are related thru spectral decomposition of G to eigensolutions of H. Quantum $G vs.\bar{G}$ duality generalizes lab-$vs.$-$body$ and $state$-$vs.$-$particle$.
The number of relevant $\bar{\gamma}^i$-parameters is reduced if a system tends to stick in states of a local symmetry subgroup $L \subset G$ so the H spectrum forms level clusters labeled by induced representations $d^{(\ell)}(L)\uparrow G$. A cluster-(ℓ) has one $E^{(\epsilon)}$-level labeled by G species (ϵ) for each L species (ℓ) in $D^\epsilon(G)\downarrow L$ by Frobenius reciprocity[d]. Then we apply *local symmetry conditions* to each irrep $D^\epsilon(\bar{\gamma}^i\bar{\mathbf{g}}_\mathbf{i})$ that has already been reduced with respect to local symmetry L. This amounts to setting each off-diagonal component $D^\epsilon_{j,k}(H)$ to zero.
Local symmetry conditions may tell which $\bar{\gamma}^i$-parameters are redundant or zero and directly determine $d^{(\ell)}\uparrow G$ tunneling matrix eigenvalues that give $E^{(\epsilon)}$-levels as well as eigenvectors. Otherwise one may need to choose a particular localizing subgroup chain $L \subset L_1 \subset L_2 ... G$ and further reduce the number of path parameters to facilitate spectral fitting.

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[a] J.T. Hougen, *2009 MSS* **RJ01**, J Mol Spect **123**, 197 (1987)
[b] W.G. Harter and J. C. Mitchell, *2009 MSS* **RJ05** (See also following talk.)
[c] R.P. Feynman, R. B. Leighton, M. Sands, *Lectures on Physics Vol.3* (Addison Wesley 1964) *p.9-1*
[d] W.G. Harter, *Principles of Symmetry, Dynamics, and Spectroscopy*, (Wiley Interscience, 1993)*p.*265