# FRACTAL DIMENSION OF MOLECULAR VIBRATIONAL LEVELS

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Fractal theory was previously developed to quantitatively describe the geometry of complicated and irregular shapes by introducing the fractional dimension. The molecular vibrational level systems can be seen as sets of a series of discrete points which show fractal properties. To characterise these fractals, we calculated the so called 'effective fractal dimensions', which behave as a function of the measuring scale, of molecular energy levels according to their spacing distributions.
The computerized box-counting method was employed in the calculation to render fractal dimension which is irrelevant to the level number. This feature is fully different from that of Cederbaum's work [a] and allows a physically meaningful connection between the fractal and statistics.
In particular, the effective fractal dimensions $D_F$ for the two limiting cases - Poisson and Wigner distributions were computed. Interestingly, there is a crossing occurring at ($r/\bar{S} = 1.0, D_F = 0.42$, where $r$ is the coarse graining size and $\bar{S}$ is the mean spacing.) which means that these two systems will geometrically appear the same when seen at a scale of their mean spacings. As a case study, the procedure was applied to the asymmetry top molecule - $SO_2$. The $U^1(4) \otimes U^2(4)$ algebraic model, which automatically embeds the stretching and bending motions, was used to calculate the vibrational levels. The Poisson- and Wigner-like level sets were chosen according to their symmetry multiplets, i.e. single or mixed Hamiltonian symmetry blocks. The obtained fractal dimensions agree well with the statistical analysis.

[a] L. S. Cederbaum, E . Haller, and P. Pfeifer, Phys. Rev. A 31, 1869 (1985).

Time required: 15 min
Session in which paper is recomended for presentation: 5