Quantum Theory of Molecular Orientations

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We formulate a quantum phase space for molecular rotational and nuclear-spin states. Taking in molecular geometry and nuclear-spin data, we reproduce a molecule's admissible angular momentum states known from spectroscopy, introduce its angular position states using quantization theory, and develop a generalized Fourier transform converting between the two. Using induced representations of the rotation group, we classify molecules into three types – asymmetric, rotationally symmetric, and perrotationally symmetric – with the last type having no macroscopic analogue due to nuclear-spin statistics constraints. We identify molecular species whose position states house an internal pseudo-spin or "fiber" degree of freedom, and the fiber's Berry phase or matrix after adiabatic changes in position yields naturally robust operations, akin to braiding anyonic quasiparticles or realizing fault-tolerant quantum gates.