Object-Oriented Approach to the Algebraic Theory of Molecules
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Motivation

A suitable potential for vibrations of a diatomic molecule is the Morse potential. This shape allows anharmonicity and the possibility for dissociation of the atoms. The phase space wave functions of the Morse Hamiltonian acquire a complicated expression in terms of Laguerre polynomials however. Fortunately the one dimensional Morse oscillator eigenstates are isomorphic to the Lie Algebra \(u(2) \supset \text{so}(2)\) basis states \(|X, m\rangle\).

State-to-State

Below we visualize initial and final states of a methane molecule. Combining the object oriented programming paradigm with abstract algebraic structures provides an elegant and powerful model for molecular spectral theory.

The instance of a molecule class can be rotated and vibrated to a final state using simple methods. This translation involves a rotation of 45 degrees around the \(z\) axis and a change of energy distribution in the bonds.

Given orientation and Morse potential well depths, the data structures and calculations for these states are made very simple with algebra instances. Transition Amplitudes \((n_1', n_2', n_3', n_4' | T | n_1, n_2, n_3, n_4\rangle\) and rotations for example become rigid hidden methods available to all instances.

Algebraic Structures

Consider the Lie algebra of creation and annihilation operators with the following commutation relation.

\[
[\hat{\sigma}, \hat{\sigma}^\dagger] = 1
\]

One can realize the structure with a set of matrices or differential operators. However, for the case of coupled Morse oscillators, a realization is not necessary for the subspaces which we construct \(u(2)\) from. This allows the subspaces to stay abstract making interfaces perfect data structures. For each bond in a molecule, we inherit the abstract properties of the subspace upon construction of the larger \(u(2)\) space for the bond:

\[
\hat{F}_+ = \hat{\sigma} \hat{\sigma}^\dagger, \quad \hat{F}_- = \hat{\sigma}^\dagger \hat{\sigma}, \quad \hat{F}_z = \hat{\sigma} \hat{\sigma}^\dagger - \hat{\sigma}^\dagger \hat{\sigma}, \quad \hat{N} = \hat{\sigma} \hat{\sigma}^\dagger + \hat{\sigma}^\dagger \hat{\sigma}
\]

Matrix representations are necessary here. We then build an even larger space combining each bond’s \(u(2)\) instance.

\[
u_1(2) \otimes u_2(2) \otimes u_3(2) \otimes u_4(2)
\]

This involves passing a vector of subalgebra instances to the algebra class’s direct product method with two possible chains. The local and normal chains are seen in the lattice of algebras:

\[
u_1(2) \otimes u_2(2) \supset \{ u_1(2) \otimes u_2(2) \supset u_3(2) \}
\]

Each with their own unique quantum numbers and basis states. Another important algebraic structure used for the orientations of the molecule is the geometric algebra \(G_3\):

\[
1, \hat{e}_1, \hat{e}_2, \hat{e}_3, \hat{e}_1 \hat{e}_2, \hat{e}_1 \hat{e}_3, \hat{e}_2 \hat{e}_3, \hat{e}_1 \hat{e}_2 \hat{e}_3
\]

With just doubles, one can instantiate G3 to represent vectors, rotation operators, planes etc. The geometric product as a generalized method of the G3 class makes it straightforward to construct methods such as rotations with rotors. In geometric algebra, a rotor and the objects it acts on live in the same space. This eliminates the need to change representations and to encode new data structures and methods.

Program Structure

This poster is focusing on a small part of a molecular collision theory as seen below.

Global Structure

Object Oriented Features

- **Inheritance**
  Since the molecule class inherits the algebra class, all methods in the subclasses inherited by the algebra class are usable by the molecule class. This offers a powerful and simple global data structure hierarchy in which algebraic operator methods may be employed at multiple levels.

- **Abstraction**
  Recognizing that the focus here is at the level of molecular properties allows abstraction at the top and bottom of the data hierarchy. Even though the boson calculus cannot be realized in matrix form its commutation properties can be encoded into an abstract data form called an interface.

- **Encapsulation**
  Methods such as the geometric product are very bulky to code so it is necessary that encapsulation protects the code. At the molecule class level only the necessary data structures are visible.

- **Polymorphism**
  Each instance of an algebra or molecule can be very different in structure. Any \(G3\) pure grade may be rotated. The methane and CO\(_2\) molecules have differing fundamental properties yet they both recognize the intensity method.

Reference

(5) Hou, Ma, *U(2) for Stretch Vibrations of tetrahedral molecules* (1997).