

Abstract Submitted
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General Symbolic Quantum Mechanics for SymPy¹ MATT CURRY, ADDISON CUGINI, BRIAN GRANGER, Cal Poly San Luis Obispo — SymPy is an open-source symbolic mathematics library for the Python programming language. In this talk we describe the general symbolic quantum mechanics capabilities that we have added to SymPy. This enables SymPy to handle the Dirac notation symbolically and includes objects that represent bras, kets, operators, inner/outer/tensor products, commutators, basis sets and Hilbert spaces. The goal of this work is to build an open-source foundation that allows a wide variety of quantum mechanical systems to be treated symbolically, from basic textbook quantum systems and atomic/molecular Hamiltonians to interacting quantum field theories and quantum computing. We will describe the different objects in the framework and how they can be combined to build and manipulate general symbolic quantum expressions. This will include examples ranging from basic states and operators to more complex usage cases involving basis sets and representations. We will briefly describe how the framework is being used to develop symbolic quantum computing and quantum many body capabilities in SymPy. Finally, we will describe some of the challenges in implementing the full Dirac notation in a symbolic computation.

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