Quantum Programming in Python

Quantum 1D Simple Harmonic Oscillator and Quantum Mapping Gate

A Senior Project

presented to

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TABLE OF CONTENTS

Section	Page	
Abstract	3	
Introduction	3	
Example Notebook for Quantum Simple Harmonic Oscillator	4	
Code for Quantum Simple Harmonic Oscillator	18	
Code for Tests of Quantum Simple Harmonic Oscillator	32	
Example Notebook for Quantum Mapping Gate	35	
Code for Quantum Mapping Gate	46	
Code for Tests of Quantum Mapping Gate	50	
Appendix	52	

ABSTRACT

A common problem when learning Quantum Mechanics is the complexity in the mathematical and physical concepts, which leads to difficulty in solving and understanding problems. Using programming languages like Python have become more and more prevalent in solving challenging physical systems. An open-source computer algebra system, SymPy, has been developed using Python to help solve these difficult systems. I have added code to the SymPy library for two different systems, a One-Dimensional Quantum Harmonic Oscillator and a Quantum Mapping Gate used in Quantum Computing.

Introduction

The goal of SymPy is "to become a full-featured computer algebra system (CAS) while keeping the code as simple as possible in order to be comprehensible and easily extensible" ("SymPy"). Through SymPy, I have submitted two projects to their library on GitHub, which "is a web-based hosting service for software development projects that use the Git revision control system" ("GitHub"). The first project is a Quantum Simple Harmonic Oscillator (QSHO), which is explained in a sample notebook using an IPython notebook. The goal of coding the QSHO is to allow others to learn how the simple harmonic oscillator is applied to a quantum system as well as allowing others to use components of the QSHO in other future projects. The second project is a Quantum Mapping Gate (QMG), which again is explained in greater detail using an IPython notebook. The QMG allows for custom creation of logic gates for quantum systems and can be used in addition to or instead of the current quantum gates. Both projects were coded using the Python language and have been added to the SymPy library.

One-Dimensional Quantum Simple Harmonic Oscillator

Imports

Before examining the Quantum 1D Simple Harmonic Oscillator, the relevant files need to be loaded to create simple harmonic oscillator states and operators.

Background

For a detailed background on the Quantum Simple Harmonic Oscillator consult Griffith's *Introduciton to Quantum Mechanics* or the Wikipedia page "Quantum Harmonic Oscillator"

Components

States

The Quantum 1D Simple Harmonic Oscillator is made up of states which can be expressed as bras and kets. And those states are acted on by different operators. Looking at the states, there are two types of states that can be made: a generic state 'n' or numerical states. Passing a string (i.e. 'n') to **SHOBra** or **SHOKet** creates a generic bra or ket state, respectively. And passing an integer to SHOBra or SHOKet creates a numerical bra or ket state.

SHOBra and SHOKet are passed the information from **SHOState** and from the Bra and Ket classes, respectively. SHOState contains the information to find the Hilbert Space of the state as well as the energy level. SHOState also has all the information and properties from State because State is passed into SHOState.

```
In [2]: b = SHOBra('b')
        b0 = SHOBra(0)
        b1 = SHOBra(1)
        k = SHOKet('k')
        k0 = SHOKet(0)
        k1 = SHOKet(1)
```

Printing

There are multiple printing methods in python: LaTeX, Pretty, repr, and srepr.

```
Bra
In [3]: b
Out[3]: (b)
In [4]: b0
Out[4]: (0
In [5]: b1
Out[5]: (1
LaTex: Gives the printing for LaTeX typesetting
In [6]: latex(b)
Out[6]: {\left\langle b\right|}
In [7]: latex(b0)
Out[7]: {\left\langle 0\right|}
In [8]: latex(b1)
Out[8]: {\left\langle 1\right|}
Pretty
In [9]: pprint(b)
         (bl
In [10]: pprint(b0)
         (01
In [11]: pprint(b1)
         (11
```

```
repr
In [12]: repr(b)
Out[12]: <b|
In [13]: repr(b0)
Out[13]: <0|
In [14]: repr(b1)
Out[14]: <1|
srepr
In [15]: srepr(b)
Out[15]: SHOBra(Symbol('b'))
In [16]: srepr(b0)
Out[16]: SHOBra(Integer(0))
In [17]: srepr(b1)
Out[17]: SHOBra(Integer(1))
Ket
In [18]: k
Out[18]: |k\rangle
In [19]: k0
Out[19]: |0\rangle
In [20]: k1
Out[20]: |1\rangle
Latex: Gives the printing for LaTeX typesetting
In [21]: latex(k)
Out[21]: {\left|k\right\rangle
```

```
In [22]: latex(k0)
Out[22]: {\left|0\right\rangle
In [23]: latex(k1)
Out[23]: {\left|1\right\rangle
Pretty
In [24]: pprint(k)
        lk)
In [25]: pprint(k0)
        10 }
In [26]: pprint(k1)
        11)
repr
In [27]: repr(k)
Out[27]: |k>
In [28]: repr(k0)
Out[28]: |0>
In [29]: repr(k1)
Out[29]: |1>
srepr
In [30]: srepr(k)
Out[30]: SHOKet(Symbol('k'))
In [31]: srepr(k0)
Out[31]: SHOKet(Integer(0))
In [32]: srepr(k1)
Out[32]: SHOKet(Integer(1))
```

Properites

```
Hilbert Space
```

```
In [33]: b.hilbert_space
Out[33]: \mathcal{C}^{\infty}
In [34]: b0.hilbert_space
Out[34]: \mathcal{C}^{\infty}
In [35]: k.hilbert_space
Out[35]: \mathcal{C}^{\infty}
In [36]: k0.hilbert_space
Out[36]: C^{\infty}
Energy Level
In [37]: b.n
Out[37]: b
In [38]: b0.n
Out[38]: 0
In [39]: b1.n
Out[39]: 1
In [40]: k.n
Out[40]: k
In [41]: k0.n
Out[41]: 0
In [42]: k1.n
Out[42]: 1
```

Operators

The states are acted upon by operators. There are four operators that act on simple harmonic kets: **RaisingOp**, **LoweringOp**, **NumberOp**, and **Hamiltonian**. The operators are created by passing a string 'n' to the operator. They can also be printed in multiple ways, but only the raising operator has a distinct difference.

Each of the operators are passed the information and properties from **SHOOp**. SHOOp contains information on the hilbert space of the operators and how the arguments are evaluated. Each of these operators are limited to one argument. The

Operatos class is passed to SHOOp, which is in turn passed to each of the four quantum harmonic oscillators.

```
In [43]: ad = RaisingOp('a')
          a = LoweringOp('a')
         N = NumberOp('N')
         H = Hamiltonian('H')
Printing
RaisingOp
In [44]: ad
Out[44]: a^{\dagger}
In [45]: latex(ad)
Out[45]: a^{\dag}
In [46]: pprint(ad)
         а
In [47]: repr(ad)
Out[47]: RaisingOp(a)
In [48]: srepr(ad)
Out[48]: RaisingOp(Symbol('a'))
LoweringOp
In [49]: a
Out[49]: a
In [50]: latex(a)
Out[50]: a
In [51]: pprint(a)
        a
In [52]: repr(a)
Out[52]: a
In [53]: srepr(a)
```

Out[53]: LoweringOp(Symbol('a'))

```
NumberOp
In [54]: N
Out[54]: N
In [55]: latex(N)
Out[55]: N
In [56]: pprint(N)
        N
In [57]: repr(N)
Out[57]: N
In [58]: srepr(N)
Out[58]: NumberOp(Symbol('N'))
Hamiltonian
In [59]: H
Out[59]: H
In [60]: latex(H)
Out[60]: H
In [61]: pprint(H)
        Н
In [62]: repr(H)
Out[62]: H
In [63]: srepr(H)
Out[63]: Hamiltonian(Symbol('H'))
Properties
Hilbert Space
In [64]: ad.hilbert_space
Out[64]: \mathcal{C}^{\infty}
```

```
In [65]: a.hilbert_space

Out[65]: C^{\infty}

In [66]: N.hilbert_space

Out[66]: C^{\infty}

In [67]: H.hilbert_space

Out[67]: C^{\infty}
```

Properties and Operations

There are a couple properties and operations of a quantum simple harmonic oscillator state that are defined. Taking the dagger of a bra returns the ket and vice versa. Using the property 'dual' returns the same value as taking the dagger. The property 'n' as seen in the State Section above returns the argument/energy level of the state, which is used when operators act on states.

```
In [68]: Dagger(b)

Out[68]: |b|

In [69]: Dagger(k)

Out[69]: |k|

In [70]: Dagger(b0)

Out[70]: |0|
```

Tests that the dagger of a bra is equal to the ket.

```
In [71]: Dagger(b0) == k0
Out[71]: True
```

Tests that the dagger of a ket is equal to the bra

```
In [72]: Dagger(k1) == b1
Out[72]: True
```

The energy level of the states must be the same for the dagger of the bra to equal the ket

```
In [73]: Dagger(b1) == k0
Out[73]: False
```

Tests that dagger(ket) = ket.dual and dagger(bra) = bra.dual

```
In [74]: k.dual
Out[74]: \langle k|
In [75]: Dagger(k) == k.dual
Out[75]: True
```

The raising operator is the dagger of the lowering operator

```
In [76]: Dagger(a)

Out[76]: a^{\dagger}

In [77]: Dagger(ad)

Out[77]: a

In [78]: Dagger(a) == ad

Out[78]: True
```

The operators can be expressed in terms of other operators. Aside from the operators stated above rewriting in terms of the position (X) and momentum operators (Px) is common. To rewrite the operators in terms of other operators, we pass a keyword that specifies which operators to rewrite in.

```
'xp' -- Position and Momentum Operators
```

'a' -- Raising and Lowering Operators

'H' -- Hamiltonian Operator

```
'N'-- Number Operator

In [79]: ad.rewrite('xp')

Out[79]: \frac{\sqrt{2}(m\omega X - \iota Px)}{2\sqrt{\hbar}\sqrt{m\omega}}

In [80]: a.rewrite('xp')

Out[80]: \frac{\sqrt{2}(m\omega X + \iota Px)}{2\sqrt{\hbar}\sqrt{m\omega}}

In [81]: N.rewrite('xp')

Out[81]: -\frac{1}{2} + \frac{m^2\omega^2(X)^2 + (Px)^2}{2\hbar m\omega}
```

```
In [82]: N.rewrite('a')

Out[82]: a^{\dagger}a

In [83]: N.rewrite('H')

Out[83]: -\frac{1}{2} + \frac{H}{\hbar \omega}

In [84]: H.rewrite('xp')

Out[84]: \frac{m^2 \omega^2(X)^2 + (Px)^2}{2m}

In [85]: H.rewrite('a')

Out[85]: \hbar \omega \left(\frac{1}{2} + a^{\dagger}a\right)

In [86]: H.rewrite('N')

Out[86]: \hbar \omega \left(\frac{1}{2} + N\right)
```

Operator Methods

Apply Operators to States: Each of the operators can act on kets using qapply.

The raising operator raises the value of the state by one as well as multiplies the state by the square root of the new state.

```
In [87]: qapply(ad*k)

Out[87]: \sqrt{k+1}|k+1\rangle
```

Two numerical examples with the ground state and first excited state.

```
In [88]: qapply(ad*k0)

Out[88]: |1>

In [89]: qapply(ad*k1)

Out[89]: \sqrt{2}|2>
```

The lowering operator lowers the value of the state by one and multiples the state by the square root of the original state. When the lowering operator acts on the ground state it returns zero because the state cannot be lowered.

```
In [90]: qapply(a*k)

Out[90]: \sqrt{k}|k-1\rangle
```

Two numerical examples with the ground state and first excited state.

The number operator is defined as the raising operator times the lowering operator. When the number operator acts on a ket it returns the same state multiplied by the value of the state. This can be checked by applying the lowering operator on a state then applying the raising operator to the result.

```
In [93]: qapply(N*k)
Out[93]: k|k>
In [94]: qapply(N*k0)
Out[94]: 0
In [95]: qapply(N*k1)
Out[95]: |1>
In [96]: result = qapply(a*k) qapply(ad*result)
Out[96]: k|k>
```

When the hamiltonian operator acts on a state it returns the energy of the state, which is equal to hbar*omega times the value of the state plus one half.

```
In [97]: qapply(H*k)

Out[97]: \hbar k\omega |k\rangle + \frac{1}{2} \hbar \omega |k\rangle

In [98]: qapply(H*k0)

Out[98]: \frac{1}{2} \hbar \omega |0\rangle

In [99]: qapply(H*k1)

Out[99]: \frac{3}{2} \hbar \omega |1\rangle
```

Commutators

A commutator is defined as [A, B] = A*B - B*A where A and B are both operators. Commutators are used to see if operators commute, which is an important property in quantum mechanics. If they commute it allows for rearranging the order operators act on states.

```
In [100]: Commutator(ad,a).doit()
Out[100]: -1
In [101]: Commutator(ad,N).doit()
Out[101]: -a<sup>†</sup>
In [102]: Commutator(a,ad).doit()
Out[102]: 1
In [103]: Commutator(a,N).doit()
Out[103]: a
```

Matrix Representation

The bras and kets can also be represented as a row or column vector, which are then used to create matrix representation of the different operators. The bras and kets must be numerical states rather than a generic *n* state

Because these vectors and matrices are mostly zeros there is a different way of creating and storing these vectors/matrices, that is to use the format scipy.sparse. The default format is sympy and another common format to use is numpy. Along with specifying the format in which the matrices are created, the dimension of the matrices can also be specified. A dimension of 4 is the default.

```
In [107]: represent(k1, ndim=5, format='numpy')
Out[107]:
             [[
             0.]
               [
             1.]
               [
             0.]
              [
             0.1
              [
             0.]]
In [108]: represent(k1, ndim=5, format='scipy.sparse')
Out[108]: (1, 0)
             1.0
Operators can be expressed as matrices using the vector representation of the bras and kets.
\langle i|N|j\rangle
The operator acts on the ket then the inner product of the bra and the new resulting ket is performed.
In [109]: represent(ad, ndim=4, format='sympy')
Out[109]: \begin{bmatrix} 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & \sqrt{2} & 0 & 0 \end{bmatrix}
             \begin{bmatrix} 0 & 0 & \sqrt{3} & 0 \end{bmatrix}
In [110]: represent(ad, format='numpy')
Out[110]: [[ 0.
                                                0.
             0.
                         ]
              [ 1.
                                 0.
                                                0.
             0.
                         ]
               [ 0.
                                 1.41421356 0.
             0.
                         ]
             [ 0.
                                0.
                                               1.73205081 0.
             ]]
In [111]: represent(ad, format='scipy.sparse', spmatrix='lil')
Out[111]:
                      (1, 0)
                (2, 1)1.41421356237
                (3, 2)1.73205080757
In [112]: str(represent(ad, format='scipy.sparse', spmatrix='lil'))
Out[112]:
                      (1, 0)
             1.0
                (2, 1)1.41421356237
                (3, 2)1.73205080757
```

```
In [113]: represent(a)

Out[113]: 
\begin{bmatrix}
0 & 1 & 0 & 0 \\
0 & 0 & \sqrt{2} & 0 \\
0 & 0 & 0 & \sqrt{3} \\
0 & 0 & 0 & 0
\end{bmatrix}

In [114]: represent(N)

Out[114]: 
\begin{bmatrix}
0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & 2 & 0 \\
0 & 0 & 0 & 3
\end{bmatrix}

In [115]: represent(H)

Out[115]: 
\begin{bmatrix}
\frac{1}{2}\hbar\omega & 0 & 0 & 0 \\
0 & \frac{3}{2}\hbar\omega & 0 & 0 \\
0 & 0 & \frac{5}{2}\hbar\omega & 0 \\
0 & 0 & 0 & \frac{7}{2}\hbar\omega
\end{bmatrix}
```

There are some interesting properties that we can test using the matrix representation, like the definition of the Number Operator.

```
In [116]: represent(N) == represent(ad) * represent(a)
Out[116]: True
```

For Additional Quantum Harmonic Oscillator Information

Griffiths, David J. Introduction to Quantum Mechanics. Upper Saddle River, NJ: Pearson Prentice Hall, 2005. Print.

http://en.wikipedia.org/wiki/Quantum_harmonic_oscillator

http://en.wikipedia.org/wiki/Harmonic_oscillator#Simple_harmonic_oscillator

```
In [ ]:
```

```
1 """Simple Harmonic Oscillator 1-Dimension"""
2
3
  from sympy import sqrt, I, Symbol, Integer, S
4 from sympy.physics.quantum.constants import hbar
5 from sympy.physics.quantum.operator import Operator
6 from sympy.physics.quantum.state import Bra, Ket, State
7 from sympy.physics.quantum.gexpr import QExpr
8 from sympy.physics.quantum.cartesian import X, Px
9 from sympy.functions.special.tensor_functions import KroneckerDelta
10 from sympy.physics.quantum.hilbert import ComplexSpace
11 from sympy.physics.quantum.matrixutils import matrix zeros
12 from sympy.physics.quantum.represent import represent
13
14 | #----
15
16 class SH00p(Operator):
       """A base class for the SHO Operators.
17
18
19
       We are limiting the number of arguments to be 1.
20
       0.00
21
22
23
       @classmethod
24
       def eval args(cls, args):
25
           args = QExpr. eval args(args)
26
           if len(args) == 1:
27
               return args
28
           else:
               raise ValueError("Too many arguments")
29
30
31
       @classmethod
32
       def eval hilbert space(cls, label):
33
           return ComplexSpace(S.Infinity)
34
35
   class RaisingOp(SHOOp):
       """The Raising Operator or a^dagger.
36
37
38
       When a^dagger acts on a state it raises the state up by one. Taking
       the adjoint of a^dagger returns 'a', the Lowering Operator. a^dagger
39
       can be rewritten in terms of postion and momentum. We can represent
40
41
       a^dagger as a matrix, which will be its default basis.
42
43
       Parameters
44
       _____
45
46
       args : tuple
47
           The list of numbers or parameters that uniquely specify the
48
           operator.
49
50
       Examples
51
       _____
```

```
52
53
        Create a Raising Operator and rewrite it in terms of positon and
        momentum, and show that taking its adjoint returns 'a':
54
55
            >>> from sympy.physics.quantum.sho1d import RaisingOp
56
57
            >>> from sympy.physics.quantum import Dagger
58
59
            >>> ad = RaisingOp('a')
            >>> ad.rewrite('xp').doit()
60
            sgrt(2)*(m*omega*X - I*Px)/(2*sgrt(hbar)*sgrt(m*omega))
61
62
63
            >>> Dagger(ad)
64
            а
65
66
        Taking the commutator of a^dagger with other Operators:
67
68
            >>> from sympy.physics.quantum import Commutator
69
            >>> from sympy.physics.quantum.shold import RaisingOp, LoweringOp
            >>> from sympy.physics.quantum.shold import NumberOp
70
71
72
            >>> ad = RaisingOp('a')
            >>> a = LoweringOp('a')
73
74
            >>> N = NumberOp('N')
75
            >>> Commutator(ad, a).doit()
76
77
            >>> Commutator(ad, N).doit()
78
            -RaisingOp(a)
79
80
        Apply a^dagger to a state:
81
82
            >>> from sympy.physics.quantum import gapply
83
            >>> from sympy.physics.quantum.sho1d import Raising0p, SH0Ket
84
85
            >>> ad = RaisingOp('a')
86
            >>> k = SH0Ket('k')
            >>> gapply(ad*k)
87
88
            sart(k + 1)*|k + 1>
89
90
        Matrix Representation
91
92
            >>> from sympy.physics.quantum.sho1d import RaisingOp
93
            >>> from sympy.physics.quantum.represent import represent
            >>> ad = RaisingOp('a')
94
            >>> represent(ad, basis=N, ndim=4, format='sympy')
95
96
            [0,
                                0, 0]
                      0,
97
            [1,
                                0, 0]
                      0,
            [0, sqrt(2),
98
99
                      0, sqrt(3), 0]
100
        .....
101
102
103
        def _eval_rewrite_as_xp(self, *args):
```

```
104
            return (Integer(1)/sqrt(Integer(2)*hbar*m*omega))*(
105
                Integer(-1)*I*Px + m*omega*X)
106
107
        def _eval_adjoint(self):
108
            return LoweringOp(*self.args)
109
110
        def _eval_commutator_LoweringOp(self, other):
111
            return Integer(-1)
112
        def _eval_commutator NumberOp(self, other):
113
            return Integer(-1)*self
114
115
116
        def apply operator SHOKet(self, ket):
            temp = ket.n + Integer(1)
117
118
            return sqrt(temp)*SHOKet(temp)
119
120
        def _represent_default_basis(self, **options):
121
            return self. represent NumberOp(None, **options)
122
        def _represent_XOp(self, basis, **options):
123
124
            # This logic is good but the underlying positon
            # representation logic is broken.
125
            # temp = self.rewrite('xp').doit()
126
            # result = represent(temp, basis=X)
127
128
            # return result
129
            raise NotImplementedError('Position representation is not
    implemented')
130
        def _represent_NumberOp(self, basis, **options):
131
            ndim info = options.get('ndim', 4)
132
            format = options.get('format','sympy')
133
            spmatrix = options.get('spmatrix', 'csr')
134
            matrix = matrix_zeros(ndim_info, ndim_info, **options)
135
            for i in range(ndim_info - 1):
136
137
                value = sqrt(i + 1)
                if format == 'scipy.sparse':
138
                    value = float(value)
139
140
                matrix[i + 1, i] = value
            if format == 'scipy.sparse':
141
142
                matrix = matrix.tocsr()
143
            return matrix
144
145
    #
        # Printing Methods
146
147
 ...
148
149
        def _print_contents(self, printer, *args):
            arg0 = printer._print(self.args[0], *args)
150
```

```
151
            return '%s(%s)' % (self.__class__._name__, arg0)
152
153
        def _print_contents_pretty(self, printer, *args):
            from sympy.printing.pretty.stringpict import prettyForm
154
155
            pform = printer._print(self.args[0], *args)
            pform = pform**prettyForm(u'\u2020')
156
157
            return pform
158
159
        def _print_contents_latex(self, printer, *args):
160
            arg = printer._print(self.args[0])
            return '%s^{\\dag}' % arg
161
162
163
    class LoweringOp(SHOOp):
        """The Lowering Operator or 'a'.
164
165
166
        When 'a' acts on a state it lowers the state up by one. Taking
        the adjoint of 'a' returns a^dagger, the Raising Operator. 'a'
167
        can be rewritten in terms of position and momentum. We can
168
169
        represent 'a' as a matrix, which will be its default basis.
170
171
        Parameters
172
        _____
173
174
        args : tuple
175
            The list of numbers or parameters that uniquely specify the
176
            operator.
177
178
        Examples
        _____
179
180
181
        Create a Lowering Operator and rewrite it in terms of positon and
182
        momentum, and show that taking its adjoint returns a dagger:
183
            >>> from sympy.physics.quantum.sho1d import LoweringOp
184
185
            >>> from sympy.physics.quantum import Dagger
186
            >>> a = LoweringOp('a')
187
            >>> a.rewrite('xp').doit()
188
189
            sqrt(2)*(m*omega*X + I*Px)/(2*sqrt(hbar)*sqrt(m*omega))
190
191
            >>> Dagger(a)
192
            RaisingOp(a)
193
194
        Taking the commutator of 'a' with other Operators:
195
196
            >>> from sympy.physics.quantum import Commutator
197
            >>> from sympy.physics.quantum.sho1d import Lowering0p, Raising0p
            >>> from sympy.physics.quantum.sho1d import NumberOp
198
199
200
            >>> a = LoweringOp('a')
            >>> ad = RaisingOp('a')
201
202
            >>> N = NumberOp('N')
```

```
203
            >>> Commutator(a, ad).doit()
204
205
            >>> Commutator(a, N).doit()
206
207
208
        Apply 'a' to a state:
209
210
            >>> from sympy.physics.quantum import qapply
211
            >>> from sympy.physics.quantum.sho1d import LoweringOp, SHOKet
212
213
            >>> a = LoweringOp('a')
214
            >>> k = SH0Ket('k')
215
            >>> gapply(a*k)
            sqrt(k)*|k - 1>
216
217
218
        Taking 'a' of the lowest state will return 0:
219
220
            >>> from sympy.physics.quantum import qapply
            >>> from sympy.physics.quantum.sho1d import LoweringOp, SHOKet
221
222
223
            >>> a = LoweringOp('a')
224
            >>> k = SH0Ket(0)
225
            >>> gapply(a*k)
226
227
228
        Matrix Representation
229
230
            >>> from sympy.physics.quantum.sho1d import LoweringOp
231
            >>> from sympy.physics.quantum.represent import represent
232
            >>> a = LoweringOp('a')
233
            >>> represent(a, basis=N, ndim=4, format='sympy')
234
            [0, 1,
                          0,
                                   01
235
            [0, 0, sart(2),
                                    01
236
                          0, sqrt(3)]
             [0, 0,
237
             [0, 0,
                          0,
                                   01
238
        1111111
239
240
241
        def _eval rewrite as xp(self, *args):
            return (Integer(1)/sqrt(Integer(2)*hbar*m*omega))*(
242
243
                 I*Px + m*omega*X)
244
245
        def _eval_adjoint(self):
246
            return RaisingOp(*self.args)
247
248
        def _eval_commutator_RaisingOp(self, other):
249
            return Integer(1)
250
251
        def _eval_commutator NumberOp(self, other):
252
            return Integer(1)*self
253
254
        def _apply_operator_SHOKet(self, ket):
```

```
255
            temp = ket.n - Integer(1)
256
            if ket.n == Integer(0):
257
                return Integer(0)
258
            else:
259
                return sqrt(ket.n)*SHOKet(temp)
260
261
        def _represent_default_basis(self, **options):
262
            return self._represent_NumberOp(None, **options)
263
        def _represent_XOp(self, basis, **options):
264
            # This logic is good but the underlying positon
265
266
            # representation logic is broken.
267
            # temp = self.rewrite('xp').doit()
            # result = represent(temp, basis=X)
268
269
            # return result
270
            raise NotImplementedError('Position representation is not
    implemented')
 ...
271
272
        def _represent_NumberOp(self, basis, **options):
            ndim_info = options.get('ndim', 4)
273
274
            format = options.get('format', 'sympy')
            spmatrix = options.get('spmatrix', 'csr')
275
276
            matrix = matrix_zeros(ndim_info, ndim_info, **options)
            for i in range(ndim info - 1):
277
278
                value = sqrt(i + 1)
279
                if format == 'scipy.sparse':
280
                    value = float(value)
281
                matrix[i,i+1] = value
            if format == 'scipy.sparse':
282
283
                matrix = matrix.tocsr()
284
            return matrix
285
286
287
    class NumberOp(SHOOp):
288
        """The Number Operator is simply a^dagger*a
289
290
        It is often useful to write a^dagger*a as simply the Number Operator
        because the Number Operator commutes with the Hamiltonian. And can be
291
292
        expressed using the Number Operator. Also the Number Operator can be
        applied to states. We can represent the Number Operator as a matrix,
293
294
        which will be its default basis.
295
296
        Parameters
297
        _____
298
299
        args : tuple
300
            The list of numbers or parameters that uniquely specify the
301
302
303
        Examples
304
        _____
305
```

```
306
        Create a Number Operator and rewrite it in terms of the ladder
307
        operators, position and momentum operators, and Hamiltonian:
308
309
            >>> from sympy.physics.quantum.sho1d import NumberOp
310
311
            >>> N = NumberOp('N')
312
            >>> N.rewrite('a').doit()
313
            Raising0p(a)*a
314
            >>> N.rewrite('xp').doit()
315
            -1/2 + (m**2*omega**2*X**2 + Px**2)/(2*hbar*m*omega)
            >>> N.rewrite('H').doit()
316
317
            -1/2 + H/(hbar*omega)
318
        Take the Commutator of the Number Operator with other Operators:
319
320
321
            >>> from sympy.physics.quantum import Commutator
            >>> from sympy.physics.quantum.sho1d import NumberOp, Hamiltonian
322
323
            >>> from sympy.physics.quantum.shold import RaisingOp, LoweringOp
324
325
            >>> N = NumberOp('N')
326
            >>> H = Hamiltonian('H')
            >>> ad = RaisingOp('a')
327
328
            >>> a = LoweringOp('a')
            >>> Commutator(N,H).doit()
329
330
            0
331
            >>> Commutator(N,ad).doit()
332
            RaisingOp(a)
333
            >>> Commutator(N,a).doit()
334
            -a
335
336
        Apply the Number Operator to a state:
337
338
            >>> from sympv.physics.quantum import gapply
339
            >>> from sympy.physics.quantum.sho1d import NumberOp, SHOKet
340
            >>> N = NumberOp('N')
341
342
            >>> k = SH0Ket('k')
343
            >>> gapply(N*k)
344
            k*|k>
345
346
        Matrix Representation
347
348
            >>> from sympy.physics.quantum.sho1d import NumberOp
349
            >>> from sympy.physics.quantum.represent import represent
350
            >>> N = Number0p('N')
351
            >>> represent(N, basis=N, ndim=4, format='sympy')
352
            [0, 0, 0, 0]
            [0, 1, 0, 0]
353
354
            [0, 0, 2, 0]
            [0, 0, 0, 3]
355
356
        1111111
357
```

```
358
359
        def _eval_rewrite_as_a(self, *args):
360
            return ad*a
361
362
        def eval rewrite as xp(self, *args):
            return (Integer(1)/(Integer(2)*m*hbar*omega))*(Px**2 + (
363
364
                m*omega*X)**2) - Integer(1)/Integer(2)
365
366
        def eval rewrite as H(self, *args):
            return H/(hbar*omega) - Integer(1)/Integer(2)
367
368
369
        def _apply_operator_SHOKet(self, ket):
370
            return ket.n*ket
371
372
        def _eval_commutator Hamiltonian(self, other):
373
            return Integer(0)
374
375
        def _eval_commutator_RaisingOp(self, other):
376
            return other
377
378
        def eval commutator LoweringOp(self, other):
            return Integer(-1)*other
379
380
381
        def _represent_default_basis(self, **options):
382
            return self. represent NumberOp(None, **options)
383
384
        def _represent_XOp(self, basis, **options):
385
            # This logic is good but the underlying positon
386
            # representation logic is broken.
387
            # temp = self.rewrite('xp').doit()
388
            # result = represent(temp, basis=X)
389
            # return result
390
            raise NotImplementedError('Position representation is not
    implemented')
391
        def _represent_NumberOp(self, basis, **options):
392
393
            ndim_info = options.get('ndim', 4)
            format = options.get('format', 'sympy')
394
395
            spmatrix = options.get('spmatrix', 'csr')
            matrix = matrix zeros(ndim info, ndim info, **options)
396
            for i in range(ndim info):
397
398
                value = i
                if format == 'scipy.sparse':
399
400
                    value = float(value)
                matrix[i,i] = value
401
            if format == 'scipy.sparse':
402
403
                matrix = matrix.tocsr()
404
            return matrix
405
406
407 class Hamiltonian(SHOOp):
        """The Hamiltonian Operator.
408
```

```
409
410
        The Hamiltonian is used to solve the time-independent Schrodinger
411
        equation. The Hamiltonian can be expressed using the ladder operators,
412
        as well as by position and momentum. We can represent the Hamiltonian
413
        Operator as a matrix, which will be its default basis.
414
415
        Parameters
416
        _____
417
418
        args : tuple
419
            The list of numbers or parameters that uniquely specify the
420
            operator.
421
422
        Examples
423
        =======
424
425
        Create a Hamiltonian Operator and rewrite it in terms of the ladder
426
        operators, position and momentum, and the Number Operator:
427
428
            >>> from sympy.physics.quantum.sho1d import Hamiltonian
429
            >>> H = Hamiltonian('H')
430
            >>> H.rewrite('a').doit()
431
432
            hbar*omega*(1/2 + RaisingOp(a)*a)
            >>> H.rewrite('xp').doit()
433
434
            (m**2*omega**2*X**2 + Px**2)/(2*m)
435
            >>> H.rewrite('N').doit()
436
            hbar*omega*(1/2 + N)
437
        Take the Commutator of the Hamiltonian and the Number Operator:
438
439
440
            >>> from sympy.physics.quantum import Commutator
441
            >>> from sympy.physics.quantum.sho1d import Hamiltonian, NumberOp
442
443
            >>> H = Hamiltonian('H')
            >>> N = NumberOp('N')
444
445
            >>> Commutator(H.N).doit()
446
            0
447
448
        Apply the Hamiltonian Operator to a state:
449
450
            >>> from sympy.physics.quantum import gapply
451
            >>> from sympy.physics.quantum.sho1d import Hamiltonian, SHOKet
452
453
            >>> H = Hamiltonian('H')
454
            >>> k = SH0Ket('k')
455
            >>> gapply(H*k)
            hbar*k*omega*|k> + hbar*omega*|k>/2
456
457
458
        Matrix Representation
459
460
            >>> from sympy.physics.quantum.sho1d import Hamiltonian
```

```
461
            >>> from sympy.physics.quantum.represent import represent
462
463
            >>> H = Hamiltonian('H')
            >>> represent(H, basis=N, ndim=4, format='sympy')
464
465
            [hbar*omega/2,
                                                                           01
                                         0.
466
                         0, 3*hbar*omega/2,
                                                          0,
                                                                           01
467
                                         0, 5*hbar*omega/2,
                                                                           01
                        0,
468
                                         0,
                                                          0, 7*hbar*omega/2]
469
        1111111
470
471
472
        def _eval_rewrite_as_a(self, *args):
473
            return hbar*omega*(ad*a + Integer(1)/Integer(2))
474
475
        def _eval rewrite as xp(self, *args):
476
            return (Integer(1)/(Integer(2)*m))*(Px**2 + (m*omega*X)**2)
477
478
        def eval rewrite as N(self, *args):
479
            return hbar*omega*(N + Integer(1)/Integer(2))
480
481
        def apply operator SHOKet(self, ket):
            return (hbar*omega*(ket.n + Integer(1)/Integer(2)))*ket
482
483
        def _eval_commutator_NumberOp(self, other):
484
485
            return Integer(0)
486
487
        def represent default basis(self, **options):
488
            return self._represent_NumberOp(None, **options)
489
490
        def _represent_XOp(self, basis, **options):
            # This logic is good but the underlying positon
491
492
            # representation logic is broken.
            # temp = self.rewrite('xp').doit()
493
494
            # result = represent(temp, basis=X)
495
            # return result
            raise NotImplementedError('Position representation is not
496
    implemented'
 ...
497
498
        def _represent_NumberOp(self, basis, **options):
            ndim_info = options.get('ndim', 4)
499
            format = options.get('format', 'sympy')
500
            spmatrix = options.get('spmatrix', 'csr')
501
            matrix = matrix zeros(ndim info, ndim info, **options)
502
503
            for i in range(ndim_info):
                value = i + Integer(1)/Integer(2)
504
                if format == 'scipy.sparse':
505
                    value = float(value)
506
                matrix[i,i] = value
507
508
            if format == 'scipy.sparse':
509
                matirx = matrix.tocsr()
510
            return hbar*omega*matrix
511
```

```
512 #----
513
514 class SHOState(State):
        """State class for SHO states"""
515
516
        @classmethod
517
518
        def _eval_hilbert_space(cls, label):
            return ComplexSpace(S.Infinity)
519
520
521
        @property
        def n(self):
522
523
            return self.args[0]
524
525
526 class SHOKet(SHOState, Ket):
527
        """1D eigenket.
528
        Inherits from SHOState and Ket.
529
530
531
        Parameters
532
        _____
533
        args : tuple
534
535
            The list of numbers or parameters that uniquely specify the ket
            This is usually its quantum numbers or its symbol.
536
537
538
        Examples
539
        =======
540
541
        Ket's know about their associated bra:
542
543
            >>> from sympy.physics.quantum.sho1d import SHOKet
544
545
            >>> k = SH0Ket('k')
546
            >>> k.dual
547
            <kl
548
            >>> k.dual class()
549
            <class 'sympy.physics.quantum.sho1d.SH0Bra'>
550
        Take the Inner Product with a bra:
551
552
553
            >>> from sympy.physics.quantum import InnerProduct
554
            >>> from sympy.physics.quantum.sho1d import SH0Ket, SH0Bra
555
556
            >>> k = SH0Ket('k')
            >>> b = SHOBra('b')
557
            >>> InnerProduct(b,k).doit()
558
559
            KroneckerDelta(k, b)
560
561
        Vector representation of a numerical state ket:
562
```

```
563
            >>> from sympy.physics.quantum.sho1d import SH0Ket, NumberOp
564
            >>> from sympy.physics.quantum.represent import represent
565
566
            >>> k = SH0Ket(3)
            >>> N = NumberOp('N')
567
568
            >>> represent(k, basis=N, ndim=4)
569
            [0]
570
            [0]
            [0]
571
            [1]
572
573
        .....
574
575
576
        @classmethod
577
        def dual_class(self):
578
            return SHOBra
579
580
        def eval innerproduct SHOBra(self, bra, **hints):
581
            result = KroneckerDelta(self.n, bra.n)
582
            return result
583
584
        def _represent_default_basis(self, **options):
            return self._represent_NumberOp(None, **options)
585
586
        def represent NumberOp(self, basis, **options):
587
588
            ndim_info = options.get('ndim', 4)
            format = options.get('format', 'sympy')
589
            options['spmatrix'] = 'lil'
590
            vector = matrix zeros(ndim info, 1, **options)
591
592
            if isinstance(self.n, Integer):
                if self.n >= ndim info:
593
                     return ValueError("N-Dimension too small")
594
595
                value = Integer(1)
                if format == 'scipy.sparse':
596
597
                    vector[int(self.n), 0] = 1.0
598
                    vector = vector.tocsr()
                elif format == 'numpy':
599
600
                    vector[int(self.n), 0] = 1.0
601
602
                    vector[self.n, 0] = Integer(1)
603
                return vector
604
            else:
                return ValueError("Not Numerical State")
605
606
607
    class SHOBra(SHOState, Bra):
608
        """A time-independent Bra in SHO.
609
610
611
        Inherits from SHOState and Bra.
612
613
        Parameters
614
        _____
```

```
615
616
        args : tuple
617
            The list of numbers or parameters that uniquely specify the ket
618
            This is usually its quantum numbers or its symbol.
619
620
        Examples
        _____
621
622
623
        Bra's know about their associated ket:
624
625
            >>> from sympy.physics.quantum.sho1d import SHOBra
626
627
            >>> b = SHOBra('b')
            >>> b.dual
628
            |b>
629
630
            >>> b.dual_class()
631
            <class 'sympy.physics.guantum.sho1d.SH0Ket'>
632
633
        Vector representation of a numerical state bra:
634
635
            >>> from sympy.physics.quantum.sho1d import SHOBra, NumberOp
636
            >>> from sympy.physics.quantum.represent import represent
637
            >>> b = SHOBra(3)
638
            >>> N = Number0p('N')
639
640
            >>> represent(b, basis=N, ndim=4)
641
            [0, 0, 0, 1]
642
        0.000
643
644
645
        @classmethod
646
        def dual_class(self):
647
            return SHOKet
648
649
        def _represent_default_basis(self, **options):
650
            return self._represent_NumberOp(None, **options)
651
652
        def _represent_NumberOp(self, basis, **options):
            ndim_info = options.get('ndim', 4)
653
            format = options.get('format', 'sympy')
opitons['spmatrix'] = 'lil'
654
655
            vector = matrix zeros(1, ndim info, **options)
656
657
            if isinstance(self.n, Integer):
658
                 if self.n >= ndim info:
                     return ValueError("N-Dimension too small")
659
                 if format == 'scipy.sparse':
660
                     vector[0, int(self.n)] = 1.0
661
662
                     vector = vector.tocsr()
663
                 elif format == 'numpy':
                     vector[0, int(self.n)] = 1.0
664
665
                 else:
666
                     vector[0, self.n] = Integer(1)
```

```
return vector
else:
return ValueError("Not Numerical State")

ad = RaisingOp('a')
a = LoweringOp('a')
H = Hamiltonian('H')
N = NumberOp('N')
m = Symbol('omega')
m = Symbol('m')
```

```
1 """Tests for shold.pv"""
2
3
  from sympy import Integer, Symbol, sqrt, I, S
4 from sympy.physics.quantum import Dagger
5 from sympy physics quantum constants import hbar
6 from sympy.physics.quantum import Commutator
7 from sympy.physics.quantum.gapply import gapply
8 from sympy.physics.quantum.innerproduct import InnerProduct
9 from sympy physics quantum cartesian import X, Px
10 from sympy.functions.special.tensor_functions import KroneckerDelta
11 from sympy.physics.quantum.hilbert import ComplexSpace
12 from sympy.physics.quantum.represent import represent
13 from sympy external import import module
14 from sympy.utilities.pytest import skip
15
16 from sympy.physics.quantum.sho1d import (RaisingOp, LoweringOp,
                                            SHOKet, SHOBra,
17
                                            Hamiltonian, NumberOp)
18
19
20 ad = RaisingOp('a')
21 a = LoweringOp('a')
22 k = SH0Ket('k')
23 kz = SH0Ket(0)
24 \text{ kf} = \text{SH0Ket}(1)
25 k3 = SH0Ket(3)
26 b = SH0Bra('b')
27 | b3 = SHOBra(3)
28 H = Hamiltonian('H')
29 N = Number0p('N')
30 omega = Symbol('omega')
31 \parallel m = Symbol('m')
32 | ndim = Integer(4)
33
34 np = import_module('numpy', min_python_version=(2, 6))
35 scipy = import_module('scipy', __import__kwargs={'fromlist': ['sparse']})
36
37 ad rep sympy = represent(ad, basis=N, ndim=4, format='sympy')
38 a_rep = represent(a, basis=N, ndim=4, format='sympy')
39 N_rep = represent(N, basis=N, ndim=4, format='sympy')
40 H_rep = represent(H, basis=N, ndim=4, format='sympy')
41 k3 rep = represent(k3, basis=N, ndim=4, format='sympy')
42 b3 rep = represent(b3, basis=N, ndim=4, format='sympy')
43
44 def test_RaisingOp():
45
       assert Dagger(ad) == a
       assert Commutator(ad, a).doit() == Integer(-1)
46
       assert Commutator(ad, N).doit() == Integer(-1)*ad
47
       assert qapply(ad*k) == (sqrt(k.n + 1)*SH0Ket(k.n + 1)).expand()
48
49
       assert gapply(ad*kz) == (sqrt(kz.n + 1)*SHOKet(kz.n + 1)).expand()
50
       assert gapply(ad*kf) == (sqrt(kf.n + 1)*SHOKet(kf.n + 1)).expand()
       assert ad.rewrite('xp').doit() == \
51
           (Integer(1)/sqrt(Integer(2)*hbar*m*omega))*(Integer(-1)*I*Px +
52
```

```
52... m*omega*X)
 53
        assert ad.hilbert_space == ComplexSpace(S.Infinity)
 54
        for i in range(ndim - 1):
 55
            assert ad_rep_sympy[i + 1,i] == sqrt(i + 1)
 56
 57
        if not np:
 58
            skip("numpy not installed or Python too old.")
 59
        ad_rep_numpy = represent(ad, basis=N, ndim=4, format='numpy')
 60
 61
        for i in range(ndim - 1):
            assert ad_rep_numpy[i + 1,i] == float(sqrt(i + 1))
 62
 63
 64
        if not np:
            skip("numpy not installed or Python too old.")
 65
        if not scipy:
 66
            skip("scipy not installed.")
 67
 68
        else:
 69
            sparse = scipy.sparse
 70
 71
        ad_rep_scipy = represent(ad, basis=N, ndim=4, format='scipy.sparse',
    spmatrix='lil')
 •••
        for i in range(ndim - 1):
 72
 73
            assert ad_rep_scipy[i + 1,i] == float(sqrt(i + 1))
 74
 75
        assert ad rep numpy.dtype == 'float64'
 76
        assert ad_rep_scipy.dtype == 'float64'
 77
    def test_LoweringOp():
 78
 79
        assert Dagger(a) == ad
        assert Commutator(a, ad).doit() == Integer(1)
 80
        assert Commutator(a, N).doit() == a
 81
        assert gapply(a*k) == (sgrt(k.n)*SHOKet(k.n-Integer(1))).expand()
 82
        assert gapply(a*kz) == Integer(0)
 83
        assert gapply(a*kf) == (sgrt(kf.n)*SHOKet(kf.n-Integer(1))).expand()
 84
 85
        assert a.rewrite('xp').doit() == \
            (Integer(1)/sqrt(Integer(2)*hbar*m*omega))*(I*Px + m*omega*X)
 86
 87
        for i in range(ndim - 1):
            assert a rep[i,i + 1] == sqrt(i + 1)
 88
 89
 90
    def test_NumberOp():
        assert Commutator(N, ad).doit() == ad
 91
 92
        assert Commutator(N, a).doit() == Integer(-1)*a
        assert Commutator(N, H).doit() == Integer(0)
 93
 94
        assert gapply(N*k) == (k.n*k).expand()
 95
        assert N.rewrite('a').doit() == ad*a
 96
        assert N.rewrite('xp').doit() ==
    (Integer(1)/(Integer(2)*m*hbar*omega))*(
 •••
 97
            Px**2 + (m*omega*X)**2) - Integer(1)/Integer(2)
 98
        assert N.rewrite('H').doit() == H/(hbar*omega) - Integer(1)/Integer(2)
        for i in range(ndim):
 99
100
            assert N_rep[i,i] == i
        assert N_rep == ad_rep_sympy*a_rep
101
```

```
102
103
   def test_Hamiltonian():
        assert Commutator(H, N).doit() == Integer(0)
104
105
        assert gapply(H*k) == ((hbar*omega*(k.n +
    Integer(1)/Integer(2)))*k).expand()
        assert H.rewrite('a').doit() == hbar*omega*(ad*a +
106
    Integer(1)/Integer(2))
107
        assert H.rewrite('xp').doit() == \
            (Integer(1)/(Integer(2)*m))*(Px**2 + (m*omega*X)**2)
108
        assert H.rewrite('N').doit() == hbar*omega*(N + Integer(1)/Integer(2))
109
110
        for i in range(ndim):
111
            assert H_rep[i,i] == hbar*omega*(i + Integer(1)/Integer(2))
112
    def test_SH0Ket():
113
        assert SH0Ket('k').dual_class() == SH0Bra
114
115
        assert SHOBra('b').dual_class() == SHOKet
        assert InnerProduct(b,k).doit() == KroneckerDelta(k.n, b.n)
116
        assert k.hilbert space == ComplexSpace(S.Infinity)
117
        assert k3_rep[k3.n, 0] == Integer(1)
118
        assert b3_rep[0, b3.n] == Integer(1)
119
120
```

Mapping Gate

Imports

Before examining the Mapping Gate, the relevant files need to be loaded.

```
In [1]: %load_ext sympy.interactive.ipythonprinting
    from sympy import Symbol, Integer, I
    from sympy.core.containers import Dict
    from sympy.physics.quantum import qapply, represent
    from sympy.physics.quantum.qubit import Qubit
    from sympy.physics.quantum.mappinggate import MappingGate
```

Theory/Background

Creating a **MappingGate** can be very useful in Quantum Computing. Normally one would have to use a combination of various quantum gates to get the desired input-output state pairings. The Mapping Gate allows for user provided initial and final state pairings for every state. Then a quantum gate that has the same pairings is created.

The Mapping Gate maps an initial qubits to scalars times final qubits. If no scalar is specified one is assumed. So there are two or three arguments for the mapping gate.

```
arg[0] = initial state
arg[1] = scalar or final state
arg[2] = final state or none
```

The qubits can either be strings or qubits. The resulting arguments of the MappingGate are converted to a sympy dictionary.

There are multiple ways to specify the qubit pairings. All quantum gates have the property of being unitary, which means only half of the gate needs to be specified and the rest can be assumed and created to preserve the unitary property. When thinking about the gates as matrices, it is only required to specify half of the matrix. And if an initial state is not paired to a final state it will return itself like the Identity Gate.

The Mapping Gate can also take a Python or Sympy dictionary as its argument. The dictionary requires qubit objects rather than strings and the scalars are multiplied with the final states.

{Qubit('initial'):scalar*Qubit('final'), ...}

Creating the MappingGate

Specify all states

Here, all pairs are specified. There are 2ⁿ number of pairs, where n is the number of qubits in each state.

```
In [2]: M_all = MappingGate(('00', I, '11'), ('01', exp(I), '10'), ('10', exp(-I), '01'), ('11
In [3]: M_all.args
```

Another useful way to express a quantum gate is using outer product representation. This takes the form:

ket(final)*bra(initial) + ...

To call this, we use rewrite and pass it a keyword, in this case 'op'.

Out[3]: $(\{|00\rangle: \iota|11\rangle, |01\rangle: e^{\iota}|10\rangle, |10\rangle: e^{-\iota}|01\rangle, |11\rangle: -\iota|00\rangle\})$

```
In [4]: M_all.rewrite('op')

Out[4]: -i|00\rangle\langle 11| + e^{-i}|01\rangle\langle 10| + e^{i}|10\rangle\langle 01| + i|11\rangle\langle 00|
```

Another common way of expressing a quantum gate is in matrix form. Any term in a matrix can be identified using a bra and a ket (i.e. (0,1) is the same as bra(0) ket(1)). Using this idea a quantum gate is created by inserting the outer product in between each identifying bra and ket for each term. If the qubits in the MappingGate return themselves the resulting matrix is the identity gate.

Now taking a look at the more complex qubit mapping from above, it is clear that the outer product terms are directly related to the terms of the matrix.

Specify only half of the states and relying on the unitary property of the gate.

Here, only half of the pairs are specified because the unitary property of the gate can fill the rest. Given that *initial* = *scalar* * *final*, this implies that *final* = *conjugate*(*scalar*) * *initial*. This is what allows for only mapping the upper triangle of the matrix. The idea of only mapping the one triangle will be more easily seen when the gate is represented in matrix form

```
In [8]: M_half = MappingGate(('00', I, '11'), ('01', exp(I), '10'))
```

We can check that the mapping for this is the same as the full mapping

```
In [10]: M_half.args == M_all.args
Out[10]: True
```

Let's look at the outerproduct representation, it should be the same as above in M_all

```
In [11]: M_{\text{half.rewrite('op')}}
Out[11]: -\iota|00\rangle\langle11| + e^{-\iota}|01\rangle\langle10| + e^{\iota}|10\rangle\langle01| + \iota|11\rangle\langle00|
```

Using the matrix representation it is clear that we only mapped the terms at (3,0) and (2,1) and the terms at (0,3) and (1,2) are the conjugates of the mapped terms.

Specify only some states

Here, only some states will be specified and their compliments. Any state not specified returns itself, but is not one of the arguments of MappingGate.

```
In [13]: M_some = MappingGate(('00', I, '11'))

In [14]: M_some.args

Out[14]: (\{|00\rangle: \iota|11\rangle, |11\rangle: -\iota|00\rangle\})
```

When using the outer product representation it will be clear that non-specified states return themselves.

```
In [15]: M_some.rewrite('op')

Out[15]: |01\rangle\langle01| + |10\rangle\langle10| - \iota|00\rangle\langle11| + \iota|11\rangle\langle00|
```

States that return themselves will yield a 1 along the diaganol like the identity matrix.

Using a Python Dictionary

The MappingGate can also take dictionaries as its arguments. Passing a dictionary as the argument to MappingGate works exactly the same as seen above except for the required form of the dictionary. Where as above MappingGate accepts either strings or qubits, a dictionary must contain qubits. Again if not all states are specified they will return themselves and only half of the matrix needs to be mapped. MappingGate converts the python dictionary to a sympy dictionary.

```
In [17]: d = dict({Qubit('00'):I*Qubit('11'), Qubit('01'):exp(I)*Qubit('10')})
M_python_dict = MappingGate(d)
```

Check that the outer product and matrix are the same as the the previous gates.

```
In [19]: M_python_dict.rewrite('op')

Out[19]: -\iota|00\rangle\langle11| + e^{-\iota}|01\rangle\langle10| + e^{\iota}|10\rangle\langle01| + \iota|11\rangle\langle00|

In [20]: M_python_dict.rewrite('op') == M_half.rewrite('op') == M_all.rewrite('op')

Out[20]: True

In [21]: represent(M_python_dict)

Out[21]: \begin{bmatrix} 0 & 0 & 0 & -\iota \\ 0 & 0 & e^{-\iota} & 0 \\ 0 & e^{-\iota} & 0 & 0 \\ \iota & 0 & 0 & 0 \end{bmatrix}

In [22]: represent(M_python_dict) == represent(M_half) == represent(M_all)

Out[22]: True
```

Using a Sympy Dictionary

A sympy dictionary can also be used to specify the qubit mapping. It works the same as the python dictionary.

```
In [23]: d = Dict(\{Qubit('00'):I*Qubit('11'), Qubit('01'):exp(I)*Qubit('10')\})

M_sympy_dict = MappingGate(d)

In [24]: M_sympy_dict.args

Out[24]: (\{|00\rangle:i|11\rangle, |01\rangle:e^i|10\rangle, |10\rangle:e^{-i}|01\rangle, |11\rangle:-i|00\rangle\})

In [25]: M_sympy_dict.rewrite('op')

Out[25]: -i|00\rangle\langle 11| + e^{-i}|01\rangle\langle 10| + e^i|10\rangle\langle 01| + i|11\rangle\langle 00|
```

```
In [26]: represent(M_sympy_dict)

Out[26]: 
\begin{bmatrix}
0 & 0 & 0 & -\iota \\
0 & 0 & e^{-\iota} & 0 \\
0 & e^{\iota} & 0 & 0 \\
\iota & 0 & 0 & 0
\end{bmatrix}
```

Examples

Create an arbitrary qubit mapping and pass it to MappingGate, then check some of its properties

```
In [27]: M = MappingGate(('000', -1, '001'), ('010', I, '101'), ('100', I*exp(I), '111'))
```

Check the arguments and outer product representation make sure there are 8 terms.

Using hilbert_space checks the hilbert space of the gate.

```
In [30]: M.hilbert_space

Out[30]: C^{2\otimes 3}
```

There are three ways to get the final state from the initial state: get_final_state, mapping, and qapply. get_final_state takes either strings or qubits where both mapping and qapply require qubits.

```
In [31]: M.get_final_state('100')
Out[31]: \( ie^i | 111 \)
In [32]: M.mapping[Qubit('100')]
Out[32]: \( ie^i | 111 \)
In [33]: \( qapply(M*Qubit('100')) \)
Out[33]: \( ie^i | 111 \)
```

The MappingGate can also act on individual qubit states or multiple qubit states.

There are three formats of the matrix representation that can be used, sympy-default, numpy, and scipy.sparse. For large matrices (i.e. large number of qubits) it is common to use the scipy.sparse format.

```
In [39]: represent(M, format='numpy')
Out[39]: [[ 0.00000000+0.j
                                   -1.00000000+0.j
         0.00000000+0.j
            0.00000000+0.j
                                    0.00000000+0.j
         0.00000000+0.j
                    0.00000000+0.j
                                            0.00000000+0.j
          [-1.00000000+0.j
                                    0.00000000+0.j
         0.00000000+0.j
            0.00000000+0.j
                                    0.00000000+0.j
         0.00000000+0.j
                    0.00000000+0.i
                                            0.00000000+0.j
          [ 0.00000000+0.j
                                    0.00000000+0.j
         0.00000000+0.j
            0.00000000+0.i
                                    0.00000000+0.i
         0.00000000-1.j
                                            0.00000000+0.j
                   0.00000000+0.j
          [ 0.00000000+0.j
                                    0.00000000+0.j
         0.00000000+0.j
            1.00000000+0.j
                                    0.00000000+0.j
         0.00000000+0.j
                   0.00000000+0.j
                                            0.00000000+0.j
         1
          [ 0.00000000+0.j
                                    0.00000000+0.j
         0.00000000+0.j
            0.00000000+0.j
                                    0.00000000+0.j
         0.00000000+0.j
                    0.00000000+0.j
         -0.84147098-0.54030231j]
          [ 0.00000000+0.j
                                    0.00000000+0.j
         0.00000000+1.j
                                    0.00000000+0.j
            0.00000000+0.j
         0.00000000+0.j
                    0.00000000+0.j
                                            0.00000000+0.j
          [ 0.00000000+0.j
                                    0.00000000+0.j
         0.00000000+0.j
            0.00000000+0.j
                                    0.00000000+0.j
         0.00000000+0.j
                    1.00000000+0.j
                                            0.00000000+0.j
          [ 0.00000000+0.j
                                    0.00000000+0.j
         0.00000000+0.j
            0.00000000+0.j
                                   -0.84147098+0.54030231j
         0.00000000+0.j
                   0.00000000+0.j
                                          0.00000000+0.j
         ]]
```

Example with nqubits = 5

The matrix representation of a quantum gate is a 2ⁿ by 2ⁿ matrix, so even for relatively small states there is a lot of data stored. An example with states of 5 qubits should use scipy.sparse representation rather than the default sympy representation.

Notice that essentially the entire matrix is zeros with ones along the diagonal. Using the scipy.sparse format here will condense the result.

```
In [43]: represent(M_large, format='scipy.sparse')
Out[43]:
               (0, 1.0)
                             -1j
               (1, 0.0)
                             1j
                             (1+0j)
             (2, 31.0)
              (3, 3)
           (1+0j)
              (4, 4)
           (1+0j)
              (5, 5)
           (1+0j)
              (6, 6)
           (1+0j)
              (7, 7)
           (1+0j)
              (8, 8)
           (1+0j)
              (9, 9)
           (1+0j)
             (10, 10)
                             (1+0j)
                             (1+0j)
             (11, 11)
             (12, 12)
                             (1+0j)
             (13, 13)
                             (1+0j)
             (14, 14)
                             (1+0j)
             (15, 15)
(16, 16)
(17, 17)
                             (1+0j)
                             (1+0j)
                             (1+0j)
             (18, 18)
                             (1+0j)
             (19, 19)
                             (1+0j)
             (20, 20)
                             (1+0j)
             (21, 21)
                             (1+0j)
             (22, 22)
                             (1+0j)
             (23, 23)
(24, 24)
(25, 25)
                             (1+0j)
                             (1+0j)
                             (1+0j)
             (26, 26)
                             (1+0j)
             (27, 27)
                             (1+0j)
             (28, 28)
                             (1+0j)
             (29, 29)
                             (1+0j)
             (30, 30)
                             (1+0j)
             (31, 2.0)
                             (1+0j)
```

Creating Quantum Gates

MappingGate can be used to create any of the common quantum gates by specifying the same mappings. Let's create the ZGate, XGate, and YGate.

ZGate

```
In [44]: from sympy.physics.quantum.gate import ZGate
In [45]: Z = ZGate(0)
M_Z = MappingGate(('0', '0'), ('1', -1, '1'))
```

```
In [46]: represent(Z, nqubits=1)
Out[46]: \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}
In [47]: represent(M Z)
Out[47]: \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}
In [48]: represent(Z, nqubits=1) == represent(M_Z)
Out[48]: True
XGate
In [49]: from sympy.physics.quantum.gate import XGate
In [50]: X = XGate(0)
             M_X = MappingGate(('0', '1'))
In [51]: represent(X, nqubits=1)
Out[51]: \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}
In [52]: represent(M_X)
Out[52]: \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}
In [53]: represent(X, nqubits=1) == represent(M X)
Out[53]: True
In [54]: from sympy.physics.quantum.gate import YGate
In [55]: Y = YGate(0)
M_Y = MappingGate(('0', I, '1'))
In [56]: represent(Y, nqubits=1)
Out[56]: \begin{bmatrix} 0 & -\iota \\ \iota & 0 \end{bmatrix}
```

For Additional Quantum Gate Information

Griffiths, David J. Introduction to Quantum Mechanics. Upper Saddle River, NJ: Pearson Prentice Hall, 2005. Print. http://en.wikipedia.org/wiki/Quantum_gate

```
In [ ]:
```

```
1 """Mapping Quantum Gates
 2
 3
   - Enable sparse mappings for large numbers of qubits
 5
 6
 7 from sympy import Integer, conjugate, Add, Mul
8 from sympy.core.containers import Dict
9 from sympy.physics.quantum import Dagger
10 from sympy.physics.quantum.gate import Gate
11 from sympy.physics.quantum.qubit import Qubit, IntQubit
12 from sympy.physics.quantum.matrixutils import matrix eye
13 from sympy.physics.quantum.gexpr import split gexpr parts
14 from sympy.physics.quantum.hilbert import ComplexSpace
15
16 | #-
17
18
19
   class MappingGate(Gate):
20
21
22
       Parameters
23
24
25
       args: tuple, dict
26
27
           arg[0] = initial state
28
           arg[1] = scalar or final state
29
           arg[2] = None or final state
30
31
           The list of initial state and final state pairs. The final states a
32
           multiplied by some scalar. If no scalar is given, 1 is assumed. Onl
           supply the qubit mapping for half of the matrix representation of t
33
           Since a quantum gate is required to be unitary, the other half is c
34
35
           to ensure it is unitary. Can pass either a python or sympy dictiona
36
           already has the qubit mappings.
37
38
       Examples
39
40
41
       Creating a Mapping Gate and checking its arguments and properties. Gett
42
       state from initial state.
43
           >>> from sympy.physics.quantum.mappinggate import MappingGate
44
45
           >>> from sympy.physics.quantum.qubit import Qubit
46
           >>> from sympy import I
           >>> M = MappingGate(('00',I,'11'), ('01','10'), ('10','01'), ('11',
47
48
           >>> M.args
49
           (\{|00\rangle: I*|11\rangle, |01\rangle: |10\rangle, |10\rangle: |01\rangle, |11\rangle: -I*|00\rangle\},)
50
           >>> M.ngubits
51
52
           >>> M.mapping[Qubit('00')]
```

```
53
            I*|11>
54
            >>> M.get_final_state('00')
55
            I*|11>
56
57
        Create a Mapping Gate by only giving half of the initial and final stat
58
        the resulting arguments are the same as the example above. Also passing
59
        or sympy dictionary to MappingGate can have the same result.
60
61
            >>> from sympy.physics.quantum.mappinggate import MappingGate
            >>> from sympy import I
62
            >>> M = MappingGate(('00', I, '11'), ('01', '10'))
63
64
            >>> M.aras
65
            (\{|00\rangle: I*|11\rangle, |01\rangle: |10\rangle, |10\rangle: |01\rangle, |11\rangle: -I*|00\rangle\},)
            >>> d = dict({Qubit('00'):I*Qubit('11'), Qubit('01'):Qubit('10')})
66
67
            >>> M_dict = MappingGate(d)
68
            >>> M.args
            (\{|00\rangle: I*|11\rangle, |01\rangle: |10\rangle, |10\rangle: |01\rangle, |11\rangle: -I*|00\rangle\},)
69
70
71
        Using gapply on initial states returns the final states.
72
73
            >>> from sympy.physics.quantum.mappinggate import MappingGate
74
            >>> from sympy import I
75
            >>> from sympy.physics.quantum.qapply import qapply
            >>> from sympy.physics.quantum.qubit import Qubit
76
77
            >>> M = MappingGate(('00', I, '11'), ('01', '10'))
            >>> q = Qubit('00') + Qubit('01')
78
79
            >>> gapply(M*q)
80
            |10> + I*|11>
81
82
        The MappingGate can be rewritten as an outer product of states. We will
        examples: one where all four states are given and one where only one st
83
84
        given. If not all initial states are specified they return themselves a
85
        states.
86
87
            >>> from sympy.physics.quantum.mappinggate import MappingGate
88
            >>> from sympy import I
89
            >>> M = MappingGate(('00', I, '11'), ('01', '10'))
90
            >>> M.rewrite('op')
            |01><10| + |10><01| - I*|00>*<11| + I*|11>*<00|
91
            >>> M = MappingGate(('00', -1, '00'))
92
93
            >>> M.rewrite('op')
            |01><01| + |10><10| + |11><11| - |00>*<00|
94
95
96
        The MappingGate is also expressed as a matrix where the rows and column
97
        represent the Qubits.
98
99
            >>> from sympy.physics.quantum.mappinggate import MappingGate
100
            >>> from sympy.physics.quantum.represent import represent
101
            >>> from sympy import I
            >>> M = MappingGate(('00', I, '11'), ('01', '10'))
102
103
            >>> represent(M)
            [0, 0, 0, -I]
104
```

```
105
             [0, 0, 1,
                        01
106
             [0, 1, 0,
                        01
             [I, 0, 0,
107
                        01
108
        .....
109
110
111
        @classmethod
112
        def _eval_args(cls, args):
             if len(args) == 1 and isinstance(args[0], (dict, Dict)):
113
                 temp = \{\}
114
115
                 for i, f in args[0].items():
                     terms = split_qexpr_parts(f)
116
117
                     if len(terms[1]) == 0:
                         temp[f] = i
118
                     else:
119
                         temp[terms[1][0]] = conjugate(Mul(*terms[0]))*i
120
                     temp[i] = f
121
122
                 new args = Dict(temp)
123
            else:
124
                 temp = \{\}
125
                 for arg in args:
                     i = Qubit(arg[0])
126
                     if len(arg) == 2:
127
                         scalar = Integer(1)
128
                         f = Qubit(arg[1])
129
130
                     elif len(arg) == 3:
131
                         scalar = arg[1]
132
                         f = Qubit(arg[2])
133
                     else:
                         raise ValueError('Too many scalar arguments')
134
                     if i.nqubits != f.nqubits:
135
                         raise ValueError('Number of qubits for each state do no
136
137
                     temp[f] = conjugate(scalar)*i
                     temp[i] = scalar*f
138
139
                 new_args = Dict(temp)
             return (new_args,)
140
141
142
        @classmethod
143
        def _eval_hilbert_space(cls, args):
            return ComplexSpace(2)**args[0].keys()[0].ngubits
144
145
146
        @property
        def mapping(self):
147
148
             return self.args[0]
149
150
        @property
151
        def nqubits(self):
             """Gives the dimension of the matrix representation"""
152
153
             return self.args[0].keys()[0].nqubits
154
155
        def get_final_state(self, qubit):
156
             """Returns the final state for a given initial state, if initial st
```

```
157
            not mapped to a final state the initial state is returned."""
158
            i = Qubit(qubit)
159
            return self.mapping.get(i, i)
160
161
        def _apply_operator_Qubit(self, qubit):
162
            return self.get final state(qubit)
163
164
        def _eval_rewrite_as_op(self, *args):
            terms = []
165
            for i in range(2**self.nqubits):
166
167
                 initial = Qubit(IntQubit(i, self.ngubits))
                 fin = self.get_final_state(initial)
168
169
                 terms.append(fin*Dagger(initial))
             return Add(*terms)
170
171
        def _represent_default_basis(self, **options):
172
             return self. represent ZGate(None, **options)
173
174
        def _represent_ZGate(self, basis, **options):
175
            format = options.get('format','sympy')
176
            matrix = matrix_eye(2**self.ngubits, **options)
177
            for i, f in self.mapping.items():
178
                 col = IntQubit(i).as_int()
179
                 terms = split_qexpr_parts(f)
180
                 if len(terms[1]) == 0:
181
182
                     row = IntQubit(*terms[0]).as_int()
183
                     scalar = Integer(1)
184
                 else:
185
                     row = IntQubit(*terms[1]).as int()
186
                     scalar = Mul(*terms[0])
187
                 if format == 'scipy.sparse':
188
                     matrix = matrix.tolil()
189
                     col = float(col)
                     row = float(row)
190
191
                     scalar = complex(scalar)
                     matrix[col, col] = 0.0
192
                 matrix[row, col] = scalar
elif format == 'numpy':
193
194
195
                     scalar = complex(scalar)
196
                     matrix[col, col] = 0.0
197
                     matrix[row, col] = scalar
198
199
                     matrix[col, col] = Integer(0)
200
                     matrix[row, col] = scalar
201
             return matrix
202
```

```
1 """Tests for mappinggate.py"""
2
  from sympy import I, Integer, Mul, Add
3
4 from sympy.physics.quantum import Dagger
5 from sympy.physics.quantum.gapply import gapply
6 from sympy.physics.quantum.represent import represent
7 from sympy.physics.quantum.qexpr import split_qexpr_parts
8 from sympy.physics.quantum.hilbert import ComplexSpace
9 from sympy.physics.quantum.qubit import Qubit, IntQubit
10 from sympy.physics.quantum.mappinggate import MappingGate
11 from sympy.external import import module
12 from sympy.utilities.pytest import skip
13
14 np = import_module('numpy', min_python_version=(2, 6))
15||scipy = import_module('scipy', __import__kwargs={'fromlist': ['sparse']})
16
17 # All 3 ways produce same Qubit Mappings
18 M = MappingGate(('00', I, '11'), ('01', '10'), ('10', '01'), ('11', -I,
... | '00')
19 M_half = MappingGate(('00', I, '11'), ('01', '10'))
20 d = dict({Qubit('00'):I*Qubit('11'), Qubit('01'):Qubit('10')})
21 M dict = MappingGate(d)
22
23 M_rep = represent(M, format='sympy')
24
25 def test_MappingGate():
26
       assert M.get_final_state('00') == I*Qubit('11')
27
       assert M.mapping[Qubit('00')] == I*Qubit('11')
       assert gapply(M*Qubit('01')) == Qubit('10')
28
29
       assert M.hilbert space == ComplexSpace(2)**M.ngubits
30
       # Shows same qubit mappings
31
       assert M.args == M_half.args
32
       assert M.args == M dict.args
33
34
       terms = []
       for i in range(2**M.nqubits):
35
           initial = Qubit(IntQubit(i, M.ngubits))
36
37
           fin = M.get_final_state(initial)
38
           terms.append(fin*Dagger(initial))
       result = Add(*terms)
39
       assert M.rewrite('op') == result
40
41
       for i, f in M.mapping.items():
42
43
           col = IntQubit(i).as_int()
44
           terms = split_qexpr_parts(f)
45
           if len(terms[1]) == 0:
               row = IntQubit(*terms[0]).as int()
46
47
               scalar = Integer(1)
48
           else:
               row = IntQubit(*terms[1]).as_int()
49
50
               scalar = Mul(*terms[0])
           assert M_rep[row, col] == scalar
51
```

```
52
53
       if not np:
54
           skip("numpy not installed or Python too old.")
55
56
       M_rep_numpy = represent(M, format='numpy')
       for i, f in M.mapping.items():
57
58
           col = IntQubit(i).as_int()
59
           terms = split_qexpr_parts(f)
           if len(terms[1]) == 0:
60
               row = IntQubit(*terms[0]).as_int()
61
               scalar = Integer(1)
62
63
           else:
64
               row = IntQubit(*terms[1]).as int()
65
               scalar = Mul(*terms[0])
           assert M_rep_numpy[row, col] == complex(scalar)
66
67
68
       if not np:
69
           skip("numpy not installed or Python too old.")
70
       if not scipy:
           skip("scipy not installed.")
71
72
       else:
73
           sparse = scipy.sparse
74
75
       M_rep_scipy = represent(M, format='scipy.sparse')
       for i, f in M.mapping.items():
76
77
           col = IntQubit(i).as_int()
78
           terms = split_qexpr_parts(f)
           if len(terms[1]) == 0:
79
               row = IntQubit(*terms[0]).as int()
80
81
               scalar = Integer(1)
82
           else:
               row = IntQubit(*terms[1]).as_int()
83
84
               scalar = Mul(*terms[0])
85
           col = float(col)
86
           row = float(row)
           scalar = complex(scalar)
87
88
           assert M rep scipy[row, col] == scalar
89
```

APPENDIX

Links

The following are the addresses of the two Quantum projects on the GitHub website in the SymPy directory.

Quantum Simple Harmonic Oscillator

https://github.com/sympy/sympy/blob/master/sympy/physics/quantum/sho1d.py

Quantum Mapping Gate

https://github.com/sympy/sympy/blob/master/sympy/physics/quantum/mappinggate.py

References

 $\hbox{``GitHub."} < \hskip-.5em \hbox{$http://en.wikipedia.org/wiki/GitHub>.}$

Griffiths, David J. Introduction to Quantum Mechanics. Upper Saddle River, NJ: Pearson Prentice Hall, 2005. Print.

"SymPy." SymPy. Web. 15 Mar. 2013. http://sympy.org/en/index.html.

Appendix 52