1.1 Introduction to package qm

The qm package was written by Eric Majzoub, University of Missouri. Email: majzoube-at-umsystem.edu

The package is loaded with: load(qm);

The qm package provides functions and standard definitions to solve quantum mechanics problems in a finite dimensional Hilbert space. For example, one can calculate the outcome of Stern-Gerlach experiments using built-in definitions of the Sx, Sy, and Sz operators for arbitrary spin, e.g. $s=\{1/2, 1, 3/2, ...\}$. For spin-1/2 the standard basis states in the x, y, and z-basis are available as $\{xp,xm\}$, $\{yp,ym\}$, and $\{zp,zm\}$, respectively. One can create general ket vectors with arbitrary but finite dimension and perform standard computations such as expectation value, variance, etc. The angular momentum $|j,m\rangle$ representation of kets is also available. Tensor product states for multiparticle systems can be created to perform calculations on those systems.

Let us consider a simple example involving spin-1/2 particles. A bra vector in the **z**-basis may be written as

$$$$

The bra will be represented in Maxima by the row vector [a b], where the basis vectors are

$$\langle z+| = [1 \ 0]$$

and

$$\langle z - | = [0 \ 1].$$

1.1.1 Types of kets and bras

There are two types of kets and bras available in this package, the first type is given by a matrix representation, as in the above example. mkets are column vectors and mbras are row vectors, and their components are entered as Maxima lists in the mbra and mket functions. The second type of bra or ket is abstract; there is no matrix representation. Abstract bras and kets are entered using the bra and ket functions using Maxima lists for the elements. These general kets are displayed in Dirac notation. Abstract bras and kets are used for both the (j,m) representation of states and also for tensor products. For example, a tensor product of two ket vectors |a> and |b> is input as ket([a,b]) and displayed as

Note that abstract kets and bras are assumed to be orthonormal. These general bras and kets may be used to build arbitrarily large tensor product states. Tensor product states in the matrix representation are also available through the tpket and tpbra commands.

The following examples illustrate some of the basic capabilities of the qm package. Here both abstract, and concrete (matrix representation) kets are shown.

Note that ket([a,b]) is treated as tensor product of states a and b as shown below.

Next, tensor products of the spin-1/2 basis states $\{zp,zm\}$ are shown in the matrix representation.

Constants that multiply kets and bras must be declared complex by the user in order for the dagger function to properly conjugate such constants. The example below illustrates this behavior.

The following shows how to declare a ket with both real and complex components in the matrix representation.

```
(%i1) declare([c1,c2],complex,r,real);
(%o1)
                                      done
(%i2) k:mket([c1,c2,r]);
                                     [ c1 ]
(%o2)
                                     [ c2 ]
                                          ]
                                     [r]
(%i3) b:dagger(k);
(\%03)
                      [ conjugate(c1) conjugate(c2) r ]
(%i4) b . k;
                    2
(\%04)
                   r + c2 conjugate(c2) + c1 conjugate(c1)
```

1.2 Functions and Variables for qm

hbar

Planck's constant divided by 2*%pi. hbar is not given a floating point value, but is declared to be a real number greater than zero.

$$\texttt{ket} ([k_1,k_2,\ldots])$$

[Function]

ket creates a general state ket, or tensor product, with symbols k_i representing the states. The state kets k_i are assumed to be orthonormal.

ketp (abstract ket)

[Function]

ketp is a predicate function for abstract kets. It returns true for abstract kets and false for anything else.

bra
$$([b_1,b_2,\ldots])$$

[Function]

bra creates a general state bra, or tensor product, with symbols b_i representing the states. The state bras b_i are assumed to be orthonormal.

brap (abstract bra)

[Function]

brap is a predicate function for abstract bras. It returns true for abstract bras and false for anything else.

$$mket ([c_1,c_2,\ldots])$$

[Function]

mket creates a *column* vector of arbitrary finite dimension. The entries c_i can be any Maxima expression. The user must declare any relevant constants to be complex. For a matrix representation the elements must be entered as a list in [...] square brackets.

mketp (vector)

[Function]

mketp is a predicate function that checks if its input is an mket, in which case it returns true, else it returns false. mketp only returns true for the matrix representation of a ket.

 $mbra ([c_1,c_2,\ldots])$

[Function]

mbra creates a *row* vector of arbitrary finite dimension. The entries c_i can be any Maxima expression. The user must declare any relevant constants to be complex. For a matrix representation the elements must be entered as a list in $[\ldots]$ square brackets.

mbrap (vector)

[Function]

mbrap is a predicate function that checks if its input is an mbra, in which case it returns true, else it returns false. mbrap only returns true for the matrix representation of a bra.

Two additional functions are provided to create kets and bras in the matrix representation. These functions conveniently attempt to automatically declare constants as complex. For example, if a list entry is a*sin(x)+b*cos(x) then only a and b will be declared complex and not x.

```
autoket ([a_1, a_2, \ldots])
```

[Function]

autoket takes a list $[a_1, a_2, \ldots]$ and returns a ket with the coefficients a_i declared complex. Simple expressions such as a*sin(x)+b*cos(x) are allowed and will declare only the coefficients as complex.

```
(%i1) autoket([a,b]);
                                             [ a ]
                                             [ ]
     (%01)
                                             [ b ]
     (%i2) facts();
             [kind(hbar, real), hbar > 0, kind(a, complex), kind(b, complex)]
     (%i1) autoket([a*sin(x),b*sin(x)]);
                                         [ a sin(x) ]
     (%01)
                                         [ b sin(x) ]
     (%i2) facts();
     (%02) [kind(hbar, real), hbar > 0, kind(a, complex), kind(b, complex)]
autobra (|a_1, a_2, \ldots|)
                                                                        [Function]
     autobra takes a list [a1, a2, ...] and returns a bra with the coefficients ai declare-
     d complex. Simple expressions such as a*sin(x)+b*cos(x) are allowed and will
     declare only the coefficients as complex.
     (%i1) autobra([a,b]);
     (%o1)
                                           [a b]
     (%i2) facts();
     (%02) [kind(hbar, real), hbar > 0, kind(a, complex), kind(b, complex)]
     (\%i1) autobra([a*sin(x),b]);
                                        [a sin(x) b]
     (%o1)
     (%i2) facts();
             [kind(hbar, real), hbar > 0, kind(a, complex), kind(b, complex)]
dagger (vector)
                                                                        [Function]
     dagger is the quantum mechanical dagger function and returns the conjugate
     transpose of its input. Arbitrary constants must be declare-d complex for dagger
     to produce the conjugate.
     (%i1) dagger(mbra([%i,2]));
                                           [ - %i ]
     (%o1)
braket (psi,phi)
                                                                        [Function]
     Given two kets psi and phi, braket returns the quantum mechanical bracket
     <psi|phi>. The vector psi may be input as either a ket or bra. If it is a ket it will
     be turned into a bra with the dagger function before the inner product is taken.
     The vector phi must always be a ket.
     (%i1) declare([a,b,c],complex);
     (%o1)
                                             done
     (%i2) braket(mket([a,b,c]),mket([a,b,c]));
                     c conjugate(c) + b conjugate(b) + a conjugate(a)
     (%o2)
     (%i3) braket(ket([a1,b1,c1]),ket([a2,b2,c2]));
     (%03)
                 kron_delta(a1, a2) kron_delta(b1, b2) kron_delta(c1, c2)
```

```
norm (psi)
                                                                        [Function]
     Given a ket or bra psi, norm returns the square root of the quantum mechanical
     bracket <psi|psi>. The vector psi must always be a ket, otherwise the function
     will return false.
     (%i1) declare([a,b,c],complex);
     (%o1)
                                             done
     (%i2) norm(mket([a,b,c]));
     (\%02)
                  sqrt(c conjugate(c) + b conjugate(b) + a conjugate(a))
magsqr (c)
                                                                        [Function]
     magsqr returns conjugate(c)*c, the magnitude squared of a complex number.
     (%i1) declare([a,b,c,d],complex);
     (%o1)
     (%i2) A:braket(mket([a,b]),mket([c,d]));
     (%o2)
                               conjugate(b) d + conjugate(a) c
     (%i3) P:magsqr(A);
     (%o3) (conjugate(b) d + conjugate(a) c) (b conjugate(d) + a conjugate(c))
```

1.2.1 Handling general kets and bras

General kets and bras are, as discussed, created without using a list when giving the arguments. The following examples show how general kets and bras can be manipulated.

1.2.2 Spin-1/2 state kets and associated operators

Spin-1/2 particles are characterized by a simple 2-dimensional Hilbert space of states. It is spanned by two vectors. In the z-basis these vectors are {zp,zm}, and the basis kets in the z-basis are {xp,xm} and {yp,ym} respectively.

```
Return the |z+> ket in the z-basis.

Zm

Return the |z-> ket in the z-basis.

xp

Return the |x+> ket in the z-basis.

xm

Return the |x-> ket in the z-basis.

[Function]

Return the |x-> ket in the z-basis.

[Function]

Return the |x-> ket in the z-basis.
```

[Function] ym Return the $|y-\rangle$ ket in the z-basis. (%i1) zp; [1] (%o1) [] [0] (%i2) zm; Γ01 (%02)] [1] (%i1) yp; [sqrt(2)] (%o1) %i -----] [sqrt(2)] (%i2) ym; sqrt(2) (%o2) %i] sqrt(2)] (%i1) braket(xp,zp); 1 (%o1)

Switching bases is done in the following example where a z-basis ket is constructed and the x-basis ket is computed.

sqrt(2)

1.2.3 Pauli matrices and Sz, Sx, Sy operators

sigmax [Function]

Returns the Pauli x matrix.

sigmay

[Function]

Returns the Pauli y matrix.

sigmaz

[Function]

Returns the Pauli z matrix.

Sx

[Function]

Returns the spin-1/2 Sx matrix.

Sy

[Function]

Returns the spin-1/2 Sy matrix.

Sz

[Function]

Returns the spin-1/2 Sz matrix.

(%i1) sigmay;

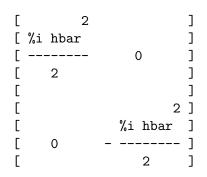
(%i2) Sy;

commutator (X,Y)

[Function]

Given two operators X and Y, return the commutator X . Y – Y . X.

(%i1) commutator(Sx,Sy);



1.2.4 SX, SY, SZ operators for any spin

SX (s)

[Function]

SX(s) for spin s returns the matrix representation of the spin operator Sx. Shortcuts for spin-1/2 are Sx,Sy,Sz, and for spin-1 are Sx1,Sy1,Sz1.

SY(s)

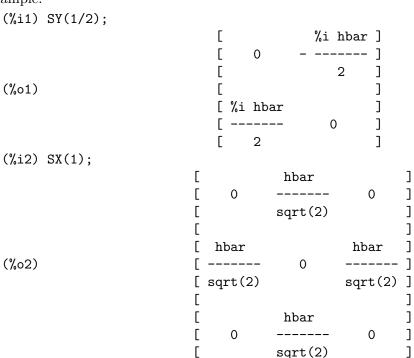
[Function]

SY(s) for spin s returns the matrix representation of the spin operator Sy. Shortcuts for spin-1/2 are Sx,Sy,Sz, and for spin-1 are Sx1,Sy1,Sz1.

SZ (s) [Function]

SZ(s) for spin s returns the matrix representation of the spin operator Sz. Shortcuts for spin-1/2 are Sx,Sy,Sz, and for spin-1 are Sx1,Sy1,Sz1.

Example:



1.2.5 Expectation value and variance

expect (0,psi) [Function]

Computes the quantum mechanical expectation value of the operator O in state psi, <psi|O|psi>.

qm_variance (0,psi)

[Function]

Computes the quantum mechanical variance of the operator O in state psi, sqrt(<psi|O²|psi> - <psi|O|psi>²).

1.2.6 Angular momentum representation of kets and bras

1.2.6.1 Matrix representation of (j,m)-kets and bras

The matrix representation of kets and bras in the qm package are represented in the z-basis. To create a matrix representation of of a ket or bra in the (j,m)-basis one uses the spin_mket and spin_mbra functions.

$$spin_mket (s, m_s, [1,2])$$

[Function]

spin_mket returns a ket in the z-basis for spin s and z-projection m_s , for axis 1=X or 2=Y.

 $spin_mbra (s, m_s, [1,2])$

(%o1)

[Function]

spin_mbra returns a bra in the z-basis for spin s and z-projection m_s , for axis 1=X or 2=Y.

(%i1) spin_mket(3/2,1/2,2);

[sqrt(3)]
[]
[3/2]
[2]
[]
[%i]
[]
[3/2]
[2]
[]
[1]
[]
[3/2]
[2]
[]
[sqrt(3) %i]
[]
[3/2]
[2]

(%i2) spin_mbra(1,1,1);

(%o2) [- ----- -] [2 sqrt(2) 2]

1.2.6.2 Abstract (j,m)-kets and bras

To create kets and bras in the $|j,m\rangle$ representation you use the abstract ket and bra functions with j,m as arguments, as in ket([j,m]) and bra([j,m]).

jmketp (jmket)

[Function]

jmketp checks to see that the ket has an m-value that is in the set $\{-j,-j+1,\ldots,+j\}$.

```
(%i1) jmketp(jmket([j,m]));
     (%o1)
                                               false
     (%i2) jmketp(jmket([3/2,1/2]));
     (%o2)
                                               true
jmbrap (jmbra)
                                                                           [Function]
     jmbrap checks to see that the bra has an m-value that is in the set \{-j,-j+1,\ldots,+j\}.
jmcheck (j,m)
                                                                           [Function]
     jmcheck checks to see that m is one of \{-j, \ldots, +j\}.
     (\%i1) jmcheck(3/2,1/2);
     (%o1)
                                               true
JP (jmket)
                                                                           [Function]
     JP is the J<sub>+</sub> operator. It takes a jmket jmket(j,m) and returns sqrt(j*(j+1)-
     m*(m+1))*hbar*jmket(j,m+1).
JM (jmket)
                                                                           [Function]
     JM is the J- operator. It takes a jmket jmket(j,m) and returns sqrt(j*(j+1)-m*(m-
     1))*hbar*jmket(j,m-1).
Jsqr (jmket)
                                                                            [Function]
     Jsqr is the J^2 operator.
                                    It takes a jmket jmket(j,m) and returns
     (j*(j+1)*hbar^2*jmket(j,m).
Jz (jmket)
                                                                            [Function]
     Jz is the J<sub>z</sub> operator. It takes a jmket jmket(j,m) and returns m*hbar*jmket(j,m).
  These functions are illustrated below.
     (%i1) k:ket([j,m]);
                                             |[j, m]>
     (%o1)
     (\%i2) JP(k);
                        hbar |[j, m + 1]\rangle sqrt(j (j + 1) - m (m + 1))
     (\%02)
     (%i3) JM(k);
                        hbar |[j, m - 1] > sqrt(j (j + 1) - (m - 1) m)
     (%03)
     (%i4) Jsqr(k);
                                   hbar j (j + 1) |[j, m]>
     (\%04)
     (%i5) Jz(k);
                                         hbar |[j, m] > m
     (%o5)
1.2.7 Angular momentum and ladder operators
```

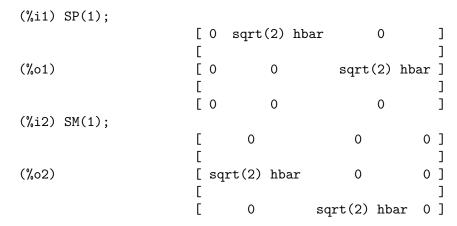
SP (s) [Function]

SP is the raising ladder operator S_{+} for spin s.

SM (s) [Function]

SM is the raising ladder operator S_{-} for spin s.

Examples of the ladder operators:



1.3 Rotation operators

RX (s,t) [Function]

 $\mathtt{RX}(\mathtt{s})$ for spin \mathtt{s} returns the matrix representation of the rotation operator \mathtt{Rx} for rotation through angle \mathtt{t} .

RY (s,t) [Function]

RY(s) for spin s returns the matrix representation of the rotation operator Ry for rotation through angle t.

RZ (s,t) [Function]

RZ(s) for spin s returns the matrix representation of the rotation operator Rz for rotation through angle t.

(%i1)
$$RZ(1/2,t)$$
;

Proviso: assuming 64*t # 0

%i t 2 [%e (%o1) %i t] 2 1 0 %e]

1.4 Time-evolution operator

UU (H,t) [Function]

UU(H,t) is the time evolution operator for Hamiltonian H. It is defined as the matrix exponential matrixexp(-%i*H*t/hbar).

1.5 Tensor products

Tensor products are represented as lists in the qm package. The ket tensor product |z+,z+> could be represented as ket([u,d]), for example, and the bra tensor product <a,b| is represented as bra([a,b]) for states a and b. For a tensor product where the identity is one of the elements of the product, substitute the string Id in the ket or bra at the desired location. See the examples below for the use of the identity in tensor products.

tpket $([k_1, k_2, \ldots])$ [Function]

tpket produces a tensor product of kets k_i . All of the elements must pass the ketp predicate test to be accepted. If a list is not used for the input kets, the tpket will be an abstract tensor product ket.

tpbra $([b_1, b_2, \ldots])$ [Function]

tpbra produces a tensor product of bras b_i . All of the elements must pass the brap predicate test to be accepted. If a list is not used for the input bras, the tpbra will be an abstract tensor product bra.

tpketp (tpket) [Function]

tpketp checks to see that the ket has the 'tpket' marker. Only the matrix representation will pass this test.

tpbrap (tpbra) [Function]

tpbrap checks to see that the bra has the 'tpbra' marker. Only the matrix representation will pass this test.

tpbraket (B,K) [Function]

tpbraket takes the inner product of the tensor products B and K. The tensor products must be of the same length (number of kets must equal the number of bras).

Examples below show how to create concrete (matrix representation) tensor products and take the bracket of tensor products.

```
(%i1) K:tpket([zp,zm]);
                                    [1] [0]
(%o1)
                           [tpket, [[ ], [ ]]]
                                    [0][1]
(%i2) zpb:dagger(zp);
(%o2)
                                  [10]
(%i3) zmb:dagger(zm);
                                  [ 0 1 ]
(%o3)
(%i4) B:tpbra([zpb,zmb]);
                        [tpbra, [[ 1 0 ], [ 0 1 ]]]
(\%04)
(%i5) tpbraket(K,B);
(%o5)
                                    false
(%i6) tpbraket(B,K);
(%06)
                                      1
```

Examples below show how to create abstract tensor products that contain the identity element Id and how to take the bracket of these tensor products.

Appendix A Function and Variable index

\mathbf{A}	\mathbf{Q}
autobra 5 autoket 4	qm_variance9
B bra	RX 12 RY 12 RZ 12
\mathbf{C}	S sigmax
commutator	sigmay 8 sigmaz 8 SM 11
D dagger5	spin_mbra 10 spin_mket 10 SP 11 Sx 8
E expect9	SX 8 Sy 8 SY 8 Sz 8 SZ 9
J	${f T}$
jmbrap 11 jmcheck 11 jmketp 10 JM 11 JP 11 Jsqr 11 Jz 11	tpbra. 13 tpbraket 13 tpbrap. 13 tpket. 13 tpketp. 13
K	U W12
ket 3 ketp 3	X
\mathbf{M}	xm 6 xp 6
magsqr 6 mbra 4 mbrap 4 mket 3 mketp 4	Y ym
N	Z
norm6	zm 6 zp 6

Appendix	A: Fun	ction	and	Variable	index