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 the built-in definition of the Sx, Sy, and Sz operators for arbitrary spin, e.g. $s=\{1/2, 1, 3/2, \ldots\}$. For spin-1/2 the standard basis states in the x, y, and z-basis are available as $\{xp,xm\}, \{yp,ym\}, \text{ and }\{zp,zm\}, \text{ respectively.}$ 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. It is also possible to create tensor product states for multiparticle systems and 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

```
<psi| = a < z+| + b < z-|.
```

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

```
<z+| = [1 \ 0] and <z-| = [0 \ 1].
```

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. kets are column vectors and bras are row vectors, and their components are entered as Maxima lists in the bra and ket functions. The second type of bra or ket is abstract; there is no matrix representation. Abstract bras and kets are entered without using lists for the elements. Thus, if one wishes to do purely symbolic calculations, then input of abstract kets, (j,m)-kets, and so forth should be done without lists. If one wishes to do numerical or component computations using the kets then enter the arguments as a list. Note that abstract kets and bras are assumed to be orthonormal.

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

Note that ket(a,b) is treated as tensor product of states a and b as shown in this example. Tensor product states within the matrix representation are shown further in the manual.

Next, tensor products of the spin-1/2 basis states {zp,zm} are shown in abstract and matrix representations.

Abstract kets and bras are assumed to be orthonormal as shown below.

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

1.2 Functions and Variables for qm

hbar [Variable]

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.

$$\text{ket }([c_1,c_2,\ldots])$$
 [Function]

ket 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. If no list is entered the ket is represented as a general ket, ket(a) will return |a>.
```

```
(%i1) kill(a);
     (%o1)
                                              done
      (%i2) ket(a);
     (\%02)
                                                la>
     (%i3) declare([c1,c2],complex);
     (\%03)
                                              done
     (%i4) ket([c1,c2]);
                                              [ c1 ]
     (\%04)
                                              [ c2 ]
      (%i5) facts();
     (%o5) [kind(hbar, real), hbar > 0, kind(c1, complex), kind(c2, complex)]
bra ([c_1, c_2, ...])
                                                                          [Function]
```

bra 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 [...] square

For a matrix representation the elements must be entered as a list in [...] square bracbras. If no list is entered the bra is represented as a general bra, bra(a) will return <a|.

ketp (vector) [Function]

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

```
(%i1) kill(a,b,k);
(%o1)
                                          done
(%i2) k:ket(a,b);
                                         |a, b>
(\%02)
(%i3) ketp(k);
(\%03)
                                          false
(%i4) k:ket([a,b]);
                                          [ a ]
(\%04)
                                              1
                                          [ b ]
(%i5) ketp(k);
(\%05)
                                          true
```

[Function]

brap (vector) [Function]

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

Two additional functions are provided to create kets and bras in the matrix representation. Additionally these functions 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 declare-d complex and not x.

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

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.

autobra takes a list $[a_1, a_2, \ldots]$ and returns a bra 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.

dagger (vector) [Function]

dagger is the quantum mechanical dagger function and returns the conjugate transpose of its input.

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.

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.

magsqr (c) [Function]

magsqr returns conjugate(c)*c, the magnitude squared of a complex number.

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.

zp	Return the $ z+\rangle$ ket in the z-basis.		[Function]
zm	Return the $ z-\rangle$ ket in the z-basis.		[Function]
хр	Return the $ x+\rangle$ ket in the z-basis.		[Function]
xm	Return the $ x-\rangle$ ket in the z-basis.		[Function]
ур	Return the $ y+\rangle$ ket in the z-basis.		[Function]
ym	Return the $ y\rangle$ ket in the z-basis.		[Function]
	(%i1) zp;		
	(%o1)	[1] [] [0]	
	(%i2) zm;		
	(%o2)	[0] [] [1]	
	(%i1) yp;		
	(%o1)	[1] [] [sqrt(2)] [%i] [] [sqrt(2)]	
	(%i2) ym;	[1]	
	(%o2)	[] [sqrt(2)] [%i] [] [sqrt(2)]	

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

1.2.3 Pauli matrices and Sz, Sx, Sy operators

[Function]

Returns the Pauli x matrix.

[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.

[%i 0]

commutator (X,Y)

[Function]

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

(%i1) commutator(Sx,Sy);

2 [%i hbar 0 2 (%o1)] 2] %i hbar 0 Г 2 ٦

for spin-1/2 are Sx,Sy,Sz, and for spin-1 are Sx1,Sy1,Sz1.

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
- 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:

(%i1) SY(1/2);

	[%i hbar]
	[0]
	[2]
(%o1)	[]
	[%i hbar]
	[0]
	[2]

(%i2) SX(1);

,]] [0	hbar sqrt(2)	0]
(%02)	[hbar sqrt(2)	0	hbar sqrt(2)]
	[0	hbar sqrt(2)	0]

1.2.5 Expectation value and variance

```
[Function]
expect (0,psi)
     Computes the quantum mechanical expectation value of the operator O in state psi,
     <psi|0|psi>.
      (%i1) ev(expect(Sy,xp+ym),ratsimp);
     (%o1)
                                               - hbar
qm_variance (0,psi)
                                                                             [Function]
     Computes the quantum mechanical variance of the operator O in state psi,
     sqrt(\langle psi|0^2|psi\rangle - \langle psi|0|psi\rangle^2).
      (%i1) ev(qm_variance(Sy,xp+ym),ratsimp);
      (%o1)
1.2.6 Angular momentum representation of kets and bras
To create kets and bras in the |j,m\rangle representation you can use the following functions.
                                                                             [Function]
jmket (j,m)
     jmket creates the ket |j,m\rangle for total spin j and z-component m.
                                                                             [Function]
jmbra (j,m)
     jmbra creates the bra \langle j,m| for total spin j and z-component m.
     (\%i1) jmbra(3/2,1/2);
      (\%01)
                                             jmbra(-, -)
      (%i2) jmbra([3/2,1/2]);
                                                   [3 1]
                                          [jmbra, [ - - ]]
      (\%02)
                                                   [22]
jmketp (jmket)
                                                                             [Function]
     jmketp checks to see that the ket has the 'jmket' marker.
      (%i1) jmketp(jmket(j,m));
      (%o1)
                                                false
      (%i2) jmketp(jmket([j,m]));
     (%o2)
                                                true
jmbrap (jmbra)
                                                                             [Function]
     jmbrap checks to see that the bra has the 'jmbra' marker.
jmcheck (j,m)
                                                                             [Function]
     jmcheck checks to see that m is one of \{-j, \ldots, +j\}.
      (\%i1) jmcheck(3/2,1/2);
      (%o1)
                                                true
```

```
jmbraket (jmbra,jmket)
                                                                         [Function]
     jmbraket takes the inner product of the jm-kets.
     (%i1) K: jmket(j1,m1);
     (%o1)
                                         jmket(j1, m1)
     (%i2) B:jmbra(j2,m2);
     (\%02)
                                         jmbra(j2, m2)
     (%i3) jmbraket(B,K);
                            kron_delta(j1, j2) kron_delta(m1, m2)
     (\%03)
     (%i4) B:jmbra(j1,m1);
     (\%04)
                                         jmbra(j1, m1)
     (%i5) jmbraket(B,K);
     (%05)
                                                1
     (%i6) K:jmket([3/2,1/2]);
                                                [3 1]
     (\%06)
                                       [jmket, [ - - ]]
                                                [22]
     (%i7) B:jmbra([3/2,1/2]);
                                                [3 1]
                                       [jmbra, [ - - ]]
     (\%07)
                                                [22]
     (%i8) jmbraket(B,K);
     (%08)
     (%i9) jmbraket(jmbra(j1,m1),jmket(j2,m2));
                            kron_delta(j1, j2) kron_delta(m1, m2)
     (%09)
JP (jmket)
                                                                         [Function]
     JP 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).
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.

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:

(%i1) SP(1); [0 sqrt(2) hbar] 0 (%o1) [0 sqrt(2) hbar] [0 0] 0 (%i2) SM(1); 0] 0 0] (%02)[sqrt(2) hbar 0 0] Г sqrt(2) hbar 0] 0

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 Γ 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

an abstract tensor product ket.

Tensor products are represented as lists in Maxima. The ket tensor product |z+,z+> is represented as [tpket,zp,zp], and the bra tensor product <a,b| is represented as [tpbra,a,b] for kets a and b. The list labels tpket and tpbra ensure calculations are performed with the correct kind of objects.

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

tpbra ([b₁, b₂, ...]) [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 repres-

entation will pass this test.

[Function]

tpbrap (tpbra)

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 abstract and concrete tensor products and take the bracket of tensor products.

```
(%i1) K:tpket(a1,b1);
(\%01)
                                 tpket(a1, b1)
(%i2) B:tpbra(a2,b2);
(%o2)
                                 tpbra(a2, b2)
(%i3) tpbraket(B,K);
(%03)
                     kron_delta(a1, a2) kron_delta(b1, b2)
(%i1) kill(a,b,c,d);
(%o1)
                                     done
(%i2) declare([a,b,c,d],complex);
(\%02)
                                     done
(%i3) tpbra([bra([a,b]),bra([c,d])]);
(\%03)
                         [tpbra, [[a b], [c d]]]
(%i4) tpbra([dagger(zp),bra([c,d])]);
(\%04)
                         [tpbra, [[ 1 0 ], [ c d ]]]
(%i1) K:tpket([zp,zm]);
                                     [1] [0]
(%o1)
                            [tpket, [[
                                         ],[]]]
                                     [0][1]
(%i2) zpb:dagger(zp);
                                   [10]
(\%02)
(%i3) zmb:dagger(zm);
(\%03)
                                   [01]
(%i4) B:tpbra([zpb,zmb]);
(\%04)
                         [tpbra, [[ 1 0 ], [ 0 1 ]]]
(%i5) tpbraket(K,B);
(%05)
                                     false
(%i6) tpbraket(B,K);
(\%06)
                                       1
```

Appendix A Function and Variable index

\mathbf{A}	\mathbf{Q}
autobra 4 autoket 4	qm_variance9
В	R
bra 3 braket 5 brap 4	RY
	\mathbf{S}
\mathbf{C}	sigmax
commutator	sigmay
D	SP
	Sx 7 SX 8 Sy 7
TO.	SY 8
\mathbf{E}	Sz 7
expect	SZ 8
J	${f T}$
jmbra 9 jmbraket 10 jmbrap 9 jmcheck 9 jmket 9 jmketp 9	tpbra. 12 tpbraket 13 tpbrap. 13 tpket 12 tpketp. 12
JM	\mathbf{U}
JP	UU
Jz	X
K	xm
ket	xp
ketp	Y
M	ym 6
magsqr	ур 6
	${f Z}$
N	zm6
norm 5	zp 6

Appendix A	A: Function	and	Variable index