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

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

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

$$$$

and

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

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. 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. 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.

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.

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

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 [...] square brackets.

(%o2) [c1 c2]

(%i3) facts();

(%o3) [kind(hbar, real), hbar > 0]

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.

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 [a1,a2,...] and returns a ket 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) autoket([a,b]);
                                              [a]
                                              [ ]
[b]
     (%o1)
     (%i2) facts();
             [kind(hbar, real), hbar > 0, kind(a, complex), kind(b, complex)]
     (%i1) autoket([a*sin(x),b*sin(x)]);
                                          [ a sin(x) ]
     (%o1)
                                          [ 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 [a_1, a_2, \ldots] and returns a bra with the coefficients a_i 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();
             [kind(hbar, real), hbar > 0, kind(a, complex), kind(b, complex)]
     (%i1) autobra([a*sin(x),b]);
     (%o1)
                                         [a sin(x) b]
     (%i2) facts();
     (%o2)
             [kind(hbar, real), hbar > 0, kind(a, complex), kind(b, complex)]
dagger (vector)
     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)
                                            Γ 2
```

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);
     (\%01)
                                             done
     (%i2) braket(mket([a,b,c]),mket([a,b,c]));
                     c conjugate(c) + b conjugate(b) + a conjugate(a)
     (\%02)
     (%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]));
                  sqrt(c conjugate(c) + b conjugate(b) + a conjugate(a))
     (\%02)
magsqr (c)
                                                                        [Function]
     magsqr returns conjugate(c)*c, the magnitude squared of a complex number.
     (%i1) declare([a,b,c,d],complex);
     (%o1)
                                             done
     (%i2) A:braket(mket([a,b]),mket([c,d]));
     (\%02)
                               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.

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

[Function]

Zm
```

Return the $|z-\rangle$ ket in the z-basis.

хр	Return the $ x+\rangle$ ket in the z-basis.		[Function]
хm	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;	r 4 7	
	(%o1)	[1]	
	(%i2) zm;	[0]	
	(%o2)	[0]	
	(%i1) yp;	[1]	
	(%o1)	[] [sqrt(2)] [
	(%i2) ym;	[1] []	
	(%o2)	<pre>[sqrt(2)] [</pre>	
	(%i1) braket(xp,zp);		
	(%o1)	1 sqrt(2)	

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

[Function]

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 Returns the spin-1/2 Sy matrix.

Sz [Function]

Returns the spin-1/2 Sz matrix.

(%i2) Sy;

commutator (X,Y) [Function]

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

(%i1) commutator(Sx,Sy);

2] [%i hbar 2]] Г 2 1 %i hbar 0 2]

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:

(%o1)

(%i1) SY(1/2);

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 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) kill(a,b,c,d);
(\%01)
                                     done
(%i2) declare([a,b,c,d],complex);
(\%02)
                                     done
(%i3) tpbra([mbra([a,b]),mbra([c,d])]);
(%03)
                         [tpbra, [[a b], [c d]]]
(%i4) tpbra([dagger(zp),mbra([c,d])]);
(\%04)
                         [tpbra, [[ 1 0 ], [ c d ]]]
(%i1) K:tpket([zp,zm]);
                                     [1] [0]
(%o1)
                            [tpket, [[ ], [
                                                ]]]
                                     [0][1]
(%i2) zpb:dagger(zp);
(\%02)
                                   [10]
(%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)
```

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}	R
autobra 4 autoket 4	RX
В	
braket	\mathbf{S}
C commutator	sigmax 7 sigmay 7 sigmaz 7 SM 11
D	SP 11 Sx 7
	SX
E	SY 8 Sz 7
	SZ 8
_	Т
J	_
jmbra 9 jmbraket 10 jmbrap 9 jmcheck 9 jmket 9 jmketp 9 JM 10	tpbra 12 tpbraket 13 tpbrap 13 tpket 12 tpketp 12
JP	\mathbf{U}
Jsqr	UU
\mathbf{M}	\mathbf{X}
magsqr 5 mbra 3 mbrap 3 mket 2	xm 6 xp 6
mketp	\mathbf{Y}
${f N}$	ут
norm	${f Z}$
Q	_
qm_variance9	zm 5 zp 5

Appendix A	A: Function	and	Variable index