### 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 kets 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 <psi| will be represented in Maxima by the row vector [a b], where the basis vectors are

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

and

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

In a Maxima session this looks like the following. The basis kets {zp,zm} are transformed into bras using the dagger function.

#### 1.1.1 Types of kets and bras

There are two types of kets and bras available in the qm package, the first type is given by a matrix representation, as returned by the functions mbra and mket. 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, while also 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.

The following examples illustrate some of the basic capabilities of the qm package. Here both abstract, and concrete (matrix representation) kets are shown. The last example shows how to contstruct an entangled Bell pair.

```
(%i1) ket([a,b])+ket([c,d]);
(%o1)
                                |[c, d]\rangle + |[a, b]\rangle
(%i2) mket([a,b]);
                                        [a]
(\%02)
                                        [ b ]
(%i3) mbra([a,b]);
(%o3)
                                      [a b]
(%i4) bell:(1/sqrt(2))*(ket([u,d])-ket([d,u]));
                                 |[u, d]> - |[d, u]>
(\%04)
                                       sqrt(2)
(%i5) dagger(bell);
                                <[u, d]| - <[d, u]|
(%05)
                                       sqrt(2)
```

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

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 (ket) [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 [...] square brackets.

mbrap (bra) [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 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
                                                                              [Function]
      Return the |z+\rangle ket in the z-basis.
                                                                              [Function]
zm
      Return the |z-\rangle ket in the z-basis.
хp
                                                                              [Function]
      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.
ym
                                                                              [Function]
      Return the |y-\rangle ket in the z-basis.
      (%i1) zp;
                                                 [1]
      (%o1)
                                                 [ 0 ]
      (%i2) zm;
                                                 [ 0 ]
      (\%02)
```

[1]

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

#### 1.2.2 Pauli matrices and Sz, Sx, Sy operators

sigmax
Returns the Pauli x matrix.

sigmay
Returns the Pauli y matrix.

sigmaz
Function
Returns the Pauli z matrix.

Sx
Returns the spin-1/2 Sx matrix.

[Function]
Returns the spin-1/2 Sy matrix.

Returns the spin-1/2 Sz matrix. [Function]

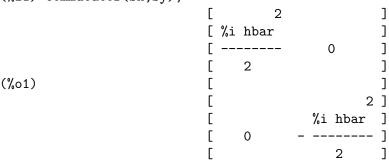
(%i1) sigmay;

(%i2) Sy;

commutator (X,Y) [Function]

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

(%i1) commutator(Sx,Sy);



anticommutator (X,Y)

[Function]

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

### 1.2.3 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) for spin s returns the matrix representation of the spin operator Sy. Shortcuts

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 ] Г ] 2 (%o1) ] [ %i hbar ] ] 0 2 (%i2) SX(1); hbar \_\_\_\_\_ 0 ] sqrt(2) ] hbar hbar (%02)0 sqrt(2) sqrt(2) ] ٦ hbar ] ] sqrt(2)

#### 1.2.4 Expectation value and variance

# 1.2.5 Angular momentum representation of kets and bras

### 1.2.5.1 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  $2=Y$ .

[Function]

 $spin_mbra (s, m_s, [1,2])$ spin\_mbra returns a bra in the z-basis for spin s and z-projection ms, for axis 1=X or 2=Y.  $(\%i1) spin_mket(3/2,1/2,2);$ sqrt(3) 3/2 2 %i 3/2 (%o1) Γ 3/2 2 [ sqrt(3) %i ] ] 3/2 2 ] (%i2) spin\_mbra(1,1,1); [ 1

### 1.2.5.2 Abstract (j,m)-kets and bras

(%o2)

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]).

[ 2 sqrt(2)

- ]

2]

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

```
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)
     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] > sqrt(j (j + 1) - m (m + 1))
      (%02)
      (%i3) JM(k);
                         hbar |[j, m - 1]\rangle sqrt(j (j + 1) - (m - 1) m)
      (%o3)
      (%i4) Jsqr(k);
                                    hbar j (j + 1) |[j, m]>
      (\%04)
      (%i5) Jz(k);
                                          hbar |[j, m] > m
      (\%05)
```

## 1.2.6 Addition of angular momentum in the (j,m)-representation

Addition of angular momentum calculations can be performed in the (j,m)-representation using the function definitions below. The internal representation of kets and bras for this purpose is the following. Given kets  $|j1,m1\rangle$  and  $|j2,m2\rangle$  a tensor product of (j,m)-kets is instantiated as:

```
[tpket,1,|j1,m1>,|j2,m2>]
```

and the corresponding bra is instantiated as:

where the factor of 1 is the multiplicative factor of the tensor product.

Using the function definitions below one must be careful to avoid errors produced by Maxima's automatic list arithmetic. For example, do not use (J1z+J2z), and instead use the defined function Jtz. Similarly for any of the operators that are added together, one should always use the total Jtxx defined function.

tpket (jmket1,jmket2)

[Function]

tpket instantiates a tensor product of two (j,m)-kets.

(%i1) tpket(ket(
$$[3/2,1/2]$$
),ket( $[1/2,1/2]$ ));

tpbra (jmbra1,jmbra2)

[Function]

tpbra instantiates a tensor product of two (j,m)-bras.

tpbraket (tpbra,tpket)

[Function]

tpbraket returns the bracket of a tpbra and a tpket.

J1z (tpket) [Function]

J1z returns the tensor product of a tpket with Jz acting on the first ket.

J2z (tpket) [Function]

J2z returns the tensor product of a tpket with Jz acting on the second ket.

(%i1) 
$$k:tpket(ket([3/2,3/2]),ket([1/2,1/2]));$$

Jtz (tpket) [Function]

Jtz is the total z-projection of spin operator acting on a tpket and returning  $(J_{1z}+J_{2z})$ .

(%i1) 
$$k:tpket(ket([3/2,3/2]),ket([1/2,1/2]));$$

```
J1sqr(tpket)
                                                                                    [Function]
      J1sqr returns Jsqr for the first ket of a tpket.
J2sqr (tpket)
                                                                                    [Function]
      J2sqr returns Jsqr for the second ket of a tpket.
J1p (tpket)
                                                                                    [Function]
      J1p returns J_+ for the first ket of a tpket.
                                                                                    [Function]
J2p (tpket)
      J2p returns J_+ for the second ket of a tpket.
Jtp (tpket)
                                                                                    [Function]
      Jtp returns (J_{1+}+J_{2+}) for the tpket.
                                                                                    [Function]
J1m (tpket)
      J1m returns J<sub>-</sub> for the first ket of a tpket.
                                                                                    [Function]
J2m (tpket)
      J2m returns J_{=} for the second ket of a tpket.
Jtm (tpket)
                                                                                    [Function]
      Jtm returns (J_{1-}+J_{2-}) for the tpket.
J1p2m (tpket)
                                                                                    [Function]
      J1p2m returns (J_{1+}J_{2-}) for the tpket.
J1m2p (tpket)
                                                                                    [Function]
      J1m2p returns (J_{1-}J_{2+}) for the tpket.
J1zJ2z (tpket)
                                                                                    [Function]
      J1zJ2z returns (J_{1z}J_{2z}) for the tpket.
                                                                                    [Function]
Jtsqr (tpket)
      Jtsqr returns (J_1^2+J_2^2+J_{1+}J_{2-}+J_{1-}J_{2+}+J_{1z}J_{2z}) for the tpket.
      (%i1) k:tpket(ket([3/2,1/2]),ket([1/2,1/2]));
                                    [tpket, 1, |[-, -]\rangle, |[-, -]\rangle]
      (%o1)
      (%i2) b:dagger(k);
                                    [tpbra, 1, <[-, -]|, <[-, -]|]
      (%o2)
      (%i3) J1p2m(k);
                                                         3 3
                           [tpket, sqrt(3) hbar , |[-, -]>, |[-, - -]>]
      (\%03)
      (%i4) J1m2p(k);
      (\%04)
                                                       0
```

$$(\%i1)$$
 k:tpket(ket([3/2,-1/2]),ket([1/2,1/2]));

(%i2) J1zJ2z(k);

(%i3) Jtsqr(k);

#### 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]

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

### 1.4 Time-evolution operator

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+> can 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.

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.

In the next example we construct the state function for an entangled Bell pair, construct the density matrix, and then trace over the first particle to obtain the density submatrix for particle 2.

# Appendix A Function and Variable index

$\mathbf{A}$	${f M}$
anticommutator       8         autobra       5         autoket       4	magsqr       6         mbra       4         mbrap       4         mket       3
В	mketp
bra       3         braket       5         brap       3	<b>N</b> norm
$\mathbf{C}$	Q
commutator	qm_variance9
D	R
dagger	RX
$\mathbf{E}$	RZ
expect	$\mathbf S$
J     J1m     13       J1m2p     13       J1p     13       J1p2m     13       J1sqr     13       J1z     12       J1zJ2z     13       J2m     13       J2p     13       J2sqr     13       J2z     12       jmbrap     11       jmcheck     11       jmketp     10       JM     11       JP     11       Jsqr     11       Jtm     13       Jtp     13       Jtp     13       Jtp     13       Jtp     13       Jtsqr     13       Jtsqr     13       Jtz     12       Jz     11	sigmax       7         sigmay       7         sigmaz       7         SM       14         spin_mbra       10         spin_mket       9         SP       14         Sx       7         SX       8         Sy       7         SY       8         Sz       8         SZ       8         T       tpbra       12         tpbraket       12         tpket       12         U       15          15
K	X
ket	xm

Y	${f Z}$
ут	
hbar 3	