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*> 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

`<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. `mket`s are column vectors and `mbra`s 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 lists for the elements. These general kets are displayed in Dirac notation. Note that abstract kets and bras are *assumed to be orthonormal*. These general bras and kets may be used as tensor product states. Tensor product states in the matrix representation are also available.

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

```
(%i1) ket([a,b])+ket([c,d]);
(%o1)                           |[c, d]> + |[a, b]>
(%i2) mket([a,b])+mket([c,d]);
                                      [ c + a ]
(%o2)                                 [       ]
                                      [ d + b ]
```

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

```
(%i1) braket(bra([a1,b1]),ket([a2,b2]));
(%o1)                kron_delta(a1, a2) kron_delta(b1, b2)
```

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

```
(%i1) tpket([zp,zm]);
                                  [ 1 ]  [ 0 ]
(%o1)                    [tpket, [[     ], [     ]]]
                                  [ 0 ]  [ 1 ]
```

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.

```
(%i1) declare([a,b],complex);
(%o1)                                done
(%i2) psi:a*ket([1])+b*ket([2]);
(%o2)                          |[2]> b + |[1]> a
(%i3) psidag:dagger(psi);
(%o3)                 <[2]| conjugate(b) + <[1]| conjugate(a)
(%i4) psidag . psi;
(%o4)                    b conjugate(b) + a conjugate(a)
```

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);
(%o3)                  [ conjugate(c1)  conjugate(c2)  r ]
(%i4) b . k;
                             2
(%o4)                       r  + c2 conjugate(c2) + c1 conjugate(c1)
```

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,...]) [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.

```
(%i1) declare([c1,c2],complex);
(%o1)                          done
(%i2) mket([c1,c2]);
                              [ c1 ]
(%o2)                         [    ]
                              [ c2 ]
(%i3) facts();
(%o3) [kind(hbar, real), hbar > 0, kind(c1, complex), kind(c2, complex)]
```

`mbra` ([c_1,c_2,...]) [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.

```
(%i1) kill(c1,c2);
(%o1)                          done
(%i2) mbra([c1,c2]);
(%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.

```
(%i1) k:ket([a,b]);
(%o1)                         |[a, b]>
(%i2) mketp(k);
(%o2)                          false
(%i3) k:mket([a,b]);
                               [ a ]
(%o3)                          [   ]
                               [ b ]
(%i4) mketp(k);
(%o4)                          true
```

`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.

```
(%i1) b:mbra([a,b]);
(%o1)                         [ a  b ]
(%i2) mbrap(b);
(%o2)                          true
```

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 `declare`-d complex and not `x`.

`autoket` ([a_1,a_2,...]) [Function]

`autoket` takes a list [a_1,a_2,...] and returns a ket 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) autoket([a,b]);
                                   [ a ]
(%o1)                              [   ]
                                   [ b ]
(%i2) facts();
(%o2)  [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();
(%o2)  [kind(hbar, real), hbar > 0, kind(a, complex), kind(b, complex)]
```

`autobra` ([a_1,a_2,...]) [Function]

`autobra` takes a list [a_1,a_2,...] 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();
(%o2)  [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*) [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)                            [      ]
                                 [   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);
(%o1)                               done
(%i2) braket(mket([a,b,c]),mket([a,b,c]));
(%o2)         c conjugate(c) + b conjugate(b) + a conjugate(a)
(%i3) braket(ket([a1,b1,c1]),ket([a2,b2,c2]));
(%o3)     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]));
(%o2)      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)                               done
(%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.

```
(%i1) ket([a])+ket([b]);
(%o1)                           |[b]> + |[a]>
(%i2) braket(bra([a]),ket([b]));
(%o2)                         kron_delta(a, b)
(%i3) braket(bra([a])+bra([c]),ket([b]));
(%o3)                 kron_delta(b, c) + kron_delta(a, b)
```

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` [Function]

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

`zm` [Function]

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

`xp` [Function]

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

xm [Function]

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

yp [Function]

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

ym [Function]

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

```
(%i1) zp;
                                        [ 1 ]
(%o1)                                   [   ]
                                        [ 0 ]
(%i2) zm;
                                        [ 0 ]
(%o2)                                   [   ]
                                        [ 1 ]
(%i1) yp;
                                     [    1    ]
                                     [ ------- ]
                                     [ sqrt(2) ]
(%o1)                                [         ]
                                     [   %i    ]
                                     [ ------- ]
                                     [ sqrt(2) ]
(%i2) ym;
                                    [     1     ]
                                    [  -------  ]
                                    [  sqrt(2)  ]
(%o2)                               [           ]
                                    [     %i    ]
                                    [ - ------- ]
                                    [   sqrt(2) ]
(%i1) braket(xp,zp);
                                        1
(%o1)                                -------
                                     sqrt(2)
```

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

```
(%i1) declare([a,b],complex);
(%o1)                                  done
(%i2) psi:mket([a,b]);
                                       [ a ]
(%o2)                                  [   ]
                                       [ b ]
(%i3) psi_x:'xp*braket(xp,psi)+'xm*braket(xm,psi);
                     b         a                 a         b
(%o3)           (------- + -------) xp + (------- - -------) xm
                 sqrt(2)   sqrt(2)        sqrt(2)   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;
                                  [ 0    - %i ]
(%o1)                             [           ]
                                  [ %i    0   ]
(%i2) Sy;
                             [            %i hbar ]
                             [    0     - ------- ]
                             [               2    ]
(%o2)                        [                    ]
                             [ %i hbar            ]
                             [ -------      0     ]
                             [    2               ]
```

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       - -------- ]
                                    [                 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:

```
(%i1) SY(1/2);
                                     [            %i hbar ]
                                     [    0     - ------- ]
                                     [               2    ]
(%o1)                                [                    ]
                                     [ %i hbar            ]
                                     [ -------      0     ]
                                     [    2               ]
(%i2) SX(1);
                                  [           hbar             ]
                                  [    0     -------      0    ]
                                  [          sqrt(2)           ]
                                  [                            ]
                                  [  hbar               hbar   ]
(%o2)                             [ -------     0      ------- ]
                                  [ sqrt(2)            sqrt(2) ]
                                  [                            ]
                                  [           hbar             ]
                                  [    0     -------      0    ]
                                  [          sqrt(2)           ]
```

1.2.5 Expectation value and variance

expect (O,psi) [Function]

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

```
(%i1) ev(expect(Sy,xp+ym),ratsimp);
(%o1)                              - hbar
```

qm_variance (O,psi) [Function]

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

```
(%i1) ev(qm_variance(Sy,xp+ym),ratsimp);
                                   %i hbar
(%o1)                              -------
                                      2
```

1.2.6 Angular momentum representation of kets and bras

To create kets and bras in the |*j*,*m*> representation you can use the following functions.

jmket (j,m) [Function]

jmket creates the ket |*j*,*m*> for total spin *j* and *z*-component *m*.

jmbra (j,m) [Function]

jmbra creates the bra <*j*,*m*| for total spin *j* and *z*-component *m*.

```
(%i1) jmbra(3/2,1/2);
                                       3  1
(%o1)                            jmbra(-, -)
                                       2  2
(%i2) jmbra([3/2,1/2]);
                                      [ 3  1 ]
(%o2)                         [jmbra, [ -  - ]]
                                      [ 2  2 ]
```

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, . . . , +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);
(%o2)                          jmbra(j2, m2)
(%i3) jmbraket(B,K);
(%o3)              kron_delta(j1, j2) kron_delta(m1, m2)
(%i4) B:jmbra(j1,m1);
(%o4)                          jmbra(j1, m1)
(%i5) jmbraket(B,K);
(%o5)                                1
(%i6) K:jmket([3/2,1/2]);
                                     [ 3  1 ]
(%o6)                        [jmket, [ -  - ]]
                                     [ 2  2 ]
(%i7) B:jmbra([3/2,1/2]);
                                     [ 3  1 ]
(%o7)                        [jmbra, [ -  - ]]
                                     [ 2  2 ]
(%i8) jmbraket(B,K);
(%o8)                                1
(%i9) jmbraket(jmbra(j1,m1),jmket(j2,m2));
(%o9)              kron_delta(j1, j2) kron_delta(m1, m2)
```

`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_z operator. It takes a `jmket` `jmket(j,m)` and returns `m*hbar*jmket(j,m)`.

These functions are illustrated below.

```
(%i1) k:jmket([j,m]);
(%o1)                          [jmket, [ j  m ]]
(%i2) JP(k);
(%o2)          hbar jmket(j, m + 1) sqrt(j (j + 1) - m (m + 1))
(%i3) JM(k);
(%o3)          hbar jmket(j, m - 1) sqrt(j (j + 1) - (m - 1) m)
(%i4) Jsqr(k);
                                2
(%o4)                      hbar  j (j + 1) jmket(j, m)
(%i5) Jz(k);
(%o5)                           hbar jmket(j, m) m
```

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       0        sqrt(2) hbar ]
                         [                               ]
                         [ 0       0             0       ]
(%i2) SM(1);
                         [      0             0        0 ]
                         [                               ]
(%o2)                    [ sqrt(2) hbar       0        0 ]
                         [                               ]
                         [      0       sqrt(2) hbar   0 ]
```

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,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          0    ]
(%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)`.

```
(%i1) UU(w*Sy,t);
Proviso: assuming 64*t*w # 0
                              [     t w         t w  ]
                              [ cos(---)  - sin(---) ]
                              [      2           2   ]
(%o1)                         [                      ]
                              [     t w        t w   ]
                              [ sin(---)   cos(---)  ]
                              [      2          2    ]
```

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`.

`tpket` ([k_1, k_2, ...]) [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, ...]) [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 abstract and concrete tensor products and take the bracket of tensor products.

```
(%i1) kill(a,b,c,d);
(%o1)                               done
(%i2) declare([a,b,c,d],complex);
(%o2)                               done
(%i3) tpbra([mbra([a,b]),mbra([c,d])]);
(%o3)                    [tpbra, [[ a  b ], [ c  d ]]]
(%i4) tpbra([dagger(zp),mbra([c,d])]);
(%o4)                    [tpbra, [[ 1  0 ], [ c  d ]]]
(%i1) K:tpket([zp,zm]);
                                    [ 1 ]  [ 0 ]
(%o1)                      [tpket, [[   ], [   ]]]
                                    [ 0 ]  [ 1 ]
(%i2) zpb:dagger(zp);
(%o2)                             [ 1  0 ]
(%i3) zmb:dagger(zm);
(%o3)                             [ 0  1 ]
(%i4) B:tpbra([zpb,zmb]);
(%o4)                    [tpbra, [[ 1  0 ], [ 0  1 ]]]
(%i5) tpbraket(K,B);
(%o5)                               false
(%i6) tpbraket(B,K);
(%o6)                                 1
```

Examples below show how to create abstract and concrete tensor products and take the bracket of tensor products.

```
(%i1) K:ket([a1,b1]);
(%o1)                             |[a1, b1]>
(%i2) B:bra([a2,b2]);
(%o2)                             <[a2, b2]|
(%i3) braket(B,K);
(%o3)                 kron_delta(a1, a2) kron_delta(b1, b2)
(%i1) bra([a1,Id,c1]) . ket([a2,b2,c2]);
(%o1)         |[-, b2, -]> kron_delta(a1, a2) kron_delta(c1, c2)
(%i2) bra([a1,b1,c1]) . ket([Id,b2,c2]);
(%o2)         <[a1, -, -]| kron_delta(b1, b2) kron_delta(c1, c2)
```

Appendix A Function and Variable index