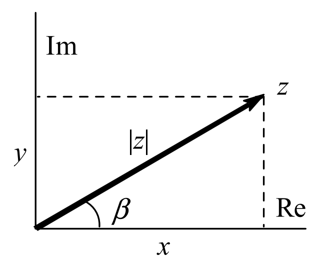
APPENDIX A: MATH REMINDER

Complex numbers

A complex number

$$z = x + iy \tag{A1}$$

can be graphically represented as in Figure A.1, where



Im is the imaginary axis
Re is the real axis
x is the real part of z
y is the coefficient of the imaginary part of z
$|z|$ is the modulus (absolute value) of z
β is the argument of z

Figure A.1. Graphic representation of a complex number $z = x+iy$. $i = \sqrt{-1}$ is the imaginary unit.

The number z is fully determined when either x and y or $|z|$ and β are known. The relations between these two pairs of variables are (see lower triangle):

$$x = |z| \cos \beta \tag{A2}$$

$$y = |z| \sin \beta \tag{A3}$$

Thus, according to (A1),

$$z = |z| \cos \beta + i |z| \sin \beta = |z| (\cos \beta + i \sin \beta) \tag{A4}$$

Using Euler's formula [see (A11)-(A16)], one obtains:

$$z = |z| \exp(i\beta) \tag{A5}$$

The complex number $z^* = x - iy = |z| \exp(-i\beta)$ is called the *complex* conjugate of z.

Elementary rotation operator

Consider a complex number r which has a modulus $|r| = 1$ and the argument α:

$$r = \exp(i\alpha) = \cos\alpha + i\sin\alpha \tag{A6}$$

Multiplying a complex number such as

$$z = |z|\exp(i\beta)$$

by r leaves the modulus of z unchanged and increases the argument by α:

$$zr = |z|e^{i\beta}e^{ia} = |z|e^{i(\beta+\alpha)} \tag{A7}$$

Equation (A7) describes the rotation of the vector Oz by an angle α (see Figure A.2). We can call r, the *elementary rotation operator*.

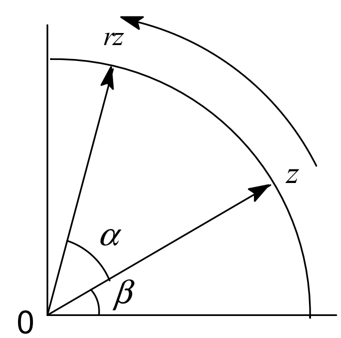


Figure A.2. Effect of the rotation operator $r = \exp(i\alpha)$ on the complex number $z = |z|\exp(i\beta)$.

Note: Although more complicated, the rotation operators in the density matrix treatment of multipulse NMR are of the same form as our elementary operator [cf.(B45)].

Example 1. A -90° (clockwise) rotation (see Figure A.3)

Let $\beta = 90^{\circ}$; $\alpha = -90^{\circ}$

Then, from (A4 and A6),

$$z = |z|(\cos 90^{\circ} + i \sin 90^{\circ}) = i|z| \tag{A8}$$

$$r = \cos(-90^{\circ}) + i \sin(-90^{\circ}) = -i \tag{A9}$$

The product

$$zr = i|z|(-i) = |z| \tag{A10}$$

is a real number (its argument is zero).

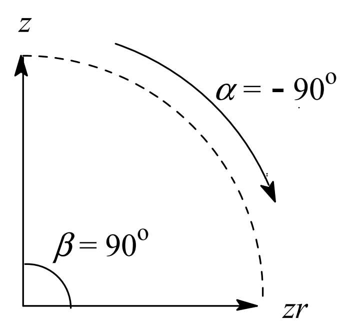


Figure A.3. Effect of the rotation operator . $-i \left(\alpha = -90^{\circ}\right)$

Equation (A10) tells us that the particular operator $-i$ effects a 90° CW (clockwise) rotation on the vector z. The operator $+i$ would rotate z by 90° CCW. Two consecutive multplications by i result in a 180° rotation. In other words, an i^2 operator (-1) orients the vector in opposite direction.

Example 2. Powers of i (the "star of i")

Since i represents a 90° CCW rotation, successive powers of i are obtained by successive 90° CCW rotations (see Figure A.4).

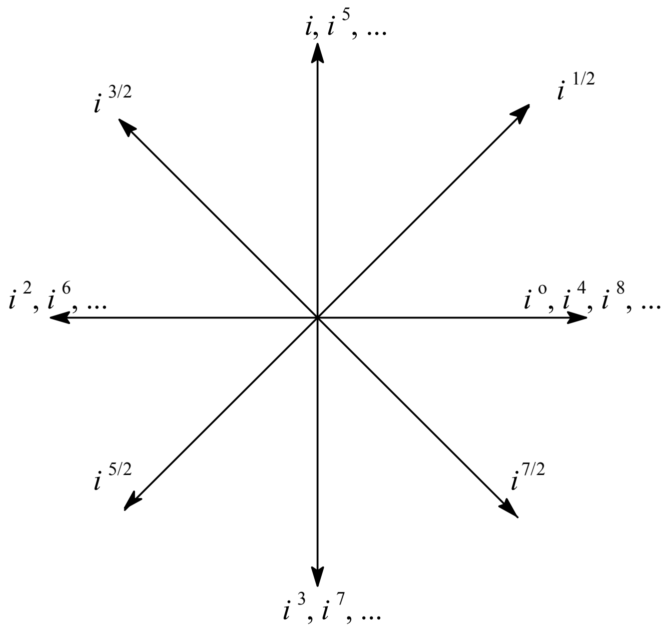


Figure A.4. The star of *i*.

Series expansion of e^x, $\sin x$, $\cos x$, and e^{ix}

The exponential function describes most everything happening in nature (including the evolution of your investment accounts). The e^x series is

$$e^x = 1 + x + x^2/2! + x^3/3! + \ldots \quad \text{(A11)}$$

The sine and cosine series are:

$$\sin x = x - x^3/3! + x^5/5! - x^7/7! + \ldots \quad \text{(A12)}$$

$$\cos x = 1 - x^2/2! + x^4/4! - x^6/6! + \ldots \quad \text{(A13)}$$

The e^{ix} series is:

$$e^{ix} = 1 + ix - x^2/2! - ix^3/3! + x^4/4! + ix^5/5! \ldots \quad \text{(A14)}$$

Separation of the real and imaginary terms gives

$$e^{ix} = 1 - x^2/2! + x^4/4! - x^6/6! + \ldots \qquad \text{(A15)}$$
$$+ i(x - x^3/3! + x^5/5! - \ldots)$$

Recognizing the sine and cosine series one obtains the Euler formula

$$e^{ix} = \cos x + i \sin x \qquad \text{(A16)}$$

Matrix algebra

Matrices are arrays of elements disposed in rows and columns; they obey specific algebraic rules for addition, multiplication and inversion. The following formats of matrices are used in quantum mechanics:

$$A = \begin{bmatrix} a_{11} & a_{12} & . & . & a_{1n} \\ a_{21} & a_{22} & . & . & a_{2n} \\ . & . & . & . & . \\ . & . & . & . & . \\ a_{n1} & a_{n2} & . & . & a_{nn} \end{bmatrix}$$

Square matrix

$$A = \begin{bmatrix} a_{11} & a_{12} & . & . & a_{1n} \end{bmatrix} \quad ; \quad A = \begin{bmatrix} a_{11} \\ a_{21} \\ . \\ . \\ a_{n1} \end{bmatrix}$$

Row matrix *Column matrix*

Row and column matrices are also called row vectors or column vectors. Note that the first subscript of each element indicates the row number and the second, the column number.

Matrix addition

Two matrices are added element by element as follows:

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} + \begin{bmatrix} b_{11} & b_{12} & b_{13} \\ b_{21} & b_{22} & b_{23} \\ b_{31} & b_{32} & b_{33} \end{bmatrix} = \begin{bmatrix} a_{11}+b_{11} & a_{12}+b_{12} & a_{13}+b_{13} \\ a_{21}+b_{21} & a_{22}+b_{22} & a_{23}+b_{23} \\ a_{31}+b_{31} & a_{32}+b_{32} & a_{33}+b_{33} \end{bmatrix}$$

Only matrices with the same number of rows and columns can be added.

Matrix multiplication

In the following are shown three typical matrix multiplications.

a) Square matrix times column matrix:

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} \times \begin{bmatrix} b_{11} \\ b_{21} \\ b_{31} \end{bmatrix} = \begin{bmatrix} c_{11} \\ c_{21} \\ c_{31} \end{bmatrix}$$

$$\begin{aligned} c_{11} &= a_{11}b_{11} + a_{12}b_{21} + a_{13}b_{31} \\ c_{21} &= a_{21}b_{11} + a_{22}b_{21} + a_{23}b_{31} \quad \text{i.e.,} \quad c_{j1} = \sum_{k=1}^{3} a_{jk}b_{k1} \qquad (j = 1,2,3) \\ c_{31} &= a_{31}b_{11} + a_{32}b_{21} + a_{33}b_{31} \end{aligned}$$

Example:

$$\begin{bmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \\ 7 & 8 & 9 \end{bmatrix} \times \begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix} = \begin{bmatrix} 14 \\ 32 \\ 50 \end{bmatrix}$$

Each element of the first line of the square matrix has been multiplied with the corresponding element of the column matrix to yield the first element of the product:

$$1 \times 1 + 2 \times 2 + 3 \times 3 = 14$$

b) Row matrix times square matrix:

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} \end{bmatrix} \times \begin{bmatrix} b_{11} & b_{12} & b_{13} \\ b_{21} & b_{22} & b_{23} \\ b_{31} & b_{32} & b_{33} \end{bmatrix} = \begin{bmatrix} c_{11} & c_{12} & c_{13} \end{bmatrix}$$

$$\begin{aligned} c_{11} &= a_{11}b_{11} + a_{12}b_{21} + a_{13}b_{31} \\ c_{12} &= a_{11}b_{12} + a_{12}b_{22} + a_{13}b_{32} \quad \text{i.e.,} \quad c_{1j} = \sum_{k=1}^{3} a_{1k}b_{kj} \qquad (j = 1, 2, 3) \\ c_{13} &= a_{11}b_{13} + a_{12}b_{23} + a_{13}b_{33} \end{aligned}$$

c) Square matrix times square matrix:

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} \times \begin{bmatrix} b_{11} & b_{12} & b_{13} \\ b_{21} & b_{22} & b_{23} \\ b_{31} & b_{32} & b_{33} \end{bmatrix} = \begin{bmatrix} c_{11} & c_{12} & c_{13} \\ c_{21} & c_{22} & c_{23} \\ c_{31} & c_{32} & c_{33} \end{bmatrix}$$

$$c_{jm} = \sum_{k=1}^{3} a_{jk}b_{km}$$

For instance, row 2 of the left hand matrix and column 3 of the right hand matrix are involved in the obtaining of the element c_{23} of the product. Example:

$$\frac{1}{\sqrt{2}}\begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix} \times \frac{1}{\sqrt{2}}\begin{bmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{bmatrix} =$$

$$\frac{1}{2}\begin{bmatrix} i & 0 & -i \\ 0 & 0 & 0 \\ i & 0 & -i \end{bmatrix} = \begin{bmatrix} i/2 & 0 & -i/2 \\ 0 & 0 & 0 \\ i/2 & 0 & -i/2 \end{bmatrix}$$

The product inherits the number of rows from the first (left) matrix and the number of columns from the second (right) matrix. The number of columns of the left matrix must match the number of rows of the right matrix.

In general the matrix multiplication is not commutative:

$$AB \neq BA \tag{A17}$$

It is associative:

$$A(BC) = (AB)C = ABC \tag{A18}$$

and distributive:

$$A(B + C) = AB + AC \tag{A19}$$

The *unit matrix* is shown below

$$[\mathbf{1}] = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \tag{A20}$$

It must be square and it can be any size. Any matrix remains unchanged when multiplied with the unit matrix:

$$[\mathbf{1}] \times A = A \times [\mathbf{1}] = A \tag{A21}$$

Matrix inversion

The inverse A^{-1} of a square matrix A is defined by the relation:

$$A \times A^{-1} = A^{-1} \times A = [\mathbf{1}] \tag{A22}$$

To find A^{-1}:

1) Replace each element of A by its signed minor determinant. The minor determinant of the matrix element a_{jk} is built with the elements of the original matrix after striking out row j and column k. To have the *signed* minor determinant, one has to multiply it by – 1 whenever the sum $j+k$ is odd.

2) Interchange the rows and the columns (this operation is called matrix transposition)

3) Divide all elements of the transposed matrix by the determinant of the original matrix A.

Example:
Find the inverse of matrix A.

$$A = \frac{1}{2}\begin{bmatrix} 1 & \sqrt{2} & 1 \\ -\sqrt{2} & 0 & \sqrt{2} \\ 1 & -\sqrt{2} & 1 \end{bmatrix} = \begin{bmatrix} 1/2 & \sqrt{2}/2 & 1/2 \\ -\sqrt{2}/2 & 0 & \sqrt{2}/2 \\ 1/2 & -\sqrt{2}/2 & 1/2 \end{bmatrix}$$

1) We replace a_{11} by

$$\begin{vmatrix} a_{22} & a_{23} \\ a_{32} & a_{33} \end{vmatrix} = \begin{vmatrix} 0 & \sqrt{2}/2 \\ -\sqrt{2}/2 & 1/2 \end{vmatrix} = 0 \times (1/2) + (\sqrt{2}/2) \times (\sqrt{2}/2) = 1/2$$

This is the minor determinant obtained by striking out row 1 and column 1 of the original matrix.

We replace a_{12} by

$$-\begin{vmatrix} a_{21} & a_{23} \\ a_{31} & a_{33} \end{vmatrix} = -\begin{vmatrix} -\sqrt{2}/2 & \sqrt{2}/2 \\ 1/2 & 1/2 \end{vmatrix}$$

$$= -[(-\sqrt{2}/2) \times (1/2) - (\sqrt{2}/2) \times (1/2)] = \sqrt{2}/2$$

and so on, obtaining:

$$\begin{bmatrix} 1/2 & \sqrt{2}/2 & 1/2 \\ -\sqrt{2}/2 & 0 & \sqrt{2}/2 \\ 1/2 & -\sqrt{2}/2 & 1/2 \end{bmatrix}$$

2) The transposition yields:

$$\begin{bmatrix} 1/2 & -\sqrt{2}/2 & 1/2 \\ \sqrt{2}/2 & 0 & -\sqrt{2}/2 \\ 1/2 & \sqrt{2}/2 & 1/2 \end{bmatrix}$$

3) Calculate the determinant of A:

$$\det(A) = 0 + (1/4) + (1/4) - 0 + (1/4) + (1/4) = 1$$

Divided by 1, the transposed matrix remains unchanged:

$$A^{-1} = \begin{bmatrix} 1/2 & -\sqrt{2}/2 & 1/2 \\ \sqrt{2}/2 & 0 & -\sqrt{2}/2 \\ 1/2 & \sqrt{2}/2 & 1/2 \end{bmatrix} = \frac{1}{2}\begin{bmatrix} 1 & -\sqrt{2} & 1 \\ \sqrt{2} & 0 & -\sqrt{2} \\ 1 & \sqrt{2} & 1 \end{bmatrix}$$

Check: $$A^{-1} \times A = [\mathbf{1}]$$

$$\frac{1}{2}\begin{bmatrix} 1 & -\sqrt{2} & 1 \\ \sqrt{2} & 0 & -\sqrt{2} \\ 1 & \sqrt{2} & 1 \end{bmatrix} \times \frac{1}{2}\begin{bmatrix} 1 & \sqrt{2} & 1 \\ -\sqrt{2} & 0 & \sqrt{2} \\ 1 & -\sqrt{2} & 1 \end{bmatrix}$$

$$= \frac{1}{4}\begin{bmatrix} 4 & 0 & 0 \\ 0 & 4 & 0 \\ 0 & 0 & 4 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} = [\mathbf{1}]$$

Note: You will be pleased to learn that:

a) There is a shortcut for the inversion of rotation operator matrices because they are of a special kind.

b) In our calculations we will need only inversions of rotation operators:

$$(R \to R^{-1})$$

Here is the shortcut:

1) Transpose *R* (vide supra)

2) Replace each element with its complex conjugate.

Example

$$R = \frac{1}{2}\begin{bmatrix} 1 & \sqrt{2} & 1 \\ -\sqrt{2} & 0 & \sqrt{2} \\ 1 & -\sqrt{2} & 1 \end{bmatrix}$$

1) Transpose:

$$\frac{1}{2}\begin{bmatrix} 1 & -\sqrt{2} & 1 \\ \sqrt{2} & 0 & -\sqrt{2} \\ 1 & \sqrt{2} & 1 \end{bmatrix}$$

2) Conjugate: Because they are all real, the matrix elements remain the same:

$$R^{-1} = \frac{1}{2}\begin{bmatrix} 1 & -\sqrt{2} & 1 \\ \sqrt{2} & 0 & -\sqrt{2} \\ 1 & \sqrt{2} & 1 \end{bmatrix}$$

Note: This is the same matrix as in the previous example; its being a rotation operator matrix, allowed us to use the shortcut procedure.

Another example:

$$R = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 0 & i & 0 \\ 0 & 1 & 0 & i \\ i & 0 & 1 & 0 \\ 0 & i & 0 & 1 \end{bmatrix}$$

(1) Transpose: you obtain the same matrix

(2) Conjugate:

$$R^{-1} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 0 & -i & 0 \\ 0 & 1 & 0 & -i \\ -i & 0 & 1 & 0 \\ 0 & -i & 0 & 1 \end{bmatrix}$$

Note: The matrix resulting from the transposition followed by complex conjugation of a given matrix A is called the <u>*adjoint*</u> <u>*matrix*</u> *A^{adj}. For all rotation operators,*

$$R^{-1} = R^{adj} \tag{A23}$$

In other words, our short cut for inversion is equivalent with finding the <u>*adjoint*</u> *of R* [see (A23)].

When $$A = A^{adj}$$

we say that the matrix A is *self adjoint* or *Hermitian*. In a Hermitian matrix, every element below the main diagonal is the complex conjugate of its symmetrical element above the diagonal

$$d_{nm} = d_{mn}^{*} \tag{A24}$$

while the diagonal elements are all real. The angular momentum, the Hamiltonian and density matrix are all Hermitian (the rotation operators never are).

The matrix algebra operations encountered in Part 1 of this book are mostly multiplications of square matrices (density matrix and product operators). Inversion is only used to find reciprocals of rotation operators, by transposition and conjugation. Frequently used is the multiplication or division of a matrix by a constant, performed by multiplying or dividing every element of the matrix. The derivative of a matrix (e.g., with respect to time) is obtained by taking the derivative of each matrix element .

Trigonometric relations

<u>Sum of squared sine and cosine</u>

$$\sin^2\alpha + \cos^2\alpha = 1 \qquad \text{(A25)}$$

Negative angles

$$\begin{aligned} \sin(-\alpha) &= -\sin\alpha \\ \cos(-\alpha) &= \ \ \cos\alpha \end{aligned} \qquad \text{(A26)}$$

Expressing sine and cosine in terms of exponentials

$$\cos\alpha = \frac{e^{i\alpha} + e^{-i\alpha}}{2} \qquad \text{(A27)}$$

$$\sin\alpha = \frac{e^{i\alpha} - e^{-i\alpha}}{2i} \qquad \text{(A28)}$$

Demo: Use Euler's formula (A16) $e^{\pm i\alpha} = \cos\alpha \pm i\sin\alpha$

Sum and difference of two angles

$$\sin(\alpha \pm \beta) = \sin\alpha\cos\beta \pm \cos\alpha\sin\beta \qquad \text{(A29)}$$
$$\cos(\alpha \pm \beta) = \cos\alpha\cos\beta \mp \sin\alpha\sin\beta \qquad \text{(A30)}$$

Demo:

$$z_1 = e^{i\alpha} = \cos\alpha + i\sin\alpha$$
$$z_2 = e^{\pm i\beta} = \cos\beta \pm i\sin\beta$$
$$z_1 z_1 = e^{i(\alpha \pm i\beta)} = (\cos\alpha + i\sin\alpha)(\cos\beta \pm i\sin\beta)$$
$$= (\cos\alpha\cos\beta \mp \sin\alpha\sin\beta) + i(\sin\alpha\cos\beta \pm \cos\alpha\sin\beta)$$
$$= \cos(\alpha \pm \beta) + i\sin(\alpha \pm \beta)$$

Angle 2α

$$\sin 2\alpha = 2\sin\alpha\cos\alpha \qquad \text{(A31)}$$

$$\cos 2\alpha = \cos^2\alpha - \sin^2\alpha = 2\cos^2\alpha - 1 \tag{A32}$$

Demo: Make $\beta = \alpha$ in (A29),(A30). Use (A25) for the last form.

Angle 3α

$$\sin 3\alpha = 3\sin\alpha - 4\sin^3\alpha \tag{A33}$$
$$\cos 3\alpha = 4\cos^3\alpha - 3\cos\alpha \tag{A34}$$

Demo: Make $\beta = 2\alpha$ in (A29),(A30), then use (A31),(A32) and eventually (A25).

Relations used for AX_2 systems

$$\cos^2\alpha = \frac{1+\cos 2\alpha}{2} = \frac{e^{2i\alpha} + 2 + e^{-2i\alpha}}{4} \tag{A35}$$
$$\cos\alpha \sin\alpha = \frac{\sin 2\alpha}{2} = \frac{e^{2i\alpha} - e^{-2i\alpha}}{4i} \tag{A36}$$

Demo: (A35) is a corollary of (A32) and (A36) is a corollary of (A31). Use (A27), (A28) to obtain the exponential form. Note the 1-2-1 triplet structure in (A 35).

Relations used for AX_3 systems

$$\cos^3\alpha = \frac{\cos 3\alpha + 3\cos\alpha}{4} = \frac{e^{3i\alpha} + 3e^{i\alpha} + 3e^{-i\alpha} + e^{-3i\alpha}}{8} \tag{A37}$$
$$\cos^2\alpha \sin\alpha = \frac{\sin 3\alpha + 3\sin\alpha}{4} = \frac{e^{3i\alpha} + e^{i\alpha} - e^{-i\alpha} - e^{-3i\alpha}}{8i} \tag{A38}$$

Demo: (A37) is a corollary of (A34). Relation (A38) can be obtained by rewriting (A33) as
$\sin 3\alpha = 3\sin\alpha - 4\sin\alpha(1-\cos^2\alpha) = 4\sin\alpha\cos^2\alpha - \sin\alpha$
Note the 1-3-3-1 quartet structure in (A37).

Relations used for AX systems

$$\cos\alpha\cos\beta = \frac{\cos(\alpha-\beta) + \cos(\alpha+\beta)}{2} \tag{A39}$$

$$\sin\alpha\sin\beta = \frac{\cos(\alpha-\beta)-\cos(\alpha+\beta)}{2} \tag{A40}$$

$$\sin\alpha\sin\beta = \frac{\cos(\alpha-\beta)-\cos(\alpha+\beta)}{2} \tag{A41}$$

$$\sin\alpha\cos\beta = \frac{\sin(\alpha-\beta)+\sin(\alpha+\beta)}{2} \tag{A42}$$

Demo: Introduce (A29) or (A30) in the second member of the equalities above.