Appendix 1: NMR Quantum Computation

$$i\frac{d\psi}{\mathrm{dt}} = \hat{H}\psi \qquad \psi = c_1[00> + c_2[01> + c_3[10> + c_4[11>$$

where the Hamiltonian operator is given by:

$$\hat{H} = g(\hat{\sigma}_1 \cdot \hat{\sigma}_2 - 3(\hat{n}\cdot\hat{\sigma}_1)(\hat{n}\cdot\hat{\sigma}_2)) - \mu_B((B_{z1}+B_{g1})\hat{\sigma}_{z1}\otimes\mathbf{1}_2 + \mathbf{1}_1\otimes(B_{z2}+B_{g2})\hat{\sigma}_{z2})$$

and the normal unit vector $\hat{n}$ is in the x- or y- direction.

Now: $\hat{\sigma}_{y1}\otimes\hat{\sigma}_{y2} = \begin{pmatrix} 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix}$ $\quad \hat{\sigma}_{x1}\otimes\hat{\sigma}_{x2} = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}$ and $\hat{\sigma}_{z1}\otimes\hat{\sigma}_{z2} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$

Defining $\hat{D}(\hat{n}) = g(\hat{\sigma}_1 \cdot \hat{\sigma}_2 - 3(\hat{n}\cdot\hat{\sigma}_1)(\hat{n}\cdot\hat{\sigma}_2))$ it is straightforward to show that:

$$\hat{D}(\hat{e}_x) = g\begin{pmatrix} 1 & 0 & 0 & -3 \\ 0 & -1 & -1 & 0 \\ 0 & -1 & -1 & 0 \\ -3 & 0 & 0 & 1 \end{pmatrix}$$

and

$$\hat{D}(\hat{e}_y) = g\begin{pmatrix} 1 & 0 & 0 & 3 \\ 0 & -1 & -1 & 0 \\ 0 & -1 & -1 & 0 \\ 3 & 0 & 0 & 1 \end{pmatrix}$$

Also, given that $\hat{U} = -\mu_B((B_{z1}+B_{g1})\hat{\sigma}_{z1}\otimes\mathbf{1}_2 + \mathbf{1}_1\otimes(B_{z2}+B_{g2})\hat{\sigma}_{z2})$ and $B_i = B_{\mathrm{zi}} + B_{\mathrm{gi}}$ it is possible to write:

$$\hat{U} = -\mu_B\begin{pmatrix} B_1+B_2 & 0 & 0 & 0 \\ 0 & B_1-B_2 & 0 & 0 \\ 0 & 0 & -B_1+B_2 & 0 \\ 0 & 0 & 0 & -B_1-B_2 \end{pmatrix} = \begin{pmatrix} m_1 & 0 & 0 & 0 \\ 0 & m_2 & 0 & 0 \\ 0 & 0 & -m_2 & 0 \\ 0 & 0 & 0 & -m_1 \end{pmatrix}$$

Hence:

$$\hat{H} = \hat{D}(\hat{e}_x) + \hat{U} = \begin{pmatrix} g+m_1 & 0 & 0 & -3g \\ 0 & -g+m_2 & -g & 0 \\ 0 & -g & -g-m_2 & 0 \\ -3g & 0 & 0 & g-m_1 \end{pmatrix}$$

Then

$$i\frac{d}{\mathrm{dt}}\begin{pmatrix} c_1 \\ c_2 \\ c_3 \\ c_4 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 \end{pmatrix}\begin{pmatrix} (g\mathbf{1} - 3g\hat{\sigma}_x + m_1\hat{\sigma}_z) & \mathbf{0} \\ \mathbf{0} & (-g\mathbf{1} - g\hat{\sigma}_x + m_2\hat{\sigma}_z) \end{pmatrix}\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}\begin{pmatrix} c_1 \\ c_2 \\ c_3 \\ c_4 \end{pmatrix}$$

which can be written as

$$i\frac{d\tilde{\psi}}{\mathrm{dt}} = (\hat{C}^{-1}\hat{H}_p\hat{C})\tilde{\psi} \qquad \text{where} \qquad \hat{C}^{+} = \hat{C}^{-1} = \hat{C}^{T}$$

and

$$\hat{U}(t)\tilde{\psi}(0)=\tilde{\psi}(t) \quad \text{with} \quad \hat{U}(t)=\exp(-i\int_0^t \mathrm{ds}\,\hat{C}^{-1}\hat{H}_p\hat{C})=\hat{C}^{-1}\exp(-i\int_0^t \mathrm{ds}\,\hat{H}_p)\hat{C}$$

where

$$\hat{H}_p=\begin{pmatrix} (g\mathbf{1}-3g\hat{\sigma}_x+m_1\hat{\sigma}_z) & \mathbf{0} \\ \mathbf{0} & (-g\mathbf{1}-g\hat{\sigma}_x+m_2\hat{\sigma}_z) \end{pmatrix}$$

which can be written as

$$\tilde{\psi}(t)=(\hat{C}^{-1}\hat{T}(t)\hat{C})\tilde{\psi}(0)$$

Defining $\tilde{\phi}(t)=\hat{C}\tilde{\psi}(t)$ then this evolves in time according to

$\tilde{\phi}(t)=\hat{T}(t)\tilde{\phi}(0)$ where $\hat{T}(\tau)=\exp(-i\tau(\hat{E}_+\otimes\hat{A}_1+\hat{E}_-\otimes\hat{A}_2))$ and $\hat{E}_+=\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \hat{E}_-=\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$

with $\hat{A}_1, \hat{A}_2$ given by the matrices

$$\hat{A}_1=\begin{pmatrix} g+m_1 & -3g \\ -3g & g-m_1 \end{pmatrix} \quad \text{and} \quad \hat{A}_2=\begin{pmatrix} -g+m_2 & -g \\ -g & -g-m_2 \end{pmatrix}$$

Now it is permissible to write that:

$$\exp(\hat{E}_\pm\otimes\hat{M})=\hat{E}_\pm\otimes\exp(\hat{M}) \quad \text{hence} \quad \hat{T}(\tau)=\hat{E}_+\otimes\exp(-i\tau\hat{A}_1)+\hat{E}_-\otimes\exp(-i\tau\hat{A}_2)$$

which is given by the matrix formula

$$\hat{T}(\tau)=\begin{pmatrix} e^{-i\tau\hat{A}_1} & \mathbf{0} \\ \mathbf{0} & e^{-i\tau\hat{A}_2} \end{pmatrix}$$

Now, writing that

$$\tilde{\psi}(t+d\tau)=(\hat{C}^{-1}\hat{T}(d\tau)\hat{C})\tilde{\psi}(t) \qquad \text{with} \qquad \hat{T}(d\tau)=\hat{I}-i\cdot d\tau\begin{pmatrix} \hat{A}_1 & \mathbf{0} \\ \mathbf{0} & \hat{A}_2 \end{pmatrix}$$

the evolution equation reads as:

$$\tilde{\psi}(t+d\tau)=\left[\hat{I}-i\cdot d\tau\hat{C}^{-1}\begin{pmatrix} \hat{A}_1 & \mathbf{0} \\ \mathbf{0} & \hat{A}_2 \end{pmatrix}\hat{C}\right]\tilde{\psi}(t) \qquad \text{where} \quad \hat{C}^{-1}\hat{I}\hat{C}=\hat{I}$$

Hence

$$\frac{\lim}{d\tau\to 0} \quad \frac{\tilde{\psi}(t+d\tau)-\tilde{\psi}(t)}{d\tau}=\frac{d\tilde{\psi}}{\mathrm{dt}}=-i(\hat{C}^{-1}\begin{pmatrix} \hat{A}_1 & \mathbf{0} \\ \mathbf{0} & \hat{A}_2 \end{pmatrix}\hat{C})\tilde{\psi}(t)$$

$$\text{with} \quad \hat{C}^{-1}\begin{pmatrix} \hat{A}_1 & \mathbf{0} \\ \mathbf{0} & \hat{A}_2 \end{pmatrix}\hat{C}=\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 \end{pmatrix}\begin{pmatrix} g+m_1 & 0 & 0 & -3g \\ -3g & 0 & 0 & g-m_1 \\ 0 & -g+m_2 & -g & 0 \\ 0 & -g & -g-m_2 & 0 \end{pmatrix}$$

$$=\begin{pmatrix} g+m_1 & 0 & 0 & -3g \\ 0 & -g+m_2 & -g & 0 \\ 0 & -g & -g-m_2 & 0 \\ -3g & 0 & 0 & g-m_1 \end{pmatrix}=\hat{H}$$

as required.

Corollary 1: Composition of CNOT

$$\hat{C}_{\rm NOT} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \otimes \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

Defining

$$\hat{E}_+ = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} = \frac{1}{2}(\mathbf{1} + \hat{\sigma}_z) \quad \text{and} \quad \hat{E}_- = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} = \frac{1}{2}(\mathbf{1} - \hat{\sigma}_z)$$

we can write

$$\hat{C}_{\rm NOT} = \frac{1}{2}[\mathbf{1}_4 + \boldsymbol{FLIP2} + \hat{\sigma}_{z1} \otimes (\mathbf{1} - \hat{\sigma}_x)]$$

which can be simplified as

$$\hat{C}_{\rm NOT} = \frac{1}{2}[\mathbf{1} \otimes \mathbf{1} + \mathbf{1} \otimes \hat{\sigma}_x + \hat{\sigma}_z \otimes \mathbf{1} - \hat{\sigma}_z \otimes \hat{\sigma}_x]$$

Denoting our operators as

$$\mathbf{1} \otimes \mathbf{1} = \mathbf{1}_4 \quad \mathbf{1} \otimes \hat{\sigma}_x = \hat{a} \quad \hat{\sigma}_z \otimes \mathbf{1} = \hat{b}$$

our decomposition reads as

$$\hat{C}_{\rm NOT} = \frac{1}{2}[\mathbf{1}_4 + \hat{a} + \hat{b} + \frac{1}{2}\{\hat{a}, \hat{b}\}]$$

where the curly brackets mean the anticommutator as usual.

Writing the anticommutator in the form:

$$\hat{c} = \frac{1}{2}\{\hat{a}, \hat{b}\} \qquad \text{we can write } a \text{ series of expressions such as} \qquad [\hat{a}, \hat{b}] = [\hat{a}, \hat{c}] = [\hat{b}, \hat{c}] = 0$$

as well as a group given by the relations

$$\frac{1}{2}\{\hat{a}, \hat{b}\} = \hat{c} \qquad \frac{1}{2}\{\hat{a}, \hat{c}\} = \hat{b} \quad \text{and} \quad \frac{1}{2}\{\hat{b}, \hat{c}\} = \hat{a}$$

$$\hat{a}^2 = \hat{b}^2 = \hat{c}^2 = \mathbf{1}_4$$

This group is not isomorphic to the Pauli spin algebra.

Corollary 2: Concurrence Formula

Define the concurrence of a state vector as:

$$C(\psi) = \frac{|\langle\psi|\hat{\sigma}_{y1}\hat{\sigma}_{y2}|\psi^+\rangle|}{|\langle\psi|\psi\rangle|^2}$$

where $|\psi^+\rangle = C.C.(|\psi\rangle)$.

$$\hat{\sigma}_{y1} \otimes \hat{\sigma}_{y2} = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \otimes \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = \begin{pmatrix} \mathbf{0} & & & -1 \\ & & 1 & \\ & 1 & & \\ -1 & & & \mathbf{0} \end{pmatrix}$$

$$|\psi\rangle = c_1|00\rangle + c_2|01\rangle + c_3|10\rangle + c_4|11\rangle$$

$$= \begin{pmatrix} c_1 \\ c_2 \\ c_3 \\ c_4 \end{pmatrix}$$

and therefore $[\psi^+ >$ is equivalent to the vector $\begin{pmatrix} c_1^+ \\ c_2^+ \\ c_3^+ \\ c_4^+ \end{pmatrix}$ where $'+'$ is complex conjugate

Hence our expression for the concurrence reads as:

$$C(\psi) = \frac{1}{|c_1|^2 + |c_2|^2 + |c_3|^2 + |c_4|^2} \cdot \left(\; c_1^+, c_2^+, c_3^+, c_4^+ \; \right) \begin{pmatrix} \mathbf{0} & & & -1 \\ & & 1 & \\ & 1 & & \\ -1 & & & \mathbf{0} \end{pmatrix} \begin{pmatrix} c_1^+ \\ c_2^+ \\ c_3^+ \\ c_4^+ \end{pmatrix}$$

which simplifies to the equation

$$C(\psi) = \frac{2\left| c_2^+ c_3^+ - c_1^+ c_4^+ \right|}{|c_1|^2 + |c_2|^2 + |c_3|^2 + |c_4|^2}$$

Corollary 3: Phase Gate Calculations

Consider the phase gate given by:

$$\hat{C}_Z = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$$

as well as two 2x2 matrices with arbitary complex co-efficients, given by

$$\hat{U} = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \quad \text{and} \quad \hat{V} = \begin{pmatrix} e & f \\ g & h \end{pmatrix}$$

We are seeking factorisations of controlled-NOT of the form:

$$\hat{C}_{\text{NOT}} = (\hat{U} \otimes \hat{U}) \hat{C}_Z (\hat{V} \otimes \hat{V}) \qquad [1]$$

$$\hat{C}_{\text{NOT}} = (\hat{U} \otimes \hat{V}) \hat{C}_Z (\hat{U} \otimes \hat{V}) \qquad [2]$$

It can be show using MAPLE that [1] has no solutions due to a contradiction. [2] has the well-known solution given by:

$$\hat{U} = \mathbf{1} \quad \text{and} \quad \hat{V} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

Also, the concurrence is maximised in the system [1] for the matrices

$$\hat{U} = 0.6228 \times 10^{-6} \begin{pmatrix} 0 & 0.235 \\ 0.235 & 1 \end{pmatrix} \quad \text{and} \quad \hat{V} = -\,0.8041 \times 10^{-6} \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$$

which are non-Hermitian in character.