Phase shifted pulses for QFT operations with paramagnetic ions.

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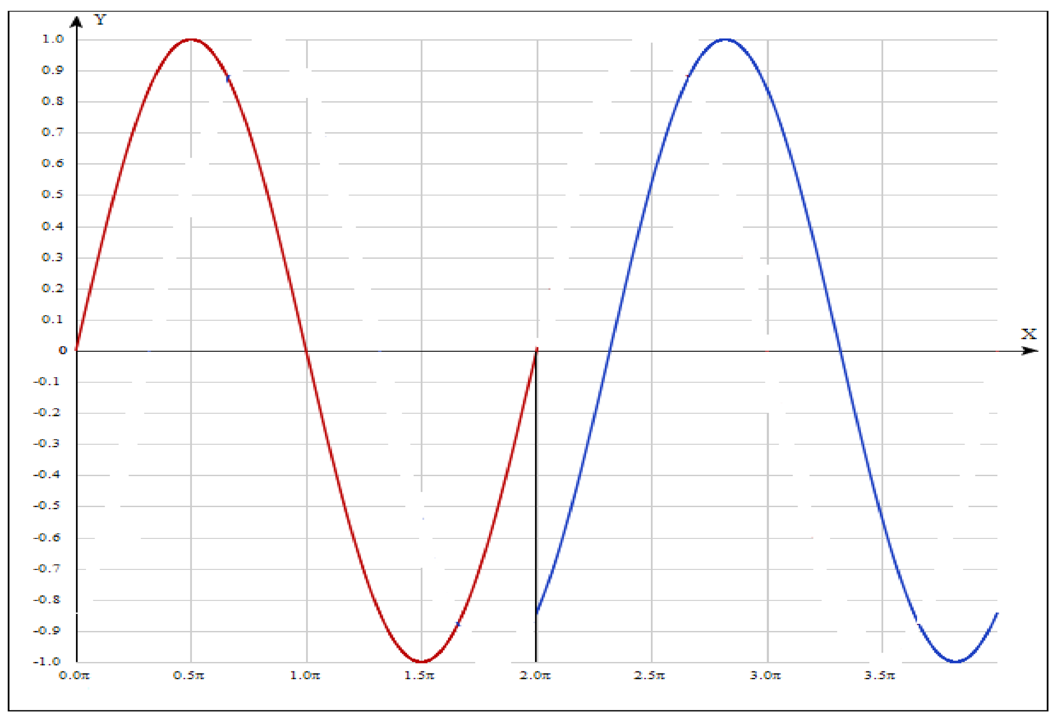
Motivation : To perform QFT an operator $S = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\varphi} \end{pmatrix}$ should be applied to a quantum system.

For this purpose a microvawe phase shifted pulses applied to two spin (two qubit) systems are suggested. Triplet molecules, biradicals and paramagnetic d2 –ions are suggested to perform QFT without permanent magnetic field.

Phase shifted microvawe (or radiofrequency) pulse.



$$H_1(t) = 2H_{1x}\cos(\omega_\Gamma t) \qquad 0 < t < \tau$$

$$H_1(t) = 2H_{1x}\cos(\omega_\Gamma t - \delta) \qquad \tau < t < \tau_2$$

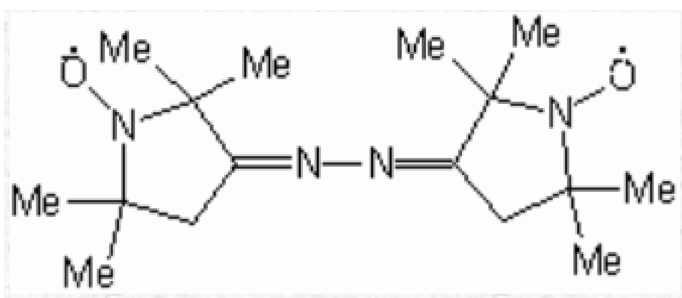
$$\omega\tau = \pi; \frac{\pi}{2}$$

$$H = \hat{H}_0 + H(t) \qquad H = g\beta H_1(t)(\sigma_{1X} + \sigma_{2X})$$

Two spin particles

1. Triplet molecules

2. Biradical



3. Paramagnetic d2 – ions (Ni (I=0), Fe2+, V3+ (I≠0))

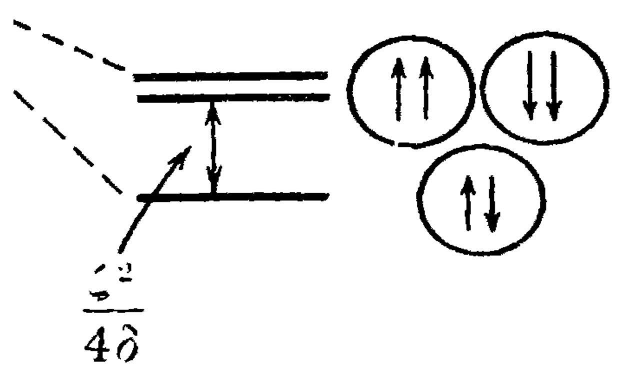
Spin-Hamiltonian at zero magnetic field a zero field splitting is valid $H = \frac{1}{2}D \cdot \sigma_{1Z}\sigma_{2Z}$

Eigenvectors and eigenvalues

$$|T_+\rangle = 2^{-1/2}|\alpha_i\alpha_j + \beta_i\beta_j\rangle$$

$$|T_-\rangle = 2^{-1/2}|\alpha_i\alpha_j - \beta_i\beta_j\rangle$$

$$|T_0\rangle = 2^{-1/2}|\alpha_i\beta_j + \beta_i\alpha_j\rangle$$



$$|\Psi(t)\rangle = U|\Psi(0)\rangle$$

$$H_1(t) = H_1(\sigma_{1X} + \sigma_{2X})\cos(\omega_\Gamma t)$$

$$U_1 = \exp(-i\frac{\theta}{2}(\sigma_{X1} + \sigma_{X2}) =$$

$$= (\cos\frac{\theta}{2} - i\sigma_{X1}\sin\frac{\theta}{2})(\cos\frac{\theta}{2} - i\sigma_{X1}\sin\frac{\theta}{2})$$

$$H_1 = H_1(\sigma_{1X} + \sigma_{2X})\cos(\omega_\Gamma t - \delta)$$

$$U_2 = \exp(-i\frac{\theta}{2}(\cos\delta \cdot \sigma_{X1} \cdot I_2 + \sigma_{Y1} \cdot \sigma_{Z2}\sin\delta))$$

$$\cdot \exp(-i\frac{\theta}{2}(\cos\delta \cdot \sigma_{X_2} \cdot I_1 + \sigma_{Y_2} \cdot \sigma_{Z_1}\sin\delta))$$

Rotation operators U

$$\delta = 0$$

$$U = \exp(-i\frac{\omega_1 t}{2}(\sigma_X)$$

$$|\alpha\rangle \to |\beta\rangle \quad |\alpha\rangle \to \frac{1}{\sqrt{2}}(|\alpha\rangle - |\beta\rangle)$$

$$\delta \neq 0$$

$$U = \exp(-i\frac{H_1 t}{2}(\vec{n} \cdot \hat{\sigma})) =$$

$$= \frac{H_1}{2}(\sigma_x\cos\delta + \sigma_y\sin\delta)$$

$$U_1(\theta = \pi/2)|T_0\rangle \to |T_+\rangle$$

$$U_2(\theta = \frac{\pi}{2}, \delta = \frac{\pi}{2})|T_0\rangle \to i|T_-\rangle$$

$$U = U_2(\theta = \frac{\pi}{2}) \cdot U_1(\theta = \frac{\pi}{2})|T_0\rangle \to \exp(i\delta(\sigma_{Z_1} + \sigma_{Z_2}))$$

$$U|T_0\rangle \to |T_0\rangle$$

$$U|T_+\rangle \to \cos\delta|T_+\rangle + i\sin\delta|T_-\rangle$$

$$S = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\varphi} \end{pmatrix}$$

Conclusions

1. Paramagnetic d2-ions and two spin molecules are new promising objects for quantum calculations
2. Phase shiftted microvawe pulses may be useful for quantum calculation algorithms

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