A Simple and Convenient Measure of NMR Rotor Fidelity

M. D. Bowdrey

Oxford Centre for Quantum Computation, Clarendon Laboratory, Parks Road, Oxford OX1 3PU, UK
E-mail: mark.bowdrey@qubit.org

J. A. Jones¹

Oxford Centre for Quantum Computation, Clarendon Laboratory, Parks Road, Oxford OX1 3PU, UK, and
Oxford Centre for Molecular Sciences, New Chemistry Laboratory, South Parks Road, Oxford, OX1 3QT, UK
E-mail: jonathan.jones@qubit.org

We describe a simple scheme for calculating the fidelity of a composite pulse when considered as a universal rotor.

Key Words: NMR, quantum computation, composite pulse, universal rotor, fidelity.

1. INTRODUCTION

Composite pulses [1, 2, 3] play an important role in many NMR experiments, as they allow the effects of experimental imperfections, such as pulse length errors and off-resonance effects, to be reduced. In conventional NMR experiments these pulses are used to implement particular transformations on the Bloch sphere, such as inversion, and their quality can be easily assessed by determining the efficiency with which some known starting state is transferred to the desired final state. Furthermore, the transfer efficiency can be both calculated and measured, allowing a simple comparison between theory and experiment.

An alternative approach to composite pulses, developed by Tycko [4], seeks to design general rotors, that is, pulses which perform well for any initial starting state. Composite pulses of this kind, which are sometimes called Class A composite pulses [2], are rarely (if ever) needed for conventional NMR experiments, but are useful in NMR implementations of quantum computation [2, 3, 4, 5], where they act to reduce systematic errors in quantum logic gates [6]. With pulses of this kind conventional measures of transfer efficiency are inappropriate, and it is necessary to consider the overall fidelity of the composite pulse sequence when viewed as a general rotor.

A solution to this problem was provided by Levitt [2], who defined the rotor fidelity by the dot product of the quaternions describing the composite pulse and the desired ideal rotation, and it is this approach which has been used to date [6, 7]. This definition, however, has one major disadvantage: while it is fairly easy to calculate it cannot be measured experimentally. It would be desirable to find a measure of rotor fidelity which, like conventional quality measures, permits theory and experiment to be compared.

One possible approach would be to use a conventional measure of pulse sequence quality and to average this over a range of starting states. Intuitively this seems reasonable, but it is not clear that such a method has any formal basis. Here we show how that this approach can, in fact, be derived from the definition of propagator fidelity widely used in quantum information theory [12].

2. RESULTS

A reasonable measure for the similarity of two pure quantum states is the square of the overlap between them,

$$\langle \psi_1 | \psi_2 \rangle^2.$$  (1)

State overlap also provides a means to compare two different propagators, $U$ and $V$, acting on the same state by considering the overlap of their final states. The fidelity of the two propagators (that is, the extent to which they are the same) can then be obtained by averaging over all initial states:

$$f = \frac{|\langle \psi | UV | \psi \rangle|^2}{\text{tr}(U | \langle \psi | UV | \psi \rangle | V \rangle).}$$  (2)

When considering a single spin-$\frac{1}{2}$ particle this expression can be greatly simplified. Any pure state of such a particle corresponds to a point on the surface of the Bloch
sphere, and the corresponding density matrix $\rho(\theta, \phi)$ can be expanded as a sum of the conventional $I_x$, $I_y$, and $I_z$ product operators \[13\] and $I_0$ (half the identity matrix, more normally written $\frac{1}{2}E$).

$$\rho(\theta, \phi) = \frac{1}{2} \mathbf{1} + \frac{1}{2} \begin{pmatrix} \cos \theta & \sin \theta e^{-i\phi} \\ \sin \theta e^{i\phi} & -\cos \theta \end{pmatrix}$$

$$= I_0 + \sin \theta \cos \phi I_x + \sin \theta \sin \phi I_y + \cos \theta I_z \quad (3)$$

= \sum_{j=0, x, y, z} c_j(\theta, \phi) I_j.

The propagator fidelity can be obtained by integrating over the Bloch sphere.

$$f = \frac{1}{4\pi} \int_0^{2\pi} \int_0^\pi f(\theta, \phi) \sin \theta \, d\theta \, d\phi \quad (4)$$

where the fidelity at any point on the sphere, $f(\theta, \phi)$, is given by

$$f(\theta, \phi) = \text{tr} \left( U \sum_j c_j(\theta, \phi) I_j U^\dagger V \sum_k c_k(\theta, \phi) I_k V^\dagger \right)$$

$$= \sum_{j,k} c_j(\theta, \phi) c_k(\theta, \phi) \text{tr} \left( U I_j U^\dagger V I_k V^\dagger \right). \quad (5)$$

When integrated over the Bloch sphere, the coefficients of terms containing different product operators sum to zero, while the diagonal terms survive:

$$\frac{1}{4\pi} \int_0^{2\pi} \int_0^\pi c_j(\theta, \phi) c_j(\theta, \phi) \sin \theta \, d\theta \, d\phi = \frac{\delta_{ij}}{3} + \frac{2\delta_{ij}\delta_{j0}}{3}. \quad (6)$$

Note that $I_0$ (which is a multiple of the identity matrix) commutes with any propagator, and so

$$\text{tr} \left( U I_0 U^\dagger V I_0 V^\dagger \right) = \text{tr} \left( I_0 U U^\dagger I_0 V V^\dagger \right)$$

$$= \text{tr} \left( I_0^2 \right) = \frac{1}{2}. \quad (7)$$

Hence the propagator fidelity is reduced to

$$f = \frac{1}{2} + \frac{1}{3} \sum_{j=x,y,z} \text{tr} \left( U I_j U^\dagger V I_j V^\dagger \right). \quad (8)$$

For an isolated spin-\(\frac{1}{2}\) particle any unitary propagator can be considered as a rotation, and the rotor fidelity of a pulse sequence can be taken as the fidelity of the corresponding propagator. As NMR experiments are usually conducted at high temperature, the spin is not described by a pure state, as assumed above, but by a highly mixed state. This state can, however, be considered as a mixture of the unit matrix and a deviation density matrix corresponding to a pure state,

$$|\psi^\prime\rangle\langle\psi^\prime| = (1 - \epsilon) \frac{1}{2} \mathbf{1} + \epsilon |\psi\rangle\langle\psi|$$

and in most situations we are only interested in the deviation matrix $|\psi\rangle\langle\psi|$. (In the language of NMR quantum computation this is referred to as the pseudo pure state approach \[14\,15\]; this is also the approach adopted in conventional NMR studies except that the contribution of $I_0$ to the deviation matrix is rarely considered).

Examining the behaviour of the deviation matrix leads to the same results as for a pure state except for a scaling factor of $\epsilon^2$, and since $\epsilon$ is in effect a measure of signal strength we follow common NMR practice and set $\epsilon = 1$. Thus the rotor fidelity is given by the previous expression for the propagator fidelity, equation \[8\]. Finally we note that $\text{tr}(U I_j U^\dagger V I_j V^\dagger)$ is simply half of the efficiency with which the propagator $V$ transfers the initial state $I_j$ to the desired final state $U I_j U^\dagger$. Thus, neglecting a scaling factor of one half and an offset of one half, the rotor fidelity is equal to the conventional transfer efficiency averaged over the three starting states $I_x$, $I_y$ and $I_z$.

3. CONCLUSIONS

The propagator fidelity provides a simple and convenient measure of rotor fidelity which can be used to assess the quality of NMR composite pulses designed to act as general rotors. Unlike the quaternion measure introduced by Levitt \[2\] the propagator fidelity can be both calculated using equation \[8\] and measured experimentally (by averaging the conventional transfer efficiency over the three starting states $I_x$, $I_y$ and $I_z$).

ACKNOWLEDGMENTS

We thank E. Galvão, L. Hardy, D. Oi and T. Short for helpful conversations. M.D.B. thanks EPSRC (UK) for a research fellowship. J.A.J. is a Royal Society University Research Fellow. This is a contribution from the Oxford Centre for Molecular Sciences, which is supported by the UK EPSRC, BBSRC, and MRC.

REFERENCES

1. M. H. Levitt and R. Freeman, J. Magn. Reson. 33, 473 (1979).
2. M. H. Levitt, Prog. NMR Spectrosc. 18, 61 (1986).
3. R. Freeman, “Spin Choreography”, Spektrum, Oxford, (1997).
4. R. Tycko, Phys. Rev. Lett. 51, 775 (1983).
5. D. G. Cory, A. F. Fahmy and T. F. Havel, in “PhysComp ’96” (T. Toffoli, M. Biafore, and J. Leão, Eds.), pp. 87–91, New England Complex Systems Institute (1996).
6. D. G. Cory, A. F. Fahmy, and T. F. Havel, Proc. Nat. Acad. Sci. USA 94, 1634 (1997).
7. N. A. Gershenfeld and I. L. Chuang, Science 275, 350 (1997).
8. J. A. Jones and M. Mosca, J. Chem. Phys. 109, 1648 (1998).
9. J. A. Jones, R. H. Hansen, and M. Mosca, J. Magn. Reson. 135, 353 (1998).
10. H. K. Cummins and J. A. Jones, New J. Phys. 2.6, 1 (2000).
11. H. K. Cummins and J. A. Jones, J. Magn. Reson. 148, 338 (2001).
12. M. Nielsen and I. Chuang, “Quantum Computation and Quantum Information”, Cambridge University Press (2000).
13. O. W. Sorensen, G. W. Eich, M. H. Levitt, G. Bodenhausen and R. R. Ernst, Prog. NMR Spectrosc. 16, 163 (1983).