Quantum Computing and Nuclear Magnetic Resonance

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Outline

- What is quantum computing?
- How to do quantum computing with NMR
- What has been done?
- What are we trying to do?
- How far can we go?

- J. A. Jones, *PhysChemComm* **11** (2001)
- J. A. Jones, *Prog. NMR Spectrosc*. **38,** 325 (2001)

Qubits & quantum registers

Classical Bit

0 or 1

Quantum Bit

0 or 1 or 0 1

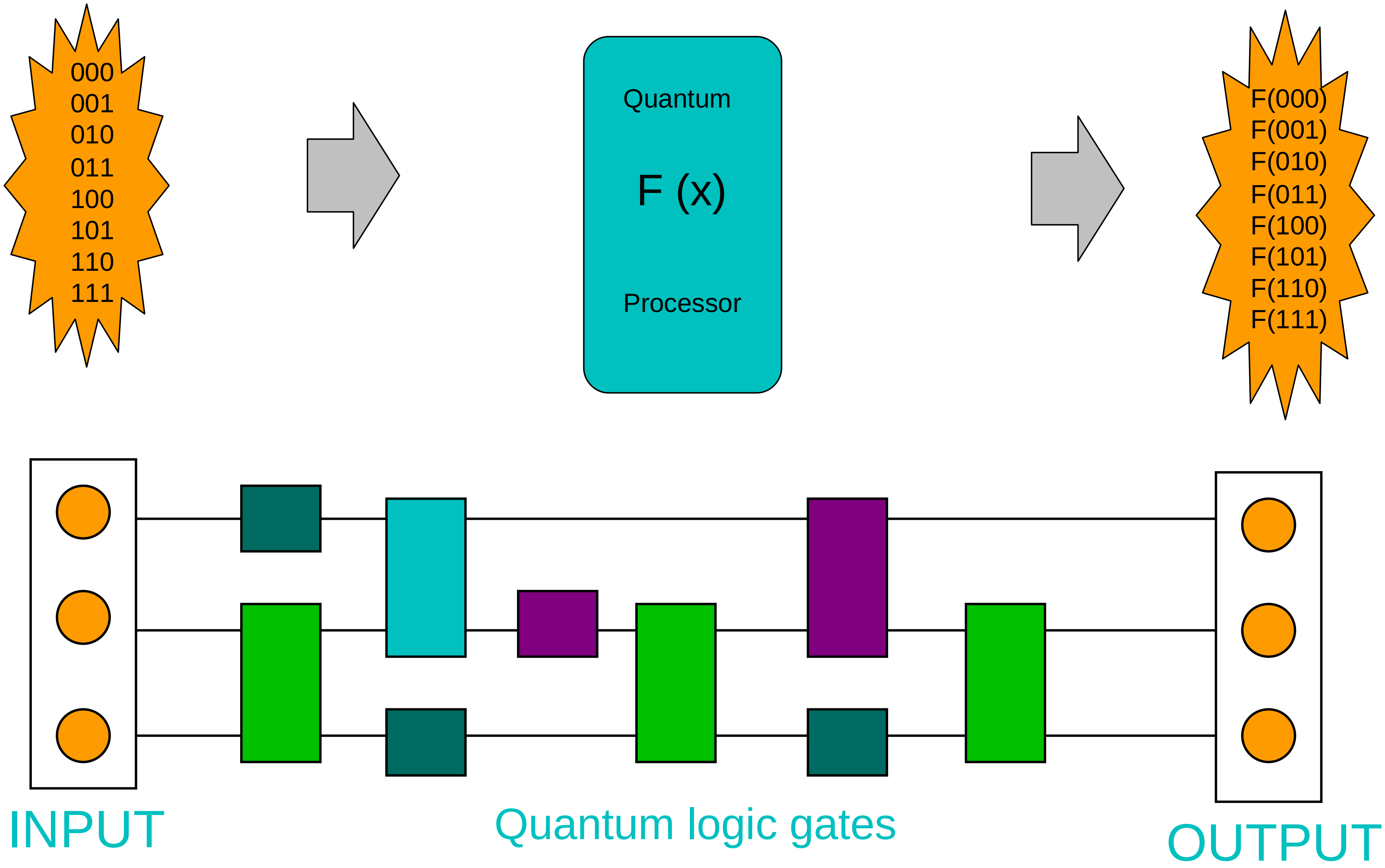
Classical register

101

Quantum register

000 001 010 011
100 101 110 111

Quantum parallel processing



What could we do with one?

- Easy to do the calculations, but hard to get the answers out from the resulting superposition!

- Simulate quantum mechanics
- Factor numbers: Shor's algorithm
  - » The end of public key cryptography?
  - » Generalises to the Abelian Hidden Subgroup problem
- Speed up searches: Grover's algorithm

- QC is not the answer to everything!

How might we build one?

- To build a quantum computer you need

- quantum two level systems (qubits),
- interacting strongly with one another,
- isolated from the environment, but
- accessible for read out of answers *etc*.

- See *Fortschritte der Physik* **48**, 767-1138 (2000)
  - » Scalable Quantum Computers - Paving the Way to Realization, S. L. Braunstein and H.-K. Lo

Nuclear Magnetic Resonance

- Conventional liquid state NMR systems (common in chemistry and biochemistry labs)
- Use two spin states of spin-1/2 nuclei (^{1}H, ^{13}C, ^{15}N, ^{19}F, ^{31}P) as a qubit
- Address and observe them with RF radiation
- Nuclei communicate by J couplings
- Conventional multi-pulse NMR techniques allow gates to be implemented
- Actually have a hot thermal ensemble of computers

NMR experiments

NMR Hamiltonians

- Usually written using “product operators”. For two coupled spins

$$H = 2\pi\nu_I I_z + 2\pi\nu_S S_z + 2\pi J_{IS} I \cdot S$$
$$\approx 2\pi\nu_I I_z + 2\pi\nu_S S_z + \pi J_{IS} 2 I_z S_z$$

- Can apply RF pulses, with good control of amplitude, frequency and phase. Normally work in a frame rotating at the RF frequency. For a single spin

$$H = 2\pi\delta_I I_z + 2\pi\nu_1 \left(I_x \cos\phi + I_y \sin\phi \right)$$

Typical frequencies (14.4T)

- For a ^{1}H nucleus (magnets are usually described by their 1H NMR frequency)

$$\nu_0 = 600\,\mathrm{MHz} \pm 3\,\mathrm{kHz}, \quad \nu_1 \leq 25\,\mathrm{kHz}$$

- For a ^{13}C nucleus

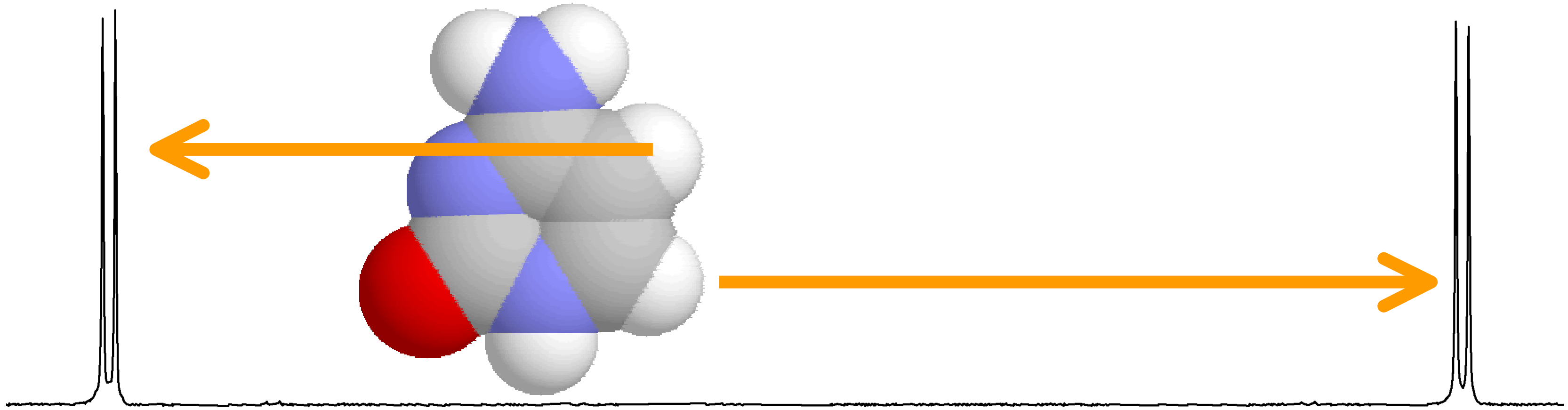
$$\nu_0 = 150\,\mathrm{MHz} \pm 15\,\mathrm{kHz}, \quad \nu_1 \leq 15\,\mathrm{kHz}$$

- For a ^{19}F nucleus

$$\nu_0 = 565\,\mathrm{MHz} \pm 50\,\mathrm{kHz}, \quad \nu_1 \leq 25\,\mathrm{kHz}$$

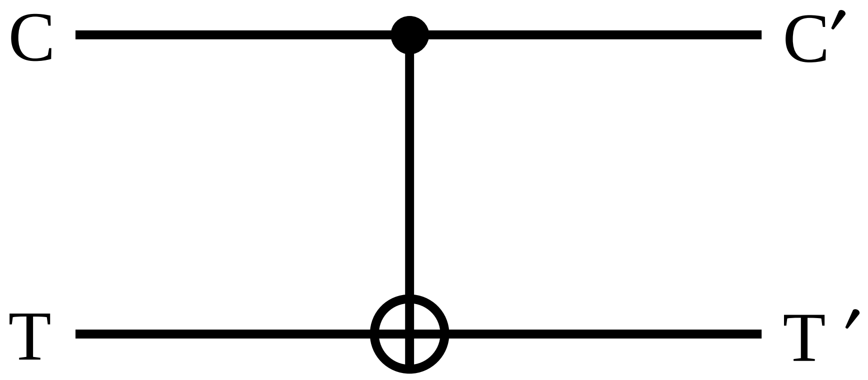
- J couplings lie in the range of 1Hz–1kHz

Single Qubit Rotations



- Single spin rotations are implemented using resonant RF pulses
- Different spins have different resonance frequencies and so can be selectively addressed
- Frequency space can become quite crowded, especially for ^{1}H (other nuclei are much better)

Controlled-NOT (CNOT) gates



$C' = C$

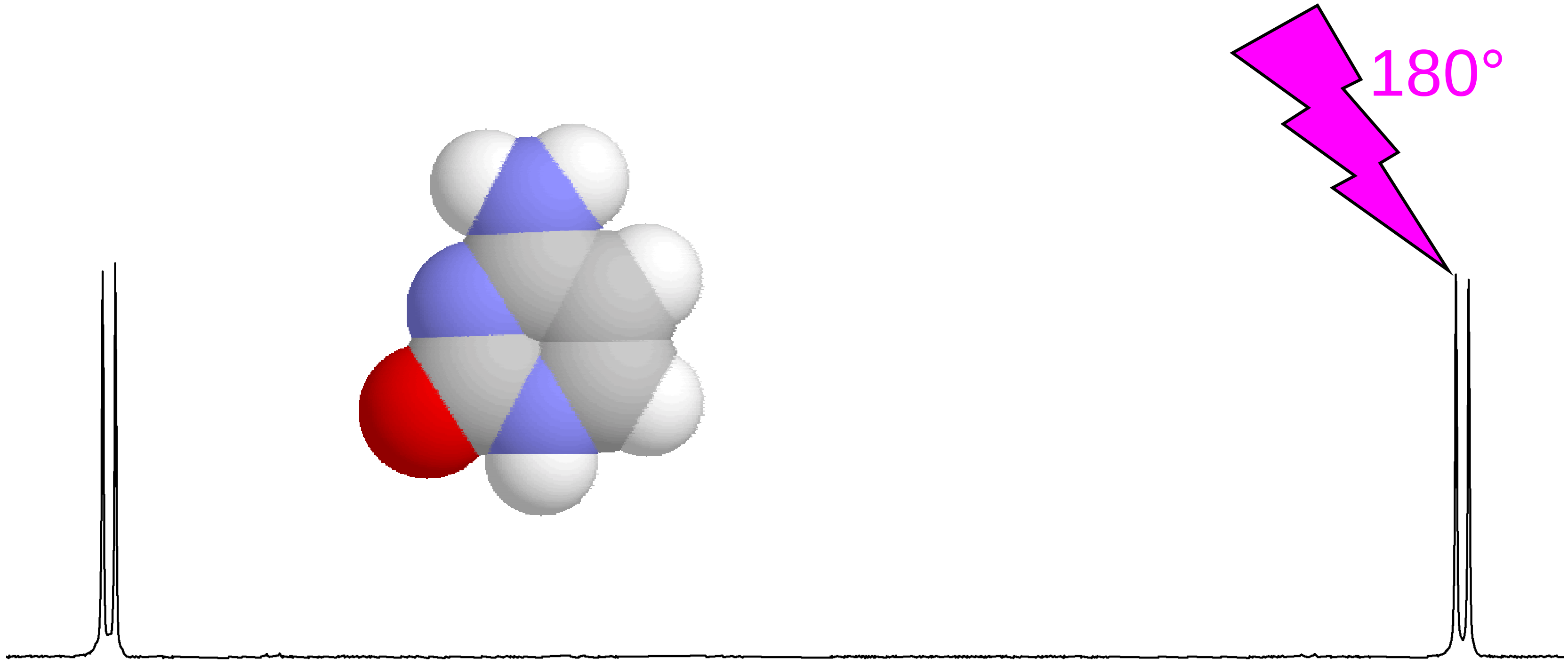
$T' = T \oplus C$

(Exclusive-OR)

- The controlled-NOT gate flips the target bit (T) if the control bit (C) is set to 1

C	T	C′	T′
0	0	0	0
0	1	0	1
1	0	1	1
1	1	1	0

CNOT and SPI (1973)



Selective Population Inversion: a 180° pulse applied to one line in a doublet is essentially equivalent to CNOT

Hamiltonian Sculpting

- Combine periods of evolution under the background Hamiltonian with periods when various RF pulses are also applied
- The Average Hamiltonian over the entire pulse sequence can be manipulated
- In general terms can be scaled down or removed at will, and desired forms can be implemented
- Highly developed NMR technique
- Ultimately equivalent to building circuits out of gates

The spin echo

- Most NMR pulse sequences are built around spin echoes which refocus Zeeman interactions
- Often thought to be unique to NMR, but in fact an entirely general quantum property

$$\alpha|0\rangle+\beta|1\rangle \xrightarrow{\tau} \alpha|0\rangle+\beta e^{i\omega\tau}|1\rangle \xrightarrow{180_x} \alpha|1\rangle+\beta e^{i\omega\tau}|0\rangle$$

$$\xrightarrow{\tau} \alpha e^{i\omega\tau}|1\rangle+\beta e^{i\omega\tau}|0\rangle \xrightarrow{180_x} \alpha e^{i\omega\tau}|0\rangle+\beta e^{i\omega\tau}|1\rangle$$

$$= e^{i\omega\tau}\left[\alpha|0\rangle+\beta|1\rangle\right]$$

- Interaction refocused up to a global phase

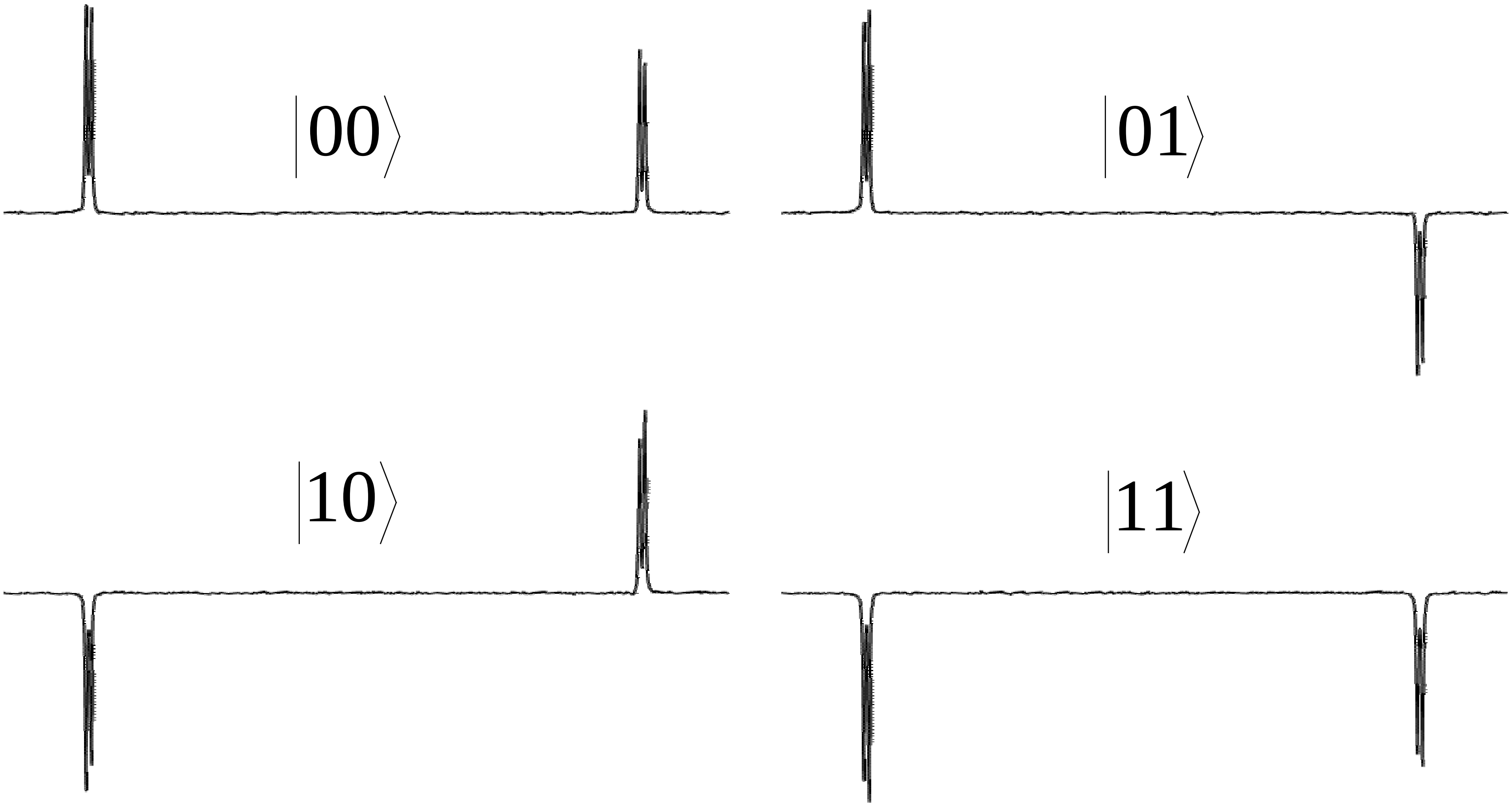
CNOT and INEPT (1979)

The CNOT propagator can be expanded as a sequence of pulses and delays using a standard NMR approach…

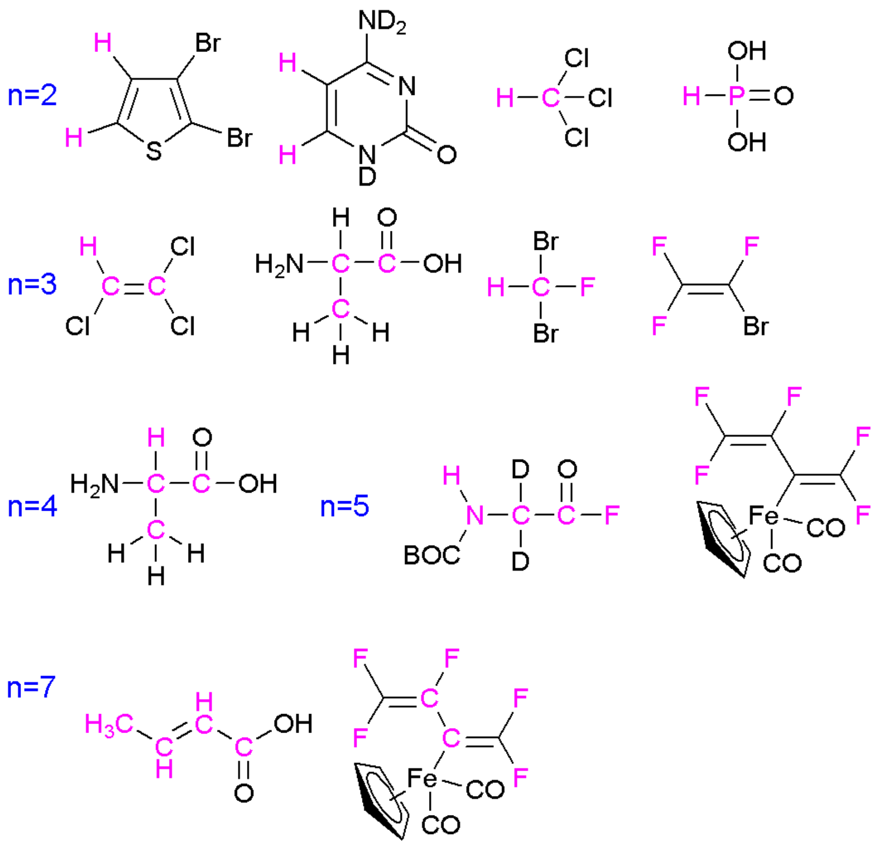
$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} = \begin{array}{l} \\ \\ 90_{-y} \end{array} \boxed{\begin{array}{cccc} & 180_x & & 90_{-y} \\ \tau = \frac{1}{4J} & & \tau = \frac{1}{4J} & \\ & 180_x & & 90_{-y} \end{array}} \begin{array}{l} 90_x \, 90_{-y} \\ \\ 90_x \end{array}$$

… to give a pulse sequence very similar to an INEPT coherence transfer experiment

Example results



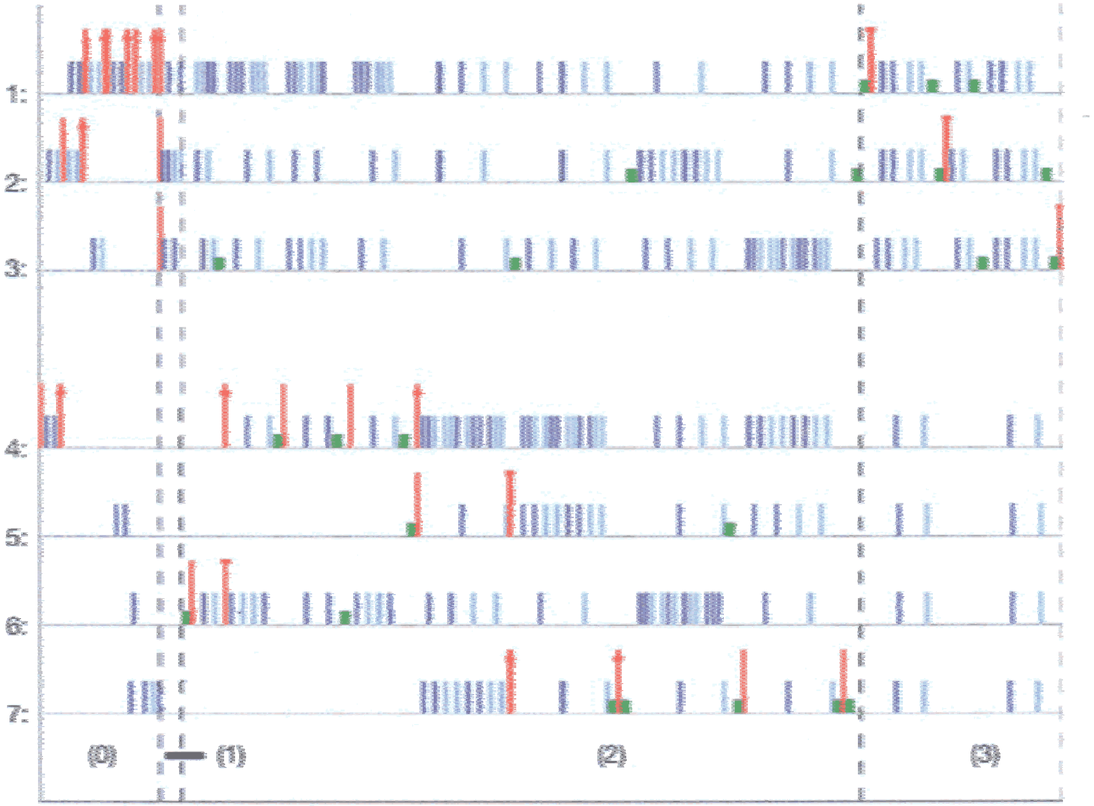
Molecules and algorithms

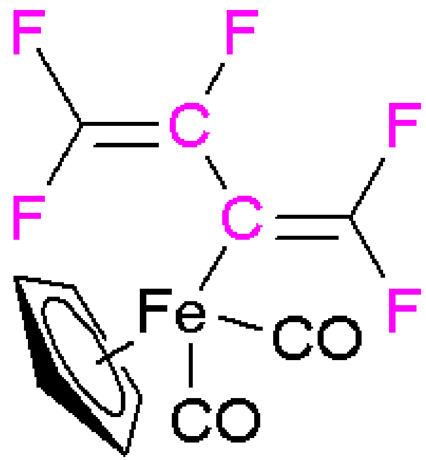


- A wide range of molecules have been used with ^{1}H, ^{13}C, ^{15}N, ^{19}F and ^{31}P nuclei
- A wide range of quantum algorithms have been implemented
- Some basic quantum phenomena have been demonstrated

State of the art

- Shor's quantum factoring algorithm to factor 15





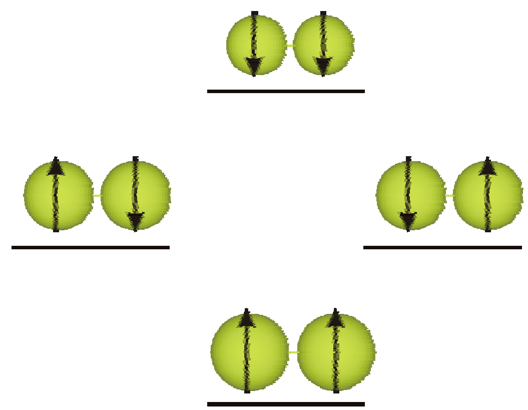
Nature **414**, 883 (2001)

The initialisation problem

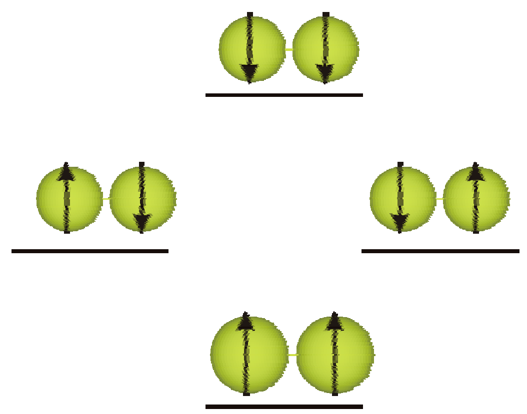
- Conventional QCs use single quantum systems which start in a well defined state
- NMR QCs use an ensemble of molecules which start in a hot thermal state
- Can create a “pseudo-pure” initial state from the thermal state: exponentially inefficient
- Better approach: use *para*-hydrogen!

Two spin system

- A homonuclear system of two spin 1/2 nuclei: four energy levels with nearly equal populations



- Equalise the populations of the upper states leaving a small excess in the lowest level



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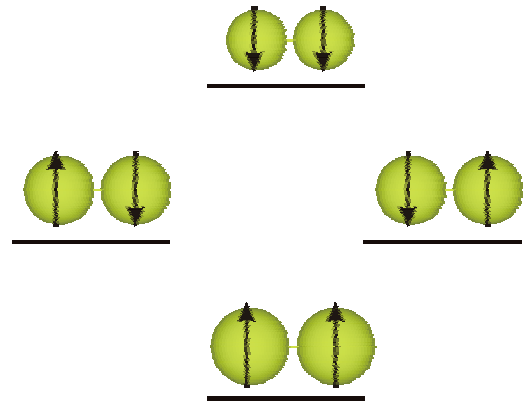

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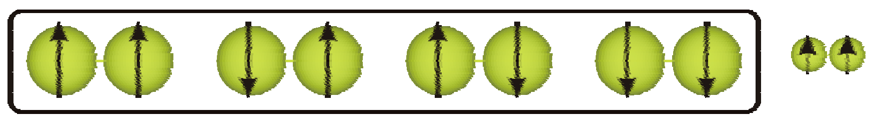


A “pseudo-pure” state

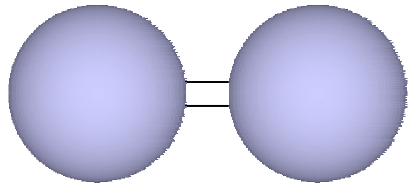
Excess population is exponentially small

para-hydrogen

- The rotational and nuclear spin states of H_2 molecules are inextricably connected by the Pauli principle
- Cooling to the J=0 state would give pure *para*-hydrogen with a singlet spin state
- Cooling below 150K in the presence of an *ortho/para* catalyst gives significant enhancement of the *para* population
- Enhancement is retained on warming if the *ortho/para* catalyst is removed

Using *para*-hydrogen

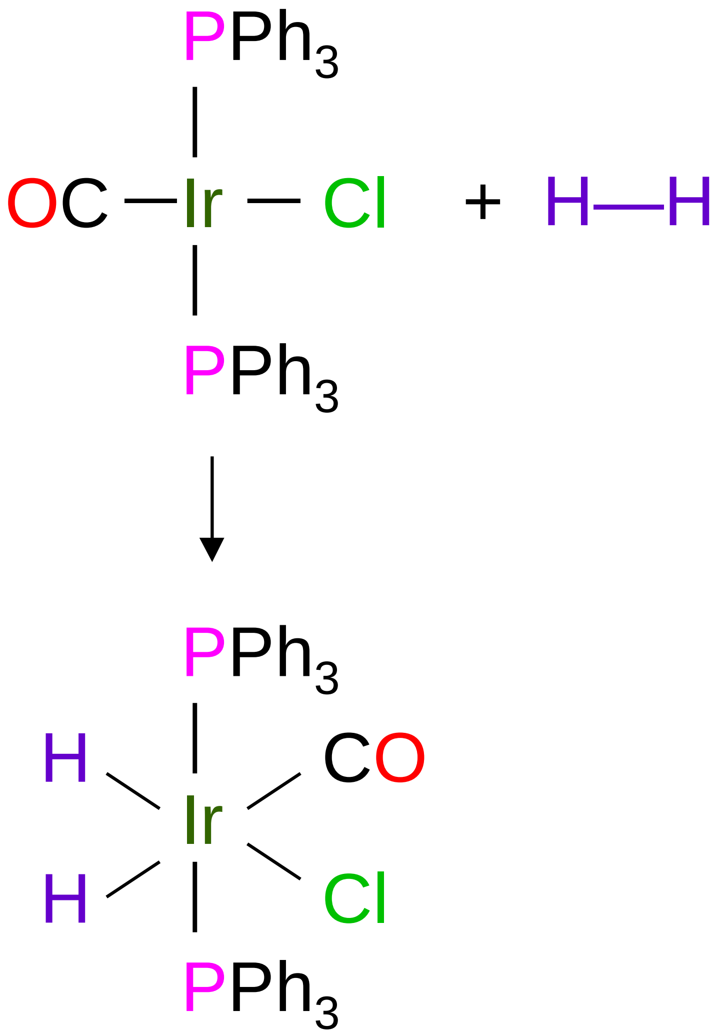
- *para*-hydrogen has a pure singlet nuclear spin state



$$\left|\psi^{-}\right\rangle = \frac{|\alpha\rangle|\beta\rangle - |\beta\rangle|\alpha\rangle}{\sqrt{2}} = \frac{|01\rangle - |10\rangle}{\sqrt{2}}$$

- Can't do computing with this directly because the H_2 molecule is too symmetric: we need to break the symmetry so that we can address the two nuclei individually

Vaska's catalyst



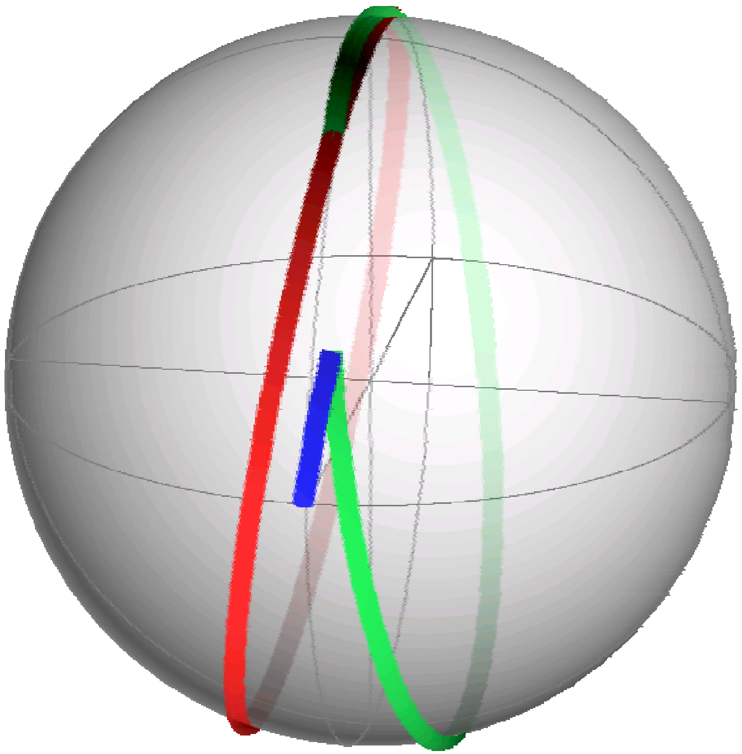
- Add the *p*-H_2 to some other molecule, e.g. Vaska's catalyst
- The two ^1H nuclei now have different chemical shifts and so can be separately addressed

Tackling systematic errors

- Quantum computers are vulnerable to errors
- *Random* errors can be tackled using advanced forms of error correcting codes
- *Systematic* errors can be tackled using various approaches for robust coherent control

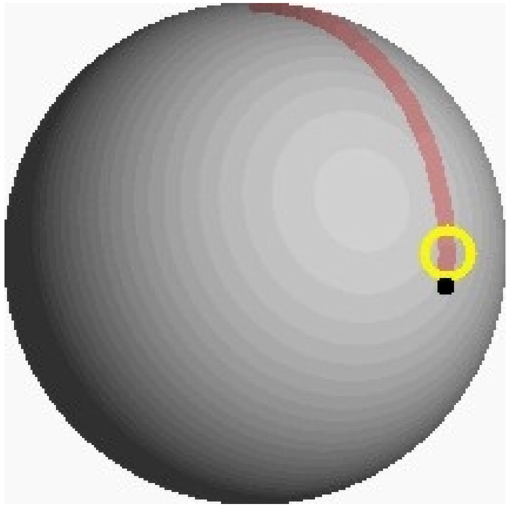
- The traditional NMR approach (composite pulses) has already proved productive

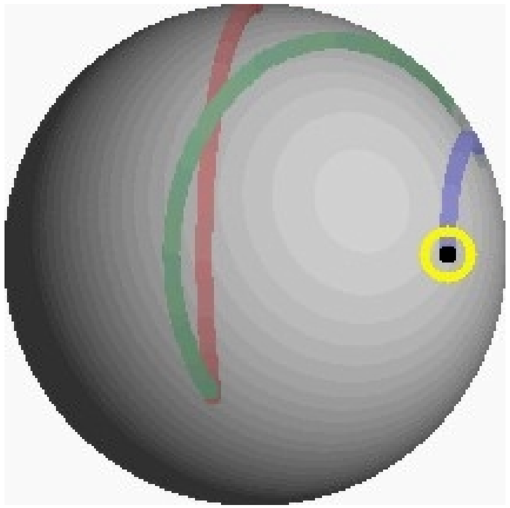
Tycko composite 90 sequence



- Tycko's composite 90° pulse $385_0 \cdot 320_{180} \cdot 25_0$ gives good compensation for small off-resonance errors
- Works well for *any* initial state, not just for *z*
- Now generalised to arbitrary angles
- *New J. Phys.* **2.6** (2000)

Pulse length errors





- The composite 90° pulse $115_{62} \cdot 180_{281} \cdot 115_{62}$ corrects for pulse length errors
- Works well for *any* initial state, not just *z*
- Generalises to arbitrary angles
- More complex sequences give even better results
- quant-ph/0208092

How far can we go with NMR?

- NMR QCs with 2–3 qubits are routine
- Experiments have been performed with up to 7 qubits; 10 qubits is in sight
- Beyond 10 qubits it will get very tricky!
  - » Exponentially small signal size
  - » Selective excitation in a crowded frequency space
  - » Decoherence (relaxation)
  - » Lack of selective reinitialisation
  - » Lack of projective measurements
  - » *Fortschritte der Physik* **48**, 909-924 (2000)

Thanks to…