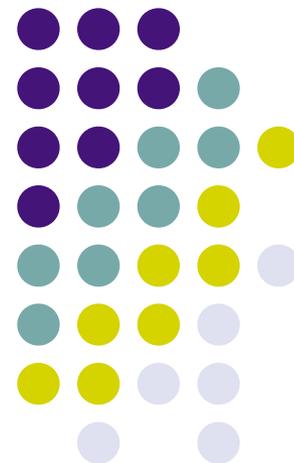


# Molecular Magnets in the Field of Quantum Computing

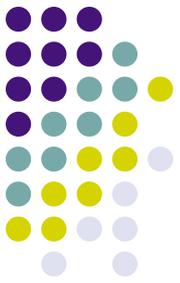


By Richard Cresswell  
Addison Huegel





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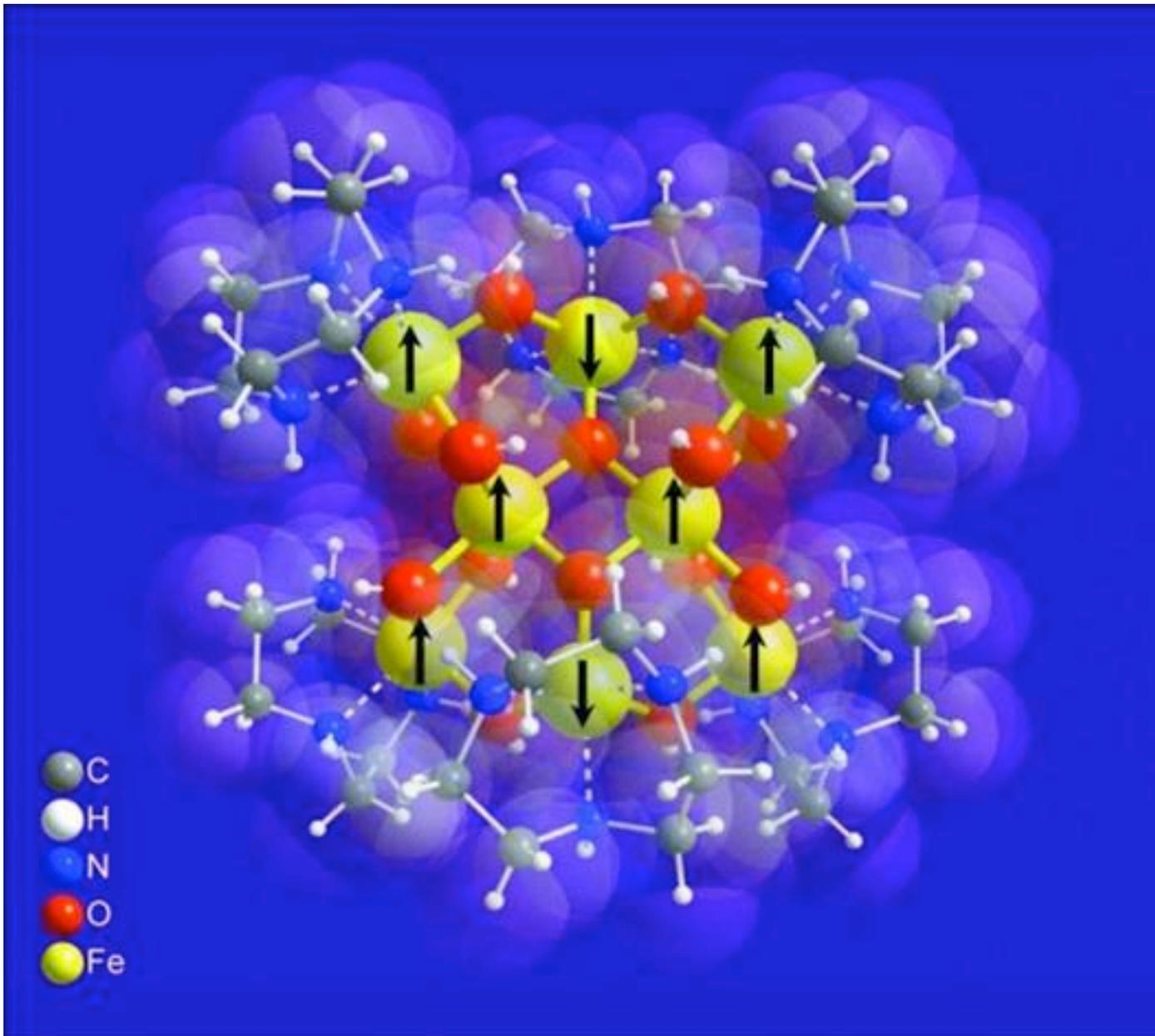


- Introduction
- Methods of Using Molecular Magnets as Qubits
- Improved Data Storage with Grover's Algorithm
- Di Vincenzo Evaluation
- Criticism

# Criteria for Molecular Magnets

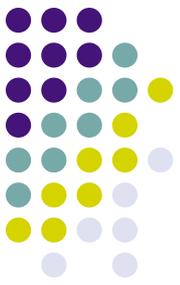


- Large Molecules – Little intermolecular interaction
- High total spin ( $S$ )
- High magnetic anisotropy (directional dependence)
- $\text{Fe}_8$ ,  $\text{Mn}_{12}$  are both  $S=10$



**Fig 1: View of the structure of the Fe<sub>8</sub> molecular cluster. The iron atoms (yellow) carry the magnetic moments that in the ground state are arranged to give  $S=10$ .**

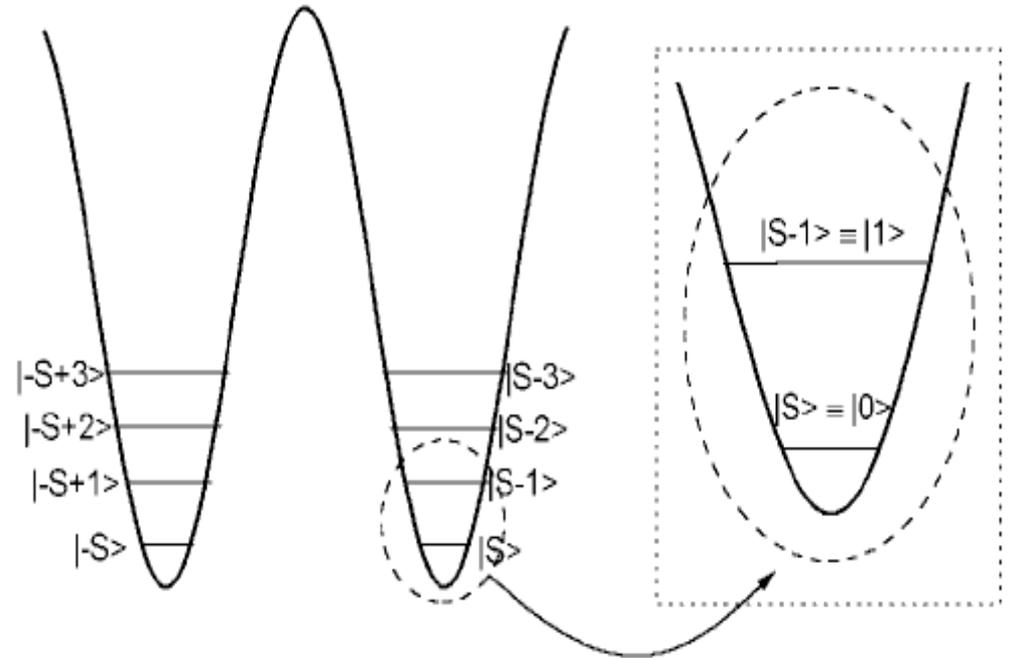
*R. Sessoli, Europhysics News 34, 2 (2003)*



# Using MM's as Qubits

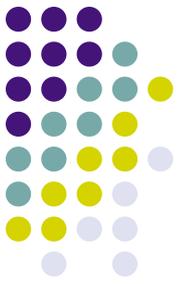
## Case 1: Suppressed Spin Tunneling

**Fig 2:  $|0\rangle$  is the ground state in one of the wells and  $|1\rangle$  is the first excited state, separated by an energy gap set by the ferromagnetic resonance frequency.**



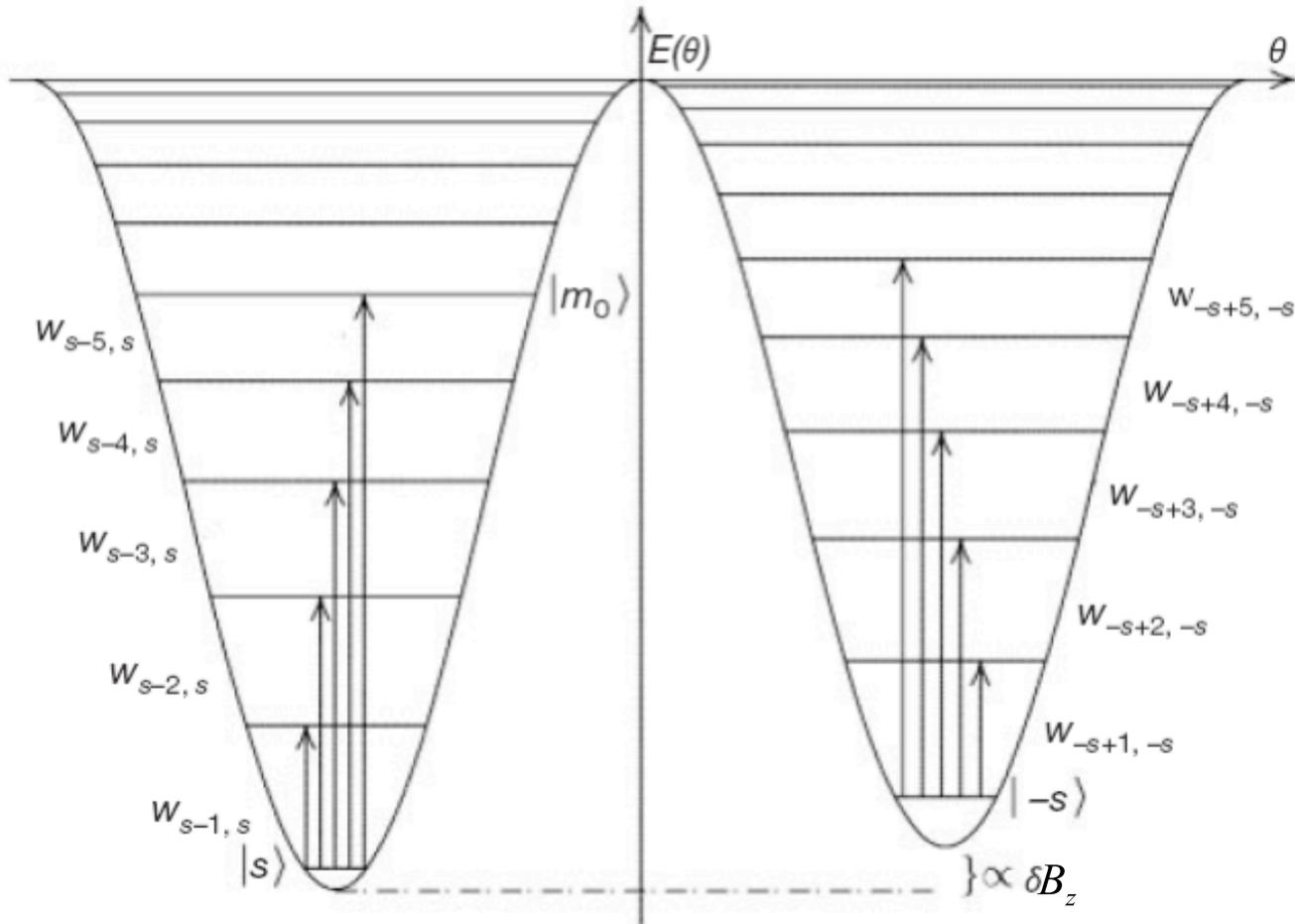
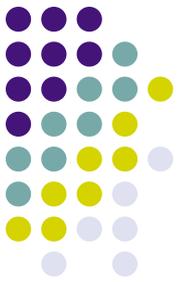
*J. Tejada et al, Nanotechnology 12, 181-186 (2001)*

# Using MM's as Qubits



## Case 2: Spin Tunneling

- High magnetic anisotropy  $\rightarrow S_z$
- Applying a longitudinal magnetic field ( $B_z$ ) in the easy axis will result in a shift in the potential wells.



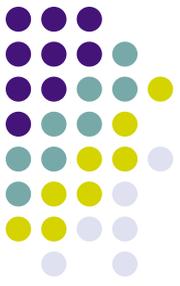
**Fig 3: Application of a longitudinal magnetic field causes a shift in the potential wells.**

# Spin Tunneling



- **Additionally, we apply a transverse magnetic field (  $B_x$  )**
- **For molecules like  $Mn_{12}$  and  $Fe_8$  the spin Hamiltonian (at low temperatures) is:**

# Spin Tunneling



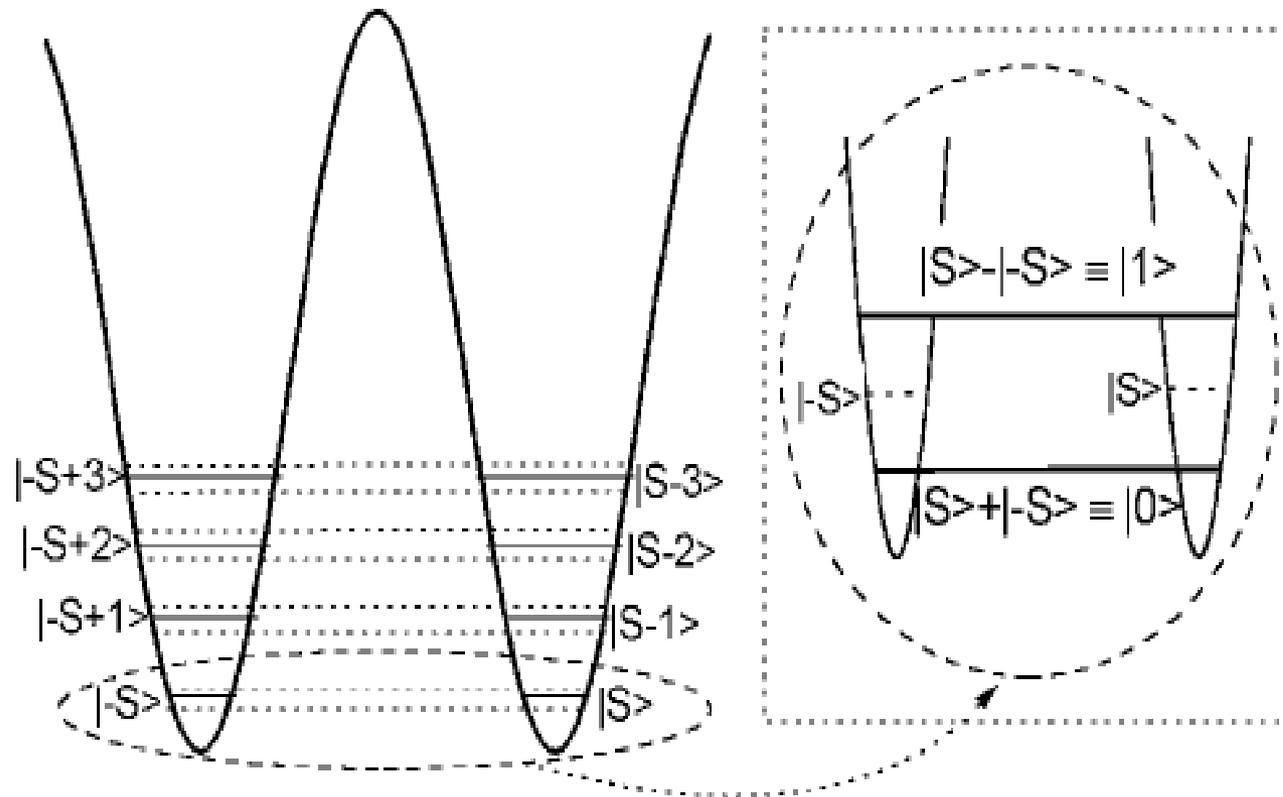
$$H = H_a + H_z + H'$$

- Where:

$$H_a = -AS_z^2 - BS_z^4$$

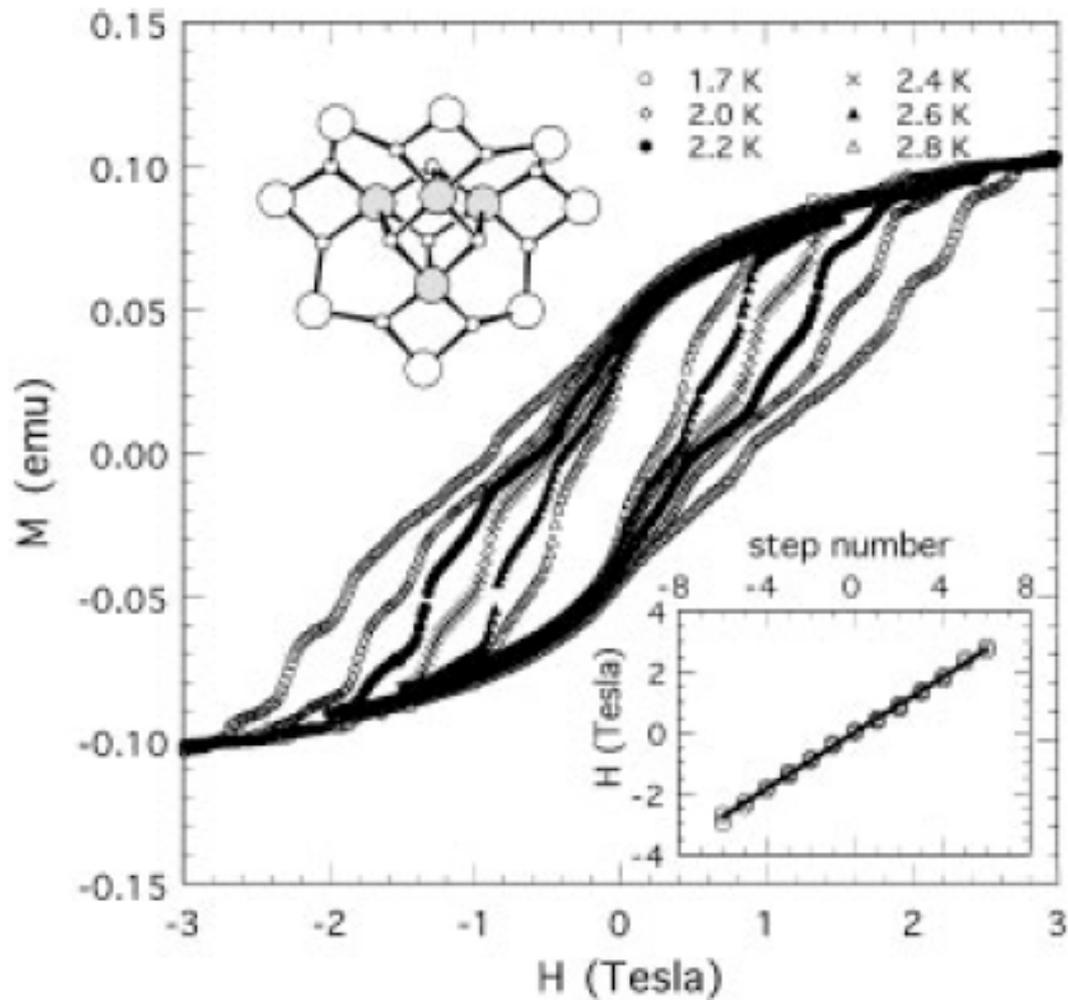
$$H_z = g\mu_B B_z S_z \quad \text{Longitudinal Field}$$

$$H' = g\mu_B B_x S_x \quad \text{Transverse Field}$$



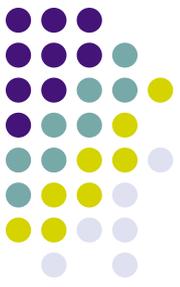
*J. Tejada et al, Nanotechnology 12, 181-186 (2001)*

**Fig 4:** The qubit states are the symmetric,  $|0\rangle$  and anti-symmetric,  $|1\rangle$  combinations of the twofold degenerate ground state  $S_z = S$ . The energy splitting between the qubit states depends on the spin tunnelling frequency and can be tuned using an external magnetic field perpendicular to the easy axis of the molecular cluster.



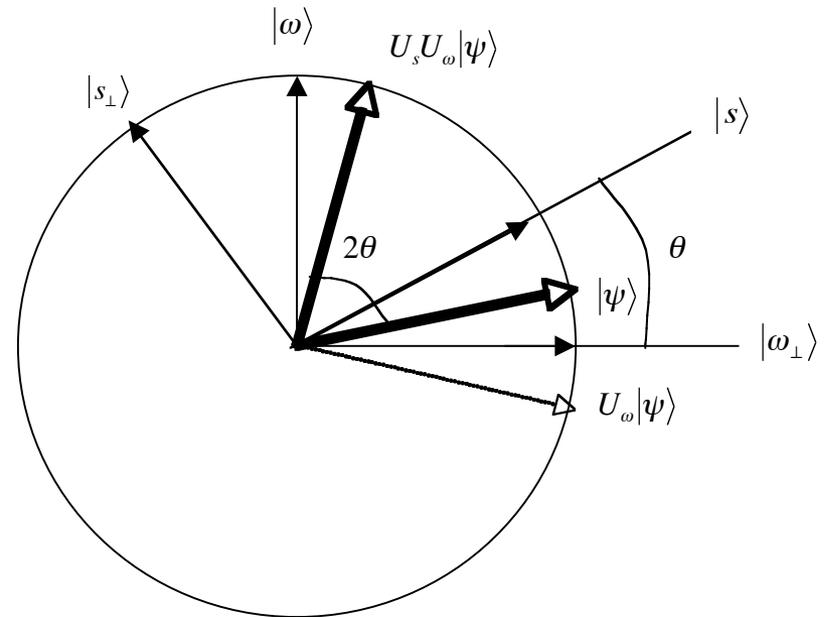
**Fig 5: Magnetisation of Mn<sub>12</sub> as a function of magnetic field at six different temperatures.**

*R. Friedman et al, Phys. Rev. Let. 76, 20 (1996)*

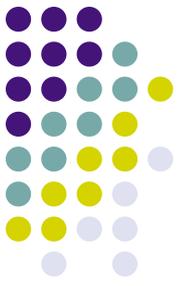


# Review of Grover's Algorithm

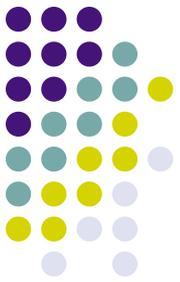
- Improves on classical database search  $O(N)$  to  $O(N^{1/2})$
- Algorithm iterated until system vector lies near to desired state
- Probability of measuring state close to unity



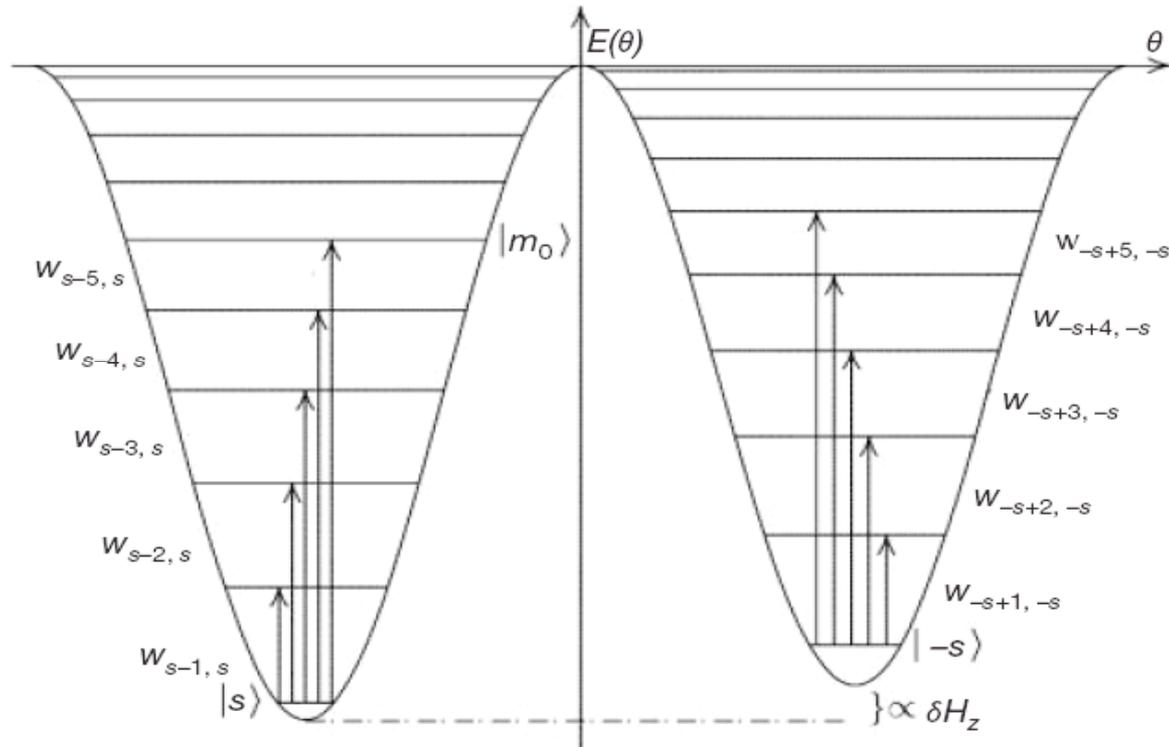
# Molecular Magnets As A Quantum Memory Device



- Utilize the spin eigenstates as qubits
- Each eigenstate represents a different binary unit i.e.  $2^0$ ,  $2^1$ ,  $2^2$ .....
- Apply a strong magnetic field along Z axis to initialise, then decrease to bias strength
- Use modified Grover scheme as described by Ahn, Weinacht and Bucksbaum, *Science* 287, 463-465 (2000) and Grover, *Phys Rev Letters*, 79, 4709-4712 (1997)

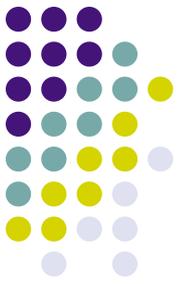


# Potential Well and Spin Eigenstates



Leuenberger and Loss, *Nature*, 410, 789-793 (2001)

# Superposition of States

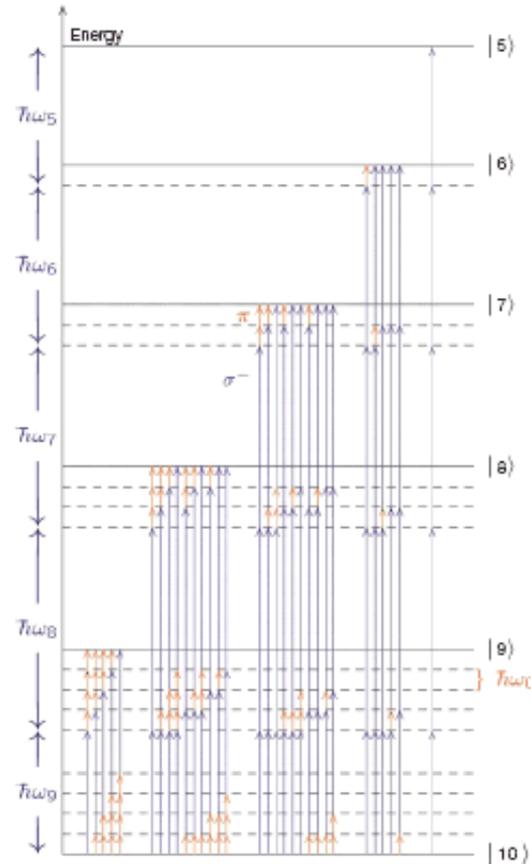
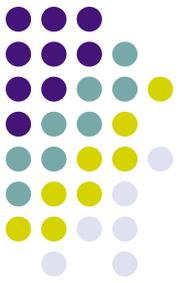


- Apply two magnetic fields to induce transitions between eigenstates

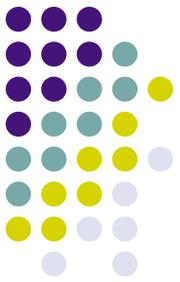
$$H_m(t) \left[ \cos(\omega_m t + \varphi_m) S_X - \sin(\omega_m t + \varphi_m) S_Y \right] \\ g\mu_B H_0(t) \cos(\omega_0 t) S_Z$$

- Perturbation theory determines field frequencies and strengths
- Non-equidistant energy level spacing means individual frequencies do not interact
- $\sigma$ -transitions and  $\pi$ -transitions populate all levels coherently with equal transition amplitudes as required by Grover's algorithm

# Transitions Between Spin Eigenstates



Leuenberger and Loss, *Nature*, 410, 789-793 (2001)

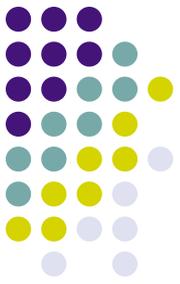


# Data Read-in

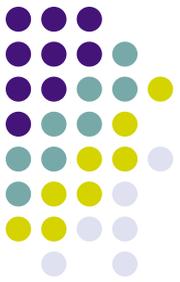
- Circularly polarised field adds individual phases to each transition amplitude (0 or  $\pi$ )
- $13_{10}=1101_2$  requires phases  $\varphi_9=\varphi_8=\varphi_7=0$ ,  
 $\varphi_6=\varphi_5=\pi$ , as different states require different numbers of  $\sigma$  photons
- Transition amplitudes are then  $\varphi_m$  and form the basis of a quantum data register,  
$$|\psi\rangle = \sum_{m=m_0}^s a_m |m\rangle$$



# Decoding Data

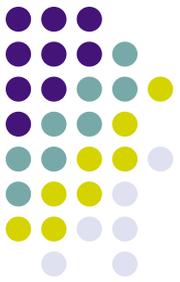


- Magnetic pulses similar to the encoding process are applied but with different phases
- Phases are independent of stored data, as the pulse acts as a unitary transform on the system. So for previous example  $\varphi_9 = \varphi_7 = \varphi_5 = 0$  and  $\varphi_6 = \varphi_8 = \pi$
- Transform amplifies flipped bits, other bits are suppressed, marking up the state
- Transforms amplitude of states by  $\eta$



# Data Read-out

- Irradiate system with pulse containing frequencies  $\omega_{m-1,m}$
- Induce transitions between populated levels and neighbouring states
- Non-equidistant energy levels give characteristic spectrum



# The Capabilities of This Device

- Capable of storing numbers as large as  $2^{2s-2}$  if both wells are utilised
- Even as high as  $M^{2s-2}$  if M phases are distinguishable
- Read-in, decode, read-out time of  $10^{-10}$  s
- Measurement of spins made easier by ensemble nature of molecular crystals
- Crystals of length  $10 \mu\text{m}$  easily grown naturally



# Limitations?

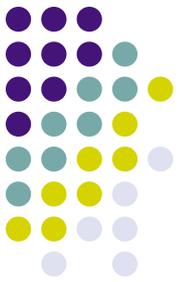
- Cannot scale to arbitrarily high spins - decoheres to classical physics
- Hence limited number storage
- Requires the control of  $\log_M N$  frequencies



# Di Vincenzo Evaluation

*[1] Identifiable Qubits:*

- Case (1): In the suppressed tunneling method GS and 1<sup>st</sup> excited state are separated by an energy equivalent to the ferromagnetic resonance frequency.
- Case (2): Must be arranged in a controlled manner.

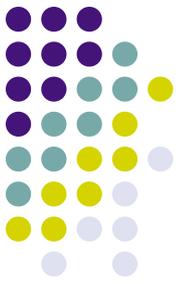


# Di Vincenzo Evaluation

*[2] State Preparation:*

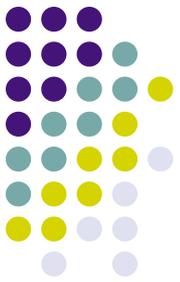
- Case (1):  $T$  much less than the energy gap ( $\sim 4\text{K}$ ).
- Case (2): Equilibrium at very low temperature (mK) in a transverse field.

# Di Vincenzo Evaluation



*[3] Decoherence:*

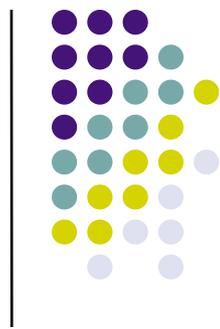
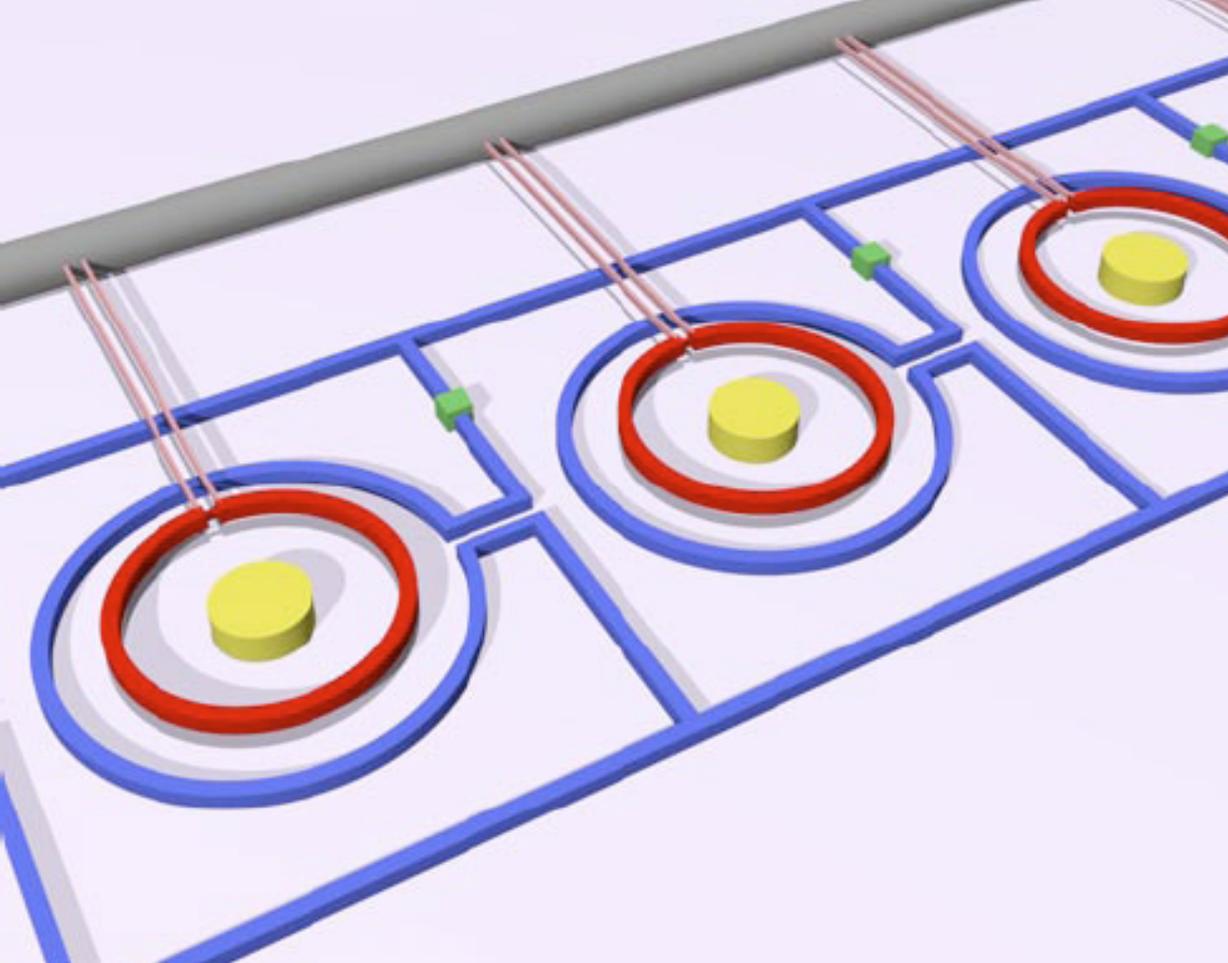
- Resonance experiments have shown that quantum coherence can be maintained for at least 10ns.
- Corresponding quality factor (Q) of  $10^6$ .
- Note that the decay of an excited state cannot come through the spontaneous emission of a photon.



# Di Vincenzo Evaluation

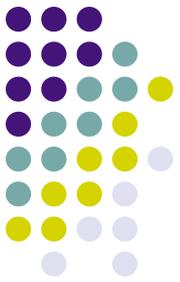
*[4] Quantum Gates:*

- Realisation of single qubit gates can be done by achieving Rabi oscillations between the GS and the 1st excited state.
- Two qubit gates can be achieved by coupling neighbouring qubits through superconducting loops possibly with Josephson switches.



*J. Tejada et al, Nanotechnology 12, 181-186 (2001)*

**Fig 6:** A schematic example of the coupled controlled qubit realization. The magnetic qubits (clusters/particles, yellow) are arranged in a one-dimensional lattice and coupled to the superconducting loops of micro-SQUID (red) circuits as shown. The coupling circuits (blue) contain Josephson switches (green).



# Di Vincenzo Evaluation

*[5] Measurement:*

- Individual microSQUIDs are needed to measure the spin state of the system.
- Limitation of technology  $\sim S=10,000$

# Criticism

- T dependence
- Individual system isolation
- Very low noise



# Thanks for Listening

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