Molecular Magnets and Quantum Resonant Tunneling

Hua Chen

Solid State Physics II
Magnetism at Different Scales

permanent magnets  micron particles  nanoparticles  clusters  molecular Magnets  Individual spins

100 nm  10 nm  1 nm

$S = 10^{23} \quad 10^{10} \quad 10^8 \quad 10^6 \quad 10^5 \quad 10^4 \quad 10^3 \quad 10^2 \quad 10 \quad 1$

multi-domain
Motion of domain walls

single-domain
uniform rotation

single molecule
quantum tunneling
Single-Domain Nanomagnets: Classical Stoner Particles

- **Origin of Hysteresis:** Irreversibility

Macroscopic Magnets: Crystal disorder

Single-Domain Nanoparticles: Bi-stability from anisotropy

![Energy diagram showing the state transition from up to down](image)
Molecular Magnets

\[ \text{Mn}_{12} \quad S = 10 \]

\[ \text{Ni}_{12} \quad S = 12 \]

\[ \text{Mn}_{84} \quad S \approx 6 \]

\[ \text{V}_{15} \quad S = \frac{1}{2} \]

\[ \text{Fe}_8 \quad S = 10 \]

Lis, 1980

Müller, 1993

Winpenny, 1999

Christou, 2004

Wiegart, 1984
The First Single Molecule Magnet: 
Mn$_{12}$-acetate

Lis, 1980

$[\text{Mn}_{12}\text{O}_{12}(\text{CH}_3\text{COO})_{16}(\text{H}_2\text{O})_4]\cdot2\text{CH}_3\text{COOH}\cdot4\text{H}_2\text{O}$

Mn$^{3+}$  \hspace{1cm} $S = 2$

Mn$^{4+}$  \hspace{1cm} $S = 3/2$

Oxygen

Carbon

Well defined giant spin ($S = 10$) at low temperatures ($T < 35$ K)
Strongly superexchange-coupled through oxygen bridges ($J \sim 100$ K)
Uncommon Hysteresis

- Magnetization versus applied field. Inset shows values of field where jumps in the magnetization are observed.

Macrospin Model

\[ H = -D S_z^2 - g\mu_B S_z H_z + H' \]

- Anisotropy
- Zeeman
- Tunneling

Lifted by external field

\( m = S \cdot 2 \)
\( m = S \cdot 1 \)
\( m = S \)
\( m = -S + 2 \)
\( m = -S + 1 \)
\( m = -S \)
**Origin of Steps: Resonant Tunneling**

\[
H = -DS_z^2 - g\mu_B S_z H_z + H'
\]

\[
H_z = -Dn/g\mu_B
\]
What Causes Tunneling?

\[ H = -DS_z^2 - g\mu_B S_z H_z + H' \]

• For Fe\textsubscript{8} : Transverse anisotropy energy

\[ H' = E(S_x^2 - S_y^2) \]

• For Mn\textsubscript{12} : Not clear
Energy Spectrum of Fe$_8$

Probability of NO Crossing:
Landau-Zener formula

$$P = 1 - \exp\left(-\frac{\pi \Delta^2}{\beta}\right)$$

No Crossing Means Tunneling

Possible Origins of Tunneling in Mn$_{12}$

- Transverse external field
- Fourth order transverse anisotropy
- Spin-phonon interaction
- Dipolar interactions between neighboring molecules
- Hyperfine interaction with the Mn and other nuclei in the system
- ....
One Possible Application: Quantum Computing

Michael N. Leuenberger & Daniel Loss
NATURE, 410, 791 (2001)

- implementation of Grover's algorithm
- storage unit of a dynamic random access memory device.
- fast electron spin resonance pulses can be used to decode and read out stored numbers of up to $10^5$ with access times as short as 0.1 nanoseconds.
Thank You