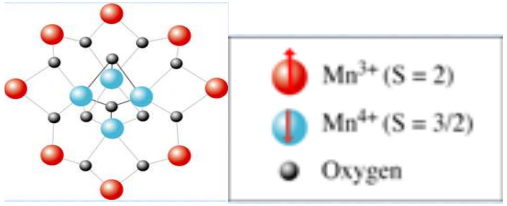
# Quantum Magnetic Deflagration in $Mn_{12}$-acetate

Reem Jaafar, Eugene Chudnovsky, Dmitri Garanin, Lehman College.

## Molecular Structure of $Mn_{12}$-acetate



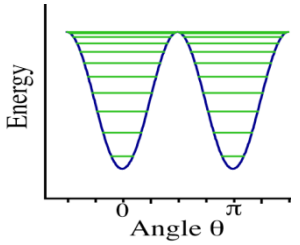

Low Temperature.
Strong antiferromagnetic exchange coupling
through the oxygen bridges
Large uniaxial anisotropy ~ 60K

## SMM: Basic Characteristics

**They are organic materials which contain a large number of identical magnetic molecules.**
**They contain magnetic clusters composed of several or many magnetic atoms coupled together at low T to form a cluster of moderate to large total spin.**
**The net spin of each molecule is determined by the exchange interaction between the magnetic moments of the atoms in the molecule.**
**At sufficiently low T, the individual magnetic moments couple together to form a composite spin particle or "single molecule magnet".**
**Mn-12 first synthesized by Liz in 1980, and characterized by X ray diffraction. (Reference 1a )**

## Spin Hamiltonian for $Mn_{12}$-acetate

$$\hat{\mathcal{H}} = -DS_z^2 - AS_z^4 - g\mu_B H_z S_z + V_T$$




$D = 0.54K$

$A = 1.1mK$

$g = 1.94$

## Quantum Tunneling of Magnetization

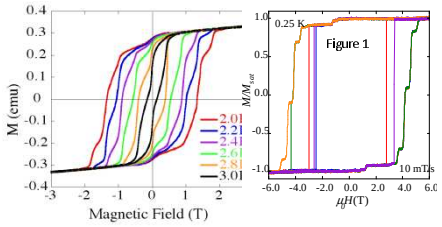
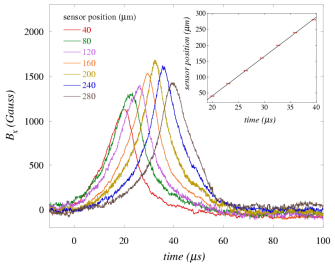


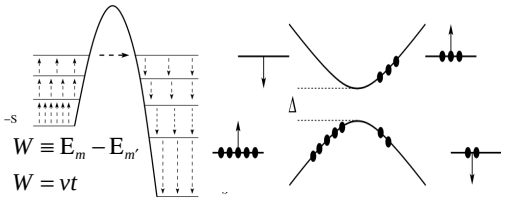

Figure 1

Instead of having well defined steps in the magnetization curve, there could be a sudden jump in the magnetization for a certain values of the field. This is an avalanche, as shown in the red and purple curves in figure 1.
Experiments have been performed to find the velocity of propagation of the avalanche and a theory has been developed to elucidate and the criteria of ignition.

To find the velocity of propagation of the avalanche, Suzuki et al. (Reference 2) has timed the arrival time of the avalanche as it propagates through the sample by placing hall sensors along the c-axis of the sample.



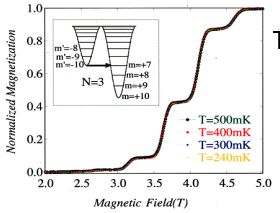

## Landau - Zener effect




$$W \equiv E_m - E_{m'}$$

$$W = vt$$

$$E_+ - E_- = \sqrt{W^2 + \Delta^2}$$



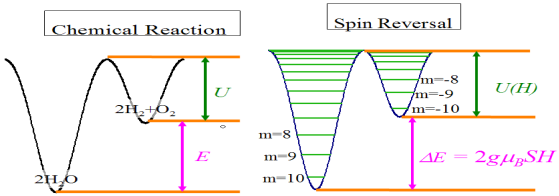

### Transition probability

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

K. M. Mertes, Yoko Suzuki, M. P. Sarachik, et al. cond-mat/0106579

## Avalanches

In this fast reversal of the magnetization, called avalanche, the relaxation of the magnetization towards the direction of the field results in the release of heat. This process is analogous to the propagation of a flame front through a flammable chemical substance (Deflagration).




The velocity of propagation of the avalanche as done by Suzuki et al. (Reference 2) is shown in figure 2. Subsequent measurements done by A. Hernandez-Minguez et al. showed a peak for certain values of the field (Figure 3, Reference). This has been attributed to "Quantum magnetic deflagration."

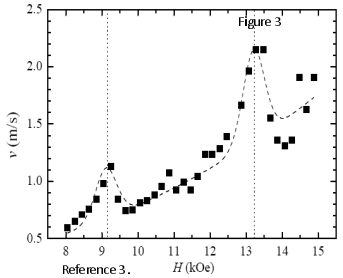



Figure 3

Reference 3.

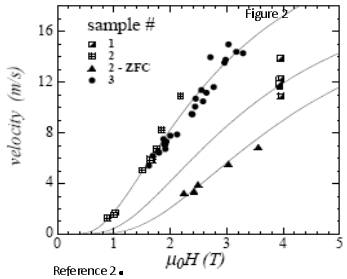



Figure 2

Reference 2.

E.Chudnovsky and D. Garanin developed a theory of the magnetic deflagration in molecular magnets (Reference 4). In contrast with chemical deflagration, magnetic deflagration is reversible, a front can be ignited many times in a sample without destroying it. This raises several questions: what are the right combinations of parameters (field and temperature) that would cause a sample to avalanche and what is the speed of the deflagration front?

According to Reference 4, deflagration begins as a thermal runaway in part of a sample that has a lower barrier U or a higher temperature T than the surrounding area. The ignition time is the time it takes for the thermal runaway to develop. A parameter δ, which defines the ignition of the deflagration, is proportional to U, the barrier, n, the initial value of the metastable population and to Γ, the ignition rate. It is inversely proportional to κ0, thermal diffusivity.
In the case of uniform energy barrier and constant temperature maintained at the boundaries, a plot of the field that ignites the avalanche versus the temperature of the sample gives the plot below (Figure 4).

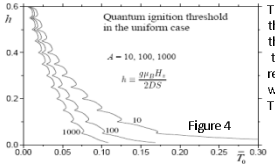
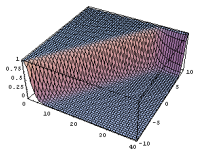


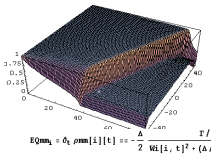

Figure 4

The plot and the theory above are for the case of static field. We'd like to solve the problem by taking into account the field dynamics at any particular moment and the influence of the dipolar field. So far, relaxation problems have been studied using the secular approximation which breaks down at resonance. To properly study magnetic relaxation, we need to study the system of molecular magnets in the non secular case which is always valid.
To achieve that, we need to use the density matrix theory.

The density Matrix theory is used to describe a system that is a part of a larger system with which in interacts (Reference 5). Here, we have a system of S = 10 molecules which interacts with a bath of phonons.
According to reference 4, the width of the deflagration front is given by: $l_d = \sqrt{\frac{\kappa_0}{\Gamma_f}}$
The relaxation rate Γ is a function of E, the phonon energy.
Using density matrix theory, we set Γ as a function of E and W (as opposed to Γ being a function of E only) , W being the energy bias for a given resonance. Then Γ(E,W) is calculated numerically from the density matrix theory and is interpolated to form a given function. Then we add the dipolar bias to find the new form of the deflagration front.



A propagating front (n vs x and t) when the temperature of the left hand side of the sample rises quickly and that of the right hand side is maintained at fixed T, without taking into account the dipolar field.



Another example of a front propagating for the case including he internal dipolar field. It is obtained by solving the equation below for a fixed rate Γ.

The next step would be to use the rate Γ found numerically from density matrix theory to find the new shape of the front and see how the dipolar field and the field dynamics affect the deflagration front.

1a) T. Lis, Acta Cryst. B69, 2042 (1980).
1b) J. R. Friedman et al. Phys. Rev. Lett. 76, 3830 (1996).
2) Y. Suzuki et al. Phys. Rev. Lett. 95, 147201 (2005).
3) A. Hernandez-Minguez et al. Phys. Rev. Lett. 95, 217205 (2005).
4) D. A. Garanin and E. M. Chudnovsky, Phys. Rev. B 76,054410 (2007).
5) D.A. Garanin, arxiv: 0805.0391.