Quantum fragmentation and classical restoration of spins

Consider a small ferromagnetic particle — so small that it contains just a single magnetic domain — placed in a magnetic field. If one reverses the direction of the magnetic field, how fast and via what path does the magnetisation change direction? This problem of classical physics was treated in 1948 by E. Stoner and E. Wohlfarth. Their model, which calculates the (zero-Kelvin) free energy of the particle, has been applied to ensembles of small magnetic particles in many areas of physics, chemistry or metallurgy such as magnetic metal alloys and glasses, mineral solid solutions, steels, gels, ceramics, and the tiny bits on computer hard-disks... More recently, similar models have been developed for nanoparticles and single-molecule magnets, objects so small that their magnetic energy is quantized into discrete values. Here we discuss a fundamental question: Can one link these two very different views of the magnetism of small particles, *i.e.* the classical and quantum physics ones?

Imagine a ferromagnetic nano-scale object, at zero K, with some tens or hundreds of spins coupled to make a large total spin S with a preferential orientation (its anisotropy axis Oz). The spin S, projected on this axis, has $2S+1$ sub-states, M_z. We have investigated, numerically, a theoretical model that has a parabolic energy barrier against spin reversal, a fixed perpendicular field H_x and a sweeping longitudinal field H_z. Fig. 1 shows one example, the 41 energy levels of a spin $S=20$. We have fixed $H_x=1$ and H_z sweeps from +1 at the right of the Figure to -1 at the left, at a constant rate c. The resultant field rotates from +45° to -45°. (Our Hamiltonian is, in reduced units, $H=-Ds_z^2-H_xs_x-H_z(t).s_z$, with the anisotropy parameter $D=1$ and with reduced spins $s_x=S_x/S$, $s_y=S_y/S$, $s_z=S_z/S$ to catch the proper limit as S approaches infinity.)

Starting from large positive H_z at the right of Fig. 1, the ground-state $M_z=20$, well separated from the higher levels with $M_z=19, 18...$, is essentially not mixed (it is quasi-classical) and, since $T=0$ K, its probability of occupation is 100%. This ground state remains fully occupied until $H_z=0$ where the first level-crossing between S and $-S$ is reached. Because of the perturbative effect of H_x, this is an avoided level crossing (an "anticrossing") so the system can, in principle, switch from $M_z=+20$ to $M_z=-20$, but the probability of this is vanishingly small for these large M_z states, even at very low sweeping rates.

For $H_z<0$ (at the left in Fig. 1), the state $M_z=S=20$ is no longer the ground state. We now call it the metastable state — or metastable branch. As the field-sweep continues, this state crosses the levels $M_z=-19$, ..., $-S+k$, ... The exponential increase of the successive anti-crossing gaps (which are proportional to $(H_x/DS)^{2S-k}$) makes spin-reversals and spin-mixtures more and more probable until the semi-classical spin S scatters along the different states below the metastable branch. We now call this spin "fragmented".

In collaboration with colleagues in Japan, we have calculated, numerically, the Quantum Dynamics of such a system at zero Kelvin with S ranging from 20 up to 320. More particularly, we have calculated for each spin value the integrated probability of spin-reversals associated with full field-sweeps, going from large positive to large negative fields H_z. We showed that all the data can be merged on to a single scaled dynamical curve as a function of S and $H-H_{SW}$ (Fig. 3 of Hatomura *et al.* 2016). Interestingly, this scaling curve valid for large quantum spins up to infinite (*i.e.* classical) spin shows that quantum dynamics is permitted for any field H_z between zero and H_{SW}. However, as expected, the probability of spin reversal goes to strictly zero there as S approaches infinity, except at the threshold $H=H_{SW}$ where spin reversal onsets very sharply in these calculations, as in the classical-physics model.

Furthermore, this function turns out to be identical to the scaling curve of the so-called "Spinodal" Phase Transition, a very general process in physics, where this function represents the probability to find "non-yet-flipped" particles in an ensemble of N diffusing particles subjected to external (usually thermal) fluctuations. This suggests that a large quantum spin S could be regarded as an ensemble of N = 2S spins ½ (↑ and ↓) having the possibility of one or more spins flipping from ↑ to ↓ at the different anti-crossings of the metastable branch. The integrated probability of spin-reversals near and at the Stoner-Wohlfarth reversal field H_{SW} (the red vertical bar in Fig. 1), our spinodal phase transition, can then simply be associated with the "fragmented" spin resulting from the spin-flips at the successive $S \rightarrow -S+k$ anti-crossings (k spin-flips).

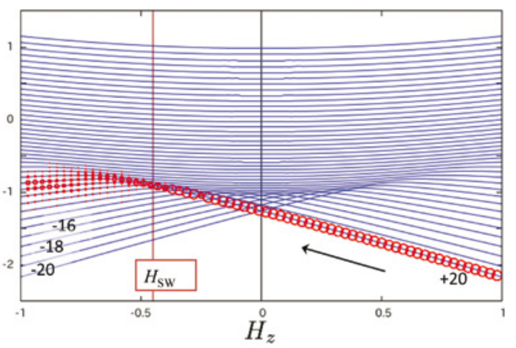

***Fig. 1**: Energy spectrum for a spin S=20. The longitudinal field H_z sweeps from right to left, which leads to spin-reversals from the ascending energy level (m =+20) to the descending levels when H_z is negative and large enough. The gaps at each avoided level crossing cannot be seen at the scale of the Figure. The sizes of the red circles indicate the probabilities of occupation of the states at zero Kelvin.*

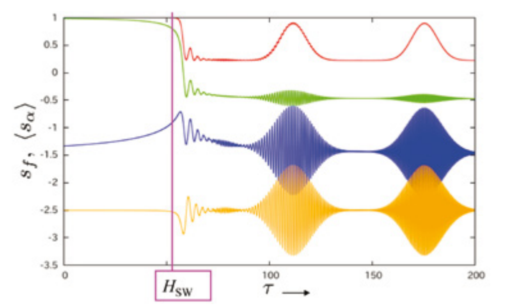

***Fig. 2**: As the field sweep continues (from left to right at constant rate c) beyond the Stoner-Wohlfarth transition at H_{SW}, the calculations yield temporal beats of (from bottom to top) the expectation values of S_x, S_y, S_z and the spin length. This beating represents the long-range spinodal modulations of the Stoner-Wohlfarth model.*

Since a consequence of the spinodal phase transition is an onset of a modulation of the order parameter, one should expect the emergence of a stable sinusoidal modulation of the spin dynamics as a function of H_z (and so with time) as H_z is swept (at constant rate c) more negative than H_{SW}. This is precisely what we found (in the absence of damping/decoherence): The calculations show long-period modulations of the "restored", *i.e.* no longer "fragmented" precession of the whole spin S, see Fig. 2. Constituting a new characteristic of Quantum Dynamics, these spin beats can also be viewed as resulting from classical interferences of the superposed spin-states ($M=-S, -S+1, -S+2, ..., S$).

Experiments are planned to observe the spinodal dynamical scaling, and also the spin beating (though this would be harder). Among the numerous outlooks of this study, the most obvious one is achieving better understanding of the nature of the quantum to classical transition.

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FURTHER READING...

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