CONDENSED MATTER THEORY (CMT)

PHENOMENOLOGIC VERSUS MICROSCOPIC DESCRIPTION OF THE NANOPARTICLE MAGNETIZATION

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One of the main reasons behind the widespread use of phenomenologic approaches for the description of nano-structures is the higher degree of complexity of the physical mechanisms acting at the nano-scale when compared to the "thermodynamic limit". As concerns magnetization of ferromagnetic nano-particles, it is common to rely on a generalization of the well known Bloch "$T^{3/2}$" law where the power of temperature becomes a parameter determined by comparison to experimental data or numerical cluster simulations:

$$M(T) = M(0)\left(1-\gamma T^{\alpha}\right) \qquad (1)$$

In an earlier paper, [1], we have shown that although due to its flexibility this expression is indeed successful in fitting the observed behavior, it nevertheless suffers from serious inconsistencies concerning its physical content. Based on the spin-S Heisenberg model with nearest neighbor exchange J coupling we have proposed a new microscopic approach which has lead to a different form of the Bloch law generalized to a finite size ferromagnet. We have shown that experimental data are reproduced equally well, but in this case the physical behavior can be understood in terms of the magnon gas concept. In the present work a further development of the microscopic approach has allowed us to explain another "puzzle" generated by the phenomenological description. Thus, when for samples of a decreasing size (below 10 nm) one finds values of the parameters in Eq. (1) which deviate form those of the bulk limit in an apparently chaotic pattern. We explain this behavior by taking into account the shape effect of the synthesized nano-particles on the temperature dependence of their magnetization

$$\begin{aligned}
N \le L \quad &: \frac{M(T)}{M(0)} \cong 1-\zeta(3/2)\times\left(k_B T / J4\pi S\right)^{3/2}/S + \frac{4-L/N}{N}\times k_B T/\left(J4\pi S^2\right) \\
N \ge L \quad &: \frac{M(T)}{M(0)} \cong 1-\zeta(3/2)\times\left(k_B T / J4\pi S\right)^{3/2}/S + \frac{3-2\ln(N/L)}{L}\times k_B T/\left(J4\pi S^2\right)
\end{aligned} \qquad (2)$$

In the above example we have a rectangular sample $N\times N\times L$ of an elongated and an oblate shapes (ion spacing is set to *1*, formula contains Riemann ζ-function and Boltzmann constant). As can be seen, the magnetization of a more symmetric sample (e.g. cubic) is above that of a bulk, while for a deformed sample the deviation from the bulk value can have opposite sign.

Our microscopic approach allows to describe in an explicit form the boundary and surface effects as well, which till were only investigated by methods of numerical simulation of small clusters.

[1] S. Cojocaru. *Solid State Comm.* **151** (2011) 1780–1783.