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I started my Ph.D. one year ago. So far, my research activity has dealt with ab-initio simulations in solid-state physics.
The main subject of my Ph.D. is the Spin-Seebeck effect (SSE), a new and astonishing result which could lead to a better understanding of fundamental microscopic magnetic properties of matter and to applications in Spintronics, Caloritronics and Thermoelectrics. In previous works, I dealt with crystallographic phase transitions in Calcium and the low temperature behavior of Finite-Size Spin-Glass.

Ab-inito study of SSE in ferromagnetic metals

SSE was experimentally discovered in 2008 by Uchida et al. [17] and opens new streets in the field of renewable energy technologies, in particular for what concerns the reuse of heat dissipated by current technologies and the efficiency of future technologies. Understanding of the SSE is a fundamental step in the development of Spintronics, which uses spin-dependent electron transport phenomena for carrier propagation in solid-state devices. It is the basis of a new field of research called Caloritronics, which introduces thermal aspects in this scheme, in particular magnetic heat transport, magneto-thermal response, and spin-related thermoelectric effects.
The SSE converts a heat current into a spin current. Spin currents propagates the spin degree of freedom, and can be used instead of electrical currents in electronic devices, reducing the energy necessary for transmitting information.
Together with other innovative effects discovered recently (i.e. Inverse spin Hall effect), SSE can be used to generate electrical voltages from a temperature difference [2].
After Uchida and his collaborators, other groups found experimental evidence of SSE in different classes of ferromagnetic materials. In particular, Jaworski et al. highlighted the presence of SSE in ferromagnetic GaMnAs semiconductors [11] and then, Kajiwara et al. [12] first and then Uchida et al. [18] revealed SSE in magnetic insulators.
In all these experiments, similar characteristics were found for the different classes of materials, both qualitatively and quantitatively (characteristic lengths, dependence on the temperature gradient).

So far, no fully satisfactory theoretical explanation exists, since it is difficult to reconcile the many new and astonishing results with a single theory. The microscopic mechanism leading to the SSE is expected to be independent of the features of the particular material studied (i.e. energy bandgap).
On the contrary, the leading hypothesis considered in SSE theoretical models is the collective motion of spins, which can propagate also in insulators. Thus, the ideal candidates for the propagation of spin currents in materials are magnons, or quantized spin-waves.

On October, 21, 2011, I presented a research project on SSE to the Education Ministry of the Belgian French community which was approved (Ref. F 3/5/5-MCF/ROI/BC-20.004).
Over the next 3 years my research will deal with spin currents in ferromagnetic materials. In particular, I will simulate by ab-initio DFT metal alloys which are close to the real alloys used in Ref.[17]. A complete study of the structure will be carried out, and standard spin diffusion will be analyzed. In a second step, the behavior of magnetic excitations, which are not yet systematically introduced in ab-initio calculations, will be analyzed.
The outcome of the Ph.D. project is to clarify how magnons interact with other excitations in the system, and how the temperature influences this interaction.

Stability of Calcium high pressure phase

Calcium undergoes a sequence of phase transitions which was discovered for the first time in 1983 by H.Olijnyk and W.B. Holzapfel [13] and was confirmed by Q. F. Gu et al. in 2009 [8]. In 2005 Yabuuchi et al. [15] pressurized Calcium further and highlighted the existence of others high-pressure phases with new and interesting physical properties. As an example, superconductivity was observed in Calcium at 50 GPa with critical temperature $T_c = 1.2K$. The critical temperature increase linearly up to reach the highest value ever registered (25K at 161GPa for the so-called CaV phase of Calcium).

The phase transition pattern followed is:

$$\begin{aligned} fcc(0-19.8GPa) \rightarrow bcc(19.8-33GPa) \rightarrow sc(33-113GPa) \\ \rightarrow CaIV(113-127GPa) \rightarrow CaV(127-139GPa) \rightarrow ... \end{aligned} \tag{1}$$

This behavior is counter-intuitive, in fact, one expect that, by applying an increasing pressure, the coordination number (i.e. the number of first neighbors) would increase as well, but, thanks to an hybridization of the s and d orbitals due to Calcium band-structure, electrons are transferred to the d orbital, so this number decreases under pressure.

Different attempts were carried out to understand what determines such an unusual behavior, nevertheless a real agreement between theory and experiment is still missing. Indeed, the latest theoretical phase transition pattern for Calcium is [9]:

$$
\begin{aligned}
fcc(0-3.5GPa) &\rightarrow bcc(3.5-35.7GPa) \rightarrow Cmcm(35.7-52GPa) \\
&\rightarrow P4_32_12(52-109GPa) \rightarrow Cmca(109-117.4GPa) \\
&\rightarrow Pnma(117.4-134.6GPa) \rightarrow I4/mcm(00\frac{4}{3})(134.6GPa-...)
\end{aligned}
\tag{2}
$$

where different structures are considered (the orthorhombic Cmcm, Cmca [16] and Pnma [20], the tetragonal $P4_32_12$ [10] and $I4/mcm(00\frac{4}{3})$ [14]). None of these works predict the existence of a stable simple cubic phase for Calcium in the 33-113 GPa phase range, giving imaginary frequencies for the *sc* structures which is stable at room temperature according to experiments.

This problem is probably due to phonon anharmonicity, which must be included in order to obtain consistent results in finite temperature ab-initio DFT. These effects are important for the correct determination of the most stable structure at room temperature in the high pressure zone ($P > 30GPa$).

Some clues in this direction have been given by molecular dynamic simulations which naturally incorporate anharmonic contributions: for instance, Yao et al. showed that as the temperature increases from 5 to 300K, the favored phase goes form $I4_1\backslash amd$ to *sc* [19]

In our work [4], we consider the harmonic and anharmonic contribution to the total energy of the system calculated explicitly. Anharmonic contributions becomes more and more important when temperature increases. They should be then systematically introduced in ab-initio calculations for materials carried out at finite temperature. Moreover, we calculate the phononic entropy (which is important but not determinant to a corrected phase diagram) and we carry out electron-phonon coupling calculations at 35 GPa, which allow us to compute the transport properties of the system, such as the electrical resistivity, and to compare with experimental results.

Replica trick in a Finite Size Spin-Glass

My first scientific work [3] is my Master's thesis which dealt with finite size effect in Spin-Glass.

Spin Glasses are magnetic alloys in which a large quantity of impurities is spread at random. This system presents quenched disorder, with frustrated inter-atomic interactions.

In the thermodynamic limit, no conventional long-range order can be established (neither ferromagnetic nor anti-ferromagnetic). Nevertheless, for low-temperatures, the system exhibits a phase transition towards a new kind of order in which the spins are aligned in random directions. This new phase is called the "Spin-glass phase", and spins seem to remain out of equilibrium even if they are left to relax under constant experimental conditions for days or weeks. This is a metastable phase that can be observed, for example, in real glasses. This behavior is due to the fact that spins "freeze" according to extremely complex ordering patterns. In spite of this, it is believed that the equilibrium

properties of the low-temperature phase controls their non-equilibrium behavior. All these features can be interpreted simply if we suppose that an extremely large number of pure states (or phases) exist for very large systems. Replicas have been proposed as a crucial tool in the study of spin glass systems [1], and a correct solution for the infinite spin glass has been found (Parisi's Replica Symmetry Breaking [5],[7],[6]) with a successful Ansatz (mean field approximation).
Due to its generality, the Spin-Glass model is particularly convenient for the modeling of different kinds of disordered systems (structural glasses in condensed-matter physics, optimization in computer science, quantum information, econophysics, etc) and useful for many applications: i.e. decreasing noise in signal transmission without increasing the signal source power.
In this work I analyzed the simplest non-trivial finite size spin glass, i.e., the system with $N = 3$ spins. For this system the partition function can be computed exactly, so the analytic result is known. Using the symmetric replica approach, we showed that good predictions for the free energy of the system can be obtained within the limit of low temperatures, without explicitly computing the partition function. We also illustrate a generalization of our approach, which yields an efficient rule for the calculation of the free energy of an arbitrary N -spin system.

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