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Magnetic and vibration excitations induced by collision in ferromagnetic cluster

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Abstract. We investigate the excitations induced by the diffusion of a spin polarized projectile on a ferromagnetic spin polarized cluster. The interaction between the projectile and the target is described with a Heisenberg Hamiltonian which excludes the charge degree of freedom during the process. The repulsion between the nucleus has a Born-Meyer form. Our calculation includes both a real time description of the spins of the two interacting systems and also the atomic motion of the cluster atoms. The spin excitations induced are studied versus the cluster size and the trajectory conditions. The effects of the phonons on the spin excitations will be discussed. The collision transfer energy between the target and the projectile presents some resonances versus the velocity of the projectile. The nonadiabatic behaviour during the collision has been characterized by the spin temperature at the end of the the collision.

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1 Introduction

A lot of papers have been devoted to the experimental study of the interaction between a fast atomic particle with a metallic cluster. The collisions could induce fragmentation and various kinds of non-adiabatic effects such as electronic excitation, ionization and capture [1]. Theoretical papers on these various phenomena have been published [2].

Up to now spin diffusion have been only performed on magnetic bulk targets. Similar experiments could be made in the next future on finite media or aggregates. The spin transfer induced by collision has not been intensively studied. Let us mention a previous work on the spin transfer in low-energy collisions of a colinear meta-stable Na_3^+ with a Na atom [3].

In this paper we intend to develop a theoretical description of this kind of phenomenon. The spin diffusion on a ferromagnetic cluster induces electronic, spin and vibration excitations which have different dynamics time scales. We restrict to low target velocity to avoid in this work the electronic excitations. We will use a time dependent Heisenberg formalism which will be presented in Section 2. The atomic motion in the cluster is treated classically and the forces are derived with the Hellmann theorem. In Section 3 we discuss our results on the spin diffusion on cluster and on the coupling between the magnetic excitation and the vibration in the cluster induced by the collision.

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2 The Heisenberg Hamiltonian

The Heisenberg Hamiltonian has been widely used in solid state physics, it has also been employed for aggregates, in particular to investigate the π electron magnetic properties in polyenes [4]. It can be written

$$H^{Heis} = -\sum_{i,j} J_{ij} \boldsymbol{S}_i \boldsymbol{S}_j \tag{1}$$

where S_i refer to the spin of particle i. In the present study of a spin diffusion on a spin polarized system, one of the sites, say site 1, is moving along a given trajectory. Before collision the target atoms are frozen. At the beginning of the collision the target has only magnetic excitations. Then in a second step the magnetic energy stored in the cluster leads to the target nucleus motion. Before the collision, between two nearest target atoms the J_{ij} interaction term is constant and worth J_o. The dependence of J_{ij} on the r_{ij} distance between the atoms i and j can taken as:

$$J_{ij} = J_o^{'} \exp\left(-\frac{r_{ij}}{r_o}\right) \tag{2}$$

$J_o^{'}$ has been chosen in our calculation such that when r_{ij} is equal to the nearest target distance before collision, J_{ij} is equal to J_o. $r_o \cong 1$ Å is a typical interaction length. In the first collision step, only the various r_{1i} distances between the incident and the target particles depend on time t.

To the Heisenberg magnetic energy obtained from equation (1), a repulsion energy term between nucleus is added and is assumed to have a Born-Meyer potential form:

$$E^{Rep} = \sum_{i,j} A \exp\left(-\frac{r_{ij}}{r_o^{'}}\right) \tag{3}$$

A is a constant obtained by assuming that the bond length in the cluster before collision is 2 Å and moreover $r_o^{'} = 2r_o$. We will assume that in the studied speed range, the particle 1 motion has a linear trajectory with an initial velocity v_o before collision. The atom motions are treated classically and no constrain is assumed on their motions. The force on them are the repulsion forces and the attractive component which is derived from the Heisenberg Hamiltonian using the Hellmann theorem like in the CarrParrinello procedure.

3 Results of the Heisenberg model for small aggregates

We consider the collision of an up incident spin on a ferromagnetic down spin target both initially polarized along the z-axis. Before the collision the cluster atoms are frozen. Hence in the first collision step only the magnetic excitations in the target are created and by consequent the interaction between target atoms could be considered constant and worth J_o. Notice that the initial state of the target is the groundstate of the Hamiltonian. The target, called C_n is a linear chain of n atoms along the y-axis. Before collision the nearest neighbour distance in the target is 2 Å. The target atoms are located at sites 2, 4, ... $2(n+1)$ Å. The projectile trajectory is parallel to the initial chain direction.

The wave function $|\Phi\rangle$ is written as:

$$|\Phi\rangle = \sum_i \alpha_i |\phi_i\rangle \tag{4}$$

$\{|\phi_i\rangle\}$ are the states $|\uparrow;\downarrow,...,\downarrow\rangle$, $|\downarrow;\uparrow,\downarrow,...,\downarrow\rangle$ ... with only one up spin for the projectile and cluster system (the first spin is referred to the projectile one). The time dependence of the coefficients α_i are obtained by solving numerically the Schrödinger equation with for the initial configuration $|\uparrow;\downarrow,...,\downarrow\rangle$. At every time of the dynamics the conservation of the total spin S_z and S^2 of the projectile and cluster has been checked. In Figure 1 we report 3 different behaviours of S_z^i for the projectile and atom cluster spin versus the projectile initial velocity v_o corresponding to an energy for a silver atom of 20 keV, 2 keV and 400 eV (i.e. respectively $v_o = 1.88 \times 10^5$ m/s, $v_o = 0.597 \times 10^5$ m/s and $v_o = 0.26 \times 10^5$ m/s) with an impact parameter $b = 2$ Å. During a first phase T_1, the projectile spin and the cluster spins are in interaction. In a second phase T_2 the projectile is no more in interaction with the cluster, so only the excited cluster has its spins varying. The T_1 and T_2 phases are marked in Figure 1. Notice that for this velocity range, during T_1 the cluster atom

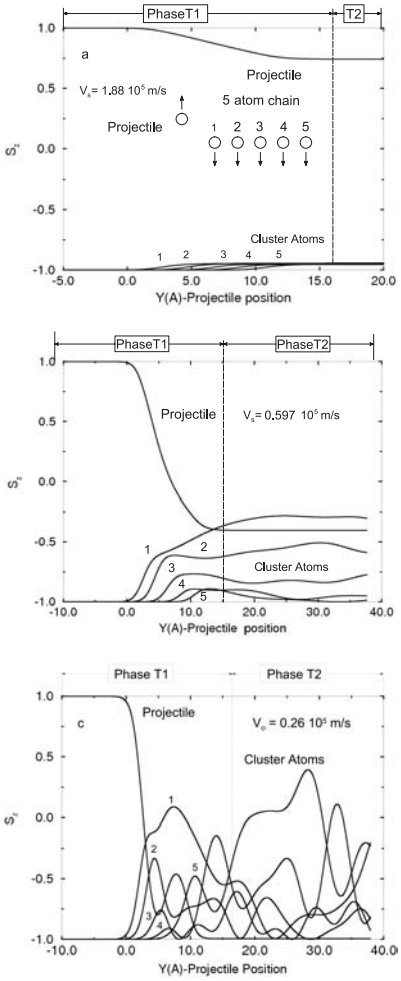

Fig. 1. Evolution of the z spin component S_z for the projectile and the atoms of the 5 atom chain C_5 versus different initial projectile velocity v_o. Y is the projectile position for an arbitrary trajectory parallel to the y-axis with an impact parameter $b = 2$ Å. The phases $T_1(T_2)$ during which the projectile is (no more) in interaction with the target are reported.

positions are still frozen and by consequent J between chain atoms is still constant. For discussing these results we need two characteristic times $\tau = \hbar/J_o = 4.6 \times 10^{-14}$ s which describes intra atomic cluster spin propagation and $\tau^{'}(v_o)$ the travelling time along one atomic distance. For $\tau^{'} < \tau$ (Fig. 1a), the target spins vary when the projectile is above them. Each site behave as if it were isolated. For $\tau^{'} \cong \tau$ (Fig. 1b), the spin amplitudes of variation are larger due to a larger projectile-site interaction. For $\tau^{'} > \tau$ (Fig. 1c), the incident spin flip almost completely. The target spin has a complex evolution. The projectile is interacting with a fully excited target.

The excitation potential energy E_x is defined as $E - E_{ad}$ where E is given by $\langle\Phi|H|\Phi\rangle$ and E_{ad} is the potential energy of the adiabatic state associated to the initial configuration state. In Figure 2a the time evolution of E_x is displayed during the T_1 phase. Its time evolution is quite complex. At some moment the projectile gives (receives) energy to (from) the cluster. It is showed that the system

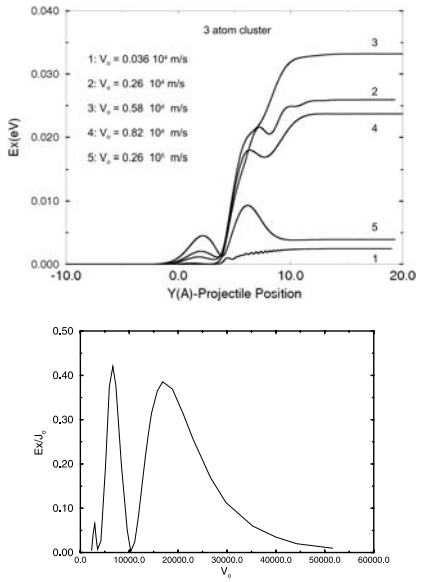

Fig. 2. Excitation potential energy evolution during collision between a 3 atom chain cluster and a projectile (Fig. 2a) and transfer excitation energy (in J_o unit) in the cluster due to the collision versus the initial projectile velocity v_o(m/s) (Fig. 2b). The initial spin configuration is displayed in Figure 1. The impact parameter $b = 2$ Å (2.5 Å) in a (b).

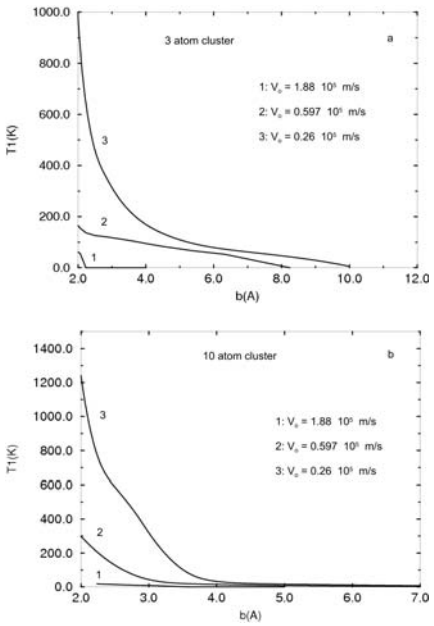

Fig. 3. Spin temperature in the cluster at the end of the collision in the 3 or 10 atom chain atoms versus the impact parameter b and versus the projectile velocity v_o. The initial spin configuration is displayed in Figure 1a.

is perturbated nonadiabatically. In Figure 2b the transfer potential energy from the projectile to the cluster at the end of the collision shows versus the initial projectile velocity some peaks at $v_o = 17100$ m/s, $v_o = 6750$ m/s, and $v_o = 3000$ m/s (for time computing problems we limit our work to $v_o > 2300$ m/s). This peaks are associated to resonances. The peak at $v_o = 17100$ m/s is associated to the spin flip between the projectile and each isolated chain atom spin. The others are linked with resonances associated to the flip between the projectile spin and the full spin system in the cluster. The E_x behaviour is a reminiscence of the spin evolution given in Figure 1.

The spin temperature in the cluster at the end of the phase T_1 is another way of characterizing the excitation in the system. Let E^{fs} be the energy stored in the cluster at the end of the phase T_1, the spin temperature T_1 is obtained from:

$$E^{fs} = \sum_i E_i \exp\left(-\frac{E_i}{kT_1}\right) / \sum_i \exp\left(-\frac{E_i}{k_b T_1}\right) \qquad (5)$$

where E_i are energy eigenvalues of the system. In Figure 3. the spin temperature is displayed versus the impact parameter. The spin temperature is increasing when b is decreasing. For large b, at high velocity, as the transfer is small, the spin temperature is also small. In the case of the 10 atom chain the temperature is significant for $b < 4.5$ Å as for for the 3 atom chain it is for $b < 10$ Å. It is due to the fact that when n is increasing the number of adiabatic levels is increasing and the difference between two levels is decreasing. For small b the collision is highly nonadiabatic and leads to two remarks firstly the spin temperature is large even for intermediate velocity and secondly the energy transfer has not smooth behaviour with respect to the number of atoms in the chain what explains the larger spin temperature in C_3 than in C_{10} for $b \cong 2$ Å.

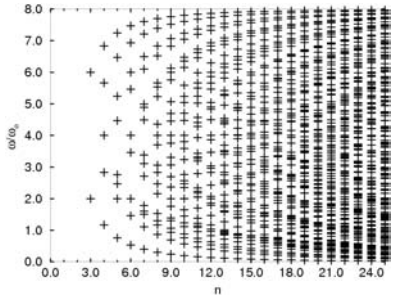

Fig. 4. The full excitation spectrum of the Heisenberg Hamiltonian produced in the cluster at the beginning of phase T_1 versus the size of the cluster ($\omega_o = J_o/4\hbar$).

For the studied range of initial projectile velocity, at the end of phase T_1, the cluster is only spin excited if the projectile is too small. The full excitation spectrum of the Heisenberg Hamiltonian produced in the cluster is reported in Figure 4 versus the cluster size. Increasing n, the excitation spectra forms a band varying between 0 and $8\omega_o$ ($\omega_o = J/4\hbar$) which is associated to the classical chain spin wave dispersion ϵ_k:

$$\epsilon_k = 4JS(1 - \cos(ka)). \qquad (6)$$

The lowest frequency ω_{min} of the spectra goes to zero with n. ω_{min} could be derived from equation (6) by introducing an infrared cut-off $k_c = 2\pi/L$ (L being the cluster size).

Depending on the collision conditions (trajectory, ...), during the collision a part of the spectrum is only

Table 1. Ratio of the excitation frequencies ω_6/ω_2 at the end of the phase T_1 in the 3 atom chain versus the impact parameter b and the projectile velocity v_o (in $\times 10^5$ m/s unit). The collision trajectory is parallel (perpendicular) to the cluster axis in a (b).

(a)

ω_6/ω_2	$b = 2$ Å	$b = 3$ Å	$b = 4$ Å	$b = 5$ Å	$b = 6$ Å
$V = 0.26$	00.52	00.57	00.23	00.15	00.11
$V = 0.59$	00.35	00.52	00.30	00.25	00.23
$V = 1.88$	00.00	00.00	00.00	00.00	00.00

(b)

ω_6/ω_2	$b = 2$ Å	$b = 3$ Å	$b = 4$ Å	$b = 5$ Å	$b = 6$ Å
$V = 0.26$	0.20	0.10	0.09	0.05	0.00
$V = 0.59$	0.22	0.21	0.18	0.17	0.16
$V = 1.88$	0.24	0.24	0.29	0.24	0.21

excited. Let us illustrate this fact with the 3 atom chain. In this case only two frequencies are possible $\omega_2 = 2\omega_o$ and $\omega_6 = 6\omega_o$ for the spin excitations of the two atoms located at the two ends of the chain and only the frequency ω_6 for the atom in the centre of the chain. In Table 1 the contribution ratio of the excitation frequencies ω_6/ω_2 for the atoms at the ends of the chain is reported versus the collision impact parameter and the initial projectile velocity v_o (either for a trajectory along the chain axis or perpendicular but always in the cluster plane). For large v_o, if the the trajectory is along the chain axis only the frequency ω_2 is involved in the process. It is not the case for the perpendicular case. In fact in the first case each spin of the cluster is excited by projectile nearly at the time in the same way and as it were isolated, hence only ω_2 is involved. But in the perpendicular case at the beginning of the collision only one of the atom located at the cluster end is excited and the excitation is propagated to the 2 other atoms and provokes the presence of ω_6. Note that the ratio ω_6/ω_2 is increasing when b is decreasing.

Let us discuss what is happening in the cluster during the phase T_2. For our studied v_o-range, during the phase T_1 the cluster is only spin excited. During the phase T_2 the excess of excitation energy of the spin system is distributed to the vibration degrees of freedom i.e.: the nucleus are no more frozen. This phenomena generate a coupling between the magnon and the phonon. In our calculation the nucleus have been treated classically. A part

Table 2. Phonon pulsation ω_{ph} ($\times 10^{12}$ s^{-1}) and spin temperature $T^{2in}(T^{2f})$ just at the beginning of the phase T_2 or after thermalisation for a 3 atom chain versus the impact parameter b with an initial projectile velocity $v_o = 0.44 \times 10^5$ m/s. The initial collision configurations are reported in Figure 1.

	$b = 2$ Å	$b = 3$ Å	$b = 4$ Å	$b = 5$ Å	$b = 6$ Å
$T^{2in}(K)$	293	172	121	87.5	65.5
$T^{2f}(K)$	268.5	166	118.5	86	64
ω_{ph}	1.39	1.46	1.49	1.495	1.5

of the spin excitations is transformed into vibration. The effect of the phonon-magnon is to induce stretching vibration mode in the cluster for our trajectory. The main feature is that the atoms are no more oscillating around their stable positions before the collision but their bond length is increasing: the larger the transfer energy E_x the longer the bond length. The first consequence is that the atomic vibration pulsation is decreasing when E_x increase or when b is decreasing see Table 2. An other consequence of the increasing of the bond length is that the time-average J in the target is decreasing as the magnetic energy and the spin temperature. In Table 2 we report the spin temperature T^{2in} at the beginning of the phase T^{in} and T^{2f} the spin temperature when the spin system has reached its new equilibrium. Note that the temperature difference $T^{in} - T^{2f}$ is decreasing when E_x decreases.

4 Conclusion

The present article has shown the importance of the coupling of the magnetic excitation to the cluster atomic vibration.

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