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Spin diffusion on a linear spin polarised chain

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Abstract. We investigate the diffusion of a spin polarised projectile (silver atom) on a ferromagnetic spin polarised chain. The interaction between the projectile and the chain is described with a Heisenberg Hamiltonian which implied that we exclude the head-on collision which provokes strong electron exchange and fragmentation. We make a real time description of the spin of two interacting systems. We deduce from it the polarisation change of the projectile and the excitation in the chain *versus* the chain length, the impact parameter and the kinetic energy of the projectile. We analyse 3 different behaviors of the system according to whether the intra-chain excitation propagates slower or faster than the projectile.

PACS. 36.40.-c Atomic and molecular clusters – 36.40.Cg Electronic and magnetic properties of cluster

1 Introduction

The non-adiabatic response of bulk system to a time dependent perturbation is an old solid state physics problem,in the last years experiments on cluster or on solid at the scale of the femtosecond gives a new interest to the fundamental subject of the time dependent response theory where non-adiabatic phenomena are important. Let us mention some of them: charge capture and collision between fast incident ion and a cluster [1] and femtosecond neutralisation dynamics [2]... Now some experiments which involves the surface magnetism have been undertaken with femtosecond laser. The laser irradiation perturbates strongly the system leading to a better knowledge on the response by the determination of the time evolution of the electron, spin and lattice temperatures [3]. Finally let us mention some studies; one on the spin motion of low energy polarised electron passing through a ferromagnet which measures the depolarisation phenomena [4] and another experiment on the ultra fast spin dependent electron dynamics in cobalt using both the time and spin resolved two photon photoemission technics [5].

Before studying the the electronic response of a magnetic cluster to a femtosecond perturbation. Let us discuss a simpler model which has also the advantage of being experimentally controlled. Instead of examining the behavior of the diffusion of a polarised electron on a ferromagnetic system, let us modelling with a spin system the diffusion of a polarised spin silver atom on a ferromagnetic system. To obtain more insights consider a cluster with a simple geometry form like the linear ferromagnetic atom chain. Such geometry is possible by the technics of deposition of atom on surface like a Si surface following by an heating leading to the atom diffusion and formation along the atomic step defect a chain pattern [6].

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2 The model

Let us for the moment suppose that the silver atom spin has been prepared such that its spin direction (down) is opposite to the chain spin direction (up) and moreover its motion is parallel to the chain one.

As we are investigated the spin diffusion on a spin chain, the Heisenberg Hamiltonian H will be the good tool to derive the physics:

$$H = -\sum_{i,j} J\boldsymbol{S}_i\boldsymbol{S}_j - \sum_i J_{iA}\boldsymbol{S}_i\boldsymbol{S}_A. \qquad (1)$$

The Heisenberg Hamiltonian has been used to study linear, cyclic and branched polyenes [7]. The first term is the contribution given by atoms of the chains and the second is the one between one atom of the chain and the silver atom A. J is the ferro-exchange integral between chain atoms ($J = 0.1$ eV) and J_{iA} is the one between the silver atom and one atom of the chain giving the time dependence to H, its distance dependence is the following:

$$J_{iA} = J_o \exp -\frac{r}{r_o} \cdot \qquad (2)$$

In Fig. 1a, the spin geometry before the diffusion is displayed. When the silver atom is near the chain, the interaction between it and the nearest chain atom is effective and a spin flip occurs between it and the chain leading to a first excitation of the chain (Fig. 1b). Then a propagation of the excitation in the chain by flip of spins of two nearest chain atoms (Fig. 1c) another phenomena happening

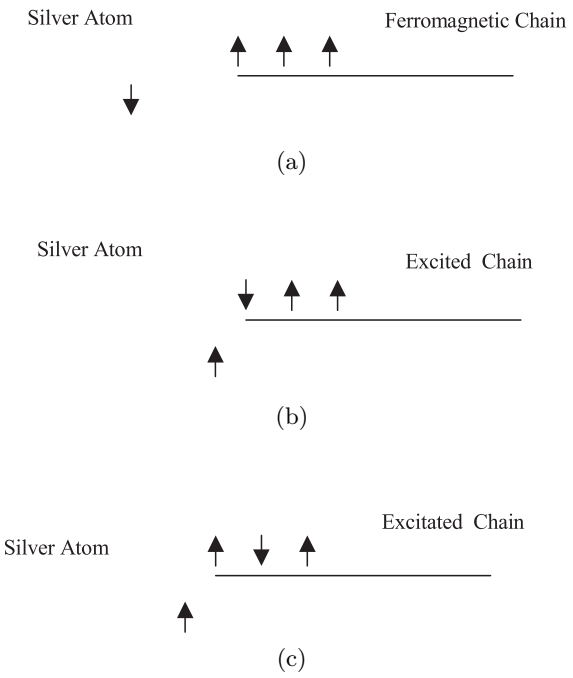

Fig. 1. Excitation process in the spin chain: (a) initial spin geometry, (b) spin flip between the projectile and one chain atom, (c) spin flip between two nearest atoms in the chain.

which is a sign of the non-adiabatic process is a flip of the silver atom with one atom of the chain. In the following we will also examine the effect of the size of the chain and the influence of the kinetic energy of the silver atom on the dynamics.

3 Time evolution of the spin system

In Fig. 2, we report the depolarisation of the spin component of the silver atom (Figs. 2a, 2c, 2e) and of the atoms of the chain (Figs. 2b, 2d, 2f) for an impact parameter of 1.5 Å and for respectively 3 kinetic energies of the silver atom (20 keV, 2 keV and 400 eV) corresponding to 3 typical response of the spin system, the x-axis is the position of silver atom which is considered parallel to the chain, therefore only one variable described the trajectory moreover the atoms of the chain are distant of 2 Å and are located at $x = 2$, 4 Å... and the y-axis is either the down spin contribution to the silver atom state or the up spin contribution for the chain atoms.

To understand the physics of the problem, two times are important: $\frac{\hbar}{J}(0.62\times10^{-14}$ s) which describes the propagation of the intra chain spin excitation and τ the time to the silver atom to go from one chain atom interaction to another. For $E = 20$ keV τ ($\tau = 1.65 \times 10^{-14}$ s) is smaller than $\frac{\hbar}{J}$. It means that the intra-chain excitation propagates slower than the silver atom and by consequent the silver atom interacts always for this speed with chain atoms having a up spin component.

Let us firstly discuss our results on the time dependence in the spin of target atoms i ($i = 1, 2...10$) for a 10 atom chain (Fig. 2b) and for $E = 20$ keV. All the curves exhibit an elbow with firstly a steep decrease (feature (1)) followed by an almost linear curve (feature (2)) whose slope near the elbow is negative for atom 1 and positive for atom 10. Near the elbow we notice that the slopes are nearly zero for the other atoms 4 to 8.

Feature (1) is a consequence of the interaction with the incident down spin which tends to inverse the initial atomic up spins. As the incident spin takes at each interaction an increasing up component, its efficiency for inverting the target atom spins decreases from atom 1 to 10, which appears clearly in Fig. 2a (its efficiency is 10 per cent of the silver atom spin at the shock moment). As the silver atom spin is not fully reversed at the end of the process, its evolution is along the whole chain length (Fig. 2a).

Feature (2) is due to the intra-target spin interaction. At the time when the elbow occurs for atom 1, atom 2 begins to get a down spin component due to its interaction with the incident spin. This partial down spin character of atom 2 tends to add a down spin character to atom 1 due to the chain excitation. Due to the same spin-flip interaction a up-spin character is taken by atom 2. Let us illustrate this phenomena by the chain with 2 atoms: feature (2) would be a down spin increase for atom 1 and a up-spin increase for atom 2. This is shown in Fig. 3. Come back to the 10 atom chain, we indeed observe a down spin increase for atom 1 but to explaining the atom 2 almost zero slope (near the elbow) we have to take into account its other neighbor, *i.e.* atom 3 which (in the same way as atom 2 for atom 1) tends to give it a down spin character. By adding the opposite up and down contributions to atom 2, we understand the nearly zero slope behavior. The same argument explains that the atom 10 spin behaves as the case of atom 2 spin in the 2 atom target atom (increasing of up-spin behavior). Finally for $x > 22$ Å although the interaction between the silver atom and the chain is finished, the chain always evolutes, in fact the shock between the silver atom and the chain provokes spin wave excitation which will be discussed at the end.

For $E = 2$ keV, τ ($\tau = 3.34\times10^{-14}$ s) is always smaller than $\frac{\hbar}{J}$. The evolution of the silver spin is happening for x between 0 and 17 Å and at the end of the process the silver spin will be up (Fig. 2c). The interaction of the silver atom with atom 1 displays a sudden drop of the spin change like in the feature (1) (Fig. 2d), the interaction is always essentially between these two atoms (during this first sudden drop the spin evolution of the second chain atom just begins). But as the motion is slower than in the case $E = 20$ keV the interaction between the silver atom and atom 1 takes place during a longer time, therefore the spin change is larger (0.6 unit). Then it interacts more effectively with the second atom of the chain at this end of this interaction the silver atom would be nearly up. Notice that the spin of atom 3 remains up when the silver atom is in the region where it could interact. But it does not interact because the two spins involved in the interaction

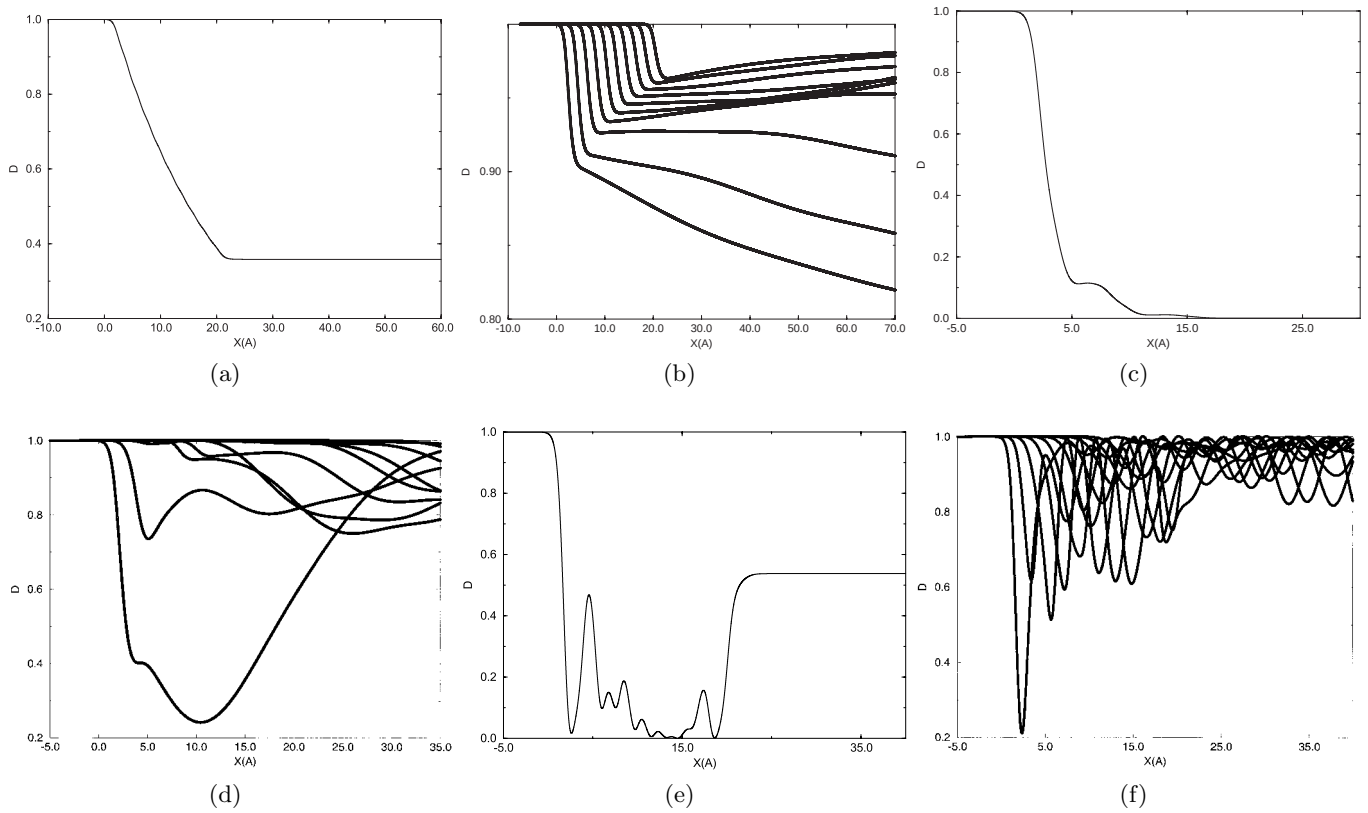

Fig. 2. Time evolution of the projectile (chain atoms) spin in a, c, e (b, d, f) for different projectile energy E. The x-axis is the projectile position, the y-axis is either the down spin contribution of the silver atom state or the up spin contribution for the chain atoms (the chain has ten atoms located at $x = 2, 4, ...20$ Å). $E = 20$ keV (a, b), $E = 2$ keV (c, d) and $E = 400$ keV (e, f).

are essentially up. The silver spin remains constant in this zone. The reason why the spin of atom 3 remains up is the same than the one given above for the feature (2) (*i.e.* the interaction between 2 and 3 tends to increase the up component of the righter atom and therefore the spin on atom 3 remains constant). The spin of atom 4 could change because the phenomena described in feature (2) does not occur for it. It is what it is happening. After that the silver atom interacts with atoms 4-8, its spin component is fully up nearby the atom 8. As the excitation in the chain propagates slower than the silver atom, it sees atoms 9 and 10 with up spin and it cannot change its spin. But as in the previous case the silver spin diffusion has excited the chain to create spin wave.

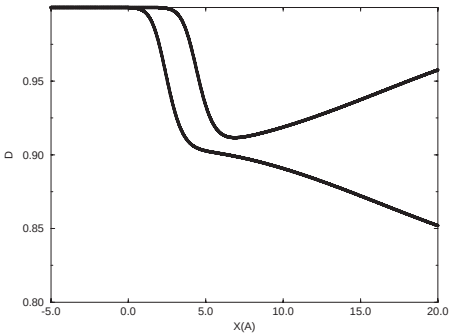

Fig. 3. Time evolution of the two atom spin chain for $E = 20$ keV. The atom are located at $x = 2$ and 4 Å.

For $E = 400$ eV, the silver atom spin time evolution looks more randomly. Now τ ($\tau = 7.49 \times 10^{-14}$ s) is larger than $\frac{\hbar}{J}$, by consequent the excitation in the chain will be very important. We could however explain the beginning of the process. In fact the silver atom in the interaction with the first atom chain flips nearly totally its spin (*i.e.* its spin is nearly up) (Fig. 2e). But now the silver atom motion is slow, the second atom which has a up spin could interact with the first atom which has an essentially down spin,they can flip their spin. Therefore the first increase of the silver spin is linked with the flip between the silver and the second chain atom. The silver atom is in fact interacting with a fully excited spin chain (Fig. 2f). It explains the apparent chaotic behavior of the time evolution. For low speed the silver spin value at the end of the process is not at predictible: this phenomena is illustrated in Fig. 4 where we reported the remained down component of the silver spin (D) at the end of the process at low energy *versus* the energy for a impact parameter of 1 and 1.5 Å (this effect is more important when the impact parameter is decreasing because the chain is more excited). D is also displayed in Fig. 5 for a chain with $n = 2$ or 10 atoms *versus* the energy for different impact y parameters.

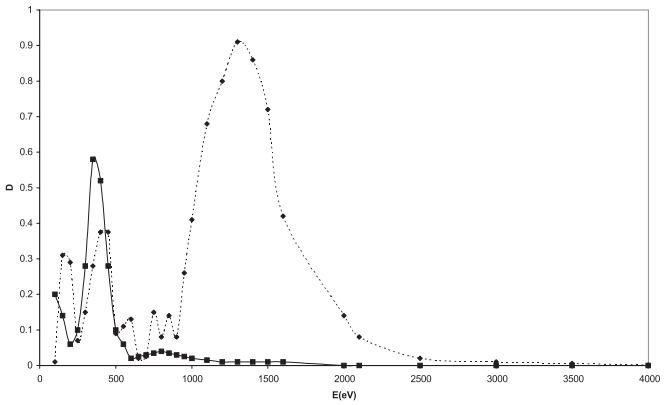

Fig. 4. Remained down spin component of the silver atom D *versus* the projectile energy for an impact parameter of $y = 1$ Å (dashed line) and $y = 1.5$ Å (solid line) for a ten atom chain.

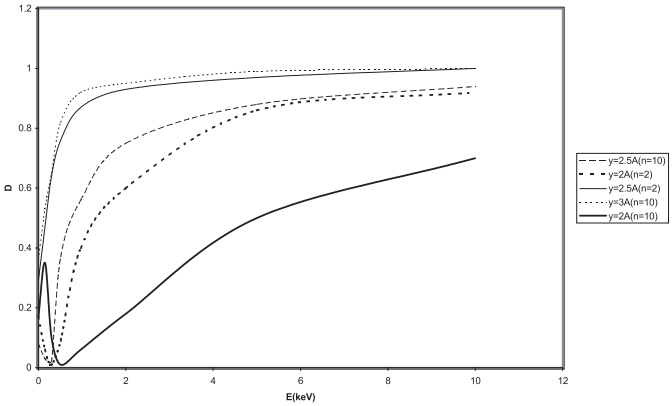

Fig. 5. Remained down spin component of the silver atom D *versus* the projectile energy for different impact parameter y and chain length n.

D is decreasing with the chain size for large speed (because the interaction is longer effective the depolarisation is more important). Moreover we notice that as the speed is decreasing D is decreasing due to the excitation in the chain as we have yet seen.

Finally let us say some words on the excitation in the chain provoked by the silver atom diffusion. We have seen that the diffusion creates some spin wave excitations. To study them we could characterize them by studying the spectral components of the spin of one atom in the chain, the excitation will be given by the Laplace transform. But the problem is not trivial. To illustrate it let us study the case of the two atom chain. When the interaction between the chain and the silver atom is finished the two chain atom spin evolute like a sine function (Fig. 6), the period

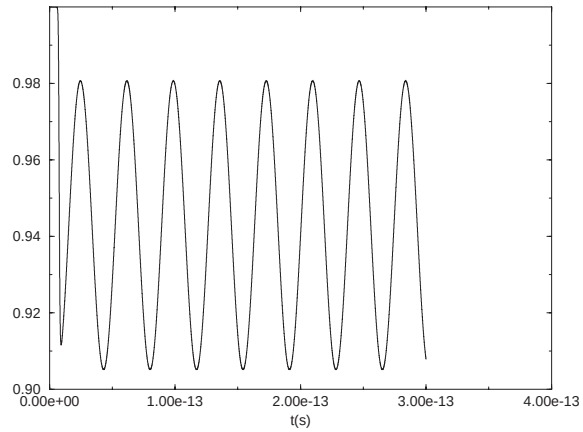

Fig. 6. Time evolution of the spin of atom 1 for $E = 20$ keV and for an impact parameters $y = 1.5$ Å.

T is independent of the impact parameter y ($T = 3.75 \times 10^{-14}$ s). This value is not linked with the expected value of 7.85×10^{-14} s associated with the magnon. In fact the interaction is so strong and perhaps some self-consistent magnons are formed.

4 Conclusion

The present article has shown the importance of the excitation of the chain in the process. An interesting study would be to investigate the excitation created by the diffusion in function of the chain size and the impact parameter. A further study would be the cluster case with ring or spherical structure.

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