Room Temperature Properties of the Quasi-0D Quantum Spin-Switching Device

Y. Hancock

School of Physics and Materials Engineering, Monash University, Victoria 3800, Australia.

The finite temperature behaviour of the quasi-zero dimensional (0D) spin-switching system of type NMMMMMN has been investigated. Here N and M respectively refer to non-magnetic and magnetic atoms of a 7-site finite linear chain. The spin-switching is determined by inspection of the 2-site spin-correlation results, which have been calculated by exact diagonalization of the single-band Hubbard Hamiltonian with external magnetic field. The maximum reduction in the magnitude of the spin-switching profile is ~ 60% at room temperature (T=303K) compared to the T=0K result. Minor 'tweaking' of the external field is used to optimize the spin-switching properties.

1. Introduction and Theoretical Method

Magnetic clusters are known to be highly sensitive to changes in size, composition and geometry [1]. Experimental advances in the fabrication of low dimensional structures have therefore meant unparalleled opportunity for exploring their properties for the purpose of device application [2,3]. Such research provides much impetus to understand these systems from a fundamental theoretical perspective. With this in mind, recent theoretical investigations have been undertaken to determine the local magnetic properties of inhomogeneous, quasi-zero dimensional (0D) clusters of the generic NMMMMMN type [4,5,6]. Here N and M respectively refer to non-magnetic and magnetic atoms of a 7-site finite linear chain. Application of an external magnetic field has been found to induce localized spin-switching in these systems as a function of electron filling with respect to the interface N/M sites [7]. To provide a more realistic basis for understanding this effect, the finite temperature properties of the spin-switching system are determined.

The calculations have been performed by exact diagonalization of the single-band Hubbard Model [8] with external field,

$$H = \sum_{i\sigma} E_i c^+{}_{i\sigma} c_{i\sigma} - \sum_{ij\sigma} t_{ij} c^+{}_{i\sigma} c_{j\sigma} + \sum_i U_i n_{i\uparrow} n_{i\downarrow} - h \sum_i (n_{i\uparrow} - n_{i\downarrow}), \quad \text{Eq. (1)}$$

where, E_i is the on-site energy corresponding to site i, t_{ij} is the hopping energy between nearest neighbour sites i and j, and $n_{i\sigma} = c^+{}_{i\sigma} c_{i\sigma}$, is the site dependent number operator. Here, $\sigma = \{\uparrow, \downarrow\}$, refers to the electron spin. Within the context of the Hubbard Model, U_i is finite on the active (magnetic) M sites and equal to zero on the non-active (non-magnetic) N sites. The parameters are expressed in arbitrary units of energy. The last term in Eq. (1) accounts for the external magnetic field, via the Zeeman energy, h. This term reduces the energy of the system when the condition $n_{i\uparrow} > n_{i\downarrow}$ is satisfied, therefore biasing the ground state in favour of configurations where $n_{i\uparrow}$ is more predominant. The spin-switching is determined by inspection of the 2-site spin correlation results, $\langle S^z_i S^z_j \rangle = \frac{1}{4} \langle m_i m_j \rangle$, as a function of electron filling, N_e. Here, $m = n_{i\uparrow} - n_{i\downarrow}$, defines the local magnetization operator at site i. The results are obtained for the 7-site NMMMMMN system, in the 'potential barrier' configuration where $(E_1 = E_7 = E_N) < (E_2 \ldots E_6 = E_M)$. The thermal average for the spin-correlation function is calculated within the Canonical ensemble using Boltzmann statistics [9].

2. Results and Discussion

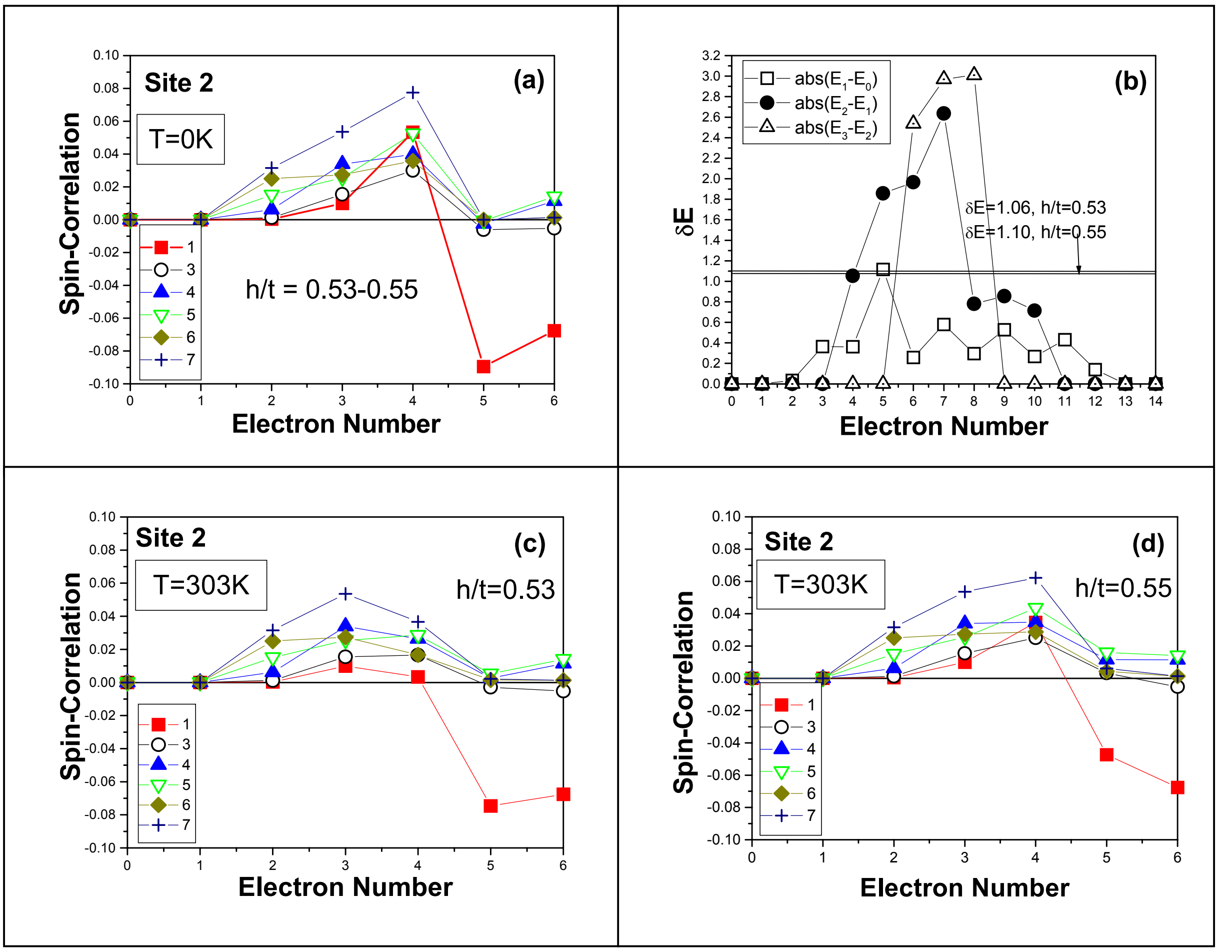

Fig. 1. 2-site spin correlation profiles, $\langle S^z_i S^z_j \rangle$, as a function of electron filling, N_e for site 2 (the M interface site) at (a) T=0K, h/t=0.53-0.55 for the NMMMMMN 'potential barrier' system at U/t=8. The spin-switching profile $\langle S^z_2 S^z_1 \rangle$ is shown in red. The corresponding energy separations between the lowest energy spin states as a function of electron filling are given in (b). In (c) and (d) the finite temperature (T=303K) results are shown for h/t=0.53 and h/t=0.55 respectively. The magnitude of the spin-switching profile is substantially reduced in (c) due to temperature effects. Minimal tweaking of the field can be used to recover some of this magnitude as indicated in (d). As the system is symmetric about its centre the spin-correlation profiles also correspond to the interface M site at site 6.

Fig. 1(a) shows the 2-site spin correlation profiles at T=0K for site 2 as a function of electron filling. The h/t=0.53-0.55 range of magnetic field is required to select the (4↑,0↓) and (3↑,2↓) spin states at N_e=4 and 5 respectively. This is indicated in Fig. 1(b), which shows the energy separation between the lowest energy spin states as a function of electron filling. The horizontal lines represent the h/t=0.53-0.55 applied field. Upon its application the topmost states on or below these lines will therefore be selected. In accordance with the Lieb-Mattis theorem, the ground state solutions for the Hubbard model at h/t=0 are those with minimum spin [10]. Thus at N_e=4, the corresponding spin configurations in order of increasing energy are E_0=(2↑,2↓), E_1=(3↑,1↓)=(1↑,3↓), E_2=(4↑,0↓)=(0↑,4) respectively. In Fig. 1(b) the application of the external field would therefore raise the (2↑,2↓) ground state to the (4↑,0↓) result. At N_e=5, the selection of the (3↑,2↓) configuration and introduction of minority spin results in an ejection of negative spin to the non-magnetic sites. This causes the positive to negative switching of the $<S^z_2S^z_1>$ profile seen at N_e=4-5 in Fig. 1(a). The switching occurs due to 'double occupancy' avoidance (spin-up and spin-down on site *i*) in the magnetic region of the chain. In accordance with Eq. (1) this results in a minimal contribution of the Hubbard U to the total energy of the system.

The applied field is found to increase the density of low lying excited states thus making the system more susceptible to finite temperature effects [11]. This becomes relevant at N_e = 4 and 5, at which points the applied field has specifically been selected for spin-switching purposes. Fig. 1(c) shows that at T=303K, h/t=0.53, the magnitude of the spin-switching profile at N_e = 4 - 5 has been substantially reduced, with a maximum reduction of ~ 90% occurring at N_e=4. By increasing the external field to the upper limit of the h/t range (i.e., to h/t=0.55) the spin-switching magnitude at N_e=4 can be partially recovered. This is shown in Fig. 1(d). In this case the spin-switching is reduced by ~ 30% compared to the T=0K result. The increase in magnetic field to h/t=0.55 causes a further reduction at N_e=5 in the spin-correlation magnitude. At this point there is a 50% drop in the negative spin-switching magnitude relative to the T=0K result. Over the h/t=0.53-0.55 range the average (maximum) reduction in spin-correlation is therefore expected to be ~ 60%. Although the range of h/t=0.53-0.55 produces the profile shown in Fig. 1(a) at T=0K, the finite temperature result indicates the true sensitivity of the spin-switching effect with respect to small changes in applied field perturbation.

3. Conclusion

The room temperature behaviour of the NMMMMMN 'potential barrier' spin-switching device has been determined. Application of the h/t=0.53-0.55 external magnetic field results in the switching points being particularly susceptible to finite temperature effects. A ~ 60% reduction in the spin-switching magnitude relative to the T=0K result occurs. Minor 'tweaking' of the applied field can be used to optimize the spin-switching properties.

Acknowledgments

The author gratefully acknowledges the financial support of the School of Physics and Materials Engineering at Monash University.

References

[1] M.A. Ojeda, J. Dorantes-Davila and G.M. Pastor, *Phys. Rev. B* **60**, 612 (1999).

[2] P. Gambardella, A. Dallmeyer, K. Maiti, M.C. Malagoli, W. Eberhardt, K. Kern and C. Carbone, *Nature* **405**, 899 (2000)

[3] F.J. Himpsel, *J. Phys.: Conds. Matter* **11**, 9483 (1999)

[4] Y. Hancock and A.E. Smith, *Phys. Lett. A* **300**, 491 (2002)

[5] Y. Hancock and A.E. Smith, *Physica E, In press.*

[6] Y. Hancock and A.E. Smith, *Condensed Matter Theories, Vol. 117. Proceedings of the Twenty-Fifth International Workshop,* Nova Science, New York (2002).

[7] Y. Hancock, *Proceedings of the Biannual Australian Institute of Physics Congress, Sydney, Australia,* "In Search of a Quasi-0D Quantum Spin-Switching Device" (2002)

[8] J. Hubbard, *Proc. R. Soc. London, Ser. A* **276**, 238 (1963).

[9] K. Huang, *Statistical Mechanics, 2^{nd} Edn.,* Wiley International, New York, London (1987).

[10] E. Lieb and D. Mattis, *Phys. Rev.* **125**, 164 (1962)

[11] Y. Hancock, "Application of the Hubbard Model to Low Dimensional Inhomogeneous Systems", Thesis, Monash University, Australia, in preparation.