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A family of spin-switching, inhomogeneous Hubbard chains

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HIGHLIGHTS

- This paper proposes a family of finite, inhomogeneous Hubbard chains with tunable spin-switching properties.
- Spin-switching occurs by external magnetic field and electron addition therefore enabling single electron detection via a change in the spinstructure.
- The physics of these systems can be mapped to a coupled quantum dot array.
- The underlying quantum mechanisms may be applicable in the future design of tunable, high-density reading and storage devices.

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1. Introduction

ABSTRACT

A family of spin-switching, inhomogeneous, Hubbard-type systems is proposed consisting of finite chains of nonmagnetic *N*-atoms separated by a magnetic *M*-atom spacer. Due to the extended *N*-atom region, multiple spin-switching events can be activated upon application of an external magnetic field and as a function of the electron filling. Varying the external magnetic field strength enables spin-switching to be triggered by the addition of a single electron. Extended Coulomb interactions are used to produce a greater range of spin-switching signals. The potential to tune the spin-switching as a function of the *N/M* atom ratio and model parameterization is also demonstrated.

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Inhomogeneous, low-dimensional systems consisting of nonmagnetic and magnetic layers of atoms have had important applications as high-memory reading and storage devices. The giant magnetoresistance (GMR) effect [1,2] is one such example, where the application of an external magnetic field can cause up to 150% maximum change in electrical resistance across a magnetic–nonmagnetic–magnetic multilayer device [3]. This impressive change in resistance is achieved by using an external magnetic field to switch the spin alignment in the magnetic region from antiferromagnetic to ferromagnetic across the nonmagnetic spacer [4].

Realizing spin-switching effects on a much smaller scale would offer a substantial increase in reading and storage densities. A potential candidate for low-dimensional spin-switching is the *NMMMMMN* finite chain consisting of two nonmagnetic *N*-atoms separated by a magnetic *M*-atom spacer [5]. Localized spin-switching occurs at the N/M atom interface activated by an

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external magnetic field and as a function of the electron filling, with a possible realization of this system being a coupled, quantum dot array [6].

Further investigation into the physics of *N* and *M* inhomogeneous Hubbard chains has led to the proposal, in this paper, of a family of tunable, spin-switching systems that are made possible by including arbitrary numbers of nonmagnetic atoms at the edges of the finite chain, extended Coulomb interactions and different *N/M* atom ratios. These extensions have resulted in a greater range of spin-switching events, as well as two types of multiple spin-switching made possible by the extended *N*-atom region, namely: (i) fixed-field (sequential) spin-switching, where the number of multiple spin-switching events for increasing electron filling equals the number of *N*-atoms at each end of the chain, and (ii) multi-field spin-switching, which occurs by changing the external magnetic field strength and upon adding a single electron into the chain.

There is extensive literature to support the mapping of an extended Hubbard model with inter-dot repulsion to a coupled quantum dot array—see for example, Refs. [7–9]. The physical realization of a coupled quantum dot array consists of quantum dots that are connected by tunable tunnel barriers [7,10]. The electron–electron (Coulomb) interactions physically manifest as





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capacitances defined locally on each dot, resulting in a intra-dot charging energy that maps to the Hubbard U, or between dots, with the capacitive coupling energy mapping to inter-dot interactions [7,8,11,12]. The capacitances, and hence electron addition, are controlled by external gate voltages.

The paper is organized as follows. Section 2 describes the theoretical method and extended, inhomogeneous Hubbard Hamiltonian that is used to model these systems. Section 3 contains the results for (i) the zero-field, ground-state spin solutions for the 2*N*-edge, 7-site *NNMMMNN* system, the concepts of (ii) fixed-field (sequential) spin-switching and (iii) multi-field spin-switching, (iv) the proposal of a family of multi-*N*-end atom inhomogeneous Hubbard spin-switches, and (v) the effect of extended interactions on these systems and demonstration of a range of tunable spin properties.

2. Theoretical method

The inhomogeneous, multi-*N*-edge atom chains are modeled using an extended, single-band Hubbard model written in second

quantization representation:

$$H = \sum_{i\sigma} E_i c_{i\sigma}^{\dagger} c_{i\sigma} - t \sum_{ij\sigma} (c_{i\sigma}^{\dagger} c_{j\sigma} + H.c.) + \sum_i U_i n_{i\uparrow} n_{i\downarrow} + D \left(\sum_{ij\sigma} v_1 n_{i\sigma} n_{j\sigma} + v_2 n_{i\sigma} n_{j(-\sigma)} \right) - h \sum_i (n_{i\uparrow} - n_{i\downarrow}),$$
(1)

and solved by exact diagonalization using the Lanczos algorithm [13].

Here, $c_{i\sigma}^{\dagger}$ ($c_{i\sigma}$) are the creation (annihilation) operators, which create (destroy) a fermion with spin $\sigma = \uparrow, \downarrow$ in the local state *i*, and $n_{i\sigma} = c_{i\sigma}^{\dagger}c_{i\sigma}$ is the site-dependent number operator. The site-index is enumerated from the left of the finite chain from *i*=1 to *L*, where *L* denotes chain length.

The hopping term, *t*, occurs between nearest-neighbor sites *i* and *j* and is assumed to be a positive, real number. Inhomogeneity is introduced through two site-dependent terms, the local Coulomb interaction term (the Hubbard *U*), and the on-site energy *E*. The Hubbard *U* is active under the condition of 'double occupancy', *i.e.*, when $n_{i1}n_{i1} = 1$. For the inhomogeneous system, $U_i > 0$ for magnetic *M*-sites and $U_i = 0$ for nonmagnetic *N*-sites. The on-site energies for the inhomogeneous chain are denoted E_N and E_M for nonmagnetic and magnetic sites, respectively.



Fig. 1. The two-site, spin-correlation as a function of the electron filling at sites 1–4 for the NNMMMNN system with U/t = 8, $E_N/t = -0.5$, $E_M/t = 0.5$ and h/t = 0.5

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