Spin Shift Register from a One-Dimensional Atomic Chain

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A spin shift register is described. It is composed of a one-dimensional chain of N identical atoms which each have an electronic spin state with $S = 1/2$. When an additional electron is conducted down the chain, it shifts the spin information by one atom. The spin shift register (SSR) can be used as a computer memory device.

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A spin shift register is described [1]. It is composed of an one-dimensional chain of N-identical atoms which each have an electronic spin state with $S = 1/2$. In the ground state, each atom has one electron, and the electronic band is half-full. In solving the Hubbard model, it is shown that when an additional electron is conducted down the chain, it shifts the spin states by one atom. This behavior acts as a shift register.

There is much interest in spintronics: developing spin states as computer memories and processors [2–4]. A shift register is used as a computer memory, but has traditionally been made from buckets of charge. Making a shift register from a line of atoms reduces the spatial dimension by 1 order of magnitude.

For practical reasons, the line of spins would probably be located on a surface. Recently, there has been much progress in measuring and manipulating the properties of spins chains on a surface [5–10]. The proposed shift register could be constructed and tested using these new techniques.

The atoms must have correlated electron states. They must be from the transition-metal or rare-earth-metal series. Then the motion of electrons is described by the one-dimensional Hubbard model [11]

$$H = t\sum_{j\delta\sigma} C^{\dagger}_{j+\delta,\sigma} C_{j\sigma} + U\sum_{j} n_{j\uparrow} n_{j\downarrow}, \tag{1}$$

where t is the tight-binding hopping term, and U is the onsite Coulomb energy. The summations are over j lattice sites, δ neighbors of j, and spin σ. We make the usual assumption that $t \ll U$. The atoms must have the property that the spin state behaves as a spin singlet, and the ground state has one electron in it. An example is the copper atom in a crystal where the normal valence is Cu^{2+}, which is a state of one d hole. Adding another electron creates the Cu^{+} state which is a full shell. There are many other examples among the rare-earth-metal series: cerium and ytterbium are examples.

We denote this as the $N + 1$ problem. The ground state has N electrons: one per atom. We prove that the additional electron (+ 1) can move freely down the chain, regardless of the spin arrangements. In this free motion, it advances the spin states by one atom. When $U \gg t$ the energy bands split in two. The lower Hubbard band, in which there are no doubly occupied sites, is occupied when the number of electrons is less than the number of sites ($N_e < N$). The upper Hubbard band is starting to be filled when $N_e > N$. Then there are doubly occupied sites, so this band is higher in energy by U. The case we discuss has one electron in the upper Hubbard band.

If there is only one electron in the chain of N atoms, the eigenvalues are

$$\varepsilon(\alpha) = 2t\cos(k_\alpha), \qquad k_\alpha = \frac{\pi\alpha}{N+1}. \tag{2}$$

When we have N electrons in a chain of N atoms, the ground state will have one electron at each site, and the electronic energy band is half full. Each atom has one electron, which can be either in the spin up ($\sigma = +$) or down ($\sigma = -$) positions. There is an energy gain of $-J \equiv -t^2/U$ if neighboring spins are antiparallel, due to short-range fluctuations. In one dimension there is no long-range order of the spin ordering. These are well-known properties of the Hubbard model [11].

For the operation of the shift register, the computer operator will determine the arrangement of the spin ordering in the chain. The temperature must obey the relationship $k_B T \ll J$ in order that thermal fluctuations do not change the spin ordering to a lower energy configuration. The values of U for the rare-earth-metal atoms are well known [12]. The values of the hopping t are quite variable. There are many different solids, with many different facets, and the atoms can be put in different lines on these different crystal faces. So the values of J can be chosen to give suitable properties.

The operation of the shift register is quite simple. Denote the initial spin ordering as $|\sigma_1\sigma_2\cdots\sigma_N\rangle$. An additional electron is injected at one end, say the site 1, from the left-hand lead. The spin arrangment is now $|d_1\sigma_2\cdots\sigma_N\rangle$, where d_j denotes double occupancy, and that site is a closed shell. Denote $\bar{\sigma}_j = -\sigma_j$. The next action is an electron hops from site one to site two. Since site two has a spin with σ_2, the electron that hops must be in the state with $\bar{\sigma}_2$. That leaves in site one the spin σ_2. So

after one hop the configuration is $|\sigma_2 d_2 \sigma_3 \cdots \sigma_N\rangle$. The next hop is to site three, and the electron that hops must have spin $\bar{\sigma}_3$, leaving σ_3 in site two. The hopping creates the chain of states

$$|d_1 \sigma_2 \cdots \sigma_N\rangle \rightarrow |\sigma_2 d_2 \sigma_3 \cdots \sigma_N\rangle \rightarrow |\sigma_2 \sigma_3 d_3 \sigma_4 \cdots \sigma_N\rangle \cdots . \quad (3)$$

The $N-1$ hop takes one to the state $|\sigma_2 \sigma_3 \cdots \sigma_N d_N\rangle$. The final hop takes the electron to the right-hand lead. The computer operator can control the spin state of the lead, in order to leave a state σ'_N in the last atom. The effect of an electron being transported down the wire is that the spin information is shifted by one atom, all along the chain of atoms, in the opposite direction of the electron motion. This motion is a coherent process, and has the same eigenvalue as Eq. (2). If one sets up a Hilbert space with all of the above-mentioned eigenstates, one has a tridiagonal matrix whose eigenvalues are identical to those of one electron traveling down an otherwise empty band. The tridiagonal matrix has off-diagonal elements of t, diagonal elements of $E_0 = 0$, and its eigenvalues and eigenfunctions are given in Ref. [13]. The spin shift register operates coherently and rapidly.

In order to store information, one must be able to control the spin configuration of the electrons in one lead. This is a magnetic conductor whose ferromagetic order parameter is switchable. Spin-filter tunneling is one option [14].

The above analysis includes effects in the first order of perturbation theory. One can also include effects in second order in the term of J, which we assume is small compared to t. Each pair of antiparallel neighboring spins has a ground state energy of -2J, while parallel pairs do not. When the extra electron hops onto a site that is part of an antiparallel pair; it may change this ground state energy by $\pm 2J$. The tridagonal matrix mentioned above has diagonal site energies of the form $2s_j J$ where $s_j = (-1, 0, 1)$. The second-order energy is

$$\Sigma^{(2)}(k) = \frac{2J}{N+1} \sum_{j=1}^{N} s_j \sin^2(jk). \quad (4)$$

Neglecting end effects, s_j has as many plus values as negative values, so that the above expression winds up being of order $O(J/N)$. The second-order effects appear to be small. Such fluctuating site energies are similar to the Anderson model of localization. However, localization is not a factor in relatively short, finite, chains.

The above analysis is for electron transport down a linear chain of N atoms. There are several related physical systems. One is an electron moving on the Bethe lattice [11] when all sites already have one electron bound to it. It is easy to show that the extra electron has exactly the same self-energy as an electron moving on an empty lattice. The feature that the spin of the electron that moves is flipping does not change the dispersion relation, nor the density of state.

Another related physical system is the transport of electrons in a periodic system of N atoms, as when they are in a ring. This cannot be used as a memory device, but has interesting eigenstates. As the result is unexpected, we first solve a simple example. At the end we generalize to any chain with any spin arrangement. In all cases we consider the $N+1$ problem.

If the chain had only one electron, the eigenvalues are similar to Eq. (2), except that

$$k_\alpha = \frac{2\pi\alpha}{N}, \qquad \alpha = 0, \pm 1, \pm 2 \cdots . \quad (5)$$

The result is similar with $N+1$ electrons but with a twist.

Consider a periodic chain of $N = 7$ atoms with eight electrons. Initially, the first site is doubly occupied, while the other sites have three spins up, and three down, in the arrangement $|d_1 \uparrow\uparrow\uparrow\downarrow\downarrow\downarrow\rangle$. After the extra electron has gone around the circle once, say in the clockwise direction, the arrangement is $|d_1 \uparrow\uparrow\downarrow\downarrow\downarrow\uparrow\rangle$. The other six spins have shifted positions. After going around twice the arrangement is $|d_1 \uparrow\downarrow\downarrow\downarrow\uparrow\uparrow\rangle$. The extra electron has to go around 6 times to return the other six spins to the original configuration. The Hilbert space has $6 \times 7 = 42$ states. The "twist" is that the eigenvalues have $N = 42$ in Eq. (5), rather than $N = 7$. The following two initial arrangements also generate a Hilbert space with $N = 42$:

$$|d_1 \uparrow\uparrow\downarrow\downarrow\uparrow\downarrow\rangle, \qquad |d_1 \uparrow\downarrow\downarrow\uparrow\uparrow\downarrow\rangle. \quad (6)$$

The following arrangement generates a Hilbert space of $N = 14$

$$|d_1 \uparrow\downarrow\uparrow\downarrow\uparrow\downarrow\rangle. \quad (7)$$

These four arrangements, and their cyclic permutations, compose the total number of $140 = 7!/(3!)^2$ different spin arrangements when there are three up spins and three down spins. In general, for a chain of N atoms, with $N+1$ electrons, the number of different arrangements is $N!/(N_\uparrow! N_\downarrow!)$, where $N_\uparrow + N_\downarrow = N - 1$. They are divided into different Hilbert spaces depending on the type of cyclic arrangment. Many have dimension of $N(N-1)$. A ferromagnetic chain has a Hilbert space of N, which is the minimum number.

[1] Shift registers are described at several web sites: (i) en.wikipedia.org and (ii) www.allaboutcircuits.com.

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