Ratchet Cellular Automata for Colloids in Dynamic Traps

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Abstract. – We numerically investigate the transport of kinks in a ratchet cellular automata geometry for colloids interacting with dynamical traps. We find that thermal effects can enhance the transport efficiency in agreement with recent experiments. At high temperatures we observe the creation and annihilation of thermally induced kinks that degrade the signal transmission. We consider both the deterministic and stochastic cases and show how the trap geometry can be adjusted to switch between these two cases. The operation of the dynamical trap geometry can be achieved with the adjustment of fewer parameters than ratchet cellular automata constructed using static traps.

Recently, a ratchet mechanism was proposed for propagating logic states in a clocked manner through a system of vortices in nanostructured type-II superconductors [1]. Since the operation of the device depends on the discrete positions of the vortices, the system was termed a ratchet cellular automata (RCA). It has been demonstrated that a complete logic architecture can be constructed using the RCA, so that variations of RCAs constructed in different systems might offer a promising alternative to the current microelectronic logic architectures based on silicon MOSFETs [1, 2]. The use of discrete particles to store logic states or perform logic operations has been studied previously in various forms including the quantum dot cellular automata [3] and magnetic dot cellular automata [4]. In contrast to these systems, which work in the adiabatic limit, an RCA operates when the system is far from equilibrium.

The original RCA geometry was proposed for vortices in a type-II superconductor with nanostructured pinning sites. The vortices act like repulsive particles and adopt one of two possible configurations in the static pinning sites. In order to propagate a logic signal through the device, an alternating external driving force must be applied, such as by inducing an oscillating Lorentz force on the vortices by means of an alternating current. The basic concept of the RCA should be applicable to any system of particles which have a repulsive interaction with each other, such as ions in optical traps, classical electrons, vortices in Bose-Einstein condensates with optical arrays of traps [5], or colloids interacting with arrangements of optical traps [7]. In many of these systems, such as for the colloids, it is already experimentally possible to create dynamical traps; in this case, an external applied drive may not be necessary.
In the original RCA geometry, the basic structural unit consists of three elongated static traps, each containing a single vortex. The three traps have different widths and biases in order to break the spatial symmetry of the system. In each trap, the vortex sits either at the top or the bottom of the trap and represents either state 0 or 1. A three-stage alternating external drive is then applied which shifts the vortices to the left and right inside the traps. The trap designs are chosen such that the result of these shifts is to alter the distance between vortices in neighboring traps so that two out of every three vortices are close to one neighboring vortex and far from the other. The resulting asymmetry permits propagation of the logic signal, which would otherwise not occur in this overdamped system. With this geometry, a kink corresponding to a change in logic state can be propagated along a chain of traps. The bare RCA functions at finite temperatures in a stochastic mode since a small barrier remains at the center of each trap which must be overcome thermally. If an additional potential is superimposed on the wells to counteract this barrier, the RCA can operate in a completely deterministic mode and can also run at $T = 0$.

Recently, an experimental version of RCA has been realized for colloids confined to two dimensions and interacting with optical traps [6, 7]. The colloids are micron-sized particles with repulsive Yukawa or screened Coulomb interactions. In this case, a series of optical traps are prepared and the wells are labeled as sites A, B, and C in a pattern that repeats across all of the wells. Each trap is composed of a double well potential created by two optical tweezers, so the colloidal particles sit either in the up or down position inside each trap. Unlike the original RCA, in the colloidal realization each trap is identical in shape. The ratchet effect is induced by dynamically relocating the positions of the wells periodically. The wells labeled B are moved to the right and left, and separately the wells labeled C are also moved to the right and left, so that the net effect is the same alternation of spacing between neighboring colloids that was achieved by means of three well shapes and a three-stage alternating drive in the vortex system of Ref. [1].

For example, a colloid in well B1 is initially close to the colloid in well A1 and far from the colloid in well C1, shown in Fig. 1. When the position of the colloid in well A1 is switched from the up to the down position, then the position of the colloid in well B1 flips from the down to the up position. The signal does not propagate any further until the wells in group C are moved to the new position marked by dashed lines in Fig. 1 and labeled (B/C). This brings colloids B1 and C1 close together while placing colloids C1 and A2 far apart, so that colloid C1 flips to the new state. In the next stage, the wells in groups B and C are simultaneously shifted to the right so that the wells in group C occupy their original positions while the wells in group B occupy the position labeled (B/C). This brings colloids C1 and A2 close together while moving B2 far from A2, and permits colloid A2 to switch. The wells in group B are moved back to their original positions and the process is repeated with the change in colloid position propagating as a dislocation which follows the far spacing of the wells.

The colloidal version of the RCA which has been experimentally realized will be a useful system for studying alternative geometries and further properties of the RCA. The colloidal version of RCA can also provide a valuable system with which to understand transport in noisy environments, which has connections to stochastic resonance. Several important issues have not been studied directly in the experiments, such as explicitly changing the temperature or the clock frequency, as well as understanding the role of thermally induced kink and anti-kink creation in the signal propagation. It would be valuable to probe the effect of trap geometry on the transition between the thermally dominated and deterministic or clocked regimes. Here, we explore all of these possibilities through simulations.

**Simulation**: We consider a quasi one-dimensional geometry of $N_c = 144$ traps with open boundary conditions, in analogy with the geometry considered in the experiments of Ref. [7].
Fig. 1 – Image of the system showing colloid positions (black dots) inside the three sets of wells marked $A$, $B$ and $C$ at the stage of the ratchet cycle where the far spacing is between wells $B$ and $C$. Wells $A$ are stationary, while the wells in sets $B$ and $C$ move back and forth to the dashed locations.

Each trap contains a single colloid which is modeled as an overdamped particle confined to two dimensions and interacting with the other colloids via a Yukawa potential

$$U(r_{ij}) = \frac{q^2}{r_{ij}} \exp(-\kappa r_{ij})$$

Here $\kappa = 1$ is the inverse screening length and $q$ is the colloid charge measured in dimensionless units. The equation of motion for a colloid $i$ is

$$\eta \dot{v}_i = F_i = F_{cc}^i + F_{\text{trap}}^i + F_T^i.$$  \hspace{1cm} (1)

Here $\eta$ is the damping constant from the surrounding fluid which is set to unity. The colloid-colloid force $F_{cc}^i = -\sum_{j \neq i} N_c \nabla_i U(r_{ij})$. Since the colloid interaction force falls off exponentially for large $r$ we place a cutoff on the interaction at $r = 4$, further than the screening length, for computational efficiency. Taking a longer cutoff produces the same results. The temperature is applied as random Langevin kicks $F_T$ with the statistical properties $\langle f_T(t) \rangle = 0$ and $\langle f_T(t) f_T(t') \rangle = 2\eta k_B T \delta(t - t')$. The trap force $F_{\text{trap}}^i$ is produced by lozenge shaped pins, each of which is composed of two half-parabolic traps separated by an elongated region that confines only in the $x$ direction. The aspect ratio of the pins is 3 to 1, with the long direction running along the $y$ axis perpendicular to the line of pins, as in Fig. 1. The pinning strength $f_p = 11.0$. The lozenge shapes of the traps were chosen to model the experiments closely. The positions of the wells in group $A$ is fixed in time, and the distance between the wells in group $A$, which corresponds to the lattice constant of the ratchet device, is 5.0. The wells $B$ and $C$ are moved back and forth periodically in three stages. In the first stage, both wells $B$ and $C$ are shifted to the right by a distance of 1.0. In the second stage, the wells in group $B$ are moved back by a distance of 1.0 to the leftmost position. In the third stage, the wells in group $C$ are moved back by a distance of 1.0 to the leftmost position. The cycle then repeats beginning with both wells $B$ and $C$ in their leftmost positions. The total length of time spent by the wells in one of the three stages is reported as the clock period $\tau$. A kink in the form of a change in logic state is produced by moving the leftmost colloid from the up to the down position at time $t = 0$. The system operates stochastically due to the presence of a finite barrier at the center of each well, generated by interparticle interactions, and at $T = 0$ there is no transmission of kinks. At finite $T$ the kink propagates and the system can exhibit either a clocked or deterministic behavior.

In Fig. 2(a) we plot the location of a kink that was inserted at the edge of the sample at $t = 0$ as a function of time for $T = 0.4$ in a system with $q^2 = 0.5$ and $\tau = 10000$. At this temperature, the kink moves in a clocked manner through the entire system of 144 dots, and there are no thermally created kinks or anti-kinks. The kink propagates at a constant speed, as indicated by the linear slope. We observe a similar clocked motion at lower temperatures until $T < 0.1$. Below this temperature the kink becomes pinned near its entry point and does not propagate across the system. For $T = 1.15$ for the same system, shown in Fig. 2(b), thermally induced kinks can appear. The kink moves in a clocked manner through the entire system of 144 dots, and the ratcheting mechanism propagates both species of kinks in the same direction. Kinks and anti-kinks collide and annihilate when the leading
kink takes a thermally induced step backwards and the anti-kink is able to catch it. In other cases the kinks and anti-kinks travel the length of the system without annihilating.

In Fig. 3(a), we show the same system at $T = 1.3$. In this case the thermal fluctuations are sufficiently strong that the induced kink does not move linearly but shows occasional steps backward so the motion is no longer completely clocked. A significant number of thermally induced kink anti-kink pairs form and also show occasional steps backwards. As the temperature increases the average number of thermally created pairs increases and the average lifetime of a given pair decreases. Figure 3(b) illustrates the system at $T = 1.4$, where thermally created pairs proliferate rapidly and the initially introduced kink is both hard to distinguish and short-lived. For $T > 1.4$ the thermal fluctuations are so strong that the colloids can hop out of the individual wells.

The kink motion can also be characterized by measuring the transmission efficiency $\eta$, which is defined in terms of the time $\tau_{\text{det}}$ it would take for a kink in the completely deterministic system to travel the length of the system. The actual travel time for a kink is given by $\tau_{\text{kink}}$, so the efficiency $\eta = \tau_{\text{kink}} / \tau_{\text{det}}$. If the kink travels at the clocked pace, $\eta = 1$. If the kink takes steps backward, gets stalled, or annihilates with a thermally activated anti-kink, $\eta < 1$.

In Fig. 4(a) we plot $\eta$ vs $T$ for fixed $q^2 = 0.5$, $f_p = 11.0$, and different frequencies or clocking speeds. Each point has been averaged over five realizations of thermal disorder. In this system the kinks are motionless for $T < 0.1$ since the particle-particle interactions induce a barrier at the center of the pinning sites that must be overcome by a small amount of thermal activation. For $T \geq 0.1$, there are enough thermal fluctuations to overcome the barrier and

\begin{figure}[ht]
\centering
\includegraphics[width=\linewidth]{fig2.png}
\caption{(a) The kink position vs time for a system with $\tau = 10000$ at $T = 0.4$. (b) The same system at $T = 1.15$. Dark dots indicate propagation of the originally introduced kink, while light dots show the formation and propagation of thermally activated kink-anti-kink pairs.}
\end{figure}

\begin{figure}[ht]
\centering
\includegraphics[width=\linewidth]{fig3.png}
\caption{The same system as in Fig. 2 for (a) $T = 1.3$; (b) $T = 1.4$. Dark dots: the originally introduced kink; light dots: thermally activated kink-anti-kink pairs.}
\end{figure}
the kinks begin to propagate. For $\tau > 10000$, kinks can propagate deterministically, and $\eta = 1$ over a wide range of temperatures. The efficiency begins to drop when $T > 0.8$ since there are excessive thermal fluctuations that cause the kinks to take occasional steps backward rather than forward. In the experiments of Ref. [7], there was also a certain range of parameters over which the system operated deterministically and $\eta = 1$. For shorter clock periods, $\tau_{det}$ decreases and the kink should in principle move through the chain at a faster rate. Instead, as the clock frequency increases, the colloids are no longer able to respond and the efficiency decreases. Fig. 4(a) shows that as the clock period decreases, the temperature at which the system reaches a deterministic mode increases. For $\tau < 10000$ the system is never able to enter the fully deterministic region. There is an upper bound on the temperature that can be applied to this system, since for $T > 1.4$ the colloids begin to jump completely out of the wells by thermal activation and the ratchet device is destroyed. In Fig. 4(b) we show the efficiency vs clock frequency $\nu$ for fixed $T = 0.5$. There is a plateau of $\eta = 1$ at low clock frequencies followed by an exponential decrease of $\eta$ with increasing $\nu$ which is cut off at the highest frequencies.

In the experimental work of Ref. [7], it was argued that increasing the strength of the central trap in each pin has an effect that is similar to decreasing the temperature. This implies that if the central trap strength is fixed, then there should be an optimal temperature range for deterministic transport of logic signals. The results in Fig. 4 support this conclusion. The effect of temperature is more pronounced at the lower clock periods $\tau$ and the temperature window in which deterministic behavior occurs shrinks with decreasing $\tau$. In the case of

Fig. 5 – (a) Efficiency vs $q^2$ for constant $T$ and fixed $\tau = 5000$. Diamonds: $T = 1.0$. Open squares: $T = 0.75$. Filled circles: $T = 0.5$. (b) Efficiency vs $T$ for elliptical traps at $\tau = 5000$. Filled circles: $q^2 = 18$. Open squares: $q^2 = 18.5$. Filled diamonds: $q^2 = 19$. 
\(\tau = 5000\) in Fig. 4(a), there is a peak value of \(\eta\) near \(T = 0.9\).

In our model, varying the trap strength \(f_p\) does not affect the ratchet efficiency. This is because it is the interaction forces between the colloids that control both the strength of the induced barrier at the center of a pin as well as the magnitude of the force that leads to propagation of the logic signal from pin to pin. We have tested both larger and smaller values of \(f_p\) and find that the pinning can be made arbitrarily strong without affecting our results. In the experimental system, there is a practical limit on the amount of laser power that can be provided to the sample in order to form the optical traps. There is also a physical limit to the amount of energy that can be absorbed by the colloids and the bath medium over a given time period before damage occurs. For smaller values of \(f_p\), which can be accessed readily in experiment by reducing the laser power, we find that the system is limited by the requirement of keeping the colloids inside the pinning sites at all times. The colloids may depin if the colloid-colloid interaction force overcomes the pinning force, if thermal activation out of the pins becomes possible, or if a combination of these two effects occur. Once the colloids depin, the ratchet is destroyed.

We have considered the effect of varying the strength of the colloid-colloid interaction, \(q^2\), as shown in Fig. 5(a) for different temperatures at \(\tau = 5000\). If \(q^2\) is reduced toward zero, there is insufficient coupling between the colloids for the ratchet mechanism to function, and \(\eta\) drops to zero. As \(q^2\) increases, the system enters the deterministic regime with \(\eta = 1\). At \(q^2 = 0.5\), the same system with clock period \(\tau = 5000\) was shown in Fig. 4(a) never to reach \(\eta = 1\) even as \(T\) is increased. Fig. 5(a) indicates that for this clock speed, the system can enter the deterministic limit if \(q^2\) is increased to a value of at least 1. If \(q^2\) is increased too much, however, the efficiency drops again when the thermal fluctuations that are required for operation of the ratchet are washed out by the very strong colloid-colloid interaction forces. We show the decrease in \(\eta\) at higher values of \(q^2\) in Fig. 5(a). At the lower temperature \(T = 0.5\), \(\eta\) drops below 1 once \(q^2 > 1.6\), while for the higher temperature \(T = 1.0\), thermal fluctuations are not washed out until \(q^2 > 5.5\).

In the experiments of Ref. [7], the traps used to construct the ratchet had a multi-well shape which we have represented in our model by a lozenge-shaped pin. The same ratchet mechanism can also operate for other types of wells. To test this, we have considered a much simpler model for the traps consisting of elliptical pins. These are simply parabolic traps with unequal aspect ratios in the \(x\) and \(y\) directions. Unlike the lozenge-shaped pins, which have a central region that is flat in the \(y\) direction and confines only in the \(x\) direction, the elliptical pins have a minimum in both the \(x\) and \(y\) directions at the center of the pin. If the ratio of the pinning force to the colloid-colloid interaction force is too small in the elliptical pin case, the system loses its two logic states and all the colloids sit in the center of the wells. On the other hand, when the colloid-colloid interaction force is strong enough that the alternating up-down configuration appears in the elliptical pin system, the ratchet mechanism can operate in a fully deterministic mode even when \(T = 0\). This is illustrated in Fig. 5(b) where we plot \(\eta\) as a function of \(T\) for elliptical wells with \(f_p = 11.0\), \(\tau = 5000\), and \(q^2 = 18, 18.5, \) and 19. Here, we see that \(\eta = 1\) all the way down to and including \(T = 0\), in contrast to the case in Fig. 4(a) where \(\eta\) drops to zero at \(T = 0\). The central minimum in the elliptical pins compensates for the potential barrier at the center of the pin induced by the colloid-colloid interaction forces. There is no benefit to adding temperature to a system with elliptical pinning sites. For low \(T\), \(\eta = 1\), but as \(T\) increases, thermally activated kinks and antikinks appear and interfere with the signal transmission, causing \(\eta\) to drop. Unlike the case shown in Fig. 3 for the lozenge-shaped pins, where thermally activated kinks tended to ratchet at nearly the clock speed through the system, in the case of elliptical pins the thermally activated kinks tend to diffuse and are much more likely to travel backwards than the kinks in the lozenge-shaped
pins. Fig. 5(b) also demonstrates that the transport efficiency of the elliptical traps at elevated temperatures is strongly sensitive to the value of $q^2$.

We note that the RCA constructed using dynamical traps has several advantages over the originally proposed RCA which involved static traps in combination with an external drive. The static trap RCA requires three different trap geometries to be constructed in the same system. In order to achieve deterministic kink propagation without temperature, an additional attractive potential must be added to the center of each trap to compensate for the barrier in the middle of the trap caused by particle-particle interactions. Finally, a three stage external drive must be applied. In the dynamical trap RCA, many of these extra parameters are eliminated, making it easier to adjust the system into a deterministic mode of operation. In the simplest case of elliptical traps, the system can function deterministically even without thermal fluctuations. We also note that it may be possible to create dynamical traps for vortices in type-II superconductors, the system in which the RCA was first proposed. It has been suggested recently that if artificial magnetic pinning sites are created in a superconducting sample, then the strength and shapes of the pinning can be changed dynamically by applying time dependent magnetic fields [8].

In conclusion, we have numerically investigated ratchet cellular automata constructed for colloidal particles using dynamic traps. Our results are in good agreement with the recent experiments of Ref. [7]. We considered the effects of changing several parameters that have not been explored experimentally, including temperature, colloid-colloid interaction strength, clock frequency, and the influence of the trap geometry. We find that temperature can enhance the transport of kinks and can permit the RCA to operate in the deterministic limit even without the addition of an attractive potential to compensate for the barrier created at the center of each pin by particle-particle interactions. We also examined the proliferation of kink-antikink pairs which are created at higher temperatures. These pairs can be transported by the ratchet effect and can recombine and annihilate. At high clock frequencies, the efficiency of the ratchet transport is degraded since the colloids can no longer fully respond to the ratchet mechanism. We also identify the existence of optimal temperature regimes and particle interaction regimes for signal transport. In the case of elliptical traps, we show that the system can operate deterministically even in the $T = 0$ limit.

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