Using ATOMIX in its horizontal configuration

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ATOMIX is a system consisting of 2878 ball bearings enclosed in a $90mm$ by $90mm$ acrylic cavity. In this paper the ATOMIX system is examined in its horizontal configuration. The pair-distribution of the ATOMIX system is compared to a Boltzmann, Logistic, and Gumbel distribution. The flaws and imperfections in the ATOMIX system are identified and characterized. Further, a method to calculate the entropy of the system is defined and utilized to show definitively that sparsely populated areas are more disorderly than densely populated regions.

I. INTRODUCTION

The ATOMIX system consists of 2878 metallic ball bearings with a diameter of $1.406\pm0.016mm$, constrained in a $90mm \times 90mm$ acrylic cavity. Thus the ATOMIX system is essentially a 2D system of circles of equal radius (henceforth referred to as balls). When placed in a vertical configuration, ATOMIX may be used to simulate and thus study the formation of crystals, crystal defects, and other related phenomena such as crystal planes. In the horizontal configuration, ATOMIX may be used to simulate the motion of a gas experiencing friction (or perhaps, the flow of a fluid). It is important to remember that ATOMIX has significant deviations from experience, as a consequence of the fact that it is a finite element simulation with spheres of constant and equal radius, quite unlike most things we see in reality.

In this paper, only the results obtained from the horizontal configuration of ATOMIX will be explored. Incidentally, similar structures have been observed by investigators in the field of random/spherical packing (see [1], [2], or [3]). It is also evident from [2] and [4] that attempts at a mathematical model have been made and that a logistic distribution is a possible candidate for distribution of the distances between all the particles in the structure ($N \times N$ pair distance values henceforth called the l-distribution or l-dist for short). From the classical theory of gases it is apparent that the Boltzmann distribution is another possible candidate.

Certain aspects of the ATOMIX system (see Figure 1) are obvious before any analysis need be completed. It is plain to see that the l-dist will not have any distances beyond $90\sqrt{2}mm$ or $128\sqrt{2}$ radii. In a similar manner, it is also apparent that there will be a drastic reduction in the frequency of pair-distance values beyond $90mm$ or 128 radii (beyond this point the l-dist focuses on the 'corners' of the ATOMIX system where balls are less common). It is also deducible that initially the frequency of pair-distribution values will be increasing rapidly (doubling between the 1st and 2nd values). This can be ascribed to a simple phenomenon: the very first l-dist value is a direct consequence of balls being packed close to each other - touching their neighbors. The tightest such configuration is hexagonal packing which will also be the most common (since it is the most stable configuration arising often in random packing see [4]). In such a case each ball has 6 nearest neighbors and thus the l-dist value should be around $6N$. The next l-dist value is a consequence of 'neighbors-once-removed' of which there are ~ 12 thus the l-dist value is $12N$, which in turn explains the doubling. Initially there are so few edge cases that they may be ignored, but as the pair-distance value increases, edge cases will start to dominate at which point the frequency of said value occurring will decrease. All of this can be seen in Figure 7.

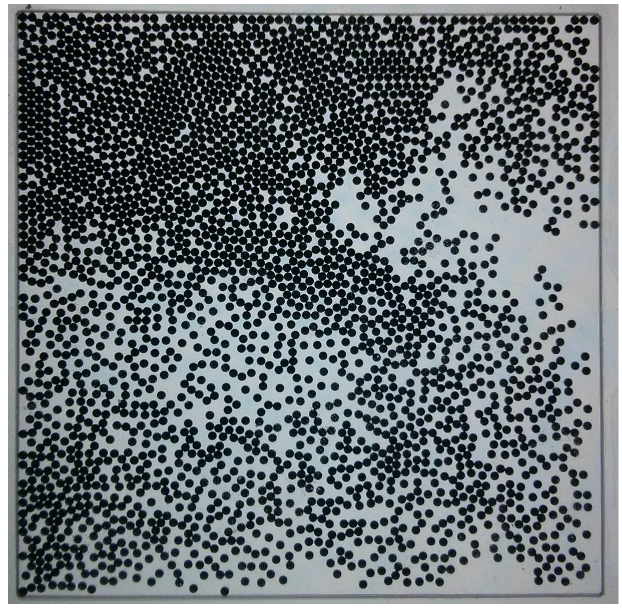

FIG. 1. Figure showing an example of the ATOMIX system in the horizontal configuration.

It should also be noted that beyond the natural variations (due to the fact that the ATOMIX system is not identical to any real phenomenon), it must also be noted that the cavity itself has many imperfections. The nature and consequences of said imperfections will be examined in this paper as well.

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II. METHODS

II.1. Capturing the positions of the balls in ATOMIX

Due to the large number of balls within the ATOMIX system, it is practically impossible to explore the system manually. It is far more efficient to apply computer vision algorithms to figure out the positions of each of the balls in the ATOMIX system. This recognition system was implemented using "OpenCV 3.0.0 Beta" with the aid of morphological transformations (such as erode and dilate) and morphological structuring elements (such as elliptical kernels). Essentially an image of the ATOMIX system is input, converted to black and white (using a moving bilateral filter), smoothed out (to remove effects of pixilation in the image) after which vision algorithms are used to detect all closed contours that match an ellipse or a circle, and to return the centers of said contours normalized against the average ball radius. From here on 1 unit will be taken to mean r (the average radius of the balls).

This method required that the input image have high contrast and as such the images were taken against a pure-white LCD Screen at full brightness. Further, as a result of the image being taken with an 8MP phone camera, there was a small consistent systematic error due to a few balls near the edges of the image-capturing frame being blurred. The error rate for the vision detection system never exceeds 1.5% and is usually around 0.7%. This corresponds to ~ 20 balls out of 2878 being incorrectly recognized. Of that 20, some balls were detected where there was just empty space, and some balls were not detected at all.

II.2. Analyzing the position of the balls

Once the positions of the balls (in unit radii) have been determined, there are many different parameters that can be calculated or many different functions that can be plotted. One such function has been mentioned before and is the l-dist. Other parameters/functions that are interesting are the x-profile, the y-profile, the density distribution, and the entropy. Definitions of the same are provided below:

- X-profile: a moving window (10 units wide) traverses the image scanning different values of the x-axis and collecting the number of balls at a given value. The step size is 1 unit. Thus, if the x-axis goes from 0 to 100, a total of 91 measurements will be taken. When plotting, the value is ascribed to the mid-point of the window used.

- Y-profile: same as X-profile but with the y-axis.

- Entropy: a random selection of N pair-dist values that are taken from N^2 values available in l-dist. The standard deviation of those values is said to be the 'entropy' associated with the system. Since N is relatively large, the N values form a representative sample from which the 'length scale' associated with the system may be extracted. The standard deviation in this value provides a measure of the uncertainty inherent in the underlying length scale. The larger the disorder in the system, the larger this uncertainty and thus we may use it as a measure of entropy. The standard deviation is normalized against the length scale of the system to ensure consistency.

II.3. Image and Simulation Axes

Due to the way in which "OpenCV 3.0.0" works, the x-axis for the image increases going from left to right but the y-axis for the image increases going from top to bottom. Essentially the origin is in the top-left corner for the image and then increases from there on.

The Simulation does not follow a similar labeling protocol. The origin for the simulation's results is in the bottom-left corner of the image as expected.

This variation in protocol is fine since actual results and simulation results are only ever compared qualitatively or in a manner which is dependent upon the absolute distance between points (not such much on the actual position of the points).

The only graph that is affected is the y-profile graph. The y-profile graph for the image should be read from right to left (in decreasing y) whilst the y-profile graph for the simulation should be read left to right (in increasing y). This is a minute detail and doesn't play a significant role in the analysis of the ATOMIX system.

II.4. Experimental Method

It is important to note that all of the experiments in this section (section II.4) were repeated multiple times (typically 5 'measurements' were taken).

II.4.1. Orientation Effects

An 'L' junction was made using books to denote the edges along which the ATOMIX system was moved. The L-junction was of a fixed length of $26 \pm 0.5cm$. The time taken by ATOMIX to traverse this path was 1 ± 0.1 seconds this was achieved by playing a metronome in the background at $60bpm$. The ATOMIX system started at the inner 'corner' of the L-junction and was moved by hand towards the outer edges where it was finally brought to rest. This meant that the ATOMIX system achieved its maximum velocity about 13cm into its path before it was decelerated to rest at the end of the 26cm track.

There were 2 orientations so tested and both had to do with the way in which balls were aligned. The method to set-up the ATOMIX system was to initially set it up in its vertical configuration (thus causing the balls to rest against the bottom) after which the ATOMIX was carefully laid on its side such that the majority of balls were still resting against one of the walls of the cavity. The two configurations thus set-up and tested were: the balls initially resting against the far side of the ATOMIX system (relative to the direction of motion); and the balls initially resting on the near side of the ATOMIX system (relative to the direction of motion).

A simulation that underwent similar circumstances was generated. It is important to note that the simulation took into account both the constant frictional force (proportional to the mass of the balls) and the energy loss due to collisions. The simulation was used to find out which of the acquired results were a consequence of the ATOMIX system, as opposed to its defects/imperfections.

II.4.2. Sharp Stop

For this experiment the ATOMIX was set-up as before (see section II.4.1) with the balls initially resting on the far side of the ATOMIX system (relative to the direction of motion). The ATOMIX system started at the far edge of the L-junction and then found its way to the inner-corner where it was brought to an abrupt halt. The distance traveled and the time taken were the same as before. It is important to note that here the maximum velocity is reached at the 'moment of impact'. A metronome was used to keep time accurately. A similar simulation was run for comparison.

II.4.3. Forcing Motion

This experiment was extremely similar to the 'Sharp Stop' experiment in section II.4.2. The only difference was that instead of being brought to a sharp halt, ATOMIX was brought to a gentle stop at the end of its motion, and then pulled back to the outer edge, and then the cycle repeated. This is similar to forcing the ATOMIX system sinusoidally with an amplitude of 13cm. The distance traveled was still 26cm (up and down) traversed 5 times over the course of 10 seconds. A metronome was used to keep time accurately. A similar simulation was not run due to the computational cost. Ultimately it was not needed for comparison.

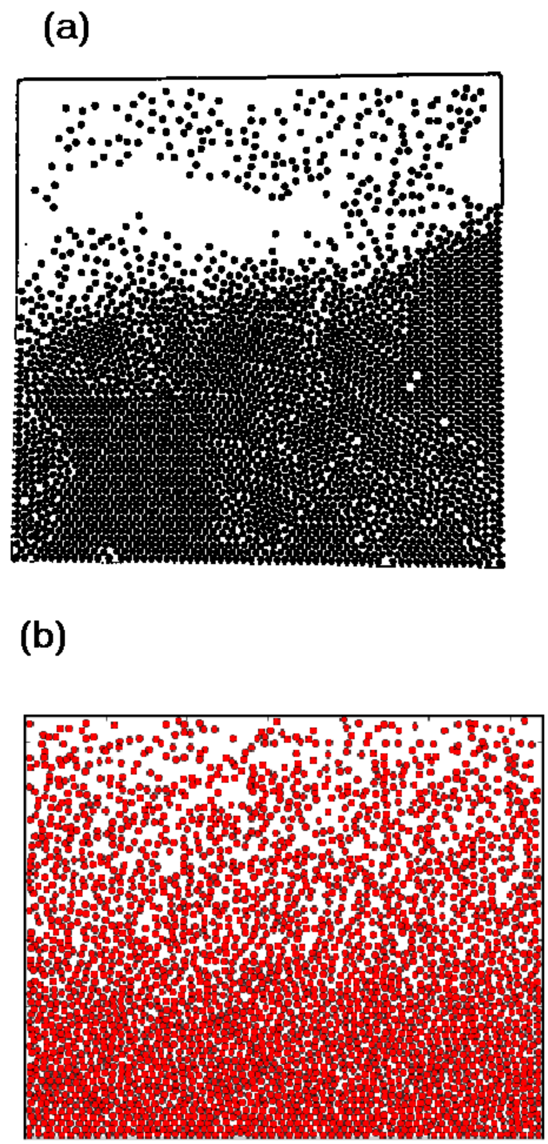

FIG. 2. (a) Figure showing final resting state of actual ATOMIX system after undergoing the experiment in section II.4.1 (b) Simulation of final resting state of ATOMIX system after undergoing similar circumstances.

III. RESULTS AND DISCUSSION

III.1. Orientation Effects

The results of this experiment (described in section II.4.1) were quite surprising in that they showed that it did not matter what the initial configuration of the balls, the final configuration was the balls resting against the near edge of the system (relative to the direction of motion), when brought to a rest. A sample simulation result and a sample experimental result are shown in Figure 2.

The x-profile, y-profile and corresponding entropy for the actual and simulated ATOMIX systems are shown in Figure 3. The standard deviation for the entropy (calcu-

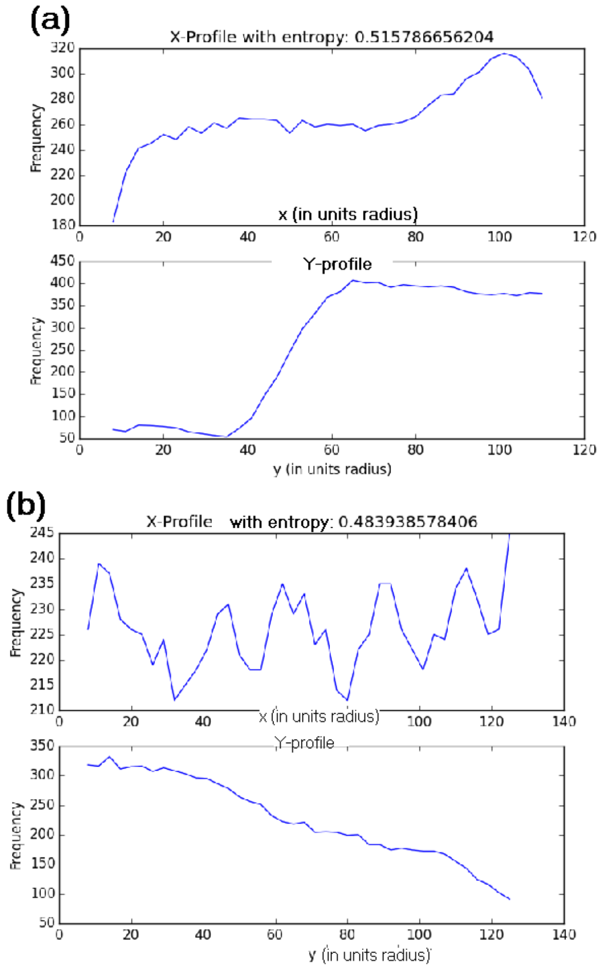

FIG. 3. (a) Figure showing entropy, x-profile and y-profile of actual ATOMIX system (b) Figure showing entropy, x-profile and y-profile of simulated system.

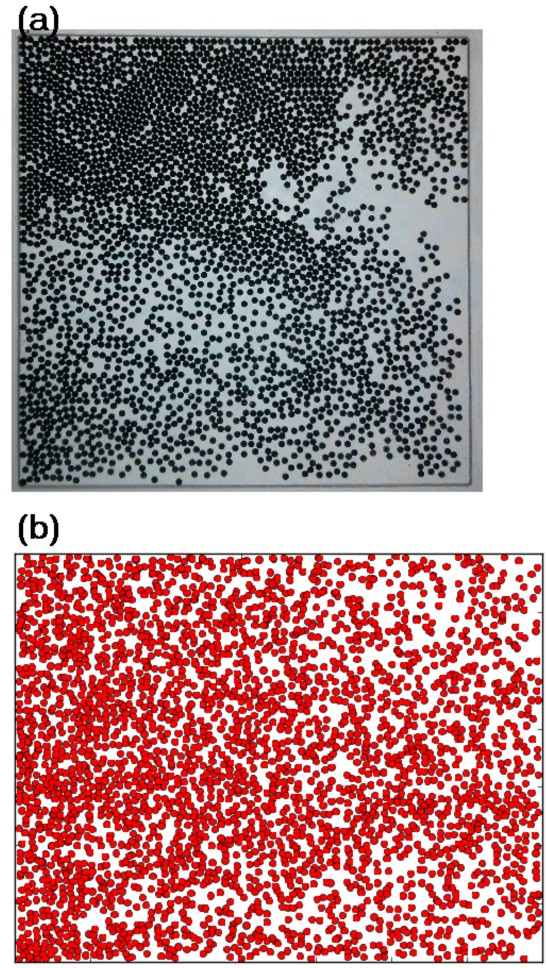

FIG. 4. (a) Figure showing final resting state of actual ATOMIX system after undergoing the experiment described in section II.4.2 (b) Simulation of final resting state of ATOMIX system after undergoing similar circumstances.

lated over multiple runs) is 0.03 for both experiment and simulation, and thus the two entropy values (for experiment and simulation) are in agreement with each other.

Certain key facts are visible from Figure 3. It is immediately apparent that the x-profiles of each roughly mirror the densely packed vs. sparsely packed interface of each. This is an trivial result; it essentially states that the x-profile, of both the image and simulation, is dictated by the densely packed areas as opposed to the sparsely packed regions. It is also apparent that the clear divide between the densely and sparsely packed areas (as shown in Figure 3 (a): y-profile) is a consequence of more than just the simple ball-ball interactions within ATOMIX, since it is not replicated in the simulation. In the simulation the y-profile decreases slowly and in a linear fashion whilst for the image the y-profile experiences a sharp transition at $y = 50$ (from the top of the image - see section II.3). It may be that the balls are slightly charged or magnetized so as to make it favorable for them to group together. It may also be a consequence of surface defects within the ATOMIX cavity. The clear divide at $y = 50$ in Figure 3 (a) could be attributed to a raised protrusion along $y = 50$, causing this y-value to be an unfavorable final resting position for the balls. This will be explored later in greater detail. The corresponding l-dist plots are discussed in section III.4.

III.2. Sharp Stop

For this experiment (described in section II.4.2) the results were not so surprising and agreed with the simulation pretty well, at least qualitatively. The results are visible in Figure 4 from which we see that the general structure for both the simulation and the ATOMIX are the same. There is a densely packed corner along with a sparsely packed corner (both opposite each other).

The x-profile, y-profile and entropy for simulation and experiment are shown in Figure 5. The standard deviation for the entropy (calculated over multiple runs) is 0.02, and thus the results are in agreement with each other. Beyond this we can only state that qualitatively

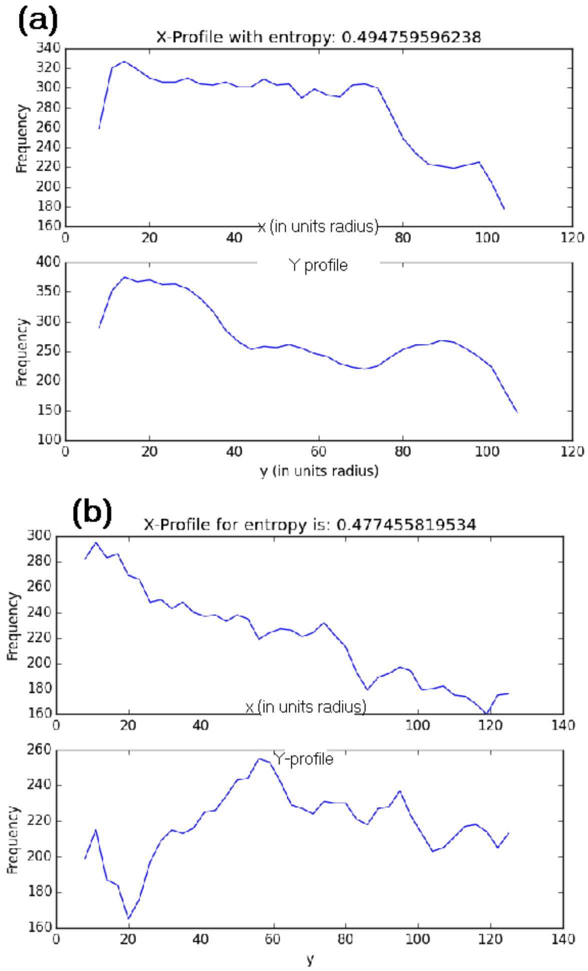

FIG. 5. (a) Figure showing entropy, x-profile and y-profile of the actual ATOMIX system (b) Figure showing entropy, x-profile and y-profile of simulated system.

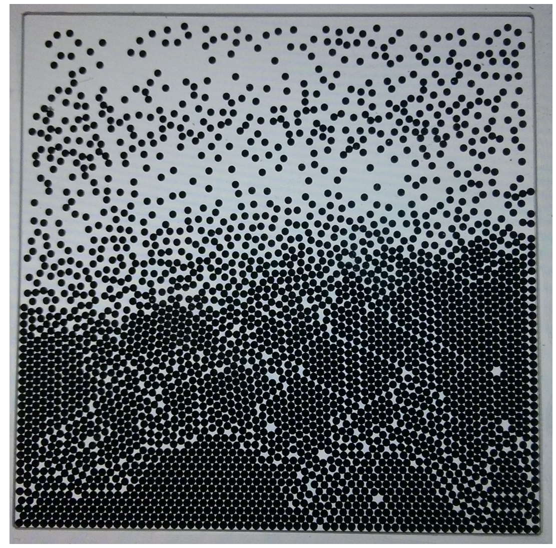

FIG. 6. Figure showing the resting state of the ATOMIX system after the experiment described in II.4.3 was run.

the x-profiles for both simulation and result are quite similar. The y-profiles are not similar to each other in any significant way. It is however interesting to examine the y-profile in Figure 5(a). The y-profile for the actual image is clearly split into three regions: $5 < y < 40$, $40 < y < 75$, and $75 < y < 110$. The regions have the same approximate width of 35. This seems to weaken the hypothesis that the balls might be charged or magnetized. It is plausible that if the balls were magnetized or charged they might form 3 separate clumps but it seems unlikely that the clumps would each be the same size.

III.3. Forcing Motion

For this experiment the results were surprising in that they were pretty identical to those seen in section III.1 as shown in Figure 6. Due to hardware limitations, the simulation caused a buffer-overflow and could not be run.

Regardless, the experiment is useful in that it adds credibility to the surface defects hypothesis which could have caused the clear divide between densely and sparsely packed regions. There is a clear divide about $\frac{2}{3}$rds of the way up which suggests that during the sinusoidal motion of the ATOMIX, some of the balls were confined to the top $\frac{1}{3}$rd of the image. This suggest that there was something energetically unfavorable about going past the divide, thus suggesting a surface protrusion. Further, the divide cannot be caused by resonance effects since ATOMIX was moved by hand with a metronome. There is no way that resonance could have been achieved for any significant period of time. This result further discredits the magnetized or charged ball hypothesis. If the balls were charged or magnetized then clumps of balls might be observable but there is no reason for them to be oriented horizontally (a result which occurs multiple times).

III.4. Global l-dist Results

The l-distribution for all experiments (see Figure 7 for an example) was fitted against a Boltzmann distribution, a Logistic distribution, and a Gumbel distribution (a variation on the logistic except with some skew). A similar fitting was done for all experiments, except ignoring edge effects, and the average R^2 values for both fittings were calculated and presented below in Table I. These results are mirrored in the l-dist for all simulations. The standard deviation in these results is ± 0.003. It is also important to note from Figure 7 that the l-distribution of the particles exhibits significant skew.

Certain key features may be noted. Regardless of whether edges effects are included or not, the Boltzmann distribution is by far the worst at fitting the data. The Logistic distribution is as good as the Gumbel when it comes to fitting data including edge effects. The Gumbel Distribution is however superior at fitting data excluding edge effects.

	Boltzmann	Logistic	Gumbel
Including Edge Effects	0.957	0.989	0.988
Ignoring Edge Effects	0.942	0.993	1.000

TABLE I. Table showing average R^2 values for different fits made to generated l-dist graphs, from ATOMIX data, both including and ignoring edge effects.

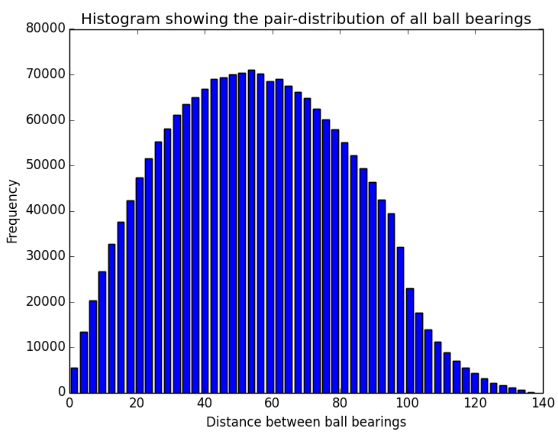

FIG. 7. A sample l-distribution showing edge effects clearly.

III.5. Sparse vs. Overall Entropy

All of sparsely populated areas from all of the experiments and simulations were isolated by eye. The entropy for all such areas was calculated and as expected was found to be higher than the entropy of the over-all structure (which includes both sparsely and densely populated areas - e.g. entropy values shown in Figure 3). This was expected since the overall structure also includes more dense, and hence more orderly, areas.

The difference between the entropy of the sparsely populated areas and the overall structures was calculated separately for simulation and experiments and then compared. There was an extraordinary level of agreement between the two as shown in Table II. The remarkable agreement in both the entropy difference, and the standard error in the mean of the entropy difference (SEM), is a testament to the quality of the simulation. The SEM should be read as the uncertainty in the entropy difference values.

Further, the reason the standard deviation of entropy difference values is extremely large, is that there are a significant number of densely packed pockets within the sparsely populated areas. This causes the local entropy to fluctuate wildly which is reflected in the large standard deviation.

III.6. Surface Protrusions

The analysis of the clear divides (observed on multiple occasions) is more easily accomplished in the sparsely populated regions of the images, thus the sparsely populated regions extracted for analysis in section III.5 were examined more closely. An example of such a region is provided in Figure 8. From here-on the divides will be assumed to be caused by surface defects/protrusions (which will be supported in the following sections).

	Simulation	Experiment
Entropy Difference	0.0460	0.0457
Std. Dev. of Entropy Diff.	0.0211	0.0200
Std. Error in the Mean	0.0040	0.0037

TABLE II. Table showing entropy difference for simulation and for experiment and the astounding agreement between the two. 28 measurements were taken from the experiment data, and 30 measurements were taken from the simulation data.

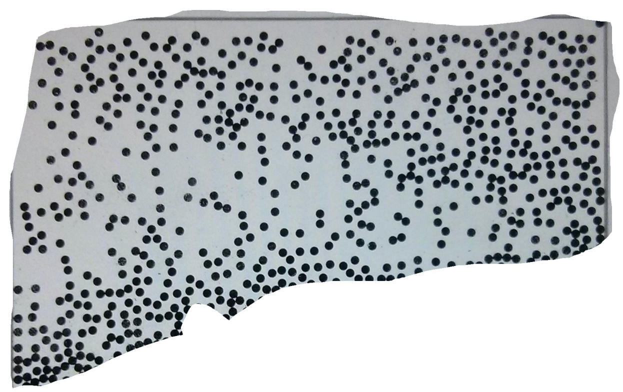

FIG. 8. Example of a sparsely populated region within an image isolated by eye.

III.6.1. Constant-X Protrusions

These protrusions occurred at $x = const.$ values and are henceforth called constant-X protrusions. Whilst many plots showed evidence of protrusion in the x-axis, 2 were prominent and are shown in Figure 9. Both have two dips around $x = 40$ and $x = 60$. The fact that the dip occurs multiple times at $x = 40$ and $x = 60$ is not something that can be easily attributed to magnetized or charged balls.

III.6.2. Constant-Y Protrusions

These protrusions occurred at $y = const.$ values and are henceforth called constant-Y protrusions. Whilst many plots showed evidence of protrusion in the y-axis, 3 were prominent and are shown in Figure 10. All have a dip at around $y = 40$. The multiple occurrences of a dip at $y = 40$ quite significantly weaken the charged/magnetized ball hypothesis.

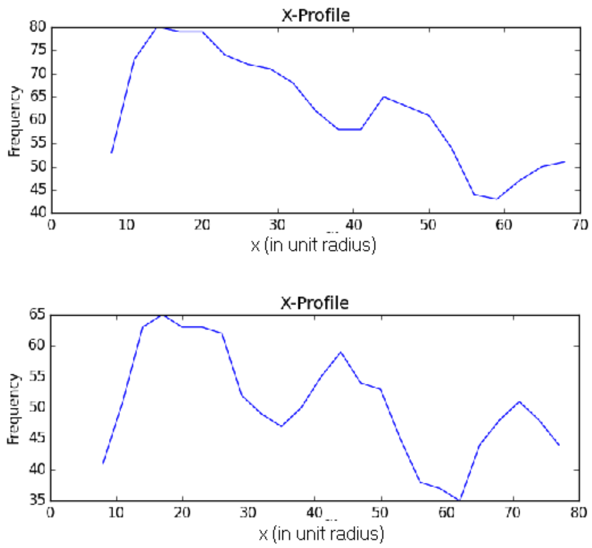

FIG. 9. Figure showing evidence of Constant-X Protrusions.

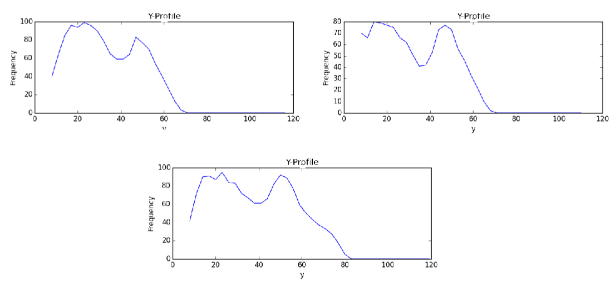

FIG. 10. Figure showing evidence of Constant-Y Protrusions.

IV. CONCLUSION

In this paper the ATOMIX system in its horizontal configuration was explored and a few key facts identified. Firstly, it was shown that the orientation of the balls in the experiment 'Orientation Effects' (descried in section II.4.1) was irrelevant and did not in any way affect the final distribution of balls within ATOMIX. Similarly it was shown that the majority of features detected in the results of the experiment 'Sharp Stop' (described in section II.4.2) were not simply the consequence of ball-ball interactions and were hence not reproducible via simulation. Further, it was shown that when the ATOMIX system is forced sinusoidally (as described in section II.4.3) the results are similar to the results of the experiment 'Orientation Effects'.

It was also shown that the Gumbel distribution is best at fitting the l-dist of the ATOMIX system including and excluding edge effects. It is important to stress that this result is supported by theory (as can be seen from [2]) since the Gumbel is essentially the logistic distribution with skew. The Logistic distribution also fits data well but does not account for skewed-nature of the results at all (as expected).

It was also shown that for the ATOMIX system, the entropy of sparse regions is ~ 0.046 units larger than the entropy for the overall structure. Since this was replicated in simulations this is probably an emergent feature from ball-ball interactions.

Finally, it was shown that the ATOMIX system had surface defects (also called surface protrusions) that caused certain positions of balls to be unfavorable, which were visible in the results of the experiments performed. The amount of data that opposes the magnetized/charged ball hypothesis is quite substantial making the hypothesis seem extremely unlikely, and as such it can be rejected quite definitively.

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