Multi-Species Screening in Anti-Ferromagnetic Pair-Annihilation Model Simulations

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ABSTRACT

Pair-annihilation process models capture the behaviour of important reactions amongst fundamental physical but also chemical systems. We develop a lattice-based pair-annihilation model based on Kawasaki exchange dynamics and with diffusion properties controlled by a lattice-gas temperature. We investigate the effect of multi-species screening in the model when anti-ferromagnetic repulsive coupling forces are used. We find a phase transition manifested by an annihilation induced population collapse around $T=0.22$ and an additional phase transition in the number of species present around $Q=5$. We describe a number of quantitative metrics based on graph component labeling and contrast the behaviours of the ferromagnetic and anti-ferromagnetic variants of the model.

KEY WORDS

pair annihilation; simulation; complex systems; phase transition.

1 Introduction

Simulation modelling is still a widely used and indeed necessary tool in developing an understanding of phase transitions and critical phenomena that occur in many physical, chemical and materials systems. Non equilibrium systems that do not have transition rates satisfying a microscopic detailed-balance condition [4] need to be studied on incomplete time-scales where the dynamics forms the basis of the analysis. It is possible however to search for parts of such systems’ phases spaces where trajectories are attracted and for which some approximation of the long term behaviour is possible.

There is continued interest in the critical systems literature in models that combine diffusion with multi-species rules and for which processes support or compete. One such model is the pair-annihilation model (PAM) which can be used to study processes where two particles meet and mutually annihilate. This is often denoted as $A + A \rightarrow 0$ and is typical of some chemical reaction processes where pairs of molecules combine to leave behind an inert product that plays no further part in the reaction [17, 34]. Annihilation models also play a useful part in understanding more fundamental physical interactions.

The pair-annihilation model [10] has been studied in a number of contexts including: segregation [20]; birth and death combinations [18]; wave pattern formation [1]; asymmetric reactions [3]; and diffusion in various forms [7,12,29] and comparisons with other models [2], and with various diffusion mechanisms explored [9]. The PAM has been studied extensively at a theoretical level [31] and with simulations in one dimension [5, 30]. In such cases it models a queue or channel of interacting particles and has relevance for comparisons with theory but is otherwise not particularly representative of any real physical system. A two dimensional system modelling a sheet of interacting particles on a surface is more interesting – but more computationally difficult to simulate.

Many simulation model like the PAM are constructed in terms of lattice simulations with interacting particles at nearest-neighbour interaction ranges [6, 26]. The PAM is usually parameterised in terms of a diffusion rate and particle annihilation and production rates. We find that the Kawasaki site-exchange model [22, 23] is a useful way to formulate the diffusion process in a more realistic way by
linking it to a temperature. The Kawasaki model [24] is based on the Ising model [21] but with exchange diffusion dynamics and is effectively a lattice gas model [16] if there are vacancies [8] 2011 present. Details of this are given below in Section 2 but in summary we obtain a model where Q species of lattice cell site diffuse around according to a simple coupling model that is controlled by temperature. Any two particles of the same species that met annihilate one another.

The PAM has been extensively studied with one and two species and some work has explored three states [11]. We are not aware of many higher number of species or states having been explored however – possibly because for normal ferromagnetic coupling systems there does not appear to be any new behaviours for higher Q [19].

When a ferromagnetic coupling model like that of the normal Ising, Potts [27, 33] or Kawasaki model is employed particle populations steadily decline according to a well known exponential law. However, our particular new finding, reported in this present article, is that when an anti-ferromagnetic coupling is employed, then like-like particles repel and elaborate interleaving checkerboard structures form whereby one species of particle effectively shields others from mutual annihilation. We find a phase transition in temperature and another in the number of species of particle present. Particles of different species cannot occupy the same space but otherwise do not couple with one another. We model our system with initial fraction \(1/Q\) of each species and we treat one of the species - "state 0" as the vacancies or null reaction products of the pair annihilations [28].

Our Multiple species Pair-Annihilation Model (MPAM) was studied through computer simulations on a square lattice model for 2,000 time steps where each site was updated on average once per step. Some snapshots of the anti-ferromagnetic model are shown in Figure 1 which shows the interleaving shielding checker-board structures forming at cold temperatures, but breaking up at temperatures above the critical temperature which we found to be around \(T_c \approx 0.22\). Using graph component labelling [14] and other metrics we investigated the formation of clusters or droplets [13] of non-vacant particles in the system. We also studied different number of species and found an additional transition in \(Q \approx 5\) where in our model the vacancies are considered to be one of the \(Q\) species present.

Our article is structured as follows: In Section 2 we summarise the multi-species pair-annihilation model and the manner in which we implement it on a lattice. We present various screen-shots and quantitative metrics from the simulations in Section 3. In Section 4 we offer a discussion of the implications of the model and results alongside with some conclusions and areas for further work in Section 5.

Figure 2: Exchange Mesh showing how A and B exchange, interacting with their nearest neighbours, or C and D do.

2 Multi-Species Pair-Annihilation

Although a number of authors have reported simulation work on the pair annihilation model, no work that we are aware of has studied the effect of anti-ferromagnetic (repulsive) couplings.

The PAM is implemented on a two dimensional lattice with a site exchange diffusion mechanism similar to Kawasaki spin-exchange dynamical model, which itself is based on the Ising model notion of nearest neighbour couplings between sites. Figure 2 shows how two sites arranged horizontally (A-B) or vertically (C-D) interact with their collective six nearest neighbours. At each step of the model the sites are “hit” randomly and the evolutionary process described in Algorithm 1 is followed.

The bonds between sites are supposed to model an interactive coupling between nearest neighbour sites of the form of the Hamiltonian:

\[
\mathcal{H} = -\frac{1}{2N} \sum_{\langle i,j \rangle} J_{i,j} \sigma_i \sigma_j
\]  

with the summation over nearest neighbouring sites of which there are four on a two-dimensional square lattice. We take the site variables \(\sigma \in \{\pm 1\}\) and the coupling parameter \(J\) to be uniform everywhere and a unit of Boltzmann’s constant \(k_B\) throughout.

Changes in the Hamiltonian \(\mathcal{H}\) that result in a lowering of energy (increased bond count) are always accepted and the swap of sites \(i, j\) made, but even changes that imply a small increase in energy are accepted stochastically, and this models the effect of thermal fluctuations. The Boltzmann probability condition for testing against a random number is:

\[
\mathcal{P} = \exp(-\Delta E/k_B T)
\]

To all intents and purposes have a single parameter model – the temperature \(T\) if we measure changes in energy as changes in the number of bonds and use \(k_B\) units for \(J\).
In the work reported below we experiment with the anti-pattern due to prior annihilations. Completely avoiding any nearest neighbour interactions. More this gives rise to a checkerboard pattern with species components like and the species arrange themselves to avoid other sites of the same species annihilate one another completely. There are three metrics that we can also track the number of distinct (non-vacancy) cluster components in the system. Using a computational algorithm we can also track the population track of a representative species as the system progresses from its initial random state. Since we treat all non-vacant species the same, it is sufficient to track the population of species-1. The population of monomer particles - that is particles with no non-vacant neighbouring particles - is also relatively simple to compute. Using a component labelling algorithm we can also track the number of distinct (non-vacancy) cluster components in the system. These three metrics are shown plotted against time (on a logarithmic scale) for both an anti-ferromagnetic coupling version of the Kawasaki dynamics, operated alongside a like-like pair annihilation process.

3 Experimental Simulation Results

Unless otherwise stated, the systems reported are based on a periodic wrap around geometry on a square lattice of size \( N = 256^2 \) sites and initialised randomly with average initial fraction \( f_Q = \frac{N}{Q} \) of each species - including vacancies. The model system is evolved for 2,000 time steps for the data presented, and various snapshots and quantitative metrics are reported.

Figure 1 shows the key result for a small system. The anti-ferromagnetic couplings make the individual species repel one another at nearest neighbour interaction lengths and the surviving particles arrange themselves on checkerboard patterns in which they can maintain themselves for a long time without meeting and annihilating with a particle of the same species. When the temperature is slowly raised however, more thermal fluctuations in the form of particles that have temporarily hopped off the checkerboard and are therefore prone to meeting an annihilation partner particle of the same species. The results are seen at a high temperature, the population of particles starts to drop significantly as particles are no longer screened by the low temperature frozen-in interleaving checkerboard patterns.

This effect is seen manifest in systems at various number of species \( Q \). Figure 3 shows the effect for \( Q = 3, 4, 5, 6 \). In this illustration we have coloured all non-vacancies a shade of red as this emphasises the long range structure of defects amongst the interleaving checkerboards that have arisen from the anti-ferromagnetic couplings. We have not illustrated the model for ferromagnetic couplings as particles annihilate very rapidly and the long-term (uninteresting) picture is of a very few isolated particles in a sea of vacancies.

There are a number of useful quantitative metrics that we report for both ferromagnetic and anti-ferromagnetic coupled systems however. The simplest to record is a population track of a representative species as the system progresses from its initial random state. Since we treat all non-vacant species the same, it is sufficient to track the population of species-1. The population of monomer particles - that is particles with no non-vacant neighbouring particles - is also relatively simple to compute. Using a component labelling algorithm we can also track the number of distinct (non-vacancy) cluster components in the system. These three metrics are shown plotted against time (on a logarithmic scale) for both an anti-ferromagnetic coupling simulation (left) and a ferromagnetic one (right).

Figure 4 shows the dramatic difference between the ferromagnetic and anti-ferromagnetic couplings on the PAM. The anti-ferromagnetism essentially creates a screening effect so
that members of the same species can be held apart long enough for intricate interleaved checker-boarding patterns to form and prevent a wholesale mutual annihilation of like-like species. In the data shown in Figure 4 we hold the system cold with temperature $T = 0$. This lets us study the progress from random initial population to long term behaviour.

In the case of the ferromagnetic model, with particle production mutual annihilation progressively removes almost all particles, and those few remaining only survive because of the lowered probability of finding an annihilation partner in the space. The anti ferromagnetic system however allows particles to survive and a steady non zero population fraction, fraction of monomers and number of non-vacancy clusters all result. We can see that at zero temperature, the number of species does not have any obvious complex effect. Increasing Q means the partial volume fraction available to each species is reduced, but also allows species to more effectively “hide from their own” and to survive annihilation for longer based upon the frozen-in long range spatial checker-boarding patterns.

A series of systems were simulated at different temperatures to study the effect of the increasing thermal fluctuations.
Figure 4: Metrics for the $256^2$ system for anti-ferromagnetic coupling (left) and ferromagnetic (right) at Temperature $T=0$, and for various number of species $Q$ values.

Figure 5 shows a plot of the final value (after 2,000 steps) of the population fraction of representative species number 1, plotted against the diffusion-controlling temperature (on a logarithmic scale) and with different curves for each of the different $Q$ values.

One interesting result is the existence of a marked phase transition for all $Q$ values at temperature $T_c \approx 0.22$. This corresponds to there being sufficient thermal energy for particles to hop out of or across the nearest neighbour checkerboard screening them from their fellows and mutually annihilating. The population drops rapidly above this critical temperature. A more subtle result is that of a second
Figure 6: Limiting low-temperature intercept population fractions for various numbers $Q$ of species present.

Figure 7: Fitted straight line to the data from Figure 6 plotted vs $1/Q$.

partial drop in the populations at temperature $T^* \approx 0.13$ for $Q \geq 5$. The existence of this suggests a richer set of phases corresponding to mutually screening structures at higher $Q$ values. This may also correspond with the known behaviour of the multi-species Ising model (known as the Potts model [27]) whose phase transition changes its characteristic behaviour around $Q = 5$.

We attempt to investigate how systematic the transition in $Q$ is by plotting the limiting values of the population fractions for each different $Q$ value at low temperatures.

This is shown in Figure 6 where the near horizontal straight line limits suggest they can be characterized by a fitted intercept to each straight line. These intercepts are themselves plotted as a function of $1/Q$ and are shown in Figure 7. There appears to be a straight line relationship with $1/Q$ to within the bounds of experimental error from the experiments reported here.

4 Discussion

We have determined that under anti-ferromagnetic coupling the MPAM model has a richer set of critical transitions than might have been expected. We identified one in the temperature and another in the number of species present which also manifests itself in a different temperature range.

Our simulations were on a $256^2$ square lattice which as large enough to support the long range checker-board structures observed. Small systems of for example $< 50^2$ where not large enough to support these for any observable times. It is possible that there may be more sophisticated interleaving shielding structures relevant to much higher $Q$ values, that only manifest themselves at larger lattice sizes.

Our simulations were performed using a custom simulation code written in Java with associated Java Swing 2D Graphics. This was sufficiently fast to obtain the results presented in this paper over a few days worth of processing effort. To study larger systems or to obtain more independent runs at each $T$ or $Q$ parameter scan, faster compute resources would be necessary. This sort of model would parallelise very well and would be well suited to the use of a data parallel accelerator such as a Graphical Processing Unit (GPU). Various parallel strategies such as multi spin coding [25] and GPU parallelism [32] have been reported as successful for this sort of model already.

We have focused on two-dimensional systems - largely due to computational limitations - but the model would extend in principle to three dimensions. There is scope for studying layering or other three dimensional structures in Kawasaki exchange dynamics based models [15].

5 Conclusions

We have extended the pair-annihilation model to multiple species and have explored up to nine different species present on a square lattice through computer simulation. We have based our diffusion mechanism on the temperature coupling of the Kawasaki model. We explored the anti-ferromagnetic coupling regime as well as the more normal ferromagnetic one and have observed long range interleaved screening structures form in the model to allow species to survive annihilation much longer than they would in the ferromagnetic system.

We have found and approximately located the phase transition temperature at which these long range structures are broken up by particles hopping across them as at around $T_c \approx 0.22$. We have also identified a change in behaviour at around $Q \approx 5$ which we believe is linked to a more subtle interaction between the mutual shielding behaviour at high $Q$. We hypothesis a relationship between the low temperature limit behaviour of the system and the reciprocal of
the number of species present Q.
There is scope to investigate these phenomena in more statistical detail and potentially to obtain a full and complete phase diagram of the anti ferromagnetic multiple species pair-annihilation model (MPAM). There is further scope to extend the model to three dimensions where more complex face-centred or body-centred shield structure might form.

References