Dissipation Learning in Active Matter

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INTRODUCTION

Active matter is, broadly, a subcategory of condensed matter systems, distinguished primarily by energy input distributed across all constituents (agents) of the system, which in turn set their own self-propelled motion across a medium. The agents therefore have *direct* access to inputs of externalenergy, and use it to autonomously propel and direct themselves (with different models and situations allowing for various degrees of freedom) [1]. The study of active matter is generally grounded in (but not limited to) the observed behaviour of biological agents, as they are the primary examples of active matter in nature.

An important motivation for studying active matter is that it helps understand biological behaviours and, therefore, the world of living organisms, where energy is constantly dissipated in order to perform various biological functions. Macroscopically, the construction of theoretical models can help explain, and to a limited degree predict, the behaviour of animals undergoing emergent swarming behaviours (where each animal can be treated as its own autonomous agent, sharing the same generally stable 'rules' of altering speed and orientation while interacting with each other and the environment)[2]. This biological emulation through physical models is not limited to what can be termed as 'simple' behaviour; human behaviour can be partially mapped and understood within physically-indexed accounts of autonomous choices within (overtly or suggestively) constrained collective action. Interesting examples are swarming behaviours identified in traffic, crowd disasters and concerts[3].

Outside of biology, active matter research serves to emulate, or otherwise learn from, naturally occurring behaviours in order to analyse a potentially more general thermodynamic framework. Due to the necessarily dissipative use of energy within self-organised agents, and their internally-induced behaviour, active matter is not described by the statistical mechanics of equilibrium states. The question then arises whether, through quantitative computation and qualitative modelling/theorising, the thermodynamic laws of equilibrium can be modified and generalised to non-equilibrium states. Exploring how these generalisations would hold as the system further departs from equillibrium through various means is then paramount[4][5][6]. These generalisations would, ideally, collapse into the known statistical thermodynamics states within the equilibrium limit.

The feature in active matter of converting stored and available energy, such as chemical potential, into mechanical work is also of great importance to the field. Energy dissipation can be utilised to do work performed by self-organised agents or collective; this is a key pursuit of nanotechnology.[7]. Statistical and computational models can lend insight into individual and collective dynamics, and in turn, give way to new experimental designs of nano/micromechanical systems. These insights, then, would facilitate the creation of synthetic active matter, whose potential ranges from the biomedical application of nanomachine acive-targeted drug delivery[8] to the location-mapping application of nanoscopic/microscopic environmental sensing[9], such as in fire rescue[10] and space exploration[11].

Note, however, that physical models are sometimes challenged in literature due to potential oversimplifications, such as the cognitive heuristics (the autonomous individual behaviour) of humans. Under duress, human agents might deal holistically, rather than individually, with each other[12]. The issue is that most active matter systems only form individual relationships between agents, and do not account for the way an agent interacts with the group as a whole - the resulting individual behaviour is merely a summation of the agent's response to each other agent around it. There are psychological arguments that this is not the case, and that instead humans might, under duress, conceptualise crowds as a collective, and take actions in relation to the collective itself. This objection rests on the assumption that this holistic heuristic does not *emerge* from individual relations, of course (in which case mapping relationships strictly between individuals is unproblematic).

These insights lead to the exploration of various models. For flocks of birds or swarms of locusts, individual cognitive heuristics tend to suffice - self-propelled particles with adaptive movement patterns based on neighbours can accurately reproduce some migrational patterns [13][14]. Microscopically, active matter models offer insight into understanding how hierarchically-organised emergence happens within cell tissues, and how it may be leveraged by medicine[15]. Bacteria lend a great example for exploring the intertwining of phenomena to be emulated by active matter. Some strains (such as *Bacillus subtilis*) can be modelled using both direct physical interaction (between individuals) and long-distance biochemical signalling (within the collective), with complexity and clustering developing in response to harsh external conditions [16]. The latter interaction is called quorum sensing, the adaptation of the individual to local population density; this has developed into its own active matter branch of individual-to-collective behaviour [17]. Using such models, it is possible to recover the aforementioned human holistic cognitive heuristics [18].

ACTIVE MATTER MODELS

Modelling active matter is useful for delineating the important features of physical systems and how they quantitatively influence behaviour. Of note are particle-based systems, which establish behaviour of individual particles, such as through Active Brownian Particles and/or field theory models. **These can be examined in on-lattice or off-latice systems**.

Active Brownian Particles (ABPs) are self-propelled particles (SPPs) interacting strictly through (soft or hard) repulsive collisions and affected by friction within the medium[19]. This model emerges from classical Brownian motion, the latter constituting a stochastic, but passive, system of collisions; unlike active matter systems, Brownian motion has no active supply of energy to the particles, and particles are placed within an energy equilibrium with their surrounding medium, expressed by a fluctuation-dissipation theorem[20]. By contrast, this theorem does not apply to ABPs, since the latter exhibit an autonomous force. The most frequent models have the acting force on and subsequent velocity of the particle be constant, such that terminal velocity is instantly exhibited, although recently there have been generalised extensions which account for deviations from stationary velocity[20][21].

A feature of self-propelled particles such as ABPs is that it replicates thermal phase separation through altering movement parameters: this is known as *motility-induced phase separation* (MIPS). In ABPs, this manifests above certain packing fractions, as physical borders between which freedom of movement for autonomous particles is significantly different (such as solidlike and gaslike regions) [22].

Active field models subject autonomous agents to external fields which influence and restrict movement; they distinguish themselves from passive field models by breaking time-reversal symmetry. The latter can be expressed through the *principle of detailed balance* (PDB), which states that the probability of seeing a system transition between two states (through any chosen path) is precisely the probability of observing the reverse process[23]. These models can be constructed both top-down or bottom-up, but the latter is more relevant to this project - by coarse-graining a model at the particle level, the final theory obtains definite parameter values which can be examined. These are, however, not guaranteed to generate all the important terms in the final theory[23].

A method of emulating simplified particle behaviour is through *lattice models*: these suppress the pseudo-infinite location and orientation possibilities (only limited by floating point operators) to an established positional grid. This discretised distribution represents a limitation of degrees of freedom, in the interests of obtaining a better focus on essential aspects of motion by coarse-graining. Furthermore, it simplifies the computational burden and therefore allows for the consideration of a wider sample size with the same resources.

There are two important principles that can be applied to lattice models: the zero range process (ZRP) and the simple exclusion interaction (SEI). The former is concerned with movement - an integer number of particles can occupy a site, and each particle can 'hop' to a neighbouring site at a rate that usually scales in some way with the amount of particles present in the site it is leaving[24]. The latter, on the other hand, is concerned with prohibiting movement - it broadly forbids a particle from occupying a lattice site that is already occupied[25].

Alongside these two principles, a run-and-tumble behavioural pattern can be employed: a certain particle speed distribution is supplemented by a 'tumbling rate', which can periodically cause agents to change orientation. This inherently breaks the PDB due to altering of the persistence length of particles, which no longer matches that of thermal fluctuations - the latter can only be emulated by run-and-tumble systems with constant tumbling.

PERSISTENT EXCLUSION PROCESS

As such, we can employ run-and-tumble particles (RTPs) with the principles of ZRP and SEI on a lattice model to obtain the **persistence exclusion process** (PEP). It is essentially a single-occupancy, multi-particle lattice structure with autonomous orientation changing and propulsion ('random walks') that operates without velocity-altering collision: a particle maintains its speed and orientation upon contact, but it does not move or push the particle it is facing towards. There are a few alterable properties: the density ρ of the system alongside the lattice size N (the latter naturally influencing the former), as well as the tumbling probability P_{tumble}, which influences departure from equilibrium[26].

The model utilised here is a PEP model in two-dimensions, characterised by the reduced unit a indicating the length of a square lattice site. The particles are randomly distributed across the lattice. The update rule is randomly sequential, and thus asynchronous, in order to avoid overlap or phasing through between neighbours (thus applying SEI properly). This method of evolution has an initially chaotic behaviour which is expected to stabilise into steady states, as particles start constraining each others' movements and undergo clustering behaviour.

The main background results of this model were achieved by Soto and Golestanian, in their one and two-dimensional application of PEP. They showed clustering behaviour occurring under three processes: cluster formation through particle collision, cluster growth by absorbing new particles at boundaries, and cluster reduction through 'evaporation' at boundaries, as particles tumble outwards and away from the structure[26]. Quantitative analysis of cluster size distributions and persistence length-dependent cluster formation alongside statistical analysis of overlap functions and stopping times was also thoroughly done[26].

In the model, the lattice site number N_{total} is kept constant at 128x128. The density ρ, the lattice site number and the total particle number N_p form the following relation:

$$N_p = \rho N_{total} = \rho N_x N_y \tag{1}$$

where N_x and N_y are the number of lattice sites along the horizontal and vertical directions, respectively. Density is thus defined through lattice square units.

NEURAL NETWORKS AND TRACKING DISSIPATION

The main interest of this project is tracking the relationship between energy dissipation and structure within the PEP model. Microscopic energy dissipation has been shown to track departure from equilibrium in active matter[27], and here it will be monitored through the breaking of detailed balance. We can take $P_{tumble} = 1$ to be the situation of a thermal system with constant fluctuations; as such, lowering the tumbling rate means increasing the departure from thermodynamic equilibrium, and consequently the increase in energy dissipation.

Pair correlations in isotropic active matter systems have been shown to correlate to energy dissipation with driving forces acting as active temperature[28]. This can be applied to our case by treating the constant speed as a steady work function, or a 'negative friction' force.

The first step of this project is to establish a characterisation of the PEP system outlined above. This involves an analysis of cluster distribution, quantitative influence or varying P_{tumble} and ρ, percolation and pair-correlations, with a dissipative interpretation of the latter.

The second step is to begin working on a minimal Convolutional Neural Network (CNN) model and train it on identifying clusters and dissipation in our PEP systems. It should have access to an experiment-like data set (ignoring orientations) which it can then interpret to trace out the resulting behaviour. The CNN architecture must be considered and validated (e.g. amount of CNN layers, minimal data required, extrapolation method).

Finally, these results must be retroactively explainable through the qualitative characterisation done in the first step: the CNN performs local measuremets to retrieve physical properties from data analysis, while the characterisation sets the landscape of these physical properties in the first place.

The end goal is to successfully build and train a CNN model to effectuate cluster analysis and derive dissipation relations from the PEP model. This analysis is initially intended to be done on steady-state regions of time within PEP evolution. An interesting extension would be training the CNN to track dissipation *before the steady-state* is reached. With sufficient time, this process could also be extended to off-lattice systems: lifting the coarse-graining premise leads to more degrees of freedom, and thus the CNN would presumably require more data to train on.

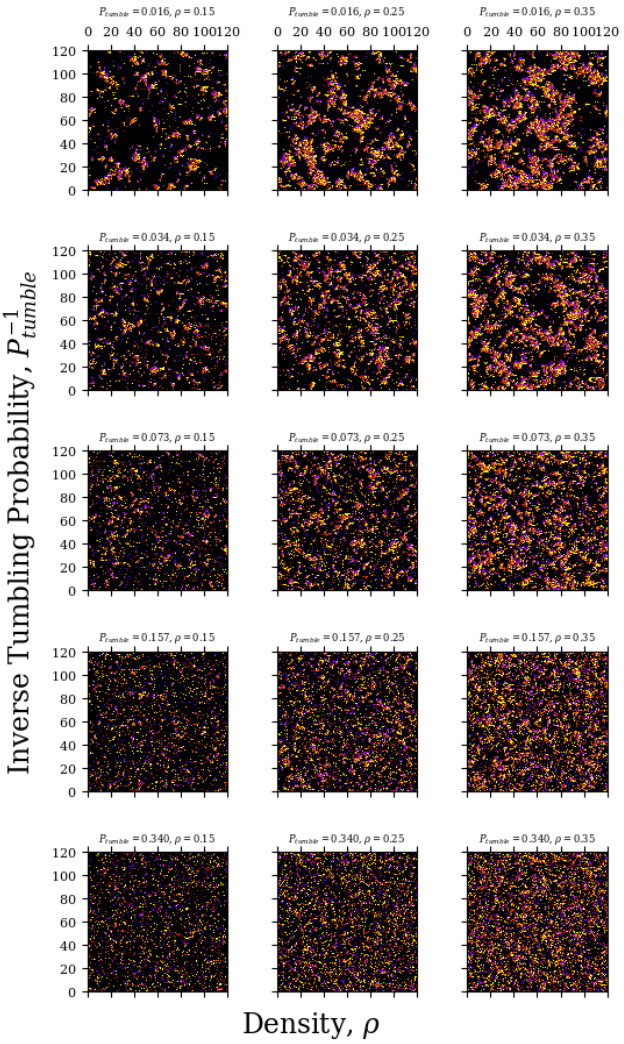

FIG. 1. Grid plot of 2D persistent exclusion process snapshots taken at the same time with varying densities (increasing from left to right) and tumbling probabilities (increasing downwards). Particle colours represent orientation.

CURRENT PROGRESS

The current goal of this project is to experiment with and modify the in-house PEP code in order to contrast and compare it with the Soto and Golestanian analysis mentioned above. The in-house code is a hybrid Python-C two-dimensional application of persistent exclusion process as outlined in the above section. As it stands, the tumbling rate P_{tumble} and density ρ have been tuned to experiment with how the system distribution qualitatively changes.

Some qualitative analysis can be derived from Figure 1. At low densities, no meaningful clustering occurs irrespective of P_{tumble}, as there are not enough particles occupying the sites: $N_p \ll N_{total}$. At very high densities (where $N_p < N_{total}$ still), clusters are not meaningfully separated from each other - this is the range of percolation. For intermediate densities,

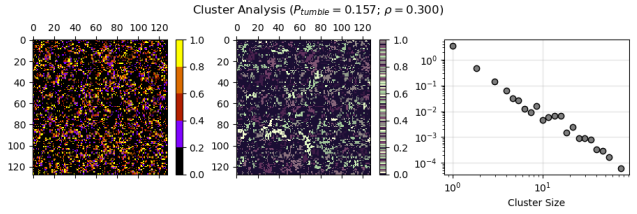

FIG. 2. Three graphs showing cluster analysis method. Graph on the left displays the PEP particles coloured by orientation, as shown by adjacent colour map; graph in the middle colour-codes particles based on clusters they belong to, emphasised by adjacent colour map; graph on the right displays a log fit (base 2) of cluster sizes.

clustering occurs with a sufficiently small P_{tumble}, and in fact the cluster sizes are inversely proportional to the tumbling rate. Too high a P_{tumble} will not allow clustering to form, as there is not enough time for outer particles to confine inner particles before direction is changed as the emerging cluster is dissipated. In Soto and Golestanian's terms[26], the clusters require a certain tumbling rate (dependent on the total system density) in order to form, and once formed, in order to statistically balance out the cluster evaporation with cluster growth.

Phase separations can begin to be observed for higher densities using analysis such as Figure 1. Unlike in ABPs, MIPS is obtained not due to repulsive forces, but due to a combination of tumbling rate P_{tumble} and SEI; both of them are nonetheless contingent on large enough densities ρ to facilitate enough particle interactions.

Having obtained snapshots (as well as animations) of PEP simulations, basic cluster analysis can then be conducted. Such a process is shown in Figure 2, for $\rho = 0.3$ and $P_{tumble} = 0.157$, still keeping N_{total} as 128x128. The snapshot is already sorted using a colour map by orientation (with the background being set to black), and its colour map is converted to colour particles by the cluster they belong to - these clusters are delimited by the adjacency of vertical or horizontal neighbours. The obtained separated clusters are then mapped in a histogram against their size, fitted logarithmically in base 2. Preliminary analysis finds agreement with Soto and Golestanian's paper[26], though more detailed data comparison is required. An initial grid of clustering as density and tumbling rate are varied (with the same values as in Figure 1) is given in Figure 3. These are taken on snapshots which are certainly in the steady-state time region, in order to ensure most clustering behaviour has already occurred.

The number of clusters broadly increases with density as expected, though this applies only up to a point where clusters begin merging due to the sheer particle number in a constrained space (this is where MIPS could begin to form). Lower tumbling rate likewise indicates an increase in cluster amount, as particles begin coalescing spontaneously - this is a breaking of detailed balance, and therefore an increase in dissipation.

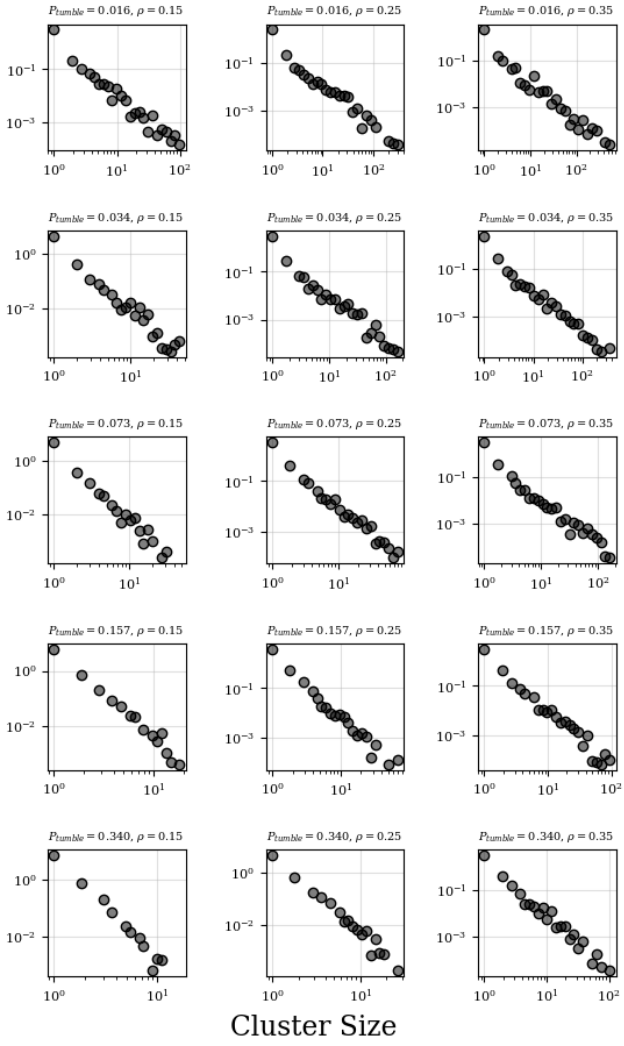

FIG. 3. Grid plot of 2D persistent exclusion process cluster sizes against counts analysed in the steady-state region for varying densities (increasing from left to right) and tumbling probabilities (increasing downwards).

DISCUSSION

The immediate future goals are to establish a method of tracking dissipation through pair-correlation, as well as analyse percolation at high densities. From there, research into the fundamental principles of CNNs and understanding how to implement them (and how implementation can be subsequently tuned) follow.

Beyond the plans discussed above, there is an interesting potential to extend these models in three dimensions (on-lattice and off-lattice). A natural problem arises here in the (two-dimensional) visual images fed to the CNN, and the further complexity of discerning depth in time.

[1] E. Flenner and G. Szamel, Active matter: quantifying the departure from equilibrium, Physical Review E **102**, 022607 (2020), arXiv:2004.11925 [cond-mat].

[2] A. Okubo, Dynamical aspects of animal grouping: Swarms, schools, flocks, and herds, Advances in Biophysics **22**, 1 (1986).

[3] J. L. Silverberg, M. Bierbaum, J. P. Sethna, and I. Cohen, Collective Motion of Humans in Mosh and Circle Pits at Heavy Metal Concerts, Physical Review Letters **110**, 228701 (2013), publisher: American Physical Society.

[4] F. Turci and N. B. Wilding, enPhase Separation and Multibody Effects in Three-Dimensional Active Brownian Particles, Physical Review Letters **126**, 038002 (2021).

[5] Fodor, C. Nardini, M. E. Cates, J. Tailleur, P. Visco, and F. Van Wijland, enHow Far from Equilibrium Is Active Matter?, Physical Review Letters **117**, 038103 (2016).

[6] A. G. Thompson, J. Tailleur, M. E. Cates, and R. A. Blythe, enLattice models of nonequilibrium bacterial dynamics, Journal of Statistical Mechanics: Theory and Experiment **2011**, P02029 (2011).

[7] W. F. Paxton, K. C. Kistler, C. C. Olmeda, A. Sen, S. K. St. Angelo, Y. Cao, T. E. Mallouk, P. E. Lammert, and V. H. Crespi, Catalytic Nanomotors: Autonomous Movement of Striped Nanorods, Journal of the American Chemical Society **126**, 13424 (2004), publisher: American Chemical Society.

[8] N. R. Stillman, M. Kovacevic, I. Balaz, and S. Hauert, enIn silico modelling of cancer nanomedicine, across scales and transport barriers, npj Computational Materials **6**, 1 (2020), number: 1 Publisher: Nature Publishing Group.

[9] C. Lv, Y. Yang, and B. Li, enNano/Micromotors in Active Matter, Micromachines **13**, 307 (2022), number: 2 Publisher: Multidisciplinary Digital Publishing Institute.

[10] J. Penders, L. Alboul, U. Witkowski, A. Naghsh, J. Saez-Pons, S. Herbrechtsmeier, and M. El-Habbal, A Robot Swarm Assisting a Human Fire-Fighter, Advanced Robotics **25**, 93 (2011), publisher: Taylor & Francis _eprint: https://doi.org/10.1163/016918610X538507.

[11] E. Vassev, R. Sterritt, C. Rouff, and M. Hinchey, Swarm Technology at NASA: Building Resilient Systems, IT Professional **14**, 36 (2012), conference Name: IT Professional.

[12] M. Moussaïd, D. Helbing, and G. Theraulaz, How simple rules determine pedestrian behavior and crowd disasters, Proceedings of the National Academy of Sciences **108**, 6884 (2011), publisher: Proceedings of the National Academy of Sciences.

[13] T. Vicsek, A. Czirók, E. Ben-Jacob, I. Cohen, and O. Shochet, enNovel Type of Phase Transition in a System of Self-Driven Particles, **75**, 1226 (1995).

[14] J. Buhl, D. J. T. Sumpter, I. D. Couzin, J. J. Hale, E. Despland, E. R. Miller, and S. J. Simpson, From Disorder to Order in Marching Locusts, Science **312**, 1402 (2006), publisher: American Association for the Advancement of Science.

[15] D. Needleman and Z. Dogic, enActive matter at the interface between materials science and cell biology, Nature Reviews Materials **2**, 1 (2017), number: 9 Publisher: Nature Publishing Group.

[16] A. Czirók, E. Ben-Jacob, I. Cohen, and T. Vicsek, enFormation of complex bacterial colonies via self-generated vortices, Physical Review E **54**, 1791 (1996).

[17] T. Bäuerle, A. Fischer, T. Speck, and C. Bechinger, enSelf-organization of active particles by quorum sensing rules, Nature Communications **9**, 3232 (2018), number: 1 Publisher: Nature Publishing Group.

[18] S. Moreno-Gámez, M. E. Hochberg, and G. S. van Doorn, enQuorum sensing as a mechanism to harness the wisdom of the crowds, Nature Communications **14**, 3415 (2023), number: 1 Publisher: Nature Publishing Group.

[19] M. C. Marchetti, Y. Fily, S. Henkes, A. Patch, and D. Yllanes, Minimal model of active colloids highlights the role of mechanical interactions in controlling the emergent behavior of active matter, Current Opinion in Colloid & Interface Science **21**, 34 (2016), arXiv:1510.00425 [cond-mat].

[20] P. Romanczuk, M. Bär, W. Ebeling, B. Lindner, and L. Schimansky-Geier, enActive Brownian particles, The European Physical Journal Special Topics **202**, 1 (2012).

[21] G. Gompper, R. G. Winkler, T. Speck, A. Solon, C. Nardini, F. Peruani, H. Löwen, R. Golestanian, U. B. Kaupp, L. Alvarez, T. Kiørboe, E. Lauga, W. C. K. Poon, A. DeSimone, S. Muiños-Landin, A. Fischer, N. A. Söker, F. Cichos, R. Kapral, P. Gaspard, M. Ripoll, F. Sagues, A. Doostmohammadi, J. M. Yeomans, I. S. Aranson, C. Bechinger, H. Stark, C. K. Hemelrijk, F. J. Nedelec, T. Sarkar, T. Aryaksama, M. Lacroix, G. Duclos, V. Yashunsky, P. Silberzan, M. Arroyo, and S. Kale, enThe 2020 motile active matter roadmap, Journal of Physics: Condensed Matter **32**, 193001 (2020).

[22] Y. Fily and M. C. Marchetti, Athermal Phase Separation of Self-Propelled Particles with No Alignment, Physical Review Letters **108**, 235702 (2012), publisher: American Physical Society.

[23] M. E. Cates, enActive Field Theories (2019), arXiv:1904.01330 [cond-mat].

[24] M. R. Evans and T. Hanney, enNonequilibrium statistical mechanics of the zero-range process and related models, Journal of Physics A: Mathematical and General **38**, R195 (2005).

[25] F. Spitzer, Interaction of Markov processes, Advances in Mathematics **5**, 246 (1970).

[26] R. Soto and R. Golestanian, enRun-and-tumble dynamics in a crowded environment: Persistent exclusion process for swimmers, Physical Review E **89**, 012706 (2014).

[27] C. del Junco, L. Tociu, and S. Vaikuntanathan, Energy dissipation and fluctuations in a driven liquid, Proceedings of the National Academy of Sciences **115**, 3569 (2018), publisher: Proceedings of the National Academy of Sciences.

[28] G. Rassolov, L. Tociu, Fodor, and S. Vaikuntanathan, enFrom predicting to learning dissipation from pair correlations of active liquids, The Journal of Chemical Physics **157**, 054901 (2022).