Monte Carlo method for active particle dynamics with thermodynamic consistency

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Active particles maintain themselves far from equilibrium by converting ambient or stored energy into self-propulsion. They are known to exhibit various novel collective phenomena, such as motility-induced phase separation, flocking, and current rectification. Recently, there has been a surge of interest in identifying the role of energy dissipation in maintaining such large-scale nonequilibrium structures. Since the models of active particles are typically very challenging to solve analytically, developing an efficient numerical method for investigating their properties is a task of great importance.

Lattice-based Monte Carlo methods provide efficient means of computing the universal scaling properties of many-particle systems. For equilibrium systems, there are well-established Monte Carlo methods based on the ensemble theories. In contrast, for active particles, the lack of ensemble theories means that one must rely on the kinetic Monte Carlo (KMC) methods that properly discretize the dynamics in space and time so that the continuum description is restored in an appropriate limit. A recently proposed KMC method achieves this goal by probabilistically mixing 'passive' steps with active ones. However, the method focuses only on the kinetics of the system, completely ignoring its energetics. If one is also interested in calculating the thermodynamic cost of maintaining a certain dissipative structure, a KMC method with well-defined energetics is needed.

In this study, we present a thermodynamically consistent KMC algorithm describing both kinetics and energetics of active particles. Towards this purpose, we construct a model of active lattice gas whose jump probability does not only satisfy the local detailed balance condition but also involves the prefactor which explicitly depends on the self-propulsion. The model correctly reproduces the continuum dynamics in the proper limit, all the while allowing us to quantify how far from equilibrium the system is by calculating the energy dissipation.

We demonstrate that the characteristic phenomena of active matter, such as motility-induced phase separation, current rectification, and accelerated phase segregation are well reproduced by our model. Moreover, our method reveals which part of the system dissipates more energy as the active particles maintain a nonequilibrium structure. These results are compared with those of previous studies that used effective field theories.