Colored Noise Models of Active Particles

I. *Multidimensional stationary probability distribution for interacting active particles.*
C. Maggi, U.M.B. Marconi, N. Gnan, and R. Di Leonardo, Scientific Reports, **5** 10742 (2015)

II *Effective interactions in active Brownian suspensions.*
T.F.F. Farage, P. Krinninger, and J.M. Brader, Physical Review E **91** 042310 (2015)

Recommended with a commentary by Mike Cates, University of Cambridge, and Cesare Nardini, University of Edinburgh

Active matter is, by definition, out of equilibrium: for example, in active colloids or motile bacteria, a continuous flow of energy permits particles to self-propel. This energy flux involves microscopic currents which violate time reversal symmetry at the microscale. However, there are situations where no macroscopic net currents are observed in steady state, in stark contrast with most non-equilibrium systems, for instance fluids subjected to shear flow. This raises the issue of whether and how an effective equilibrium description, albeit valid only at a macroscopic level [1], might actually be found. The two papers discussed here have recently made significant progress in this direction.

Both Maggi et al. [paper I] and Farage et al. [paper II] consider a minimal model for active particle systems. Specifically, they consider systems composed of overdamped interacting particles driven by persistent ("colored") noise: a noise whose temporal correlation decays exponentially. Without interactions, the noise fixes directly the velocity of each active particle, which acquires a finite correlation time. Detailed balance, which stems from microscopic time-reversal symmetry, is violated because the noise is persistent while the damping is instantaneous – in breach of the fluctuation-dissipation theorem. The colored noise model can be seen as an approximate description of active Brownian colloids with a fixed magnitude of propulsive force (hence, in the dilute limit, fixed speed) [paper II]; but it can also be viewed as a benchmark model in its own right. Unlike active Brownian colloids, the colored noise model makes sense even in 1D.

The colored noise model breaks detailed balance already in the simplest case of a single particle in an external potential ϕ. As is typical for non-equilibrium systems, it is not possible in general to find the exact stationary probability distribution function (PDF) for the particle position. However, an interesting exact limit arises when the persistence time vanishes ($\tau \to 0$) and the (root-mean-square) self-propulsion speed diverges ($u_0 \to \infty$) such that the macroscopic diffusivity $D \propto u_0^2\tau$ remains finite. In this limit, the noise becomes white in time and the stationary PDF approaches the Boltzmann equilibrium measure $P_s \propto \exp(-\phi/D)$. (Units are chosen so that the drag coefficient is unity; hence D has the units of k_BT.) A natural question then arises: what if τ is small but finite? Can an effectively Markovian description be given?

Interestingly, much work was done in the 1980s to build effective Markovian approximations for one-particle colored-noise systems. At the time, these models were of interest for their applications to dye lasers, not active matter. Two approaches are particularly relevant to this commentary: the theory of Fox [2] and the 'universal colored noise approximation', UCNA [3]. These provides two different Markovian effective descriptions, but predict very similar stationary properties; for example their steady-state PDFs for a single particle in an external potential are identical. A very interesting observation is that these effective descriptions contain terms of all orders in τ. One might thus hope that, even if they are obtained in the small τ limit, they remain useful even away from that limit. For those interested in connections to the older literature, we recommend the review by Hanggi [4].

The main result of Maggi et al. in paper I is a generalization of UCNA to more than one interacting particle, creating a new tool to address the collective properties of active matter through construction of an effective free energy that governs steady states. It is thus possible in principle to write explicitly the full PDF for the positions of particles in terms of an effective potential: $P_s \propto \exp(-\phi_{\text{eff}}/D)$. Here ϕ_{eff} describes a set of effective interactions, in an equilibrium system whose PDF is the same as the active one.

However, the UCNA approximates not just steady states but the entire dynamics. Here, advancing beyond paper I, very recent work by two groups has confirmed a stronger result [5, 6]. Namely, UCNA results in an effective description that is not only Markovian, but also respects detailed balance. It therefore maps the active system onto an effectively passive one (with new and perhaps complicated interactions, see below) not just for steady states but for dynamics.

Although the approximation is hard to justify beyond the small τ limit, UCNA is able to capture steady-state phenomena that are clearly due to activity, such as accumulation of particles near the boundaries of their container. Moreover, even when τ is not small, UCNA gives in various cases very good quantitative predictions for the density profiles. While paper I only consider systems composed of one and two active particles, the same authors have now started to investigate many body systems within their approach [5].

The second work we highlight here, by Farage et al. [paper II], goes much further than paper I in addressing many-body systems, this time using Fox theory to calculate an effective potential ϕ_{eff} for steady states. A major difficulty is that the effective equilibrium system is extremely complex: ϕ_{eff} contains many-body and long-ranged terms. In paper II this difficulty is set aside by only retaining the two body interactions, and then employing liquid state integral equation theory. Although the two-body approximation is far from under control at finite densities (and notwithstanding a technical error in the calculations [9]) many of the predictions are impressively good when compared with direct numerical simulations.

The methods of paper II confirm existing qualitative insights, and also provide new ones. With a purely repulsive bare inter-particle potential ϕ, the effective two-body interactions are attractive at large distances, so that the system separates in high and low density phases. This is the now-familiar phenomenon of motility-induced phase separation [1]. More intriguingly, with attractive ϕ, the effective interactions can be repulsive at large distance, creating at two-body level a complex phase diagram with phase separated, mixed and finite-cluster phases.

An important theoretical distinction is that paper I uses the UCNA while paper II uses Fox theory. When τ is small but finite the two schemes give identical stationary distributions for many-body systems [6] as they do in the single-particle case. However, the time evolution equations do not coincide. Since papers I and II compare only stationary properties to direct numerical simulations, we do not know yet which is preferable dynamically. Indeed, it is an open question whether either approach is really good for dynamics, and this is poorly understood even for one-particle systems. There has been confusion on this topic since the 1980s [4, 7, 8] largely due to poorly resolved numerical simulations. We believe that this is an interesting open question that merits detailed attention.

In summary, the two papers recommended here each provide an explicit but approximate steady-state mapping of a simple but nontrivial active model onto an effective equilibrium system. These theories do not contain any fitting parameter and provide excellent predictions for density profiles and two-body correlations. In principle, they provide much more: the full many-body PDF for particle positions (just as Boltzmann-Gibbs does for a standard equilibrium system). In practice, however, the effective equilibrium system has many-body, long-range interactions that may resist analysis. Accordingly there are many open questions. Do the many-body effective interactions matter? Do they matter even at qualitative level? Is it even useful to have a mapping onto equilibrium if the resulting system is so complicated?

As a final remark, we underline once again that these approximation schemes map an initially non-equilibrium descripition into an equilibrium one. Accordingly, macroscopic steady-state fluxes are ruled out, and neither Fox theory nor UCNA can accurately describe situations where such fluxes do, after all, arise. We are far from having a clear set of conditions under which that happens; without it, use of either approximation risks neglecting important aspects of the active physics.

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[9] The effective Markovian dynamics written in paper II (eqs. (5)-(8)) is incorrect due to an error in Appendix B. However, the authors use their result only in low density limit (eqs. (9)-(13)) where correcting this error amounts to replacing τ by 2τ. Hence the main results of the paper are qualitatively unaffected [TFF Farage and JM Brader, private communication]. The authors do not discuss detailed balance; further work shows that only the corrected effective Markovian dynamics obeys it [6].