Partitioning by collision

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Shaking a can of mixed nuts sorts them according to size. Mixtures of self-propelling particles of equal size can also undergo demixing, provided they differ in their diffusivities.

An ensemble consisting of a binary mixture of particles of equal size can partition itself into its component fractions - provided that the two species differ in their diffusion constants.

If you shake a can of mixed nuts before opening it, you can count on finding the walnuts on top and the peanuts at the bottom. This is an everyday example of the "spontaneous", demixing of heterogeneously sized particles, popularly known as the Brazil Nut effect. The phenomenon is observed in all granular systems consisting of particles of unequal sizes, where the imposition of an undirected force results in random active movements of its constituents. However, computer simulations performed by a group led by Ludwig-Maximilans-Universitaet (LMU) in Munich physicist Erwin Frey have now shown that mixtures of equally sized particles in solution will sort themselves out, provided that the components differ in diffusivity. "Based on the results of our simulations, we now provide a theoretical explanation for this phenomenon, which has never been investigated before. Our model indicates that the random motions of the particles involved play an important role in the demixing process," says Frey. The new study appears in the journal *Physical Review Letters*.

Soluble substances normally become evenly distributed throughout the solvent medium, thanks to passive molecular diffusion. The rate at which this occurs depends on the diffusion constant of the molecule concerned, whose magnitude increases with the temperature. In mixtures that have attained thermal equilibrium, particles of equal size normally exhibit the same diffusion constant. "We were interested in what happens when particles of equal size differ in their diffusion constants," says Simon Weber, first author on the new paper. Since such a situation can only arise in non-equilibrium systems which contain actively driven particles, we chose a system in which some of the particles exhibit irregular active motion. These motions are characterized by their so-called persistence length, which describes the average path length traversed by a particle in a given direction before it careers off in a different direction."

Simulations of particle motions in such a system indicate that a binary mixture consisting of rapidly moving 'hot' particles and passively diffusing 'cold' particles will undergo spontaneous partitioning if the persistence length for the self-propelled particles is very short. This is the case for motile bacterial cells, for example, for which the persistence length is less than the cell diameter. "Demixing occurs because the passive particles are constantly being buffeted by the active species," Frey explains. "This results in an effective attraction between the passive particles, such that, in the long term, they congregate into a single cluster. The active particles become distributed uniformly around the cluster, essentially acting as a cage within which the cluster is confined.

However, the fractionation effect is only observed if both the total number of particles and the difference between the diffusion constants of the particle species are sufficiently large - and even then, demixing is a slow process. "It takes a long time for a population of particles to be distributed uniformly in a given volume of space by means of diffusive motion. And the fact that the diffusive motions of the passive particles are primarily driven by collisions with the active particles makes the process even slower," Weber says. "We believe that the reason why this sort of cluster formation by the passive particles has never been reported before is that the relevant simulations were broken off too early." The next chapter in this story will be concerned with the experimental verification of the effect predicted by the simulations described in the new paper.

More information: Simon N. Weber et al. Binary Mixtures of Particles with Different Diffusivities Demix, *Physical Review Letters* (2016). DOI: 10.1103/PhysRevLett.116.058301

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