Superadiabatic forces in overdamped Brownian dynamics

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Power functional theory (PFT) [1] is an exact generalization of equilibrium density functional theory to nonequilibrium Brownian dynamics.

In PFT the exact dynamics of overdamped Brownian particles is described by a unique time-dependent power functional that depends on both the one-body density distribution and the one-body current. By construction, the functional attains a minimum with respect to the current at the physical time evolution of the system.

PFT goes beyond the adiabatic approximation implicit in dynamic density functional theory [2] by including superadiabatic forces. The superadiabatic forces are generated via functional differentiation of the excess (over ideal gas) power functional, which plays the analogous role as the excess free energy functional in equilibrium density functional theory.

We present an explicit and simple approximation for the superadiabatic excess power functional based on the local velocity gradient [3]. The resulting superadiabatic forces, obtained via functional differentiation, are in very good agreement with Brownian dynamics simulations, and explain a broad range of phenomena, such as viscous forces, structural forces, lane formation in colloidal systems, shear migration, and motility induced phase separation in active systems.

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[1] M. Schmidt and J. M. Brader, J. Chem. Phys. **138**, 214101 (2013).

[2] U. M. B. Marconi and P. Tarazona, J. Chem. Phys. **110**, 8032 (1999).

[3] D. de las Heras and M. Schmidt, Phys. Rev. Lett. **120**, 028001 (2018).