

Long-lived non-equilibrium state in a molecular fluid with non-linear drag

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Glassy behaviour is typically associated with systems with many distinctly interacting units, which give rise to a complex energy landscape with multiple minima separated by barriers. The typical phenomenology of glassy systems includes, among other aspects, strongly non-exponential relaxation. Here, we study the dynamical evolution of a fluid with non-linear drag, for which binary collisions are elastic, described at the kinetic level by the Enskog-Fokker-Planck (EFP) equation

$$\partial_t f = \frac{\partial}{\partial \mathbf{v}} \cdot \left[\zeta(v) \left(\mathbf{v} + \frac{k_B T_s}{m} \frac{\partial}{\partial \mathbf{v}} \right) f \right] + J[\mathbf{v}|f, f]. \quad (1)$$

In the above, $f = f(\mathbf{v}, t)$ is the one-particle velocity distribution function (VDF), k_B the Boltzmann's constant, T_s the bath temperature, m the mass of the fluid particles, $J[\mathbf{v}|f, f]$ the Enskog collision operator, and

$$\zeta(v) = \zeta_0 \left(1 + \gamma \frac{mv^2}{k_B T_s} \right) \quad (2)$$

the non-linear drag coefficient [1]. In the latter, γ measures the degree of non-linearity of the drag force.

The dynamical state of the system is determined via the physical variables $(T, \{a_l\}_{l=2}^{\infty})$, where $T(t)$ is the kinetic temperature, and $a_l(t)$ are the so-called Sonine coefficients, which measure deviations from the local equilibrium Maxwellian distribution

$$f_{LE}(\mathbf{v}, T(t)) = \left(\frac{m}{2k_B T(t)} \right)^{\frac{d}{2}} e^{-\frac{mv^2}{2k_B T(t)}}, \quad (3)$$

i.e. $a_l(t) = 0$, for all l , if $f = f_{LE}$.

We observe that a non-exponential relaxation function for the kinetic temperature appears when the system is quenched to low enough temperatures, such that $\theta_i \equiv T_i/T_s \gg 1$, with θ_i being the ratio between the initial and final temperatures. This relaxation is universal in the sense that, after a suitable rescaling of the variables, it does not depend on the initial and final temperatures, nor on the degree of non-linearity, nor on the relevance of the collision term. This phenomenon is related to the existence of a long-lived non-equilibrium state (LLNES), in which the Sonine coefficients approach large stationary values a_l^r . In such state, the temperature decays algebraically, specifically

$$T(s) = \frac{T_i}{1 + 2(d+2)(1+a_2^r)s}, \quad (4)$$

with $s \equiv \gamma\theta_i t$ being a new timescale. Figure 1 shows the comparison between our theoretical prediction for the relaxation function and different sets of data obtained through

Direct Simulation Monte Carlo (DSMC), which allows to solve the EFP equation numerically. As one may observe, the agreement between simulations and theory is excellent.

The physical picture behind the LLNES is appealing. The limit $\theta_i \gg 1$ is roughly equivalent to setting $T_s \rightarrow 0$, which removes the diffusion, stochastic term from the EFP equation. Thus, in the absence of collisions, the system behaviour is purely governed by the non-linear drag, and the dynamics of the particles become deterministic. In fact, we show that the VDF at the LLNES becomes a Dirac delta function in velocity space,

$$f_{LLNES}(\mathbf{v}, t) \propto \delta\left(v^2 - \frac{dk_B T(t)}{m}\right), \quad (5)$$

where we may identify $v_T(t) \equiv \sqrt{2k_B T(t)/m}$ as the thermal velocity. Thus, in this regime, the motion of the particles is completely determined by the kinetic temperature.

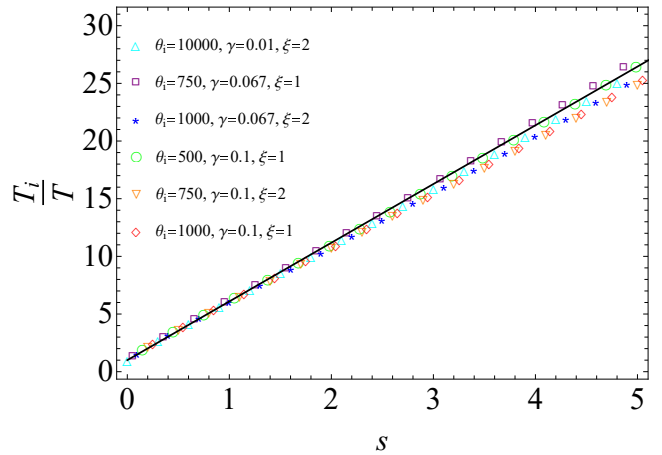


Fig. 1. Relaxation after a quench to a low temperature. Specifically, we plot T_i/T as a function of the scaled time $s = \gamma\theta_i t$. Data from DSMC correspond to parameters (θ_i, γ, ξ) , as specified in the legend, and $d = 2$. In the above, ξ stands for the inverse collision rate ($\xi \rightarrow +\infty$ corresponds to the collisionless case). The linear behaviour in T_i/T implies that the temperature relaxes algebraically, basically as t^{-1} , as theoretically predicted by Eq. (4) (solid line).

[1] A. Patrón, B. Sánchez-Rey, and A. Prados, *Strong non-exponential relaxation and memory effects in a fluid with non-linear drag*, Phys. Rev. E **104**, 064127 (2021).