Time-irreversibility in the classical many-body system in the hydrodynamic limit

Gyula I. Tóth

Interdisciplinary Centre for Mathematical Modelling, and Department of Mathematical Sciences, Loughborough University, LE11 3TU Loughborough, United Kingdom

Abstract

In this paper, exact continuum equations are derived to the classical many-body system in the hydrodynamic limit without the utilisation of statistical mechanics. It is shown that the resulting equations are universal for a class of pair potentials, and, unlike in statistical mechanics based coarse-grained models, the momentum density field carries the temperature. Evidence for the presence of pseudo time-irreversible equilibration, heat and momentum transport is provided by analysing numerical solutions of the dynamical equations. The numerical solutions further indicate the presence of non-diffusional relaxation of the macroscopic order, which raises questions about the completeness of the classical many-body dynamics in regards of the second law of thermodynamics. 

Keywords: classical n-body problem, hydrodynamic limit, Loschmidt’s paradox, irreversibility

1. Introduction

One of the most exciting unsolved problems in fundamental physics that has been puzzling physicists for almost one and half centuries is the origin of the thermodynamic arrow of time provided by the second law of thermodynamics. In particular, while the fundamental microscopic mathematical models of matter only provide time-reversible solutions, spatial order in a closed macroscopic system is known to solely decay in spontaneous temporal processes, which results in a contradiction known as Loschmidt’s paradox [1]. It is obvious that the time-
symmetry of the general solution of a dynamical system is not affected by the number of degrees of freedom, and therefore a closed Hamiltonian many-body dynamics is time reversible. Nevertheless, solutions exhibiting pseudo time-irreversibility may emerge due to the chaotic nature of the dynamics. The most widely accepted interpretation of the emergence of these solutions is linked to Poincaré’s recurrence theorem [2]. One can argue that even though the dynamics is recurring, the recurrence time for certain initial conditions are larger than the estimated age of the Universe, and therefore the time evolution of the system on practical time scales is irreversible [2, 3]. While it is plausible to accept that non-linearities transfer energy from small wave numbers to large ones in a system exhibiting macroscopic order alongside with microscopic randomness, the recurrence theorem provides no guarantee for the diffusive spatio-temporal relaxation of mass, momentum and kinetic energy on macroscopic scales, which are the primary manifestations of the second law of thermodynamics. The problem has been partially resolved in the framework of statistical mechanics. Although the Liouville equation is also time-reversible for a time-reversible microscopic dynamics, its exact-non equilibrium solutions are unknown in general, which leaves room to construct time-symmetry breaking ensembles by using the so-called Markovian approximation. The most common example is the derivation of the Boltzmann Kinetic Equation, where the Hypothesis of Molecular Chaos is used to resolve the two-particle distribution function in the Bogoliubov–Born–Green–Kirkwood–Yvon hierarchy [4]. Another famous example is the Zwanzig-Mori projection formalism, where the Markovian approximation is utilised to resolve a complicated convolution term [5]. The extension of the Dynamical Density Functional Theory for viscous liquids is also an illustrative example [5], where the Taylor expansion of the Maxwell-Boltzmann one-particle distribution is used around Local Thermodynamic Equilibrium [7]. In a recent approach, an almost exact derivation of the Navier-Stokes equations was provided for initially locally Gibbsian ensembles [8]. In this framework, viscosity emerges as the first finite-scale correction to the ideal hydrodynamic limit. Diffusion can also be incorporated directly in a dynamical system by adding a time-
continuous stochastic noise to the equations \([9, 10]\). Furthermore, it is known from the analysis of weakly perturbed Hamiltonian systems that incorporating a Markovian stochastic component operating even on a single degree of freedom is enough to break the time reversibility of the dynamics \([11, 12, 13]\). This is quite similar in molecular simulations \([14]\), since thermostats being utilised to control the temperature in these simulations \([15]\) makes the otherwise non-ergodic Hamiltonian dynamics \([16, 17, 18]\) ergodic \([19]\), which therefore converges to a statistical mechanical-compatible equilibrium. Although the results of statistical mechanical based approaches are in excellent agreement with experimental observations, one must not forget that obtaining the desired result may justify, but never proves the exactness of the assumption that lead to it. Accordingly, the existence of pseudo time-irreversible solutions and the fashion of relaxation processes in deterministic systems can only be investigated directly, i.e., without the utilisation of statistical tools and approximations. Such studies are available for fully chaotic maps, where a statistical phenomenon called “deterministic diffusion” has been discovered \([20]\). Regarding the closed Hamiltonian many-body problem, it has already been shown that this system, when supplemented with a certain weak Markovian noise, satisfies the Euler equations in the hydrodynamic limit \([21]\). Later, a direct derivation of the Euler equations were also given for simple closed Hamiltonian particle systems \([22]\). In the spirit of these works, here we propose universal continuum equations to the closed many-body system of pair interacting particles for a class of pair potentials in the exact hydrodynamic limit.

2. Theory

2.1. Microscopic continuum dynamics

The time evolution of a system of \(N\) identical, point-like classical particles interacting via the isotropic pair potential \(u(r) \equiv \varepsilon \tilde{u}(r/\sigma)\) (where \(\varepsilon\) and \(\sigma\) are the fundamental energy and length scales, respectively) is governed by the canonical equations \(\dot{\mathbf{r}}_i = \partial_{\mathbf{p}_i} \mathcal{H}\) and \(\dot{\mathbf{p}}_i = -\partial_{\mathbf{r}_i} \mathcal{H}\), where \(\mathcal{H} = \sum_i \frac{|\mathbf{p}_i|^2}{2m} + \frac{1}{2} \sum_{i,j} u(|\mathbf{r}_i - \mathbf{r}_j|)\).
$r_j$ is the Hamiltonian of the system, $r_i(t)$ and $p_i(t)$ are the position and momentum of particle $i$, respectively, and $m$ is the particle mass. To re-cast the canonical equations in continuum form, we introduce the \textit{microscopic} mass and momentum densities

$$\hat{\rho}(r, t) \equiv \sum_i m \delta[r - r_i(t)],$$

$$\hat{g}(r, t) \equiv \sum_i p_i(t) \delta[r - r_i(t)],$$

respectively, where $\delta(r) = \delta(x)\delta(y)\delta(z)$ is the three-dimensional Dirac-delta distribution. Assuming that the Fourier Transform of the pair potential exists, following the methodology of Zaccarelli et al. \cite{23, 24, 25}, then non-dimensionalising the equations by introducing the dimensional unit length $\lambda \equiv \bar{l} \sigma$, time $\tau \equiv \lambda \sqrt{m/\varepsilon}$, and mass density $\rho_0$ (where $\bar{l} = \bar{n}^{-1/3}$ with $\bar{n} = \rho_0(\sigma^3/m)$, and $\rho_0$ is the dimensional average mass density of the system) result in the following dimensionless microscopic continuum equations (See Appendix A for the detailed derivation):

$$\partial_t \hat{\rho} + \nabla \cdot \hat{g} = 0 ;$$

$$\partial_t \hat{g} + \nabla \cdot \hat{K} = \hat{\rho} (f \ast \hat{\rho}) ;$$

$$\hat{\rho} \hat{K} = \hat{g} \otimes \hat{g},$$

where $f(r) = -\nabla v(r)$ is the particle force field with $v(r) = \tilde{u}(\bar{l}r)$, while the symbols $\ast$ and $\otimes$ stand for convolution in space and dyadic product, respectively. Furthermore, $\hat{\rho}(r, t) = \sum_i \delta[r - r_i(t)], \hat{g}(r, t) = \sum_i v_i(t) \delta[r - r_i(t)]$, and $\hat{K}(r, t) = \sum_i v_i(t) \otimes v_i(t) \delta[r - r_i(t)]$ are the dimensionless mass, momentum and kinetic stress densities, respectively, where $r_i(t)$ is the dimensionless particle position and $v_i(t)$ the dimensionless particle velocity. It is important to note that since the Hamiltonian particle dynamics is closed for the positions and momenta, the exact microscopic continuum equations are also closed for the mass and momentum densities, and there is no need to introduce further densities at this stage. Finally we mention that the right-hand side of Eq. (4) is the microscopic analogue of the local Gibbs-Duhem relation known from Dynamical Density
Functional Theory [6] or phenomenological continuum models [26, 27, 28] for the following reason. The potential energy of the system can be written as:

$$V = \frac{1}{2} \sum_{i,j} u(|r_i - r_j|) = \frac{1}{2} \int d\mathbf{r} \left\{ \hat{\rho} \left( \frac{u}{m^2} \ast \hat{\rho} \right) \right\} .$$  \hspace{1cm} (6)

Since $u(r)$ is isotropic, the first functional derivative of the potential energy w.r.t. the mass density reads $\delta U / \delta \hat{\rho} = \frac{u}{m^2} \ast \hat{\rho}$, and therefore Eq. (4) can be written as

$$\partial_t \hat{\chi} + \nabla \cdot \hat{\mathbf{K}} = -\hat{\rho} \nabla \frac{\delta V}{\delta \hat{\rho}} .$$  \hspace{1cm} (7)

It has been shown recently that the Navier-Stokes equation can be derived by applying a statistical mechanical coarse-graining on Eq. (7) [25]. Nevertheless, our goal here is to avoid utilising statistical methods for the reasons discussed in the introduction.

### 2.2. Exact hydrodynamic limit

The practical value of Eqs. (3)-(5) is strongly limited, mainly due to the fact that the transformation is exact, and therefore the solutions of the Hamiltonian dynamics and the microscopic continuum model coincide. Addressing the macroscopic-scale behaviour of the system can be done by utilising an equivalence transformation. The solution of the dynamical equations for particle mass $m_\kappa \equiv \kappa^3 m$, pair potential $u_\kappa(r) \equiv \kappa^3 u(r/\kappa)$, and dimensional average number density $\bar{n}_\kappa \equiv \kappa^{-3} \bar{n}_0$ (called the $\kappa$-system henceforth) can be expressed as

$$\chi_\kappa(r,t) = \hat{\chi}(r/\kappa,t) \text{ (see Appendix B)},$$

where $\hat{\chi}(r,t)$ stands for the solution in the original system with $\chi = \rho, g, K$. The scaling relation

$$\hat{\chi}(r,t) = \chi_\kappa(\kappa r, \kappa t)$$  \hspace{1cm} (8)

indicates that the $O(1)$-scale dynamics in the $\kappa$-system corresponds to the $O(1/\kappa)$-scale dynamics in the original one. Consequently, the macroscopic dynamics of the original system can then be studied by considering the $O(1)$-scale dynamics in the $\kappa \to 0$ system. In this limit, one can assume that $\rho(r,t) \equiv \lim_{\kappa \to 0} \rho_\kappa(r,t)$ and $g(r,t) \equiv \lim_{\kappa \to 0} g_\kappa(r,t)$ become bounded functions.
Table 1: Macroscopic limit for the collision, Yukawa, screened inverse power, and the Hartree-Fock dispersion B potentials (from top to bottom), as defined by Eq. (9).

| $\tilde{u}(r)$ | $a_0$ |
|----------------|-------|
| $\delta(r)$   | 1     |
| $\exp(-\alpha r)/r$ | $4\pi/\alpha^2$ |
| $\{|[1 - \exp(-\alpha r)]/r\}^n$ | $A_n \alpha^{n-3}$ |
| $\exp(-\alpha r - \beta r^2)$ | $[\pi^{3/2}/(2 \beta^{5/2})] \exp[\alpha^2/(4\beta)]$ |
|                  | $\times (\alpha^2 + 2\beta) \text{erfc}[\alpha/(2\sqrt{\beta})] - \pi \alpha/\beta^2$ |

(see the argumentation later). Consequently, the kinetic stress can be expressed from the closure relation: $K = (g \otimes g)/\rho$, where $K(\mathbf{r}, t) = \lim_{\kappa \to 0} \mathbb{K}_\kappa(\mathbf{r}, t)$, and the dynamical equations for the $\kappa \to 0$ system then read: $\partial_t \rho + \nabla \cdot (\rho \mathbf{v}) = 0$ and $\partial_t \mathbf{v} + \mathbf{v} \cdot \nabla \mathbf{v} = -\nabla (v_0 * \rho)$, where $\mathbf{v}(\mathbf{r}, t) = g(\mathbf{r}, t)/\rho(\mathbf{r}, t)$ is the velocity field, while $v_0(\mathbf{r}) = \tilde{n} \lim_{\kappa \to 0} \{[\kappa^{-3}\tilde{u}(r/\kappa)]$. Using the Fourier Transform representation of the pair potential, it can be shown (see Appendix B for details) that

$$v_0(\mathbf{r}) = \tilde{n} a_0 \delta(\mathbf{r})$$

(9) for common pair potentials listed in Table 1. Using Eq. (9) in the momentum equation, then eliminating the group velocity $c_0^2 = \tilde{n} a_0$ by re-scaling time yield the following universal exact macroscopic continuum equations to the Hamiltonian system of pair interacting classical particles:

$$\partial_t \rho + \nabla \cdot (\rho \mathbf{v}) = 0 ;$$

$$\partial_t \mathbf{v} + \mathbf{v} \cdot \nabla \mathbf{v} + \nabla \rho = 0 ,$$

(10) (11)

where the spatial average of $\rho(\mathbf{r}, t)$ is unity.

### 2.3. Boundedness of the densities in the hydrodynamic limit

Before proceeding to the analysis of the numerical solution of Eqs. (10) and (11), we discuss two important aspects of the equations. Firstly, the equations are only valid if $\rho(\mathbf{r}, t)$ and $g(\mathbf{r}, t)$ are bounded functions, which can be demonstrated as follows. Without the loss of generality, the dimensionless particle
Figure 1: Schematic illustration of Eqs. (7) and (8) in a two-dimensional system. The component of the density varying on length scale \( \kappa \) is illustrated by the smoothly deformed grid, while the actual particle positions are indicated by the off-grid dots.

positions and momenta can be decomposed as (see Figure 1):

\[
\begin{align*}
\mathbf{r}_{j(i)}(t) &= \mathbf{r}_i^0 + \mathbf{u}(\kappa \mathbf{r}_i^0, \kappa t)/\kappa + \Delta \mathbf{r}_{j(i)}(t); \\
\mathbf{v}_{j(i)}(t) &= \mathbf{w}(\kappa \mathbf{r}_i^0, \kappa t) + \Delta \mathbf{v}_{j(i)}(t),
\end{align*}
\]

where \( \mathbf{r}_i^0 \in \mathbb{Z}^3 \) spans a uniform grid with unit grid spacing, \( \mathbf{u}(\mathbf{r}, t) \) and \( \mathbf{w}(\mathbf{r}, t) \) are sufficiently smooth, zero-average vector fields describing spatio-temporal variations of the mass and momentum densities on some \( \kappa \ll 1 \) scale, respectively, while \( \Delta \mathbf{r}_{j(i)}(t) \) and \( \Delta \mathbf{v}_{j(i)}(t) \) carry all other details (see Figure 2). Furthermore, \( j(i) \) is an instantaneous map between the lattice sites (indexed by \( i \in \mathbb{N} \)) and the particles (indexed by \( j \in \mathbb{N} \)). Considering only one spatial dimension, substituting Eqs. 12 and 13 into Eq. 1 yields (see Appendix C for a detailed derivation):

\[
\rho(x, t) = 1 + \sum_{p=1}^{\infty} \frac{1}{p!} (-\partial_x)^p [u^p(x, t)].
\]

A similar calculation can be performed for the momentum density, thus yielding:

\[
g(x, t) = \sum_{p=0}^{\infty} \frac{1}{p!} (-\partial_x)^p [\omega(x, t) u^p(x, t)].
\]
where $\omega(x,t) = w(x,t) + \xi(x,t)$ with $\xi(x,t) = \lim_{\kappa \to 0} \Delta v_i([x/\kappa])(t/\kappa)$ with $[x]$ denoting the floor of $x$. Eqs. (14) and (15) indicate that $\rho(x,t)$ and $g(x,t)$ can be bounded functions. The boundedness of $g(x,t)$ in case of $v_i(t) \neq 0$ can be argued on the basis of the invariance of the dimensionless particle velocities in the equivalent systems.

2.4. Temperature

In addition to the boundedness of the momentum density in the $\kappa \to 0$ system, an important feature of Eq. (15) is that $\Delta v_i(t)$ persists in $\omega(x,t)$, thus suggesting that the velocity field in Eqs. (10) and (11) carries the temperature in the form of a pseudo-noise. This can be verified by calculating the instantaneous dimensionless temperature of the $\kappa = 1$ system: $\tilde{T}(t) \equiv T(t)/T_0 = \frac{1}{3} \langle \text{Tr} \nabla (r,t) \rangle$, where $\langle \cdot \rangle$ stands for spatial average, $T(t) \equiv (3k_B N m)^{-1} \sum_i |p_i|^2$ is the dimensional temperature, and $T_0 = \epsilon/k_B$. Since the spatial averages of the corresponding microscopic densities coincide in the equivalent systems, the temperature can be expressed in terms of the continuum fields in the $\kappa \to 0$ system as:

$$\Theta(t) \equiv 3 \tilde{T}(t)/(a_0 \bar{n}) = \langle \rho(r,t) |v(r,t)|^2 \rangle,$$

where $\rho(r,t)$ and $v(r,t)$ are the solution of Eqs. (10) and (11). Eq. (16) shows that the interpretation of Eqs. (10) and (11) is cardinally different from that of the traditional hydrodynamic equations, which describe the spatio-temporal evolution of slowly varying fields only. In contrast, the derivation of Eqs. (10) and (11) from the many-body dynamics is exact, and therefore they are expected to preserve the microscopic details. Accordingly, the stationary solution $\rho(r,t) = 1$ and $v(r,t) = 0$ of Eqs. (10) and (11) corresponds to $T = 0 K$, as it is indicated by Eq. (16). Consequently, only solutions Eqs. (10) and (11) with non-vanishing velocity field can represent finite temperature systems. It is important to note that this idea is not exactly new. Recent results indicated the presence of quasi-equilibration in the Burgers equation, which simply describes the macroscopic dynamics of non-interacting systems. Interestingly, we have numerical evidence that irreversibility is also present in these systems [29, 30, 31].
To investigate the physically relevant solutions of Eqs. (10) and (11), first we investigate the structure of the equations. Since the derivation of the equations from the many-body dynamics is exact, time reversibility of the solution is naturally preserved, and therefore any apparent irreversibility emerges from the special choice of the initial conditions. Assuming that Eqs. (12) and (13) hold, Eqs. (15) and (16) indicate \( \rho(r,t) = 1 \) and \( g(r,t) \approx \xi(r,t) \) (spatio-temporal noise), which corresponds to thermodynamic equilibrium at finite temperature.

In thermodynamic equilibrium, the momentum is expected to spread evenly across the Fourier modes, which emerges from \( \Theta(t) \approx \sum_k |v_k(t)|^2 \approx \sum_k |g_k(t)|^2 \) for \( \rho(r,t) \approx 1 \). The hypothesis of spectral equipartition reads:

\[
\Theta_\infty \equiv \lim_{t \to \infty} \frac{1}{t} \int_0^t d\tau \Theta(\tau) = N_k V_\infty^2,
\]

where \( V_\infty^2 = \frac{1}{t} \int_0^t d\tau |\tilde{v}_k(\tau)|^2 \) (constant), and \( N_k \) is the number of Fourier modes.

3. Numerical results

3.1. Equilibration and equipartition

To validate the hypothesis of spectral equipartition, numerical simulations were performed for \( \Theta_0 = 5 \times 10^{-4} \) initial temperature, mimicking liquid Argon below its boiling point [32, 33]. To exploit the conservation of mass and momentum, the numerical implementation of Eqs. (10) and (11) was done for the mass-momentum formalism \( \partial_t \rho + \nabla \cdot g = 0 \) and \( \partial_t g + \nabla \cdot [(g \otimes g)/\rho + \rho \nabla \rho] = 0 \) by using a flux-consistent finite-volume scheme and forward Euler time discretisation [34] on a two-dimensional uniform grid with grid size \( N = 1024 \), grid spacing \( h = 1 \) and time step \( \Delta = 10^{-4} \) (see Appendix D for further details).

We applied periodic boundary conditions, thus resulting in a discrete Fourier space with resolution \( \Delta k = 2\pi/1024 \). In the first numerical simulation, the initial conditions \( \rho(r,0) = 1 \) and \( \tilde{g}_k(0) = A f(k) (I - n_k \otimes n_k) \cdot \tilde{\xi}_k \) were used, where \( \tilde{\xi}_k \) is an uncorrelated Gaussian random vector field, \( A = (\pi/N)\sqrt{6 \Theta_0/I} \) and \( I = \int_0^\pi (2\pi k \, dk) f^2(k) \). The out-of-equilibrium initial condition was assured
Figure 2: Fourier amplitudes (logarithmic scale) of the momentum density in the range $[-\pi, \pi] \times [-\pi, \pi]$ at (a) $t = 0$ and (b) $t = 10^4$; (c) Time dependence of spectral momentum components at $k = (40 \Delta k n, 0)$, where $n = 1, 2, \ldots, 12$ (from top to bottom, respectively).

by choosing $f(k) = \text{sinc}^{16}(k) \theta(\pi - k)$. The time evolution of the system was studied for $n = 10^8$ time steps. While the spectral components of the momentum (denoted by $|g_k(t)|^2$) were fast decaying around $k = 0$ at $t = 0$, by the end of the simulation the momentum had spread across the available wave numbers [see Figs. 2(a) and 2(b)]. The time evolution of the square magnitude of 12 different Fourier components of the momentum density are shown in Fig. 2(c). The figure indicates that Fourier amplitudes initially spanning an 11 orders of magnitude range “converge” for large times in the sense that their maxima tend to be in the same order of magnitude (indicated by the thick horizontal line in the figure). In addition, since the relative density and temperature fluctuations remained in the range of $\pm 0.5\%$ and $\pm 0.025\%$, respectively, the results provide evidence for the presence of thermodynamic equilibrium with spectral equipartition defined by Eq. (17).
Figure 3: Kinetic energy density in real space at (a) $t = 0$ and (b) $t = 5 \times 10^3$; (c) Time evolution of the Fourier coefficients of $e(r, t)$ for $k = (\Delta k n, 0)$, where $n = 1, 3, 5, \ldots, 19$ (from top to bottom).

3.2. Heat conduction

In the second numerical simulation, heat transport was investigated by bringing two equilibrated systems with temperatures $T_1 = 10^{-3}$ and $T_2 = T_1/2$ into contact as shown in Fig 2(a). (In the equilibration process of the sub-systems a homogeneous thermostat was applied in every $10^5$ time steps to prevent the system from overheating due to Galerkin truncation.) The temperature difference between the regimes of different temperatures started to decrease gradually in an equalization process, and almost completely vanished by $t = 5 \times 10^3$ [see Figs. 3(b) and 3(c)], thus confirming the presence of heat condition. Nevertheless, Fig. 3(d) shows the time evolution of the magnitude of some Fourier coefficients of the kinetic energy density $e(r, t) = (1/2) \rho(r, t)|v(r, t)|^2$ (or local temperature). The figure indicates exponential relaxation of the Fourier modes with roughly the same relaxation time, which suggests a pseudo-irreversible process with a local relaxation dynamics $\partial_t \Theta(r, t) = -\alpha[\Theta(r, t) - \Theta_\infty]$ rather than diffusion emerging from the phenomenological Fourier’s law.
3.3. Viscous flow

In our last numerical experiment, viscous momentum transport was studied by bringing two equilibrated systems of average densities $\rho_1 = 0.99$ and $\rho_2 = 1.01$ into contact at $\Theta_0 = 10^{-3}/3$ [see Fig. 4(a)]. To prevent the system from overheating, we applied a homogeneous thermostat in every $N_T = 10^4$ steps, in which the temperature was reduced by a 0.01%. In addition, the temperature was brought back to $\Theta_0$ in every $N_P = 512/\Delta t$ time steps. With these techniques, the temperature was kept within the relative range $\pm 6\%$ [see Fig. 4(c)]. As indicated by Fig. 4(c), the temperature started to oscillate at angular frequency $\omega_T = 2\pi/512$, which more resembles the FPUT-type recurrence rather than pseudo-irreversibility emerging from a diverging Poincaré recurrence time. The decay of the macroscopic order in the density field is indicated by Figs. 4(b) and 4(d). As shown in Fig. 4(d), the long wavelength Fourier amplitudes of the density evolved in the fashion of $|\delta P(k,t)| \propto \cos^2(\omega_k t)\{1 + \alpha [\sin(\Omega_k t)/(\Omega_k t)]^p\}$ (where $\omega_k = \Delta k \sqrt{2n+1}$ for $k = \Delta n, n = 1, 3, 5, \ldots$), which indicates the decay of the initial macroscopic
order in the studied time interval. However, despite the relatively small difference of the average densities of the two initial sub-systems, the dynamics of the relaxation is different compared to the diffusive relaxation provided by the linearisation of the Navier-Stokes equations, which provides $|\delta P(k, t)|^2 \propto e^{-\mu k^2 t}$ for a viscous one-dimensional ideal gas (where $\mu$ is the viscosity).

4. Summary

Summarising the results, we presented the derivation of exact continuum equations to the classical many-body system of pair-interacting particles in the hydrodynamic limit. The derivation relied only on the assumption that the sum of infinitely many, infinitely small-amplitude Dirac-delta distributions located infinitely close to each other is a bounded function, for which evidence has been provided. The emerging equations are time-reversible, similarly to those derived by Olla, Varadhan and Yau in 1993 [21], and also universal for pair potentials being nascent to the Dirac-delta distribution. Since the Dirac-delta potential is a fixed point of the similarity transformation, our equations clearly indicate the difference between interacting and non-interacting systems in the hydrodynamic limit. Since the continuum equations are not coarse-grained equations (which can be obtained in the framework of statistical physics), the temperature is carried by the momentum density. Since in the hydrodynamic limit the volume element contains infinitely many particles, the temperature manifests as a pseudo-random noise in the momentum field. Consequently, equilibration and heat transport can be addressed without developing an additional transport equation for the energy. Numerical evidence has been provided for the emergence of pseudo thermal equilibrium in the Galerkin truncated equations. The results of numerical simulations also revealed the presence of non-diffusive pseudo-irreversible macroscopic-scale transport of heat and momentum in the hydrodynamic limit. The presence of thermodynamic equilibrium, together with the deviations from the well-known diffusion laws raises serious questions. There
can be various reasons of the discrepancy, including (i) the lack of finite-scale
terms (dissipative terms are also absent in the equations of Olla, Varadhan and
Yau referring to the hydrodynamic limit [21], and such terms emerge as the first
finite-scale correction in the statistical theory of Sasa [8], or (ii) the incom-
pleteness of the classical microscopic model, which is supported by quantum
mechanical arguments [35, 36]. The latter suggests that a Markovian stochastic
component might be missing in the Hamiltonian particle dynamics [37], which
would naturally ensure irreversibility, and might result in diffusive relaxation
on macroscopic scales. Nevertheless, we have demonstrated that pseudo ir-
reversibility is present in the closed Hamiltonian many-body dynamics in the
exact hydrodynamic limit, which is the first step towards a direct resolution of
Loschmidt’s paradox.

Acknowledgements

The author wishes to thank M. te Vrugt (University of Münster, Germany),
A. J. Archer and K. Khusnutdinova (Loughborough University, UK) for their
valuable comments.

Appendix A. Microscopic dynamical equation

Appendix A.1. Definitions

The analytical calculations refer to 3 spatial dimensions. Accordingly, the
Fourier/inverse Fourier transforms and the Dirac-delta distribution are defined
as:

- Fourier transform: \( F(k) \equiv \frac{1}{(2\pi)^3} \int dr \{ f(r)e^{-i\mathbf{k}\cdot\mathbf{r}} \}; \)
- Inverse Fourier transform: \( f(r) \equiv \int dk \{ F(k)e^{i\mathbf{k}\cdot\mathbf{r}} \}; \)
- 3-dimensional Dirac-delta: \( \delta(r) \equiv \delta(x)\delta(y)\delta(z) = \frac{1}{(2\pi)^3} \int dk \{ e^{i\mathbf{k}\cdot\mathbf{r}} \}; \)
- The Fourier transform of \( f(r) \equiv \delta(\mathbf{r} - \mathbf{a}) \) reads: \( F(k) = \frac{1}{(2\pi)^3} e^{-i\mathbf{k}\cdot\mathbf{a}} \).
Appendix A.2. Conservation of mass and momentum

Let \( m \) be the particle mass, and let \( \mathbf{r}_i(t) \) and \( \mathbf{p}_i(t) \) be the position and momentum of particle \( i \), respectively. The microscopic mass and momentum densities read:

- Mass density: \( \hat{\rho}(r, t) = m \sum_i \delta[\mathbf{r} - \mathbf{r}_i(t)]; \)
  Fourier transform: \( \hat{\mathbf{P}}(k, t) = \frac{m}{(2\pi)^3} \sum_i e^{-i\mathbf{k} \cdot \mathbf{r}_i(t)}; \)

- Momentum density: \( \hat{\mathbf{g}}(r, t) = \sum_i \mathbf{p}_i(t) \delta[\mathbf{r} - \mathbf{r}_i(t)]; \)
  Fourier transform: \( \hat{\mathbf{G}}(k, t) = \frac{1}{(2\pi)^3} \sum_i \mathbf{p}_i(t) e^{-i\mathbf{k} \cdot \mathbf{r}_i(t)}; \)

In the derivation of the microscopic continuum equations, we use the canonical equations \( \mathbf{p}_i(t) = m \dot{\mathbf{r}}_i(t) \) and \( \mathbf{p}_i(t) = -\partial V/\partial \mathbf{r}_i(t) \), where \( V = \frac{1}{2} \sum_{i,j} u(|\mathbf{r}_i(t) - \mathbf{r}_j(t)|) \) is the potential energy, and \( u(r) \) the isotropic pair potential. The time derivative of the Fourier transform of the microscopic mass density reads:

\[
\frac{\partial \hat{\rho}(k, t)}{\partial t} = -\frac{i\mathbf{k}}{(2\pi)^3} \cdot \sum_i m \dot{\mathbf{r}}_i(t) e^{-i\mathbf{k} \cdot \mathbf{r}_i(t)} = -i\mathbf{k} \cdot \hat{\mathbf{G}}(k, t), \quad (A.1)
\]

thus indicating

\[
\frac{\partial \hat{\rho}(k, t)}{\partial t} + i\mathbf{k} \cdot \hat{\mathbf{G}}(k, t) = 0 \quad \Rightarrow \quad \frac{\partial \hat{\rho}(r, t)}{\partial t} + \nabla \cdot \hat{\mathbf{G}}(r, t) = 0. \quad (A.2)
\]

The time derivative of the Fourier transform of the microscopic momentum density reads:

\[
\frac{\partial \hat{\mathbf{G}}(k, t)}{\partial t} = \frac{1}{(2\pi)^3} \sum_i \{ \dot{\mathbf{p}}_i(t) - [i\mathbf{k} \cdot \dot{\mathbf{r}}_i(t)] \mathbf{p}_i(t) \} e^{-i\mathbf{k} \cdot \mathbf{r}_i(t)} \quad , \quad (A.3)
\]

thus yielding

\[
\frac{\partial \hat{\mathbf{G}}(k, t)}{\partial t} + \frac{i\mathbf{k}}{(2\pi)^3} \sum_i \mathbf{p}_i(t) \otimes \mathbf{p}_i(t) e^{-i\mathbf{k} \cdot \mathbf{r}_i(t)} = -\frac{1}{(2\pi)^3} \sum_i \frac{\partial V}{\partial \mathbf{r}_i(t)} e^{-i\mathbf{k} \cdot \mathbf{r}_i(t)}. \quad (A.4)
\]

Assuming that the Fourier transform of the pair potential [denoted by \( U(k) \)] exists, the pair potential can be written as: \( u(r) = \int d\mathbf{k} \{ U(k) e^{i\mathbf{k} \cdot \mathbf{r}} \}. \) Conse-
quently,

$$\frac{\partial V}{\partial r_i(t)} = \frac{\partial}{\partial r_i(t)} \left( \frac{1}{2} \sum_{m,n} d\mathbf{q} \left\{ U(q) e^{i \mathbf{q} \cdot (\mathbf{r}_m(t) - \mathbf{r}_n(t))} \right\} \right)$$

$$= \frac{1}{2} \int d\mathbf{q} \left\{ U(q) \sum_{m,n} i \mathbf{q} (\delta_{m,i} - \delta_{n,i}) e^{i \mathbf{q} \cdot (\mathbf{r}_m(t) - \mathbf{r}_n(t))} \right\}$$

$$= \int d\mathbf{q} \left\{ i \mathbf{q} U(q) \sum_j e^{i \mathbf{q} \cdot (\mathbf{r}_i(t) - \mathbf{r}_j(t))} \right\} . \tag{A.5}$$

Introducing \( \hat{K}(\mathbf{k},t) \equiv \frac{1}{(2\pi)^3} \sum_i \frac{\mathbf{P}_i(t) \otimes \mathbf{P}_i(t)}{m} e^{-i \mathbf{k} \cdot \mathbf{r}_i(t)} \), and using the above expression in the spectral momentum equation yield:

$$\frac{\partial \hat{G}(\mathbf{k},t)}{\partial t} + i \mathbf{k} \cdot \hat{K}(\mathbf{k},t) = \frac{1}{(2\pi)^3} \int d\mathbf{q} \left\{ i \mathbf{q} U(q) \sum_{i,j} e^{-i (\mathbf{k} - \mathbf{q}) \cdot (\mathbf{r}_i(t) - \mathbf{r}_j(t))} \right\}$$

$$= -\frac{(2\pi)^3}{m^2} \int d\mathbf{q} \left\{ i \mathbf{q} U(q) \hat{\mathbf{P}}(\mathbf{q},t) \hat{\mathbf{P}}(\mathbf{k} - \mathbf{q},t) \right\} . \tag{A.6}$$

Calculating the inverse Fourier transform of both sides yields:

$$\frac{\partial \hat{g}(\mathbf{r},t)}{\partial t} + \nabla \cdot \hat{\mathbf{K}}(\mathbf{r},t) = -\hat{\rho}(\mathbf{r},t) \nabla \int d\mathbf{r'} \left\{ \frac{v(\mathbf{r'})}{m^2} \hat{\rho}(\mathbf{r} - \mathbf{r'},t) \right\} , \tag{A.7}$$

where \( \hat{\mathbf{K}}(\mathbf{r},t) = \sum_i \frac{\mathbf{P}_i(t) \otimes \mathbf{P}_i(t)}{m} \delta[\mathbf{r} - \mathbf{r}_i(t)] \) is the microscopic kinetic stress tensor. To show that Eq. (A.7) conserves momentum, we start from an equivalent formulation of Eq. (A.6):

$$\frac{\partial \hat{G}}{\partial t} + i \mathbf{k} \cdot \hat{K} = (2\pi)^3 [(\mathbf{F} \hat{P}) \ast \hat{P}] , \tag{A.8}$$

where \( \mathbf{F}(\mathbf{k}) = -i \mathbf{k} U(\mathbf{k})/m^2 \), and \( \ast \) stands for convolution in the wave number space. Using the convolution theorem, the right-hand side can be written as:

$$[(\mathbf{F} \hat{P}) \ast \hat{P}](\mathbf{k},t) =$$

$$\frac{1}{2} \int d\mathbf{q} \left\{ \mathbf{F}(\mathbf{q}) \hat{P}(\mathbf{q},t) \hat{P}(\mathbf{k} - \mathbf{q},t) + \mathbf{F}(\mathbf{k} - \mathbf{q}) \hat{P}(\mathbf{k} - \mathbf{q},t) \hat{P}(\mathbf{q},t) \right\} . \tag{A.9}$$

Setting \( \mathbf{k} \equiv 0 \) in the equation yields:

$$[(\mathbf{F} \hat{P}) \ast \hat{P}](\mathbf{0},t) = \frac{1}{2} \int d\mathbf{q} \left\{ [\mathbf{F}(\mathbf{q}) + \mathbf{F}(-\mathbf{q})] [\hat{P}(\mathbf{q},t)]^2 \right\} = 0 , \tag{A.10}$$
since \( \mathbf{F}(q) + \mathbf{F}(-q) = 0 \) (reflecting Newton’s third law). Setting \( k = 0 \) in Eq. (A.8) then yields
\[
\frac{d\mathbf{G}(0,t)}{dt} = 0 .
\] (A.11)

Since the total momentum of the system is \( \mathbf{P}(t) = (2\pi)^3\mathbf{G}(0,t) \), the time derivative of the total momentum is zero: \( d\mathbf{P}(t)/dt = 0 \), i.e., the total momentum of the system is conserved.

Appendix A.3. Microscopic closure relation

To find a closure relation for the microscopic kinetic stress, we show that \( \mathbf{\dot{K}}(r,t) \) can be related to \( \mathbf{\dot{p}}(r,t) \) and \( \mathbf{\dot{g}}(r,t) \):
\[
\mathbf{\dot{p}}(r,t) \mathbf{\dot{K}}(r,t) - \mathbf{\dot{g}}(r,t) \otimes \mathbf{\dot{g}}(r,t)
= \sum_{i,j} [\mathbf{p}_i(t) \otimes \mathbf{p}_j(t) - \mathbf{p}_i(t) \otimes \mathbf{p}_j(t)] \delta[r - r_i(t)] \delta[r - r_j(t)]
= \frac{1}{2} \sum_{i,j} [\Delta \mathbf{p}_{i\bar{j}}(t) \otimes \Delta \mathbf{p}_{j\bar{i}}(t)] \delta[r - r_i(t)] \delta[r - r_j(t)]
= \frac{1}{2} \sum_{i,j} [\Delta \mathbf{p}_{i\bar{j}}(t) \otimes \Delta \mathbf{p}_{j\bar{i}}(t)] \delta[\Delta \mathbf{r}_{i\bar{j}}(t)] \delta[r - \bar{r}_{i\bar{j}}(t)] ,
\] (A.12)

where \( \Delta \mathbf{p}_{i\bar{j}}(t) = \mathbf{p}_i(t) - \mathbf{p}_j(t) \), \( \Delta \mathbf{r}_{i\bar{j}}(t) = \mathbf{r}_i(t) - \mathbf{r}_j(t) \), \( \bar{r}_{i\bar{j}}(t) = [\mathbf{r}_i(t) + \mathbf{r}_j(t)]/2 \), and we used the identity \( \delta(x - a) \delta(x - b) = \delta(a - b) \delta(x - (a + b)/2) \). This identity can be proven by interpreting the product of Dirac-delta functions as
\[
\delta(x - a) \delta(x - b) = \lim_{\sigma \to 0} G_\sigma(x - a) G_\sigma(x - b),
\]
where \( G_\sigma(x) \) is any nascent function to the Dirac-delta, i.e., \( \delta(x) \equiv \lim_{\sigma \to 0} G_\sigma(x) \). Choosing \( G_\sigma(x) \equiv \frac{1}{\sigma \sqrt{2\pi}} e^{-x^2/(2\sigma^2)} \), for instance, and introducing \( s_\sigma(x) \equiv G_\sigma(x - a)G_\sigma(x - b) \) results in
\[
S_\sigma(k) = \frac{1}{2\pi} \left\{ \frac{1}{\sqrt{4\pi \sigma^2}} e^{-\frac{(a-b)^2}{4\sigma^2}} \right\} e^{-\frac{i(x+k)}{L r}} e^{-\frac{i(x-k)}{L r}}
\Rightarrow \lim_{\sigma \to 0} S_\sigma(k) = \frac{1}{2\pi} \delta(a - b) e^{-\frac{i(x+k)}{L r}}
\] (A.13)

which is the Fourier transform of \( \delta(a - b) \delta[x - (a+b)/2] \). Assuming that the order of the integration and the limit are interchangeable, it follows that \( \delta(x - a) \delta(x - b) \to \delta(x - a) \delta(x - b) \).
\[ b = \delta(a-b)\delta[x-(a+b)/2]. \]

Introducing \( \hat{R}(r, t) = \tilde{\rho}(r, t) \tilde{K}(r, t) - \hat{g}(r, t) \otimes \hat{g}(r, t) \) then yields:

\[
\hat{R}(k, t) = \frac{1}{(2\pi)^3} \frac{1}{2} \sum_{i,j} [\Delta p_{ij}(t) \otimes \Delta p_{ij}(t)] \delta[r_i(t) - r_j(t)] e^{-ik \cdot \bar{r}_{ij}(t)} . \quad (A.14)
\]

Since \( r_i(t) \neq r_j(t) \) for any \( i \neq j \) (i.e., the particles cannot occupy the same position coincidentally), \( \Delta p_{ij}(t) \equiv 0 \) for \( i = j \), and \( x \delta(x) = 0 \) everywhere, the above expression is identically zero, which results in the microscopic closure relation

\[
\hat{\rho}(r, t) \tilde{K}(r, t) = \hat{g}(r, t) \otimes \hat{g}(r, t) . \quad (A.15)
\]

**Appendix A.4. Non-dimensionalisation**

Let \( u(r) = \epsilon \tilde{u}(r/\sigma) \) be the pair potential, where \( \epsilon \) is energy, while \( \sigma \) the characteristic microscopic length scale (typically the location of the minimum of the pair potential). Measuring length in \( \sigma \) units, time in \( \tau \) units (to be determined later), \( \hat{\rho}(r, t) \) in \( m/\sigma^3 \) units, and \( \hat{g}(r, t) \) in \( m/(\sigma^2 \tau) \) units results in the dimensionless continuity equation:

\[
\partial_t \hat{\rho}' + \nabla' \cdot \hat{g}' = 0 , \quad (A.16)
\]

where \( \hat{\rho}'(r', t') = \sum_i \delta[r' - r'_i(t')] \) and \( \hat{g}'(r', t') = \sum_i v'_i(t') \delta[r' - r'_i(t')] \) are the dimensionless mass and momentum densities, while \( r'_i(t') = r_i(t' \tau)/\sigma \) and \( v'_i(t') = v_i(t' \tau)/(\tau/\sigma) \) are the dimensionless particle position and velocity, respectively. Furthermore, measuring \( K(r, t) \) in \( m/(\sigma^2 \tau) \) units results in the dimensionless microscopic momentum equation

\[
\partial_t \hat{g}' + \nabla' \cdot \hat{K}' = -\hat{\rho}' \nabla'(v' \ast' \hat{\rho}') , \quad (A.17)
\]

where \( \hat{K}(r', t') = \sum_i [v'_i(t') \otimes v'_i(t')] \delta[r' - r'_i(t')] \) is the dimensionless kinetic stress tensor, \( \ast' \) denotes a spatial convolution in the dimensionless length, while \( v'(r') = \frac{\tau^2}{m \sigma^4} \tilde{u}(r') \) is the dimensionless pair potential. Setting \( \tau \equiv \sigma \sqrt{m/\epsilon} \) then gives

\[
v'(r') = \tilde{u}(r') . \quad (A.18)
\]
The dimensionless microscopic closure equation simply reads:

\[ \hat{\rho}' \hat{K}' = \hat{g}' \otimes \hat{g}' . \]  

(A.19)

Prescribing 0 average for the momentum components (no drift), the model has two parameters: the dimensionless average density \( \bar{n} \equiv \rho_0(\sigma^3/m) \), where \( \rho_0 \) is the dimensional average mass density, and the dimensionless pair potential \( \tilde{u}(r) \). Measuring the dimensionless length and time in \( \bar{l} \equiv 1/\bar{n}^{1/3} \) units, the dimensionless mass and momentum densities, and the dimensionless kinetic stress tensor in \( \bar{n} \) units results in:

\[ \partial_t \hat{\rho}'' + \nabla'' \cdot \hat{g}'' = 0 \quad \text{(A.20)} \]

\[ \partial_t \hat{g}'' + \nabla'' \cdot \hat{K}'' = -\hat{\rho}'' \hat{\nabla}''(\hat{v}'' \otimes \hat{\rho}'') , \quad \text{(A.21)} \]

where \( \hat{\rho}''(r'') = \tilde{u}((\bar{l} r'')) \), while

- \( \hat{\rho}''(r'', t'') = \hat{\rho}'((\bar{l} r''), (\bar{l} t''))/\bar{n} = \sum_i \delta[r'' - r''_i(t'')] \);  
- \( \hat{g}''(r'', t'') = \hat{g}'((\bar{l} r''), (\bar{l} t''))/\bar{n} = \sum_i v'_i((\bar{l} t')) \delta[r'' - r''_i(t'')] \);  
- \( \hat{K}''(r'', t'') = \hat{K}'((\bar{l} r''), (\bar{l} t''))/\bar{n} = \sum_i [v'_i((\bar{l} t')) \otimes v'_i((\bar{l} t'))] \delta[r'' - r''_i(t'')] \),

where \( r''_i(t'') = r''_i((\bar{l} t''))/\bar{l} \). This step scales the average mass density to unity, while preserves the dimensionless velocity magnitudes: \( |v''_i(t'')| = |v'_i((\bar{l} t''))|^2 \).

The microscopic closure relation simply transform as:

\[ \hat{\rho}''(r, t) \hat{K}''(r, t) = \hat{g}''(r, t) \otimes \hat{g}''(r, t) . \]  

(A.22)

\textbf{Appendix A.5. Instantaneous temperature}

The dimensional instantaneous temperature of the system is defined as:

\[ T(t) \equiv \frac{2}{3} \frac{K(t)}{k_B N} , \]  

(A.23)

where \( K(t) = \sum_i \frac{|p_i(t)|^2}{2m} \) is the instantaneous kinetic energy of the system. By introducing the microscopic kinetic energy density \( \hat{\epsilon}(r, t) \equiv \sum_i \frac{|p_i(t)|^2}{2m} \delta[r - r_i(t)] \), the temperature can be expressed as

\[ T(t) = \frac{2}{3} \frac{k_B}{N} \int_V dr \hat{\epsilon}(r, t) = \frac{m}{3k_B \rho_0} \left[ \frac{1}{V} \int \int V \hat{K}(r, t) \right] , \]  

(A.24)
where we used that the kinetic energy density is related to the kinetic stress tensor via \( \dot{e}(r, t) = \frac{1}{2} \operatorname{Tr} \dot{K}(r, t) \). Applying the non-dimensionalisation yields:

\[
\dot{T}(t'') = \frac{1}{3} \langle \operatorname{Tr} \dot{K}''(r'', t'') \rangle ,
\]

(Eq. A.25)

where \( \langle \cdot \rangle \) stands for spatial average, and \( T_0 = \epsilon/k_B \) is the temperature scale.

For the sake of simplicity, we omit the \( ()'' \) notation henceforth.

### Appendix B. Hydrodynamic limit

#### Appendix B.1. Dynamical equations

Here we consider a system (called \( \kappa \)-system henceforth) with particle mass \( \kappa^3 m \), pair potential \( \kappa^3 u(r/\kappa) \), and the number density \( n_0/\kappa^3 \), where \( \kappa \) is positive real. Using the same units as in case of the original system results in the following dimensionless dynamical equations:

\[
\begin{align*}
\partial_{\tilde{t}} \rho_\kappa + \tilde{\nabla} \cdot \tilde{g}_\kappa &= 0 \quad (B.1) \\
\partial_{\tilde{t}} \tilde{g}_\kappa + \tilde{\nabla} \cdot \tilde{K}_\kappa &= -\rho_\kappa \tilde{\nabla}(v_\kappa \tilde{g}_\kappa) \quad (B.2)
\end{align*}
\]

where

\[
v_\kappa(\tilde{r}) = \tilde{u}(\tilde{l}/\kappa)/\kappa^3 .
\]

(B.3)

The closure relation reads:

\[
\rho_\kappa(\tilde{r}, \tilde{t})\tilde{K}_\kappa(\tilde{r}, \tilde{t}) = \tilde{g}_\kappa(\tilde{r}, \tilde{t}) \otimes \tilde{g}_\kappa(\tilde{r}, \tilde{t}) .
\]

(B.4)

It is trivial to see that the \( \kappa \)-system is equivalent to the original system under space-time rescaling, i.e., \( \rho_\kappa(\hat{r}, \hat{t}) = \hat{\rho}''(\hat{r}/\kappa, \hat{t}/\kappa) \), \( \tilde{g}_\kappa(\hat{r}, \hat{t}) = \hat{g}''(\hat{r}/\kappa, \hat{t}/\kappa) \) and \( \tilde{K}_\kappa(\hat{r}, \hat{t}) = \hat{K}''(\hat{r}/\kappa, \hat{t}/\kappa) \), where the double-primed quantities are the solution of Eqs. (A.20)-(A.22). In addition, the spatial averages of the densities are preserved:

\[
\langle A_\kappa(\hat{r}, \hat{t}) \rangle = \frac{1}{V} \int_V d\hat{r} A_\kappa(\hat{r}, \hat{t}) = \frac{1}{V} \int_V d\hat{r} \hat{A}(\hat{r}/\kappa, \hat{t}/\kappa)
\]

\[
= \frac{1}{V/\kappa^3} \int_{V/\kappa^3} dr \hat{A}(r, t) = \langle \hat{A}(r, t) \rangle,
\]

(B.5)
where \( A = \rho, g \) or \( \mathbb{K} \). Consequently, the temperature is also preserved, since

\[
\bar{T}(t) = \frac{1}{3} \langle \text{Tr} \hat{\mathbb{K}}(\mathbf{r}, t) \rangle = \frac{1}{3} \text{Tr} \langle \mathbb{K}(\mathbf{r}, t) \rangle = \frac{1}{3} \text{Tr} \langle \mathbb{K}_\kappa(\tilde{\mathbf{r}}, \kappa t) \rangle = \frac{1}{3} \text{Tr} \langle \mathbb{K}_\kappa(\tilde{\mathbf{r}}, \kappa t) \rangle
\]

(B.6)

for arbitrary \( \kappa \). The key point of this re-scaling is that the physical quantities (mass and momentum densities, and the temperature) remain finite as \( \kappa \) converges to 0. The equivalence transformation indicates that the \( O(\xi) \)-scale dynamics of the \( \kappa \)-system corresponds to the \( O(\xi/\kappa) \)-scale dynamics of the original system. Consequently, the \( O(\infty) \) (macroscopic) scale dynamics of the original system can be studied by studying the \( O(1) \)-scale dynamics of the \( \kappa \)-system in the \( \kappa \to 0 \) limit. Omitting the \( \tilde{\cdot} \) notation in the arguments this results in:

\[
\begin{align*}
\partial_t \rho + \nabla \cdot g &= 0 \quad \text{(B.7)} \\
\partial_t g + \nabla \cdot \mathbb{K} &= -\rho \nabla (u_0 * \rho) \quad , \quad \text{(B.8)}
\end{align*}
\]

where \( A(\mathbf{r}, t) \equiv \lim_{\kappa \to 0} A_\kappa(\mathbf{r}, t) \) (with \( A = \rho, g \) and \( \mathbb{K} \)), while

\[
\begin{align*}
u_0(r) &= \lim_{\kappa \to 0} \left[ \frac{1}{\kappa^3} \tilde{u} \left( \frac{\tilde{l} r}{\kappa} \right) \right] . \quad \text{(B.9)}
\end{align*}
\]

The macroscopic closure relation reads:

\[
\lim_{\kappa \to 0} \left[ \rho_\kappa(\mathbf{r}, t) \mathbb{K}_\kappa(\mathbf{r}, t) \right] = \lim_{\kappa \to 0} \left[ g_\kappa(\mathbf{r}, t) \otimes g_\kappa(\mathbf{r}, t) \right] . \quad \text{(B.10)}
\]

If \( \rho(\mathbf{r}, t) = \lim_{\kappa \to 0} \rho_\kappa(\mathbf{r}, t) \) and \( g(\mathbf{r}, t) = \lim_{\kappa \to 0} g_\kappa(\mathbf{r}, t) \) are bounded functions, then the above equation indicates that \( \mathbb{K}(\mathbf{r}, t) = \lim_{\kappa \to 0} \mathbb{K}_\kappa(\mathbf{r}, t) \) is also bounded, and

\[
\rho(\mathbf{r}, t) \mathbb{K}(\mathbf{r}, t) = g(\mathbf{r}, t) \otimes g(\mathbf{r}, t) . \quad \text{(B.11)}
\]

If, in addition, \( \rho(\mathbf{r}, t) > 0 \), the kinetic stress can be explicitly expressed in terms of the mass and momentum densities:

\[
\mathbb{K}(\mathbf{r}, t) = \frac{g(\mathbf{r}, t) \otimes g(\mathbf{r}, t)}{\rho(\mathbf{r}, t)} . \quad \text{(B.12)}
\]

Alternatively, it is possible to introduce the macroscopic velocity field as the ratio of the macroscopic momentum and density fields: \( \mathbf{v}(\mathbf{r}, t) \equiv g(\mathbf{r}, t)/\rho(\mathbf{r}, t) \).
Eqs. (B.7) and (B.8) can be re-formulated as:

\[ \frac{\partial}{\partial t} \rho + \nabla \cdot (\rho \mathbf{v}) = 0; \quad (B.13) \]

\[ \frac{\partial}{\partial t} \mathbf{v} + \mathbf{v} \cdot \nabla \mathbf{v} = -\nabla (u_0 \ast \rho). \quad (B.14) \]

Finally, using Eq. (B.12) in Eq. (B.6) results in:

\[ \tilde{T} = \frac{1}{3} \langle \rho | \mathbf{v}^2 \rangle. \quad (B.15) \]

**Appendix B.2. Scaling limit of the pair potential**

The scaling limit of the pair potential is given by Eq. (B.9). Introducing \( \alpha \equiv \kappa / \bar{l} \) (where \( 0 < \bar{l} < \infty \)) results in:

\[ u_0(r) = \bar{n} \lim_{\alpha \to 0} \left[ \tilde{u}(r/\alpha) / \alpha^3 \right]. \quad (B.16) \]

The limit is evaluated as follows. The Fourier transform of \( u_0(r) \) can be written as

\[ U_0(k) = \frac{\bar{n}}{(2\pi)^3} \lim_{\alpha \to 0} F_\alpha(k), \quad (B.17) \]

where

\[ F_\alpha(k) = \int_0^\infty dr \left\{ (4\pi r^2) \left[ \frac{1}{\alpha^3} \tilde{u} \left( \frac{r}{\alpha} \right) \left( \frac{\sin(kr)}{kr} \right) \right] \right\}, \quad (B.18) \]

where we utilised that the pair potential has radial symmetry. If

\[ \lim_{\alpha \to 0} F_\alpha(k) = a_0 \quad \text{(constant)}, \quad (B.19) \]

then

\[ u_0(r) = \bar{n} a_0 \delta(r). \quad (B.20) \]

We note that the notation \( \delta(r) \) in Eq. (B.20) is consistent, since the three-dimensional Dirac-delta distribution is radially symmetric. This can be shown by considering the radial Dirac-delta in three dimensions as the limit of a radially symmetric nascent function:

\[ \delta(r) \equiv \lim_{\sigma \to 0} g_\sigma(r), \quad (B.21) \]

where \( g_\sigma(r) = \frac{1}{(\sigma \sqrt{2\pi})^3} e^{-\frac{r^2}{2\sigma^2}}, \) for instance. Since \( \lim_{\sigma \to 0} G_\sigma(k) = 1/(2\pi)^3, \) which is the Fourier transform of \( \delta(x)\delta(y)\delta(z), \delta(r) \equiv \delta(r). \) The same result
can be obtained by using radial Fourier transform in general, however, one must be careful and bare in mind that \( \int_0^\infty (4\pi r^2 dr) \delta(r) = 1 \), and therefore the Fourier transform of \( \delta(r) \) is \( \Delta(k) = \frac{1}{(2\pi)^2} \lim_{r \to 0} \frac{\sin(kr)}{kr} = \frac{1}{(2\pi)^2} \). As an example for the scaling limit of the par potential, we consider the Yukawa potential: \( \tilde{u}(r) = \exp(-\gamma r)/r \). For this potential, \( a_0 = \lim_{\alpha \to 0} F_\alpha(k) = \lim_{\alpha \to 0} \frac{4\pi}{(k\alpha)^2 + \gamma^2} = \frac{4\pi}{\gamma^2} \) \( (B.22) \)

Similarly, for the Hartee-Fock B potential \( \tilde{u}(r) = \exp(-\gamma r^2 - \delta r) \) the limit reads:

\[
F_\alpha(k) = \frac{(\pi/\delta)^{3/2}}{2 k'} e^{-\frac{(\gamma - ik')^2}{4\delta}} \\
\times \left\{ (k' - i\gamma)e^{\frac{ik'}{\delta}} \text{erfc} \left( \frac{\gamma + ik'}{2\sqrt{\delta}} \right) - (\gamma - ik') \left[ \text{erfi} \left( \frac{k' + i\gamma}{2\sqrt{\delta}} \right) - i \right] \right\} ,
\]

(B.23)

where \( k' = \alpha k \). This indicates

\[
a_0 = \lim_{\alpha \to 0} F_\alpha(k) = \frac{\pi^{3/2}}{2 \delta^{5/2}} e^{-\frac{\gamma^2 + 2\delta}{2\delta}} \text{erfc} \left( \frac{\gamma}{2\sqrt{\delta}} \right) - \frac{\pi \gamma}{\delta^2} , \quad (B.24)
\]

which is also finite. More complex integrals can be evaluated using computer software (such as Mathematica). For any pair potential for which \( u_0(r) = \bar{n} a_0 \delta(r) \) holds, Eqs. (38) and (39) indicate

\[
\partial_t \rho + \nabla \cdot (\rho \mathbf{v}) = 0 ; \quad (B.25)
\]

\[
\partial_t \mathbf{v} + \mathbf{v} \cdot \nabla \mathbf{v} = -c_0^2 \nabla \rho , \quad (B.26)
\]

were \( c_0 = \sqrt{\bar{n}/a_0} \) is the group speed. Eliminating \( c_0 \) by measuring time in \( \tau = 1/c_0 \) units results in the universal macroscopic continuum equations:

\[
\partial_t \rho + \nabla \cdot (\rho \mathbf{v}) = 0 \quad \text{and} \quad \partial_t \mathbf{v} + \mathbf{v} \cdot \nabla \mathbf{v} + \nabla \rho = 0 , \quad (B.27)
\]

where the spatial average of \( \rho(\mathbf{r}, t) \) is unity. Finally, using the re-scaling in Eq. (25) results in the instantaneous dimensionless temperature

\[
\Theta(t) \equiv \frac{3 \tilde{T}(t)}{\bar{n}/a_0} = \langle \rho \mathbf{v}^2 \rangle . \quad (B.28)
\]

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Appendix  C. Boundedness of the densities in the hydrodynamic limit

The validity of the macroscopic equations depends on the existence of the macroscopic mass and momentum densities \( \rho(\mathbf{r}, t) \equiv \lim_{\kappa \to 0} \hat{\rho}_\kappa(\mathbf{r}, t) \) and \( \mathbf{g}(\mathbf{r}, t) \equiv \lim_{\kappa \to 0} \hat{\mathbf{g}}_\kappa(\mathbf{r}, t) \), respectively. We consider a one-dimensional system where \( p_i = 0 \) and

\[
x_i = \begin{cases} 
  i/(1 - \Delta) & \text{for } i < 0 \\
  0 & \text{for } i = 0 \\
  i/(1 + \Delta) & \text{for } i > 0 
\end{cases} 
\]  

(C.1)

In this system, the average density is trivially \( 1 - \Delta \) for \( x < 0 \) and \( 1 + \Delta \) for \( x > 0 \), respectively. This result can be recovered by taking the macroscopic limit of the microscopic mass density. The microscopic mass density of the system reads

\[
\hat{\rho}(x) = \sum_{i=-\infty}^{\infty} \delta(x - x_i).
\]

The average density of the system reads:

\[
\bar{\rho} = \lim_{L \to \infty} \frac{1}{2L} \int_{-L}^{+L} dx \hat{\rho}(x) = 1 - \lim_{L \to \infty} \frac{\{L(1 - \Delta)\} + \{L(1 + \Delta)\} - 1}{2L} = 1 ,
\]

(C.2)

where \( \{.\} \) stands for the fractional part (since the nominator in the limit is bounded, the limit is zero). The density difference is defined as

\[
\delta\hat{\rho}(x) = \delta\hat{\rho} - \bar{\rho} = \sum_{i=-\infty}^{\infty} \delta(x - x_i) - 1 ,
\]

(C.3)

which guarantees \( \int_{-\infty}^{\infty} dx \delta\hat{\rho}(x) = 0 \). Using Eq. (C.1) in Eq. (C.3), the Fourier transform of \( \delta\rho_\kappa(x) \equiv \delta\hat{\rho}(x/\kappa) \) reads:

\[
\delta P_\kappa(k) = \frac{\kappa}{2\pi} \sum_{i=-\infty}^{\infty} e^{-ik\kappa x_i} = \frac{i\kappa}{4\pi} \csc \left( \frac{\kappa k}{2(\Delta - 1)} \right) \csc \left( \frac{\kappa k}{2(\Delta + 1)} \right) \sin \left( \frac{k \Delta \kappa}{\Delta^2 - 1} \right) ,
\]

(C.4)

for \( k \neq 0 \), while \( \delta P(0) = 0 \). From Eq. (C.4),

\[
\delta P(k) = \lim_{\kappa \to 0} \delta P_\kappa(k) = \frac{i \Delta}{k \pi} ,
\]

(C.5)

and therefore \( \delta\rho(x) = \lim_{\kappa \to 0} \delta\rho_\kappa(x) = \Delta \text{sgn}(x) \). Finally, the macroscopic density reads:

\[
\rho(x) = 1 + \delta\rho(x) = \begin{cases} 
  1 - \Delta & \text{for } x < 0 \\
  1 & \text{for } x = 0 \\
  1 + \Delta & \text{for } x > 0 
\end{cases} 
\]

(C.6)

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as expected. The key result here is that the macroscopic density $\rho(x)$, which is an exact limit of the microscopic one, is a bounded function. Without loss of generality, we consider the following from of the dimensionless positions and momenta of the particles, respectively (see Fig. 1):

$$r_{j(i)}(t) = r_0^i + u(\kappa r_0^i, \kappa t)/\kappa + \Delta r_{j(i)}(t) \quad (C.7)$$

$$p_{j(i)}(t) = w(\kappa r_0^i, \kappa t) + \Delta p_{j(i)}(t) \quad (C.8)$$

where $r_0^i \in \mathbb{Z}^d$ is a lattice site on a $d$-dimensional uniform grid with grid spacing $h = 1$ (the whole grid is covered as $i$ runs for the natural numbers), $u(\cdot, \cdot)$ and $w(\cdot, \cdot)$ are smooth, zero-average vector fields generating the slowly varying components of the density and the momentum fields for $\kappa \ll 1$, $j(i)$ is an instantaneous map between the lattice sites and the particle positions (a particle is assigned to the closest grid point on the deformed grid $r_0^i + u(\kappa r_0^i, \kappa t)/\kappa$), while $\Delta r_{j(i)}(t)$ and $\Delta p_{j(i)}(t)$ carry the microscopic details. The Fourier transform of $\delta \rho(\kappa r, t) \equiv \hat{\delta \rho}(r/\kappa, t/\kappa)$ - where $\hat{\delta \rho}(r, t) = -1 + \sum_i \delta[r - r_i(t)]$ - reads:

$$\delta P_\kappa(k, t) = \left(\frac{\kappa}{2\pi}\right)^3 \sum_i e^{-i\cdot(k\cdot r_i(t/\kappa)} - \frac{1}{(2\pi)^3} \int dr e^{-i\cdot kr}$$

$$= \frac{1}{(2\pi)^3} \left\{ \sum_n e^{-i\cdot k} \left[ \delta[\kappa n + u(\kappa n, t) + \kappa \Delta r_{j(n)}(t/\kappa)] - \int dr e^{-i\cdot kr} \right] \right\}, \quad (C.9)$$

where $n = (n_1, n_2, n_3) \in \mathbb{Z}^3$. Eq. (C.9) indicates

$$\lim_{\kappa \to 0} \delta P_\kappa(k, t) = \frac{1}{(2\pi)^3} \int dr \left[ e^{-i\cdot k u(r, t)} - 1 \right] e^{-i\cdot kr}, \quad (C.10)$$

where we used that $\Delta r_{j(n)}(t)$ is finite. The key idea in Eq. (C.10) is that the summation for the particles is converted into the Fourier transform in the zero Knudsen number limit. In one spatial dimension the argument reads:

$$e^{-i\cdot k u(r, t)} - 1 = \sum_{p=1}^{\infty} \frac{[-i\cdot k u(x, t)]^p}{p!} = (-i\cdot k) u(x, t) + \frac{1}{2} (-i\cdot k)^2 u^2(x, t) + \ldots, \quad (C.11)$$

thus indicating

$$\delta \rho(x, t) = \sum_{p=1}^{\infty} \frac{(-1)^p}{p!} \partial_x^p [u^p(x, t)] \quad (C.12)$$

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We note here that Eq. (C.11) is different in multiple dimensions, where matrix algebraic identities must be used to expand $(k \cdot u)^p$. For $p = 2$, for instance, the general form is $(i k \cdot u)^2 = (i k) \cdot [(i k) \cdot (u \otimes u)]$, and therefore the corresponding real-space operation is $\nabla \cdot [\nabla \cdot (u \otimes u)]$, and so on. The key point in calculating the macroscopic limit of the mass density using Eq. (C.7) is that the microscopic details $\Delta r_j(t)$ cancel in the macroscopic density. This, however, does not apply to the macroscopic momentum density. Using Eq. (C.8) in $g_\kappa(r, t) = \hat{g}(r/\kappa, t/\kappa)$, where $\hat{g}(r, t) = \sum_i v_i(t) \delta[r - r_i(t)]$ is the microscopic momentum, yields:

$$G_\kappa(k, t) = \left(\frac{\kappa}{2\pi}\right)^3 \sum_i \left[ w(\kappa n, t) + \Delta v_{j(n)}(t/\kappa) \right] e^{-i k \cdot [\kappa n + u(\kappa n, t) + \kappa \Delta r_{j(n)}(t/\kappa)]} .$$

(C.13)

Taking the $\kappa \to 0$ limit results in:

$$G_\kappa(k, t) = \frac{1}{(2\pi)^3} \int dr \left\{ \left[ w(r, t) + \tilde{\xi}(r, t) \right] e^{-i k \cdot u(r, t)} \right\} e^{-i k \cdot r} ,$$

(C.14)

where $\tilde{\xi}(r, t) = \lim_{\kappa \to 0} \Delta v_{j(\lfloor r/\kappa \rfloor)}(t/\kappa)$. Considering only one spatial dimension and using Eq. (C.7), the macroscopic momentum density reads:

$$G(x, t) = \sum_{p=0}^\infty \frac{(-1)^p}{p!} \partial_x^p \left[ \left\{ w(x, t) + \xi(x, t) \right\} u^p(x, t) \right] .$$

(C.15)

**Appendix D. Numerical simulations**

Eqs. (B.27) were implemented on a two-dimensional collocated grid with grid spacing $h = 1$ by using finite volume method and forward Euler time stepping scheme. To avoid $2h$-type spatial derivatives, together with keeping the benefits of conservation laws, first we re-write Eqs. (B.27) as:

$$\partial_t \rho = -\nabla \cdot (\rho \mathbf{v}) ,$$

(D.1)

$$\partial_t \mathbf{g} = -\nabla \cdot [\rho \mathbf{v} \otimes \mathbf{v} + (\rho^2/2)\mathbf{I}] ,$$

(D.2)
where \( v = g / \rho \). Integrating the equations for cell \((i, j)\) results in:

\[
\frac{d\Delta M_{ij}(t)}{dt} = - \int_{A_{ij}} \{ \nabla \cdot (\rho v) \} = - \oint_{\Gamma_{ij}} d\Gamma \cdot \{ \rho v \} \,
\]

\[
\frac{d\Delta P_{ij}(t)}{dt} = - \int_{A_{ij}} \{ \nabla \cdot [\rho v \otimes v + (\rho^2/2)I] \} = - \oint_{\Gamma_{ij}} d\Gamma \cdot \{ \rho v \otimes v + (\rho^2/2)I \}
\]

where \( \Delta M_{ij}(t) \approx h^2 \rho_{ij}(t) \) and \( \Delta P_{ij}(t) \approx h^2 \mathbf{g}_{ij}(t) \) are the mass and momentum in cell \((i, j)\), respectively. Using the notation \( v = (u, v) \), the boundary integrals can be approximated as

\[
\oint_{\Gamma_{ij}} d\Gamma \cdot \{ \rho v \} \approx h [(\rho_e u_e - \rho_w u_w) + (\rho_n v_n - \rho_s v_s)]
\]

\[
\oint_{\Gamma_{ij}} d\Gamma \cdot \{ \rho u v + (\rho^2/2) v \} \approx h \left\{ \rho_e^2 - \rho_w^2 \right\} + \left[ (\rho_e u_e^2 - \rho_w u_w^2) + (\rho_n u_n v_n - \rho_s v_s u_s) \right] \,
\]

\[
\oint_{\Gamma_{ij}} d\Gamma \cdot \{ \rho v v + (\rho^2/2) u \} \approx h \left\{ \rho_n^2 - \rho_s^2 \right\} + \left[ (\rho_n v_n^2 - \rho_s v_s^2) + (\rho_e u_e v_e - \rho_w u_w v_w) \right]
\]

where \( \chi_e = (\chi_{i,j} + \chi_{i+1,j})/2 \), \( \chi_w = (\chi_{i-1,j} + \chi_{i,j})/2 \), \( \chi_n = (\chi_{i,j} + \chi_{i,j+1})/2 \), and \( \chi_s = (\chi_{i,j-1} + \chi_{i,j})/2 \) are the mid-cell wall values \((\chi = \rho, u, v)\). Introducing \( g = (p, q) \) and using the forward Euler time stepping scheme and \( h = 1 \) yield:

\[
\rho_{ij}^{t+\Delta t} = \rho_{ij}^t - \Delta t \left\{ (\rho_e u_e^t - \rho_w u_w^t) + (\rho_n v_n^t - \rho_s v_s^t) \right\}
\]

\[
\rho_{ij}^{t+\Delta t} = \rho_{ij}^t - \Delta t \left\{ (\rho_e^2 - \rho_w^2) \right\} + \left[ (\rho_e u_e^t)^2 - (\rho_w u_w^t)^2 \right] \,
\]

\[
q_{ij}^{t+\Delta t} = q_{ij}^t - \Delta t \left\{ (\rho_e^t v_e^t - \rho_w^t v_w^t) \right\} + \left[ (\rho_e^t v_e^t)^2 - (\rho_w^t v_w^t)^2 \right]
\]

where \( u_{ij}^t = \rho_{ij}^t / \rho_{ij}^t \) and \( v_{ij}^t = q_{ij}^t / \rho_{ij}^t \). This scheme avoids \( 2h \)-type central differences together with keeping flux consistency by utilising finite volume scheme, and therefore is expected to be stable and mass and momentum conserving (up
Implementing the equations in single floating point precision, however, can result in the accumulation of numerical error for long simulations (including typically billions of time steps), which might be further enhanced by the Galerkin truncation in case of a scale-free equation, where all wave numbers are equally "loaded". In our calculations, we prevented the system from overheating by applying a homogeneous thermostat $g_{ij} \rightarrow \sqrt{T_2/T_1} g_{ij}$ (where $T_1$ is the actual and $T_2$ the desired temperature) at every $N_T$ (typically in the order of $10^4$) time steps. The instantaneous temperature of the system is given by Eq. (B.28). Setting $\rho(r,0) \equiv 1$ and using $\Theta(t) = 3 \tilde{T}(t)/(a_0 \bar{n})$ gives

$$\Theta(0) = \langle |g(r,0)|^2 \rangle = \sum_k G_k^*(0) \cdot G_k(0) ,$$  

(D.11)

where $G_k(t) = (1/V) \int dr \{ g(r,t) e^{-i \mathbf{k} \cdot \mathbf{r}} \}$ is the Fourier coefficient of the (periodic) momentum density $g(r,t) = \sum_k G_k(t) e^{i \mathbf{k} \cdot \mathbf{r}}$. To start a simulation from a nearly equilibrated state, we choose a spatially correlated, incompressible isotropic Gaussian random vector field:

$$G_k(0) \equiv A f(k) (I - n_k \otimes n_k) \cdot \tilde{\xi}(k) ,$$  

(D.12)

where $n_k = k/k$ is a unit vector, $f(k)$ is responsible for spatial correlations, and $\tilde{\xi}(k) \in \mathbb{C}^d$ a $d$-dimensional complex random vector field, where the independent components follow standard normal distribution in both the (also independent) real and imaginary parts, while the wave numbers are also uncorrelated (apart from the Hermitian symmetry $\tilde{\xi}_{-k} \equiv \tilde{\xi}_{k}^*$). The expected value of the initial temperature can be calculated by plugging Eq. (D.12) into Eq. (D.11), yielding:

$$E[\Theta(0)] = 2(d-1) A^2 \sum_k f^2(k) .$$  

(D.13)

Using the approximation $\sum_k f^2(k) \approx (L/\pi)^d I$ with $I = \int d\mathbf{k} \{ f^2(k) \}$, where $L = N h$ is the linear size of the $d$-dimensional domain, $N$ the number of points, and $h$ the grid spacing, results in

$$A = \sqrt{\frac{\Theta_0}{2(d-1) I \left( \frac{2 \pi}{N h} \right)^d}} ,$$  

(D.14)
where $\Theta_0 = \mathbb{E}[\Theta(0)]$ is fixed. In $d = 2$, for $h = 1$ Eq. (D.14) reduces to
\[
A = \frac{\pi N}{N} \sqrt{\frac{6 \Theta_0}{I}}.
\]

References

[1] J. Loschmidt, "Uber den zustand des wärmegleichgewichtes eines systems von körpern mit rücksicht auf die schwerkraft, Sitzungsber. Kais. Akad. Wiss. Wien, Math. Naturwiss. (1876) 128—142.

[2] L. BARREIRA, Poincaré recurrence: old and new pp. 415–422. doi:10.1142/9789812704016_0039.

URL https://www.worldscientific.com/doi/abs/10.1142/9789812704016_0039

[3] W. M. Haddad, V. Chellaboina, S. G. Nersesov, Time-reversal symmetry, poincaré recurrence, irreversibility, and the entropic arrow of time: From mechanics to system thermodynamics, in: Proceedings of the 44th IEEE Conference on Decision and Control, 2005, pp. 5995–6002. doi:10.1109/CDC.2005.1583121

[4] V. Ardourel, Irreversibility in the derivation of the boltzmann equation Foundations of Physics 47 (4) (2017) 471–489. doi:10.1007/s10701-017-0072-9.

URL https://doi.org/10.1007/s10701-017-0072-9

[5] M. te Vrugt, R. Wittkowski, Projection operators in statistical mechanics: a pedagogical approach European Journal of Physics 41 (4) (2020) 045101. doi:10.1088/1361-6404/ab8e28.

URL https://doi.org/10.1088/1361-6404/ab8e28

[6] E. S. Kikkinides, P. A. Monson, Dynamic density functional theory with hydrodynamic interactions: Theoretical development and application in the study of phase separation in gas-liquid systems. The Journal of Chemical Physics 142 (9) (2015) 094706. arXiv:https://doi.org/10.1063/1.
[7] H. Kreuzer, *Nonequilibrium Thermodynamics and Its Statistical Foundations*, Monographs on the physics and chemistry of materials, Clarendon Press, 1983.

URL https://books.google.co.uk/books?id=JoB9QgAACAAJ

[8] S.-i. Sasa, *Derivation of hydrodynamics from the hamiltonian description of particle systems*, Phys. Rev. Lett. 112 (2014) 100602. doi:10.1103/PhysRevLett.112.100602

URL https://link.aps.org/doi/10.1103/PhysRevLett.112.100602

[9] E. Platen, Ikeda, n. / watanabe, s., *stochastic differential equations and diffusion processes*. north-holland mathematical library 24. amsterdam-new york, north-holland publ. co. 1981. 480 s., us $ 85.25. dfl. 175.00. isbn 0-444-86172-6, ZAMM - Journal of Applied Mathematics and Mechanics / Zeitschrift für Angewandte Mathematik und Mechanik 62 (12) (1982) 713–713. doi:https://doi.org/10.1002/zamm.19820621219

[10] A. Bazzani, O. Mazzarisi, M. Giovannozzi, E. Maclean, *Diffusion in stochastically perturbed Hamiltonian systems with applications to the recent LHC dynamic aperture experiments*, pp. 70–85. doi:10.1142/9789813279612_0005

[11] A. A. Lykov, V. A. Malyshev, *A new approach to boltzmann’s ergodic hypothesis*, Doklady Mathematics 92 (2) (2015) 624–626. doi:10.1134/S1064562415050269

URL https://doi.org/10.1134/S1064562415050269

[12] A. Lykov, V. Malyshev, *Convergence to equilibrium for many particle systems*, in: V. Panov (Ed.), *Modern Problems of Stochastic Analysis and Statistics*, Springer International Publishing, Cham, 2017, pp. 271–301.
[13] N. Cuneo, J.-P. Eckmann, M. Hairer, L. Rey-Bellet, Non-equilibrium steady states for networks of oscillators, Electronic Journal of Probability 23 (none) (2018) 1 – 28. doi:10.1214/18-EJP177
URL https://doi.org/10.1214/18-EJP177

[14] A. Dhar, H. Spohn, Fourier’s law based on microscopic dynamics, Comptes Rendus Physique 20 (5) (2019) 393–401, fourier and the science of today / Fourier et la science d’aujourd’hui. doi:https://doi.org/10.1016/j.crhy.2019.08.004
URL https://www.sciencedirect.com/science/article/pii/S1631070519301100

[15] P. H. Hüenberger, Thermostat Algorithms for Molecular Dynamics Simulations, Springer Berlin Heidelberg, Berlin, Heidelberg, 2005, pp. 105–149. doi:10.1007/b99427
URL https://doi.org/10.1007/b99427

[16] L. Markus, K. Meyer, Generic hamiltonian dynamical systems are neither integrable nor ergodic, Mem. Am. Math. Soc. 144 (1974) 1—-52.

[17] V. Arnold, V. Kozlov, A. Neishtadt, Mathematical Aspects of Classical and Celestial Mechanics, 2nd Edition, Springer-Verlag Berlin Heidelberg, 1997. doi:10.1007/978-3-642-61237-4

[18] L. Chierchia, G. Pinzari, The planetary n-body problem: symplectic foliation, reductions and invariant tori, Inventiones mathematicae 186 (1) (2011) 1–77. doi:10.1007/s00222-011-0313-z
URL https://doi.org/10.1007/s00222-011-0313-z

[19] X. Yong, L. T. Zhang, Thermostats and thermostat strategies for molecular dynamics simulations of nanofluidics, The Journal of Chemical Physics 138 (8) (2013) 084503. arXiv:https://doi.org/10.1063/1.4792202
doi:10.1063/1.4792202
URL https://doi.org/10.1063/1.4792202
[20] D. J. Driebe, Deterministic Diffusion, Springer Netherlands, Dordrecht, 1999, pp. 93–114. doi:10.1007/978-94-017-1628-4_6
URL https://doi.org/10.1007/978-94-017-1628-4_6

[21] S. Olla, S. R. S. Varadhan, H. T. Yau, Hydrodynamical limit for a hamiltonian system with weak noise, Communications in Mathematical Physics 155 (3) (1993) 523–560. doi:10.1007/BF02096727
URL https://doi.org/10.1007/BF02096727

[22] A. A. Lykov, V. A. Malyshev, From the n-body problem to euler equations, Russian Journal of Mathematical Physics 24 (1) (2017) 79–95. doi:10.1134/S106192081701006X
URL https://doi.org/10.1134/S106192081701006X

[23] E. Zaccarelli, G. Foffi, P. D. Gregorio, F. Sciortino, P. Tartaglia, K. A. Dawson, Dynamics of supercooled liquids: density fluctuations and mode coupling theory, Journal of Physics: Condensed Matter 14 (9) (2002) 2413–2437. doi:10.1088/0953-8984/14/9/330
URL https://doi.org/10.1088%2F0953-8984%2F14%2F9%2F330

[24] A. J. Archer, Dynamical density functional theory for dense atomic liquids, Journal of Physics: Condensed Matter 18 (24) (2006) 5617–5628. doi:10.1088/0953-8984/18/24/004
URL https://doi.org/10.1088%2F0953-8984%2F18%2F24%2F004

[25] G. I. Tóth, W. Ma, Phase-field modelling of the effect of density change on solidification revisited: model development and analytical solutions for single component materials, Journal of Physics: Condensed Matter 32 (20) (2020) 205402. doi:10.1088/1361-648x/ab670e
URL https://doi.org/10.1088%2F1361-648x%2Fab670e

[26] A. A. Wheeler, G. B. McFadden, On the notion of a $\xi$-vector and a stress tensor for a general class of anisotropic diffuse interface models, Proc. Roy. Soc. London A 453 (1963) (1997) 1611–1630. doi:10.1098/rspa.1997.
[27] D. M. Anderson, G. B. McFadden, A. A. Wheeler, Diffuse-interface methods in fluid mechanics, Annu. Rev. Fluid Mech. 30 (1) (1998) 139–165. doi:10.1146/annurev.fluid.30.1.139.
URL http://dx.doi.org/10.1146/annurev.fluid.30.1.139

[28] D. Anderson, G. McFadden, A. Wheeler, A phase-field model of solidification with convection, Physica D 135 (1–2) (2000) 175 – 194. doi:http://dx.doi.org/10.1016/S0167-2789(99)00109-8
URL http://www.sciencedirect.com/science/article/pii/S0167278999001098

[29] S. Ray, U. Frisch, S. Nazarenko, T. Matsumoto, Resonance phenomenon for the galerkin-truncated burgers and euler equations, Physical review. E, Statistical, nonlinear, and soft matter physics 84 (2011) 016301. doi:10.1103/PhysRevE.84.016301

[30] D. Venkataraman, S. Sankar Ray, The onset of thermalization in finite-dimensional equations of hydrodynamics: insights from the burgers equation, Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences 473 (2197) (2017) 20160585. doi:10.1098/rspa.2016.0585

[31] S. S. RAY, Thermalized solutions, statistical mechanics and turbulence: An overview of some recent results, Pramana 84 (3) (2015) 395–407. doi:10.1007/s12043-014-0928-x
URL https://doi.org/10.1007/s12043-014-0928-x

[32] R. A. Aziz, M. J. Slaman, The repulsive wall of the ar-ar interatomic potential reexamined, The Journal of Chemical Physics 92 (2) (1990) 1030–1035. arXiv:https://doi.org/10.1063/1.458165, doi:10.1063/1.458165
URL https://doi.org/10.1063/1.458165
[33] R. A. Aziz, A highly accurate interatomic potential for argon, The Journal of Chemical Physics 99 (6) (1993) 4518–4525. arXiv:https://doi.org/10.1063/1.466051 URL https://doi.org/10.1063/1.466051

[34] P. Chandrashekar, Kinetic energy preserving and entropy stable finite volume schemes for compressible euler and navier-stokes equations, Communications in Computational Physics 14 (5) (2013) 1252–1286. doi:10.4208/cicp.170712.010313a

[35] G. C. Ghirardi, P. Pearle, A. Rimini, Markov processes in hilbert space and continuous spontaneous localization of systems of identical particles, Phys. Rev. A 42 (1990) 78–89. doi:10.1103/PhysRevA.42.78 URL https://link.aps.org/doi/10.1103/PhysRevA.42.78

[36] L. Diósi, Models for universal reduction of macroscopic quantum fluctuations, Phys. Rev. A 40 (1989) 1165–1174. doi:10.1103/PhysRevA.40.1165 URL https://link.aps.org/doi/10.1103/PhysRevA.40.1165

[37] M. te Vrugt, G. I. Toth, R. Wittkowski, Master equations for wigner functions with spontaneous collapse and their relation to thermodynamic irreversibility, submitted to the Journal of Computational Electronics (2021). URL https://arxiv.org/abs/2106.00137