Journal of Statistical Physics (2026) 193:59
https://doi.org/10.1007/s10955-026-03618-x

Foundation of classical dynamical density functional theory: uniqueness of time-dependent density–potential mappings

Michael Andreas Klatt[1,2,3] · **Christian Bair**[3] · **Hartmut Löwen**[3] · **René Wittmann**[3,4]

Received: 22 July 2025 / Accepted: 7 April 2026

Abstract
When can we map a classical density profile to an external potential? In equilibrium, without time dependence, the one-body density is known to specify the external potential that is applied to the many-body system. This mapping from a density to the potential is the cornerstone of classical density functional theory (DFT). Here, we consider non-equilibrium, time-dependent many-body systems that evolve from a given initial condition. We derive explicit conditions, for example, no flux at the boundary, that ensure that the mapping from the density to a time-dependent external potential is unique. We thus prove the underlying assertion of dynamical density functional theory (DDFT) — without resorting to the so-called adiabatic approximation often used in applications. By ascertaining uniqueness for all n-body densities, we ensure that the proof — and the physical conclusions drawn from it — hold for general *superadiabatic* dynamics of interacting systems even in the presence of (known) non-conservative forces.

1 Introduction

The foundation of classical density functional theory (DFT) [20, 21, 40, 65] rests on the fact that the one-body density determines the external potential and hence the underlying Hamiltonian if the interaction potential is known. In essentially all relevant cases, there exists a unique mapping from the one-body density $\rho(x)$ to an external potential $V(x)$ for $x \in \Omega$ in d-dimensional Euclidean space $\Omega \subset \mathbb{R}^d$ and for a given interaction potential, temperature, and number of particles (or chemical potential). Remarkably, because of this

Communicated by Bruno Nachtergaele.

✉ Michael Andreas Klatt
michael.klatt@dlr.de

1 German Aerospace Center (DLR), Institute for AI Safety and Security, Wilhelm-Runge-Str. 10, 89081 Ulm, Germany

2 German Aerospace Center (DLR), Institute of Frontier Materials on Earth and in Space Functional, Granular, and Composite Materials, 51170 Cologne, Germany

3 Institut für Theoretische Physik II: Weiche Materie, Heinrich-Heine-Universität Düsseldorf, 40225 Düsseldorf, Germany

4 Institut für tierische Lebensmittel, Max Rubner-Institut, 95326 Kulmbach, Germany

unique mapping, the one-body density fully specifies a many-body system in equilibrium if the interparticle interactions are known. The existence of such a unique density–potential mapping was first proven in the context of quantum mechanics by Hohenberg and Kohn [28], Kohn and Sham [30], and Mermin [40]. Mermin's generalized arguments can be directly applied to classical many-body systems as elaborated by Evans [20] and later rigorously confirmed by Chayes, Chayes, and Lieb [9]. The unique mapping exists under mild and natural conditions on the density and interparticle interactions that essentially assume finite energies. Among others, this result implies a formal equivalence of Mermin-Evans DFT to the alternative framework [17] based on Levy's constrained search [31] (which does not a priori restrict to density profiles that are realizable by an external potential).

Here, we are interested in the generalization of these density–potential mappings to the dynamical case, in which all functions additionally depend on time $t \in [0, \infty)$. If such a mapping exists, it is the foundation of classical dynamical density functional theory (DDFT) [5, 38, 53], as first derived by Marconi and Tarazona [38] from the stochastic Langevin equation and later by Archer and Evans [5] from the corresponding Smoluchowski equation or by Español and Löwen using the projection operator formalism [18]. More specifically, we study the fundamental relation between the time-dependent one-body density $\rho(x, t)$ and external potential $V(x, t)$. These considerations also elucidate the role of the one-body current $j(x, t)$.

The central question of this paper is: under which conditions can we map a classical time-dependent density $\rho : \Omega \times [0, \infty) \to \mathbb{R}$ to an external potential $V : \Omega \times [0, \infty) \to \mathbb{R}$? Such a mapping always refers to the functions and not their instantaneous value at time t, and it presupposes some well-specified initial conditions. Importantly, in this context of statistical physics, a *unique* mapping from ρ to V implies that the density ρ can only be realized by the external potential V and not by another potential $V' \neq V$. Hence, the question is whether a mapping from the density to the external potential is well defined not whether it is injective. (In equilibrium, injectivity fails at phase coexistence, but the dynamical problem is conceptually different due to a deterministic time evolution starting from given initial conditions.)

As in the case of equilibrium DFT, once we have proven the existence of a unique density–potential mapping for a given interaction pair potential U and temperature T, we can assert that the full knowledge of the density profile $\rho : \Omega \times [0, \infty) \to \mathbb{R}$ at all times specifies the forces driving the entire dynamics. Hence, it contains all relevant information about the system, including correlations of any order. Hence, our central question is of both fundamental importance and practical relevance to the study of time-dependent many-body systems.

We, therefore, consider the exact dynamics driven by the full non-equilibrium interaction force, i.e., we do not rely on an "adiabatic" approximation that equates equilibrium and non-equilibrium correlations (which is usually required for explicit calculations in DDFT) [5, 38]. Consequently, our results also pertain to the recently developed superadiabatic-DDFT [55, 57] as well as to the framework of power functional theory (PFT) [50, 51]. Both approaches incorporate "superadiabatic" forces [22] that are neglected in standard (adiabatic) DDFT approximations. The underlying variational principle of PFT, based on Levy's constrained search [31], entails the existence of a unique mapping from the two functions $\rho(x, t)$ and $j(x, t)$ to the function $V(x, t)$. A recent reformulation of the PFT formalism suggests that the only relevant field is $j(x, t)$ [36]. Since our pursuit of unique density–potential mappings neither requires an approximation nor a specific framework, our results shed light on the relation between DDFT and PFT on a formal level and help, in particular, to better understand the role of the current.

In quantum mechanics, an argument for the unique mapping from time-dependent densities $\rho(x, t)$ to potentials $V(x, t)$ was provided by Runge and Gross in 1984 [46], which became the

foundation of time-dependent density functional theory (TDDFT). Assuming time-analytic potentials and smooth densities, they linked the quest for uniqueness of the density–potential mapping to that of the solution for an elliptic partial differential equation (PDE). However, as pointed out later [15, 25, 26, 66], this solution is unique only under certain conditions on both $\rho(x,t)$ and $V(x,t)$. These joint assumptions on the density and potential are more complex than in equilibrium, where the conditions for a unique $V(x)$ only depend on $\rho(x)$ [9]. Intuitively speaking, these more intricate assumptions arise in the time-dependent case because more states are allowed than in equilibrium.

For classical systems, Chan and Finken [8] asserted uniqueness following the idea of Runge and Gross [46]. However, because the evolution of two- and higher-body densities were not explicitly taken into account, the argument so far holds only for noninteracting particles or under the adiabatic approximation. Moreover, no conditions have hitherto been stated for the uniqueness of classical density–potential mappings. In fact, this omission is more critical in the classical setting than it would be in the quantum case since, for the latter, loopholes to unique mappings are considered to be "largely unphysical" [26] and are hence often neglected. By contrast, diverging potentials are not only relevant but even common in classical statistical physics.

In this work, we begin to close these two gaps by proving explicit conditions for the uniqueness of classical density–potential mappings based on an exact hierarchy for the n-body densities. Thus, our conditions are independent of the adiabatic approximation, and, somewhat surprisingly, they also allow for (known) non-conservative forces. Thus, we begin to provide a rigorous foundation of classical DDFT. Since we follow the proof of Runge and Gross [46], we have to assume time-analytic potentials and smooth densities. We thus provide only sufficient conditions for uniqueness. In the outlook, we briefly discuss the general case as an open problem for further research in mathematical physics.

To this end, we first specify our setting in Sec. 2 and derive the hierarchy of reduced Smoluchowski equations for all time-dependent n-body densities $\rho_n(x_1,\dots,x_n,t)$ in Sec. 3; see Theorem 3.1. Since we are concerned with possibly diverging potentials, we accurately derive the boundary contributions and find that all corresponding terms vanish if and only if the Yvon-Born-Green (YBG)-hierarchy holds on average at the boundary (for which we also provide a physical intuitive condition).

Then, we prove our main results in Sec. 4, i.e., we derive generic conditions that guarantee that two given external potentials $V(x,t)$ and $V'(x,t)$ do not yield the same time-dependent one-body density $\rho(x,t)$. We use this general result to specifically show that the density–potential mapping is unique for no-flux boundary conditions. More specifically, similar to the idea of Runge and Gross (or Chan and Finken) [8, 46], we assume analytic potentials and can, therefore, reduce the uniqueness of the mapping to the uniqueness of a solution to a (semi-)elliptic PDE. In contradistinction to the available proofs in quantum mechanics [25, 26, 45, 46], we here use the hierarchy of reduced Smoluchowski equations. Our proof of Theorem 4.5, therefore, requires no approximation of n-body correlations; in particular, our uniqueness theorems are not restricted to adiabatic DDFT. Moreover, our rephrasing of the problem allows us to obtain a physically intuitive condition for uniqueness. Theorem 4.6 asserts that a unique solution can be guaranteed for no-flux boundary conditions or, in fact, any specified flux in or out of the system.

In Sec. 5, we demonstrate that such a simultaneous condition on the density and potential is inevitable. More specifically, we present explicit loopholes to uniqueness where the same $\rho(x,t)$ is attained for two different external potentials. Obviously, these examples violate the conditions of our theorems. For an exponentially fast decaying density profile, a non-unique external potential must necessarily include an exponential divergence (in space). In contrast,

if the density profile has heavy tails, already a polynomial divergence of $V(x,t)$ can lead to non-unique mappings. Hence, the conditions on the asymptotic behavior have to depend on both $\rho(x,t)$ and $V(x,t)$.

To conclude the discussion of loopholes in Sec. 5, we embed our findings in the framework of PFT. A unique mapping to an external potential implies a unique current $j(x,t)$. In contrast, if a suitable external potential $V'(x,t)$ that violates our conditions is added, it causes a divergence-free current $j'(x,t)$ that does not change the density $\rho(x,t)$. Such loopholes have been simulated via a numerical procedure known as *custom flow* [11, 14] that determines, in line with PFT, the unique external force field as a functional of $\rho(x,t)$ and $j(x,t)$. The hierarchy of Smoluchowski equations from Theorem 3.1 emphasizes the necessity of this approach for interacting systems. For the ideal gas (or under the adiabatic approximation), our analytic formula (5.2) can be applied for a systematic construction of non-unique density–potential mappings for effectively one-dimensional systems.

Our mathematical findings are summarized and interpreted in physical terms in Section 6, where we focus on the insights in view of necessary approximations required for explicit predictive calculations using DDFT and related theories. Finally, in Section 7, we conclude and discuss open mathematical questions. We also offer pathways towards further uniqueness theorems for a broad class of soft matter systems.

2 Densities and Smoluchowski operators

We here consider an overdamped many-body system with a fixed number of indistinguishable particles $N > 0$ in an open, bounded domain $\Omega \subseteq \mathbb{R}^d$, $d \geq 1$. Furthermore, we assume for convenience that Ω is connected and has a smooth boundary $\partial\Omega$. The position of a particle is here typically denoted by a d-dimensional vector $x \in \Omega$.

We characterize our system by its time-dependent symmetric N-body probability density

$$P_N : \Omega^N \times [0,\infty) \to [0,\infty); \quad (x^N, t) \mapsto P_N(x^N, t).$$

In the following, we will write x^N as a shorthand notation for a collection of positions $x_1, \ldots, x_N \in \Omega$, and time is denoted by $t \geq 0$. Note that P_N is a simple function of time t but a probability density in the spatial coordinates x^N, i.e., $P_N(x^N, t)$ is the probability density of finding particles at positions x^N at time t. Hence, at any time $t \geq 0$, the integral over Ω^N is normalized,

$$\int P_N(x^N, t)\, dx^N = 1. \tag{2.1}$$

Here and in the following, each unspecified integral is over the full domain.

We obtain the (reduced) n-body densities $\rho_n : \Omega^n \times [0,\infty) \to [0,\infty)$ with $n \leq N$ from the symmetric N-body probability density P_N by applying the n-body density operator:

$$\begin{aligned}
\rho_n(x^n, t) &:= \int P_N(y^N, t) \sum_{i_1 \neq i_2 \neq \cdots \neq i_n} \delta(x_1 - y_{i_1}) \ldots \delta(x_n - y_{i_n})\, dy^N \\
&= \frac{N!}{(N-n)!} \int P_N(y^N, t) \delta(x_1 - y_1) \ldots \delta(x_n - y_n)\, dy^N \\
&= \frac{N!}{(N-n)!} \int P_N(x^n, y^{N-n}, t)\, dy^{N-n},
\end{aligned} \tag{2.2}$$

where δ denotes a Dirac delta distribution. In the following we use the usual shorthand notation for the number density $\rho := \rho_1$.

The interaction between the particles is given by a two-body force $K_2 : \Omega^2 \to \mathbb{R}^d$, which consists of a (time-independent) pair potential $U : \Omega^2 \to \mathbb{R}$ and a divergence-free, non-conservative force $Q : \Omega^2 \to \mathbb{R}^d$, i.e., $K_2(x, y) := -\nabla_x U(x, y) + Q(x, y)$, where $Q(x, y)$ and $K_2(x, y)$ denote forces of a particle at y acting on a particle at x, and ∇_x denotes the differential operator nabla with respect to the x coordinate. As usual, the pair potential is symmetric and only depends on the relative distance, i.e., we define $U(x - y) := U(x - y, 0) = U(x, y)$ for $x, y \in \Omega$. We assume that $K_2 \in C^1(\Omega^2)$ and that K_2 is continuously extensible to $\partial\Omega$ (and hence also bounded).

The many-body system is also subject to an external potential $V : \Omega \times [0,\infty) \to \mathbb{R}$ that is twice continuously differentiable in space (i.e., for $t \geq 0$, the function $V_t : \Omega \to \mathbb{R}, x \mapsto V(x, t)$ is in $C^2(\Omega)$) such that $\nabla_x V_t : \Omega \to \mathbb{R}^d$, $x \mapsto \nabla_x V(x, t)$ is continuously extensible to $\partial\Omega$. (Note, however, that our bounded system can be physically interpreted as being confined within hard walls via the boundary conditions that may be interpreted as an infinitely steep potential on $\partial\Omega$ in addition to V.) Furthermore, we consider a divergence-free, non-conservative, one-body, time-dependent external force $R : \Omega \times [0, \infty) \to \mathbb{R}^d$. We again assume that $R_t : \Omega \to \mathbb{R}^d, x \mapsto R(x, t)$ is in $C^1(\Omega)$ and continuously extensible to $\partial\Omega$. We combine these contributions in the definition of the external one-body force $K_1(x, t) := -\nabla_x V(x, t) + R(x, t)$.

The evolution of P_N under these forces obeys the following N-body Smoluchowski equation:

$$\partial_t P_N(x^N, t) = D \sum_{i=1}^{N} \nabla_{x_i}^2 P_N(x^N, t) - D\beta \sum_{i=1}^{N} \nabla_{x_i} \Big[P_N(x^N, t) F_{N,i}(x^N, t) \Big], \tag{2.3}$$

where the inverse temperature β and diffusion constant D are fixed and the total force $F_{N,i} : \Omega^N \times [0, \infty) \to \mathbb{R}^d$ on particle $i \in \{1, 2, \ldots, N\}$ is defined as

$$F_{N,i}(x^N, t) := K_1(x_i, t) + \sum_{\substack{j=1 \\ j\neq i}}^{N} K_2(x_i, x_j). \tag{2.4}$$

The same definition of $F_{N,i}$ holds for any number of particles, say $n < N$. Let us also point out here that the index i always refers to the ith argument, e.g., $F_{n+1,n+1}(x^n, y, t) = K_1(y, t) + \sum_{j=1}^{n} K_2(y, x_j)$.

In shorthand notation, we combine all forces into a single vector $F_N : \Omega^N \times [0,\infty) \to \mathbb{R}^{dN}$ (and analogously define the differential operator nabla ∇_{x^N}). We, moreover, define the N-body current field $J_N : \Omega^N \times [0, \infty) \to \mathbb{R}^{dN}$ as

$$J_N(x^N, t) := -D\nabla_{x^N} P_N(x^N, t) + D\beta P_N(x^N, t) F_N(x^N, t)$$

that obeys the continuity equation

$$\partial_t P_N(x^N, t) = -\nabla_{x^N} J_N(x^N, t), \tag{2.5}$$

which is then equivalent to the Smoluchowski equation. By defining the Smoluchowski operator

$$\hat{\mathcal{O}}_N := D \sum_{i=1}^{N} \nabla_{x_i} \Big[\nabla_{x_i} - \beta F_{N,i}(x^N, t) \Big],$$

we can write the Smoluchowski equation (2.3) more succinctly as

$$\partial_t P_N(x^N, t) = \hat{\mathcal{O}}_N P_N(x^N, t). \tag{2.6}$$

For our derivation of a reduced Smoluchowski equation for $\rho_n(x^n, t)$ in the next section, it is useful to define *partial* Smoluchowski operators as

$$\hat{\mathcal{O}}^-_{n,N} := D \sum_{i=1}^{n} \nabla_{x_i} \left\{ \nabla_{x_i} - \beta F_{N,i}(x^N, t) \right\},$$
$$\hat{\mathcal{O}}^+_{n,N} := D \sum_{i=n+1}^{N} \nabla_{x_i} \left\{ \nabla_{x_i} - \beta F_{N,i}(x^N, t) \right\}.$$

The behavior of the system is determined by an initial value boundary problem that, in our case, is defined by the Smoluchowski equation (2.6), the initial condition $P_N^{(0)} : \Omega^N \to \mathbb{R}, x^N \mapsto P_N^{(0)}(x^N) := P_N(x^N, 0)$ at time $t = 0$ (for all spatial coordinates), and a boundary condition on $\partial\Omega$ (for all times). Since we here consider a system with a fixed number of particles, a natural choice is that there is no N-body flux in or out of the system, i.e.,

$$n(x^N) J_N(x^N, t) = 0, \text{ for all } x^N \in \partial\Omega^N, \tag{2.7}$$

where $n(x^N)$ denotes the outward unit normal on $\partial\Omega^N$. Another prominent example (especially for simulations) are periodic boundary conditions. In both examples, the number of particles is conserved.

We say that a solution P_N is *well behaved* if it has the following properties:

(*i*) $P_N \in C^2(\Omega^N \times [0, \infty))$, i.e., for $t = 0$ twice differentiable from the right-hand side;
(*ii*) P_N and $\nabla_{x^N} P_N$ are continuously extensible to $\partial\Omega^N$;
(*iii*) $\partial_t P_N$, $\hat{\mathcal{O}}_n P_N$, $\hat{\mathcal{O}}^{\pm}_{n,N} P_N$, $\nabla_x K_2(x, y)$ and $\nabla_{x^N} P_N$ are bounded for all $n = 1, 2, \ldots N$;
(*iv*) the average n-body interaction force $E_{n,i} : \Omega^n \times [0, \infty) \to \mathbb{R}$ on particle $i \in \{1, \ldots, n\}$ that is defined by

$$E_{n,i}(x^n, t) := \int \rho_{n+1}(x^n, y, t) K_2(x_i, y)\, dy \tag{2.8}$$

exists and is continuously differentiable on Ω^n and for $t \geq 0$. For convenience, we also define $E_{n,i} \equiv 0$ for $n \geq N$. The index is analogously defined to that of the force $F_{n,i}$.

Here, we always assume the existence and uniqueness of a well-behaved solution. Even though a proof of existence and uniqueness is beyond the scope of this paper, we briefly discuss a possible approach at least for a proof of existence and conditions that can be expected in the outlook.

The main question of this paper can now be summarized as follows. Consider N particles with known interparticle interactions and non-conservative forces. Given the initial conditions $P_N^{(0)}$, does the density ρ as a function of time and space uniquely specify the potential V, or in more mathematical terms, is a mapping from ρ to V well defined? As noted in the introduction, the question about a "unique potential" here refers to whether the density–potential mapping is well defined (not whether it is injective).

3 Hierarchy of reduced Smoluchowski equations

In the physics literature, boundary terms are often neglected in the derivation of a reduced Smoluchowski equation [34]. These boundary terms may be essential, however, to derive necessary conditions for a unique density–potential mapping (since non-unique loopholes involve diverging external potentials).

We, therefore, first derive a reduced Smoluchowski equation paying special attention to the boundary terms. Moreover, since we do not rely on the adiabatic approximation but instead consider the exact dependencies between n-body densities, we derive a complete set of reduced Smoluchowski equations for all orders.

Theorem 3.1 *The reduced n-body density ρ_n with $1 \leq n < N$ obeys the following reduced Smoluchowski equation:*

$$\begin{aligned}\partial_t \rho_n(x^n,t) = D\sum_{i=1}^{n}\nabla_{x_i}\left\{\left[\nabla_{x_i}-\beta F_{n,i}(x^n,t)\right]\rho_n(x^n,t)-\beta E_{n,i}(x^n,t)\right\}\\ + D\oint_{\partial\Omega}\left\{\left[\nabla_y-\beta F_{n+1,n+1}(x^n,y,t)\right]\rho_{n+1}(x^n,y,t)-\beta E_{n+1,n+1}(x^n,y,t)\right\}dS(y),\end{aligned} \tag{3.1}$$

where the last term represents a surface integral with respect to the outward unit normal vector.

Proof Under our assumptions, we can apply the n-body density operator to the N-body Smoluchowski differential equation (2.6). First, we use

$$\partial_t \rho_n(x^n,t) = \frac{N!}{(N-n)!}\int \partial_t P_N(x^n,y^{N-n},t)\,dy^{N-n}$$

and $\hat{\mathcal{O}}_N = \hat{\mathcal{O}}^-_{n,N} + \hat{\mathcal{O}}^+_{n,N}$ to obtain

$$\begin{aligned}\partial_t \rho_n(x^n,t) = \frac{N!}{(N-n)!}\int \hat{\mathcal{O}}^-_{n,N} P_N(x^n,y^{N-n},t)\,dy^{N-n}\\ + \frac{N!}{(N-n)!}\int \hat{\mathcal{O}}^+_{n,N} P_N(x^n,y^{N-n},t)\,dy^{N-n}.\end{aligned} \tag{3.2}$$

To simplify the first term on the right-hand side, we note that

$$\hat{\mathcal{O}}^-_{n,N} = \hat{\mathcal{O}}_n - D\beta\sum_{i=1}^{n}\nabla_{x_i}\left[\sum_{j=1}^{N-n}K_2(x_i,y_j)\right]$$

and hence

$$\begin{aligned}\frac{N!}{(N-n)!}\int \hat{\mathcal{O}}^-_{n,N} P_N(x^n,y^{N-n},t)\,dy^{N-n} = \hat{\mathcal{O}}_n\rho_n(x^n,t)\\ - D\beta\frac{N!}{(N-n)!}\int\sum_{i=1}^{n}\nabla_{x_i}\left[P_N(x^n,y^{N-n},t)\sum_{j=1}^{N-n}K_2(x_i,y_j)\right]dy^{N-n}.\end{aligned} \tag{3.3}$$

Using the average n-body interaction force $E_{n,i}$ from (2.8), we can further simplify the remaining integral:

$$\begin{aligned}
&\frac{N!}{(N-n)!}\int \sum_{i=1}^{n}\nabla_{x_i}\left[P_N(x^n,y^{N-n},t)\sum_{j=1}^{N-n}K_2(x_i,y_j)\right]dy^{N-n}\\
&\quad=\sum_{i=1}^{n}\nabla_{x_i}\int\sum_{j=1}^{N-n}\frac{N!}{(N-n)!}P_N(x^n,y^{N-n},t)K_2(x_i,y_j)\,dy^{N-n}\\
&\quad=\sum_{i=1}^{n}\nabla_{x_i}\int\frac{N!}{[N-(n+1)]!}\int P_N(x^n,y,z^{N-(n+1)},t)\,dz^{N-(n+1)}K_2(x_i,y)\,dy\\
&\quad=\sum_{i=1}^{n}\nabla_{x_i}E_{n,i}(x^n,t).
\end{aligned}$$

Inserting this result in (3.3) and finally in (3.2), we have

$$\partial_t\rho_n(x^n,t)=\hat{\mathcal{O}}_n\rho_n(x^n,t)-D\beta\sum_{i=1}^{n}\nabla_{x_i}E_{n,i}(x^n,t)+B(x^n,t),$$

where we define the *boundary term* by

$$\begin{aligned}
B(x^n,t)&:=\frac{N!}{(N-n)!}\int\hat{\mathcal{O}}^{+}_{n,N}P_N(x^n,y^{N-n},t)\,dy^{N-n}\\
&=D\frac{N!}{(N-n)!}\int\sum_{i=1}^{N-n}\nabla_{y_i}\left\{\nabla_{y_i}-\beta F_{N,n+i}(x^n,y^{N-n},t)\right\}P_N(x^n,y^{N-n},t)\,dy^{N-n}\\
&=D\frac{N!}{[N-(n+1)]!}\oint_{\partial\Omega}\int\left\{\nabla_y-\beta F_{N,n+1}(x^n,y,z^{N-(n+1)},t)\right\}\\
&\quad\times P_N(x^n,y,z^{N-(n+1)},t)\,dz^{N-(n+1)}\,dS(y).
\end{aligned}$$

The last equality holds by the divergence theorem. To prove (3.1), it remains to show that

$$\begin{aligned}
&\frac{N!}{[N-(n+1)]!}\int\left\{\nabla_y-\beta F_{N,n+1}(x^n,y,z^{N-(n+1)},t)\right\}P_N(x^n,y,z^{N-(n+1)},t)\,dz^{N-(n+1)}\\
&\qquad=\left[\nabla_y-\beta F_{n+1,n+1}(x^n,y,t)\right]\rho_{n+1}(x^n,y,t)-\beta E_{n+1,n+1}(x^n,y,t).
\end{aligned}$$

This assertion follows from the fact that

$$F_{N,n+1}(x^n,y,z^{N-(n+1)},t)=F_{n+1,n+1}(x^n,y,t)+\sum_{j=1}^{N-(n+1)}K_2(y,z_j)$$

and (for $n<N-1$)

$$\begin{aligned}
&\frac{N!}{[N-(n+1)]!}\int\sum_{j=1}^{N-(n+1)}K_2(y,z_j)P_N(x^n,y,z^{N-(n+1)},t)\,dz^{N-(n+1)}\\
&\qquad=\frac{N!}{[N-(n+2)]!}\int K_2(y,z)\int P_N(x^n,y,z,v^{N-(n+2)},t)\,dv^{N-(n+2)}\,dz,
\end{aligned}$$

where the last expression is, by definition, equal to $E_{n+1,n+1}(x^n,y,t)$. □

Remark 3.2 The two expressions in curly brackets in the first and second line of the reduced Smoluchowski equation (3.1) for ρ_n are those of the YBG hierarchy [27, Sec. 4.2] for order n and $n+1$, respectively. In equilibrium, the two expressions always vanish, which is in agreement with $\partial_t \rho_n(x^n, t) = 0$ for all $x^n \in \Omega^n$ and $t \geq 0$. Out of equilibrium, the boundary terms vanish for all orders if and only if the YBG hierarchy holds *on average* at the boundary.

We can formally extend the reduced Smoluchowski equation (3.1) to $n = 0$, where $\rho_0 \propto N$ corresponds to the number N of particles and the right-hand side only consists of the boundary term, which then corresponds to the first member of the YBG hierarchy. If this boundary term vanishes, the equation $\partial N/\partial t = 0$ directly reflects particle conservation.

In the following, we denote the components of J_N that correspond to the ith particle by $J_{N,i} : \Omega^N \times [0, \infty) \to \mathbb{R}^d$ (with $i = 1, \ldots, N$). We are interested in physically relevant boundary problems for which the following condition holds

$$\int \nabla_{x_i} J_{N,i}(x^N, t)\, dx_i = \oint_{\partial\Omega} J_{N,i}(x^N, t)\, dS(x_i) = 0, \text{ for all } i = 1, \ldots N. \tag{3.4}$$

This condition guarantees that a time-dependent version of the YGB hierarchy holds on average at the boundary for all orders.

Proposition 3.3 *If (3.4) holds, then the boundary term in (3.1) vanishes for all $n < N$.*

Proof Combining $F_{n,1}, \ldots F_{n,n}$ into one vector-valued function $F_n : \Omega^n \times [0, \infty) \to \mathbb{R}^{dn}$ (analogous to F_N) and $E_{n,1}, \ldots E_{n,n}$ into $E_n : \Omega^n \times [0, \infty) \to \mathbb{R}^{dn}$, we define the n-body current $J_n : \Omega^n \times [0, \infty) \to \mathbb{R}^{dn}$ as

$$J_n(x^n, t) := -D\nabla_{x^n} \rho_n(x^n, t) + \beta D \rho_n(x^n, t) F_n(x^n, t) + \beta D E_n(x^n, t).$$

We use the similar notation as by $J_{N,i}$. Then (3.1) can then be rewritten as

$$\partial_t \rho_n(x^n, t) = -\nabla_{x^n} J_n(x^n, t) - \oint_{\partial\Omega} J_{n+1,n+1}(x^n, y, t)\, dS(y). \tag{3.5}$$

Analogous to the proof of Theorem 3.1, we obtain for $i = 1, \ldots, n$

$$\int J_{N,i}(x^n, y^{N-n}, t)\, dy^{N-n} = \frac{(N-n)!}{N!} J_{n,i}(x^n, t)$$

and thus obtain for the boundary term in (3.5):

$$\begin{aligned} &\oint_{\partial\Omega} J_{n+1,n+1}(x^n, y, t)\, dS(y) \\ &= \frac{N!}{(N-n)!} \int \oint_{\partial\Omega} J_{N,n+1}(x^n, y, z^{N-n-1}, t)\, dS(y) dz^{N-n-1} = 0, \end{aligned}$$

where the last equation holds due to (3.4). □

In the following, we always assume that (3.4) holds. For example, this condition is guaranteed both by (2.7) or by periodic boundary conditions. Thus, we recover the well-known (reduced) Smoluchowski equation for the one-body density:

$$\begin{aligned} \partial_t \rho(x, t) = D\nabla_x \Big\{ &\nabla_x \rho(x, t) + \beta \rho(x, t) \nabla_x V(x, t) - \beta \rho(x, t) R(x, t) \\ &- \beta \int \rho_2(x, y, t) K_2(x, y)\, dy \Big\}. \end{aligned} \tag{3.6}$$

More generally, for the n-body densities, we obtain:

$$\partial_t \rho_n(x^n,t) = D\sum_{i=1}^{n}\nabla_{x_i}\Big\{\nabla_{x_i}\rho_n(x^n,t) + \beta\rho_n(x^n,t)\nabla_{x_i}V(x_i,t) - \beta\rho_n(x^n,t)R(x_i,t) - \beta\rho_n(x^n,t)\sum_{\substack{j=1\\ j\neq i}}^{n}K_2(x_i,x_j) - \beta\int\rho_{n+1}(x^n,y,t)K_2(x_i,y)\,dy\Big\}. \tag{3.7}$$

Based on (3.6), we define the one-body current $j:\Omega\times[0,\infty)\to\mathbb{R}^d$ as

$$j(x,t) := -D\nabla_x\rho(x,t) - D\beta\rho(x,t)\nabla_x V(x,t) + D\beta\rho(x,t)R(x,t) + D\beta\int\rho_2(x,y,t)K_2(x,y)\,dy, \tag{3.8}$$

so that it obeys the following continuity equation

$$\partial_t\rho(x,t) = -\nabla_x j(x,t).$$

Our definition (3.8) is equivalent to the ensemble average of a current operator [50].

We define the normal one-body current $j_\perp:\partial\Omega\times[0,\infty)\to\mathbb{R}$ at the boundary via an extension of j from (3.8) to $\partial\Omega$:

$$\begin{aligned} j_\perp(x,t) &:= n(x)j(x,t)\\ &= -n(x)D\nabla_x\rho(x,t) - n(x)D\beta\rho(x,t)\nabla_x V(x,t)\\ &\quad + n(x)D\beta\rho(x,t)R(x,t) + n(x)D\beta\int\rho_2(x,y,t)K_2(x,y)\,dy, \end{aligned} \tag{3.9}$$

where $n(x)$ denotes the outward unit normal on $\partial\Omega$ at x. By property (iii) of a well-behaved solution and by the type of forces that we consider, $j_\perp$ is well defined. As before, the product of vectors is consistently interpreted as a scalar product.

Boundary condition (2.7) of a vanishing normal N-body flux also implies a corresponding condition on the one-body current:

$$j_\perp(x,t) = 0 \quad \text{for all } x\in\partial\Omega, t\geq 0. \tag{3.10}$$

Intuitively speaking, the normal component of the one-body current field vanishes at the boundary $\partial\Omega$. It is a common boundary condition in physics. In the following, any boundary condition that implies (3.10) is called a *no-flux boundary condition*.

4 Uniqueness theorems

We now turn to the central question of this paper. Given an initial condition $P_N^{(0)}$, does ρ uniquely specify V, i.e., is a mapping from ρ to V well defined?

There are two obvious limitations to uniqueness. First, the mapping can only be unique for $x\in\Omega$ where and when $\rho(x,t)>0$. Variations in V outside the support of ρ, i.e., within the complement of the set $\mathrm{supp}(\rho) := \{(x,t)\in\Omega\times[0,\infty) : \rho(x,t)>0\}$, do not change the time evolution of the system as determined by the Smoluchowski equation. Secondly, adding a time-dependent constant to the potential does not change the time evolution either.

We can combine both limitations in a single statement, i.e., if the difference of the potentials is a time-dependent constant on the support of ρ, then it has no effect on the density.

Definition 4.1 Two external potentials V and V' are said to be *diffusion equivalent*, $V \sim V'$, for a given one-body density ρ if the difference $d_V : \Omega \times [0, \infty) \to \mathbb{R}; (x, t) \mapsto d_V(x, t) := V(x, t) - V'(x, t)$ is only a function of time on $\mathrm{supp}(\rho)$.

(For example, for $d = 1$ and $\rho(x, t) \equiv 1$, $V(x, t) \equiv 0$ is diffusion equivalent to $V'(x, t) = \sin(t)$ but not to $V''(x, t) = \sin(x)$.) This definition allows us to formulate our strategy of proof more specifically. In the following, we consider two systems with densities ρ and ρ' and with external potentials V and V'. Both systems start from the same initial condition $P_N^{(0)}$, and they have the same boundary conditions, pair potentials, and non-conservative forces.

Our aim is to derive conditions for which an equivalence of ρ and ρ' implies diffusion equivalence of V and V', or in other words that the difference

$$d_V(x, t) := V(x, t) - V'(x, t) \tag{4.1}$$

is diffusion equivalent to a function that is identically zero. For convenience, we will actually show the contrapositive. If the two potentials are not diffusion equivalent, then the densities must differ, and thus ρ determines V.

A key step in the proof is to reduce the question of a unique mapping to that of the unique solvability of a (semi-)elliptic PDE. As discussed in the introduction, this approach is partly similar to the argument by Runge and Gross (or Chan and Finken) [8, 46], but it differs in that we use the hierarchy of reduced Smoluchowski equations from Theorem 3.1. We also pay close attention to a rigorous treatment of the boundary terms. Additionally, we prove that a no-flux boundary condition always implies uniqueness.

The main advantage of our strategy is a physically intuitive proof that helps to clarify the essential physical questions. This intuition comes at the price of two additional assumptions that could possibly be avoided by alternative methods, like a fix-point scheme that has already been employed in the quantum case [44, 45]. We summarize these two assumptions via the following definition.

Definition 4.2 We call a many-body system *analytically accessible* if the following conditions hold:

(A1) the external potential V is real analytic in time for $t \geq 0$, and for each $k \in \mathbb{N}_0$, $\partial_t^k V \in C^2(\Omega \times [0, \infty))$, and $\partial_t^k V(\cdot, t = 0)$ is continuously extensible to $\partial\Omega$;

(A2) the n-body densities ρ_n for all $n = 1, 2, \ldots N$ and non-conservative one-body forces R are infinitely often differentiable in time from the right at $t = 0$, and for each $k \in \mathbb{N}_0$, $\partial_t^k \rho_n \in C^2(\Omega^n \times [0, \infty))$, and $\partial_t^k \rho_n$ is bounded, and $\partial_t^k R \in C^1(\Omega \times [0, \infty))$.

More specifically, concerning conditions (A1), by including the start time $t = 0$, we assume that the potential is right differentiable; and since for each $x \in \Omega$, the function $V_x : [0, \infty) \to \mathbb{R}, t \mapsto V(x, t)$ is real analytic, the corresponding Taylor series at the origin converges in some neighborhood of 0. Hence, the derivatives at the origin uniquely specify the potential at all times (according to the identity theorem for analytic functions). With regards to conditions (A2), note that we do not require ρ_n to be time analytic.

Proposition 4.3 *The N-body probability density $P_N(x^N, t) > 0$ for $x^N \in \Omega^N$ and $t > 0$.*

Proof Due to (2.1) for $t = 0$, $\int P_N^{(0)}(x^N)\,dx^N = 1$ and since $P_N^{(0)}(x^N) \geq 0$, the support of $P_N^{(0)}$ is not empty and there exist a $x_1^N \in \Omega^N$ with $P_N^{(0)}(x_1^N) > 0$. Suppose $P_N(x_0^N, t_0) = 0$ for one $x_0^N \in \Omega^N$ and $t_0 > 0$. Since Ω is open and connected, there is a connected domain D compactly contained in Ω ($\bar{D} \subset \Omega$) with $x_0^N, x_1^N \in D^N$. From $P_N(x_0^N, t_0) = 0$ follows $\inf_{x^N \in D^N} P_N(x^N, t_0) = 0$.

According to Theorem 10 in [19, Chapter 7.1], we obtain for $0 < t < t_0$ that

$$\sup_{x^N \in D^N} P_N(x^N, t) \leq C \inf_{x^N \in D^N} P_N(x^N, t_0) = 0 \tag{4.2}$$

with a constant C that depends on D^N, t, t_0, and the coefficients of $\hat{\mathcal{O}}_N$. Theorem 10 in [19, Chapter 7.1] assumes continuous coefficients of the parabolic differential equation, i.e., the assertion only holds for potentials $V \in C^2(\Omega)$, $R \in C(\Omega)$, and $K_2 \in C(\Omega^2 \times [0, \infty))$, and diverging potentials are excluded; all of which is in agreement with our assumptions in Sec. 2.

By (4.2), $P_N(x^N, t) = 0$ for all $x^N \in D^N$ and $0 < t < t_0$ and specifically $P_N(x_1^N, t) = 0$. Since $P_N \in C(\Omega^N \times [0, \infty))$, we have $P_N(x_1^N, 0) = P_N^{(0)}(x_1^N) = 0$, which is a contradiction to $P_N^{(0)}(x_1^N) > 0$. Therefore, $P_N(x^N, t) > 0$ and accordingly $\rho(x, t) > 0$ for all $x^N \in \Omega^N$, $x \in \Omega$ and $t > 0$. □

To simplify our proofs, we assume in the following that $P_N^{(0)}(x^N) > 0$ holds for all $x^N \in \Omega^N$, which we here denote by $P_N^{(0)} > 0$. With Proposition 4.3, this assumption is innocuous from a physical point of view.

Since we assume that the potentials are analytic, we will consider the time derivatives of their difference, i.e., we define $d_V^{(k)} : \Omega \to \mathbb{R}$ for $k \in \mathbb{N}_0$:

$$x \mapsto d_V^{(k)}(x) := \partial_t^k d_V(x, t)\Big|_{t=0}.$$

Because V and V' are analytic in time and $\mathrm{supp}(\rho) = \Omega \times [0, \infty)$, V and V' are diffusion equivalent if and only if $\nabla_x d_V(x, t) = 0$ for all $x \in \Omega$ and $t \geq 0$, which is equivalent to $\nabla_x d_V^{(k)}(x) = 0$ for all $x \in \Omega$ and $k \in \mathbb{N}_0$. Let V and V' be not diffusion equivalent; then there exists a smallest non-negative integer, say l, for which $\nabla d_V^{(l)} \not\equiv 0$.

The proof of our theorems rests on the following lemma. Importantly, it allows an exact treatment of the average n-body interaction forces for all orders of n (via the hierarchy of reduced Smoluchowski equations).

Lemma 4.4 *Given two analytically-accessible many-body systems with identical initial conditions $P_N^{(0)} > 0$ and boundary conditions. Let their external potentials V and V' be not diffusion equivalent, and denote by $l \in \mathbb{N}_0$ the smallest integer for which $\nabla d_V^{(l)} \not\equiv 0$. Then*

$$\partial_t^k \left[\rho_n(x^n, t) - \rho_n'(x^n, t)\right]\Big|_{t=0} \equiv 0 \quad \text{for all } n = 1, 2, \ldots, N \text{ and } k = 0, 1, \ldots, l \tag{4.3}$$

and

$$\partial_t^{l+1} \left[\rho(x, t) - \rho'(x, t)\right]\Big|_{t=0} = D\beta\nabla_x \left[\rho(x, 0)\nabla_x d_V^{(l)}(x)\right]. \tag{4.4}$$

Proof We first prove (4.3) by an induction-like argument. This equation obviously holds for $k = 0$ by (2.2) because both many-body systems start from the same initial condition $P_N^{(0)}$. In the case $l > 0$, assume that (4.3) holds for all $k = 0, 1, \ldots, m$ for some $m < l$. We must now verify that (4.3) also holds for $k = m + 1$. Therefore, we subtract the reduced Smoluchowski

equations (3.7) for the n-body densities of the two many-body systems, take m additional time derivatives and evaluate the derivatives at $t = 0$:

$$\partial_t^{m+1}\left[\,\rho_n(x^n,t)-\rho_n'(x^n,t)\right]\Big|_{t=0} = D\sum_{i=1}^{n}\nabla_{x_i}^2\,\partial_t^m\left[\rho_n(x^n,t)-\rho_n'(x^n,t)\right]\Big|_{t=0} \tag{4.5a}$$

$$+\,D\beta\sum_{i=1}^{n}\nabla_{x_i}\partial_t^m\left[\rho_n(x^n,t)\nabla_{x_i}V(x_i,t)-\rho_n'(x^n,t)\nabla_{x_i}V'(x_i,t)\right]\Big|_{t=0} \tag{4.5b}$$

$$-\,D\beta\sum_{i=1}^{n}\nabla_{x_i}\partial_t^m\left[\rho_n(x^n,t)-\rho_n'(x^n,t)\right]R(x_i,t)\Big|_{t=0} \tag{4.5c}$$

$$-\,D\beta\sum_{\substack{i,j=1\\ j\neq i}}^{n}\nabla_{x_i}\left\{\partial_t^m\left[\rho_n(x^n,t)-\rho_n'(x^n,t)\right]\Big|_{t=0}K_2(x_i,x_j)\right\} \tag{4.5d}$$

$$-\,D\beta\sum_{i=1}^{n}\nabla_{x_i}\int\partial_t^m\left[\rho_{n+1}(x^n,y,t)-\rho_{n+1}'(x^n,y,t)\right]\Big|_{t=0}K_2(x_i,y)\,dy. \tag{4.5e}$$

The terms (4.5a) on the right-hand side, (4.5d) and (4.5e) vanish directly since (4.3) holds for $k = m$ by our induction hypothesis. For the remaining derivative in the second term (4.5b), we have

$$\begin{aligned}
&\partial_t^m\left[\rho_n(x^n,t)\nabla_{x_i}V(x_i,t)-\rho_n'(x^n,t)\nabla_{x_i}V'(x_i,t)\right]\Big|_{t=0}\\
&=\sum_{k=0}^{m}\binom{m}{k}\left[\partial_t^k\rho_n(x^n,t)\Big|_{t=0}\nabla_{x_i}\partial_t^{m-k}V(x_i,t)\Big|_{t=0}-\partial_t^k\rho_n'(x^n,t)\Big|_{t=0}\nabla_{x_i}\partial_t^{m-k}V'(x_i,t)\Big|_{t=0}\right]\\
&=\sum_{k=0}^{m}\binom{m}{k}\left[\partial_t^k\rho_n(x^n,t)\Big|_{t=0}\nabla_{x_i}d_V^{(m-k)}(x_i)\right],
\end{aligned} \tag{4.6}$$

where the last equality holds again because of our induction hypothesis, i.e., we apply (4.3) for $k \le m$. Now, since $\nabla d_V^{(k)} \equiv 0$ for all $k \le m < l$, assertion (4.3) follows for all $k = 0, 1, \ldots, l$. For (4.5c), we consider

$$\begin{aligned}
&\partial_t^m\left[\rho_n(x^n,t)-\rho_n'(x^n,t)\right]R(x_i,t)\Big|_{t=0}\\
&\quad=\sum_{k=0}^{m}\binom{m}{k}\partial_t^k\left[\rho_n(x^n,t)-\rho_n'(x^n,t)\right]\Big|_{t=0}\partial_t^{m-k}R(x_i,t)\Big|_{t=0}\overset{(4.3)}{=}0.
\end{aligned}$$

To prove (4.4), we subtract the reduced Smoluchowski equations (3.6) for the one-body densities of the two many-body systems, take l additional time derivatives and evaluate the result at $t = 0$:

$$\begin{aligned}
\partial_t^{l+1}\left[\rho(x,t)-\rho'(x,t)\right]\Big|_{t=0} &= D\,\nabla_x^2\partial_t^l\left[\rho(x,t)-\rho'(x,t)\right]\Big|_{t=0}\\
&\quad+D\beta\,\nabla_x\partial_t^l\left[\rho(x,t)\nabla_xV(x,t)-\rho'(x,t)\nabla_xV'(x,t)\right]\Big|_{t=0}\\
&\quad-D\beta\,\nabla_x\partial_t^l\left[\rho(x,t)-\rho'(x,t)\right]R(x,t)\Big|_{t=0}\\
&\quad-D\beta\,\nabla_x\int\partial_t^l\left[\rho_2(x,y,t)-\rho_2'(x,y,t)\right]\Big|_{t=0}K_2(x,y)\,dy.
\end{aligned}$$

The first and last term on the right-hand side vanish by (4.3) and the third term vanishes like (4.5c). Thus, we have

$$\begin{aligned}\partial_t^{l+1}\left[\rho(x,t)-\rho'(x,t)\right]\Big|_{t=0} &= D\beta\,\nabla_x\partial_t^l\left[\rho(x,t)\nabla_x V(x,t)-\rho'(x,t)\nabla_x V'(x,t)\right]\Big|_{t=0}\\ &= D\beta\,\nabla_x\sum_{k=0}^{l}\binom{l}{k}\left[\partial_t^k\rho(x,t)\Big|_{t=0}\nabla_x\partial_t^{l-k}V(x,t)\Big|_{t=0}-\partial_t^k\rho'(x,t)\Big|_{t=0}\nabla_x\partial_t^{l-k}V'(x,t)\Big|_{t=0}\right]\\ &= D\beta\,\nabla_x\sum_{k=0}^{l}\binom{l}{k}\left[\partial_t^k\rho(x,t)\Big|_{t=0}\nabla_x d_V^{(l-k)}(x)\right],\end{aligned}$$

where the last equality holds again by (4.3). Since $\nabla d_V^{(l-k)}\equiv 0$ for all $0<k\le l$, we have proven (4.4) which concludes the proof. □

The n-body densities ρ_n with $n>1$ are highly relevant for the correct time evolution of the one-body density ρ. The preceding lemma provides control over these contributions since (4.3) holds for all $n\ge 1$ and their derivatives up to order l. As an important consequence, (4.4) and hence our final results on uniqueness have no explicit condition on ρ_n. Our proof via an induction-like argument reflects the hierarchical structure of the reduced Smoluchowski equations for ρ_n.

Next, we state and prove our first main Theorem 4.5 with a general and quite formal condition for uniqueness. We then verify this condition for no-flux boundary conditions in our central Theorem 4.6. The general condition of Theorem 4.5 is still useful to easily adapt the proof to other boundary conditions as in Corollary 4.8.

Theorem 4.5 *Given two analytically-accessible many-body systems with identical initial conditions $P_N^{(0)}>0$ and boundary conditions. Let their external potentials V and V' be not diffusion equivalent, and denote by $l\in\mathbb{N}_0$ the smallest integer for which $\nabla_x d_V^{(l)}\not\equiv 0$.*

If

$$\oint_{\partial\Omega}\rho(x,0)d_V^{(l)}(x)\nabla_x d_V^{(l)}(x)dS(x)=0, \tag{4.7}$$

then the two resulting densities are different, i.e., $\rho\not\equiv\rho'$.

Proof By condition (A2), all time derivatives of ρ and ρ' exist. Thus if

$$\partial_t^k\left[\rho(x,t)-\rho'(x,t)\right]\Big|_{t=0}\not\equiv 0,$$

for some $k\in\mathbb{N}$, then the densities are different. Consider the case $k=l+1$. According to (4.4) from Lemma 4.4, it suffices to show that

$$\nabla_x\left[\rho(x,0)\nabla_x d_V^{(l)}(x)\right]\not\equiv 0. \tag{4.8}$$

Suppose, on the contrary, that $d_V^{(l)}(x)\not\equiv 0$ is a non-trivial solution of the PDE:

$$\nabla_x\left[\rho(x,0)\nabla_x d_V^{(l)}(x)\right]\equiv 0. \tag{4.9}$$

Now, consider the following integral

$$\int d_V^{(l)}(x)\nabla_x\left[\rho(x,0)\nabla_x d_V^{(l)}(x)\right]dx$$

$$= -\int \rho(x,0)\left[\nabla_x d_V^{(l)}(x)\right]^2 dx + \oint_{\partial\Omega} \rho(x,0) d_V^{(l)}(x)\nabla_x d_V^{(l)}(x)\, dS(x)$$

using partial integration. By our assumption, the surface term vanishes, and we obtain

$$\int d_V^{(l)}(x)\nabla_x\left[\rho(x,0)\nabla_x d_V^{(l)}(x)\right] dx = -\int \rho(x,0)\left[\nabla_x d_V^{(l)}(x)\right]^2 dx.$$

Since $\nabla d_V^{(l)} \not\equiv 0$ and $\rho(x,0) > 0$, the right-hand side is strictly negative. Therefore, the integrand on the left-hand side cannot vanish for all $x \in \Omega$, which in turn implies (4.8). □

From Theorem 4.5, we can distinguish different cases of uniqueness based on the behavior of ρ close to the boundary. In fact, condition (4.7) could, in principle, allow for diverging densities if the gradient of the potential difference vanishes fast enough. We will discuss such cases in the next section. Note, moreover, that condition (4.7) can be immediately generalized to a non-positive surface integral (which is, however, less physically intuitive).

Now, we consider the physically-intuitive no-flux boundary condition from (3.10) and show that it guarantees condition (4.7) from Theorem 4.5 for any V and V' which are not diffusion equivalent. This proof allows for an explicit uniqueness theorem.

Theorem 4.6 *For an analytically-accessible many-body system with initial condition $P_N^{(0)} > 0$ and no normal flux $j_\perp$ at the boundary $\partial\Omega$, the density ρ uniquely determines the external potential V (up to diffusion equivalence).*

Proof As discussed above, we want to show that the density–potential mapping is unique, i.e., $\rho \equiv \rho'$ implies $V \sim V'$, by proving the contrapositive, i.e., if V and V' are not diffusion equivalent, then $\rho(x,t)$ must differ from $\rho'(x,t)$ for some $x \in \Omega$ and $t > 0$.

Let $V \nsim V'$ and l denote the smallest integer for which $\nabla d_V^{(l)} \not\equiv 0$, as in Theorem 4.5. To show that $\rho \not\equiv \rho'$, we have to show that condition (4.7) holds. Since the normal flux is zero for the two many-body systems, subtracting (3.9) for the two systems yields

$$\begin{aligned} 0 = &- Dn(x)\nabla_x[\rho(x,t) - \rho'(x,t)] \\ &- D\beta n(x)[\rho(x,t)\nabla_x V(x,t) - \rho'(x,t)\nabla_x V'(x,t)] \\ &+ D\beta n(x)[\rho(x,t) - \rho'(x,t)]R(x,t) \\ &+ D\beta n(x)\int [\rho_2(x,y,t) - \rho_2'(x,y,t)]K_2(x,y)\, dy \end{aligned}$$

for all $x \in \partial\Omega$. By applying l subsequent time derivatives and (4.3), we get

$$n(x)\partial_t^l[\rho(x,t)\nabla_x V(x,t) - \rho'(x,t)\nabla_x V'(x,t)]\Big|_{t=0} = 0,$$

and

$$n(x)\rho(x,0)\nabla_x d_V^{(l)}(x) \equiv 0$$

follows by the same argumentation as in (4.6).

Since $\partial_t^l V(x,t)\big|_{t=0}$ and $\partial_t^l V'(x,t)\big|_{t=0}$ are continuously extensible to $\partial\Omega$, and since Ω is bounded, $d_V^{(l)}$ is bounded on $\partial\Omega$. Thus, we obtain:

$$n(x)\rho(x,0)d_V^{(l)}(x)\nabla_x d_V^{(l)}(x) = 0$$

for all $x \in \partial\Omega$. Therefore the integrand of equation (4.7) vanishes, which proves the assertion. □

Remark 4.7 Theorem 4.6 can be readily extended to other boundary conditions that prescribe the normal flux at $\partial\Omega$, provided that the boundary terms in (3.1) remain zero. However, when applying such conditions to our general N-body framework, where each particle is conserved according to the Smoluchowski equation, one must carefully verify that these conditions are physically meaningful and well-defined.

In general, such nonzero boundary fluxes would require source and sink terms already in the N-body Smoluchowski equation (2.3). Alternatively, a prominent example where (dynamic) flux through the boundary can be considered a common behavior of the evolving system are periodic boundary conditions (in which case the Smoluchowski equation would not need to be modified). Such boundary conditions are typically used in computer simulations.

Theorem 4.6 together with Remark 4.7 capture a generic case where the density and the normal flux at the boundary together uniquely specify the external potential and hence all higher-order correlations. This assertion is consistent with the PFT framework, where the density and current together yield a complete statistical description of a time-dependent many-body system [50, 51]. However, our result is less restrictive since we only need to fix the normal flux at the boundary. In fact, an alternative formulation of our uniqueness theorem is possible, which only involves the current without further assumptions on the boundary condition.

Corollary 4.8 *For an analytically-accessible many-body system with initial condition $P_N^{(0)} > 0$, the one-body current j uniquely determines the external potential V (up to diffusion equivalence).*

Proof Consider two potentials $V \nsim V'$ and l denote the smallest integer for which $\nabla d_V^{(l)} \not\equiv 0$. Now let ρ and ρ' be the densities that result with the external potentials V and V' with initial condition $P_N^{(0)}$ and identical boundary conditions, which satisfying conditions (A1) and (A2). By (3.8), we have

$$\begin{aligned} j(x,t) - j'(x,t) = &- D\nabla_x \left[\rho(x,t) - \rho'(x,t)\right] \\ &- D\beta\rho(x,t)\nabla_x d_V(x,t) - D\beta\left[\rho(x,t) - \rho'(x,t)\right]\nabla_x V'(x,t) \\ &+ D\beta\left[\rho(x,t) - \rho'(x,t)\right]R(x,t) \\ &+ D\beta\int\left[\rho_2(x,y,t) - \rho_2'(x,y,t)\right]K_2(x,y)\,dy. \end{aligned}$$

Now consider

$$\begin{aligned} \partial_t^l\left[j(x,t) - j'(x,t)\right]\Big|_{t=0} = -D\Bigg[&\partial_t^l\left[\rho(x,t) - \rho'(x,t)\right]\Big|_{t=0} \\ &+ \beta\sum_{k=0}^{l}\binom{l}{k}\partial_t^{l-k}\rho(x,t)\Big|_{t=0}\nabla_x d_V^{(k)}(x) \\ &+ \beta\sum_{k=0}^{l}\binom{l}{k}\partial_t^{l-k}\left[\rho(x,t) - \rho'(x,t)\right]\Big|_{t=0}\nabla_x\partial_t^k V'(x,t)\Big|_{t=0} \\ &- \beta\sum_{k=0}^{l}\binom{l}{k}\partial_t^{l-k}\left[\rho(x,t) - \rho'(x,t)\right]\Big|_{t=0}\partial_t^k R(x,t)\Big|_{t=0} \\ &- \beta\int\partial_t^l\left[\rho_2(x,y,t) - \rho_2'(x,y,t)\right]\Big|_{t=0}K_2(x,y)\,dy\Bigg]. \end{aligned}$$

From Lemma 4.4 and $\rho(x,0) > 0$ follows

$$\partial_t^l \left[j(x,t) - j'(x,t) \right] \Big|_{t=0} = -D\beta\rho(x,0)\nabla_x d_V^{(l)} \not\equiv 0.$$

Thus, following the proof of Theorem 4.5, we have $j \not\equiv j'$. □

Remark 4.9 The condition (4.7) for uniqueness in Theorem 4.5 depends on the difference d_V of the potentials, as expected from the arguments in quantum mechanics [45, 46]. Intuitively speaking, the uniqueness of the potential V that realizes ρ is stated (only) in a "neighborhood" of V, i.e., within a space of admissible potentials defined by (4.7).

In contrast, Theorem 4.6 and Corollary 4.8 make no explicit assumption on d_V. Instead, the conditions on the current (at the boundary) allow for a "global" statement because they exclude all potentials outside this "neighborhood" of V. (There is, of course, still the additional assumption of smooth potentials according to our method of proof following Runge and Gross [46].)

Since we assume in condition (A1) in Definition 4.2 that the potential and its time derivatives are continuously extensible to $\partial\Omega$, we exclude potentials that diverge at the boundary $\partial\Omega$, but recall that hard walls, which are a common choice for an external potential in physics, are here represented via our bounded domain Ω and the no-flux boundary conditions. Definition 4.2 only restricts any additional (time-dependent) potential within the domain. For unbounded systems, it will be interesting to relax condition (A1) in future work (e.g., via a limit for infinite system sizes).

Note that in the proof of Theorem 4.6, the only explicit requirement is that the difference $d_V^{(l)}$ does not diverge on $\partial\Omega$. Hence, it is promising to consider a larger space of external potentials, in the sense of Remark 4.9, where V and V' may diverge at the boundary while their difference $d_V^{(l)}$ remains finite on $\partial\Omega$ so that uniqueness is still preserved in a neighborhood of V. Moreover, we expect that our results can also be generalized to non-integrable density profiles to include such a simple case as the homogeneous bulk. We illustrate these scenarios in the examples below.

5 Loopholes to uniqueness

Our explicit conditions for uniqueness imply cases where a violation directly results in non-unique potentials, i.e., a density profile that can be realized by two different external potentials (which are not diffusion equivalent). According to Remark 4.9, such non-unique potentials have to differ strongly, in the sense that they violate (4.7). Theorem 4.5 obviously makes no direct statement about how to construct such potentials. However, the proof structure provides cues on their existence, as the uniqueness of the density–potential mapping is essentially equivalent to having only trivial solutions of the elliptic PDE (4.9). This insight allows us to specify a constructive method of non-unique potentials for the ideal gas or, more generally, under the adiabatic approximation [5, 38, 53]. The latter assumes that the two-body density $\rho_2(x,y,t)$ is a functional of the one-body density $\rho(x,t)$ at the same time t. The resulting "loopholes" can also be illustrated for unbounded systems and non-integrable densities.

A generic procedure to construct explicit loopholes to uniqueness that violate (4.7) follows directly from (3.6) and the assumption that ρ_2 is a functional of ρ. In that case, (3.6) is a closed equation in the sense that it only depends on ρ and not on ρ_n with $n > 1$. By taking

the difference for two systems with distinct external potentials V' and V, we obtain a PDE similar to (4.9) but for d_V, as defined in (4.1), instead of its expansion coefficients:

$$\nabla_x[\rho(x,t)\nabla_x d_V(x,t)] = 0 \text{ for all } x \in \Omega, t \geq 0. \tag{5.1}$$

Precisely, we start with a system with given external potential V' and a prescribed boundary condition on the normal flux according to Remark 4.7. Then, we can add to V' a nontrivial solution of (5.1) without changing the density profile, i.e., the resulting potential V of the new system gives rise to $\rho(x,t) = \rho'(x,t)$. However, the expression in (5.1) results in a divergence-free difference $j(x,t) - j'(x,t) = -D\beta\rho(x,t)\nabla_x d_V(x,t)$ of the one-body currents in the two systems. By construction, this distinct current j of the new system violates our condition for uniqueness in Theorem 4.5 (and also contradicts our requirement in Theorem 4.6 and Remark 4.7), so that, consistently, the external potential can no longer be expected to be unique.

The construction of loopholes according to (5.1) can be made even more explicit if the density is effectively one-dimensional (i.e., homogeneous in all coordinates but one). In that case, the elliptic PDE (5.1) reduces to a Sturm-Liouville problem [59], which can be solved explicitly:

$$d_V(x,t) = \int_{x_0}^{x} \frac{c(t)}{\rho'(y,t)}\, dy \tag{5.2}$$

with $x_0 \in \Omega$ and $c(t)$ being a purely time-dependent constant. This additional external potential leads to the new (effectively) one-dimensional current

$$j(x,t) = j'(x,t) - D\beta c(t)$$

in x-direction. Only $c(t) \equiv 0$ results in a potential that does not violate condition (A1), and in that case, the additional current vanishes, $-D\beta c(t) = 0$.

The procedure to construct non-unique potentials for an ideal gas (5.2) is carried out in the following example, inspired by [37], where we consider the bounded domain $\Omega = [-\pi/2, \pi/2] \subset \mathbb{R}$. For the rest of this section, we set all constants to one by our choice of units (i.e., without loss of generality).

Example 5.1 *(Bounded systems)* Consider an ideal gas in (effectively) one dimension that is trapped in a bounded domain $\Omega = [-\pi/2, \pi/2]$, e.g., via hard walls, but without an additional potential inside the domain, i.e., $V'(x,t) \equiv 0$. Since the system is in equilibrium, there is no current $j'(x,t) \equiv 0$, and the density $\rho'(x,t) \equiv 1$ is constant in space and time; see Fig. 1 (a).

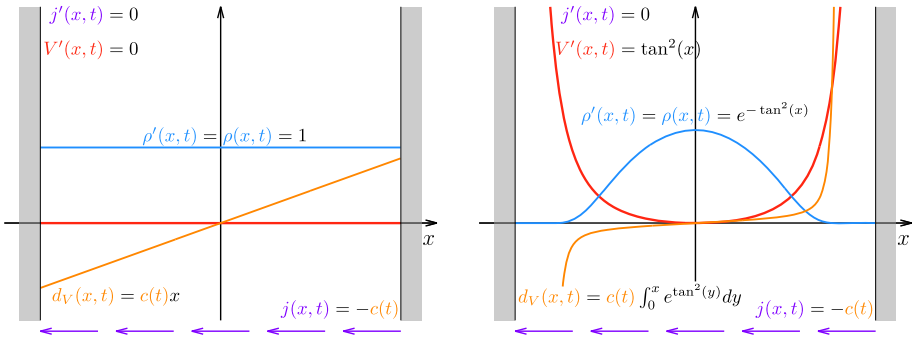
If we add an external potential according to (5.2),

$$d_V(x,t) = c(t)x,$$

the potential gives rise to a current $j'(x,t) \equiv -c(t)$, which may vary in time, but which is spatially homogeneous. Therefore, it preserves the homogeneous density $\rho(x,t) \equiv 1$ even though particles get transported through the system.

Obviously, such a current violates the no-flux boundary condition of hard walls (but it may be realized by periodic boundary conditions, as discussed below).

Now, we consider another system, where the ideal gas is bounded by the diverging potential $V'(x,t) = \tan^2(x)$. Its density is given by $\rho'(x,t) = e^{-\tan^2(x)}$. To obtain a homogeneous current that preserves the density profile, the added external potential d_V has to diverge even



(a) Bounded potentials (b) Diverging potentials

Fig. 1 Schematics of non-unique potentials for bounded domains (illustrated as within hard walls): We start from the equilibrium solution $\rho'(x,t)$ for non-interacting particles (a) without an external potential, i.e., $V'(x,t)=0$; or (b) with a diverging potential $V'(x,t)=\tan^2(x)$. Since the systems are in equilibrium, $j'(x,t)=0$. When a time-dependent potential $d_V(x,t)$ is added to the system (with $c(t)>0$), the density profile remains unchanged, $\rho(x,t)\equiv\rho'(x,t)$, but we obtain a spatially constant current $j(x,t)\not\equiv 0$, as indicated by the arrows at the bottom). Such a current requires a source and sink at the boundary, in violation of our conditions in Theorem 4.6; see also Remark 4.7

stronger than the original potential, i.e.,

$$d_V(x,t)=c(t)\int_0^x e^{\tan^2(y)}\,dy;$$

see Fig. 1 (b).

The preceding example illustrates a general principle. If the density vanishes at the boundary, then the nontrivial solution d_V must diverge. By construction, this results in a constant current that preserves the density profile $\rho=\rho'$. Intuitively speaking, the trick is that the new external force is inversely proportional to ρ, i.e., it pulls stronger where the density is lower. According to Remark 4.7, the new current requires appropriate source and sink terms at the boundary. Thus, in fact, there is no loophole for the original N-body Smoluchowski equation.

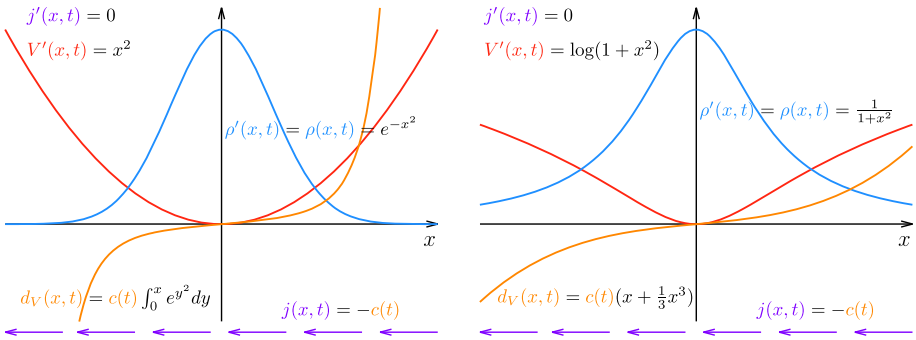
Similar physically intuitive examples are available for an unbounded domain, i.e., $\Omega=\mathbb{R}$. Note that whether Ω is (un-)bounded is not essential to the question of uniqueness, as discussed above at the end of Sec. 4.

Example 5.2 *(Unbounded systems with localized density profiles)* Consider an (effectively) one-dimensional ideal gas that is trapped in a harmonic potential, i.e., subject to an external potential $V'(x,t)=x^2$ so that $\rho'(x,t)=e^{-x^2}$; see Fig. 2 (a). The system is again in equilibrium, and hence $j'(x,t)\equiv 0$.

An additional external potential according to (5.2),

$$d_V(x,t)=c(t)\int_0^x e^{y^2}\,dy, \tag{5.3}$$

quickly diverges for $x\to\pm\infty$. In (5.3), the potential d_V has to diverge exponentially fast to obtain the same density with different potentials. A slower divergence of d_V suffices if the density profile has a heavy tail, e.g., $\rho'(x,t)=1/(1+x^2)$ for $V'(x,t)=\log(1+x^2)$, in which case $d_V(x,t)=O(x^3)$ for $x\to\pm\infty$, see Fig. 2 (b).



(a) Exponentially diverging potentials (b) Polynomially diverging potentials

Fig. 2 Schematics of non-unique potentials for *unbounded* domains, analogous to Fig. 1 but now with potentials (a) $V'(x,t) = x^2$ and (b) $V'(x,t) = \log(1+x^2)$

Even though a constant ρ' defined on $\Omega = \mathbb{R}^d$ is, strictly speaking, excluded from our setting (which assumes $N < \infty$), the construction principle according to (5.1) and (5.2) still works. It provides an obvious loophole to uniqueness via a constant force.

Example 5.3 *(Homogeneous bulk)* Consider a homogeneous ideal gas in bulk with $\rho'(x,t) \equiv 1$ and, analogous to the first case in Example 5.1, add an (effectively) one-dimensional potential $d_V(x,t) = c(t)x$. Thus, we obtain a constant force that results in a constant current proportional to $c(t)$ through the homogeneous system. This argumentation could also hold for interacting systems. However, a no-flux boundary condition again excludes such a loophole to uniqueness.

Our procedure based on (5.1) and (5.2) can also be applied to systems with periodic boundary conditions (representing a flat torus). In this case, the flux is typically not fixed at the periodic boundary, but can change over time due to the intrinsic dynamics.

Example 5.4 *(Periodic systems)* Consider again an (effectively) one-dimensional ideal gas. If the system is defined on a flat torus, the additional potential $d_V(x,t)$ is periodic and, hence, discontinuous (at the boundary). This discontinuity is at odds with our setting of a Smoluchowski equation with differentiable potentials. In contrast, the corresponding force will be continuous. Such an example has already been numerically studied in simulations of interacting particles, going beyond the adiabatic approximation, within the framework of PFT and custom flow [11, 14]. In our case, the new potential violates our conditions for uniqueness, as the resulting spatially constant change of the current also affects its value at the periodic boundary.

While the density does not uniquely specify the potential in any of the aforementioned examples, the one-body current does so, as the underlying principle of Corollary 4.8 still applies in each case (as knowing the initial one-body density in our examples for an ideal gas implies knowing the full initial N-body probability density). In this strict mathematical sense, it is thus enough to know the current (together with the initial density), even if it takes a simple form like $j(x,t) = -D\beta c(t)$.

For general interaction potentials, ρ_2 will no longer be a functional of ρ, and our simple procedure from (5.1) and (5.2) breaks down. Instead, the entire hierarchy of n-body correlations from Theorem 3.1 has to be considered, in line with our proof of uniqueness through Lemma 4.4. This necessity to properly account for superadiabatic forces [22] can be easily

overlooked in the proof because it does not impose additional conditions on the uniqueness theorem itself.

A practical way to resolve this problem of loopholes for systems with superadiabatic forces is the so-called *custom flow* procedure [11]. It employs many-particle Brownian dynamics simulations to numerically determine for a given density the potential (or, more generally, even non-conservative forces) required to obtain a predefined flow profile; see also [14].

6 Physical implications

We have shown that the uniqueness of the potential can be inferred (i) from the density alone, according to Theorem 4.6, see also Remark 4.7, or (ii) from the current alone, according to Corollary 4.8. In both cases $P_N^{(0)}$ must be known since this initial condition is obviously required for a well-defined behavior of an interacting many-particle system. What specifies appropriate boundary conditions at the N-body level in general is related to the divergence theorem and the continuity equation (2.5). Let P_N and P_N' be different N-body probability densities that evolve from the same initial condition but differ in their time derivatives. According to the divergence theorem and (2.5), an integral of $\partial_t(P_N - P_N')$ over Ω^N is equivalent to an integral of $n(x^N)(J_N - J_N')$ over $\partial\Omega^N$. Therefore, different probability densities correspond to different normal fluxes, which means that a well-posed initial-value-boundary problem requires an appropriate condition on the normal flux at the boundary. Surprisingly, even in the presence of (known) non-conservative forces, the one-body density suffices to formally recover the N-body dynamics under physically meaningful boundary conditions, such as no flux, or, more generally, a fixed normal one-body flux.

Closely related to the necessity of full N-body initial conditions is our notion of a *non-instantaneous* density–potential mapping in the following sense. Uniqueness here means that $V(x,t)$ for a certain point $x \in \Omega$ and at a certain time t is determined only if the values $\rho(y,s)$ (or $j(y,s)$) are given for all $y \in \Omega$ and $0 \le s \le t$. The mapping is thus not instantaneous (in the physical sense that only the quantities at time t were known and not their time derivatives). By requiring that our systems are analytically accessible, we imply that ρ is specified throughout; in that sense, the potential at all times is determined by the one-body density at all times.

Importantly, our results imply the existence of a theory solely based on the one-body density (or current) which contains all higher-order information on the dynamical system. While our method of proof does not provide a constructive recipe of an explicit theory, we can use the insight gained to answer the following three essential questions on the adiabatic assumption underlying standard DDFT and the general nature of an appropriate theoretical framework.

Do our uniqueness theorems hold under the adiabatic approximation? First note that establishing a uniqueness theorem or assessing the performance of a density-based approximation are two separate problems. In particular, the proof of uniqueness requires a well specified model (and then no further approximations). Hence, we can distinguish two different points of view: (i) Adiabatic dynamics are utterly flawed for interacting systems and the question is uninteresting since the density obtained from solving the approximate PDE does not reflect the actual physical system. Our rigorous statements are made for the exact dynamics. Hence the question of applicability to an imprecise approximation is ill posed. (ii) If we take the approximate adiabatic dynamics as the actual mathematical model to be studied, then our theorems hold accordingly and their proofs shorten considerably. By definition, the adiabatic

approximation assumes that the information contained in ρ determines P_N at all times. Thus, the proof of Lemma 4.4 considerably simplifies to the argumentation required for an ideal gas because the induction step for showing (4.3) only needs to be laid out for $n = 1$ when we use the functional chain rule. Likewise, simple analytic counterexamples can be derived through (5.1) under the adiabatic assumption or for an ideal gas, see Sec. 5. In contrast, our hierarchical proof of Lemma 4.4 is essential for the general problem and (5.2) cannot be used to construct general loopholes because the actual dynamics of interacting particles is always superadiabatic and the assumptions used to derive (5.1) do not apply.

In how far are the known drawbacks of adiabatic DDFT reflected in our proof? The adiabatic approximation only uses the instantaneous density, which neither maps to the instantaneous potential nor provides accurate dynamics in general. To see this, we need to consider explicitly what happens when solving Eq. (3.6). Our proof, with the help of Lemma 4.4, explicitly takes into account the full hierarchy of ρ_n, which ensures a proper transfer of the full information contained in $P_N(\cdot, t)$ to $P_N(\cdot, t')$ at any later time $t' > t$, i.e., it reflects the exact dynamics. In contrast, the adiabatic approximation amounts to express the right-hand side of Eq. (3.6) in terms of a functional of the instantaneous one-body density ρ, such that it does not contain the full information on its history. Formally, this approximation only allows to propagate in time the information contained in ρ but not P_N, which is equivalent to only knowing the initial condition $\rho(\cdot, 0)$ instead of $P_N^{(0)}$. Strictly speaking, all $P_N^{(0)}$ which are not given by a unique expression $P_N^{(0)}[\rho(\cdot, 0)]$ provided by the presumed underlying equilibrium mapping (to an effective adiabatic potential [10]) cannot be represented at all. With this loss of generality, the density is not sufficient to properly describe the N-body dynamics in the framework of adiabatic DDFT.

How can our results contribute to going beyond adiabatic DDFT? While our Theorems assume the exact dynamics of the N-body system, any practical theory must operate on a reduced set of variables, which usually requires a closure to remove the implicit (hierarchical) dependence on other variables. Since our proofs are non-constructive, they do not directly translate into an improved theory. Nevertheless, both our theorems and our proof strategy help to clarify certain requirements. Based on our results, an appropriate DDFT (i.e., a theory, solely built on the one-body density, that is fully closed in both space and time) should, in general, use the full history of ρ to model the propagation in time. This indispensably requires a (generally unknown) memory kernel. Generalized versions of DDFT utilizing such a flow kernel have already been constructed for fluids under shear [7, 48, 49]. Likewise, the framework of PFT formally introduces memory through the excess dissipation functional as an extension of DDFT [50]. Explicit PFT approximations are provided in the form of a functional of both the density and the current (or rather the velocity field), which is nonlocal in space and time [12, 54] and a combination of PFT and neural networks can be used to characterize memory effects [68]. In our induction argument for proofing Lemma 4.4, the information on the N-body initial condition $P_N^{(0)}$ is propagated in time implicitly through the n-body densities ρ_n and no explicit account of the system history is needed (for analytically accessible systems). Specifically, the knowledge of $\rho_n(\cdot, 0)$ ensures a correct description of $\partial_t^{n-1}\rho(\cdot, t)$ at $t = 0$ and can thus account for differences in the external potentials up to order $d_V^{(n-2)}$ in (4.4). Our proof thus illustrates that the full hierarchy of reduced Smoluchowski equations feeds back on the time evolution of the one-body density in a unique way. This argument suggests a minimal (or systematic) extension of adiabatic DDFT to include memory on a time-local level by explicitly considering the dynamics of ρ_2 (or further higher-order densities). A practical recipe to do so is provided by superadiabatic-DDFT [55–57], recently introduced by Tschopp and Brader, who arrive by a different line of argument at the same

conclusion. In [57], they argue that *"within superadiabatic-DDFT the flow history of the system is encoded in the current value of the nonequilibrium two-body density, without the need for a memory kernel"*. Following our argumentation in response to the previous question, such a theory would formally propagate in time the information contained in the initial $\rho_2(\cdot, 0)$ and thus represent these superadiabatic correlations, as $P_N^{(0)}[\rho_2(\cdot, 0)]$ is no longer enslaved by $\rho(\cdot, 0)$, and thus provide a very good description for systems interacting with pair potentials, which evolve according to Eq. (3.6). Indeed, this superadiabatic-DDFT has been shown to yield significant improvement over standard adiabatic DDFT [55–57].

To conclude, the drawbacks of adiabatic DDFT are not related to violating uniqueness but can be understood and overcome when considering the details of the proof related to superadiabatic correlations, see Lemma 4.4. Hence, while the density alone is often sufficient to uniquely determine the generating forces, it is not a suitable basis (with currently available methods) to construct a workable theory for obtaining reliable predictions. In turn, the current approaches beyond DDFT can stimulate further interesting mathematical questions. For example, one could investigate whether our inclusion of nonconservative forces provides additional insight into the PFT-based structure-flow splitting of [13]. An alternative setting of our problem, along the lines of superadiabatic-DDFT, is to find alternative conditions for uniqueness using the two-body density instead of boundary currents.

7 Outlook

In this paper, we derive explicit conditions for a well-defined density–potential mapping under the assumptions of analytical potentials and smooth densities. Given a well-posed initial value boundary problem for the N-particle system, the external potential is determined by the one-body density under a fixed boundary condition for the normal flux or, alternatively, from the one-body current alone. We crucially supplement the argumentation of Chan and Finken [8] by Lemma 4.4 and highlight the central role of initial- and boundary conditions. Our rigorous proof thus provides the foundation of dynamical density functional theory (DDFT) and clarifies the relation to its recent extensions.

A useful extension will be to include non-integrable density profiles, which should require a mere technical adaption of the setting and the proof. Another open problem is to drop the condition of analytic potentials. As mentioned above, a fixed-point approach as in [43, 45] could avoid this restriction. Such a generalization could also include time-dependent diverging potentials (i.e., beyond static hard walls that can already be encoded in our setting via no-flux boundary conditions). Relatedly, our chosen restriction to a simply-connected domain and finite interaction forces ensures that the particles can instantaneously reach each point in the available space. Hence the density becomes positive in the whole domain. It will be interesting to loosen these assumptions in future work (similar to Example 9.1 in [9]) especially in view of scenarios involving strong localization or caging of individual hard particles, where the (canonical) density remains constantly zero in certain regions of space; such scenarios are of particular interest in the context of (D)DFT [35, 52, 61].

So far, we have also assumed the existence and uniqueness of a well-behaved solution $P_N(x^N, t)$. A proof of existence could be constructed similarly to our proof of uniqueness following ideas of van Leeuwen [58]. The existence of a suitable potential will then require the solution to an inhomogeneous PDE analogous to (4.9). The resulting conditions on the density and interaction potential should include, as a special case, the known conditions for systems in equilibrium [9]. Similar questions have recently been discussed in quantum mechanics

[64]. The assumed uniqueness of the solution implies that the density–potential mapping is injective, which is not essential to our proof but physically reasonable for given initial conditions. In contrast, for (grand-canonical) equilibrium DFT without initial conditions, the mapping is not injective, e.g., at phase coexistence two different densities $\rho \neq \rho'$ can be realized by the same potential V.

Our method of proof has been chosen to provide physical intuitive conclusions and may serve as the basis for investigating a broad range of related problems. In particular, whenever we can derive a condition of the form (4.9) the rest of the proof follows analogously. Therefore, in future work, the rigorous search for unique density–potential mappings should also be extended to more general interactions and external influences, such as the following examples. (i) Our strategy of proof can be straightforwardly applied to particles with inertia, as originally considered by Chan and Finken [8]. (ii) Triplet or higher-order potentials [16, 33, 47], as well as, time-dependent interactions [4, 63, 67], result in additional and more complex contributions to the average interaction force but should not change the structure of proof. (iii) Similarly, our approach should be generalizable to marked particles, where the marks may represent different particle shapes, sizes, and orientations [42, 60, 62]. (iv) A position-dependent mobility tensor should lead to a PDE analogous to (4.9), while $\rho(x,t)$ will be multiplied with this tensor. This PDE will then be elliptic if and only if the tensor is positive definite and symmetric, which is the case in models for hydrodynamic interactions [6, 39, 41]; see also [23, 24]. Asymmetric tensors that give rise to odd diffusivity [29] are, however, of growing interest in physics, as they, for example, can be used to model the effect of Lorentz forces [1, 2]. The corresponding non-elliptic PDE might result in more involved conditions for uniqueness of density–potential mappings in odd-DDFT [3]. (v) We further expect that our uniqueness theorems could also hold in the additional presence of a (known) mechanism of self-propulsion that constantly drives the system out of equilibrium [32, 39, 60]. This activity generates an additional non-conservative force field in (2.4) that also depends on the orientational dynamics and is thus not known *a priori*. Thus, this interplay needs to be separately accounted for in the proof of Lemma 4.4 to ensure that superadiabatic properties of the system are described appropriately, as in the case of known non-conservative forces. It will be interesting to check whether the uniqueness of the density–potential mapping would follow under (slightly) modified conditions for these intrinsically non-equilibrium systems.

Acknowledgements The authors are very grateful to Axel Grünrock, Daniel de las Heras, and the anonymous referees for valuable pointers, and the authors also thank Joseph Brader, Tobias Kuna, Tanniemola B. Liverpool, and Salomée Tschopp for stimulating discussions.

Funding Open Access funding enabled and organized by Projekt DEAL. This work was supported by the Initiative and Networking Fund of the Helmholtz Association under the call Helmholtz Young Investigator Groups (VH-NG-19-34, DataMat) and by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation), through the SPP 2265, under Grant Nos. KL 3391/2-2, WI 5527/1-2, and LO 418/25-2.

Data Availability No datasets were generated or analyzed for this work.

Declarations

Competing interests All authors declare that they have no conflicts of interest.

References

1. Abdoli, I., Vuijk, H.D., Sommer, J.U., Brader, J.M., Sharma, A.: Nondiffusive Fluxes in a Brownian System with Lorentz Force. Phys. Rev. E **101**, 012120 (2020)
2. Abdoli, I., Vuijk, H.D., Wittmann, R., Sommer, J.U., Brader, J.M., Sharma, A.: Stationary State in Brownian Systems with Lorentz Force. Phys. Rev. Res. **2**, 023381 (2020)
3. Abdoli, I., Wittmann, R., Löwen, H.: Dynamical density functional theory for dense odd-diffusive fluids. J. Phys. Chem. B **130**, 4672–4682 (2026)
4. Al-Saedi, H.M., Archer, A.J., Ward, J.: Dynamical Density-Functional-Theory-Based Modeling of Tissue Dynamics: Application to Tumor Growth. Phys. Rev. E **98**, 022407 (2018)
5. Archer, A.J., Evans, R.: Dynamical Density Functional Theory and Its Application to Spinodal Decomposition. J. Chem. Phys. **121**, 4246–4254 (2004)
6. Bleibel, J., Domínguez, A., Oettel, M.: A Dynamic DFT Approach to Generalized Diffusion Equations in a System with Long-Ranged and Hydrodynamic Interactions. J. Phys.: Condens. Matter **28**, 244021 (2016)
7. Brader, J.M., Krüger, M.: Density Profiles of a Colloidal Liquid at a Wall under Shear Flow. Mol. Phys. **109**, 1029–1041 (2011)
8. Chan, G.K.-L., Finken, R.: Time-Dependent Density Functional Theory of Classical Fluids. Phys. Rev. Lett. **94**, 183001 (2005)
9. Chayes, J.T., Chayes, L., Lieb, E.H.: The Inverse Problem in Classical Statistical Mechanics. Commun. Math. Phys. **93**, 57–121 (1984)
10. de Las Heras, D., Brader, J.M., Fortini, A., Schmidt, M.: Particle conservation in dynamical density functional theory. J. Phys.: Condens. Matter **28**(24), 244024 (2016)
11. de Las Heras, D., Renner, J., Schmidt, M.: Custom Flow in Overdamped Brownian Dynamics. Phys. Rev. E **99**, 023306 (2019)
12. de las Heras, D., Schmidt, M.: Velocity Gradient Power Functional for Brownian Dynamics. Phys. Rev. Lett. **120**, 028001 (2018)
13. de las Heras, D., Schmidt, M.: Flow and Structure in Nonequilibrium Brownian Many-Body Systems. Phys. Rev. Lett. **125**, 018001 (2020)
14. de Las Heras, D., Zimmermann, T., Sammüller, F., Hermann, S., Schmidt, M.: Perspective: How to Overcome Dynamical Density Functional Theory. J. Phys.: Condens. Matter, 35:271501, (2023)
15. Dhara, A.K., Ghosh, S.K.: Density-Functional Theory for Time-Dependent Systems. Phys. Rev. A **35**, 442–444 (1987)
16. Dobnikar, J., Brunner, M., von Grünberg, H.-H., Bechinger, C.: Three-Body Interactions in Colloidal Systems. Phys. Rev. E: Stat., Nonlin, Soft Matter Phys. **69**, 031402 (2004)
17. Dwandaru, W.S.B., Schmidt, M.: Variational Principle of Classical Density Functional Theory via Levy's Constrained Search Method. Phys. Rev. E **83**, 061133 (2011)
18. Español, P., Löwen, H.: Derivation of Dynamical Density Functional Theory Using the Projection Operator Technique. J. Chem. Phys. **131**, 244101 (2009)
19. Evans, L.C.: Partial Differential Equations. American Mathematical Society, Providence, second edition edition (2010)
20. Evans, R.: The Nature of the Liquid-Vapour Interface and Other Topics in the Statistical Mechanics of Non-Uniform. Classical Fluids. Adv. Phys. **28**, 143–200 (1979)
21. Evans, R.: Density Functionals in the Theory of Non-Uniform Fluids. In D Henderson, editor, Fundamentals of Inhomogeneous Fluids, pages 85–175. Marcel Dekker, (1992)
22. Fortini, A., Heras, D.D.L., Brader, J.M., Schmidt, M.: Superadiabatic forces in Brownian many-body dynamics. Phys. Rev. Lett. **113**(16), 167801 (2014)
23. Goddard, B.D., Mills-Williams, R.D., Ottobre, M., Pavliotis, G.: Well-Posedness and Equilibrium Behaviour of Overdamped Dynamic Density Functional Theory (2021)
24. Goddard, B.D., Nold, A., Savva, N., Pavliotis, G.A., Kalliadasis, S.: General Dynamical Density Functional Theory for Classical Fluids. Phys. Rev. Lett. **109**, 120603 (2012)

25. Gross, E.K.U., Kohn, W.: Time-Dependent Density-Functional Theory. In Per-Olov Löwdin, editor, Advances in Quantum Chemistry, volume 21 of Density Functional Theory of Many-Fermion Systems, pages 255–291. Academic Press (1990)
26. Gross, E.K.U., Maitra, N.T.: Introduction to TDDFT. In Miguel A.L. Marques, Neepa T. Maitra, Fernando M.S. Nogueira, E.K.U. Gross, and Angel Rubio, editors, Fundamentals of Time-Dependent Density Functional Theory, Lecture Notes in Physics, pages 53–99. Springer, Berlin, Heidelberg, (2012)
27. Hansen, J.-P., McDonald, I.R.: Theory of Simple Liquids: With Applications to Soft Matter, 4th edn. Academic Press, Amsterdam (2013)
28. Hohenberg, P., Kohn, W.: Inhomogeneous Electron Gas. Phys. Rev. **136**, B864–B871 (1964)
29. Kalz, E., Vuijk, H.D., Abdoli, I., Sommer, J.-U., Löwen, H., Sharma, A.: Collisions Enhance Self-Diffusion in Odd-Diffusive Systems. Phys. Rev. Lett. **129**, 090601 (2022)
30. Kohn, W., Sham, L.J.: Self-Consistent Equations Including Exchange and Correlation Effects. Phys. Rev. **140**, A1133–A1138 (1965)
31. Levy, M.: Universal Variational Functionals of Electron Densities, First-Order Density Matrices, and Natural Spin-Orbitals and Solution of the v-Representability Problem. Proc. Natl. Acad. Sci. **76**, 6062–6065 (1979)
32. Liverpool, T.B.: Steady-State Distributions and Nonsteady Dynamics in Nonequilibrium Systems. Phys. Rev. E **101**, 042107 (2020)
33. Löwen, H., Allahyarov, E.: The Role of Effective Triplet Interactions in Charged Colloidal Suspensions. J. Phys.: Condens. Matter **10**, 4147 (1998)
34. Löwen, H.: Dynamical Density Functional Theory for Brownian Dynamics of Colloidal Particles. In: Jianzhong, W. (ed.) Variational Methods in Molecular Modeling. Molecular Modeling and Simulation, pp. 255–284. Springer, Singapore (2017)
35. Lutsko, J.F.: Classical density functional theory in the canonical ensemble. Phys. Rev. E **105**, 034120 (2022)
36. Lutsko, J.F., Oettel, M.: Reconsidering power functional theory. J. Chem. Phys. **155**(9), 094901 (2021)
37. Maitra, N.T., Burke, K.: Demonstration of Initial-State Dependence in Time-Dependent Density-Functional Theory. Phys. Rev. A **63**, 042501 (2001)
38. Marconi, U.M.B., Tarazona, P.: Dynamic Density Functional Theory of Fluids. J. Chem. Phys. **110**, 8032–8044 (1999)
39. Menzel, A.M., Saha, A., Hoell, C., Löwen, H.: Dynamical Density Functional Theory for Microswimmers. J. Chem. Phys. **144**, 024115 (2016)
40. David Mermin, N.: Thermal Properties of the Inhomogeneous Electron Gas. Phys. Rev. **137**, A1441–A1443 (1965)
41. Rex, M., Löwen, H.: Dynamical Density Functional Theory with Hydrodynamic Interactions and Colloids in Unstable Traps. Phys. Rev. Lett. **101**, 148302 (2008)
42. Rex, M., Wensink, H.H., Löwen, H.: Dynamical Density Functional Theory for Anisotropic Colloidal Particles. Phys. Rev. E **76**, 021403 (2007)
43. Ruggenthaler, M., Giesbertz, K.J.H., Penz, M., van Leeuwen, R.: Density-Potential Mappings in Quantum Dynamics. Phys. Rev. A **85**, 052504 (2012)
44. Ruggenthaler, M., van Leeuwen, R.: Global Fixed-Point Proof of Time-Dependent Density-Functional Theory. EPL **95**, 13001 (2011)
45. Ruggenthaler, M., Penz, M., van Leeuwen, R.: Existence, Uniqueness, and Construction of the Density-Potential Mapping in Time-Dependent Density-Functional Theory. J. Phys.: Condens. Matter **27**, 203202 (2015)
46. Runge, E., Gross, E.K.U.: Density-Functional Theory for Time-Dependent Systems. Phys. Rev. Lett. **52**, 997–1000 (1984)
47. Sammüller, F., de Las Heras, D., Schmidt, M.: Inhomogeneous Steady Shear Dynamics of a Three-Body Colloidal Gel Former. J. Chem. Phys. **158**, 054908 (2023)
48. Scacchi, A., Archer, A.J., Brader, J.M.: Dynamical density functional theory analysis of the laning instability in sheared soft matter. Phys. Rev. E **96**, 062616 (2017)
49. Scacchi, A., Krüger, M., Brader, J.M.: Driven Colloidal Fluids: Construction of Dynamical Density Functional Theories from Exactly Solvable Limits. J. Phys.: Condens. Matter **28**, 244023 (2016)
50. Schmidt, M.: Power Functional Theory for Many-Body Dynamics. Rev. Mod. Phys. **94**, 015007 (2022)
51. Schmidt, M., Brader, J.M.: Power Functional Theory for Brownian Dynamics. J. Chem. Phys. **138**, 214101 (2013)
52. Tarazona, P., Rosenfeld, Y.: From zero-dimension cavities to free-energy functionals for hard disks and hard spheres. Phys. Rev. E **55**, R4873–R4876 (1997)
53. te Vrugt, M., Löwen, H., Wittkowski, R.: Classical Dynamical Density Functional Theory: From Fundamentals to Applications. Adv. Phys. **69**, 121–247 (2020)

54. Treffenstädt, L.L., Schmidt, M.: Memory-induced motion reversal in Brownian liquids. Soft Matter **16**, 1518–1526 (2020)
55. Tschopp, S.M., Brader, J.M.: First-Principles Superadiabatic Theory for the Dynamics of Inhomogeneous Fluids. J. Chem. Phys. **157**, 234108 (2022)
56. Tschopp, S.M., Brader, J.M.: Superadiabatic dynamical density functional theory for colloidal suspensions under homogeneous steady-shear. J. Chem. Phys. **160**(21), 214124 (2024)
57. Tschopp, S.M., Vuijk, H.D., Brader, J.M.: Superadiabatic dynamical density functional study of Brownian hard-spheres in time-dependent external potentials. J. Chem. Phys. **158**(23), 234904 (2023)
58. van Leeuwen, R.: Mapping from Densities to Potentials in Time-Dependent Density-Functional Theory. Phys. Rev. Lett. **82**, 3863–3866 (1999)
59. Walter, W.: Gewöhnliche Differentialgleichungen, 7th edn. Springer-Lehrbuch. Springer, Berlin Heidelberg, Berlin, Heidelberg (2000)
60. Wittkowski, R., Löwen, H.: Dynamical Density Functional Theory for Colloidal Particles with Arbitrary Shape. Mol. Phys. **109**, 2935–2943 (2011)
61. Wittmann, R., Löwen, H., Brader, J.M.: Order-preserving dynamics in one dimension – single-file diffusion and caging from the perspective of dynamical density functional theory. Mol. Phys. **119**(15–16), e1867250 (2021)
62. Wittmann, R., Marechal, M., Mecke, K.: Fundamental Measure Theory for Non-Spherical Hard Particles: Predicting Liquid Crystal Properties from the Particle Shape. J. Phys.: Condens. Matter **28**, 244003 (2016)
63. Wittmann, R., Nguyen, G.H.P., Löwen, H., Schwarzendahl, F.J., Sengupta, A.: Collective mechano-response dynamically tunes cell-size distributions in growing bacterial colonies. Communications Physics **6**(1), 331 (2023)
64. Wrighton, J., Albavera-Mata, A., Rodríguez, H.F., Tan, T.S., Cancio, A.C., Dufty, J.W., Trickey, S.B.: Some Problems in Density Functional Theory. Lett. Math. Phys. **113**, 41 (2023)
65. Jianzhong, W.: Density Functional Theory for Chemical Engineering: From Capillarity to Soft Materials. AIChE J. **52**, 1169–1193 (2006)
66. Bu-Xing, X., Rajagopal, A.K.: Current-Density-Functional Theory for Time-Dependent Systems. Phys. Rev. A **31**, 2682–2684 (1985)
67. Zhang, Y., Fodor, É.: Pulsating Active Matter. Phys. Rev. Lett. **131**, 238302 (2023)
68. Zimmermann, T., Sammüller, F., Hermann, S., Schmidt, M., de las Heras, D.: Neural force functional for non-equilibrium many-body colloidal systems. Machine Learning: Science and Technology **5**, 035062 (2024)