Derivation of Hydrodynamics from the Hamiltonian Description of Particle Systems

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Hamiltonian particle systems may exhibit nonlinear hydrodynamic phenomena as the time evolution of the density fields of energy, momentum, and mass. In this Letter, an exact equation describing the time evolution is derived assuming the local Gibbs distribution at initial time. The key concept in the derivation is an identity similar to the fluctuation theorems. The Navier-Stokes equation is obtained as a result of simple perturbation expansions in a small parameter that represents the scale separation.

Introduction.—Let us consider a large number of interacting particles that obey a classical Hamiltonian equation as an isolated system. The initial condition is assumed to provide spatial variation in the macroscopic density fields. Examples include turbulent configurations of the momentum density field. Through time evolution of the particles, the density fields exhibit interesting space-time structures, and the system eventually relaxes to an equilibrium state. This process is believed to be described universally by hydrodynamic equations of the density fields for liquids and gases [1]. As a stimulating numerical experiment of a Hamiltonian particle system, quite recently, the Kolmogorov spectrum has been observed in a transient state [2]. However, it remains unclear whether the hydrodynamic description of such violent time evolution can be understood on the basis of Hamiltonian particle systems.

The problem of deriving the hydrodynamic equations has been studied over the last century by various approaches such as the analysis of the Boltzmann equation [3], the calculation on the basis of local equilibrium distributions [4,5], and the derivation from hypothetical nonequilibrium ensembles [6–9]. However, nonlinear hydrodynamic phenomena of liquids are out of the scope of these classical works, because the Boltzmann equation applies to only dilute gases, the local equilibrium distributions cannot describe dissipation effects, and the hypothetical ensembles are not justified beyond the linear response regime from a global equilibrium state [10].

Nevertheless, a physical intuition of the hydrodynamic description in particle systems is simple, and it has been known as follows. When the length scale of the spatial variation of the density fields is much larger than the particle scales, the particle distribution may be characterized by a local equilibrium distribution with local thermodynamic variables. If such local equilibrium propagates in time, the solution of the Liouville equation may be close to the local equilibrium distribution [11]. For example, turbulence is a strongly nonlinear phenomenon described by a deterministic equation for the density fields, whereas the particle distribution in the turbulent state is still near local equilibrium. Thus, the nonlinear hydrodynamic equations may be derived by developing a perturbation theory with a small parameter representing the scale separation.

As one attempt that follows the physical intuition, a perturbation theory leading to the incompressible Navier-Stokes equation was presented with the assumption of the propagation of local equilibrium [12]. Since this study attempts to construct solutions of the Liouville equation without specifying the initial condition, it seems difficult to investigate the validity of the assumption. Rather, in order to obtain a definite result, it may be necessary that a special class of initial conditions is focused on.

Such a situation can be seen in the statistical mechanical derivation of the second law of thermodynamics. If an initial distribution satisfies some conditions, the second law of thermodynamics can be derived [13,14]. In particular, if the canonical distribution is assumed initially, the proof of the second law becomes quite simple by utilizing the Jarzynski equality [15]. These results obtained for special but familiar initial distributions provide key insights into the second law of thermodynamics.

In this Letter, as an extension of these studies, the nonlinear hydrodynamic equations are derived in a quite compact manner for an isolated Hamiltonian system (i.e., a purely mechanical system) with an initial condition given by the local Gibbs distribution. The crucial step in the derivation is to find a universal relation similar to the fluctuation theorems [16–23], by which an exact expression for the time evolution of the density fields is obtained. Furthermore, a straightforward perturbation leads to the Navier-Stokes equation after introducing a scale separation parameter that is assumed to be small.

Framework.—Let \( r_i \) and \( p_i \) (\( 1 \leq i \leq N \)) be the position and the momentum of \( i \)th particle with the mass \( m \). The short-range interaction potential between \( i \)th and \( j \)th particles is expressed as \( V(|r_{ij}|) \), where \( r_{ij} = r_i - r_j \). The phase space coordinate of the system is a collection of \( (r_i, p_i) \), which is denoted by \( \Gamma \). The particles are confined in a cube \( \Omega \) with length \( L \). For simplicity, periodic boundary conditions are assumed. The time evolution of
the system is described by the Hamiltonian equation. The solution of the equation for an initial state $\Gamma$ is simply denoted as $\Gamma_t$, for any real number $t$. That is, $\Gamma_{t+s} = (\Gamma_t)_s$ for any $t$ and $s$.

There are five conserved quantities: the total mass, the total momentum, and the total energy. It is assumed that there are no other independent conserved quantities and that there are no soft modes arising from symmetry breaking. Corresponding to the conserved quantities, the following microscopic density fields are defined:

$$\rho(r; \Gamma) = \sum_i m \delta(r - r_i), \quad \pi(r; \Gamma) = \sum_i m \delta(r - r_i),$$

where $m$ is a constant. The density fields $\rho(r; \Gamma)$ satisfy

$$\partial_t \rho(r; \Gamma) + \nabla \cdot \mathbf{J} = 0,$$

where the microscopic currents $\mathbf{J} = \mathbf{f} \cdot \mathbf{r}$. The expectation value of the functional $\langle \mathbf{J} \rangle$ is derived as

$$\langle \mathbf{J} \rangle = \left. \frac{\partial}{\partial \lambda} \langle \mathbf{J} \rangle \right|_{\lambda=0}.$$

The main assumption in this Letter is that initial states $\Gamma$ at $t = 0$ are chosen according to the local Gibbs (LG) distribution

$$P_{LG}(\Gamma; \lambda) = e^{-\lambda_t \cdot \hat{C}_t},$$

where the position dependent parameter $\lambda_t(r)$ characterizes the inhomogeneous distribution of the density fields. The normalization condition of the probability determines the functional $\Psi(\lambda)$ for the Hamiltonian. Let us call $\lambda$ and $\Psi(\lambda)$ the conjugate field and the Mathieu functional, respectively, although these names may not be accurate except for the limited case where $\lambda$ is spatially homogeneous. $\Psi(\lambda)$ is assumed to be a convex functional of $\lambda$ as a natural extension from the spatially homogeneous case. One example of initial states may be a snapshot of the molecular configuration in a turbulent state.

The local Gibbs distribution describes an inhomogeneous equilibrium state in the moving frame with the local velocity $\mathbf{u} = -\lambda_t/\lambda_t$. Indeed, let $\Gamma_t$ be the phase space coordinate obtained from $\Gamma$ by transforming $p_i$ in $\Gamma$ to $p_i - m \mathbf{u}(r_i)$. In general, a dynamical variable in the moving frame is defined as $\hat{A}^t(\Gamma) = \hat{A}(\Gamma^t)$ for any dynamical variable $\hat{A}$. Then, $\lambda_t^a \cdot \hat{C}_t^a$ is written as

$$\lambda_t^a \cdot \hat{C}_t^a = \lambda_t^0 \cdot \hat{h} + \left( \lambda_t^a - \frac{1}{2} \frac{|\lambda|^2}{\lambda_t^0} \right) \cdot \hat{\rho},$$

which implies that $\lambda_t^0(r)$ and $\lambda_t^a(r)$ are related to inhomogeneous inverse temperature and a one-body potential function. It should be noted that $\hat{h}$ is interpreted as the internal energy density field.

The expectation value of the density field $\hat{C}(r; \Gamma_t)$ at time $t$ with respect to the initial distribution is given by $\int d\Gamma P_{LG}(\Gamma; \lambda) \hat{C}(r; \Gamma_t)$. It is further written as $\int d\Gamma P_t(\Gamma) \hat{C}(r; \Gamma_t)$, where

$$P_t(\Gamma) = e^{-\lambda_t^a \cdot \hat{C}_t^a(\Gamma)}.$$
may be an extension of the entropy to that for nonequilibrium states characterized by the density field, but no thermodynamic interpretation is given yet. The important thing here is that the quantity $S(C)$ is determined from the Hamiltonian under consideration. Then, for a given density field $C_t(r)$, the conjugate field $λ_t(r)$ is calculated by

$$λ_t(r) = \frac{δS(C)}{δC(r)}|_{C=C_t},$$

which is the second identity. At this stage, let us remember that $C_t$ and $λ_t$ are determined uniquely from the time evolution and the initial distribution.

The third identity is a variant of the so-called fluctuation theorems. In order to obtain it, (5) is formally rewritten as

$$P_t(Γ) = e^{-\tilde{J}^t(Γ) - Ψ(λ_t) + \tilde{Σ}_t(Γ)},$$

where

$$\tilde{Σ}_t(Γ) = \int_0^t ds \partial_1[λ^s \cdot \tilde{C}^t(Γ_{s-r}) + Ψ(λ_s)].$$

By comparing (12) with (5), it is found for any dynamical variable $\tilde{A}(Γ)$ that

$$\langle \tilde{A} \rangle_t = \langle \tilde{A} e^{\tilde{Σ}_t} \rangle_L^G,$$

which is the third identity. Various nontrivial relations of statistical quantities can be derived from this identity. As an example, (14) with $\tilde{A} = e^{-\tilde{Σ}}$ becomes $\langle e^{-\tilde{Σ}} \rangle_t = 1$, which corresponds to an integral fluctuation theorem. With a trivial inequality $e^{-x} ≥ 1 - x$, the integral fluctuation theorem leads to the inequality $\langle \tilde{Σ}_t \rangle_t ≥ 0$. Since (13) gives $\langle \tilde{Σ}_t \rangle_t = S(C_t) - S(C_0)$, $\langle \tilde{Σ}_t \rangle_t ≥ 0$ implies $S(C_t) ≥ S(C_0)$ for any $t$. This can be related to the second law of thermodynamics for some special cases.

These three identities provide a useful representation of the time evolution. Given $C_t$ for $s \in [0, t]$, one determines $λ_t$ by the second identity (11). Then, the third identity (14) leads to

$$J_{\tilde{t}}^{\tilde{a}a}(r) = \langle \tilde{J}^{\tilde{a}a}(r) e^{\tilde{Σ}} \rangle_L^G,$$

with

$$\tilde{Σ}_t(Γ) = \int_0^t ds[\partial_\tilde{s}λ^s \cdot \delta \tilde{J}^{\tilde{a}a}(r) + (\partial_\tilde{s}λ^s) \cdot \delta \tilde{C}^t].$$

According to thermodynamics, the inverse temperature and the chemical potential are defined by $β = \partial S_{th}(h', ρ)/\partial h'$ and $μ = -β^{-1}∂S_{th}(h', ρ)/∂ρ$, respectively. Through this relation, $β_t(r)$ and $μ_t(r)$ are determined from $C_t(r)$. Then, from (11) and (17), $β_t$ and $μ_t$ are related to the conjugate fields as $β_t = λ_0 + O(ε^2)$ and $β_t μ_t = -λ^2 + β_t |μ_t|^2/2 + O(ε^2)$, and the straightforward calculation [24] using a thermodynamic relation yields

$$S(0)(C) = ∫_Ω d^3r s_{th}(h'(r), ρ(r)).$$

(17)
\[
(\partial^a \lambda^a_s) J_{sa} = (\partial^a \beta_s) J_{sa}^{\text{nat}} - (\beta_s \partial^a u^a_s) (J_{sa}^{\text{lab}} - p_s \delta^{ab}) + O(\epsilon^3), \tag{18}
\]

where \(p(r)\) is the thermodynamic pressure determined from \(s_0(h'(r), \rho(r))\).

Next, since \(\Sigma_{t}^{(1)}\) in (16) is estimated as \(O(\epsilon)\), it is found from (15) that \(J_{t}^{(u)}(0) = (J_{t}^{\text{nu}})^{\text{LG}}\). From the isotropic property, \(J_{t}^{(u)}(0)^{\text{LG}} = 0\) and \(J_{t}^{(ab)}(0)^{\text{LG}} = \phi_0 \delta^{ab}\), where \(\phi(r)\) is a scalar field. Then, the combination of (7) with (18) leads to \(\beta \partial^a u^a \cdot (\phi - \rho) = 0\). Since \(\phi - \rho\) is independent of \(u\), \(\phi = \rho\) is obtained. The result was in fact derived by the direct calculation [4]. It is thus concluded that \(J_{t}^{(u)}(0) = (h + p)u^a\), \(J_{t}^{(a)}(0) = \rho \partial^a \phi + pu^a \delta^a\), and \(J_{t}^{(a)} = J_{t}^{(a)}(0) = \rho u^a\), where the relation \(J_{t}^{(a)}\) and \(J_{t}^{(a)}\) has been used [24]. The hydrodynamic equation \(\partial_\xi C_i^t + \partial^a J_{t}^{(a)}(0) = 0\) is the Euler equation. (See Ref. [25] for the mathematical derivation of the Euler equation.)

Furthermore, from (15), it is found that \(J_{t}^{(a)}(1) = \langle J_{t}^{(a)}(1) \rangle^{\text{LG}}\), where \(\langle J_{t}^{(a)}(1) \rangle^{\text{LG}}\) represents the estimation that \(\partial_\xi \lambda^a_s\) in \(\Sigma_{t}^{(1)}\) is given by the Euler equation. Then, \(\Sigma_{t}^{(1)}\) is calculated as [24]

\[
\Sigma_{t}^{(1)}(\Gamma) = \int_0^\tau ds \left[ \langle \partial \beta_s \rangle \cdot \tilde{q}^a(\Gamma_{\tau-s}) - (\beta_s \partial^a \phi_s) \cdot \tilde{q}^{ab}(\Gamma_{\tau-s}) \right], \tag{19}
\]

where

\[
\tilde{q}^a \equiv J_{t}^{(u)} - \frac{h^t + p}{\rho} \tilde{u}^a, \tag{20}
\]

\[
\tilde{q}^{ab} \equiv \delta J_{t}^{(a)} - \left[ \left( \frac{\partial h^t}{\partial h^t} \right) \delta h_t + \left( \frac{\partial h^t}{\partial \rho} \right) \delta \rho_t \right] \delta^{ab}. \tag{21}
\]

\(\tilde{q}^a\) and \(\tilde{q}^{ab}\) are interpreted as the irreducible part of the energy and momentum fluxes in the moving frame with the local velocity, in which the contribution from fluctuations of the density fields are subtracted from the energy and momentum fluxes. By combining (20) and (21) with the relation between \(J_{t}^{(a)}\) and \(J_{t}^{(a)}\), it is obtained that \(J_{t}^{(a)}(1) = \tau_{t}^{(1)} u^a + \tilde{q}_t^{(1)}(a)\) and \(J_{t}^{(ab)}(1) = \tau_{t}^{(ab)}(1)\). Here, it is assumed that the characteristic length and time scales of \(C^a\) are much larger than the correlation length and time of \(\tilde{q}^{ab}(1)\) and \(\tilde{q}^{ab}(1)\). This enables us to replace \(C_i^t(\rho)\) in the space-time integration of \(\langle \tilde{q}^{(a)}(\Sigma_{t}^{(1)})^{\text{LG}}\rangle\) by \(C_i^t(\Gamma)\). By noting the isotropic property of the system, it is finally derived that \(q_t^{(1)} = k(\partial^a \beta_s)\) and

\[
\tau_{t}^{(ab)}(1) = -\eta (\partial^a u^b + \partial^b u^a) - \left( \frac{\epsilon - 2\eta}{\eta} \right) \partial^a u^b \tilde{q}^{ab}, \tag{22}
\]

with the Green-Kubo formula [26]
problem, and a new concept would be necessary for a breakthrough. In particular, a role of the local equilibrium distributions may be clarified more. Regarding this difficulty, neither a proof of the nondecreasing property of $S(C)$ nor a counterexample is obtained, whereas $S^{0}(C)$ is found to be nondecreasing when the Navier-Stokes equation is considered. The understanding of $S(C)$ beyond $S^{0}(C)$ may be connected to steady-state thermodynamics.

I hope that the formulation described in this Letter will be developed further in order to discover the relationship between the macroscopic and microscopic descriptions.

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