Kinetic derivation of the hydrodynamic equations for capillary fluids

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(Received 6 May 2004; published 13 December 2004)

Based on the generalized kinetic equation for the one-particle distribution function with a small source, the transition from the kinetic to the hydrodynamic description of many-particle systems is performed. The basic feature of this interesting technique to obtain the hydrodynamic limit is that the latter has been partially incorporated into the kinetic equation itself. The hydrodynamic equations for capillary fluids are derived from the characteristic function for the local moments of the distribution function. Fick's law appears as a consequence of the transformation law for the hydrodynamic quantities under time inversion.

DOI: 10.1103/PhysRevE.70.067301 PACS number(s): 47.10.+g, 05.20.Dd, 05.40.Jc

I. INTRODUCTION

The most simple and comprehensive model in the physics of interfaces and capillarity is described by the following hydrodynamic equations:

$$\frac{\partial \varrho}{\partial t} + \boldsymbol{\nabla} \cdot (\varrho \mathbf{V}) = 0, \tag{1}$$

$$\frac{\partial \mathbf{V}}{\partial t} + (\mathbf{V} \cdot \boldsymbol{\nabla})\mathbf{V} = - \boldsymbol{\nabla} \left[\frac{\delta(\varrho \mathcal{F})}{\delta \varrho} \right], \tag{2}$$

where $\mathcal{F}(\varrho, \alpha)$ is a function of the density ϱ and of $\alpha = (1/2)|\nabla \rho|^2$ and $\mathbf{V}$ is the current velocity [1]. This formulation of the van der Waals theory was originally due to Korteweg [2], who proposed a continuum mechanical model in which the Cauchy stress tensor apart from the standard Cauchy-Poisson term contains an additional term defined as

$$\mathbf{T} = (-p + \alpha \nabla^2 \varrho(\mathbf{x};t) + \beta |\boldsymbol{\nabla} \varrho(\mathbf{x};t)|^2)\mathbf{1} + \delta \boldsymbol{\nabla} \varrho(\mathbf{x};t) \otimes \boldsymbol{\nabla} \varrho(\mathbf{x};t) + \gamma (\boldsymbol{\nabla} \otimes \boldsymbol{\nabla}) \varrho(\mathbf{x};t), \tag{3}$$

where **1** is the unit tensor. As already mentioned by Dunn and Serrin [3], the modern terminology concerning the Korteweg model refers to elastic materials of grade n, where the particular case of $n=3$ has been well studied in recent years [4].

Equations (1) and (2) have been linked recently [5,6] to a nonlinear Schrödinger equation and its hydrodynamics counterpart, i.e., nonlinear Madelung fluid [7,8]. This link between capillarity and the Schrödinger equation can shed more light onto the so-called quantumlike approach to many-particle systems such as beams in particle accelerators and beam-plasma systems. The standard procedure in this direction is to approximate the physical systems characterized by an overall interaction with a suitable mean field theory. To avoid misunderstanding, it is worthwhile to note that the Schrödinger equation alone does not provide an entire quantum mechanical picture. It should be necessarily supplemented by a theory of quantum measurement and consequently by a proper physical interpretation of wave packets. In the quantumlike approach, the many-particle systems are described in an effective way as a whole. Based on the above considerations, it appears interesting to explore the possibility of a derivation from kinetic theory of the general hydrodynamic picture thus discussed. The analysis performed in this paper can be outlined as follows: starting from the equation for the one-particle distribution function, we consider a stochastic contribution from an additional collision term (small source). To estimate this term, we use the Kramers-Moyal expansion truncated at second order (diffusion processes). The final step constituting the hydrodynamic marginalization is performed in the third section. Taking into account a special class of diffusion processes, the so-called Nelson diffusion [11,8], this step recovers as expected the standard time-reversal invariance of hydrodynamic equations.

II. GENERAL FRAMEWORK

The starting point of our analysis is the equation for the microscopic phase space density $N_M(\mathbf{x}, \mathbf{p}; t)$

$$\frac{\partial N_M}{\partial t} + \frac{1}{m} \boldsymbol{\nabla} \cdot (\mathbf{p} N_M) + \vec{\partial}_{\mathbf{p}} \cdot [\mathbf{F}_M(\mathbf{x}, \mathbf{p}; t) N_M] = 0, \tag{4}$$

for a system consisting of N particles, which occupies volume V in the configuration space. Here $\mathbf{x}$ and $\mathbf{p}$ are the coordinates and the canonically conjugate momenta, m is the particle mass, and $\mathbf{F}_M(\mathbf{x}, \mathbf{p}; t)$ is the microscopic force, which apart from the external force includes a part specifying the type of interaction between particles. Suppose that at some initial time t_0 the microscopic phase space density is known to be $N_{M0}(\mathbf{x}, \mathbf{p}; t_0)$. Then, the formal solution of Eq. (4) for arbitrary time t can be written as

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$$N_M(\mathbf{x},\mathbf{p};t) = \hat{\mathcal{S}}(t;t_0)N_{M0}(\mathbf{x},\mathbf{p};t_0), \tag{5}$$

where $\hat{\mathcal{S}}(t;t_0)$ is the evolution operator, specifying the Hamiltonian flow.

The choice of the initial $N_{M0}(\mathbf{x},\mathbf{p};t_0)$ is based on the knowledge of the microscopic characteristics of the system. Due to the extremely complex particles' dynamics, full consistent description is not feasible. Therefore the detailed information on the microscopic level is incomplete. If our system is a complex one in the sense that both the external forces and the collective forces are highly nonlinear, a dynamic instability of motion is likely to occur on a characteristic time scale τ. The only information available to an outside observer by means of a macroscopic measuring device is a coarse-grained density distribution with a smoothing function, which takes into account the dynamic instability of motion. Thus we assume

$$N_{M0}(\mathbf{x};t_0) = \widetilde{N}_M(\mathbf{x};t_0) = \int d^3\mathbf{z}G(\mathbf{x};t_0|\mathbf{z})N_M(\mathbf{z};t_0), \tag{6}$$

where for simplicity the explicit dependence on the momentum variables $\mathbf{p}$ has been suppressed. To take into account the initial preparation of the system, one has to displace the initial time t_0 at $-\infty$ and perform an average over the past history of the system. Then Eq. (4) becomes [9]

$$\frac{\partial N_M}{\partial t} + \frac{1}{m}\boldsymbol{\nabla}\cdot(\mathbf{p}N_M) + \vec{\partial}_{\mathbf{p}}\cdot[\mathbf{F}_M(\mathbf{x},\mathbf{p};t)N_M] = \frac{1}{\tau}(\widetilde{N}_M - N_M). \tag{7}$$

Since the collision time is supposed to be much smaller than the time τ, the standard collision integral which appears in kinetic theory can be dropped and the kinetic equation for the one-particle distribution function $f(\mathbf{x},\mathbf{p};t)$ can be written as

$$\frac{\partial f}{\partial t} + \frac{\mathbf{p}}{m}\cdot\boldsymbol{\nabla} f + \mathbf{F}(\mathbf{x},\mathbf{p};t)\cdot\vec{\partial}_{\mathbf{p}} f = \frac{1}{\tau}(\tilde{f} - f). \tag{8}$$

The right-hand-side of Eq. (8) is regarded as a "collision integral" and using the Kramers-Moyal expansion, it can be expressed as

$$\frac{1}{\tau}(\tilde{f} - f) = \sum_{l=1}^{\infty}\sum_{\substack{n_1,n_2,\ldots,n_k=0 \\ n_1+n_2+\cdots+n_k=l}}^{l}\frac{(-1)^l}{n_1!\,n_2!\cdots n_k!} \times \frac{\partial^l}{\partial x_1^{n_1}\cdots\partial x_k^{n_k}}[\mathcal{D}^{(l)}_{n_1 n_2\cdots n_k}(\mathbf{x};t)f], \tag{9}$$

where

$$\mathcal{D}^{(l)}_{n_1 n_2\cdots n_k}(\mathbf{x};t) = \frac{1}{\tau}\int d^3\mathbf{z}\Delta z_1^{n_1}\Delta z_2^{n_2}\cdots\Delta z_k^{n_k}G(\mathbf{z};t|\mathbf{x}) = \frac{1}{\tau}\langle\Delta z_1^{n_1}\Delta z_2^{n_2}\cdots\Delta z_k^{n_k}\rangle^{(G)}_{\mathbf{x},t}, \tag{10}$$

with $\Delta\mathbf{z}=\mathbf{z}-\mathbf{x}$. As a first very interesting step, we consider the diffusion approximation

$$\frac{1}{\tau}(\tilde{f} - f) = -\nabla_k[A_k(\mathbf{x};t)f] + \frac{1}{2}\nabla_k\nabla_l[B_{kl}(\mathbf{x};t)f], \tag{11}$$

where

$$A_k(\mathbf{x};t) = \frac{1}{\tau}\langle\Delta z_k\rangle^{(G)}_{\mathbf{x},t}, \quad B_{kl}(\mathbf{x};t) = \frac{1}{\tau}\langle\Delta z_k\Delta z_l\rangle^{(G)}_{\mathbf{x},t}, \tag{12}$$

and a summation over repeated indices is implied. For Hamiltonian systems the well-known relation

$$A_k(\mathbf{x};t) = \frac{1}{2}\nabla_l B_{kl}(\mathbf{x};t) \tag{13}$$

holds, which gives $\mathbf{A}=0$ for $B_{kl}=\text{const}$.

In passing, it is worthwhile to mention that using the principle of maximum information entropy formulated by Jaynes, it can be shown [9] that the smoothing function $G(\mathbf{z};t|\mathbf{x})$ is of the form

$$G(\mathbf{z};t|\mathbf{x}) = \frac{1}{\pi^{3/2}\sqrt{|\det\hat{\mathcal{C}}|}}\exp[-(\mathbf{z}-\langle\mathbf{z}\rangle^{(G)}_{\mathbf{x},t})^T \times\hat{\mathcal{C}}^{-1}(\mathbf{x};t)(\mathbf{z}-\langle\mathbf{z}\rangle^{(G)}_{\mathbf{x},t})]. \tag{14}$$

The quantities

$$\langle z_k\rangle^{(G)}_{\mathbf{x},t}, \quad \langle z_k z_l\rangle^{(G)}_{\mathbf{x},t}, \tag{15}$$

are the first and the second moment of $\mathbf{z}$ at the instant of time $t+\tau$, provided that $\mathbf{z}$ measured at the instant t equals $\mathbf{x}$ [i.e., $\mathbf{z}(t)=\mathbf{x}$]. In addition, $\hat{\mathcal{C}}(\mathbf{x};t)$ is the covariance matrix defined as

$$\mathcal{C}_{kl}(\mathbf{x},t) = 2[\langle z_k z_l\rangle^{(G)}_{\mathbf{x},t} - \langle z_k\rangle^{(G)}_{\mathbf{x},t}\langle z_l\rangle^{(G)}_{\mathbf{x},t}]. \tag{16}$$

The generalized kinetic equation (8) has a form analogous to the Bhatnagar-Gross-Krook (BGK) equation, widely used in the kinetic theory of gases [10]. There is, however, an important conceptual difference between the two equations. In the BGK equation the function $\tilde{f}$ should be replaced by the equilibrium distribution function f_0 describing the global equilibrium and the characteristic time τ should be replaced by the corresponding relaxation time. The smoothed distribution function in Eq. (8) characterizes a local quasiequilibrium state within the smallest unit cell of continuous medium, while τ is the corresponding time scale.

III. HYDRODYNAMIC APPROXIMATION

Rather than following the standard approach in deriving the hydrodynamic picture, we introduce the characteristic function

$$\mathcal{G}(\mathbf{x},\mathbf{w};t) = \int d^3\mathbf{p}f(\mathbf{x},\mathbf{p};t)e^{-i\mathbf{w}\cdot\mathbf{p}}, \tag{17}$$

instead. It is straightforward to verify that $\mathcal{G}$ satisfies the following equation:

$$\frac{\partial \mathcal{G}}{\partial t} + \frac{i}{m}\boldsymbol{\nabla}\cdot\vec{\partial}_{\mathbf{w}}\mathcal{G} + i\mathbf{w}\cdot\mathbf{F}\mathcal{G} = -\boldsymbol{\nabla}\cdot(\mathbf{A}\mathcal{G}) + \frac{1}{2}\nabla_n\nabla_s(B_{ns}\mathcal{G}). \tag{18}$$

Note that the local moments $\langle p_1^{n_1}p_2^{n_2}\cdots p_k^{n_k}\rangle$ can be obtained from the characteristic function according to the relation

$$\langle p_1^{n_1}p_2^{n_2}\cdots p_k^{n_k}\rangle = i^l \left.\frac{\partial^l \mathcal{G}}{\partial w_1^{n_1}\partial w_2^{n_2}\cdots\partial w_k^{n_k}}\right|_{\mathbf{w}=0}, \tag{19}$$

where $n_1+n_2+\cdots+n_k=l$. The well-known hydrodynamic quantities, such as the mass density ϱ, the mean velocity $\mathbf{V}_{(+)}$ of a fluid element, and the hydrodynamic stress tensor Π_{kl} can be defined as

$$\varrho(\mathbf{x};t) = mn\mathcal{G}(\mathbf{x},0;t) = mn\int d^3\mathbf{p} f(\mathbf{x},\mathbf{p};t), \tag{20}$$

$$\varrho(\mathbf{x};t)\mathbf{V}_{(+)}(\mathbf{x};t) = in\partial_{\mathbf{w}}\mathcal{G}\big|_{\mathbf{w}=0} = n\int d^3\mathbf{p}\mathbf{p} f(\mathbf{x},\mathbf{p};t), \tag{21}$$

$$\Pi_{kl}(\mathbf{x};t) = -\frac{n}{m}\left.\frac{\partial^2\mathcal{G}}{\partial w_k\partial w_l}\right|_{\mathbf{w}=0} = \frac{n}{m}\int d^3\mathbf{p} p_k p_l f(\mathbf{x},\mathbf{p};t), \tag{22}$$

Here, $n=\lim_{N,V\to\infty}(N/V)$ implies the thermodynamic limit. Defining also the deviation from the mean velocity as

$$m\mathbf{c}_{(+)} = \mathbf{p} - m\mathbf{V}_{(+)}, \tag{23}$$

and using the evident relation

$$\int d^3\mathbf{p}\mathbf{c}_{(+)}(\mathbf{x},\mathbf{p};t) f(\mathbf{x},\mathbf{p};t) = 0,$$

we can represent the stress tensor Π_{mn} according to the relation

$$\Pi_{mn} = \varrho V_{(+)m}V_{(+)n} + \mathcal{P}_{mn}. \tag{24}$$

Here

$$\mathcal{P}_{kl}(\mathbf{x};t) = mn\int d^3\mathbf{p} c_{(+)k}c_{(+)l} f(\mathbf{x},\mathbf{p};t) \tag{25}$$

is the internal stress tensor.

Equation (18) and the one obtained after differentiating with respect to w_k evaluated at $\mathbf{w}=0$, yield the Smoluchowski equation and the equation for the momentum balance, respectively. These can be written in the form

$$\frac{\partial\varrho}{\partial t} + \boldsymbol{\nabla}\cdot[\varrho(\mathbf{V}_{(+)}+\mathbf{A})] = \frac{1}{2}\nabla_k\nabla_l(B_{kl}\varrho), \tag{26}$$

$$\frac{\partial}{\partial t}(\varrho V_{(+)k}) + \nabla_l(\varrho V_{(+)k}V_{(+)l}) = \frac{\varrho}{m}F_k - \boldsymbol{\nabla}\cdot(\mathbf{A}\varrho V_{(+)k}) - \nabla_l\mathcal{P}_{kl} + \frac{1}{2}\nabla_l\nabla_n(B_{ln}\varrho V_{(+)k}). \tag{27}$$

Let us consider the time inversion transformation specified by [9,11] $t\to\tilde{t}=-t$, $\mathbf{x}\to\tilde{\mathbf{x}}=\mathbf{x}$ and $\mathbf{p}\to\tilde{\mathbf{p}}=-\mathbf{p}$. We argue that there exists a backward velocity $\mathbf{V}_{(-)}(\mathbf{x},t)$ such that

$$\widetilde{\mathbf{V}}_{(+)}(\mathbf{x},-t) = -\mathbf{V}_{(-)}(\mathbf{x},t). \tag{28}$$

The transformed Smoluchowski equation (26) can be represented according to

$$\frac{\partial\varrho}{\partial t} - \boldsymbol{\nabla}\cdot[\varrho(-\mathbf{V}_{(-)}+\mathbf{A})] = -\frac{1}{2}\nabla_k\nabla_l(B_{kl}\varrho). \tag{29}$$

Summing up and subtracting Eqs. (26) and (27), we obtain the continuity equation

$$\frac{\partial\varrho}{\partial t} + \boldsymbol{\nabla}\cdot(\varrho\mathbf{V}) = 0, \tag{30}$$

and the Fick's law

$$U_k = -A_k + \frac{1}{2\varrho}\nabla_l(B_{kl}\varrho). \tag{31}$$

Here

$$\mathbf{V} = \frac{1}{2}(\mathbf{V}_{(+)}+\mathbf{V}_{(-)}), \quad \mathbf{U} = \frac{1}{2}(\mathbf{V}_{(+)}-\mathbf{V}_{(-)}), \tag{32}$$

are the current and the osmotic velocity, respectively. It is worthwhile to mention that since the mean velocity of a fluid element is a generic function of time t, it can be split into odd and even parts. Note that from Eq. (32) it follows that $\mathbf{V}_{(+)}=\mathbf{V}+\mathbf{U}$, where $\mathbf{V}$ is the odd part, while $\mathbf{U}$ is the even part. Equation (27) for the balance of momentum can be written alternatively as

$$\frac{\partial V_{(+)k}}{\partial t} + V_{(-)l}\nabla_l V_{(+)k} = \frac{F_k}{m} + A_l\nabla_l V_{(+)k} - \frac{1}{\varrho}\nabla_l\mathcal{P}_{kl} + \frac{B_{ln}}{2}\nabla_l\nabla_n V_{(+)k}. \tag{33}$$

After performing a time inversion in Eq. (33), we obtain

$$\frac{\partial V_{(-)k}}{\partial t} + V_{(+)l}\nabla_l V_{(-)k} = \frac{F_k}{m} - A_l\nabla_l V_{(-)k} - \frac{1}{\varrho}\nabla_l\widetilde{\mathcal{P}}_{kl} - \frac{B_{ln}}{2}\nabla_l\nabla_n V_{(-)k}, \tag{34}$$

where $\widetilde{\mathcal{P}}_{kl}$ denotes the transformed internal stress tensor after performing the time inversion. Summing up the last two equations, we arrive at the sought-for equation for the current velocity,

$$\frac{\partial V_k}{\partial t} + V_l\nabla_l V_k = \frac{F_k}{m} + A_l\nabla_l U_k - \frac{1}{\varrho}\nabla_l\overline{\mathcal{P}}_{lk} + U_l\nabla_l U_k + \frac{B_{ln}}{2}\nabla_l\nabla_n U_k, \tag{35}$$

where

$$\overline{\mathcal{P}}_{kn} = \frac{1}{2}(\mathcal{P}_{kn} + \widetilde{\mathcal{P}}_{kn}). \tag{36}$$

In order to find the explicit form of the internal stress tensor (25), we observe that the maximum entropy of the system is realized, provided the small source in the generalized kinetic equation (8) vanishes. This condition is equivalent to the condition of detailed balance in the case, where the collision integral (small source) is approximated by a Fokker-Planck operator. The condition of detailed balance implies that the distribution function factorizes in the form

$$f_{eq}(\mathbf{x},\mathbf{p};t) = \frac{\varrho(\mathbf{x};t)}{mn}\mathcal{F}(\mathbf{p};t), \tag{37}$$

where $\mathcal{F}(\mathbf{p};t)$ is a normalizable function. From the above considerations, it follows directly that

$$\mathcal{P}_{kl}(\mathbf{x};t) = \frac{3k_BT}{m}\varrho(\mathbf{x};t)\delta_{kl}, \tag{38}$$

where k_B is the Boltzmann constant and T is the temperature.

In the simplest case, where the external force vanishes and the diffusion tensor is diagonal and isotropic, $B_{kl}=\beta\delta_{kl}$, we obtain

$$\frac{\partial \mathbf{V}}{\partial t} + (\mathbf{V}\cdot\boldsymbol{\nabla})\mathbf{V} = -\boldsymbol{\nabla}\left(\alpha \ln \varrho - \frac{\beta^2}{2}\frac{\nabla^2\sqrt{\varrho}}{\sqrt{\varrho}}\right), \tag{39}$$

where $\alpha=3k_BT/m$. Thus the hydrodynamic equations describing a free capillary fluid have been recovered.

In the case, where an external force is applied, the Korteweg stress tensor contains an additional term proportional to the drift coefficient **A**. On the other hand, from the principle of detailed balance, it follows that the drift coefficient is proportional to the external force. The physical implication of the latter is that the additional term in the Korteweg stress tensor can be regarded as a coupling between the external field and the mean field of purely hydrodynamical origin.

IV. CONCLUSION

Since detailed information about the system on the microscopic level is incomplete, one possible way to take into account its initial preparation, i.e., an eventual dynamic instability of motion that might have set in and/or other large-scale characteristics, is to introduce a suitable smoothing procedure. As a result, the kinetic equation providing a unified kinetic, hydrodynamic, and diffusion description contains a small source and is therefore irreversible. Although the effective collision integral (small source) can be represented as a Kramers-Moyal expansion, for the purposes of the present paper it suffices to consider the right-hand side of the generalized kinetic equation as approximated with a properly defined Fokker-Planck operator. The latter form of the collision term is adopted as a starting point in the derivation of the hydrodynamic equations for capillary fluids. The hydrodynamic approximation is further obtained in a standard manner from the characteristic function for the local moments of the distribution function. An important feature of the approach is that Fick's law emerges naturally from the transformation properties of the hydrodynamic quantities under time inversion. The osmotic velocity is uniquely specified by the first two infinitesimal moments of the smoothing function and in a sense is a measure of the irreversibility.

The main result of the analysis performed in this paper, the hydrodynamic equations for free capillary fluids, has been derived from kinetic theory. If an external force is present, the Korteweg stress tensor has to be modified accordingly. An additional term proportional to the drift coefficient emerges implying a coupling between the external field and the mean field of purely hydrodynamical origin.

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