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Review

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Review

Generalized Equations in Quantum Mechanics and Brownian Theory

Pierre-Henri Chavanis

Laboratoire de Physique Théorique, Université de Toulouse, CNRS, UPS, 31062 Toulouse, France; chavanis@irsamc.ups-tlse.fr

Abstract: We discuss formal analogies between a nonlinear Schrödinger equation derived by the author from the theory of scale relativity and the equations of Brownian theory. By using the Madelung transformation, the nonlinear Schrödinger equation takes the form of hydrodynamic equations involving a friction force, an effective thermal pressure, a pressure due to the self-interaction, and a quantum potential. These hydrodynamic equations have a form similar to the damped Euler equations obtained for self-interacting Brownian particles in the theory of simple liquids. In that case, the temperature is due to thermal motion and the pressure arises from spatial correlations between the particles. More generally, the correlations can be accounted for by using the dynamical density functional theory. We determine the excess free energy of Brownian particles that reproduces the standard quantum potential. We then consider a more general form of excess free energy functionals and propose a new class of generalized Schrödinger equations. For a certain form of excess free energy, we recover the generalized Schrödinger equation associated with the Tsallis entropy considered in a previous paper.

Keywords: kinetic theory; quantum mechanics; Brownian motion

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1. Introduction

The theory of Brownian motion and the quantum theory were two great revolutions in physics at the beginning of the twentieth century.

Brownian motion was discovered by the Scottish botanist Robert Brown [1] in 1827 by observing the erratic motion of small grains of pollen suspended in a fluid. It was explained by Einstein [2,3] in 1905 who understood that the motion of small particles suspended in a solvent was caused by thermal fluctuations due to the molecular movement of the liquid[1]. He showed that a Brownian particle has a diffusive motion and proposed a probabilistic derivation of the diffusion equation based on microscopic processes[2]. He solved the diffusion equation, finding a self-similar Gaussian distribution, and showed that the mean square displacement of the Brownian particle is given by $\overline{x^2} = 2Dt$. He also obtained a relation between the diffusion coefficient D, the mobility of the particle $\mu = 1/(\xi m)$, and the temperature T:

$$D = \frac{k_B T}{\xi m}. \tag{1}$$

This is the celebrated Einstein relation. To obtain this relation he used heuristic arguments based on a hydrodynamic approach. He considered a Brownian particle submitted to an external force and wrote the equilibrium condition in two different manners: one describing the balance between the external force and the osmotic pressure (hydrostatic equilibrium) and the other describing the balance between the drift due to the external force and the diffusion current. Actually, the Einstein relation had been previously derived in an even more general form by Sutherland [20] using a direct method that does not require the introduction of an external force, by simply equating the friction force (Stokes law) and the osmotic pressure force. Smoluchowski [21] also obtained a similar relation with, however, a different prefactor by using a random walk approach[3]. The Einstein relation was later rederived by Langevin [27] from a stochastic differential equation (generalizing Newton's equation) incorporating a random noise term modeling the collisions between the Brownian particles and the molecules of the surrounding fluid. The validity of the Einstein relation and the reality of the atoms were experimentally confirmed by Perrin [28,29] in 1909. The case of a Brownian particle moving in an external potential was considered by Smoluchowski [30] who derived a drift-diffusion equation for the probability density of finding the particle in $\mathbf{r}$ at time t. The Smoluchowski equation can be viewed as a Fokker–Planck equation in position space. It relaxes towards the Boltzmann distribution. The theories of Einstein and Smoluchowski are valid for Brownian particles in the strong friction limit $\xi \to +\infty$ (overdamped motion). The case of inertial Brownian particles moving in an external potential was considered by Klein [11], Kramers [12], and Chandrasekhar [13] who derived a Fokker–Planck equation in phase space involving a linear friction. This is the so-called Kramers equation. It relaxes towards the Maxwell–Boltzmann distribution[4]. If we take the moments of the Kramers equation and close the hierarchy of hydrodynamic equations with a local thermodynamic equilibrium (LTE) condition, we obtain the damped Euler equation including a pressure force associated with the ideal equation of state $P_{\rm id} = \rho k_B T/m$ and a friction force $-\xi\mathbf{u}$ proportional and opposite to the velocity [32]. In the strong friction limit $\xi \to +\infty$, we recover the Smoluchowski equation and the Einstein relation[5]. The equations of Brownian theory were later used in the theory of simple liquids [33]. In that case, one has to take into account nontrivial correlations between the particles due to their self-interactions. This can be done by introducing an excess free energy $F_{\rm ex}[\rho]$. The excess free energy can be calculated at equilibrium by using the density functional theory (DFT) [34]. It is then assumed that the same functional can be used out-of-equilibrium in the kinetic equations. This is the so-called dynamic density functional theory (DDFT) [35]. In certain cases, the excess free energy accounts for an excess pressure $P_{\rm ex}$. For systems with long-range interactions, the correlations between the particles can be neglected in the large N limit, implying that the mean field approximation becomes exact in a proper thermodynamic limit $N \to +\infty$ [36]. If the Brownian particles have both short-range and long-range interactions [37], the damped Euler equations take the form

$$\frac{\partial\rho}{\partial t} + \nabla\cdot(\rho\mathbf{u}) = 0, \tag{2}$$

$$\rho\left[\frac{\partial\mathbf{u}}{\partial t} + (\mathbf{u}\cdot\nabla)\mathbf{u}\right] = -\frac{k_B T}{m}\nabla\rho - \rho\nabla\frac{\delta F_{\rm ex}}{\delta\rho} - \rho\nabla\Phi - \rho\nabla\Phi_{\rm ext} - \xi\rho\mathbf{u}, \tag{3}$$

$$\Phi(\mathbf{r},t) = \int u_{\rm LR}(|\mathbf{r}-\mathbf{r}'|)\rho(\mathbf{r}',t)\,d\mathbf{r}'. \tag{4}$$

In the strong friction limit $\xi \to +\infty$, they reduce to the Smoluchowski equation

$$\xi\frac{\partial\rho}{\partial t} = \nabla\cdot\left(\frac{k_B T}{m}\nabla\rho + \rho\nabla\frac{\delta F_{\rm ex}}{\delta\rho} + \rho\nabla\Phi + \rho\nabla\Phi_{\rm ext}\right). \tag{5}$$

These equations describe a system of self-interacting Brownian particles in contact with a heat bath fixing the temperature. They decrease the free energy F monotonically and, if the free energy is bounded from below, relax towards an equilibrium state, which minimizes the free energy at fixed mass. This provides an H-theorem in the canonical ensemble. As discussed in [17,38], these equations can describe Brownian charges that interact through the repulsive electric force (Nernst–Planck and Debye–Hückel models of electrolytes) [39–43], the chemotaxis of bacterial populations (Keller–Segel model) [44], self-gravitating Brownian particles (Smoluchowski–Poisson equations) [45], colloid particles at a fluid interface [46], superconductors of type II [47], nucleation of colloids and macromolecules in solution [48], two-dimensional Brownian point vortices [49], the Brownian mean field (BMF) model [50], and other systems.

Wave mechanics started with the pioneering work of de Broglie [51] who proposed associating a wave to a particle through the correspondences $E = \hbar\omega$ and $\mathbf{p} = \hbar\mathbf{k}$ (wave–particle duality). Schrödinger [52–55] developed the ideas of de Broglie about matter waves. He introduced an equation (the celebrated Schrödinger equation) for a complex wave function $\psi(\mathbf{r}, t)$ and showed that its solution can account for the energy spectrum of the hydrogen atom in the nonrelativistic limit, thereby recovering and enlarging the results of the planetary Bohr [56,57] model[6]. Madelung [63] showed that the Schrödinger equation for the electron could be formally transformed into fluid equations similar to the continuity equation and the pressureless Euler equation but involving an additional quantum potential proportional to $\hbar^2$. These results were rediscovered later by Bohm [64,65] in his theory of "hidden" variables. Nonlinear Schrödinger equations including a self-interaction potential were introduced in relation to particle physics (solitons) [66], nonlinear optics (e.g., the Townes soliton) [67], or superfluidity and Bose–Einstein condensates (BECs) [68–72]. They have the form of Gross–Pitaevskii (GP) or generalized GP equations[7]. If we perform the Madelung transformation on these equations, we obtain a quantum Euler equation including, in addition to the quantum potential, a pressure force determined by the self-interaction potential.

In a recent paper [74], we derived a nonlinear Schrödinger equation by extending the formalism of Nottale's theory of scale relativity [75] to the case of dissipative systems. This equation involves a logarithmic nonlinearity with a complex friction coefficient. When transformed into fluid equations, the complex logarithmic potential gives rise to a linear friction force and an effective thermal pressure force. These two terms arise simultaneously from the complex nature of the friction coefficient (they are "twins"). We generalized this equation further by introducing a self-interaction potential (taking into account short-range interactions) and a long-range potential of interaction [76]. This leads to a generalized GP equation of the form

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\Delta\psi + m\Phi\psi + m\Phi_{\rm ext}\psi + m\frac{dV_{\rm int}}{d|\psi|^2}\psi$$
$$+2k_B T\ln|\psi|\,\psi - i\frac{\hbar}{2}\xi\left[\ln\left(\frac{\psi}{\psi^*}\right) - \left\langle\ln\left(\frac{\psi}{\psi^*}\right)\right\rangle\right]\psi, \tag{6}$$

$$\Phi(\mathbf{r}, t) = \int u(|\mathbf{r} - \mathbf{r}'|)|\psi|^2(\mathbf{r}', t)\,d\mathbf{r}'. \tag{7}$$

This equation incorporates an arbitrary nonlinearity, an effective temperature, and a source of dissipation. As discussed in [76,77], this equation can describe dark matter halos made of self-gravitating bosons or self-gravitating fermions [78–80][8], the fermionic and bosonic Hamiltonian mean field (HMF) models [106,107], fermions and bosons with electrostatic interaction [77,108], etc. Interestingly, if we perform the Madelung transformation on this equation, we obtain fluid equations, which are similar to the damped Euler Equations (2)–(4) obtained in the case of Brownian particles in interaction. This analogy between generalized quantum equations and generalized Brownian equations was mentioned in our previous works [76,77] and is here reviewed with some amplification. It is not clear if this analogy is purely formal or if it bears more physical significance than is apparent at first sight. We determine the excess free energy of Brownian particles that reproduces the standard quantum potential. We then consider a more general form of excess free energy functionals and propose a new class of generalized Schrödinger equations. For a certain form of excess free energy, we recover the generalized Schrödinger equation associated with the Tsallis entropy considered in a previous paper [16].

The paper is organized as follows. In Section 2, we derive a generalized Schrödinger equation from the theory of scale relativity by considering dissipative systems. In Section 3, we introduce a self-interaction term in that equation and obtain a generalized GP equation governing the evolution of a dissipative BEC. In Section 4, we develop an effective thermodynamical formalism associated with the generalized GP equation. We then consider a system of classical Brownian particles in interaction. We discuss their statistical equilibrium state in Section 5 and their kinetic theory in Section 6. In Section 7, we explain how one can close the equations of the kinetic theory by using the DDFT. In Section 8, we show that the hydrodynamic equations of classical Brownian particles in interaction are similar to the hydrodynamic equations obtained from the generalized GP equation. The quantum potential corresponds to a special form of excess free energy (i.e., to a special form of correlations). We can thus derive an equation similar to the Schrödinger equation from the hydrodynamic equations of Brownian particles in interaction. We then propose a generalized class of Schrödinger equations associated with other forms of excess free energy. The general case is treated in Section 9 where we introduce a generalized Schrödinger equation incorporating an arbitrary excess free energy in addition to the usual quantum terms.

2. Derivation of a Generalized Schrödinger Equation from the Theory of Scale Relativity

In this section, we recall the derivation of the generalized Schrödinger equation obtained in ref. [74] by extending the theory of scale relativity [75] to the case of dissipative systems.

2.1. Basics Results in the Theory of Scale Relativity

The theory of scale relativity elaborated by Nottale [75] assumes that the trajectories of the particles are intrinsically nondifferentiable. The nondifferentiable nature of space-time gives rise to quantum mechanics. When a trajectory is nondifferentiable, the derivative $d\mathbf{r}/dt$ is not defined (contrary to classical mechanics) and one has to introduce two velocities: $\mathbf{u}_+(\mathbf{r}(t),t)$ and $\mathbf{u}_-(\mathbf{r}(t),t)$, defined from $t-dt$ to t for $\mathbf{u}_-$ and from t to $t+dt$ for $\mathbf{u}_+$. The breaking of the symmetry $dt \leftrightarrow -dt$ leading to the two-valuedness character of the velocity is at the origin of complex numbers in quantum mechanics. The elementary displacement $d\mathbf{r}_\pm$ for both processes has a differential part $d\mathbf{r}_\pm = \mathbf{u}_\pm\, dt$ and a nondifferentiable part $d\mathbf{b}_\pm$, which can be described by a stochastic variable of zero mean $\langle d\mathbf{b}_\pm\rangle = \mathbf{0}$. It can be interpreted as a scale-dependent fractal fluctuation. Quantum mechanics has a fractal dimension $D_{\rm F} = 2$ [109,110] similar to that of Brownian motion or more generally to Markov processes. Therefore, we can write

$$d\mathbf{r}_\pm = \mathbf{u}_\pm\, dt + d\mathbf{b}_\pm \tag{8}$$

with

$$\langle d\mathbf{b}_\pm\rangle = \mathbf{0}, \qquad \langle db_{\pm i} db_{\pm j}\rangle = \pm 2\mathcal{D}\delta_{ij}dt, \tag{9}$$

where $\mathcal{D}$ is the quantum diffusion coefficient measuring the covariance of the noise. It characterizes the amplitude of the fractal fluctuations. We can also introduce two classical derivative operators d_+/dt and d_-/dt, which yield the twin classical velocities when they are applied to the position vector $\mathbf{r}$, namely,

$$\frac{d_+\mathbf{r}}{dt} = \mathbf{u}_+, \qquad \frac{d_-\mathbf{r}}{dt} = \mathbf{u}_-. \tag{10}$$

It is convenient to replace the twin velocities $(\mathbf{u}_+, \mathbf{u}_-)$ with the couple $(\mathbf{u}, \mathbf{u}_Q)$ where

$$\mathbf{u} = \frac{\mathbf{u}_+ + \mathbf{u}_-}{2}, \qquad \mathbf{u}_Q = \frac{\mathbf{u}_+ - \mathbf{u}_-}{2}. \tag{11}$$

With these two velocities, we can form a complex velocity

$$\mathbf{U} = \mathbf{u} - i\mathbf{u}_Q. \tag{12}$$

The velocity $\mathbf{u}$ can be interpreted as the classical velocity and the velocity $\mathbf{u}_Q$ as the quantum velocity. In the classical limit, where the trajectories of the particles are differentiable, we have $\mathbf{u}_+ = \mathbf{u}_- = \mathbf{u}$ and $\mathbf{u}_Q = \mathbf{0}$. The quantum velocity is at the origin of the complex number i in the equations of quantum mechanics. We can also define a complex derivative operator

$$\frac{D}{Dt}=\frac{d_{+}+d_{-}}{2dt}-i\frac{d_{+}-d_{-}}{2dt}\tag{13}$$

in terms of which

$$\frac{D\mathbf{r}}{Dt}=\mathbf{U}.\tag{14}$$

The total derivative with respect to the time of a function $f(\mathbf{r}(t),t)$ of fractal dimension $D_{\rm F}=2$ reads

$$\frac{df}{dt}=\frac{\partial f}{\partial t}+\nabla f\cdot\frac{d\mathbf{r}}{dt}+\frac{1}{2}\sum_{i,j}\frac{\partial^2 f}{\partial x_i\partial x_j}\frac{dx_i dx_j}{dt}.\tag{15}$$

Using Equation (9), we find that the classical (differentiable) part of this expression is

$$\frac{d_{\pm}f}{dt}=\frac{\partial f}{\partial t}+\mathbf{u}_{\pm}\cdot\nabla f\pm\mathcal{D}\Delta f.\tag{16}$$

Substituting Equation (16) into Equation (13), we obtain the expression of the complex time derivative operator [75]:

$$\frac{D}{Dt}=\frac{\partial}{\partial t}+\mathbf{U}\cdot\nabla-i\mathcal{D}\Delta.\tag{17}$$

The fundamental postulate of Nottale's theory of scale relativity [75] is that the equations of quantum mechanics (where the trajectories of the particles are nondifferentiable) can be obtained from the equations of classical mechanics (where the trajectories of the particles are differentiable) by replacing the standard velocity $\mathbf{u}$ with the complex velocity $\mathbf{U}$ and the standard time derivative d/dt with the complex time derivative D/Dt. In other words, D/Dt plays the role of a "covariant derivative operator". It is assumed that, when expressed in terms of this derivative operator, the fundamental equations of physics keep the same form in the classical and quantum regimes. This is similar to the principle of covariance in Einstein's theory of relativity according to which the form of the equations of physics should be preserved under a change of coordinates.

2.2. Generalized Schrödinger Equation

Nottale [75] showed that the standard Schrödinger equation could be derived from Newton's law of motion by using the principle of scale covariance. Below, we extend this procedure to the case of dissipative systems and derive a generalized Schrödinger equation [74].

In classical mechanics, the equation of motion of a damped particle submitted to an external potential $\Phi_{\rm ext}$ reads

$$\frac{d\mathbf{v}}{dt}=-\nabla\Phi_{\rm ext}-\xi\mathbf{v},\tag{18}$$

where we assume a linear friction force $-\xi\mathbf{v}$. Following Nottale's method of quantization, we transpose the equation of motion (18) into

$$\frac{D\mathbf{U}}{Dt}=-\nabla\Phi_{\rm ext}-{\rm Re}(\gamma\mathbf{U}),\tag{19}$$

where $\mathbf{U}(\mathbf{r},t)$ and D/Dt are the complex velocity and the covariant derivative operator defined above and γ is a complex friction coefficient. As explained in [74], it is necessary to take the real part of the complex friction force in Equation (19) in order to guarantee the local conservation of the normalization condition. Using the expression (17) of the covariant derivative, Equation (19) can be rewritten as a damped complex viscous Burgers equation

$$\frac{\partial \mathbf{U}}{\partial t}+(\mathbf{U}\cdot\nabla)\mathbf{U}=i\mathcal{D}\Delta\mathbf{U}-\nabla\Phi_{\rm ext}-{\rm Re}(\gamma\mathbf{U}) \tag{20}$$

with an imaginary viscosity $\nu=i\mathcal{D}$. From the Lagrangian formalism, it can be shown [75] that the complex velocity field $\mathbf{U}$, or more precisely the impulse $\mathbf{P}=m\mathbf{U}$, can be written as the gradient of a complex action:

$$\mathbf{U}=\frac{\nabla\mathcal{S}}{m}. \tag{21}$$

This defines a potential flow. As a consequence, the flow is irrotational: $\nabla\times\mathbf{U}=\mathbf{0}$. Using the well-known identities of fluid mechanics $(\mathbf{U}\cdot\nabla)\mathbf{U}=\nabla(\mathbf{U}^2/2)-\mathbf{U}\times(\nabla\times\mathbf{U})$ and $\Delta\mathbf{U}=\nabla(\nabla\cdot\mathbf{U})-\nabla\times(\nabla\times\mathbf{U})$, which reduce to $(\mathbf{U}\cdot\nabla)\mathbf{U}=\nabla(\mathbf{U}^2/2)$ and $\Delta\mathbf{U}=\nabla(\nabla\cdot\mathbf{U})$ for an irrotational flow, and using the identity $\nabla\cdot\mathbf{U}=\Delta\mathcal{S}/m$ resulting from Equation (21), we find that Equation (20) is equivalent to the complex quantum Hamilton–Jacobi (or Bernoulli) equation

$$\frac{\partial\mathcal{S}}{\partial t}+\frac{1}{2m}(\nabla\mathcal{S})^2-i\mathcal{D}\Delta\mathcal{S}+m\Phi_{\rm ext}+V(t)+{\rm Re}(\gamma\mathcal{S})=0, \tag{22}$$

where $V(t)$ is a "constant" of integration that may depend on time. By analogy with the Burgers equation in hydrodynamics, we introduce a complex function $\psi(\mathbf{r},t)$ through the Cole–Hopf transformation[9]

$$\mathcal{S}=-2im\mathcal{D}\ln\psi. \tag{23}$$

This equation can be rewritten in a form equivalent to the WKB formula in quantum mechanics

$$\psi=e^{i\mathcal{S}/\hbar} \tag{24}$$

provided that we make the identification

$$\mathcal{D}=\frac{\hbar}{2m}. \tag{25}$$

Therefore, the complex function $\psi(\mathbf{r},t)$ represents the wave function of the particle. The relation (25) between the diffusion coefficient $\mathcal{D}$ and the mass m of the particle is sometimes called the Nelson [111] relation[10]. Substituting Equation (23) into Equation (22), and using the identity

$$\Delta(\ln\psi)=\frac{\Delta\psi}{\psi}-\frac{1}{\psi^2}(\nabla\psi)^2, \tag{26}$$

we obtain the nonlinear wave equation [74]

$$i\hbar\frac{\partial\psi}{\partial t}=-\frac{\hbar^2}{2m}\Delta\psi+m\Phi_{\rm ext}\psi+V\psi+\hbar\,{\rm Im}(\gamma\ln\psi)\psi. \tag{27}$$

When $\gamma=0$, we recover the standard Schrödinger equation. Writing $\gamma=\gamma_R+i\gamma_I$, where γ_R is the classical friction coefficient and γ_I is the quantum friction coefficient, and using the identity

$${\rm Im}(\gamma\ln\psi)=\gamma_I\ln|\psi|-\frac{1}{2}i\gamma_R\ln\left(\frac{\psi}{\psi^*}\right), \tag{28}$$

we can rewrite Equation (27) in the equivalent form

$$i\hbar\frac{\partial\psi}{\partial t}=-\frac{\hbar^2}{2m}\Delta\psi+m\Phi_{\rm ext}\psi+V\psi+\hbar\gamma_I\ln|\psi|\,\psi-i\frac{\hbar}{2}\gamma_R\ln\left(\frac{\psi}{\psi^*}\right)\psi. \tag{29}$$

Introducing the notations

$$\gamma_R = \xi, \qquad \gamma_I = \frac{2k_B T}{\hbar}, \tag{30}$$

the generalized Schrödinger Equation (29) becomes

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\Delta\psi + m\Phi_{\rm ext}\psi + V\psi + 2k_B T\ln|\psi|\,\psi - i\frac{\hbar}{2}\xi\ln\left(\frac{\psi}{\psi^*}\right)\psi. \tag{31}$$

As shown in [74] (see also Section 3.2), ξ plays the role of an ordinary friction coefficient, while T plays the role of an effective temperature. Since the temperature is effective, it can be positive or negative. Finally, we choose the function $V(t)$ so that the average value of the friction term proportional to ξ is equal to zero. This gives

$$V(t) = i\frac{\hbar}{2}\xi\left\langle\ln\left(\frac{\psi}{\psi^*}\right)\right\rangle, \tag{32}$$

where $\langle X\rangle = \int \rho X\, d\mathbf{r}$ is a spatial average. Then, the generalized Schrödinger Equation (31) takes the form [74]

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\Delta\psi + m\Phi_{\rm ext}\psi + 2k_B T\ln|\psi|\,\psi - i\frac{\hbar}{2}\xi\left[\ln\left(\frac{\psi}{\psi^*}\right) - \left\langle\ln\left(\frac{\psi}{\psi^*}\right)\right\rangle\right]\psi. \tag{33}$$

When $T = 0$, we recover the nonlinear wave equation introduced by Kostin [118], and when $\xi = 0$ and $k_B T = -b < 0$, we recover the nonlinear wave equation introduced by Bialynicki–Birula and Mycielski [119]. The nonlinear wave Equation (33) is equivalent to the equation of motion (19). It is interesting to note that the complex nature of the friction coefficient

$$\gamma = \xi + i\frac{2k_B T}{\hbar} \tag{34}$$

leads to a generalized Schrödinger equation simultaneously exhibiting a friction term ξ and an effective temperature term $k_B T$. They correspond to the real and imaginary parts of γ. In this sense, they are twins. This may be viewed as a new form of fluctuation–dissipation theorem. As a result, the generalized Schrödinger Equation (33) connects the generalized Schrödinger equation introduced by Kostin [118] and the generalized Schrödinger equation introduced by Bialynicki–Birula and Mycielski [119]. Remarkably, the generalized Schrödinger Equation (33) can be obtained from a unique equation of motion, Equation (19), by using the formalism of scale relativity [75].

Remark 1. *If we equate the Einstein relation (1) and the Nelson relation (25), we obtain* $\xi = 2k_B T/\hbar$*, which corresponds to the quantum friction coefficient* γ_I*. It is not clear if this relation is just a result of dimensional analysis or if it bears a deeper significance.*

3. Generalized Gross–Pitaevskii Equation for Bose–Einstein Condensates

3.1. Generalized Gross–Pitaevskii Equation

We now introduce additional nonlinearities in the generalized Schrödinger Equation (33) and consider a generalized GP equation of the form [76]

$$\begin{aligned} i\hbar\frac{\partial\psi}{\partial t} &= -\frac{\hbar^2}{2m}\Delta\psi + m\left[\Phi + \frac{dV_{\rm int}}{d|\psi|^2} + \Phi_{\rm ext}\right]\psi \\ &+2k_B T\ln|\psi|\,\psi - i\frac{\hbar}{2}\xi\left[\ln\left(\frac{\psi}{\psi^*}\right) - \left\langle\ln\left(\frac{\psi}{\psi^*}\right)\right\rangle\right]\psi \end{aligned} \tag{35}$$

with

$$\Phi(\mathbf{r},t) = \int u(|\mathbf{r}-\mathbf{r}'|)|\psi|^2(\mathbf{r}',t)\,d\mathbf{r}'. \tag{36}$$

This generalized GP equation governs the evolution of BECs at zero thermodynamic temperature ($T_{\rm thermo} = 0$), where all the bosons are in the same quantum state described by a single wavefunction $\psi(\mathbf{r}, t)$. The spatial density of the bosons is $\rho(\mathbf{r}, t) = |\psi(\mathbf{r}, t)|^2$. The generalized GP equation conserves the mass $M = \int |\psi|^2 \, d\mathbf{r}$. Here, $V_{\rm int}(|\psi|^2)$ represents the self-interaction potential of the bosons (taking into account short-range interactions) and $u(|\mathbf{r} - \mathbf{r}'|)$ represents a long-range potential of interaction between the bosons (e.g., the gravitational interaction for cosmic BECs [96,97]). Equation (35) with $\xi = T = 0$ is the standard GP equation extended here to an arbitrary nonlinearity. When coupled to an attractive long-range potential of interaction (like the gravitational potential), this equation exhibits a complicated process of gravitational cooling [120,121] and violent relaxation [122,123]. This process is fundamental to understanding the structure of dark matter halos made of BECs. As discussed in [77], the generalized GP Equation (35) with a friction $\xi > 0$ and an effective temperature $T > 0$ could provide a heuristic parametrization of the process of violent relaxation and gravitational cooling on a coarse-grained scale[11]. It leads to equilibrium states with a core–envelope structure, namely, a quantum core surrounded by an isothermal envelope [77–79]. The quantum core (soliton) corresponds to the ground state of the GP equation and the (isothermal) envelope accounts for quantum interferences of excited states. This core–envelope structure has been evidenced in numerical simulations of the Schrödinger–Poisson equations [93,94,98–105] and is consistent with the structure of dark matter halos (see the reviews [81–89] on this topic). The quantum core may solve the core–cusp problem [124] of the cold dark matter (CDM) model and the isothermal envelope, which is similar to a Navarro–Frenk–White (NFW) profile [125], accounts for the flat rotation curves of the galaxies. The generalized GP Equation (35) can, therefore, find applications in the context of BEC dark matter.

If we introduce the total potential $V = V_{\rm id} + V_{\rm int}$, where

$$V_{\rm id}(|\psi|^2) = \frac{k_B T}{m} |\psi|^2 \left(\ln |\psi|^2 - 1 \right) \tag{37}$$

is the effective thermal potential of an ideal gas (see Section 2) and $V_{\rm int}$ is the self-interaction potential of the bosons, we can rewrite the generalized GP Equation (35) as

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \Delta \psi + m \left[\Phi + \frac{dV}{d|\psi|^2} + \Phi_{\rm ext} \right] \psi - i \frac{\hbar}{2} \xi \left[\ln\left(\frac{\psi}{\psi^*} \right) - \left\langle \ln\left(\frac{\psi}{\psi^*} \right) \right\rangle \right] \psi. \tag{38}$$

The generalized GP equation can also be written as

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \Delta \psi + m[\Phi + h(|\psi|^2) + \Phi_{\rm ext}] \psi - i \frac{\hbar}{2} \xi \left[\ln\left(\frac{\psi}{\psi^*} \right) - \left\langle \ln\left(\frac{\psi}{\psi^*} \right) \right\rangle \right] \psi, \tag{39}$$

where the function $h(|\psi|^2)$ is related to the potential $V(|\psi|^2)$ by

$$h(|\psi|^2) = \frac{dV}{d|\psi|^2}, \qquad \text{i.e.,} \qquad h(\rho) = V'(\rho). \tag{40}$$

It can be decomposed into $h = h_{\rm id} + h_{\rm int}$ with

$$h_{\rm id}(\rho) = V'_{\rm id}(\rho) = \frac{k_B T}{m} \ln \rho \quad \text{and} \quad h_{\rm int}(\rho) = V'_{\rm int}(\rho). \tag{41}$$

Remark 2. *For a standard BEC [126], the self-interaction potential $V_{\rm int}$ and the function $h_{\rm int}$ are*

$$V_{\rm int}(|\psi|^2) = \frac{2\pi a_s \hbar^2}{m^3} |\psi|^4, \qquad h_{\rm int}(|\psi|^2) = \frac{4\pi a_s \hbar^2}{m^3} |\psi|^2, \tag{42}$$

where a_s is the scattering length of the bosons (when $a_s > 0$, the self-interaction is repulsive, and when $a_s < 0$, the self-interaction is attractive). In that case, the generalized GP Equation (35) takes the form

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\Delta\psi + m\Phi\psi + \frac{4\pi a_s\hbar^2}{m^2}|\psi|^2\psi + m\Phi_{\rm ext}\psi \\ +2k_B T\ln|\psi|\,\psi - i\frac{\hbar}{2}\xi\left[\ln\left(\frac{\psi}{\psi^*}\right) - \left\langle\ln\left(\frac{\psi}{\psi^*}\right)\right\rangle\right]\psi. \tag{43}$$

3.2. Madelung Transformation

We use the Madelung [63] transformation to rewrite the generalized GP Equation (39) in the form of hydrodynamic equations. We write the wave function as

$$\psi(\mathbf{r},t) = \sqrt{\rho(\mathbf{r},t)}e^{iS(\mathbf{r},t)/\hbar}, \tag{44}$$

where $\rho(\mathbf{r},t)$ is the density and $S(\mathbf{r},t)$ is the real action. They are given in terms of the wave function by

$$\rho = |\psi|^2 \qquad \text{and} \qquad S = -i\frac{\hbar}{2}\ln\left(\frac{\psi}{\psi^*}\right). \tag{45}$$

We note that the dissipative term in the GP Equation (39) can be written as $\xi(S - \langle S\rangle)\psi$. Following Madelung, we introduce the velocity field

$$\mathbf{u} = \frac{\nabla S}{m}. \tag{46}$$

Since the velocity is potential, the flow is irrotational: $\nabla\times\mathbf{u} = \mathbf{0}$. Substituting Equation (44) into Equation (39) and separating the real and imaginary parts, we obtain

$$\frac{\partial\rho}{\partial t} + \nabla\cdot(\rho\mathbf{u}) = 0, \tag{47}$$

$$\frac{\partial S}{\partial t} + \frac{1}{2m}(\nabla S)^2 + m[\Phi + h(\rho) + \Phi_{\rm ext}] + Q + \xi(S - \langle S\rangle) = 0, \tag{48}$$

where

$$Q = -\frac{\hbar^2}{2m}\frac{\Delta\sqrt{\rho}}{\sqrt{\rho}} = -\frac{\hbar^2}{4m}\left[\frac{\Delta\rho}{\rho} - \frac{1}{2}\frac{(\nabla\rho)^2}{\rho^2}\right] \tag{49}$$

is the quantum potential, which takes into account the Heisenberg uncertainty principle (the kinetic term in the GP equation)[12]. The first equation is similar to the equation of continuity in hydrodynamics. It accounts for the local conservation of mass $M = \int\rho\,d\mathbf{r}$. The second equation has a form similar to the classical Hamilton–Jacobi equation with an additional quantum potential and a source of dissipation. It can also be interpreted as a generalized Bernoulli equation for a potential flow. Taking the gradient of Equation (48) and using the well-known identity of vector analysis $(\mathbf{u}\cdot\nabla)\mathbf{u} = \nabla(\mathbf{u}^2/2) - \mathbf{u}\times(\nabla\times\mathbf{u})$, which reduces to $(\mathbf{u}\cdot\nabla)\mathbf{u} = \nabla(\mathbf{u}^2/2)$ for an irrotational flow, we obtain an equation similar to the Euler equation with a linear friction and a quantum force

$$\frac{\partial\mathbf{u}}{\partial t} + (\mathbf{u}\cdot\nabla)\mathbf{u} = -\nabla h - \nabla\Phi - \nabla\Phi_{\rm ext} - \frac{1}{m}\nabla Q - \xi\mathbf{u}. \tag{50}$$

We can also write Equation (50) in the form

$$\frac{\partial\mathbf{u}}{\partial t} + (\mathbf{u}\cdot\nabla)\mathbf{u} = -\frac{1}{\rho}\nabla P - \nabla\Phi - \nabla\Phi_{\rm ext} - \frac{1}{m}\nabla Q - \xi\mathbf{u}, \tag{51}$$

where $P(\mathbf{r},t)$ is a pressure. Since $h(\mathbf{r},t)=h[\rho(\mathbf{r},t)]$, the pressure $P(\mathbf{r},t)=P[\rho(\mathbf{r},t)]$ is a function of the density, i.e., the flow is barotropic. The equation of state $P(\rho)$ is determined by the function $h(\rho)$ through the relation

$$h'(\rho)=\frac{P'(\rho)}{\rho}. \tag{52}$$

Equation (52) can be integrated into

$$P(\rho)=\rho h(\rho)-V(\rho)=\rho V'(\rho)-V(\rho)=\rho^2\left[\frac{V(\rho)}{\rho}\right]', \tag{53}$$

where V is a primitive of h. It actually corresponds to the total potential $V(|\psi|^2)$ in the GP Equation (38) (see Equation (40)). We have the relation

$$h(\rho)=\frac{P(\rho)+V(\rho)}{\rho}. \tag{54}$$

Equation (53) determines the equation of state $P(\rho)$ for a given potential $V(\rho)$. Conversely, for a given equation of state, the potential is given by

$$V(\rho)=\rho\int\frac{P(\rho)}{\rho^2}\,d\rho. \tag{55}$$

We can add a term of the form $A\rho$ in the potential without changing the pressure. The squared speed of sound is given by

$$c_s^2=P'(\rho)=\rho V''(\rho). \tag{56}$$

In conclusion, the generalized GPP equations are equivalent to the hydrodynamic equations[13]

$$\frac{\partial\rho}{\partial t}+\nabla\cdot(\rho\mathbf{u})=0, \tag{57}$$

$$\frac{\partial\mathbf{u}}{\partial t}+(\mathbf{u}\cdot\nabla)\mathbf{u}=-\frac{1}{\rho}\nabla P-\nabla\Phi-\nabla\Phi_{\rm ext}-\frac{1}{m}\nabla Q-\xi\mathbf{u}, \tag{58}$$

$$\Phi(\mathbf{r},t)=\int u(|\mathbf{r}-\mathbf{r}'|)\rho(\mathbf{r}',t)\,d\mathbf{r}'. \tag{59}$$

The total pressure can be written as $P=P_{\rm id}+P_{\rm int}$ with

$$P_{\rm id}=\rho V_{\rm id}'(\rho)-V_{\rm id}(\rho)=\rho\frac{k_BT}{m}\quad\text{and}\quad P_{\rm int}=\rho V_{\rm int}'(\rho)-V_{\rm int}(\rho). \tag{60}$$

The first term is the equation of state $P_{\rm id}=k_BT\rho/m$ of a perfect gas. In the noninteracting (ideal) case, where $P_{\rm int}=0$, the quantum Euler equation reduces to

$$\frac{\partial\mathbf{u}}{\partial t}+(\mathbf{u}\cdot\nabla)\mathbf{u}=-\frac{k_BT}{m}\nabla\ln\rho-\nabla\Phi-\nabla\Phi_{\rm ext}-\frac{1}{m}\nabla Q-\xi\mathbf{u}. \tag{61}$$

We shall refer to Equations (57)–(59) as the quantum damped Euler equations [76]. We note that these hydrodynamic equations do not involve viscous terms since they are equivalent to the GP equation. As a result, they describe a superfluid. When the quantum potential can be neglected ($Q=0$), we recover the classical damped Euler equations. For dissipationless systems ($\xi=0$), they reduce to the quantum and classical Euler equations.

Remark 3. *As shown in Appendix A, the self-interaction potential V coincides with the density of internal energy u and the function $h=V'(\rho)=(P+V)/\rho$ coincides with the enthalpy $h=(P+u)/\rho$ of a cold gas ($T_{\rm thermo}=0$). The enthalpy is equal to the local chemical potential by* *unit of mass ($h = \mu/m$). This is one component of the total chemical potential (see Equation (110) below). Equations (52) and (53) can be written $dP = \rho dh = n d\mu$ (where $n = \rho/m$ is the numerical density) and $d(u/\rho) = -Pd(1/\rho)$. They correspond to the local Gibbs–Duhem relation and the local first law of thermodynamics for a barotropic gas at $T_{\rm thermo} = 0$. For a given self-interaction potential $V(\rho)$, the enthalpy $h(\rho)$ and the pressure $P(\rho)$ are completely determined by Equations (40) and (53). Explicit results for the standard BEC are given in Appendix A. In particular, $P_{\rm int} = (2\pi a_s \hbar^2/m^3)\rho^2$. Together with the isothermal term, this leads to an equation of state of the form $P = \rho k_B T/m + (2\pi a_s \hbar^2/m^3)\rho^2$, which can describe the structure of dark matter halos [79].*

3.3. Generalized Quantum Smoluchowski Equation

Using the continuity Equation (57), the quantum Euler Equation (58) can be rewritten as

$$\frac{\partial}{\partial t}(\rho \mathbf{u}) + \nabla(\rho \mathbf{u} \otimes \mathbf{u}) = -\nabla P - \rho \nabla \Phi - \rho \nabla \Phi_{\rm ext} - \frac{\rho}{m}\nabla Q - \xi \rho \mathbf{u}. \tag{62}$$

In the overdamped limit $\xi \to +\infty$, we can formally neglect the inertia of the particles in Equation (62) and write

$$\xi \mathbf{u} \simeq -\frac{1}{\rho}\nabla P - \nabla \Phi - \nabla \Phi_{\rm ext} - \frac{1}{m}\nabla Q. \tag{63}$$

Substituting this relation into the continuity Equation (57), we obtain the quantum barotropic Smoluchowski equation [76,128]:

$$\xi \frac{\partial \rho}{\partial t} = \nabla \cdot \left(\nabla P + \rho \nabla \Phi + \rho \nabla \Phi_{\rm ext} + \frac{\rho}{m}\nabla Q \right). \tag{64}$$

When the quantum potential can be neglected, we recover the classical barotropic Smoluchowski equation. Finally, if we neglect the advection term $\nabla(\rho \mathbf{u} \otimes \mathbf{u})$ in Equation (62), but retain the term $\partial(\rho \mathbf{u})/\partial t$ and combine the resulting expression with the continuity Equation (57), we obtain the quantum barotropic telegraph equation

$$\frac{\partial^2 \rho}{\partial t^2} + \xi \frac{\partial \rho}{\partial t} = \nabla \cdot \left(\nabla P + \rho \nabla \Phi + \rho \nabla \Phi_{\rm ext} + \frac{\rho}{m}\nabla Q \right). \tag{65}$$

It can be seen as a generalization of the quantum barotropic Smoluchowski Equation (64) taking inertial (or memory) effects into account [76].

In the noninteracting (ideal) case, where $P_{\rm int} = 0$, the quantum Smoluchowski equation and the telegraph equation reduce to

$$\xi \frac{\partial \rho}{\partial t} = \nabla \cdot \left(\frac{k_B T}{m}\nabla \rho + \rho \nabla \Phi + \rho \nabla \Phi_{\rm ext} + \frac{\rho}{m}\nabla Q \right) \tag{66}$$

and

$$\frac{\partial^2 \rho}{\partial t^2} + \xi \frac{\partial \rho}{\partial t} = \nabla \cdot \left(\frac{k_B T}{m}\nabla \rho + \rho \nabla \Phi + \rho \nabla \Phi_{\rm ext} + \frac{\rho}{m}\nabla Q \right). \tag{67}$$

The classical diffusion coefficient is given by the Einstein relation (1).

3.4. Quantum Force

The quantum potential (49) first appeared in the work of Madelung [63] and was rediscovered later by Bohm [64,65]. For that reason, it is sometimes called "the Bohm potential". The quantum force by unit of mass reads

$$\mathbf{F}_Q = -\frac{1}{m}\nabla Q. \tag{68}$$

It can be written in the form

$$(F_Q)_i = -\frac{1}{m}\partial_i Q = -\frac{1}{\rho}\partial_j P_{ij}, \tag{69}$$

where P_{ij} is a tensor defined by

$$P_{ij}^{(1)} = -\frac{\hbar^2}{4m^2}\rho\,\partial_i\partial_j \ln\rho = \frac{\hbar^2}{4m^2}\left(\frac{1}{\rho}\partial_i\rho\partial_j\rho - \partial_i\partial_j\rho\right) \tag{70}$$

or

$$P_{ij}^{(2)} = \frac{\hbar^2}{4m^2}\left(\frac{1}{\rho}\partial_i\rho\partial_j\rho - \delta_{ij}\Delta\rho\right). \tag{71}$$

This tensor is manifestly symmetric: $P_{ij} = P_{ji}$. It is called the quantum stress (or pressure) tensor [129]. Equation (69) shows that the quantum force $-\nabla Q$ is equivalent to the force produced by an anisotropic pressure tensor P_{ij}. In comparison, the force $-m\nabla h$ due to the self-interaction is equivalent to the force produced by an isotropic pressure $P(\rho)$.

3.5. Time-Independent GP Equation

A wave function of the form

$$\psi(\mathbf{r},t) = \phi(\mathbf{r})e^{-iEt/\hbar}, \tag{72}$$

where $\phi(\mathbf{r}) = \sqrt{\rho(\mathbf{r})}$ and E are real, is a stationary solution of the GP Equation (39). Substituting Equation (72) into Equations (36) and (39), we obtain the time-independent GP equation

$$-\frac{\hbar^2}{2m}\Delta\phi + m(\Phi + h(\rho) + \Phi_{\rm ext})\phi = E\phi \tag{73}$$

with

$$\Phi(\mathbf{r}) = \int u(|\mathbf{r}-\mathbf{r}'|)\phi^2(\mathbf{r}')\,d\mathbf{r}'. \tag{74}$$

Equations (73) and (74) define a nonlinear eigenvalue problem for the wave function $\phi(\mathbf{r})$, where the eigenvalue E is the energy (eigenenergy). Dividing Equation (73) by $\phi(\mathbf{r})$ and recalling that $\rho = \phi^2$, we obtain

$$m\Phi + mh(\rho) + m\Phi_{\rm ext} + Q = E. \tag{75}$$

This relation can also be derived from the quantum damped Hamilton–Jacobi Equation (48) by writing $S = -Et$.

3.6. Hydrostatic Equilibrium

The time-independent GP Equation (75) can also be obtained from the quantum damped barotropic Euler Equation (51) since it is equivalent to the generalized GP Equation (39). The equilibrium state of the quantum damped barotropic Euler Equation (51), obtained by taking $\partial_t = 0$ and $\mathbf{u} = \mathbf{0}$, satisfies the condition of quantum hydrostatic equilibrium

$$\nabla P + \rho\nabla\Phi + \rho\nabla\Phi_{\rm ext} + \frac{\rho}{m}\nabla Q = \mathbf{0}. \tag{76}$$

Equation (76) describes the balance between the pressure due to effective thermal effects (quantum interferences of excited states) and self-interaction (scattering), the long-range potential, the external potential, and the quantum potential arising from the Heisenberg uncertainty principle. This equation is equivalent to Equation (75). Indeed, integrating

Equation (76) using Equation (52), we obtain Equation (75), where the eigenenergy E appears as a constant of integration.

4. Generalized Thermodynamics

In this section, we develop a thermodynamical formalism associated with the generalized GP Equations (35) and (36). We stress from the start that this thermodynamical formalism is effective since we are basically considering a boson gas at zero thermodynamic temperature ($T_{\rm thermo} = 0$). However, a deep analogy with thermodynamics arises from the presence of the nonlinear term in the generalized GP Equation (35) giving rise to a pressure force in the quantum Euler Equation (58). We must keep in mind that this pressure does not have a true thermal origin. In particular, the temperature T, which occurs in the ideal equation of state $P_{\rm id} = \rho k_B T/m$, should be considered as an effective temperature $T_{\rm eff}$, not as the true thermodynamical temperature (see [76,77] for a more detailed discussion on that point). As we shall see, this thermodynamical formalism is closely related to the one developed in refs. [17,37,38,130,131] in connection with nonlinear Fokker–Planck equations [132] and the theory of simple liquids [33].

4.1. Free Energy

The free energy associated with the generalized GP Equations (35) and (36), or equivalently with the quantum damped barotropic Euler Equations (57)–(59), can be written as

$$F_{\rm tot} = \Theta_c + \Theta_Q + U + W + W_{\rm ext}. \tag{77}$$

The first two terms in Equation (77) correspond to the total kinetic energy

$$\Theta = \frac{\hbar^2}{2m^2}\int |\nabla\psi|^2\, d\mathbf{r}. \tag{78}$$

Using the Madelung transformation, the kinetic energy $\Theta = \Theta_c + \Theta_Q$ can be decomposed into the classical kinetic energy

$$\Theta_c = \int \rho \frac{\mathbf{u}^2}{2}\, d\mathbf{r} \tag{79}$$

and the quantum kinetic energy (or the von Weizsäcker [133] functional)

$$\Theta_Q = \frac{\hbar^2}{8m^2}\int \frac{(\nabla\rho)^2}{\rho}\, d\mathbf{r} = \frac{1}{m}\int \rho Q\, d\mathbf{r}. \tag{80}$$

The third term in Equation (77) is the internal energy

$$U = \int V(\rho)\, d\mathbf{r} = \int \rho \int^{\rho} \frac{P(\rho')}{\rho'^2}\, d\rho'\, d\mathbf{r}. \tag{81}$$

Using Equation (37), it can be decomposed into $U = U_{\rm id} + U_{\rm int}$ with

$$U_{\rm id} = \frac{k_B T}{m}\int \rho(\ln\rho - 1)\, d\mathbf{r} \quad \text{and} \quad U_{\rm int} = \int V_{\rm int}(\rho)\, d\mathbf{r}. \tag{82}$$

The first term is the ideal (Boltzmann) internal energy and the second term is the internal energy associated with the self-interaction[14]. The fourth term in Equation (77) is the potential energy of long-range interactions

$$W = \frac{1}{2}\int \rho\Phi\, d\mathbf{r}. \tag{83}$$

The fifth term in Equation (77) is the external potential energy

$$W_{\rm ext}=\int \rho\Phi_{\rm ext}\, d\mathbf{r}. \tag{84}$$

Regrouping all these terms, the total free energy can be explicitly written as

$$F_{\rm tot}=\frac{\hbar^2}{2m^2}\int |\nabla\psi|^2\, d\mathbf{r}+\int V(|\psi|^2)\, d\mathbf{r}+\frac{1}{2}\int |\psi|^2\Phi\, d\mathbf{r}+\int |\psi|^2\Phi_{\rm ext}\, d\mathbf{r} \tag{85}$$

or, in terms of hydrodynamic variables, as

$$F_{\rm tot}=\int \rho\frac{\mathbf{u}^2}{2}\, d\mathbf{r}+\frac{1}{m}\int \rho Q\, d\mathbf{r}+\int V(\rho)\, d\mathbf{r}+\frac{1}{2}\int \rho\Phi\, d\mathbf{r}+\int \rho\Phi_{\rm ext}\, d\mathbf{r}. \tag{86}$$

It is convenient to write

$$F_{\rm tot}=\Theta_c+F, \tag{87}$$

where Θ_c is the classical kinetic energy and

$$F=\Theta_Q+U+W+W_{\rm ext} \tag{88}$$

is the sum of the quantum kinetic energy, the internal energy, the potential energy of long-range interactions, and the external potential energy. Explicitly,

$$F=\frac{1}{m}\int \rho Q\, d\mathbf{r}+\int V(\rho)\, d\mathbf{r}+\frac{1}{2}\int \rho\Phi\, d\mathbf{r}+\int \rho\Phi_{\rm ext}\, d\mathbf{r}. \tag{89}$$

This is the free energy associated with the quantum barotropic Smoluchowski Equation (64) since the classical kinetic energy Θ_c, which is of order $O(\xi^{-2})$, can be neglected in the overdamped limit $\xi\rightarrow+\infty$.

For future reference, we also perform the decomposition

$$F_{\rm tot}=\Theta+\mathcal{F}\qquad \text{or}\qquad F=\Theta_Q+\mathcal{F}, \tag{90}$$

where Θ is the total kinetic energy (classical + quantum) and

$$\mathcal{F}=U+W+W_{\rm ext} \tag{91}$$

is the sum of the internal energy, the potential energy of long-range interactions, and the external potential energy.

4.2. H-Theorem

It is shown in [76] that the time derivative of the free energy (77) satisfies the identity

$$\dot{F}_{\rm tot}=-\xi\int \rho\mathbf{u}^2\, d\mathbf{r}=-2\xi\Theta_c. \tag{92}$$

For dissipationless BECs ($\xi=0$), the free energy is conserved: $\dot{F}_{\rm tot}=0$. In that case, it can be shown from general arguments [134] that a minimum of free energy at fixed mass determines a steady state of the GP equations, or a steady state of the quantum barotropic Euler equations, which is formally nonlinearly dynamically stable.

For dissipative BECs ($\xi>0$), Equation (92) forms an H-theorem for the generalized GP equations or for the quantum damped barotropic Euler equations: $\dot{F}_{\rm tot}\le 0$. In that case, it can be shown from Lyapunov's direct method that the system relaxes towards a minimum of free energy at fixed mass (provided that the free energy is bounded from below). This equilibrium state is nonlinearly dynamically stable.

In the strong friction limit, the H-theorem for the quantum Smoluchowski equation reads [76]

$$\dot{F} = -\frac{1}{\xi}\int \frac{1}{\rho}\left(\nabla P + \rho\nabla\Phi + \rho\nabla\Phi_{\rm ext} + \frac{\rho}{m}\nabla Q\right)^2 d\mathbf{r} \le 0. \tag{93}$$

4.3. Equilibrium State

According to the previous discussion, the equilibrium state of the (generalized) GP equations, or quantum (damped) barotropic Euler equations, is the solution of the minimization problem

$$F_{\rm tot}(M) = \min_{\rho,\mathbf{u}}\{F_{\rm tot}[\rho,\mathbf{u}] \quad | \quad M \quad \text{fixed}\}. \tag{94}$$

An extremum of free energy at fixed mass is determined by the variational principle

$$\delta F_{\rm tot} - \frac{\mu}{m}\delta M = 0, \tag{95}$$

where μ is a Lagrange multiplier taking into account the mass constraint. It can be interpreted as a global chemical potential. Using the results of Appendix B, this variational principle gives $\mathbf{u} = \mathbf{0}$ (the equilibrium state is static) and the relation

$$m\Phi + m\Phi_{\rm ext} + mh(\rho) + Q = \mu. \tag{96}$$

This relation can be interpreted as a quantum Gibbs condition expressing the fact that the gravitational potential Φ plus the external potential $\Phi_{\rm ext}$ plus the enthalpy $h = V'(\rho)$ plus the quantum potential Q/m is a constant equal to the global chemical potential by unit of mass μ/m. In this sense, the enthalpy h can be interpreted as a local chemical potential $h = \mu_{\rm loc}(\rho)/m$. Taking the gradient of Equation (96) and using Equation (52), we recover the condition of quantum hydrostatic equilibrium (76). Equation (96) is also equivalent to the time-independent GP Equation (75) provided that we make the identification

$$\mu = E. \tag{97}$$

This shows that the Lagrange multiplier μ (the global chemical potential) in the variational principle (95) associated with the minimization problem (94) can be identified with the eigenenergy E. Conversely, the eigenenergy E may be interpreted as a chemical potential. To determine the stability of the equilibrium state (if it is a minimum of the free energy at fixed mass), we can study the sign of $\delta^2 F$ or linearize the equations of motion about the equilibrium state and investigate the sign of the squared pulsation ω^2. These methods require one to solve a rather complicated eigenvalue equation. Alternatively, the stability of an equilibrium state can be settled more directly by plotting the series of equilibria and using the Poincaré criterion (see ref. [76] for more details about these different methods).

4.4. Functional Derivatives in Terms of the Hydrodynamic Variables

In this section, we show that the hydrodynamic equations associated with the generalized GP equation can be expressed in terms of functional derivatives of the free energy. Taking the functional derivative of the free energy (89) with respect to ρ, and using the relations in Appendix B, we obtain

$$\frac{\delta F}{\delta\rho} = \Phi + h(\rho) + \Phi_{\rm ext} + \frac{Q}{m}. \tag{98}$$

Taking the gradient of this relation and using Equation (52), we obtain

$$\nabla\cdot\left(\frac{\delta F}{\delta\rho}\right)=\nabla\Phi+\frac{1}{\rho}\nabla P+\nabla\Phi_{\rm ext}+\frac{1}{m}\nabla Q. \tag{99}$$

According to Equation (95), the equilibrium state is determined by the Gibbs condition

$$\frac{\delta F}{\delta\rho}=\frac{\mu}{m}, \tag{100}$$

where μ is a constant. Using Equation (98), we recover Equation (96). Taking the gradient of Equation (100), we obtain

$$\nabla\cdot\left(\frac{\delta F}{\delta\rho}\right)=\mathbf{0}. \tag{101}$$

Using Equation (99), we recover the condition of quantum hydrostatic equilibrium (76). On the other hand, the hydrodynamic Equations (57) and (58) can be written as

$$\frac{\partial\rho}{\partial t}+\nabla\cdot(\rho\mathbf{u})=0, \tag{102}$$

$$\frac{\partial\mathbf{u}}{\partial t}+(\mathbf{u}\cdot\nabla)\mathbf{u}=-\nabla\left(\frac{\delta F}{\delta\rho}\right)-\xi\mathbf{u}. \tag{103}$$

In the strong friction limit $\xi\rightarrow+\infty$, we can make the approximation

$$\xi\mathbf{u}\simeq-\nabla\left(\frac{\delta F}{\delta\rho}\right). \tag{104}$$

Substituting Equation (104) into Equation (102), we obtain

$$\xi\frac{\partial\rho}{\partial t}=\nabla\cdot\left(\rho\nabla\frac{\delta F}{\delta\rho}\right), \tag{105}$$

which corresponds to the quantum barotropic Smoluchowski Equation (64). The H-theorems for Equations (102) and (103) and for Equation (105) are derived in Appendix C. These equations relax towards a stable equilibrium state, which minimizes the free energy at fixed mass. It is determined by Equation (100).

Remark 4. *Since the flow is irrotational, we have* $(\mathbf{u}\cdot\nabla)\mathbf{u}=\nabla(\mathbf{u}^2/2)$. *Using* $\delta\Theta_c/\delta\rho=\mathbf{u}^2/2$, *Equation (103) can also be written as*

$$\frac{\partial\mathbf{u}}{\partial t}=-\nabla\left(\frac{\delta F_{\rm tot}}{\delta\rho}\right)-\xi\mathbf{u}. \tag{106}$$

The out-of-equilibrium energy is defined by

$$E(\mathbf{r},t)=m\frac{\delta F_{\rm tot}}{\delta\rho} \tag{107}$$

and the out-of-equilibrium chemical potential is defined by

$$\mu(\mathbf{r},t)=m\frac{\delta F}{\delta\rho}. \tag{108}$$

We can then write the foregoing equations in terms of $E(\mathbf{r},t)$ *and* $\mu(\mathbf{r},t)$ *instead of* $\delta F_{\rm tot}/\delta\rho$ *and* $\delta F/\delta\rho$. *Using the relations in Appendix B, we have*

$$E(\mathbf{r},t)=\frac{1}{2}m\mathbf{u}^2+m\Phi+mh(\rho)+m\Phi_{\rm ext}+Q \tag{109}$$

and

$$\mu(\mathbf{r},t) = m\Phi + mh(\rho) + m\Phi_{\rm ext} + Q, \tag{110}$$

so that

$$E(\mathbf{r},t) = \frac{1}{2}m\mathbf{u}^2 + \mu(\mathbf{r},t). \tag{111}$$

Comparing Equation (109) with Equation (48), we obtain

$$E(\mathbf{r},t) = -\frac{\partial S}{\partial t} - \xi(S - \langle S\rangle). \tag{112}$$

For dissipationless systems, this equation reduces to $E(\mathbf{r},t) = -\partial S/\partial t$. *At equilibrium,* $\mu(\mathbf{r},t) = \mu$ *and* $E(\mathbf{r},t) = E$ *are constant and* $E = \mu$.

4.5. Functional Derivatives in Terms of the Wave Function

The generalized GP Equation (35) can also be written in terms of the functional derivative of a free energy. For example, it can be written as

$$i\hbar\frac{\partial\psi}{\partial t} = m\frac{\delta F_{\rm tot}}{\delta\psi^*} - i\frac{\hbar}{2}\xi\left[\ln\left(\frac{\psi}{\psi^*}\right) - \left\langle\ln\left(\frac{\psi}{\psi^*}\right)\right\rangle\right]\psi, \tag{113}$$

where $F_{\rm tot}$ is defined by Equation (85). From Equations (85) and (113), we easily obtain the identity (see Appendix C)

$$\dot{F}_{\rm tot} = -\xi\int\frac{\hbar^2}{4m^2}|\psi|^2\left|\nabla\ln\left(\frac{\psi}{\psi^*}\right)\right|^2 d\mathbf{r}, \tag{114}$$

which coincides with the H-theorem from Equation (92). We can also write the generalized GP Equation (35) as

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\Delta\psi + m\frac{\delta\mathcal{F}}{\delta|\psi|^2}\psi - i\frac{\hbar}{2}\xi\left[\ln\left(\frac{\psi}{\psi^*}\right) - \left\langle\ln\left(\frac{\psi}{\psi^*}\right)\right\rangle\right]\psi, \tag{115}$$

where $\mathcal{F}$ is defined by Equation (91).

5. Statistical Equilibrium State of a System of Classical Brownian Particles

5.1. Gibbs Canonical Equilibrium

We consider a system of N classical Brownian particles with identical mass m interacting via a potential $U(\mathbf{r}_1,\ldots,\mathbf{r}_N)$. We assume that the potential is of the form

$$U(\mathbf{r}_1,\ldots,\mathbf{r}_N) = m^2\sum_{i<j}u_{\rm LR}(|\mathbf{r}_i - \mathbf{r}_j|) + m^2\sum_{i<j}u_{\rm SR}(|\mathbf{r}_i - \mathbf{r}_j|) + m\sum_i\Phi_{\rm ext}(\mathbf{r}_i), \tag{116}$$

where $u_{\rm LR}$ is a long-range binary potential, $u_{\rm SR}$ is a short-range binary potential, and $\Phi_{\rm ext}$ is an external potential. The Hamiltonian is

$$H = \sum_{i=1}^N\frac{1}{2}mv_i^2 + U(\mathbf{r}_1,\ldots,\mathbf{r}_N), \tag{117}$$

where the first term is the kinetic energy K and the second the potential energy U. These Brownian particles are in contact with a heat bath fixing the temperature T. Accordingly, they are described by the canonical ensemble. The statistical equilibrium state is given by the Gibbs canonical distribution

$$P_N(\mathbf{r}_1,\mathbf{v}_1,\ldots,\mathbf{r}_N,\mathbf{v}_N) = \frac{1}{Z_{\rm tot}(\beta)}e^{-\beta\left[\sum_{i=1}^N m\frac{v_i^2}{2} + U(\mathbf{r}_1,\ldots,\mathbf{r}_N)\right]}, \tag{118}$$

where $\beta = 1/(k_B T)$ is the inverse temperature. The N-body distribution $P_N(\mathbf{r}_1, \mathbf{v}_1, \ldots, \mathbf{r}_N, \mathbf{v}_N)$ gives the probability density that the first particle is at position $\mathbf{r}_1$ with velocity $\mathbf{v}_1$, the second particle at position $\mathbf{r}_2$ with velocity $\mathbf{v}_2$, etc. The normalization condition given by $\int P_N d\mathbf{r}_1 d\mathbf{v}_1 \ldots d\mathbf{r}_N d\mathbf{v}_N = 1$ determines the partition function $Z_{\rm tot}(\beta) = \int e^{-\beta H} \prod_i d\mathbf{r}_i d\mathbf{v}_i$. We introduce the free energy functional

$$F_{\rm tot}[P_N] = E_{\rm tot}[P_N] - T S_{\rm tot}[P_N], \tag{119}$$

where

$$E_{\rm tot} = \langle H \rangle = \int P_N H \, d\mathbf{r}_1 d\mathbf{v}_1 \ldots d\mathbf{r}_N d\mathbf{v}_N \tag{120}$$

is the average energy and

$$S_{\rm tot} = -k_B \int P_N \ln P_N \, d\mathbf{r}_1 d\mathbf{v}_1 \ldots d\mathbf{r}_N d\mathbf{v}_N \tag{121}$$

is the entropy. The canonical N-body distribution (118) minimizes the free energy $F_{\rm tot}[P_N]$ under the normalization constraint. Furthermore, the value of the free energy at equilibrium, obtained by substituting the Gibbs distribution (118) into Equations (120) and (121), is $F_{\rm tot}(\beta) = -(1/\beta) \ln Z_{\rm tot}(\beta)$. The average energy at equilibrium can be obtained from the relation $E_{\rm tot}(\beta) = -d \ln Z_{\rm tot}/d\beta$. The fluctuations of energy are given by $\langle (\Delta E)^2 \rangle = C/(k_B \beta^2)$, where $C = dE_{\rm tot}/dT = -k_B \beta^2 dE_{\rm tot}/d\beta$ is the specific heat. This relation was first established by Gibbs and Einstein. It shows that the specific heat is always positive in the canonical ensemble [135].

From Equation (118), we see that the velocity dependence of the N-body distribution is Gaussian. Therefore, the average kinetic energy is $\langle K \rangle = dNk_B T/2$ (where d is the dimension of space) like for a noninteracting gas. In the following, we shall mainly focus on the configurational part of the distribution function

$$P_N(\mathbf{r}_1, \ldots, \mathbf{r}_N) = \frac{1}{Z(\beta)} e^{-\beta U(\mathbf{r}_1, \ldots, \mathbf{r}_N)}, \tag{122}$$

which contains the nontrivial information on the system. The normalization condition given by $\int P_N d\mathbf{r}_1 \ldots d\mathbf{r}_N = 1$ determines the configurational partition function $Z(\beta) = \int e^{-\beta U} \prod_i d\mathbf{r}_i$. Due to the Gaussian nature of the velocity distribution, we have

$$P_N(\mathbf{r}_1, \mathbf{v}_1, \ldots, \mathbf{r}_N, \mathbf{v}_N) = \left(\frac{\beta m}{2\pi} \right)^{dN/2} e^{-\beta \sum_{i=1}^N m \frac{v_i^2}{2}} P_N(\mathbf{r}_1, \ldots, \mathbf{r}_N). \tag{123}$$

Comparing Equations (118), (122) and (123), we find that $Z_{\rm tot}(\beta) = (2\pi/\beta m)^{dN/2} Z(\beta)$. We introduce the configurational free energy

$$F[P_N] = E[P_N] - TS[P_N], \tag{124}$$

where

$$E = \langle U \rangle = \int P_N U \, d\mathbf{r}_1 \ldots d\mathbf{r}_N \tag{125}$$

is the average potential energy and

$$S = -k_B \int P_N \ln P_N \, d\mathbf{r}_1 \ldots d\mathbf{r}_N \tag{126}$$

is the configurational entropy. These expressions can be obtained by substituting Equation (123) into Equations (120) and (121). This yields additional constant terms $(d/2)Nk_B T$ and $(d/2) Nk_B \ln(2\pi k_B T/m) + (d/2)Nk_B$ in Equations (125) and (126), which we have not written [38].

The canonical N-body distribution (122) minimizes $F[P_N]$ under the normalization constraint. Furthermore, the value of the free energy at equilibrium, obtained by substituting Equation (122) into Equations (125) and (126), is $F(\beta) = -(1/\beta)\ln Z(\beta)$. The average energy and the fluctuations of energy are given by $E(\beta) = -d\ln Z/d\beta$ and $\langle(\Delta E)^2\rangle = C/(k_B\beta^2)$, where $C = dE/dT = -k_B\beta^2 dE/d\beta$ is the specific heat.

5.2. Yvon–Born–Green (YBG) Hierarchy

From the Gibbs distribution (122), we can obtain a hierarchy of equations for the reduced probability distributions (see Equation (13) in [37]). This is the so-called Yvon–Born–Green (YBG) hierarchy [136–138]. The first equation of this hierarchy can be written as

$$\frac{k_B T}{m}\nabla\rho(\mathbf{r}) = -\int \rho_2(\mathbf{r},\mathbf{r}')\nabla u(|\mathbf{r}-\mathbf{r}'|)\,d\mathbf{r}' - \rho(\mathbf{r})\nabla\Phi_{\rm ext}(\mathbf{r}), \tag{127}$$

where $\rho(\mathbf{r}) = NmP_1(\mathbf{r})$ is the spatial density (one-body probability density) and $\rho_2(\mathbf{r},\mathbf{r}') = N(N-1)m^2P_2(\mathbf{r},\mathbf{r}')$ is the two-body density (two-body probability density). This equation determines the equilibrium density profile $\rho(\mathbf{r})$ when the two-body density is known. Since the velocity distribution is Gaussian, the equilibrium distribution function in phase space $f(\mathbf{r},\mathbf{v}) = NmP_1(\mathbf{r},\mathbf{v})$ is given by

$$f(\mathbf{r},\mathbf{v}) = \left(\frac{\beta m}{2\pi}\right)^{d/2}\rho(\mathbf{r})e^{-\beta m\frac{v^2}{2}}. \tag{128}$$

Equation (127) can be written as a condition of hydrostatic equilibrium

$$\nabla P_{\rm id}(\mathbf{r}) + \int \rho_2(\mathbf{r},\mathbf{r}')\nabla u(|\mathbf{r}-\mathbf{r}'|)\,d\mathbf{r}' + \rho(\mathbf{r})\nabla\Phi_{\rm ext}(\mathbf{r}) = \mathbf{0}, \tag{129}$$

where $P_{\rm id}$ is the ideal pressure given by the isothermal equation of state

$$P_{\rm id}(\mathbf{r}) = \rho(\mathbf{r})\frac{k_B T}{m}. \tag{130}$$

This is the equation of state of a noninteracting perfect gas. The ideal pressure corresponds to the kinetic pressure defined by

$$P_{\rm id}(\mathbf{r}) = P_{\rm kin}(\mathbf{r}) = \frac{1}{d}\int f v^2\,d\mathbf{v}. \tag{131}$$

We note that the YBG hierarchy is not closed since the equation for $\rho(\mathbf{r})$ involves the equation for $\rho_2(\mathbf{r},\mathbf{r}')$ and so on. In the following sections, we explain how one can close the YBG hierarchy by making a mean field approximation for long-range interactions or by using the DFT for short-range interactions.

5.3. Long-Range Interactions: Mean Field Approximation

For long-range interactions, it has been established rigorously [139] that, in a proper thermodynamic limit $N \to +\infty$ with $m \sim 1/N$, the mean field approximation is exact: the N-body distribution function is a product of N one-body distribution functions. In particular,

$$\rho_2(\mathbf{r},\mathbf{r}') = \rho(\mathbf{r})\rho(\mathbf{r}'). \tag{132}$$

Therefore, in the mean field approximation, we have

$$\int \rho_2(\mathbf{r},\mathbf{r}')\nabla u_{\rm LR}(|\mathbf{r}-\mathbf{r}'|)\,d\mathbf{r}' = \rho(\mathbf{r})\nabla\int \rho(\mathbf{r}')u_{\rm LR}(|\mathbf{r}-\mathbf{r}'|)\,d\mathbf{r}'. \tag{133}$$

This equation can be written as

$$\int \rho_2(\mathbf{r},\mathbf{r}')\nabla u_{\rm LR}(|\mathbf{r}-\mathbf{r}'|)\,d\mathbf{r}' = \rho(\mathbf{r})\nabla\Phi(\mathbf{r}), \tag{134}$$

where

$$\Phi(\mathbf{r}) = \int \rho(\mathbf{r}')u_{\rm LR}(|\mathbf{r}-\mathbf{r}'|)\,d\mathbf{r}' \tag{135}$$

is the mean field potential produced by the smooth distribution of particles.

For a binary potential of interaction, the average potential energy (125) can be written as

$$W = \frac{1}{2}\int \rho_2(\mathbf{r},\mathbf{r}')u(|\mathbf{r}-\mathbf{r}'|)\,d\mathbf{r}d\mathbf{r}'. \tag{136}$$

For long-range interactions, we can make the mean field approximation from Equation (132) and we obtain

$$W = \frac{1}{2}\int \rho_2(\mathbf{r},\mathbf{r}')u_{\rm LR}(|\mathbf{r}-\mathbf{r}'|)\,d\mathbf{r}d\mathbf{r}' = \frac{1}{2}\int \rho(\mathbf{r})\rho(\mathbf{r}')u_{\rm LR}(|\mathbf{r}-\mathbf{r}'|)\,d\mathbf{r}d\mathbf{r}'. \tag{137}$$

Introducing the mean field potential from Equation (135), we can rewrite the potential energy as

$$W[\rho] = \frac{1}{2}\int \rho\Phi d\mathbf{r}. \tag{138}$$

On the other hand, the configurational entropy from Equation (126) becomes

$$S = -k_B\int \frac{\rho}{m}\ln\frac{\rho}{m}d\mathbf{r}. \tag{139}$$

5.4. Short-Range Interactions: Density Functional Theory

We now consider a system of Brownian particles with long-range and short-range interactions. A central result in the theory of fluids [33,34] is that, even if there exist nontrivial correlations between the particles, the equilibrium density profile $\rho(\mathbf{r})$ minimizes a free energy functional $F[\rho]$ at fixed mass. This free energy can be written as

$$F[\rho] = \int \rho\Phi_{\rm ext}d\mathbf{r} + \frac{1}{2}\int \rho\Phi\,d\mathbf{r} + k_BT\int \frac{\rho}{m}\ln\frac{\rho}{m}d\mathbf{r} + F_{\rm ex}[\rho]. \tag{140}$$

The first term is the potential energy associated with the external potential. The second term is the mean field potential energy associated with the long-range potential of interaction (see Section 5.3). The third term is the Boltzmann free energy of the ideal gas, i.e., in the absence of correlations. Finally, the fourth term is the excess free energy $F_{\rm ex}[\rho]$. This is a nontrivial functional of the density determined by the short-range interactions. All the difficulty in the theory of fluids is to find some approximate forms of this functional. Once this functional is known, the spatial density, and all the n-point correlation functions, can be obtained via functional differentiation. Inversely, the excess free energy is often obtained from the study of the correlation functions. The excess free energy $F_{\rm ex}$ is only known exactly for some simple systems, such as hard rods in one dimension [140], but very good approximations can be devised in more general cases (see [33] for some standard methods).

The fact that the spatial density minimizes a free energy functional at fixed mass implies that its first constrained variations vanish. Writing

$$\delta F - \frac{\mu}{m}\delta M = 0, \tag{141}$$

where μ (global chemical potential) is a Lagrange multiplier taking into account the conservation of mass, we obtain the Gibbs condition

$$\frac{\delta F}{\delta \rho} = \frac{\mu}{m}, \tag{142}$$

where μ is a constant[15]. With the decomposition from Equation (140) and the identities in Appendix B, the Gibbs condition (142) can be written as

$$\frac{k_B T}{m}[1 + \ln(\rho/m)] + \Phi + \Phi_{\rm ext} + \frac{\delta F_{\rm ex}}{\delta \rho} = \frac{\mu}{m}. \tag{143}$$

The equilibrium density profile is then determined by the equation

$$\rho = A e^{-\beta m \left(\Phi + \Phi_{\rm ext} + \frac{\delta F_{\rm ex}}{\delta \rho}\right)}. \tag{144}$$

We stress that the r.h.s. of this equation depends on $\rho(\mathbf{r})$ itself through Φ and $F_{\rm ex}$, so that Equation (144) is a complicated integrodifferential equation.

Taking the gradient of Equation (142), we obtain the condition of hydrostatic equilibrium

$$\nabla \left(\frac{\delta F}{\delta \rho} \right) = \mathbf{0}. \tag{145}$$

With the decomposition from Equation (140), it reads

$$\frac{k_B T}{m} \nabla \rho + \rho \nabla \frac{\delta F_{\rm ex}}{\delta \rho} + \rho \nabla \Phi + \rho \nabla \Phi_{\rm ext} = \mathbf{0}. \tag{146}$$

On the other hand, the first equation of the YBG hierarchy (see Equation (127)) including long-range and short-range interactions reads

$$\frac{k_B T}{m} \nabla \rho = -\int \rho_2(\mathbf{r}, \mathbf{r}') \nabla u_{\rm SR}(|\mathbf{r} - \mathbf{r}'|)\, d\mathbf{r}' - \rho \nabla \Phi - \rho \nabla \Phi_{\rm ext}, \tag{147}$$

where we used Equation (134) to evaluate the long-range interaction term. Comparing Equations (146) and (147), we find that

$$\int \rho_2(\mathbf{r}, \mathbf{r}') \nabla u_{\rm SR}(|\mathbf{r} - \mathbf{r}'|)\, d\mathbf{r}' = \rho(\mathbf{r}) \nabla \frac{\delta F_{\rm ex}}{\delta \rho}[\rho(\mathbf{r})]. \tag{148}$$

This relation is exact at statistical equilibrium and is a central result in the theory of fluids [33,34]. It relates the two-body density to the excess free energy functional. Then, Equation (147) can be viewed as an integrodifferential equation (equivalent to Equation (144)) determining the equilibrium density profile once the excess free energy is known.

5.5. Excess Free Energy Functional for a Barotropic Gas

For an excess free energy of the form (see Appendix D)

$$F_{\rm ex} = \int f_{\rm ex}(\rho)\, d\mathbf{r} = \int \rho \int^{\rho} \frac{P_{\rm ex}(\rho')}{\rho'^2}\, d\rho'\, d\mathbf{r}, \tag{149}$$

where $P_{\rm ex}$ is the excess pressure, the total free energy (140) becomes

$$F[\rho] = \int \rho \Phi_{\rm ext} d\mathbf{r} + \frac{1}{2} \int \rho \Phi\, d\mathbf{r} + k_B T \int \frac{\rho}{m} \ln \frac{\rho}{m} d\mathbf{r} + \int f_{\rm ex}(\rho)\, d\mathbf{r}. \tag{150}$$

Introducing the total density of free energy $f = f_{\rm id} + f_{\rm ex}$, where

$$f_{\rm id}(\rho) = \frac{k_B T}{m} \rho \ln \frac{\rho}{m} \tag{151}$$

is the ideal density of free energy and $f_{\rm ex}$ is the excess density of free energy, we can rewrite Equation (150) as

$$F[\rho] = \int \rho \Phi_{\rm ext} d\mathbf{r} + \frac{1}{2} \int \rho \Phi \, d\mathbf{r} + \int f(\rho) \, d\mathbf{r}. \tag{152}$$

The Gibbs condition (142) takes the form

$$\frac{k_B T}{m} [1 + \ln(\rho/m)] + \Phi + \Phi_{\rm ext} + f'_{\rm ex}(\rho) = \frac{\mu}{m}, \tag{153}$$

where $h_{\rm ex}(\rho) = f'_{\rm ex}(\rho)$ can be interpreted as an excess enthalpy (see Appendix D). The equilibrium density profile is determined by the equation

$$\rho = A e^{-\beta m [\Phi + \Phi_{\rm ext} + f'_{\rm ex}(\rho)]}, \tag{154}$$

where the r.h.s. depends on ρ through Φ and $f_{\rm ex}$. Using the identity (see Equation (A67))

$$\rho \nabla \frac{\delta F_{\rm ex}}{\delta \rho} = \nabla P_{\rm ex}, \tag{155}$$

the condition of hydrostatic equilibrium (145) takes the form

$$\frac{k_B T}{m} \nabla \rho + \nabla P_{\rm ex} + \rho \nabla \Phi + \rho \nabla \Phi_{\rm ext} = \mathbf{0}, \tag{156}$$

where the excess pressure $P_{\rm ex}(\rho)$ is determined from $f_{\rm ex}(\rho)$ by (see Equation (A60))

$$P_{\rm ex}(\rho) = -\frac{d(f_{\rm ex}/\rho)}{d(1/\rho)} = \rho^2 \left(\frac{f_{\rm ex}}{\rho} \right)' = \rho f'_{\rm ex}(\rho) - f_{\rm ex}(\rho). \tag{157}$$

If we introduce the total pressure

$$P = P_{\rm id} + P_{\rm ex} = \rho \frac{k_B T}{m} + P_{\rm ex}, \tag{158}$$

the condition of hydrostatic equilibrium can be written as

$$\nabla P + \rho \nabla \Phi + \rho \nabla \Phi_{\rm ext} = \mathbf{0}. \tag{159}$$

Remark 5. *For a system with long-range and short-range interactions, the first equation of the YBG hierarchy (see Equation (127)) reads*

$$\frac{k_B T}{m} \nabla \rho + \int \rho_2(\mathbf{r}, \mathbf{r}') \nabla u_{\rm SR}(|\mathbf{r} - \mathbf{r}'|) \, d\mathbf{r}' + \int \rho_2(\mathbf{r}, \mathbf{r}') \nabla u_{\rm LR}(|\mathbf{r} - \mathbf{r}'|) \, d\mathbf{r}' + \rho \nabla \Phi_{\rm ext} = \mathbf{0}. \tag{160}$$

Comparing Equations (156) and (160), we see that the long-range interactions create a mean field force $-\rho \nabla \Phi$*, while the short-range interactions create an excess pressure* $P_{\rm ex}(\mathbf{r})$ *in addition to the ideal pressure* $P_{\rm id}(\mathbf{r}) = \rho(\mathbf{r}) k_B T/m$*. Long-range and short-range interactions, therefore, have a very different effect on the system. According to Equations (156) and (160), or according to Equations (148) and (155), we have*

$$\nabla P_{\rm ex} = \int \rho_2(\mathbf{r}, \mathbf{r}') \nabla u_{\rm SR}(|\mathbf{r} - \mathbf{r}'|) \, d\mathbf{r}'. \tag{161}$$

This equation relates the two-body density to the excess pressure. Introducing the total pressure $P = P_{\rm id} + P_{\rm ex}$*, we obtain*

$$\nabla P = \frac{k_B T}{m}\nabla\rho + \int \rho_2(\mathbf{r},\mathbf{r}')\nabla u_{\rm SR}(|\mathbf{r}-\mathbf{r}'|)\, d\mathbf{r}'. \tag{162}$$

Taking the scalar product of this relation with $\mathbf{r}$*, integrating over the entire domain and integrating by parts (assuming that boundary terms can be neglected), we find that*

$$\int P\, d\mathbf{r} = Nk_B T - \frac{1}{d}\int \rho_2(\mathbf{r},\mathbf{r}')\mathbf{r}\cdot\nabla u_{\rm SR}(|\mathbf{r}-\mathbf{r}'|)\, d\mathbf{r}d\mathbf{r}'. \tag{163}$$

For a spatially uniform fluid, we recover the virial equation [33]*:*

$$\frac{\beta P}{n} = 1 - \frac{S_d}{2d}\beta n \int_0^{+\infty} g(\xi)u'_{\rm SR}(\xi)\xi^d\, d\xi, \tag{164}$$

where $n = \rho/m = N/V$ *is the number density and* $g(\xi)$ *is the radial correlation function defined by* $\rho_2(\mathbf{r},\mathbf{r}') = n^2 g(|\mathbf{r}-\mathbf{r}'|)$.

5.6. Free Energy in Phase Space

The free energy in phase space can be written as follows[16] :

$$F_{\rm tot} = \int f\frac{v^2}{2}\, d\mathbf{r}d\mathbf{v} + \int \rho\Phi_{\rm ext}\, d\mathbf{r} + \frac{1}{2}\int \rho\Phi\, d\mathbf{r} + k_B T\int \frac{f}{m}\ln\frac{f}{m}\, d\mathbf{r}d\mathbf{v} + F_{\rm ex}[\rho]. \tag{165}$$

The first term is the kinetic energy. The second term is the potential energy associated with the external potential. The third term is the mean field potential energy associated with the long-range potential of interaction (see Section 5.3). The fourth term is the free energy of the ideal gas, i.e., in the absence of correlations. Finally, the fifth term is the excess free energy $F_{\rm ex}[\rho]$. The free energy can be written as $F_{\rm tot} = E - TS$, where

$$E = \int f\frac{v^2}{2}\, d\mathbf{r}d\mathbf{v} + \frac{1}{2}\int \rho\Phi\, d\mathbf{r} + \int \rho\Phi_{\rm ext}\, d\mathbf{r} + F_{\rm ex}[\rho] \tag{166}$$

is the energy including the effect of correlations and

$$S = -k_B \int \frac{f}{m}\ln\frac{f}{m}\, d\mathbf{r}d\mathbf{v} \tag{167}$$

is the Boltzmann entropy.

The equilibrium distribution function minimizes the free energy (165) at fixed mass. Writing the variational principle for the first variations as

$$\delta F_{\rm tot} - \frac{\mu_{\rm tot}}{m}\delta M = 0, \tag{168}$$

where $\mu_{\rm tot}$ (the global chemical potential) is a Lagrange multiplier taking into account the conservation of mass, we obtain the Gibbs condition

$$\frac{\delta F_{\rm tot}}{\delta f} = \frac{\mu_{\rm tot}}{m}, \tag{169}$$

where $\mu_{\rm tot}$ is a constant. With the decomposition from Equation (165), the Gibbs condition (169) can be written as

$$\frac{v^2}{2} + \Phi + \Phi_{\rm ext} + \frac{k_B T}{m}[\ln(f/m) + 1] + \frac{\delta F_{\rm ex}}{\delta\rho} = \frac{\mu_{\rm tot}}{m}. \tag{170}$$

The equilibrium distribution function is then determined by the equation

$$f = A' e^{-\beta m \left(\frac{v^2}{2} + \Phi + \Phi_{\rm ext} + \frac{\delta F_{\rm ex}}{\delta \rho} \right)}. \tag{171}$$

The velocity distribution is Maxwellian in agreement with the general result from Section 5.1. Integrating over the velocities, we recover the spatial density from Equation (144).

Taking the spatial and velocity gradients of Equation (169), we obtain

$$\frac{\partial}{\partial \mathbf{v}} \left(\frac{\delta F_{\rm tot}}{\delta f} \right) = \mathbf{0} \qquad \text{and} \qquad \nabla \left(\frac{\delta F_{\rm tot}}{\delta f} \right) = \mathbf{0}. \tag{172}$$

With the decomposition from Equation (165), these equations take the form

$$f\mathbf{v} + \frac{k_B T}{m} \frac{\partial f}{\partial \mathbf{v}} = 0 \tag{173}$$

and

$$f \nabla \Phi + f \nabla \Phi_{\rm ext} + \frac{k_B T}{m} \frac{\partial f}{\partial \mathbf{r}} + f \nabla \frac{\delta F_{\rm ex}}{\delta \rho} = \mathbf{0}. \tag{174}$$

The first equation implies that the velocity distribution is Maxwellian. The second equation implies, after integration over $\mathbf{v}$, the condition of hydrostatic equilibrium (146) and the spatial density (144). The combination of these results returns the expression of the equilibrium distribution function from Equation (171), which is in agreement with Equation (128).

For an excess free energy of the form of Equation (149), the total free energy (165) becomes

$$F_{\rm tot} = \int f \frac{v^2}{2} \, d\mathbf{r} d\mathbf{v} + \frac{1}{2} \int \rho \Phi \, d\mathbf{r} + \int \rho \Phi_{\rm ext} \, d\mathbf{r} + k_B T \int \frac{f}{m} \ln \frac{f}{m} \, d\mathbf{r} d\mathbf{v} + \int f_{\rm ex}(\rho) \, d\mathbf{r}. \tag{175}$$

The Gibbs condition from Equation (169) takes the form

$$\frac{v^2}{2} + \Phi + \Phi_{\rm ext} + \frac{k_B T}{m} [\ln(f/m) + 1] + f'_{\rm ex}(\rho) = \frac{\mu_{\rm tot}}{m}, \tag{176}$$

leading to the equilibrium distribution function

$$f = A' e^{-\beta m \left[\frac{v^2}{2} + \Phi + \Phi_{\rm ext} + f'_{\rm ex}(\rho) \right]}. \tag{177}$$

Repeating the above calculations, we recover the spatial density from Equation (154) and the condition of hydrostatic equilibrium from Equation (159).

6. Kinetic Theory of Brownian Particles in Interaction

6.1. N-Body Langevin Equations

We consider N Brownian particles in interaction described by the coupled stochastic Langevin equations [37,141]:

$$\frac{d\mathbf{r}_i}{dt} = \mathbf{v}_i, \tag{178}$$

$$\frac{d\mathbf{v}_i}{dt} = -\xi \mathbf{v}_i - \frac{1}{m} \nabla_i U(\mathbf{r}_1, \ldots, \mathbf{r}_N) + \sqrt{2D} \mathbf{R}_i(t), \tag{179}$$

where $-\xi \mathbf{v}_i$ is a friction force, D is the diffusion coefficient in velocity space, and $\mathbf{R}_i(t)$ is a Gaussian white noise such that $\langle \mathbf{R}_i(t) \rangle = \mathbf{0}$ and $\langle R_i^\alpha(t) R_j^\beta(t') \rangle = \delta_{ij} \delta_{\alpha\beta} \delta(t - t')$. Here,

$i = 1, \ldots, N$ label the particles and $\alpha = 1, \ldots, d$ the coordinates of space. The diffusion coefficient in velocity space D is related to the friction coefficient ξ, the particle mass m, and the temperature T by the Einstein relation[17]

$$D = \frac{\xi k_B T}{m}. \tag{180}$$

This system is described by the canonical ensemble where the temperature T measures the strength of the stochastic force (since $D \sim T$). The stochastic processes (178) and (179) extend the standard Brownian model [142] to the case of particles in interaction. In this context, the friction force is due to the presence of an inert fluid in which the particles move and the stochastic force is due to Brownian motion, turbulence, or any other stochastic effect. The friction and the noise can also mimic the overall influence of an external medium with which the particles interact. This is the notion of "thermal bath".

6.2. N-Body Kramers Equation

The evolution of the N-body distribution function $P_N(\mathbf{r}_1, \mathbf{v}_1, \ldots, \mathbf{r}_N, \mathbf{v}_N, t)$ is governed by the N-body Fokker–Planck equation

$$\frac{\partial P_N}{\partial t} + \sum_{i=1}^{N} \left(\mathbf{v}_i \cdot \frac{\partial P_N}{\partial \mathbf{r}_i} + \mathbf{F}_i \cdot \frac{\partial P_N}{\partial \mathbf{v}_i} \right) = \xi \sum_{i=1}^{N} \frac{\partial}{\partial \mathbf{v}_i} \cdot \left(\frac{k_B T}{m} \frac{\partial P_N}{\partial \mathbf{v}_i} + P_N \mathbf{v}_i \right), \tag{181}$$

where $\mathbf{F}_i = -\frac{1}{m} \nabla_i U(\mathbf{r}_1, \ldots, \mathbf{r}_N)$ is the force by unit of mass acting on the i-th particle. This particular Fokker–Planck equation is called the N-body Kramers equation. For $\xi = D = 0$, it reduces to the Liouville equation, which governs the evolution of an isolated Hamiltonian system in the microcanonical ensemble [141]. The N-body Kramers equation monotonically dissipates the free energy (119). Indeed, a direct calculation yields the canonical H-theorem:

$$\dot{F}_{\rm tot} = -\sum_{i=1}^{N} \int \frac{\xi m}{P_N} \left(\frac{k_B T}{m} \frac{\partial P_N}{\partial \mathbf{v}_i} + P_N \mathbf{v}_i \right)^2 d\mathbf{r}_1 d\mathbf{v}_1 \ldots d\mathbf{r}_N d\mathbf{v}_N \leq 0. \tag{182}$$

For a steady state, $\dot{F}_{\rm tot} = 0$, the term in parenthesis in Equation (182), which is the diffusion current in the Kramers Equation (181), vanishes. Since $\partial/\partial t = 0$, the advection term (l.h.s.) in Equation (181) must also vanish independently. From these two requirements, we find that the stationary solution of the N-body Fokker–Planck equation is the Gibbs canonical distribution (118). Therefore, the Brownian gas described by the stochastic Equations (178) and (179) automatically relaxes towards the Gibbs distribution (provided that the free energy is bounded from below).

6.3. BBGKY-like Hierarchy and Kramers Equation

From the N-body Kramers Equation (181), we can obtain a hierarchy of equations for the reduced distribution functions (see Equation (79) in [37]). This is the equivalent of the BBGKY hierarchy for Hamiltonian systems[18]. The first equation of this hierarchy can be written as

$$\begin{aligned} \frac{\partial f}{\partial t} + \mathbf{v} \cdot \frac{\partial f}{\partial \mathbf{r}} - \frac{\partial}{\partial \mathbf{v}} \cdot \int f_2(\mathbf{r}, \mathbf{v}, \mathbf{r}', \mathbf{v}', t) \nabla u(|\mathbf{r} - \mathbf{r}'|)\, d\mathbf{r}' d\mathbf{v}' - \nabla \Phi_{\rm ext} \cdot \frac{\partial f}{\partial \mathbf{v}} \\ = \xi \frac{\partial}{\partial \mathbf{v}} \cdot \left(\frac{k_B T}{m} \frac{\partial f}{\partial \mathbf{v}} + f \mathbf{v} \right), \end{aligned} \tag{183}$$

where $f(\mathbf{r}, \mathbf{v}, t) = N m P_1(\mathbf{r}, \mathbf{v}, t)$ is the distribution function and $f_2(\mathbf{r}, \mathbf{v}, \mathbf{r}', \mathbf{v}') = N(N-1) m^2 P_2(\mathbf{r}, \mathbf{v}, \mathbf{r}', \mathbf{v}')$ is the two-body distribution function. This is the exact Kramers equation. We note that the BBGKY-like hierarchy is not closed since the equation for $f(\mathbf{r}, \mathbf{v}, t)$ involves the equation for $f_2(\mathbf{r}, \mathbf{v}, \mathbf{r}', \mathbf{v}')$, and so on. In Section 7, we explain how one can close the

BBGKY hierarchy by making a mean field approximation for long-range interactions and by using the DDFT for short-range interactions.

Remark 6. *If we make the approximation*

$$f_2(\mathbf{r},\mathbf{v},\mathbf{r}',\mathbf{v}',t) = f(\mathbf{r},\mathbf{v},t)f(\mathbf{r}',\mathbf{v}',t)\frac{\rho_2(\mathbf{r},\mathbf{r}',t)}{\rho(\mathbf{r},t)\rho(\mathbf{r}',t)}, \tag{184}$$

which assumes that there are no correlations in velocity space (see note 16), the Kramers Equation (183) becomes

$$\frac{\partial f}{\partial t} + \mathbf{v}\cdot\frac{\partial f}{\partial \mathbf{r}} - \frac{1}{\rho(\mathbf{r},t)}\left[\int \rho_2(\mathbf{r},\mathbf{r}',t)\nabla u(|\mathbf{r}-\mathbf{r}'|)\,d\mathbf{r}'\right]\cdot\frac{\partial f}{\partial \mathbf{v}} - \nabla\Phi_{\rm ext}\cdot\frac{\partial f}{\partial \mathbf{v}} = \xi\frac{\partial}{\partial \mathbf{v}}\cdot\left(\frac{k_B T}{m}\frac{\partial f}{\partial \mathbf{v}} + f\mathbf{v}\right). \tag{185}$$

We will use this approximate equation in Sections 7.2 and 8.6. However, the results obtained in the other sections rely only on the exact Kramers Equation (183).

6.4. Damped Jeans Equations

We now develop a hydrodynamic theory of Brownian particles with long- and short-range interactions. Taking the zeroth and first hydrodynamic moments of the exact Kramers Equation (183) and proceeding as in [37], we obtain the exact equations

$$\frac{\partial \rho}{\partial t} + \nabla\cdot(\rho\mathbf{u}) = 0, \tag{186}$$

$$\rho\left[\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u}\cdot\nabla)\mathbf{u}\right] = -\frac{\partial P_{ij}}{\partial x_j} - \int \rho_2(\mathbf{r},\mathbf{r}',t)\nabla u(|\mathbf{r}-\mathbf{r}'|)\,d\mathbf{r}' - \rho\nabla\Phi_{\rm ext} - \xi\rho\mathbf{u}, \tag{187}$$

where $\rho(\mathbf{r},t) = \int f d\mathbf{v}$ is the density, $\mathbf{u}(\mathbf{r},t) = (1/\rho)\int f\mathbf{v}d\mathbf{v}$ is the local velocity, $\mathbf{w} = \mathbf{v} - \mathbf{u}(\mathbf{r},t)$ is the relative velocity, and $P_{ij} = \int f w_i w_j d\mathbf{v}$ is the kinetic pressure tensor. We also recall that the kinetic pressure is defined by $P_{\rm kin}(\mathbf{r},t) = \frac{1}{d}\int f w^2\,d\mathbf{v}$. For $\xi = 0$, and in the absence of short-range interactions, Equations (186) and (187) reduce to the so-called Jeans equations [144,145][19]. Equations (186) and (187) will be called the damped Jeans equations [37]. Using the equation of continuity (186), we obtain the identity

$$\rho\left[\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u}\cdot\nabla)\mathbf{u}\right] = \frac{\partial}{\partial t}(\rho\mathbf{u}) + \frac{\partial}{\partial x_j}(\rho u_i u_j). \tag{188}$$

Therefore, the damped Jeans Equation (187) can also be written as

$$\frac{\partial}{\partial t}(\rho\mathbf{u}) + \nabla(\rho\mathbf{u}\otimes\mathbf{u}) = -\frac{\partial P_{ij}}{\partial x_j} - \int \rho_2(\mathbf{r},\mathbf{r}',t)\nabla u(|\mathbf{r}-\mathbf{r}'|)\,d\mathbf{r}' - \rho\nabla\Phi_{\rm ext} - \xi\rho\mathbf{u}. \tag{189}$$

By taking the higher-order moments of the exact Kramers Equation (183), we can construct a hierarchy of hydrodynamic equations. This Jeans-like hierarchy is not closed since the equation for the moment of order k involves the moment of order $k+1$, and so on. Below, we explain how one can close the hierarchy of Jeans-like equations by considering the strong friction limit or by making an LTE approximation.

6.5. Strong Friction Limit: Smoluchowski Equation

The exact Smoluchowski equation can be derived from the exact Kramers Equation (183) in the strong friction limit $\xi \to +\infty$. Considering the r.h.s. of Equation (183), we note that, for $\xi \to +\infty$, the term in parenthesis must vanish so that the velocity distribution is Maxwellian:

$$f(\mathbf{r},\mathbf{v},t) = \left(\frac{\beta m}{2\pi}\right)^{d/2} \rho(\mathbf{r},t) e^{-\beta m \frac{v^2}{2}} + O(\xi^{-1}). \tag{190}$$

This implies that $\mathbf{u} = O(1/\xi)$, $P_{ij} = (\rho k_B T/m)\delta_{ij} + O(1/\xi)$ and $P_{\text{kin}} = \rho k_B T/m + O(1/\xi)$. Therefore, to leading order in $1/\xi$, the damped Jeans Equation (187) reduces to

$$\rho\mathbf{u} \simeq -\frac{1}{\xi}\left(\frac{k_B T}{m}\nabla\rho + \int \rho_2(\mathbf{r},\mathbf{r}',t)\nabla u(|\mathbf{r}-\mathbf{r}'|)\,d\mathbf{r}' + \rho\nabla\Phi_{\text{ext}}\right). \tag{191}$$

Inserting Equation (191) into the continuity Equation (186), we obtain the exact Smoluchowski equation

$$\xi\frac{\partial\rho}{\partial t} = \nabla\cdot\left[\frac{k_B T}{m}\nabla\rho + \int \rho_2(\mathbf{r},\mathbf{r}',t)\nabla u(|\mathbf{r}-\mathbf{r}'|)\,d\mathbf{r}' + \rho\nabla\Phi_{\text{ext}}\right]. \tag{192}$$

We note that the diffusion coefficient in position space is given by the usual Einstein relation from Equation (1). This approach shows that, for $\xi \to +\infty$, the velocity distribution is Maxwellian and the evolution of the spatial density $\rho(\mathbf{r},t)$ is governed by the exact Smoluchowski Equation (192). The steady state of this equation returns the first YBG Equation (127).

Remark 7. *We can take the strong friction limit directly in the N-body Langevin Equations (178) and (179) as detailed in Section 3 of [37]. The N-body Smoluchowski equation and the exact one-body Smoluchowski equation can then be obtained from this formalism.*

6.6. Local Thermodynamic Equilibrium Approximation: Damped Euler Equation

The damped Jeans Equation (187) is not closed since the pressure tensor depends on the next order moment of the velocity. Following [37,143], we propose to close the hierarchy by making an LTE approximation:

$$f_{\text{LTE}}(\mathbf{r},\mathbf{v},t) = \left(\frac{\beta m}{2\pi}\right)^{d/2} \rho(\mathbf{r},t) e^{-\frac{1}{2}\beta m(\mathbf{v}-\mathbf{u}(\mathbf{r},t))^2}. \tag{193}$$

The distribution function (193) minimizes the free energy (165) for a given value of the density $\rho(\mathbf{r},t)$ and local velocity $\mathbf{u}(\mathbf{r},t)$. With the LTE approximation, the pressure tensor takes the form

$$P_{ij} = \rho(\mathbf{r},t)\frac{k_B T}{m}\delta_{ij}. \tag{194}$$

The kinetic pressure is given by $P_{\text{kin}}(\mathbf{r},t) = \rho(\mathbf{r},t)k_B T/m$. Substituting this result into Equation (187), we obtain the damped Euler equation

$$\rho\left[\frac{\partial\mathbf{u}}{\partial t} + (\mathbf{u}\cdot\nabla)\mathbf{u}\right] = -\frac{k_B T}{m}\nabla\rho - \int \rho_2(\mathbf{r},\mathbf{r}',t)\nabla u(|\mathbf{r}-\mathbf{r}'|)\,d\mathbf{r}' - \rho\nabla\Phi_{\text{ext}} - \xi\rho\mathbf{u}. \tag{195}$$

For $\xi \to +\infty$, we can formally neglect the advection term (l.h.s.) in Equation (195) and we obtain

$$\rho\mathbf{u} \simeq -\frac{1}{\xi}\left(\frac{k_B T}{m}\nabla\rho + \int \rho_2(\mathbf{r},\mathbf{r}',t)\nabla u(|\mathbf{r}-\mathbf{r}'|)\,d\mathbf{r}' + \rho\nabla\Phi_{\text{ext}}\right). \tag{196}$$

Inserting Equation (196) into the continuity Equation (186), we recover the exact Smoluchowski Equation (192). However, we stress that this procedure cannot be considered as a derivation (even formal) of the exact Smoluchowski equation, unlike the derivation in Section 6.5, because the damped Euler Equation (195) is heuristic. Indeed, there is no rigorous justification of the LTE approximation (193) [32][20]. Accordingly, it does not appear possible to rigorously derive the damped Euler Equation (195) from the exact Kramers Equation (183).

Remark 8. *We closed the hierarchy of hydrodynamic equations at the level of the momentum equation (187) by using the LTE approximation (193) involving the (constant) temperature of the bath* T*. We can more generally derive a system of hydrodynamic equations for the density* $\rho(\mathbf{r},t)$*, the local velocity* $\mathbf{u}(\mathbf{r},t)$*, and the kinetic temperature* $T_{\rm kin}(\mathbf{r},t)$ *of the Brownian particles by closing the hierarchy of hydrodynamic equations at the level of the energy equation, as detailed in Appendix D of [37].*

6.7. Cattaneo Equation

Using the identity (188), the damped Euler Equation (195) can be rewritten as

$$\frac{\partial}{\partial t}(\rho\mathbf{u})+\nabla(\rho\mathbf{u}\otimes\mathbf{u})=-\frac{k_B T}{m}\nabla\rho-\int\rho_2(\mathbf{r},\mathbf{r}',t)\nabla u(|\mathbf{r}-\mathbf{r}'|)\,d\mathbf{r}'-\rho\nabla\Phi_{\rm ext}-\xi\rho\mathbf{u}. \quad (197)$$

This equation is hyperbolic. If we neglect the inertial term (l.h.s.) in Equation (197) and substitute the resulting expression for $\rho\mathbf{u}$ in the continuity Equation (186), we obtain the exact Smoluchowski Equation (192), which is parabolic (this is valid in the strong friction limit $\xi\to+\infty$). The Smoluchowski equation neglects memory effects and leads to infinite speed propagation. Following [37,143], we can obtain a simplified hyperbolic model taking into account memory effects and having a finite speed propagation. Indeed, if we only neglect the nonlinear term $\nabla(\rho\mathbf{u}\otimes\mathbf{u})$ in Equation (197), we obtain

$$\frac{\partial}{\partial t}(\rho\mathbf{u})=-\frac{k_B T}{m}\nabla\rho-\int\rho_2(\mathbf{r},\mathbf{r}',t)\nabla u(|\mathbf{r}-\mathbf{r}'|)\,d\mathbf{r}'-\rho\nabla\Phi_{\rm ext}-\xi\rho\mathbf{u}. \quad (198)$$

This approximation is exact in the linear regime close to equilibrium where $|\mathbf{u}|\to 0$ [143]. Taking the time derivative of Equation (186) and substituting Equation (198) into the resulting expression, we find that

$$\frac{\partial^2\rho}{\partial t^2}+\xi\frac{\partial\rho}{\partial t}=\nabla\cdot\left(\frac{k_B T}{m}\nabla\rho+\int\rho_2(\mathbf{r},\mathbf{r}',t)\nabla u(|\mathbf{r}-\mathbf{r}'|)\,d\mathbf{r}'+\rho\nabla\Phi_{\rm ext}\right). \quad (199)$$

This equation, which is second order in time, is analogous to the Cattaneo equation [147], or to the telegraph equation, which generalizes the diffusion equation by introducing memory effects and a finite speed propagation.

7. Dynamic Density Functional Theory

The hydrodynamic equations discussed previously are not closed because they involve the two-body density $\rho_2(\mathbf{r},\mathbf{r}',t)$, which is not explicitly known[21]. In the following, we explain how one can close these equations by using the DDFT.

7.1. Long- and Short-Range Interactions

For systems with long-range interactions, the mean field approximation $\rho_2(\mathbf{r},\mathbf{r}',t)=\rho(\mathbf{r},t)\rho(\mathbf{r}',t)$ is exact in a proper thermodynamic limit $N\to+\infty$ with $m\sim 1/N$. Therefore, all the results in Section 5.3 remain valid out-of-equilibrium. In particular, we have

$$\int\rho_2(\mathbf{r},\mathbf{r}',t)\nabla u_{\rm LR}(|\mathbf{r}-\mathbf{r}'|)\,d\mathbf{r}'=\rho(\mathbf{r},t)\nabla\Phi(\mathbf{r},t), \quad (200)$$

where $\Phi(\mathbf{r},t)$ is the mean field potential produced by the smooth distribution of particles $\rho(\mathbf{r},t)$ (see Equation (135)).

For systems with short-range interactions, we can use the DDFT of fluids. In this approach, the hierarchy of kinetic equations is closed by making the approximation [35]:

$$\int \rho_2(\mathbf{r},\mathbf{r}',t)\nabla u_{\rm SR}(|\mathbf{r}-\mathbf{r}'|)\,d\mathbf{r}' = \rho(\mathbf{r},t)\nabla\frac{\delta F_{\rm ex}}{\delta\rho}[\rho(\mathbf{r},t)], \tag{201}$$

where $F_{\rm ex}[\rho]$ is the excess free energy calculated at equilibrium. This relation is exact at equilibrium (see Section 5.4) and the approximation consists in extending it out-of-equilibrium with the actual density $\rho(\mathbf{r},t)$ calculated at each time t. This closure is equivalent to assuming that the two-body dynamic correlations are the same as those in an equilibrium fluid with the same one-body density profile. Although it is not possible to ascertain the validity of this approximation in the general case, it has been observed for the systems considered that this approximation gives remarkable agreement with direct Brownian N-body simulations.

In the following, we consider the general case where the potential of interaction is the sum of a long-range interaction and a short-range interaction: $u = u_{\rm LR} + u_{\rm SR}$. We treat the long-range interaction in the mean field approximation (200) and the short-range interaction with the approximation (201) of the DDFT. We note that Equation (200) can also be obtained from Equation (201) with the mean field energy functional W from Equation (138). In that case, Equation (201) with $F_{\rm ex} = W$ is exact for $N \gg 1$.

7.2. Kramers Equation

The Kramers Equation (185) can be closed by using the DDFT, yielding

$$\frac{\partial f}{\partial t} + \mathbf{v}\cdot\frac{\partial f}{\partial \mathbf{r}} - \nabla\frac{\delta F_{\rm ex}}{\delta\rho}\cdot\frac{\partial f}{\partial \mathbf{v}} - \nabla(\Phi+\Phi_{\rm ext})\cdot\frac{\partial f}{\partial \mathbf{v}} = \xi\frac{\partial}{\partial \mathbf{v}}\cdot\left(\frac{k_B T}{m}\frac{\partial f}{\partial \mathbf{v}} + f\mathbf{v}\right). \tag{202}$$

If the excess free energy is of the form of Equation (149), using the relation (155), we obtain

$$\frac{\partial f}{\partial t} + \mathbf{v}\cdot\frac{\partial f}{\partial \mathbf{r}} - \frac{\nabla P_{\rm ex}}{\rho}\cdot\frac{\partial f}{\partial \mathbf{v}} - \nabla(\Phi+\Phi_{\rm ext})\cdot\frac{\partial f}{\partial \mathbf{v}} = \xi\frac{\partial}{\partial \mathbf{v}}\cdot\left(\frac{k_B T}{m}\frac{\partial f}{\partial \mathbf{v}} + f\mathbf{v}\right). \tag{203}$$

We can write the Kramers Equation (202) in the form

$$\frac{\partial f}{\partial t} - [f,E] = \xi\frac{\partial}{\partial \mathbf{v}}\cdot\left[f\frac{\partial}{\partial \mathbf{v}}\left(\frac{\delta F_{\rm tot}}{\delta f}\right)\right], \tag{204}$$

where

$$[F,G] = \int f\left\{\frac{\delta F}{\delta f},\frac{\delta G}{\delta f}\right\}d\mathbf{r}d\mathbf{v} \tag{205}$$

is the noncanonical Poisson bracket [148] and $\{f,g\} = \nabla_{\mathbf{r}} f\cdot\nabla_{\mathbf{v}} g - \nabla_{\mathbf{v}} f\cdot\nabla_{\mathbf{r}} g$ is the usual Poisson bracket. In Equation (204), E denotes the energy functional (166) and $F_{\rm tot}$ denotes the free energy functional (165). We have the H-theorem (see Appendix C.3)

$$\dot{F}_{\rm tot} = -\int \xi f\left[\frac{\partial}{\partial \mathbf{v}}\left(\frac{\delta F_{\rm tot}}{\delta f}\right)\right]^2 d\mathbf{r}d\mathbf{v} \le 0. \tag{206}$$

It can be explicitly written as

$$\dot{F}_{\rm tot} = -\int \frac{\xi}{f}\left(\frac{k_B T}{m}\frac{\partial f}{\partial \mathbf{v}} + f\mathbf{v}\right)^2 d\mathbf{r}d\mathbf{v} \le 0. \tag{207}$$

The Kramers Equation (202) relaxes towards a stable equilibrium state, which minimizes the free energy at fixed mass (assuming that the free energy is bounded from below). This equilibrium state is determined by Equation (171).

Remark 9. *For purely long-range interactions ($u_{\rm SR} = 0$), the mean field approximation $f_2(\mathbf{r},\mathbf{v},\mathbf{r}',\mathbf{v}',t) = f(\mathbf{r},\mathbf{v},t)f(\mathbf{r}',\mathbf{v}',t)$ is exact in the limit $N \rightarrow +\infty$ with $m \sim 1/N$. This corresponds to the regime where the "collisions" between the particles can be neglected. In that case, Equation (183) reduces to the mean field Kramers equation*

$$\frac{\partial f}{\partial t} + \mathbf{v}\cdot\frac{\partial f}{\partial \mathbf{r}} - \nabla(\Phi+\Phi_{\rm ext})\cdot\frac{\partial f}{\partial \mathbf{v}} = \xi\frac{\partial}{\partial \mathbf{v}}\cdot\left(\frac{k_B T}{m}\frac{\partial f}{\partial \mathbf{v}} + f\mathbf{v}\right). \tag{208}$$

This equation can also be obtained from Equation (202) in the ideal case where $F_{\rm ex} = 0$. For $\xi = D = 0$, we recover the Vlasov equation, which describes Hamiltonian systems with long-range interactions in the collisionless limit $N \rightarrow +\infty$ with $m \sim 1/N$ [141].

7.3. Damped Jeans Equations

The damped Jeans Equations (186) and (187) can be closed by using the DDFT, yielding

$$\frac{\partial \rho}{\partial t} + \nabla\cdot(\rho\mathbf{u}) = 0, \tag{209}$$

$$\rho\left[\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u}\cdot\nabla)\mathbf{u}\right] = -\frac{\partial P_{ij}}{\partial x_j} - \rho\nabla\frac{\delta F_{\rm ex}}{\delta\rho} - \rho\nabla\Phi - \rho\nabla\Phi_{\rm ext} - \xi\rho\mathbf{u}. \tag{210}$$

If the excess free energy is of the form of Equation (149), using the relation (155), we obtain

$$\rho\left[\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u}\cdot\nabla)\mathbf{u}\right] = -\frac{\partial P_{ij}}{\partial x_j} - \nabla P_{\rm ex} - \rho\nabla\Phi - \rho\nabla\Phi_{\rm ext} - \xi\rho\mathbf{u}. \tag{211}$$

Remark 10. *In the ideal case ($F_{\rm ex} = u_{\rm SR} = 0$), i.e., for purely long-range interactions, Equation (210) reduces to the mean field damped Jeans equation*

$$\rho\left[\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u}\cdot\nabla)\mathbf{u}\right] = -\frac{\partial P_{ij}}{\partial x_j} - \rho\nabla\Phi - \rho\nabla\Phi_{\rm ext} - \xi\rho\mathbf{u}. \tag{212}$$

For $\xi = 0$, we recover the usual Jeans equation issued from the Vlasov equation, which describes Hamiltonian systems with long-range interactions in the collisionless limit $N \rightarrow +\infty$ with $m \sim 1/N$ [141].

7.4. Smoluchowski Equation

The Smoluchowski Equation (192), which is valid in the strong friction limit $\xi \rightarrow +\infty$, can be closed by using the DDFT, yielding

$$\frac{\partial \rho}{\partial t} = \nabla\cdot\left[\frac{1}{\xi}\left(\frac{k_B T}{m}\nabla\rho + \rho\nabla\frac{\delta F_{\rm ex}}{\delta\rho} + \rho\nabla\Phi + \rho\nabla\Phi_{\rm ext}\right)\right]. \tag{213}$$

For an excess free energy of the form of Equation (149), using the relation (155) and introducing the total pressure from Equation (158), we obtain

$$\frac{\partial \rho}{\partial t} = \nabla\cdot\left[\frac{1}{\xi}(\nabla P + \rho\nabla\Phi + \rho\nabla\Phi_{\rm ext})\right]. \tag{214}$$

We can write the generalized Smoluchowski Equation (213) in the form

$$\frac{\partial\rho}{\partial t}=\nabla\cdot\left(\frac{1}{\xi}\rho\nabla\frac{\delta F}{\delta\rho}\right) \tag{215}$$

with the free energy functional (140). We have the H-theorem (see Appendix C.1)

$$\dot{F}=-\int\frac{1}{\xi}\rho\left(\nabla\frac{\delta F}{\delta\rho}\right)^2 d\mathbf{r}\leq 0. \tag{216}$$

It can be explicitly written as

$$\dot{F}=-\frac{1}{\xi}\int\frac{1}{\rho}\left(\frac{k_B T}{m}\nabla\rho+\rho\nabla\frac{\delta F_{\rm ex}}{\delta\rho}+\rho\nabla\Phi+\rho\nabla\Phi_{\rm ext}\right)^2 d\mathbf{r}\leq 0. \tag{217}$$

For the free energy (152), it becomes

$$\dot{F}=-\frac{1}{\xi}\int\frac{1}{\rho}(\nabla P+\rho\nabla\Phi+\rho\nabla\Phi_{\rm ext})^2\, d\mathbf{r}\leq 0. \tag{218}$$

The Smoluchowski equation relaxes towards a stable equilibrium state, which minimizes the free energy at fixed mass (assuming that the free energy is bounded from below). This equilibrium state is determined by Equation (144).

Remark 11. *In the ideal case ($F_{\rm ex}=u_{\rm SR}=0$), i.e., for purely long-range interactions, Equation (213) reduces to the mean field Smoluchowski equation*

$$\xi\frac{\partial\rho}{\partial t}=\nabla\cdot\left(\frac{k_B T}{m}\nabla\rho+\rho\nabla\Phi+\rho\nabla\Phi_{\rm ext}\right). \tag{219}$$

7.5. Damped Euler Equation

The damped Euler Equation (195) can be closed by using the DDFT, yielding

$$\rho\left[\frac{\partial\mathbf{u}}{\partial t}+(\mathbf{u}\cdot\nabla)\mathbf{u}\right]=-\frac{k_B T}{m}\nabla\rho-\rho\nabla\frac{\delta F_{\rm ex}}{\delta\rho}-\rho\nabla\Phi-\rho\nabla\Phi_{\rm ext}-\xi\rho\mathbf{u}. \tag{220}$$

For an excess free energy of the form of Equation (149), using the relation (155) and introducing the total pressure from Equation (158), we obtain

$$\rho\left[\frac{\partial\mathbf{u}}{\partial t}+(\mathbf{u}\cdot\nabla)\mathbf{u}\right]=-\nabla P-\rho\nabla\Phi-\rho\nabla\Phi_{\rm ext}-\xi\rho\mathbf{u}. \tag{221}$$

We can write the damped Euler Equation (220) in the form

$$\rho\left[\frac{\partial\mathbf{u}}{\partial t}+(\mathbf{u}\cdot\nabla)\mathbf{u}\right]=-\rho\nabla\frac{\delta F}{\delta\rho}-\xi\rho\mathbf{u} \tag{222}$$

with the free energy functional (140). We have the H-theorem (see Appendix C.2)

$$\dot{F}_{\rm tot}=-\int\xi\rho\mathbf{u}^2 d\mathbf{r}\leq 0 \tag{223}$$

with

$$F_{\rm tot}[\rho,\mathbf{u}]=\int\rho\frac{\mathbf{u}^2}{2}d\mathbf{r}+\int\rho\Phi_{\rm ext}d\mathbf{r}+\frac{1}{2}\int\rho\Phi\, d\mathbf{r}+k_B T\int\frac{\rho}{m}\ln\frac{\rho}{m}d\mathbf{r}+F_{\rm ex}[\rho]. \tag{224}$$

The damped Euler equation relaxes towards a stable equilibrium state, which minimizes the free energy at fixed mass (assuming that the free energy is bounded from below). This equilibrium state is determined by Equation (144).

In the strong friction limit $\xi \to +\infty$, the preceding equations reduce formally to those obtained in Section 7.4. However, as we have already indicated in Section 6.6, this is not the correct way to justify the generalized Smoluchowski equation since the damped Euler Equation (220) is based on an LTE approximation, which has no rigorous foundation.

Remark 12. *In the ideal case ($F_{\rm ex} = u_{\rm SR} = 0$), i.e., for purely long-range interactions, Equation (220) reduces to the mean field damped Euler equation*

$$\rho\left[\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u}\cdot\nabla)\mathbf{u}\right] = -\frac{k_B T}{m}\nabla\rho - \rho\nabla\Phi - \rho\nabla\Phi_{\rm ext} - \xi\rho\mathbf{u}. \tag{225}$$

7.6. Cattaneo Equation

The Cattaneo Equation (199) can be closed by using the DDFT, yielding

$$\frac{\partial^2\rho}{\partial t^2} + \xi\frac{\partial\rho}{\partial t} = \nabla\cdot\left(\frac{k_B T}{m}\nabla\rho + \rho\nabla\frac{\delta F_{\rm ex}}{\delta\rho} + \rho\nabla\Phi + \rho\nabla\Phi_{\rm ext}\right). \tag{226}$$

For an excess free energy of the form of Equation (149), using the relation (155) and introducing the total pressure from Equation (158), we obtain

$$\frac{\partial^2\rho}{\partial t^2} + \xi\frac{\partial\rho}{\partial t} = \nabla\cdot(\nabla P + \rho\nabla\Phi + \rho\nabla\Phi_{\rm ext}). \tag{227}$$

We can write the Cattaneo Equation (226) in the form

$$\frac{\partial^2\rho}{\partial t^2} + \xi\frac{\partial\rho}{\partial t} = \nabla\cdot\left(\rho\nabla\frac{\delta F}{\delta\rho}\right) \tag{228}$$

with the free energy functional (140).

Remark 13. *In the ideal case ($F_{\rm ex} = u_{\rm SR} = 0$), i.e., for purely long-range interactions, Equation (226) reduces to the mean field Cattaneo equation*

$$\frac{\partial^2\rho}{\partial t^2} + \xi\frac{\partial\rho}{\partial t} = \nabla\cdot\left(\frac{k_B T}{m}\nabla\rho + \rho\nabla\Phi + \rho\nabla\Phi_{\rm ext}\right). \tag{229}$$

7.7. Stochastic Kinetic Equations

The previous equations ignore fluctuations. We can take fluctuations into account by introducing a noise term in these equations in order to satisfy the fluctuation–dissipation theorem (see [17,38,143])[22]. This procedure transforms deterministic partial differential equations into stochastic partial differential equations. It is then easy from these stochastic equations to construct the corresponding Onsager–Machlup action functional, which describes the probability density of the different paths [17,150].

The stochastic Kramers equation reads

$$\begin{aligned}\frac{\partial f}{\partial t} + \mathbf{v}\cdot\frac{\partial f}{\partial \mathbf{r}} - \frac{\partial}{\partial \mathbf{v}}\cdot\int f_2(\mathbf{r},\mathbf{v},\mathbf{r}',\mathbf{v}',t)\nabla u(|\mathbf{r}-\mathbf{r}'|)\,d\mathbf{r}'d\mathbf{v}' - \nabla\Phi_{\rm ext}\cdot\frac{\partial f}{\partial \mathbf{v}}\\ = \xi\frac{\partial}{\partial \mathbf{v}}\cdot\left(\frac{k_B T}{m}\frac{\partial f}{\partial \mathbf{v}} + f\mathbf{v}\right) + \frac{\partial}{\partial \mathbf{v}}\cdot\left(\sqrt{2\xi k_B T f}\,\mathbf{Q}(\mathbf{r},\mathbf{v},t)\right),\end{aligned} \tag{230}$$

where $\mathbf{Q}(\mathbf{r},\mathbf{v},t)$ is Gaussian white noise, satisfying the conditions $\langle\mathbf{Q}(\mathbf{r},\mathbf{v},t)\rangle = \mathbf{0}$ and $\langle Q_i(\mathbf{r},\mathbf{v},t)Q_j(\mathbf{r}',\mathbf{v}',t')\rangle = \delta(\mathbf{r}-\mathbf{r}')\delta(\mathbf{v}-\mathbf{v}')\delta(t-t')$.

The stochastic damped Jeans equation reads

$$\rho\left[\frac{\partial \mathbf{u}}{\partial t}+(\mathbf{u}\cdot\nabla)\mathbf{u}\right]=-\frac{\partial P_{ij}}{\partial x_j}-\int \rho_2(\mathbf{r},\mathbf{r}',t)\nabla u(|\mathbf{r}-\mathbf{r}'|)\,d\mathbf{r}'-\rho\nabla\Phi_{\rm ext}-\xi\rho\,\mathbf{u}$$
$$-\sqrt{2\xi k_B T\rho}\,\mathbf{R}(\mathbf{r},t), \qquad (231)$$

where $\mathbf{R}(\mathbf{r},t)$ is Gaussian white noise satisfying $\langle \mathbf{R}(\mathbf{r},t)\rangle=\mathbf{0}$ and $\langle R_i(\mathbf{r},t)R_j(\mathbf{r}',t')\rangle=\delta_{ij}\delta(\mathbf{r}-\mathbf{r}')\delta(t-t')$. We note that the continuity Equation (186) is not affected by the noise term. Using the DDFT, Equation (231) becomes

$$\rho\left[\frac{\partial \mathbf{u}}{\partial t}+(\mathbf{u}\cdot\nabla)\mathbf{u}\right]=-\frac{\partial P_{ij}}{\partial x_j}-\rho\nabla\frac{\delta F_{\rm ex}}{\delta\rho}-\rho\nabla\Phi-\rho\nabla\Phi_{\rm ext}-\xi\rho\,\mathbf{u}-\sqrt{2\xi k_B T\rho}\,\mathbf{R}(\mathbf{r},t). \qquad (232)$$

In the strong friction limit $\xi\rightarrow+\infty$, we obtain the stochastic Smoluchowski equation

$$\xi\frac{\partial\rho}{\partial t}=\nabla\cdot\left(\rho\nabla\frac{\delta F}{\delta\rho}\right)+\nabla\cdot\left(\sqrt{2\xi k_B T\rho}\mathbf{R}\right), \qquad (233)$$

where $F[\rho]$ is the free energy functional (140). We note that the noise is multiplicative since it depends on the density $\rho(\mathbf{r},t)$.

If we make the LTE approximation, Equation (232) leads to the stochastic damped Euler equation

$$\rho\left[\frac{\partial \mathbf{u}}{\partial t}+(\mathbf{u}\cdot\nabla)\mathbf{u}\right]=-\rho\nabla\frac{\delta F}{\delta\rho}-\xi\rho\,\mathbf{u}-\sqrt{2\xi k_B T\rho}\,\mathbf{R}(\mathbf{r},t). \qquad (234)$$

Finally, the stochastic Cattaneo equation reads

$$\frac{\partial^2\rho}{\partial t^2}+\xi\frac{\partial\rho}{\partial t}=\nabla\cdot\left(\rho\nabla\frac{\delta F}{\delta\rho}\right)+\nabla\cdot\left(\sqrt{2\xi k_B T\rho}\,\mathbf{R}\right). \qquad (235)$$

When the system admits several equilibrium states, i.e., when there exist stable states (global minima of free energy) and metastable states (local minima of free energy), and when the number N of particles is not too large (or if we are close to a critical point), the fluctuations are important and can induce random transitions from one (meta)stable state to another [151]. These random transitions can be studied with the stochastic kinetic equations discussed above.

Remark 14. *The stochastic damped Euler, Cattaneo, and Smoluchowski Equations (233)–(235) also apply to the quantum systems of Sections 3 and 4 by using the free energy functional from Equation (89), taking into account the quantum potential (see the analogy between Brownian and quantum systems in the following section).*

8. Back to the Generalized Schrödinger Equation

By considering a system of Brownian particles in interaction, by using the DDFT, and by making an LTE approximation, we derived a generalized damped Euler equation of the form (see Equation (220)):

$$\rho\left[\frac{\partial \mathbf{u}}{\partial t}+(\mathbf{u}\cdot\nabla)\mathbf{u}\right]=-\frac{k_B T}{m}\nabla\rho-\rho\nabla\frac{\delta F_{\rm ex}}{\delta\rho}-\rho\nabla\Phi-\rho\nabla\Phi_{\rm ext}-\xi\rho\mathbf{u}. \qquad (236)$$

It involves an ideal thermal pressure $P_{\rm id}=\rho k_B T/m$ and an effective potential $\delta F_{\rm ex}/\delta\rho$ arising from the correlations between the particles. On the other hand, by starting from the generalized Schrödinger Equation (35) and by performing the Madelung transformation, we derived a generalized quantum damped Euler equation of the form (see Equation (58)):

$$\rho\left[\frac{\partial\mathbf{u}}{\partial t}+(\mathbf{u}\cdot\nabla)\mathbf{u}\right]=-\frac{k_BT}{m}\nabla\rho-\nabla P_{\rm int}-\rho\nabla\Phi-\rho\nabla\Phi_{\rm ext}-\frac{\rho}{m}\nabla Q-\xi\rho\mathbf{u}. \tag{237}$$

It involves an effective thermal pressure $P_{\rm id}=\rho k_BT/m$, an isotropic pressure $P_{\rm int}$ due to the self-interaction of the bosons, and a quantum potential Q/m, which is equivalent to an anisotropic quantum pressure P_{ij} (see Equation (69)). We show below that we can derive Equation (237) from Equation (236) by choosing an appropriate form of excess free energy functional in Equation (236). This functional can be decomposed into

$$F_{\rm ex}=F_{\rm ex}^{\rm (SI)}+F_{\rm ex}^{\rm (Q)}, \tag{238}$$

where the first term accounts for the self-interaction of the bosons and the second term accounts for the quantum effects. Since the quantum damped Euler Equation (58) is equivalent to the generalized Schrödinger Equation (35), our procedure shows that we can derive the generalized Schrödinger Equation (35) by considering a classical system of Brownian particles in interaction with a special form of correlations. This suggests that the quantum kinetic energy may be interpreted as an excess free energy functional in the physics of simple liquids. This interpretation may be difficult (if not impossible) to justify for a single quantum particle like an electron, except if it can be treated as a "fluid" of subquantum particles as suggested by the Madelung hydrodynamic picture. The hydrodynamic interpretation of the quantum potential may be more relevant for a BEC made of many bosons in the same quantum state. In any case, there is an interesting mapping between a classical Brownian gas with a special form of correlations and the generalized Schrödinger equation. Whether this mapping is just formal or has a deeper interpretation remains a question for future investigations.

Remark 15. *There is an important difference between a quantum system described by the generalized Schrödinger Equation (35), and hence by the quantum damped Euler Equation (237), and a classical system of Brownian particles in interaction described by the damped Euler Equation (236). For quantum systems, the velocity field defined by Equation (46) is potential and irrotational (it characterizes a superfluid), while this is not necessarily the case for Brownian particles. The assumption of a potential flow is necessary to derive the generalized Schrödinger Equation (35) from the damped Euler Equation (236) by the inverse Madelung transformation (see also the quantization condition from note 13). In the following, we shall assume that the flow produced by the Brownian particles is potential but we must keep in mind that this may not always be the case. There is also another difference. For Brownian systems, the damped Euler Equation (236) is approximate since it relies on the LTE approximation, which is not rigorously justified (except in the strong friction limit), while for quantum systems the damped Euler Equation (237) is exact since it is obtained from the generalized Schrödinger Equation (35) without approximation.*

8.1. Self-Interaction Pressure

We first focus on the self-interaction term. If we consider a functional of the form of Equation (149) and use the relation (155), we can rewrite Equation (236) as

$$\rho\left[\frac{\partial\mathbf{u}}{\partial t}+(\mathbf{u}\cdot\nabla)\mathbf{u}\right]=-\frac{k_BT}{m}\nabla\rho-\nabla P_{\rm ex}-\rho\nabla\Phi-\rho\nabla\Phi_{\rm ext}-\xi\rho\mathbf{u}. \tag{239}$$

It involves an ideal thermal pressure $P_{\rm id}=\rho k_BT/m$ and an isotropic excess pressure $P_{\rm ex}$ due to the correlations of the particles. This term is similar to the self-interaction pressure $P_{\rm int}$, which occurs in the r.h.s. of Equation (237). The two terms coincide if we take the following[23]:

$$P_{\rm ex}(\rho)=P_{\rm int}(\rho),\qquad f_{\rm ex}(\rho)=V_{\rm int}(\rho). \tag{240}$$

Therefore, the self-interaction between the particles can be described by an excess free energy of the form

$$F_{\rm ex}^{\rm (SI)} = U_{\rm int} = \int V_{\rm int}(\rho)\, d\mathbf{r}. \tag{241}$$

As in Sections 3 and 5, we can combine the thermal pressure and the self-interaction (or excess) pressure into a total pressure $P = P_{\rm id} + P_{\rm int}$ (or $P = P_{\rm id} + P_{\rm ex}$). This corresponds to a total potential $V = V_{\rm id} + V_{\rm int}$ (or a total free energy density $f = f_{\rm id} + f_{\rm ex}$).

8.2. Generalized Landau Free Energy Functional

We now account for the quantum potential. For that purpose, we consider a functional of the form

$$F_{\rm ex}[\rho] = \int \left[\frac{1}{2}K(\rho)(\nabla\rho)^2 + V_{\rm int}(\rho)\right] d\mathbf{r}, \tag{242}$$

where $K(\rho)$ is a function of the density. Equation (242) can be viewed as a generalized Landau free energy functional (the Landau free energy functional is recovered for $K(\rho) = K = {\rm cst}$). The first term takes into account quantum effects, possibly in a generalized sense (see below). The second term takes into account the self-interaction of the particles as discussed in the previous section. As detailed in Appendix E, we have

$$\frac{\delta F_{\rm ex}}{\partial\rho} = -\frac{1}{2}K'(\rho)(\nabla\rho)^2 - K(\rho)\Delta\rho + V'_{\rm int}(\rho), \tag{243}$$

where we recall that $V'_{\rm int}(\rho) = h_{\rm int}(\rho)$ is the enthalpy (see Section 3). Substituting this relation into Equation (236), we obtain

$$\frac{\partial\mathbf{u}}{\partial t} + (\mathbf{u}\cdot\nabla)\mathbf{u} = -\frac{1}{\rho}\nabla P - \nabla\Phi_{\rm ext} - \nabla\Phi + \nabla[K(\rho)\Delta\rho] + \frac{1}{2}\nabla\left[K'(\rho)(\nabla\rho)^2\right] - \xi\mathbf{u}, \tag{244}$$

where $P = P_{\rm id} + P_{\rm int}$. If we introduce the K-potential (see Appendix E)

$$Q_K = -mK(\rho)\Delta\rho - \frac{1}{2}mK'(\rho)(\nabla\rho)^2, \tag{245}$$

we can rewrite Equation (244) as

$$\frac{\partial\mathbf{u}}{\partial t} + (\mathbf{u}\cdot\nabla)\mathbf{u} = -\frac{1}{\rho}\nabla P - \nabla\Phi_{\rm ext} - \nabla\Phi - \frac{1}{m}\nabla Q_K - \xi\mathbf{u}. \tag{246}$$

In the strong friction limit, we obtain the K-generalized Smoluchowski equation

$$\xi\frac{\partial\rho}{\partial t} = \nabla\cdot\left(\nabla P + \rho\nabla\Phi_{\rm ext} + \rho\nabla\Phi + \frac{\rho}{m}\nabla Q_K\right) \tag{247}$$

or, more explicitly,

$$\xi\frac{\partial\rho}{\partial t} = \nabla\cdot\left(\nabla P + \rho\nabla\Phi_{\rm ext} + \rho\nabla\Phi - \rho\nabla[K(\rho)\Delta\rho] - \frac{1}{2}\rho\nabla\left[K'(\rho)(\nabla\rho)^2\right]\right). \tag{248}$$

Remark 16. *If ρ varies slowly, we can obtain the expression (242) of the excess free energy by a systematic expansion of a general functional $F_{\rm ex}[\rho]$ in powers of the inhomogeneity. In that case, we can explicitly relate the function $K(\rho)$ to the direct correlation function $c^{(2)}(|\mathbf{r}-\mathbf{r}'|,\rho)$. One finds that $K(\rho) = \frac{1}{6\beta}\int c^{(2)}(\rho,q)q^2\, d\mathbf{q}$ [34] (see Appendix F.4). However, in the following, we shall not necessarily assume that ρ varies slowly.*

8.3. Quantum Potential

We see that the K-potential (245) appearing in Equation (246) coincides with the quantum potential (49) in Equation (237) provided that we take

$$K(\rho) = \frac{\hbar^2}{4m^2\rho}. \tag{249}$$

Indeed, in that case, we have

$$K'(\rho) = -\frac{\hbar^2}{4m^2\rho^2} = -\frac{K(\rho)}{\rho} \tag{250}$$

and

$$Q_K = -\frac{\hbar^2}{4m}\left[\frac{\Delta\rho}{\rho} - \frac{1}{2}\frac{(\nabla\rho)^2}{\rho^2}\right]. \tag{251}$$

Therefore, with this choice of the function $K(\rho)$, the K-potential from Equation (245) coincides with the quantum potential from Equation (49) and the K-functional (A73) appearing in the excess free energy (242) coincides with the quantum kinetic energy from Equation (80):

$$Q_K = Q, \qquad \Theta_Q^K = \Theta_Q. \tag{252}$$

We, thus, recovered the generalized quantum damped Euler Equation (237), which, together with the continuity Equation (209) and the assumption that the flow is potential (see the Remark at the beginning of Section 8), is equivalent through the inverse Madelung transformation to the generalized Schrödinger equation

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\Delta\psi + m\Phi\psi + m\frac{dV}{d|\psi|^2}\psi + m\Phi_{\rm ext}\psi - i\frac{\hbar}{2}\xi\left[\ln\left(\frac{\psi}{\psi^*}\right) - \left\langle\ln\left(\frac{\psi}{\psi^*}\right)\right\rangle\right]\psi. \tag{253}$$

8.4. K-Generalized Schrödinger Equation

By considering an arbitrary function $K(\rho)$, we can construct a more general Schrödinger equation. Performing the inverse Madelung transformation, we can see that Equation (246), together with the continuity Equation (209) and the assumption that the flow is potential, is equivalent to a generalized Schrödinger equation of the following form[24]:

$$\begin{aligned} i\hbar\frac{\partial\psi}{\partial t} = & -\frac{\hbar^2}{2m}\Delta\psi - Q\psi + Q_K\psi + m\Phi_{\rm ext}\psi + m\Phi\psi + m\frac{dV}{d|\psi|^2}\psi \\ & -i\frac{\hbar}{2}\xi\left[\ln\left(\frac{\psi}{\psi^*}\right) - \left\langle\ln\left(\frac{\psi}{\psi^*}\right)\right\rangle\right]\psi. \end{aligned} \tag{254}$$

We shall call it the K-generalized Schrödinger equation. Using Equations (49) and (245) with $\rho = |\psi|^2$, it can be written as

$$\begin{aligned} i\hbar\frac{\partial\psi}{\partial t} = & -\frac{\hbar^2}{2m}\Delta\psi + \frac{\hbar^2}{2m}\frac{\Delta|\psi|}{|\psi|}\psi - mK(|\psi|^2)\Delta(|\psi|^2)\psi - \frac{1}{2}mK'(|\psi|^2)(\nabla|\psi|^2)^2\psi \\ & +m\Phi_{\rm ext}\psi + m\Phi\psi + m\frac{dV}{d|\psi|^2}\psi - i\frac{\hbar}{2}\xi\left[\ln\left(\frac{\psi}{\psi^*}\right) - \left\langle\ln\left(\frac{\psi}{\psi^*}\right)\right\rangle\right]\psi. \end{aligned} \tag{255}$$

Let us give some examples:
(i) The classical case corresponds to $K = 0$ (no "quantum" correlation) leading to

$$Q_K = 0, \qquad \Theta_Q^K = 0, \tag{256}$$

$$\frac{\partial \mathbf{u}}{\partial t}+(\mathbf{u}\cdot\nabla)\mathbf{u}=-\frac{1}{\rho}\nabla P-\nabla\Phi_{\rm ext}-\nabla\Phi-\xi\mathbf{u}, \tag{257}$$

$$\begin{aligned} i\hbar\frac{\partial\psi}{\partial t}&=-\frac{\hbar^2}{2m}\Delta\psi+\frac{\hbar^2}{2m}\frac{\Delta|\psi|}{|\psi|}\psi+m\Phi\psi+m\frac{dV}{d|\psi|^2}\psi\\ &-i\frac{\hbar}{2}\xi\left[\ln\left(\frac{\psi}{\psi^*}\right)-\left\langle\ln\left(\frac{\psi}{\psi^*}\right)\right\rangle\right]\psi. \end{aligned} \tag{258}$$

In the strong friction limit, we obtain the generalized classical Smoluchowski equation

$$\xi\frac{\partial\rho}{\partial t}=\nabla\cdot(\nabla P+\rho\nabla\Phi_{\rm ext}+\rho\nabla\Phi). \tag{259}$$

(ii) The ordinary Landau functional corresponds to $K=\text{cst}$ leading to

$$Q_K=-mK\Delta\rho,\qquad \Theta_Q^K=\frac{1}{2}K\int(\nabla\rho)^2\,d\mathbf{r}, \tag{260}$$

$$\frac{\partial \mathbf{u}}{\partial t}+(\mathbf{u}\cdot\nabla)\mathbf{u}=-\frac{1}{\rho}\nabla P-\nabla\Phi_{\rm ext}-\nabla\Phi+K\nabla(\Delta\rho)-\xi\mathbf{u}, \tag{261}$$

$$\begin{aligned} i\hbar\frac{\partial\psi}{\partial t}&=-\frac{\hbar^2}{2m}\Delta\psi+\frac{\hbar^2}{2m}\frac{\Delta|\psi|}{|\psi|}\psi-mK\Delta(|\psi|^2)\psi+m\Phi_{\rm ext}\psi\\ &+m\Phi\psi+m\frac{dV}{d|\psi|^2}\psi-i\frac{\hbar}{2}\xi\left[\ln\left(\frac{\psi}{\psi^*}\right)-\left\langle\ln\left(\frac{\psi}{\psi^*}\right)\right\rangle\right]\psi. \end{aligned} \tag{262}$$

In the strong friction limit, we obtain the generalized Smoluchowski equation

$$\xi\frac{\partial\rho}{\partial t}=\nabla\cdot[\nabla P+\rho\nabla\Phi_{\rm ext}+\rho\nabla\Phi-K\rho\nabla(\Delta\rho)]. \tag{263}$$

(iii) The standard quantum case corresponds to

$$K(\rho)=\frac{\hbar^2}{4m^2\rho}, \tag{264}$$

leading to

$$Q_K=-\frac{\hbar^2}{4m}\left[\frac{\Delta\rho}{\rho}-\frac{1}{2}\frac{(\nabla\rho)^2}{\rho^2}\right]=Q,\qquad \Theta_Q^K=\frac{\hbar^2}{8m^2}\int\frac{(\nabla\rho)^2}{\rho}\,d\mathbf{r}=\int\rho\frac{Q}{m}\,d\mathbf{r}=\Theta_Q, \tag{265}$$

$$\frac{\partial \mathbf{u}}{\partial t}+(\mathbf{u}\cdot\nabla)\mathbf{u}=-\frac{1}{\rho}\nabla P-\nabla\Phi_{\rm ext}-\nabla\Phi-\frac{1}{m}\nabla Q-\xi\mathbf{u}, \tag{266}$$

$$i\hbar\frac{\partial\psi}{\partial t}=-\frac{\hbar^2}{2m}\Delta\psi+m\Phi_{\rm ext}\psi+m\Phi\psi+m\frac{dV}{d|\psi|^2}\psi-i\frac{\hbar}{2}\xi\left[\ln\left(\frac{\psi}{\psi^*}\right)-\left\langle\ln\left(\frac{\psi}{\psi^*}\right)\right\rangle\right]\psi. \tag{267}$$

In the strong friction limit, we obtain the quantum Smoluchowski equation

$$\xi\frac{\partial\rho}{\partial t}=\nabla\cdot\left(\nabla P+\rho\nabla\Phi_{\rm ext}+\rho\nabla\Phi+\frac{\rho}{m}\nabla Q\right). \tag{268}$$

(iv) An example of the K-generalized Schrödinger equation was introduced and studied in [16] in connection with Tsallis generalized thermodynamics. It corresponds to

$$K(\rho)=\frac{\hbar^2}{4m^2}\frac{q\rho_0^{1-q}}{\rho^{2-q}}, \tag{269}$$

leading to

$$Q_K = -\frac{\hbar^2}{2m}\frac{\Delta[(\rho/\rho_0)^{q/2}]}{(\rho/\rho_0)^{1-q/2}} = -\frac{\hbar^2}{4m}q\left[\frac{\Delta(\rho/\rho_0)}{(\rho/\rho_0)^{2-q}} - \frac{1}{2}(2-q)\frac{[\nabla(\rho/\rho_0)]^2}{(\rho/\rho_0)^{3-q}}\right], \tag{270}$$

$$\Theta_Q^K = \frac{\hbar^2}{8m^2}\int \frac{q\rho_0^{1-q}}{\rho^{2-q}}(\nabla\rho)^2\,d\mathbf{r} = \frac{1}{q}\int \rho\frac{Q_K}{m}\,d\mathbf{r}, \tag{271}$$

$$\frac{\partial\mathbf{u}}{\partial t} + (\mathbf{u}\cdot\nabla)\mathbf{u} = -\frac{1}{\rho}\nabla P - \nabla\Phi_{\rm ext} - \nabla\Phi - \frac{1}{m}\nabla Q_K - \xi\mathbf{u}, \tag{272}$$

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\Delta\psi + \frac{\hbar^2}{2m}\frac{\Delta|\psi|}{|\psi|}\psi - \frac{\hbar^2}{2m}\frac{\Delta[(|\psi|/\psi_0)^q]}{(|\psi|/\psi_0)^{2-q}}\psi + m\Phi_{\rm ext}\psi + m\Phi\psi + m\frac{dV}{d|\psi|^2}\psi$$
$$-i\frac{\hbar}{2}\xi\left[\ln\left(\frac{\psi}{\psi^*}\right) - \left\langle\ln\left(\frac{\psi}{\psi^*}\right)\right\rangle\right]\psi. \tag{273}$$

An interest of this nonlinear Schrödinger equation is that it admits exact self-similar solutions with a Tsallis invariant profile when the self-interaction potential is of the form $V(|\psi|^2) = \frac{K}{\gamma-1}|\psi|^{2\gamma}$ (corresponding to a polytropic equation of state $P = K\rho^\gamma$) and when the coefficients q and γ are related to each other by the relation $q = 2\gamma - 1$ [16]. For $q = 1$, we recover the generalized Schrödinger Equation (267). It admits exact self-similar solutions with a Gaussian invariant profile when the self-interaction potential is of the form $V(|\psi|^2) = \frac{k_B T}{m}|\psi|^2\big(\ln|\psi|^2 - 1\big)$ (corresponding to an isothermal equation of state $P = \rho k_B T/m$). In the strong friction limit, we obtain the generalized Smoluchowski equation

$$\xi\frac{\partial\rho}{\partial t} = \nabla\cdot\Big(\nabla P + \rho\nabla\Phi_{\rm ext} + \rho\nabla\Phi + \frac{\rho}{m}\nabla Q_K\Big). \tag{274}$$

8.5. Another Generalization

We can propose an even more general Schrödinger equation without specifying the form of the excess free energy $F_{\rm ex}$. Consider the classical damped Euler equation

$$\rho\left[\frac{\partial\mathbf{u}}{\partial t} + (\mathbf{u}\cdot\nabla)\mathbf{u}\right] = -\nabla P - \rho\nabla\frac{\delta F_{\rm ex}}{\delta\rho} - \rho\nabla\Phi - \rho\nabla\Phi_{\rm ext} - \xi\rho\mathbf{u}. \tag{275}$$

Adding and subtracting $-(1/m)\nabla Q$ in the r.h.s. of Equation (275) and performing the inverse Madelung transformation, we obtain a generalized Schrödinger equation of the form

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\Delta\psi - Q\psi + m\frac{\delta F_{\rm ex}}{\delta\rho}\psi + m\Phi_{\rm ext}\psi + m\Phi\psi + m\frac{dV}{d|\psi|^2}\psi$$
$$-i\frac{\hbar}{2}\xi\left[\ln\left(\frac{\psi}{\psi^*}\right) - \left\langle\ln\left(\frac{\psi}{\psi^*}\right)\right\rangle\right]\psi. \tag{276}$$

Using Equation (49) with $\rho = |\psi|^2$, it can be written as

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\Delta\psi + \frac{\hbar^2}{2m}\frac{\Delta|\psi|}{|\psi|}\psi + m\frac{\delta F_{\rm ex}}{\delta|\psi|^2}\psi + m\Phi_{\rm ext}\psi + m\Phi\psi + m\frac{dV}{d|\psi|^2}\psi$$
$$-i\frac{\hbar}{2}\xi\left[\ln\left(\frac{\psi}{\psi^*}\right) - \left\langle\ln\left(\frac{\psi}{\psi^*}\right)\right\rangle\right]\psi. \tag{277}$$

The excess free energy $F_{\rm ex}$ may take into account nontrivial correlations that can be of quantum or nonquantum origin. We can write the generalized Schrödinger Equation (277) in the form

$$i\hbar\frac{\partial\psi}{\partial t}=-\frac{\hbar^2}{2m}\Delta\psi+\frac{\hbar^2}{2m}\frac{\Delta|\psi|}{|\psi|}\psi+m\frac{\delta F}{\delta|\psi|^2}\psi-i\frac{\hbar}{2}\xi\left[\ln\left(\frac{\psi}{\psi^*}\right)-\left\langle\ln\left(\frac{\psi}{\psi^*}\right)\right\rangle\right]\psi, \tag{278}$$

where $F=F_{\rm ex}+W_{\rm ext}+W+U$ is the total free energy. When $F_{\rm ex}=\Theta_Q$, we recover the generalized Schrödinger Equation (253).

8.6. Vlasov–Bohm–Kramers Equation

By making the approximation from Equation (184) and by using the DDFT, we obtained the generalized Kramers equation (see Equation (202))

$$\frac{\partial f}{\partial t}+\mathbf{v}\cdot\frac{\partial f}{\partial\mathbf{r}}-\nabla\frac{\delta F_{\rm ex}}{\delta\rho}\cdot\frac{\partial f}{\partial\mathbf{v}}-\nabla(\Phi+\Phi_{\rm ext})\cdot\frac{\partial f}{\partial\mathbf{v}}=\xi\frac{\partial}{\partial\mathbf{v}}\cdot\left(\frac{k_BT}{m}\frac{\partial f}{\partial\mathbf{v}}+f\mathbf{v}\right). \tag{279}$$

If we consider an excess free energy functional of the form of Equation (242), using the identities

$$\frac{\delta F_{\rm ex}}{\delta\rho}=\frac{Q_K}{m}+V'_{\rm int}(\rho),\qquad \nabla\frac{\delta F_{\rm ex}}{\delta\rho}=\frac{1}{m}\nabla Q_K+\frac{1}{\rho}\nabla P_{\rm int}, \tag{280}$$

obtained from Equation (A78), we can rewrite Equation (279) as

$$\begin{aligned}\frac{\partial f}{\partial t}+\mathbf{v}\cdot\frac{\partial f}{\partial\mathbf{r}}-\frac{1}{m}\nabla Q_K\cdot\frac{\partial f}{\partial\mathbf{v}}-\frac{1}{\rho}\nabla P_{\rm int}\cdot\frac{\partial f}{\partial\mathbf{v}}-\nabla(\Phi+\Phi_{\rm ext})\cdot\frac{\partial f}{\partial\mathbf{v}}&\\=\xi\frac{\partial}{\partial\mathbf{v}}\cdot\left(\frac{k_BT}{m}\frac{\partial f}{\partial\mathbf{v}}+f\mathbf{v}\right).&\end{aligned} \tag{281}$$

If we ignore the dissipative term ($\xi=0$) and take $P_{\rm int}=\Phi_{\rm ext}=0$ and $Q_K=Q$, we obtain the Vlasov–Bohm equation (see Appendix F of [77])

$$\frac{\partial f}{\partial t}+\mathbf{v}\cdot\frac{\partial f}{\partial\mathbf{r}}-\frac{1}{m}\nabla Q\cdot\frac{\partial f}{\partial\mathbf{v}}-\nabla\Phi\cdot\frac{\partial f}{\partial\mathbf{v}}=0, \tag{282}$$

in which quantum effects are included in the Bohm quantum potential. The Vlasov–Bohm equation may be viewed as an approximate, or simplified, version of the Wigner equation, which is the correct quantum generalization of the Vlasov equation [152]. If we account for dissipative effects, we obtain the Vlasov–Bohm–Kramers equation

$$\frac{\partial f}{\partial t}+\mathbf{v}\cdot\frac{\partial f}{\partial\mathbf{r}}-\frac{1}{m}\nabla Q\cdot\frac{\partial f}{\partial\mathbf{v}}-\nabla\Phi\cdot\frac{\partial f}{\partial\mathbf{v}}=\xi\frac{\partial}{\partial\mathbf{v}}\cdot\left(\frac{k_BT}{m}\frac{\partial f}{\partial\mathbf{v}}+f\mathbf{v}\right), \tag{283}$$

which can be viewed as an approximate or simplified version of the Wigner–Kramers equation. The Wigner–Kramers equation and the Vlasov–Bohm–Kramers equation were introduced in [77] in the context of the violent relaxation of quantum systems with long-range interactions. If we use Q_K instead of Q, we obtain a K-generalization of the Vlasov–Bohm–Kramers equation. If we use an arbitrary excess free energy functional $F_{\rm ex}[\rho]$, we obtain an even more general form of Vlasov–Bohm–Kramers equation.

Remark 17. *By taking the hydrodynamic moments of the Vlasov–Bohm–Kramers Equation (283) and by closing the hierarchy of equations with the LTE approximation (193), we obtain the continuity Equation (209) and the quantum Euler Equation (237), which are equivalent to the generalized GP Equation (35). The same equations are obtained from the Wigner–Kramers equation when some additional approximations are implemented (see [77] for details). The Wigner–Kramers–Poisson equations can be derived, on the coarse-grained scale, from the theory of violent relaxation of self-gravitating BECs [77]. This may be a manner to justify the generalized GP Equation (35).*

9. General Case

By combining the results derived in the previous sections, we can propose a generalized Schrödinger equation of the form

$$i\hbar\frac{\partial\psi}{\partial t}=-\frac{\hbar^2}{2m}\Delta\psi+m\frac{\delta\mathcal{F}_{\rm ex}}{\delta|\psi|^2}\psi+m\Phi_{\rm ext}\psi+m\Phi\psi+m\frac{dV}{d|\psi|^2}\psi \\ -i\frac{\hbar}{2}\xi\left[\ln\left(\frac{\psi}{\psi^*}\right)-\left\langle\ln\left(\frac{\psi}{\psi^*}\right)\right\rangle\right]\psi. \quad (284)$$

We have included in the equations of Section 3 an excess free energy $\mathcal{F}_{\rm ex}[\rho]$, which can take into account nontrivial correlations between the quantum particles (and is more general than a self-interaction potential V) like in the equations in Section 7 for Brownian particles in interaction[25]. This term could be justified on a microscopic basis by developing a quantum N-body theory for a gas of bosons in interaction. This is similar in spirit to the Kohn–Sham DDFT [153] except that, in the present case, we are dealing with just one wavefunction $\psi(\mathbf{r},t)$ instead of a multistate system[26]. Performing the Madelung transformation, we obtain a quantum damped Euler equation of the form

$$\rho\left[\frac{\partial\mathbf{u}}{\partial t}+(\mathbf{u}\cdot\nabla)\mathbf{u}\right]=-\nabla P-\rho\nabla\frac{\delta\mathcal{F}_{\rm ex}}{\delta\rho}-\rho\nabla\Phi-\rho\nabla\Phi_{\rm ext}-\frac{\rho}{m}\nabla Q-\xi\rho\mathbf{u}. \quad (285)$$

If we define $F_{\rm ex}=\mathcal{F}_{\rm ex}+\Theta_Q+U_{\rm int}$, we obtain an equation equivalent the damped Euler Equation (236). Conversely, if we consider an excess free energy of the form $F_{\rm ex}=\mathcal{F}_{\rm ex}+\Theta_Q+U_{\rm int}$ in Equation (236) and assume that the velocity field is potential (see the remark at the end of Section 8), we obtain the Euler Equation (285) leading to the generalized Schrödinger Equation (284). In the strong friction limit, we obtain the generalized Smoluchowski equation

$$\xi\frac{\partial\rho}{\partial t}=\nabla\cdot\left(\nabla P+\rho\nabla\frac{\delta\mathcal{F}_{\rm ex}}{\delta\rho}+\rho\nabla\Phi+\rho\nabla\Phi_{\rm ext}+\frac{\rho}{m}\nabla Q\right). \quad (286)$$

These equations can also be obtained from the generalized Vlasov–Bohm–Kramers equation (see Section 8.6)

$$\frac{\partial f}{\partial t}+\mathbf{v}\cdot\frac{\partial f}{\partial\mathbf{r}}-\nabla\frac{\delta\mathcal{F}_{\rm ex}}{\delta\rho}\cdot\frac{\partial f}{\partial\mathbf{v}}-\frac{1}{m}\nabla Q\cdot\frac{\partial f}{\partial\mathbf{v}}-\frac{1}{\rho}\nabla P_{\rm int}\cdot\frac{\partial f}{\partial\mathbf{v}}-\nabla(\Phi+\Phi_{\rm ext})\cdot\frac{\partial f}{\partial\mathbf{v}} \\ =\xi\frac{\partial}{\partial\mathbf{v}}\cdot\left(\frac{k_BT}{m}\frac{\partial f}{\partial\mathbf{v}}+f\mathbf{v}\right). \quad (287)$$

If we define $\mathcal{F}=\mathcal{F}_{\rm ex}+U+W+W_{\rm ext}$ (this functional does not include the quantum potential), we can write the generalized Schrödinger Equation (284) as

$$i\hbar\frac{\partial\psi}{\partial t}=-\frac{\hbar^2}{2m}\Delta\psi+m\frac{\delta\mathcal{F}}{\delta|\psi|^2}\psi-i\frac{\hbar}{2}\xi\left[\ln\left(\frac{\psi}{\psi^*}\right)-\left\langle\ln\left(\frac{\psi}{\psi^*}\right)\right\rangle\right]\psi, \quad (288)$$

the damped Euler Equation (285) as

$$\rho\left[\frac{\partial\mathbf{u}}{\partial t}+(\mathbf{u}\cdot\nabla)\mathbf{u}\right]=-\rho\nabla\frac{\delta\mathcal{F}}{\delta\rho}-\frac{\rho}{m}\nabla Q-\xi\rho\mathbf{u}, \quad (289)$$

and the generalized Smoluchowski Equation (286) as

$$\xi\frac{\partial\rho}{\partial t}=\nabla\cdot\left(\rho\nabla\frac{\delta\mathcal{F}}{\delta\rho}+\frac{\rho}{m}\nabla Q\right). \quad (290)$$

If we define $F=\mathcal{F}+\Theta_Q$, we recover the structure of the damped Euler Equation (103) and the structure of the Smoluchowski Equation (105). On the other hand, Equation (288) is structurally equivalent to the Schrödinger Equation (115). If we define $F_{\rm tot} = \Theta + \mathcal{F} = \Theta_c + F$, we recover Equation (113). If we define $\mathcal{F}_0 = \mathcal{F}_{\rm ex} + U_{\rm int} + W + W_{\rm ext}$ (this functional does not include the quantum potential nor the thermal free energy), the foregoing equations can be obtained from the generalized Vlasov–Bohm–Kramers equation

$$\frac{\partial f}{\partial t} + \mathbf{v}\cdot\frac{\partial f}{\partial \mathbf{r}} - \nabla\frac{\delta\mathcal{F}_0}{\delta\rho}\cdot\frac{\partial f}{\partial \mathbf{v}} - \frac{1}{m}\nabla Q\cdot\frac{\partial f}{\partial \mathbf{v}} = \xi\frac{\partial}{\partial \mathbf{v}}\cdot\left(\frac{k_B T}{m}\frac{\partial f}{\partial \mathbf{v}} + f\mathbf{v}\right). \tag{291}$$

Alternatively, we could account for quantum effects through the exact Wigner advection operator instead of the heuristic Vlasov–Bohm advection operator (see Section 8.6).

Remark 18. *We can introduce a noise term in the previous equations in order to take into account fluctuations (arising from finite N effects or finite temperature effects) as discussed in Section 7.7.*

10. Conclusions

In this paper, we introduced generalized equations in quantum mechanics and Brownian theory and we discussed their formal analogies.

By using the formalism of scale relativity, and taking into account dissipative effects, we first derived a generalized GP equation (see Equation (33)), including a temperature term and a friction term. We then completed this equation by introducing an arbitrary potential of self-interaction and a long-range potential of interaction (see Equation (35)). By using the Madelung transformation, we wrote this equation in the form of hydrodynamic equations called the quantum damped Euler equations (see Equations (57) and (58)). In the strong friction limit, they reduce to the quantum Smoluchowski equation (see Equation (64)).

We then considered a system of classical Brownian particles with long-range and short-range interactions. Starting from the N-body Kramers equation (see Equation (181)), we obtained the exact one-body Kramers equation including the two-body correlation function (see Equation (183)). Long-range interactions can be treated with the mean field approximation (for $N \gg 1$) while short-range interactions can be treated with the DDFT. By taking the moments of the Kramers equation, we obtained the damped Jeans equations (see Equations (209) and (210)). By making the LTE approximation, this hierarchy of equations can be closed leading to the damped Euler equations (see Equations (209) and (220)). In the strong friction limit, they reduce to the Smoluchowski equation (see Equation (213)). When the excess free energy has an adequate form, these equations coincide with those obtained from the generalized GP Equation (35)[27]. In addition, the generalized Kramers Equation (202) coincides with the Vlasov–Bohm–Kramers Equation (283). We then considered more general forms of excess free energy and obtained generalized quantum equations (see Sections 8 and 9). We finally indicated how fluctuations can be taken into account in our formalism (see Section 7.7).

It is interesting to compare these results with those obtained in [77]. In that paper, we first recalled that the Schrödinger equation (see Equation (10) of [77]) can be transformed into the Wigner equation (see Equation (44) of [77]). When coupled to a long-range potential of interaction (like gravity), we argued that the quantum system undergoes a process of violent relaxation (or gravitational cooling) and that the relevant equation to consider is the Wigner–Kramers equation describing the evolution of the coarse-grained distribution function (see Equation (46) of [77]). Quantum effects are taken into account in the advection (Wigner) term and thermal effects are taken into account in the effective collision (Kramers) term. We also proposed a heuristic Vlasov–Bohm–Kramers equation (see Equation (F2) of [77]). By taking the moments of these equations, we obtained the damped quantum Jeans equations (see Equations (56) and (57) of [77]). By making the LTE approximation, this hierarchy of equations can be closed, leading to the damped quantum Euler equations (see Equations (72) and (73) of [77])[28]. In the strong friction limit, they reduce to the quantum Smoluchowski equation (see Equation (81) of [77]). By performing the inverse Madelung transformation, we obtained the generalized GP equation (see Equation (92) of [77]), which coincides with Equation (35). When applied to self-gravitating BECs, this equation leads to equilibrium states with a core–envelope structure. This core–envelope structure, made of a quantum core (soliton) surrounded by an isothermal envelope, is consistent with the structure of dark matter halos [77–79]. We refer the reader to the reviews [81–89] for more details on this topic.

Our work also suggests an interesting and original interpretation of generalized thermodynamics [154]. Complex systems are sometimes described by generalized entropies or generalized free energies [131,132,155]. In the interpretation given in the present paper, these generalized free energies correspond to what is called excess free energies in the physics of liquids and in the DFT and DDFT [33–35]. They take into account correlations between the particles arising from short-range interactions. This interpretation may demystify the notion of generalized thermodynamics. Actually, we must distinguish two different situations:

(i) In this paper, we assumed that the evolution of the N-body distribution of the Brownian system is governed by the ordinary Kramers equation (see Equation (181)). At equilibrium, we obtain the ordinary Gibbs distribution (see Equation (118)). This implies that the velocity distribution is Maxwellian. In this sense, we are fundamentally using ordinary thermodynamics for the N-body system. However, when we consider the one-body distribution in configuration space $\rho(\mathbf{r}, t)$, we have to take into account the correlation $\rho_2(\mathbf{r}, \mathbf{r}')$ between the particles due to short-range interactions. As a result, the free energy in configuration space $F[\rho]$ differs from the ideal Boltzmann free energy $F_{\rm id}[\rho]$. In the DFT and DDFT, the correlations are taken into account through an excess free energy $F_{\rm ex}[\rho]$ in configuration space, which can be interpreted as a generalized free energy. In certain cases, this excess free energy can be related to the Tsallis free energy (see Equation (A71)) but this is not universally true. In the strong friction limit, the evolution of the density $\rho(\mathbf{r}, t)$ is governed by a generalized Smoluchowski equation (see Equation (214)), including a nonlinear barotropic pressure $P(\rho)$, which is due to the spatial correlations encapsulated in the excess free energy $F_{\rm ex}[\rho]$. This equation can be viewed as a generalized Fokker–Planck equation in configuration space. In the absence of correlations, we recover the ordinary Smoluchowski Equation (219) with an isothermal (linear) equation of state associated with the Boltzmann free energy $F_{\rm id}[\rho]$.

(ii) If we come back to the foundations of generalized thermodynamics [154,155], we should modify the Kramers equation and the Gibbs distribution function for the N-body system. Developing the corresponding formalism represents, however, a formidable task. Another, more tractable, possibility is to modify the Kramers equation for the one-body distribution function $f(\mathbf{r}, \mathbf{v}, t)$ [131,132]. This leads to the notion of generalized Fokker–Planck equations in phase space associated with a generalized free energy $F[f]$ (see Section 4 of [131] and Section 6.2 of [37]). In that case, the equilibrium velocity distribution is not Maxwellian. In the strong friction limit, the generalized Kramers equation leads to a generalized Smoluchowski equation including a nonlinear barotropic pressure $P(\rho)$ determined by the generalized free energy $F[f]$. This equation can be derived rigorously from a Chapman–Enskog expansion [156]. The equation of state $P(\rho)$ is different from the isothermal (linear) equation of state even in the absence of correlations in configuration space. If there are correlations in configuration space, the pressure is due both to these correlations (as in (i)) and to the non-Boltzmannian nature of the distribution function.

Although the nonlinear Fokker–Planck equations in configuration space (the generalized Smoluchowski equation) are structurally similar in the two situations, they are derived in a completely different manner. This shows that the notion of generalized entropies and nonlinear Fokker–Planck equations may have different origins. In the theory of fluids [33,34], the distribution function is Boltzmannian and the nonlinear pressure is due to the two-body correlation function originating from short-range interactions $u_{\rm SR}$. In the generalized thermodynamics approach [131,132], the nonlinear pressure arises from the non-Boltzmannian nature of the distribution function in phase space due to the bias in the transition probabilities from one state to the other. The hydrodynamic (macroscopic) equations coincide even though the microscopic models are fundamentally different [37].

The classical Brownian equations discussed in our paper have been used in the theory of simple liquids [33–35] and in the context of generalized thermodynamics and nonlinear Fokker–Planck equations [17,37,38,130–132,155]. When coupled to the Poisson equation, they describe a system of self-gravitating Brownian particles [45], which may find applications in the context of planet formation [157]. They also describe the chemotaxis of bacterial populations within the Keller–Segel model [44]. There is a vast literature on these equations and their generalizations (see, e.g., [151] and references therein). The quantum equations discussed in our paper have been used in the context of DM made of BECs (see the reviews [81–89] on this subject). They lead to DM halos with a core–envelope structure, including a quantum core and an isothermal envelope. The quantum core may solve the core–cusp problem of the CDM model and the isothermal envelope accounts for the flat rotation curves of the galaxies. The friction term provides an H-theorem and ensures that the system converges towards this core–envelope structure. Therefore, they could provide a parametrization of the GPP equations. This is explained in detail in [77]. A predictive model of bosonic DM halos based on these equations was developed in [79]. The generalized quantum equations that we obtained in the present paper, based on the analogy between quantum and Brownian equations, could provide generalized models of DM. Since the nature of DM is still uncertain, it is always interesting to consider generalizations of the standard equations of physics in order to see if they can account for the observations. Conversely, this generalization may tell us to which extent the standard equations of physics are specific in describing the objects that we observe in nature.

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Appendix A. Thermodynamical Identities for a Cold Gas

In this Appendix, we regroup useful thermodynamical identities valid for a cold gas like a BEC at $T = 0$.

Appendix A.1. First Principle of Thermodynamics and Gibbs–Duhem Relation

The first principle of thermodynamics can be written in a local form as

$$d\left(\frac{u}{\rho}\right) = -Pd\left(\frac{1}{\rho}\right) + Td\left(\frac{s}{\rho}\right), \tag{A1}$$

where u is the density of internal energy, ρ is the mass density, P is the pressure, T is the temperature, and s is the entropy density. We also recall the local integrated Gibbs–Duhem relation

$$u = -P + Ts + \frac{\mu}{m}\rho, \tag{A2}$$

where μ is the local chemical potential.

Let us consider the situation appropriate to a cold gas such as a BEC at $T = 0$ described by the generalized GP Equation (35)[29]. If $T = 0$, the first principle of thermodynamics from Equation (A1) can be written as

$$d\left(\frac{u}{\rho}\right) = -Pd\left(\frac{1}{\rho}\right) = \frac{P}{\rho^2}d\rho. \tag{A3}$$

If we introduce the enthalpy density

$$h = \frac{P+u}{\rho}, \tag{A4}$$

then we obtain the relations

$$du = h\,d\rho \qquad \text{and} \qquad dh = \frac{dP}{\rho}. \tag{A5}$$

On the other hand, the local integrated Gibbs–Duhem relation (A2) reduces to

$$u = -P + \frac{\mu}{m}\rho. \tag{A6}$$

Comparing Equations (A4) and (A6), we find that

$$h = \frac{\mu}{m}. \tag{A7}$$

Therefore, the enthalpy $h(\mathbf{r})$ coincides with the local chemical potential $\mu(\mathbf{r})$ by unit of mass: $h(\mathbf{r}) = \mu(\mathbf{r})/m$.

Appendix A.2. Barotropic Equation of State

For a general barotropic equation of state of the form $P = P(\rho)$, the foregoing relations lead to the identities

$$\left(\frac{u}{\rho}\right)' = \frac{P(\rho)}{\rho^2}, \qquad h(\rho) = \frac{P(\rho) + u(\rho)}{\rho}, \tag{A8}$$

$$h(\rho) = u'(\rho), \qquad h'(\rho) = \frac{P'(\rho)}{\rho}, \tag{A9}$$

$$P(\rho) = \rho h(\rho) - u(\rho) = \rho u'(\rho) - u(\rho) = \rho^2 \left(\frac{u}{\rho}\right)', \tag{A10}$$

$$P'(\rho) = \rho u''(\rho). \tag{A11}$$

The first principle of thermodynamics for a cold gas (see Equation (A3)) provides a general relation between the density of internal energy $u(\rho)$ and the pressure $P(\rho)$. If we know the internal energy density $u = u(\rho)$, we can obtain the pressure by

$$P(\rho) = -\frac{d(u/\rho)}{d(1/\rho)} = \rho^2 \left(\frac{u}{\rho}\right)' = \rho u'(\rho) - u(\rho). \tag{A12}$$

Conversely, if we know the equation of state $P = P(\rho)$, we can obtain the internal energy density by

$$u(\rho) = \rho \int^{\rho} \frac{P(\rho')}{\rho'^2}\, d\rho'. \tag{A13}$$

This is the solution of the differential equation

$$\rho \frac{du}{d\rho} - u(\rho) = P(\rho). \tag{A14}$$

We also note that the enthalpy is given by

$$h(\rho) = \int^{\rho} \frac{P'(\rho')}{\rho'}\, d\rho'. \tag{A15}$$

Appendix A.3. Internal Energy Functional

For a barotropic gas, using Equation (A13), the internal energy functional is

$$U = \int u(\rho)\, d\mathbf{r} = \int \rho \int^{\rho} \frac{P(\rho')}{\rho'^2}\, d\rho'\, d\mathbf{r}. \tag{A16}$$

We have

$$\frac{\delta U}{\delta\rho}=u'(\rho)=h(\rho)=\int^{\rho}\frac{P'(\rho')}{\rho'}\,d\rho' \tag{A17}$$

and

$$\nabla\frac{\delta U}{\delta\rho}=u''(\rho)\nabla\rho=h'(\rho)\nabla\rho=\frac{P'(\rho)}{\rho}\nabla\rho. \tag{A18}$$

Therefore,

$$\rho\nabla\frac{\delta U}{\delta\rho}=\nabla P. \tag{A19}$$

We also note the identity

$$\frac{\nabla P}{\rho}=u''(\rho)\nabla\rho=h'(\rho)\nabla\rho=\nabla h. \tag{A20}$$

Appendix A.4. Polytropic Equation of State

For a polytropic equation of state of the form $P=K\rho^{\gamma}$ with $\gamma=1+1/n$, using Equation (A13), we find that the density of internal energy is given by

$$u=\frac{K}{\gamma-1}\rho^{\gamma}=\frac{P}{\gamma-1}=nP=nK\rho^{1+1/n}, \tag{A21}$$

where we set the constant of integration to zero. We can also write the density of internal energy in the form

$$u=\frac{K}{\gamma-1}(\rho^{\gamma}-\rho) \tag{A22}$$

by taking the constant of integration equal to $-K/(\gamma-1)$. In that case, the internal energy functional

$$U=\frac{K}{\gamma-1}\int(\rho^{\gamma}-\rho)\,d\mathbf{r} \tag{A23}$$

takes a form similar to the Tsallis free energy with an index γ and a generalized temperature K.

Appendix A.5. Self-Interaction Potential

Comparing Equations (40), (52)–(54) and (56) with Equations (A8)–(A11), we see that the potential $V(\rho)$ that occurs in the generalized GP Equation (38) represents the density of internal energy. We, therefore, have

$$u(\rho)=V(\rho). \tag{A24}$$

This justifies the expression of the internal energy in Equation (81).

Appendix A.6. Standard BEC

For the standard BEC with the self-interaction potential from Equation (42), we obtain

$$V=u=\frac{2\pi a_s\hbar^2}{m^3}\rho^2,\qquad U=\frac{2\pi a_s\hbar^2}{m^3}\int\rho^2\,d\mathbf{r}, \tag{A25}$$

$$h=\frac{4\pi a_s\hbar^2}{m^3}\rho,\qquad P=\frac{2\pi a_s\hbar^2}{m^3}\rho^2. \tag{A26}$$

The equation of state corresponds to a polytrope of index $\gamma=2$ (i.e., $n=1$).

Appendix B. Variation of the Energies Functionals

In this appendix, we detail the first-order variations of the different functionals that compose the free energy (77). The details of the derivation are given in Appendix C of [76].

The first-order variations of the classical kinetic energy (79) are

$$\delta\Theta_c = \int \frac{\mathbf{u}^2}{2}\delta\rho\, d\mathbf{r} + \int \rho\mathbf{u}\cdot\delta\mathbf{u}\, d\mathbf{r}. \tag{A27}$$

The first-order variations of the quantum kinetic energy (80) are

$$\delta\Theta_Q = \frac{1}{m}\int Q\delta\rho\, d\mathbf{r}. \tag{A28}$$

The first-order variations of the internal energy (81) are

$$\delta U = \int h(\rho)\delta\rho\, d\mathbf{r}. \tag{A29}$$

The first-order variations of the potential energy of long-range interactions (83) are

$$\delta W = \int \Phi\delta\rho\, d\mathbf{r}. \tag{A30}$$

The first-order variations of the external potential energy (84) are

$$\delta W_{\rm ext} = \int \Phi_{\rm ext}\delta\rho\, d\mathbf{r}. \tag{A31}$$

Appendix C. *H*-Theorems

In this Appendix, we derive the H-theorems for the generalized Smoluchowski, damped Euler and Kramers equations. We use a functional derivative approach. We refer to [17,37,38,130,131] for a more detailed discussion of the properties of nonlinear Fokker–Planck equations [132].

Appendix C.1. Smoluchowski Equation

The Smoluchowski equation can be written as

$$\frac{\partial\rho}{\partial t} = \nabla\cdot\left(\frac{1}{\xi}\rho\nabla\frac{\delta F}{\delta\rho}\right), \tag{A32}$$

where $F[\rho]$ is the free energy. The quantum Smoluchowski Equation (64) corresponds to Equation (A32) with the functional from Equation (89), the generalized Smoluchowski Equation (213) corresponds to Equation (A32) with the functional from Equation (140), and the generalized Smoluchowski Equation (214) corresponds to Equation (A32) with the functional from Equation (150). The Smoluchowski Equation (A32) monotonically dissipates the free energy functional, which plays the role of a Lyapunov functional. Indeed, a straightforward calculation leads to the H-theorem appropriate to the canonical ensemble:

$$\dot{F} = \int \frac{\delta F}{\delta\rho}\frac{\partial\rho}{\partial t}d\mathbf{r} = \int \frac{\delta F}{\delta\rho}\nabla\cdot\left(\frac{1}{\xi}\rho\nabla\frac{\delta F}{\delta\rho}\right)d\mathbf{r} = -\int \frac{1}{\xi}\rho\left(\nabla\frac{\delta F}{\delta\rho}\right)^2 d\mathbf{r} \le 0. \tag{A33}$$

For a steady state, $\dot{F} = 0$, the last term in parenthesis, which is proportional to the diffusion current in the Smoluchowski Equation (A32), vanishes so that $\delta F/\delta\rho$ is uniform:

$$\frac{\delta F}{\delta\rho} = \frac{\mu}{m}. \tag{A34}$$

This returns the Gibbs condition from Equation (100) for quantum systems and the Gibbs condition from Equation (142) for Brownian systems. Therefore, a density profile $\rho(\mathbf{r})$ is a steady state of the Smoluchowski Equation (A32) if, and only if, it is an extremum of free energy F at fixed mass. Furthermore, it can be shown that a steady state is linearly dynamically stable with respect to the Smoluchowski Equation (A32) if, and only if, it is a (local) minimum of free energy F at fixed mass [131,132]. This is consistent with the condition of thermodynamic equilibrium in the canonical ensemble (see Section 5). If F is bounded from below[30], we know from Lyapunov's direct method that the system will relax towards a (local) minimum of F at fixed mass M for $t \to +\infty$. If several (local) minima exist (metastable states), the choice of the selected equilibrium will depend on a complicated notion of basin of attraction.

Remark A1. *The Smoluchowski Equation (A32) can be justified in a phenomenological manner from the linear thermodynamics of Onsager [160,161] if we interpret it as a continuity equation* $\partial_t \rho + \nabla \cdot \mathbf{J} = 0$ *with a current* $\mathbf{J} = -(\rho/\xi)\nabla(\delta F/\delta\rho)$ *proportional to the gradient of a (chemical) potential* $\mu(\mathbf{r})/m \equiv \delta F/\delta\rho$ *that is uniform at equilibrium. We note the resemblances between the Smoluchowski Equation (A32), the Ginzburg–Landau Equation (A97) and the Cahn–Hilliard Equation (A98). There are also crucial differences between these equations. For example, in the Cahn–Hilliard Equation (A98), the current is proportional to* $\nabla(\delta F/\delta\rho)$*, whereas it is proportional to* $\rho\nabla(\delta F/\delta\rho)$ *in the Smoluchowski Equation (A32).*

Appendix C.2. Damped Euler Equations

The damped Euler equations can be written as

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0, \tag{A35}$$

$$\rho \left[\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla)\mathbf{u} \right] = -\rho \nabla \frac{\delta F}{\delta \rho} - \xi \rho \mathbf{u}, \tag{A36}$$

where $F[\rho]$ is the free energy. The quantum damped Euler Equation (58) corresponds to Equation (A36) with the functional from Equation (89), the generalized damped Euler Equation (220) corresponds to Equation (A36) with the functional from Equation (140), and the generalized damped Euler Equation (221) corresponds to Equation (A36) with the functional from Equation (150). The damped Euler Equations (A35) and (A36) satisfy an H-theorem for the total free energy $F_{\rm tot}[\mathbf{u}, \rho] = (1/2) \int \rho \mathbf{u}^2 \, d\mathbf{r} + F[\rho]$. Indeed, using the well-known identity of vector analysis $(\mathbf{u} \cdot \nabla)\mathbf{u} = \nabla(\mathbf{u}^2/2) - \mathbf{u} \times (\nabla \times \mathbf{u})$, we can write the damped Euler equations in the form

$$\frac{\partial \rho}{\partial t} = -\nabla \cdot \left(\frac{\delta F_{\rm tot}}{\delta \mathbf{u}} \right), \tag{A37}$$

$$\frac{\partial \mathbf{u}}{\partial t} - \mathbf{u} \times (\nabla \times \mathbf{u}) = -\nabla \frac{\delta F_{\rm tot}}{\delta \rho} - \xi \mathbf{u}. \tag{A38}$$

Then, using the fact that $\mathbf{u} \times (\nabla \times \mathbf{u})$ is orthogonal to $\mathbf{u}$, we find that

$$\begin{aligned} \dot{F}_{\rm tot} &= \int \frac{\delta F_{\rm tot}}{\delta \rho} \frac{\partial \rho}{\partial t} \, d\mathbf{r} + \int \frac{\delta F_{\rm tot}}{\delta \mathbf{u}} \cdot \frac{\partial \mathbf{u}}{\partial t} \, d\mathbf{r} \\ &= -\int \frac{\delta F_{\rm tot}}{\delta \rho} \nabla \cdot \left(\frac{\delta F_{\rm tot}}{\delta \mathbf{u}} \right) d\mathbf{r} - \int \frac{\delta F_{\rm tot}}{\delta \mathbf{u}} \cdot \nabla \frac{\delta F_{\rm tot}}{\delta \rho} \, d\mathbf{r} - \xi \int \frac{\delta F_{\rm tot}}{\delta \mathbf{u}} \cdot \mathbf{u} \, d\mathbf{r}. \end{aligned} \tag{A39}$$

Since the first two terms in the second equality of Equation (A39) vanish after an integration by parts, we finally obtain

$$\dot{F}_{\rm tot} = -\int \xi\rho\mathbf{u}^2 d\mathbf{r} \leq 0. \tag{A40}$$

For a steady state, $\dot{F}_{\rm tot} = 0$, the velocity vanishes ($\mathbf{u} = \mathbf{0}$). Then, Equation (A36) implies that $\delta F/\delta\rho$ is uniform leading to Equation (A34). As a result, a density profile $\rho(\mathbf{r})$ is a steady state of the damped Euler Equations (A35) and (A36) if, and only if, it is an extremum of free energy F at fixed mass. Furthermore, it is dynamically stable if, and only if, it is a (local) minimum of F at fixed mass M. More generally, the same results as those described in Appendix C.1 apply to the present situation.

Appendix C.3. Kramers Equation

The Kramers equation can be written as

$$\frac{\partial f}{\partial t} - [f, E] = \frac{\partial}{\partial \mathbf{v}}\cdot\left[\xi f \frac{\partial}{\partial \mathbf{v}}\left(\frac{\delta F_{\rm tot}}{\delta f}\right)\right], \tag{A41}$$

where $E[f]$ is the energy and $F_{\rm tot}[f] = E[f] - TS[f]$ is the free energy ($S[f]$ is the entropy). The generalized Kramers Equation (202) corresponds to Equation (A41) with the functional F from Equation (165) and the functional E from Equation (166), and the generalized Kramers Equation (203) corresponds to Equation (A41) with the functional F from Equation (175) and the functional E from Equation (166). The Vlasov–Bohm–Kramers Equation (283) is a particular case of Equation (202) with $F_{\rm ex} = \Theta_Q$.

The left-hand side of the Kramers equation (advection term) conserves the energy E and the entropy S individually. Therefore, it conserves the free energy $F_{\rm tot} = E - TS$. On the other hand, the right-hand side of the Kramers equation (diffusion term) monotonically dissipates the free energy $F_{\rm tot}$, which plays the role of a Lyapunov functional. Indeed, a straightforward calculation leads to the H-theorem appropriate to the canonical ensemble

$$\begin{aligned}\dot{F}_{\rm tot} &= \int \frac{\delta F_{\rm tot}}{\delta f}\frac{\partial f}{\partial t}\, d\mathbf{r}d\mathbf{v} = \int \frac{\delta F_{\rm tot}}{\delta f}\frac{\partial}{\partial \mathbf{v}}\cdot\left[\xi f \frac{\partial}{\partial \mathbf{v}}\left(\frac{\delta F_{\rm tot}}{\delta f}\right)\right] d\mathbf{r}d\mathbf{v} \\ &= -\int \xi f \left[\frac{\partial}{\partial \mathbf{v}}\left(\frac{\delta F_{\rm tot}}{\delta f}\right)\right]^2 d\mathbf{r}d\mathbf{v} \leq 0. \end{aligned} \tag{A42}$$

For a steady state, $\dot{F}_{\rm tot} = 0$, the last term in brackets in Equation (A42), which is proportional to the diffusion current in the Kramers Equation (A41), vanishes so that $\delta F_{\rm tot}/\delta f$ is independent of $\mathbf{v}$. We then have $\delta E/\delta f - T\delta S/\delta f = C(\mathbf{r})$, implying that $f(\mathbf{r}, \mathbf{v})$ is a function of $\delta E/\delta f - C(\mathbf{r})$. Since the right-hand side of Equation (A41) vanishes, the left-hand side must also vanish independently. Since $\partial/\partial t = 0$, we obtain $[f, E] = 0$, implying that $f(\mathbf{r}, \mathbf{v})$ is a function of $\delta E/\delta f$ alone. From these two requirements, we conclude that $C(\mathbf{r})$ is a constant; hence, $\delta F_{\rm tot}/\delta f$ is a constant:

$$\frac{\delta F_{\rm tot}}{\delta f} = \frac{\mu_{\rm tot}}{m}. \tag{A43}$$

This returns the Gibbs condition from Equation (169). Therefore, a distribution function $f(\mathbf{r}, \mathbf{v})$ is a steady state of the Kramers Equation (A41) if, and only if, it is an extremum of free energy $F_{\rm tot}$ at fixed mass. Furthermore, it can be shown that a steady state is linearly dynamically stable with respect to the Kramers Equation (A41) if, and only if, it is a (local) minimum of free energy $F_{\rm tot}$ at fixed mass [131,132]. This is consistent with the condition of thermodynamic equilibrium in the canonical ensemble (see Section 5). If $F_{\rm tot}$ is bounded from below, we know from Lyapunov's direct method that the system will relax towards a (local) minimum of F at fixed mass M for $t \to +\infty$. If several (local) minima exist (metastable states), the choice of the selected equilibrium will depend on a complicated notion of basin of attraction.

Remark A2. *The free energy* $F_{\rm tot}[\rho,\mathbf{u}]$ *associated with the damped Euler Equation (A36) can be deduced from the free energy* $F_{\rm tot}[f]$ *associated with the Kramers Equation (A41) by performing the LTE approximation; in addition, the free energy* $F[\rho]$ *associated with the Smoluchowski Equation (A32) can be deduced from the free energy* $F_{\rm tot}[\rho,\mathbf{u}]$ *associated with the damped Euler equation by neglecting the kinetic term (this is valid when* $\xi\rightarrow+\infty$*).*

Appendix C.4. Generalized GP Equation

The generalized GP Equation (35) can be written as

$$i\hbar\frac{\partial\psi}{\partial t}=m\frac{\delta F_{\rm tot}}{\delta\psi^*}-i\frac{\hbar}{2}\xi\left[\ln\left(\frac{\psi}{\psi^*}\right)-\left\langle\ln\left(\frac{\psi}{\psi^*}\right)\right\rangle\right]\psi, \tag{A44}$$

where $F_{\rm tot}[\psi,\psi^*]$ is the free energy from Equation (85). The generalized GP Equation (A44) monotonically dissipates the free energy functional, which plays the role of a Lyapunov functional. Indeed, a straightforward calculation leads to an H-theorem appropriate to the canonical ensemble. We have

$$\dot{F}_{\rm tot}=\int\frac{\delta F_{\rm tot}}{\delta\psi}\frac{\partial\psi}{\partial t}\,d\mathbf{r}+{\rm c.c.} \tag{A45}$$

Substituting Equation (A44) into Equation (A45), we obtain

$$\dot{F}_{\rm tot}=\frac{m}{i\hbar}\int\frac{\delta F_{\rm tot}}{\delta\psi}\frac{\delta F_{\rm tot}}{\delta\psi^*}\,d\mathbf{r}-\frac{1}{2}\xi\int\frac{\delta F_{\rm tot}}{\delta\psi}\left[\ln\left(\frac{\psi}{\psi^*}\right)-\left\langle\ln\left(\frac{\psi}{\psi^*}\right)\right\rangle\right]\psi\,d\mathbf{r}+{\rm c.c.} \tag{A46}$$

Using the fact that

$$\frac{\delta F_{\rm tot}}{\delta\psi}=-\frac{\hbar^2}{2m^2}\Delta\psi^*+\left[h(|\psi|^2)+\Phi+\Phi_{\rm ext}\right]\psi^*, \tag{A47}$$

and recalling that $\ln(\psi/\psi^*)$ is purely imaginary, we see that many terms vanish by symmetry with their complex conjugate. There remains

$$\dot{F}_{\rm tot}=\frac{\hbar^2}{4m^2}\xi\int\Delta\psi^*\left[\ln\left(\frac{\psi}{\psi^*}\right)-\left\langle\ln\left(\frac{\psi}{\psi^*}\right)\right\rangle\right]\psi\,d\mathbf{r}+{\rm c.c.} \tag{A48}$$

Integrating by parts and again discarding the terms that vanish as a result of symmetry with their complex conjugate, we find that

$$\dot{F}_{\rm tot}=-\frac{\hbar^2}{4m^2}\xi\int(\psi\nabla\psi^*-\psi^*\nabla\psi)\cdot\nabla\left[\ln\left(\frac{\psi}{\psi^*}\right)\right]d\mathbf{r}, \tag{A49}$$

which can be written as

$$\dot{F}_{\rm tot}=-\xi\int\frac{\hbar^2}{4m^2}|\psi|^2\left|\nabla\ln\left(\frac{\psi}{\psi^*}\right)\right|^2d\mathbf{r}\leq 0. \tag{A50}$$

This expression coincides with the H-theorem from Equation (A40).

Appendix D. Thermodynamical Identities for Brownian Particles in Contact with a Heat Bath

In this appendix, we regroup useful thermodynamical identities valid for Brownian particles in contact with a heat bath fixing the temperature ($T={\rm cst}$).

Appendix D.1. First Principle of Thermodynamics and Gibbs–Duhem Relation

If $T = \text{cst}$ (canonical ensemble), introducing the density of free energy $f = u - Ts$, the first principle of thermodynamics from Equation (A1) can be written as follows[31]:

$$d\left(\frac{f}{\rho}\right) = -P d\left(\frac{1}{\rho}\right) = \frac{P}{\rho^2} d\rho. \tag{A51}$$

If we introduce the enthalpy density

$$h = \frac{P + f}{\rho}, \tag{A52}$$

we obtain the relations

$$df = h\, d\rho \qquad \text{and} \qquad dh = \frac{dP}{\rho}. \tag{A53}$$

On the other hand, the local Gibbs–Duhem relation (A2) reduces to

$$f = -P + \frac{\mu}{m}\rho. \tag{A54}$$

Comparing Equations (A52) and (A54), we find that

$$h = \frac{\mu}{m}. \tag{A55}$$

Therefore, the enthalpy $h(\mathbf{r})$ coincides with the local chemical potential $\mu(\mathbf{r})$ by unit of mass: $h(\mathbf{r}) = \mu(\mathbf{r})/m$.

Appendix D.2. Barotropic Equation of State

In a fluid, the local pressure is of the form $P = P(\rho, T)$. Since the temperature T is fixed in the case of Brownian particles (canonical description), the pressure is barotropic and we shall simply write $P = P(\rho)$. For a general barotropic equation of state of the form $P = P(\rho)$, the foregoing relations lead to the identities

$$\left(\frac{f}{\rho}\right)' = \frac{P(\rho)}{\rho^2}, \qquad h(\rho) = \frac{P(\rho) + f(\rho)}{\rho}, \tag{A56}$$

$$h(\rho) = f'(\rho), \qquad h'(\rho) = \frac{P'(\rho)}{\rho}, \tag{A57}$$

$$P(\rho) = \rho h(\rho) - f(\rho) = \rho f'(\rho) - f(\rho) = \rho^2 \left(\frac{f}{\rho}\right)', \tag{A58}$$

$$P'(\rho) = \rho f''(\rho). \tag{A59}$$

The first principle of thermodynamics for a system of Brownian particles in contact with a heat bath (see Equation (A51)) provides a general relation between the density of free energy $f(\rho)$ and the pressure $P(\rho)$. If we know the free energy density $f = f(\rho)$, we can obtain the pressure by

$$P(\rho) = -\frac{d(f/\rho)}{d(1/\rho)} = \rho^2 \left(\frac{f}{\rho}\right)' = \rho f'(\rho) - f(\rho). \tag{A60}$$

Conversely, if we know the equation of state $P = P(\rho)$, we can obtain the free energy density by

$$f(\rho) = \rho \int^{\rho} \frac{P(\rho')}{\rho'^2}\, d\rho'. \tag{A61}$$

This is the solution of the differential equation

$$\rho \frac{df}{d\rho} - f(\rho) = P(\rho). \tag{A62}$$

We also note that the enthalpy is given by

$$h(\rho) = \int^{\rho} \frac{P'(\rho')}{\rho'} \, d\rho'. \tag{A63}$$

Appendix D.3. Free Energy Functional

For a barotropic gas, using Equation (A61), the free energy functional is

$$F = \int f(\rho) \, d\mathbf{r} = \int \rho \int^{\rho} \frac{P(\rho')}{\rho'^2} \, d\rho' \, d\mathbf{r}. \tag{A64}$$

We have

$$\frac{\delta F}{\delta \rho} = f'(\rho) = h(\rho) = \int^{\rho} \frac{P'(\rho')}{\rho'} \, d\rho' \tag{A65}$$

and

$$\nabla \frac{\delta F}{\delta \rho} = f''(\rho) \nabla \rho = h'(\rho) \nabla \rho = \frac{P'(\rho)}{\rho} \nabla \rho. \tag{A66}$$

Therefore,

$$\rho \nabla \frac{\delta F}{\delta \rho} = \nabla P. \tag{A67}$$

We also note the identity

$$\frac{\nabla P}{\rho} = f''(\rho) \nabla \rho = h'(\rho) \nabla \rho = \nabla h. \tag{A68}$$

Appendix D.4. Polytropic Equation of State

For a polytropic equation of state of the form $P = K\rho^{\gamma}$ with $\gamma = 1 + 1/n$, using Equation (A61), we find that the density of free energy is given by

$$f = \frac{K}{\gamma - 1} \rho^{\gamma} = \frac{P}{\gamma - 1} = nP = nK\rho^{1+1/n}, \tag{A69}$$

where we set the constant of integration to zero. We can also write the density of free energy in the form

$$f = \frac{K}{\gamma - 1} (\rho^{\gamma} - \rho) \tag{A70}$$

by taking the constant of integration equal to $-K/(\gamma - 1)$. In that case, the free energy functional

$$F = \frac{K}{\gamma - 1} \int (\rho^{\gamma} - \rho) \, d\mathbf{r} \tag{A71}$$

takes a form similar to the Tsallis free energy with an index γ and a generalized temperature K.

Appendix D.5. Connection with Cold Gases like BECs ($T = 0$)

Let us now consider the situation appropriate to a cold gas such as a BEC at $T = 0$ described by the generalized GP Equation (35). The previous results remain valid with

$$f = u, \qquad F = U. \tag{A72}$$

In other words, the free energy coincides with the internal energy.

Remark A3. *According to Equations (A24) and (A72), we see that the free energy $f(\rho)$, which determines the pressure in the Brownian model, coincides with the potential $V(\rho)$ that appears in the generalized GP Equation (35). This is why the two models present analogies. However, these analogies are purely formal since the quantum system is at $T_{\rm thermo} = 0$, while the Brownian model is at $T_{\rm thermo} \neq 0$. In other words, the temperature T and the free energy F that appear in the quantum model are effective temperature and effective free energy.*

Appendix E. *K*-Functional

In this appendix, we give a few properties of the K-functional

$$\Theta_Q^K = \int \frac{1}{2} K(\rho)(\nabla\rho)^2 \, d\mathbf{r} \tag{A73}$$

introduced in Section 8. A more general discussion containing additional results and details of calculations will be given in a forthcoming paper [162].

Appendix E.1. K-Potential

For a small perturbation of the form $\rho + \delta\rho$ with $\delta\rho \ll \rho$, we can make the expansion

$$\begin{aligned} \Theta_Q^K[\rho+\delta\rho] &= \int \frac{1}{2} K(\rho+\delta\rho)(\nabla\rho + \nabla\delta\rho)^2 \, d\mathbf{r} \\ &= \int \frac{1}{2} \left[K(\rho) + K'(\rho)\delta\rho + \ldots\right] \left[(\nabla\rho)^2 + 2\nabla\rho\cdot\nabla\delta\rho + \ldots\right] d\mathbf{r}. \end{aligned} \tag{A74}$$

The first-order variations of the K-functional are

$$\begin{aligned} \delta\Theta_Q^K &= \int K(\rho)\nabla\rho\cdot\nabla\delta\rho \, d\mathbf{r} + \frac{1}{2}\int K'(\rho)(\nabla\rho)^2\delta\rho \, d\mathbf{r} \\ &= -\int \nabla[K(\rho)\nabla\rho]\delta\rho \, d\mathbf{r} + \frac{1}{2}\int K'(\rho)(\nabla\rho)^2\delta\rho \, d\mathbf{r} \\ &= -\int K(\rho)\Delta\rho\delta\rho \, d\mathbf{r} - \frac{1}{2}\int K'(\rho)(\nabla\rho)^2\delta\rho \, d\mathbf{r}. \end{aligned} \tag{A75}$$

Its functional derivative is, therefore,

$$\frac{\delta\Theta_Q^K}{\partial\rho} = -\frac{1}{2}K'(\rho)(\nabla\rho)^2 - K(\rho)\Delta\rho. \tag{A76}$$

If we define the K-potential by

$$Q_K = -mK(\rho)\Delta\rho - \frac{1}{2}mK'(\rho)(\nabla\rho)^2, \tag{A77}$$

we obtain

$$\delta\Theta_Q^K = \int \frac{Q_K}{m}\delta\rho \, d\mathbf{r} \qquad \text{and} \qquad \frac{\delta\Theta_Q^K}{\delta\rho} = \frac{Q_K}{m}. \tag{A78}$$

Remark A4. *For the usual quantum potential, we recover Equation (A28).*

Appendix E.2. K-Pressure Tensor

We define the K-force by

$$\mathbf{F}_Q^K = -\frac{1}{m}\nabla Q_K. \tag{A79}$$

Using Equation (A77), we find that

$$-\frac{1}{m}\partial_i Q_K = K'(\rho)\partial_i\rho\Delta\rho + K'(\rho)\partial_{ij}\rho\partial_j\rho + \frac{1}{2}K''(\rho)\partial_i\rho(\nabla\rho)^2 + K(\rho)\partial_i\Delta\rho. \tag{A80}$$

By proceeding as in Appendix C.4 of [16], we can show that the K-force can be written as

$$(F_Q^K)_i = -\frac{1}{m}\partial_i Q_K = -\frac{1}{\rho}\partial_j P_{ij}^K, \tag{A81}$$

where P_{ij}^K is a K-pressure tensor given by

$$P_{ij}^K = A(\rho)\partial_i\rho\partial_j\rho + B(\rho)\Delta\rho\,\delta_{ij} + C(\rho)\partial_{ij}\rho + D(\rho)(\nabla\rho)^2\,\delta_{ij} \tag{A82}$$

with coefficients

$$A = \frac{1}{2}(K - \rho K') = -\frac{1}{2}\rho^2\left(\frac{K}{\rho}\right)', \tag{A83}$$

$$B = C = -\frac{1}{2}\rho K, \qquad D = 0. \tag{A84}$$

Other equivalent expressions of the K-pressure tensor are given in [162].

Let us give some examples:

(i) The classical case corresponds to $K = 0$ (no "quantum" correlation), implying

$$P_{ij}^K = 0. \tag{A85}$$

(ii) The ordinary Landau functional corresponds to $K = \text{cst}$, implying

$$P_{ij}^K = \frac{1}{2}K\partial_i\rho\partial_j\rho - \frac{1}{2}K\rho\Delta\rho\,\delta_{ij} - \frac{1}{2}K\rho\partial_{ij}\rho. \tag{A86}$$

(iii) The standard quantum case corresponds to $K(\rho) = \hbar^2/(4m^2\rho)$, implying

$$P_{ij}^K = \frac{\hbar^2}{4m^2}\left(\frac{1}{\rho}\partial_i\rho\partial_j\rho - \frac{1}{2}\Delta\rho\,\delta_{ij} - \frac{1}{2}\partial_{ij}\rho\right). \tag{A87}$$

We recover the expression (70) of the quantum pressure tensor up to a term of the form $\chi_{ij} = \delta_{ij}\Delta\rho - \partial_i\partial_j\rho$ satisfying $\partial_j\chi_{ij} = 0$.

(iv) For the function $K(\rho) = q\hbar^2\rho_0^{1-q}/(4m^2\rho^{2-q})$ associated with the Tsallis entropy [16], we obtain

$$P_{ij}^K = \frac{\hbar^2}{8m^2}q\rho_0^{1-q}(3-q)\left[\frac{1}{\rho^{2-q}}\partial_i\rho\partial_j\rho - \frac{1}{(3-q)}\frac{1}{\rho^{1-q}}\Delta\rho\,\delta_{ij} - \frac{1}{3-q}\frac{1}{\rho^{1-q}}\partial_{ij}\rho\right]. \tag{A88}$$

For $q = 1$, we recover the expression from Equation (A87).

Appendix F. Expansion of the Mean Field Potential for Weak Inhomogeneity

In this appendix, we expand the mean field potential $\Phi(\mathbf{r},t)=\int u(|\mathbf{r}-\mathbf{r}'|)\rho(\mathbf{r}',t)\,d\mathbf{r}'$ for a sufficiently weak inhomogeneity of the system with respect to the range of the interaction.

Appendix F.1. Pseudo-Potential

We first assume that the interaction between the particles corresponds to binary collisions that can be modeled by the effective (or pseudo-) potential $u=g\delta(\mathbf{r}-\mathbf{r}')$ [163,164]. This is a pair contact potential. In the case of BECs, the coupling constant g is related to the s-wave scattering length a_s of the bosons by $g=4\pi a_s\hbar^2/m^3$ [126]. Under these conditions, the mean field potential $\Phi(\mathbf{r},t)=\int u(|\mathbf{r}-\mathbf{r}'|)\rho(\mathbf{r}',t)\,d\mathbf{r}'$ is given by [69–72]

$$\Phi(\mathbf{r},t)=g\rho(\mathbf{r},t). \tag{A89}$$

The associated energy is

$$W=\frac{1}{2}g\int\rho^2\,d\mathbf{r}. \tag{A90}$$

This corresponds to a self-interaction potential V and a pressure P given by Equations (A25) and (A26) characterizing a standard BEC described by the GP Equation (43).

Appendix F.2. Square Gradient Functional

More generally, the relation from Equation (A89) represents the leading term in an expansion of the mean field potential in powers of the inhomogeneity. Below, we consider the next order term in this expansion. Setting $\mathbf{q}=\mathbf{r}'-\mathbf{r}$ and writing the mean field potential as

$$\Phi(\mathbf{r},t)=\int u(q)\rho(\mathbf{r}+\mathbf{q},t)d\mathbf{q}, \tag{A91}$$

we can Taylor expand $\rho(\mathbf{r}+\mathbf{q},t)$ to the second order in $\mathbf{q}$ to obtain

$$\rho(\mathbf{r}+\mathbf{q},t)=\rho(\mathbf{r},t)+\sum_i\frac{\partial\rho}{\partial x_i}q_i+\frac{1}{2}\sum_{i,j}\frac{\partial^2\rho}{\partial x_i\partial x_j}q_iq_j. \tag{A92}$$

Substituting this expansion into $\Phi(\mathbf{r},t)=\int u(|\mathbf{r}-\mathbf{r}'|)\rho(\mathbf{r}',t)\,d\mathbf{r}'$, we obtain

$$\Phi(\mathbf{r},t)=-a\rho(\mathbf{r},t)-K\Delta\rho(\mathbf{r},t) \tag{A93}$$

with $a=-4\pi\int_0^{+\infty}u(q)q^2\,dq$ and $K=-\frac{2\pi}{3}\int_0^{+\infty}u(q)q^4\,dq$. The case $a,K>0$ corresponds to an attractive self-interaction and the case $a,K<0$ corresponds to a repulsive self-interaction. We note that $l=(K/a)^{1/2}$ has the dimension of a length. As mentioned above, the term $-a\rho$ can be incorporated in the self-interaction potential $V(\rho)$ or in the pressure $P(\rho)$. Therefore, we shall focus below on the term $-K\Delta\rho$. We write it as

$$\Phi_{\rm K}(\mathbf{r},t)=-K\Delta\rho(\mathbf{r},t). \tag{A94}$$

This term is associated with the square gradient energy functional

$$W_{\rm K}=\frac{1}{2}K\int(\nabla\rho)^2\,d\mathbf{r}. \tag{A95}$$

This expression can be obtained by substituting Equation (A94) into Equation (83) and integrating by parts. The total free energy, including the internal energy (81) and the square gradient energy (A95), is

$$F=\int\left[\frac{1}{2}K(\nabla\rho)^2+V(\rho)\right]d\mathbf{r}. \tag{A96}$$

It has the form of a Landau free energy functional. This type of functionals appears in the Ginzburg–Landau equation [165]

$$\xi\frac{\partial\rho}{\partial t}=-\frac{\delta F}{\delta\rho}=K\Delta\rho+V'(\rho)\tag{A97}$$

and in the Cahn–Hilliard equation [166]

$$\xi\frac{\partial\rho}{\partial t}=\Delta\frac{\delta F}{\delta\rho}=-\Delta\left[K\Delta\rho+V'(\rho)\right],\tag{A98}$$

where the potential $V(\rho)$ usually has a double-well shape of the form $V(\rho)=A(\sigma^2-\rho^2)^2$ leading to phase separation[32].

Remark A5. *We note that the Landau free energy defined in Equation (A96) is a particular case of the excess free energy from Equation (242) with* $K=\mathrm{cst}$. *In that case, the K-potential* Q_K/m *from Equation (245) coincides with the potential* Φ_K *from Equation (A94), i.e., it corresponds to the Laplacian term in the expansion (A93) of the mean field potential* Φ *for weak inhomogeneity. This yields Equations (260)–(263) of Section 8.4. They can be viewed as generalized Cahn–Hilliard or generalized Ginzburg–Landau equations with the crucial differences mentioned at the end of Appendix C.1.*

Appendix F.3. Van der Waals Equation of State

Let us illustrate our formalism with the example of the van der Waals equation of state [167]. As in Section 7, we assume that the particles experience short-range and long-range interactions of microscopic origin. We write the total potential as $u=u_{\rm SR}+u_{\rm LR}$, where $u_{\rm SR}$ refers to short-range interactions and $u_{\rm LR}$ refers to long-range interactions.

Long-range interactions can be treated with the mean field approximation (for $N\gg 1$). Assuming that the density varies weakly with the position (on the scale of the microscopic interactions), we can make the approximation $\Phi_{\rm LR}(\mathbf{r},t)=-a\rho(\mathbf{r},t)$ with $a=-4\pi\int_0^{+\infty}u_{\rm LR}(q)q^2\,dq$ (see Appendix F.2). We then have

$$W=-\frac{1}{2}a\int\rho^2\,d\mathbf{r}.\tag{A99}$$

This corresponds to a free energy density $f_{\rm LR}(\rho)=-(1/2)a\rho^2$ giving a pressure (see Equation (A60))

$$P_{\rm LR}=-\frac{1}{2}a\rho^2.\tag{A100}$$

For an attractive long-range interaction, one has $a>0$, so the pressure $P_{\rm LR}$ is negative (see Appendix F.2).

Short-range interactions can be treated with an excess free energy $F_{\rm ex}$ in addition to the ideal free energy $F_{\rm id}$. The total free energy $F_{\rm id}+F_{\rm ex}$ can be written as $-TS$ where $S=-k_B\int C(\rho)\,d\mathbf{r}$ is a generalized entropy taking into account microscopic constraints [130]. In principle, it can be obtained from a combinatorial analysis (see Section 2.4 of [38]). As reported by van Kampen [168], it was first shown by Ornstein [169] in 1908 that the generalized entropy associated with the van der Waals gas is given by

$$S=-k_B\int\frac{\rho}{m}\ln\left(\frac{\rho}{\rho_*-\rho}\right)d\mathbf{r}.\tag{A101}$$

This is probably the first example of generalized entropy being introduced into physics. It corresponds to a free energy density $f_{\rm SR}(\rho)=k_BTC(\rho)$ giving a pressure (see Equation (A60))

$$P_{\rm SR}=\frac{\rho}{1-\rho/\rho_*}\frac{k_BT}{m}. \tag{A102}$$

The term in the denominator takes into account excluded volume effects due to the finite size of the molecules. The gas cannot be compressed indefinitely so that the pressure diverges when $\rho\rightarrow\rho_*$.

If we now add the pressure $P_{\rm SR}$ due to short-range interactions and the pressure $P_{\rm LR}$ due to long-range interactions, we obtain the celebrated van der Waals equation of state

$$P=\frac{\rho}{1-\rho/\rho_*}\frac{k_BT}{m}-\frac{1}{2}a\rho^2. \tag{A103}$$

This is the local form of the usual formula $(P+a/V^2)(V-b)=RT$. The first term corresponds to the ideal equation of state $P_{\rm id}=\rho k_BT/m$ modified by repulsive short-range interactions (hard sphere effects), and the second term represents the effect of attractive long-range interactions between the molecules. The van der Waals equation of state is associated to a free energy

$$F_{\rm WdW}=-\frac{1}{2}a\int\rho^2\,d\mathbf{r}+k_BT\int\frac{\rho}{m}\ln\left(\frac{\rho}{\rho_*-\rho}\right)d\mathbf{r}. \tag{A104}$$

If we use it in Equation (38), we obtain a generalized GP equation of the form

$$\begin{aligned}i\hbar\frac{\partial\psi}{\partial t}&=-\frac{\hbar^2}{2m}\Delta\psi+m\Phi\psi-am|\psi|^2\psi+m\Phi_{\rm ext}\psi\\ +k_BT\left[\ln\left(\frac{|\psi|^2}{\rho_*-|\psi|^2}\right)+\frac{\rho_*}{\rho_*-|\psi|^2}\right]\psi&-i\frac{\hbar}{2}\xi\left[\ln\left(\frac{\psi}{\psi^*}\right)-\left\langle\ln\left(\frac{\psi}{\psi^*}\right)\right\rangle\right]\psi.\end{aligned} \tag{A105}$$

In a more complete model, one should include the term coming from the square gradient energy functional defined in Equation (A96) like in Appendix F.2 (see Equation (262)).

Remark A6. *One could also consider the Fermi–Dirac entropy in position space leading to another form of exclusion constraint [170]. In that case, the free energy reads*

$$F=\frac{k_BT}{m}\rho_*\int\left\{\frac{\rho}{\rho_*}\ln\frac{\rho}{\rho_*}+\left(1-\frac{\rho}{\rho_*}\right)\ln\left(1-\frac{\rho}{\rho_*}\right)\right\}d\mathbf{r}. \tag{A106}$$

It leads to the equation of state

$$P=-\frac{k_BT}{m}\rho_*\ln\left(1-\frac{\rho}{\rho_*}\right). \tag{A107}$$

If we use it in Equation (38), we obtain a generalized GP equation of the form

$$\begin{aligned}i\hbar\frac{\partial\psi}{\partial t}&=-\frac{\hbar^2}{2m}\Delta\psi+m\Phi\psi+m\Phi_{\rm ext}\psi\\ +k_BT\ln\left(\frac{|\psi|^2}{\rho_*-|\psi|^2}\right)\psi&-i\frac{\hbar}{2}\xi\left[\ln\left(\frac{\psi}{\psi^*}\right)-\left\langle\ln\left(\frac{\psi}{\psi^*}\right)\right\rangle\right]\psi.\end{aligned} \tag{A108}$$

Appendix F.4. Weakly Inhomogeneous Systems

In Section 5.5, we gave a first simplified expression of the excess free energy, which applies to a barotropic gas. Here, we shall briefly mention another simplified expression that has been extensively used in the physics of liquids (see, e.g., Refs. [34,171,172]). If the density distribution varies slowly and exhibits small departures relative to some reference density $\overline{\rho}$, we can expand the functional $F_{\rm ex}[\rho]$ to the second order in $|\rho(\mathbf{r},t)-\overline{\rho}| \ll \overline{\rho}$, thereby obtaining

$$F_{\rm ex}[\rho] = -\frac{1}{2}k_B T \int (\rho-\overline{\rho})(\mathbf{r},t)c^{(2)}(|\mathbf{r}-\mathbf{r}'|,\overline{\rho})(\rho-\overline{\rho})(\mathbf{r}',t)\,d\mathbf{r}d\mathbf{r}', \tag{A109}$$

where $c^{(2)}(\mathbf{r},\overline{\rho})$ denotes the Ornstein–Zernike [173] direct correlation function in the homogeneous reference system

$$c^{(2)}(|\mathbf{r}-\mathbf{r}'|,\overline{\rho}) = -\beta\frac{\delta^2 F_{\rm ex}}{\delta\rho(\mathbf{r})\delta\rho(\mathbf{r}')}. \tag{A110}$$

If we introduce the one-body direct correlation function

$$c(\mathbf{r},\overline{\rho}) = -\beta\frac{\delta F_{\rm ex}}{\delta\rho(\mathbf{r})} = -\beta\frac{\mu_{\rm ex}(\mathbf{r},\overline{\rho})}{m}, \tag{A111}$$

we find that

$$c(\mathbf{r},\overline{\rho}) = \int c^{(2)}(|\mathbf{r}-\mathbf{r}'|,\overline{\rho})(\rho-\overline{\rho})(\mathbf{r}')\,d\mathbf{r}'. \tag{A112}$$

There are several methods in the physics of liquids to obtain useful approximations of the direct correlation function [33], and hence of the functional (A109). Interestingly, we note that the functional (A109) has the same form (up to a shift in density) as the mean field free energy functional (138) with Equation (135), provided that we view the direct correlation function as an effective binary potential of interaction

$$u_{\rm eff}(|\mathbf{r}-\mathbf{r}'|) = -k_B T c^{(2)}(|\mathbf{r}-\mathbf{r}'|,\overline{\rho}). \tag{A113}$$

This relation first appeared in a work of Zwanzig [174]. The direct correlation function $c^{(2)}(|\mathbf{r}-\mathbf{r}'|)$ can be obtained experimentally or theoretically. One can use, for example, the Percus–Yevick [175] integral equation. Its solution is known exactly for the special case of a fluid of hard spheres [176–178] but approximate expressions can be obtained in more general situations. It then determines the effective potential of interaction $u_{\rm eff}(|\mathbf{r}-\mathbf{r}'|)$ through Equation (A113) and the excess free energy through Equation (A109). We see that the results obtained for systems with long-range interactions in the mean field approximation can be applied to simple liquids provided that the potential of interaction $u_{\rm LR}(|\mathbf{r}-\mathbf{r}'|)$ is replaced by the effective potential of interaction $u_{\rm eff}(|\mathbf{r}-\mathbf{r}'|)$. Similarly, the one-body direct correlation function $c(\mathbf{r},\overline{\rho})$ plays the role of an effective mean field potential $\Phi_{\rm eff}(\mathbf{r})$ through the relation

$$\Phi_{\rm eff}(\mathbf{r}) = -k_B T c(\mathbf{r},\overline{\rho}). \tag{A114}$$

This makes it possible to apply the results obtained for mean field potentials to correlated systems with short-range interactions by using the correspondences from Equations (A113) and (A114).

Remark A7. *Since the density varies slowly, we can expand the excess free energy from Equation (A109) as in Appendix F.2. This yields the square gradient energy functional* $F_{\rm ex} = \frac{1}{2}K\int(\nabla\rho)^2\,d\mathbf{r}$ *with a coefficient* $K = -\frac{1}{6}\int u_{\rm eff}(q)q^2\,d\mathbf{q}$ *determined by the effective binary potential. Using Equation (A113), it can be rewritten as* $K = \frac{1}{6}k_B T\int c^{(2)}(q,\overline{\rho})q^2\,d\mathbf{q}$*, which is in agreement with the result quoted at the end of Section 8.2.*

Appendix G. Generalized Dispersion Relations

In this appendix, we consider a system described by the generalized GP Equation (284) with $\Phi_{\rm ext} = 0$ or by the generalized Vlasov–Bohm Equation (287) with $\Phi_{\rm ext} = P_{\rm int} = \xi = 0$. We discuss the dispersion relation characterizing the evolution of a small perturbation in an infinite homogeneous background. To be specific, we assume that the excess free energy $\mathcal{F}_{\rm ex}$ corresponds to the K-functional from Equation (A73). The following results apply either to quantum systems (when $\hbar \neq 0$) or to classical systems (when $\hbar = 0$).

Appendix G.1. Generalized Schrödinger Equation

The generalized GP Equation (284) is equivalent to the continuity equation and the generalized damped quantum Euler Equation (285). Considering a small perturbation with respect to an infinite homogeneous distribution and using standard methods [76,107,179], we obtain the generalized dispersion relation

$$\omega^2 + i\xi\omega = \frac{\hbar^2 k^4}{4m^2} + \rho K(\rho)k^4 + c_s^2 k^2 + (2\pi)^d \hat{u}(k)\rho k^2, \tag{A115}$$

where $c_s^2 = P'(\rho)$ is the squared speed of sound. The condition of marginal stability ($\omega = 0$) reads

$$\frac{\hbar^2 k^4}{4m^2} + \rho K(\rho)k^4 + c_s^2 k^2 + (2\pi)^d \hat{u}(k)\rho k^2 = 0. \tag{A116}$$

We see that the K-potential has the same effect as the quantum potential with a pseudo-Planck constant

$$\hbar_{\rm pseudo} = 2m\sqrt{\rho K(\rho)}. \tag{A117}$$

We can, therefore, define an effective Planck constant by

$$\hbar_{\rm eff} = \sqrt{\hbar^2 + 4m^2\rho K(\rho)}. \tag{A118}$$

The quantum potential always has a repulsive effect. When $K > 0$, the K-potential increases the effective Planck constant, and hence augments the repulsion. When $K < 0$, the K-potential decreases the effective Planck constant, and hence reduces the repulsion. The K-potential counteracts the quantum potential at the critical density ρ_c such that $\hbar^2 + 4m^2\rho_c K(\rho_c) = 0$ (provided that $K < 0$). When $\hbar^2 + 4m^2\rho K(\rho) < 0$, the effective Planck constant is imaginary, meaning that the total interaction (quantum potential + K-potential) is attractive.

Remark A8. *For a weak inhomogeneity, Equation (A94) can be Fourier transformed into* $\hat{\Phi}_{\rm K} = Kk^2\hat{\rho}$. *Compared with the relation* $\hat{\Phi} = (2\pi)^d\hat{u}(k)\hat{\rho}$ *obtained from Equation (A91), this corresponds to a self-interaction potential* $(2\pi)^d\hat{u}_{\rm K}(k) = Kk^2$, *which is the first-order term in the expansion of the potential* $\hat{u}(k)$ *for small k (long wavelengths). In that case, the interaction term* $(2\pi)^d\hat{u}(k)\rho k^2 = \rho K k^4$ *in the dispersion relation (A115) becomes equivalent to the K-potential term* $\rho K k^4$, *which is itself analogous to the quantum potential* $\hbar^2 k^4/4m^2$ *with the correspondence* $K = \hbar^2/(4m^2\rho)$ *as discussed above.*

Appendix G.2. Generalized Vlasov–Bohm Equation

We now consider the generalized Vlasov–Bohm Equation (287). Performing a small perturbation with respect to an infinite homogeneous distribution and using standard methods [180–182], we obtain the generalized dispersion relation

$$1 - \left[(2\pi)^d\hat{u}(k) + \frac{\hbar^2 k^2}{4m^2\rho} + K(\rho)k^2\right]\int \frac{f'(v)}{v - \omega/k}\,dv = 0. \tag{A119}$$

For a homogeneous distribution, we established the general identity [180–182]

$$c_s^2 = -\frac{\rho}{\int \frac{f'(v)}{v}\, dv}, \tag{A120}$$

where c_s^2 is the squared speed of sound in the corresponding barotropic gas. Using Equation (A120), we see that the condition of marginal stability ($\omega = 0$) from Equation (A119) coincides with Equation (A116). Therefore, the condition of marginal stability is the same for the Vlasov–Bohm equation and for the GP equation (or for the quantum Euler equation). However, this equivalence is lost if we use the more rigorous Wigner equation instead of the Vlasov–Bohm equation [107]. In that case, the dispersion relation reads (for $K = 0$) [107]:

$$1 + (2\pi)^d \hat{u}(k) \frac{m}{\hbar} \int \frac{f\left(v + \frac{\hbar k}{2m}\right) - f\left(v - \frac{\hbar k}{2m}\right)}{\omega - kv}\, dv = 0. \tag{A121}$$

The condition of marginal stability

$$1 - (2\pi)^d \hat{u}(k) \frac{m}{\hbar k} \int \frac{f\left(v + \frac{\hbar k}{2m}\right) - f\left(v - \frac{\hbar k}{2m}\right)}{v}\, dv = 0 \tag{A122}$$

is generally different from Equations (A116) and (A119), except in the classical limit $\hbar \to 0$, where the Wigner equation reduces to the Vlasov equation [180–182].

Notes

[1] In his first paper [2], Einstein was not sure that his theory applied to Brownian motion. But in his second paper [3], he mentioned that Siedentopf informed him that he and other physicists, notably Gouy [4], had been convinced by direct observations that Brownian motion was caused by the irregular thermal movements of the molecules of the liquid. The order of magnitude of the paths described by the particles (in particular the dependence of the intensity of motion on the particle size and on the temperature) were in agreement with Einstein's theory.

[2] Fick [5,6] introduced the diffusion equation phenomenologically in 1855 by analogy with Fourier's law of heat conduction and Ohm's law of charge transport. He considered the diffusion of salts in water and did not mention the connection with Brownian motion. The probabilistic derivation proposed by Einstein [2], which relies on the Taylor expansion of a Master equation, is essentially the same as the one used later by Fokker [7–9], Planck [10], Klein [11], Kramers [12], Chandrasekhar [13] and Moyal [14] to derive the Fokker-Planck equation through the Kramers-Moyal expansion. Actually, this method of expansion was first introduced by Lord Rayleigh [15] as early as 1891 long before all the classic works on Brownian theory. He considered the kinetic theory of massive particles bombarded by numerous small projectiles. Although Lord Rayleigh did not explicitly refer to Brownian motion, his paper can be seen as a precursor of the theory of Brownian motion that is usually considered to start with the seminal work of Einstein [2,3]. There is, however, an important difference. Lord Rayleigh [15] considered the velocity distribution $f(\mathbf{v}, t)$ of homogeneously distributed particles while Einstein [2] considered the spatial density $\rho(\mathbf{r}, t)$ of Brownian particles in the strong friction limit $\xi \to +\infty$ (or, equivalently, for large times $t \gg \xi^{-1}$). See Refs. [16–19] for additional comments about the paper of Lord Rayleigh in connection to the history of Brownian motion.

[3] The random walk approach was pioneered by Lord Rayleigh [22,23] (see [13,24–26]).

[4] This equation, without the advection term, was first derived by Lord Rayleigh [15] for a spatially homogeneous distribution of particles bombarded by numerous small projectiles (see additional comments in Refs. [16–19]). This equation was further studied by Uhlenbeck and Ornstein [31].

[5] This moment approach [32] can be seen as a formalization of the Sutherland-Einstein hydrodynamic approach [2,20]. For a finite value of the friction coefficient ξ, the LTE condition is not rigorously justified. Therefore, the damped Euler equation is at most approximate. One can show [32] that the LTE approximation becomes exact in the limit $\xi \to +\infty$. As a result, the Smoluchowski equation is rigorously justified in the strong friction limit.

[6] The Bohr model was extended in special relativity by Sommerfeld [58,59] who could explain the fine structure of the hydrogen spectrum. In unpublished notes, Schrödinger first derived a relativistic wave equation (now known as the Klein-Gordon equation) but did not recover the fine structure of the hydrogen spectrum because this equation does not account for the spin of the electron (this problem was solved later by the Dirac [60,61] equation). This is why he restricted himself to the nonrelativistic limit in his first communications [52–54] (he published the Klein-Gordon equation in his fourth communication [55] with the largest reserve).

See the introduction of Ref. [62] for a short account of the early history of wave mechanics (Schrödinger, Klein-Gordon and Dirac equations) and an exhaustive list of references.

[7] In the relativistic regime they have the form of nonlinear Klein-Gordon equations (see the introduction of Ref. [73] for a review).

[8] There is a vast literature on these equations in the case $T = \xi = 0$ (see the reviews [81–89]). For bosons without self-interaction, we get the Schrödinger-Poisson equations [90]. This leads to the fuzzy dark matter (FDM) model [91] which is also called the scalar field dark matter (SFDM) model [92] or the Bose-Einstein condensate dark matter (BECDM) model [93,94]. For self-interacting bosons, we get the Gross-Pitaevskii-Poisson (GPP) equations [95–97]. These equations have been solved numerically in Refs. [93,94,98–105].

[9] To our knowledge, the interpretation of Equation (23) in terms of a Cole-Hopf transformation was not mentioned by Nottale [75].

[10] This relation was noted by many authors [112–117] in the early years of quantum mechanics due to the formal analogy between the Schrödinger equation and the diffusion equation with an imaginary diffusion coefficient (or an imaginary time). This relation also appeared in the work of Nelson [111] who first proposed a derivation of the Schrödinger equation from Newtonian mechanics by using an entirely classical stochastic approach.

[11] The justification of Equation (35) given in Ref. [77] based on an extension of the theory of violent relaxation [122,123] to a self-gravitating boson gas (leading to a form of Wigner-Kramers equation) is physically different from the justification given in Refs. [74,78] and in Section 2 based on an extension of the theory of scale relativity [75] to the case of dissipative quantum systems. It is not clear at that point if the two approaches are related to each other.

[12] The quantum potential Q is directly related to the imaginary part $\mathbf{u}_Q$ of the complex velocity $\mathbf{U}$ in the theory of scale relativity by Equation (E.12) of [74]. The imaginary part of the velocity can also be interpreted as an "osmotic" velocity in the sense of Nelson [111] (see the discussion in Appendix E.4 of [74]).

[13] Actually, the Madelung hydrodynamic equations are not fully equivalent to the Schrödinger equation [127]. To achieve equivalence, we must assume that the velocity is equal to a gradient. Furthermore, we must add by hand a quantization condition $\oint \mathbf{u}\cdot d\mathbf{l} = n\,2\pi\hbar/m$, where n is an integer, as in the old quantum theory. This ensures that the wave function is single valued.

[14] The free energy can be written in the usual form $F_{\rm tot} = E - TS$ where $E = \Theta_c + \Theta_Q + U_{\rm int} + W + W_{\rm ext}$ is the total energy and $S = -k_B \int (\rho/m)(\ln\rho - 1)\,d\mathbf{r}$ is the Boltzmann entropy in configuration space. We recall, however, that T is an effective temperature.

[15] If we define the out-of-equilibrium chemical potential by

$$\mu(\mathbf{r},t) = m\frac{\delta F}{\delta\rho},$$

the Gibbs condition means that $\mu(\mathbf{r},t) = \mu$ is uniform at equilibrium.

[16] This expression results from Equation (119) by assuming that there are no correlations in velocity space. This is valid for $N \gg 1$.

[17] This relation ensures that the Gibbs canonical distribution (118) of statistical equilibrium is the stationary solution of the N-body Kramers Equation (181). Note that the Einstein relation (180) differs from the original Einstein relation (1) since we are considering inertial Brownian particles instead of overdamped Brownian particles.

[18] One could also start from the Dean equation in phase space which governs the evolution of the exact DF $f_d(\mathbf{r},\mathbf{v},t) = \sum_i \delta(\mathbf{r} - \mathbf{r}_i(t))\delta(\mathbf{v} - \mathbf{v}_i(t))$ [143]. This is the equivalent of the Klimontovich equation for Hamiltonian systems.

[19] These equations were first derived by Maxwell in his theory of gases [146].

[20] The LTE approximation is rigorously justified only for $\xi \to +\infty$. It may provide a good approximation when ξ is sufficiently large or when the system is sufficiently close to equilibrium (i.e. $t \gg \xi^{-1}$).

[21] This closure problem is distinct from the closure of the hierarchy of damped Jeans equations considered previously.

[22] As shown in [38,143] the expression of the noise term can be obtained from the fluctuating hydrodynamics of Landau and Lifshitz [149].

[23] This equivalence is rather obvious since we can consider that the self-interaction between the bosons corresponds to the correlations that arise from short-range interactions.

[24] To obtain Equation (254) we have added and subtracted $-(1/m)\nabla Q$ in the r.h.s. of Equation (246). This introduces a potential $Q - Q_K$ in the standard Schrödinger equation.

[25] When $\mathcal{F}_{\rm ex} = F_{\rm ex} - \Theta_Q$, we recover the equations of Section 8.5.

[26] This is related to the fact that the bosons are all condensed in the same quantum state.

[27] We can relate the temperature and the friction in the generalized GP equation to the temperature and the friction of a gas of Brownian particles. We also questioned whether it is possible to interpret the self-interaction and the quantum potential in the GP equation in terms of fluid correlations described by an appropriate excess free energy. Although there is an interesting correspondance between generalized quantum equations and Brownian equations, it is not clear if this correspondance is just a formal analogy or it if has a more profound interpretation.

[28] If we take the hydrodynamic moments of the Wigner equation, we find that the quantum pressure P_{ij} [see Equation (69)] can be written in the form $P_{ij} = \int f_W(\mathbf{v}-\mathbf{u})_i(\mathbf{v}-\mathbf{u})_j\, d\mathbf{v}$, where $f_W(\mathbf{r},\mathbf{v},t)$ is the Wigner distribution function [77]. The quantum pressure can therefore be related to the correlations of the velocity fluctuations of "particles" like in an ordinary fluid. On the other hand, in the Vlasov-Bohm equation, the quantum potential is introduced in an *ad hoc* manner in the advection term. In the interpretation that we have suggested here, it can be related to the excess free energy $F_{\rm ex}$ of a fluid, hence to the spatial correlation function of its constitutive particles.

[29] We recall that the temperature T in Equation (35) is an effective temperature which is different from the true thermodynamical temperature $T \equiv T_{\rm thermo}$ considered here.

[30] This is not always the case. For example, the free energy associated with the Smoluchowski-Poisson equations describing self-gravitating Brownian particles is not bounded from below [158]. In that case, the system can experience an isothermal collapse. However, at sufficiently high temperatures, there exist long-lived metastable states (local minima of free energy at fixed mass) on which the system can settle [159].

[31] The system evolves at fixed temperature but $P \neq \rho k_B T/m$ because of the presence of correlations among the particles.

[32] In the work of Cahn and Hilliard [166], the general free energy functional $F = \int f(\rho, \nabla\rho, \Delta\rho, ...)\, d\mathbf{r}$ is expanded in a Taylor series about $f_0(\rho)$ leading to a free energy of the form $F = \int \left[f_0(\rho) + \kappa(\nabla\rho)^2\right] d\mathbf{r}$ equivalent to Equation (A96). See also the Remark at the end of Section 8.2.

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