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On entropy production in the Madelung fluid and the role of Bohm's potential in classical diffusion

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Abstract The Madelung equations map the non-relativistic time-dependent Schrödinger equation into hydrodynamic equations of a virtual fluid. While the von Neumann entropy remains constant, we demonstrate that an increase of the Shannon entropy, associated with this Madelung fluid, is proportional to the expectation value of its velocity divergence. Hence, the Shannon entropy may grow (or decrease) due to an expansion (or compression) of the Madelung fluid. These effects result from the interference between solutions of the Schrödinger equation. Growth of the Shannon entropy due to expansion is common in diffusive processes. However, in the latter the process is irreversible while the processes in the Madelung fluid are always reversible. The relations between interference, compressibility and variation of the Shannon entropy are then examined in several simple examples. Furthermore, we demonstrate that for classical diffusive processes, the “force” accelerating diffusion has the form of the positive gradient of the quantum Bohm potential. Expressing then the diffusion coefficient in terms of the Planck constant reveals the lower bound given by the Heisenberg uncertainty principle in terms of the product between the gas mean free path and the Brownian momentum.

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1 Introduction

The Madelung equations [1] transform the non-relativistic time-dependent Schrödinger equation into hydrodynamical equations of an Eulerian fluid [2–5]. The aim of this study is to explore the entropy properties of the Madelung fluid and compare these with the ones of classical Eulerian fluids.

The hydrodynamical transformation is obtained when considering the Schrödinger equation,

$$i\hbar \frac{\partial \Psi}{\partial t} = \hat{H}\Psi = \left(\frac{\hat{p}^2}{2m} + U \right) \Psi = \left(-\frac{\hbar^2}{2m} \nabla^2 + U \right) \Psi, \quad (1)$$

for a continuous wave function $\Psi(\mathbf{r}, t) = \sqrt{\rho}(\mathbf{r}, t)e^{iS(\mathbf{r}, t)/\hbar}$ (so that $\rho = \Psi^*\Psi$) of a particle with mass m , in the presence of an external potential $U(\mathbf{r}, t)$. Using the de Broglie guiding equation, $\mathbf{u}_a = \nabla \tilde{S}$ (where the tilde superscripts represent hereinafter quantities per unit mass m), the real part of (1) becomes the continuity equation

$$\frac{\partial \rho}{\partial t} = -\nabla \cdot (\rho \mathbf{u}_a), \quad (2)$$

where the imaginary part of the Schrödinger equation becomes the Eulerian fluid momentum equation,

$$\frac{D_a}{Dt} \mathbf{u}_a = -\nabla \tilde{Q}(\rho) - \nabla \tilde{U}. \quad (3)$$

Here, $\frac{D_a}{Dt} \equiv \frac{\partial}{\partial t} + \mathbf{u}_a \cdot \nabla$, is the material (advective) time derivative of a fluid element along its trajectory and $\tilde{Q} = -\frac{\hbar^2}{2m^2} \frac{\nabla^2 \sqrt{\rho}}{\sqrt{\rho}}$ is the Bohm potential per unit mass [6] (for further relations between the Madelung formulation and the de Broglie-Bohm interpretation of quantum mechanics we refer the reader to [4, 6–8]).

In Ref. [5], it was suggested that the conservation of the domain integrated energy in (1) implies that the Madelung fluid is adiabatic. The fluid conserves the sum of the domain integrated kinetic, potential and internal energy, where the latter is given by the Fisher information. The domain averaged adiabaticity is in agreement with the conservation of the von Neumann entropy. The von Neumann entropy, i.e., the trace $Ent_{VN} = -k_B \text{Tr}[\hat{\rho} \ln \hat{\rho}]$, where k_B is the Boltzmann constant and $\hat{\rho}$ the density matrix of a closed system with a general (possibly time dependent) Hamiltonian, cannot (by virtue of unitary time evolution) change with time. One may, nevertheless, devise other illuminating entropy functionals (e.g., the “diagonal entropy” of [9]) that, even for closed systems, transparently adhere to standard thermodynamic relations (including the second law of thermodynamics). In the current work, our focus is on quantities associated with the Madelung fluid. Domain averaged adiabaticity of the Madelung fluid does not imply that entropy is materially conserved by a “fluid parcel”. This viable non-conservation differs, for instance, from the thermodynamic entropy of mono-atomic ideal gasses, $Ent_T = k_B \ln(T^{3/2}/\rho)$, which is materially conserved in adiabatic processes, $\frac{D_a}{Dt} Ent_T = 0$ [10].

We find that the classical Madelung fluid dynamics motivates the introduction of its associated “Shannon entropy” (Ent_S) [11]. For the standard density $\rho(\mathbf{r}, t) \equiv \Psi^*\Psi$ in real space we set

$$Ent_S \equiv -k_B \int \rho \ln \rho d\mathbf{r} \equiv k_B \int s d\mathbf{r}. \quad (4)$$

This Shannon entropy captures, for instance, the change in classical thermodynamic entropy during Joule free expansion of an ideal gas into a vacuum, and can be regarded as the configurational Boltzmann entropy of the Madelung fluid (as discussed in the Appendix). Ent_S may vary in time, in contrast to Ent_{VN} , which remains unchanged under unitary time evolution.

The remainder of this work is organized as follows. In Section 2, we examine the Shannon entropy production in the Madelung fluid via expansion by considering examples of both reversible and irreversible processes. In Section 3, we show that for classical diffusion the positive value of the Bohm potential gradient acts as an effective force. This implies that the Bohm potential represents diffusive processes in the Madelung fluid, as discussed in Section 4. Summary and conclusions appear in Section 5.

2 The Shannon Entropy production and compressibility effects

Within the definition of (4), the continuity equation (2) yields

$$\frac{\partial s}{\partial t} + \nabla \cdot (s \mathbf{u}_a) = \rho \nabla \cdot \mathbf{u}_a, \quad (5)$$

and if all fluxes vanish at the domain boundaries, we immediately obtain that

$$\frac{\partial}{\partial t} Ent_S = k_B \int \rho \nabla \cdot \mathbf{u}_a dV = k_B \langle \nabla \cdot \mathbf{u}_a \rangle = k_B \langle \nabla^2 \tilde{S} \rangle. \quad (6)$$

Hence, the total entropy production is equal to the expectation value of the divergence, i.e., the Shannon entropy grows through expansion of the fluid and may decay through compression. For the Madelung fluid to be compressible, the quantum action S must have a “source” in the sense that it has to satisfy some Poisson equation in the form of $\nabla^2 S \neq 0$. From the wave function perspective, compressibility results from superposition. For a single plane wave solution of the form $\Psi = \sqrt{\rho} e^{i(\mathbf{k} \cdot \mathbf{r} - \omega t)} = \sqrt{\rho} e^{iS/\hbar}$, $\mathbf{u}_a = \nabla \tilde{S} = \frac{\hbar}{m} \mathbf{k}$. Thus, the advective velocity is simply proportional to the wavenumber \mathbf{k} and $\nabla \cdot \mathbf{u}_a = 0$. However, when two plane waves or more interfere, $\nabla \cdot \mathbf{u}_a \neq 0$ in general.

In the next two simple examples we show how a superposition of plane waves triggers entropy growth. We will furthermore see how compressibility may lead to a reversible process. In the two cases we consider, the dynamics of a 1D Gaussian density solution that has been derived by [12],

$$\rho(x, t) = \frac{1}{\sigma(t)\sqrt{2\pi}} e^{-\frac{x^2}{2\sigma^2(t)}}. \quad (7)$$

Substituting (7) in the continuity equation (2) yields

$$u_a(x, t) = x \frac{\partial \ln \sigma}{\partial t} \implies \nabla \cdot \mathbf{u}_a = \frac{\partial \ln \sigma}{\partial t}. \quad (8)$$

(i) First we consider the case of a free particle. Substituting (7) and (8) in the 1D version of (3) for $\tilde{U} = 0$ yields

$$\sigma \frac{\partial^2 \sigma}{\partial t^2} = \left(\frac{\hbar}{2m\sigma} \right)^2 \implies \sigma^2 = \sigma_0^2 + \left(\frac{\hbar t}{2m\sigma_0} \right)^2. \quad (9)$$

The Shannon entropy

$$Ent_S = k_B \ln(\sigma\sqrt{2\pi e}) = Ent_{S_0} + \frac{k_B}{2} \ln \left[1 + \left(\frac{\hbar t}{2m\sigma_0^2} \right)^2 \right]. \quad (10)$$

Thus,

$$\frac{1}{k_B} \frac{\partial Ent_S}{\partial t} = \nabla \cdot \mathbf{u}_a = \frac{\partial \ln \sigma}{\partial t} = \frac{t}{\left(\frac{2m\sigma_0^2}{\hbar} \right)^2 + t^2} > 0. \quad (11)$$

These results illustrate how the superposition of plane waves in the Gaussian wave packet of Eq. (7) influences the compressibility of the Madelung fluid and how it gives rise to an increase of entropy. For a free particle, a 1D plane wave solution of (1) has the form of $\Psi = A(k)e^{ik[x - (\frac{\hbar}{2m})kt]}$, hence the dynamic Gaussian solution of (7) is a continuous superposition of plane waves whose amplitude $A(k) \propto e^{-(\sigma_0 k)^2}$, as can be verified from the Fourier transform of the square root of (7) at time $t = 0$.

(ii) As a second example we consider (7) in the presence of the harmonic potential $U = \frac{m}{2}(\omega_0 x)^2$ to obtain from (3):

$$\sigma \frac{\partial^2 \sigma}{\partial t^2} = \omega_0^2(\sigma_0^2 - \sigma^2), \quad \sigma_0^2 = \frac{\hbar}{2m\omega_0}, \quad (12)$$

which can be solved numerically. The well known stationary ground state solution (e.g. [13]) in which $\sigma = \sigma_0$, is a special case of (12) where $\rho_0 = \frac{1}{\sigma_0\sqrt{2\pi}} e^{-\frac{x^2}{2\sigma_0^2}}$, and the Shannon entropy is constant.

$$Ent_{S_0} = -k_B \int \rho_0 \ln \rho_0 dx = k_B \ln(\sigma_0\sqrt{2\pi e}). \quad (13)$$

As pointed out by [5], and is evident from (8), the only possible solution for the velocity in this case is $u_a = 0$, hence the Madelung fluid is obviously incompressible in the ground state. Consider, however, a small deviation from the ground state: $\sigma = \sigma_0 + \epsilon(t)$, where $|\epsilon|/\sigma_0 \ll 1$. Eq. (12) then yields $\frac{\partial^2 \epsilon}{\partial t^2} = -2\omega_0^2 \epsilon + O(\epsilon^2)$, so that $\epsilon(t) = \epsilon_0 \cos(\sqrt{2}\omega_0 t)$ for $O(\epsilon)$. Hence,

$$Ent_S = Ent_{S_0} + k_B \left(\frac{\epsilon}{\sigma_0} \right), \quad \frac{1}{k_B} \frac{\partial Ent_S}{\partial t} = \nabla \cdot \mathbf{u}_a = \frac{1}{\sigma_0} \frac{\partial \epsilon}{\partial t} = -\frac{\sqrt{2}\omega_0}{\sigma_0} \sin(\sqrt{2}\omega_0 t), \quad (14)$$

implying a reversible sinusoidal variation of the Shannon entropy.

For completeness we note that the action \tilde{S} , associated with the density function of (7), can be found explicitly (up to some constant) using $u_a = x \frac{\partial}{\partial t} \ln \sigma = \frac{\partial}{\partial x} \tilde{S}$ so that $\tilde{S} = \frac{x^2}{2} \frac{\partial \ln \sigma}{\partial t} + f(t)$. The time-dependent function $f(t)$, must satisfy the Hamilton-Jacobi equation (or the time-dependent Bernoulli equation in the fluid dynamics language [5]), which is the imaginary part of (1) from which (3) is derived. For the 1D version this equation becomes

$$\frac{\partial \tilde{S}}{\partial t} + \frac{1}{2} \left(\frac{\partial \tilde{S}}{\partial x} \right)^2 + \tilde{Q} + \tilde{U} = 0, \quad (15)$$

yielding $f(t) = -\left(\frac{\hbar}{2m}\right)^2 \int_{t_0}^t \frac{dt}{\sigma^2}$.

3 The role of the Bohm potential in classical diffusion

We wish to contrast the temporal evolution of the Madelung fluid's entropy with irreversible processes occurring in classical diffusion. Towards this end, we consider the standard case where the diffusive velocity \mathbf{u}_d satisfies Fick's first law:

$$\mathbf{u}_d = -D\nabla \ln \rho. \quad (16)$$

Here, \mathbf{u}_d is also referred to as the osmotic velocity [14] with D the diffusion coefficient (assumed constant for simplicity).

Changes in density result then from diffusive fluxes (rather than advective fluxes in the hydrodynamic continuity equation of (2)) as stated by Fick's second law:

$$\frac{\partial \rho}{\partial t} = -\nabla \cdot (\rho \mathbf{u}_d) = D\nabla^2 \rho. \quad (17)$$

Equation (5) still holds when \mathbf{u}_a is replaced by \mathbf{u}_d , but its domain integration yields now:

$$\frac{\partial}{\partial t} (Ent_S)_D = k_B \int \rho \nabla \cdot \mathbf{u}_d dV = k_B \langle \nabla \cdot \mathbf{u}_d \rangle = k_B D \langle (\nabla \ln \rho)^2 \rangle \geq 0, \quad (18)$$

where $Fi = \int \frac{(\nabla \rho)^2}{\rho} dV = \langle (\nabla \ln \rho)^2 \rangle$ is the Fisher information and $(Ent_S)_D$ represents the Shannon entropy undergoing a diffusion process. Hence, this well known relation (e.g. [11], for other information theory contexts) suggests that entropy increases in diffusive processes through expansion, as in the hydrodynamic case, but in contrast with the latter, the entropy increases irreversibly with time as long as density gradients exist (in agreement with the second law of thermodynamics).

Equation (17) can be transformed into a momentum like equation when defining a "material diffusive derivative" as $\frac{D_d}{Dt} \equiv \frac{\partial}{\partial t} + \mathbf{u}_d \cdot \nabla$. Then it is straightforward to show that (17) can be translated to

$$\frac{D_d}{Dt} \mathbf{u}_d = \nabla \tilde{Q}_d, \quad (19)$$

where $\tilde{Q}_d = -2D^2 \frac{\nabla^2 \sqrt{\rho}}{\sqrt{\rho}}$ may be denoted as a diffusive Bohm potential. Hence, the positive gradient (as opposed to the negative sign in (3)) of the diffusive Bohm potential acts as a "force" to accelerate the diffusion. This appearance of the quantum Bohm potential in a classical process is intriguing.

The role of the gradient of the Bohm potential as a diffusive force becomes more transparent when returning to the dynamic 1D Gaussian example. The well known solution to the 1D version of (17) (e.g., [15]) is given by

$$\rho(x, t) = \frac{1}{\sigma(t)\sqrt{2\pi}} e^{-\frac{x^2}{2\sigma^2(t)}}, \quad \sigma^2 = 2Dt, \quad u_d(x, t) = -D \frac{\partial \ln \rho}{\partial x} = x \frac{\partial \ln \sigma}{\partial t} = \frac{x}{2t}. \quad (20)$$

Hence

$$\frac{1}{k_B} \frac{\partial}{\partial t} (Ent_S)_D = \nabla \cdot \mathbf{u}_d = \frac{1}{2t}, \quad (21)$$

(note that for large t both (11) and (21) experience asymptotic entropy growth which is proportional to t^{-1}). Since $u_d = \frac{dx}{dt} = x/(2t)$ a fluid element located at

x_0 at time t_0 will be drifted at time t to $x = \left(\frac{x_0}{\sqrt{t_0}}\right) \sqrt{t}$ (random walk). Therefore, $u_d = x/(2t) = \left(\frac{x_0}{2\sqrt{t_0}}\right) / \sqrt{t}$, and the acceleration of the fluid element is

$$\frac{d}{dt}u_d = - \left(\frac{x_0\sqrt{t}}{\sqrt{t_0}}\right) \frac{1}{4t^2} = -\frac{x}{4t^2}, \quad (22)$$

where $\frac{d}{dt}u_d \equiv \frac{D_d}{Dt}u_d \equiv \frac{\partial u_d}{\partial t} + u_d \frac{\partial u_d}{\partial x}$. Thus, in this example the diffusion rate is being decelerated by the gradient of the diffusive Bohm potential

$$\frac{D_d}{Dt}u_d = \frac{\partial \tilde{Q}_d}{\partial x} = -2D^2 \frac{\partial}{\partial x} \left(\frac{x}{\sigma^2}\right)^2 = -\frac{x}{4t^2}. \quad (23)$$

4 Representation of diffusion in the Madelung fluid

The authors of [5,8,14,16] defined the complex velocity derived from the momentum operator $-i\hbar\nabla\Psi$, as

$$\mathbf{v} = [-i\frac{\hbar}{m}\nabla\ln\Psi] = \mathbf{v}_r + i\mathbf{v}_i, \quad (24)$$

so that $\mathbf{v}_r = \mathbf{u}_a = \nabla\tilde{S}$ is the advective velocity and $\mathbf{v}_i = -\frac{\hbar}{2m}\nabla(\ln\rho)$. One may interpret $\mathbf{v}_i = \mathbf{u}_d$, as in (16), suggesting the relation between the Planck constant and the diffusion coefficient to be $\frac{\hbar}{2} = mD$, so that Q_d becomes identical to the quantum Bohm potential. For the simplest case of the Einstein relations in an ideal gas, $mD = (\mathbf{l} \cdot \bar{\mathbf{p}})/3$, where $|\mathbf{l}|$ is the molecular mean free path and $|\bar{\mathbf{p}}|$ is the magnitude averaged thermal (random walk) molecular momentum in-between collisions. Isotropy results in the relation $\frac{\hbar}{2} = l_x p_x$, and indeed l_x and p_x are the basic scales obtained from statistical mechanics for deriving the kinetic theory of gases. In other words, one cannot resolve the ideal gas dynamics within length scales smaller than l_x or for momenta smaller than p_x . As pointed out by [17, 18], it is intriguing that these two fundamental scales form the canonical variables which set the exact limiting case of the Heisenberg uncertainty principle.

Finally, incorporating (2) with (16) we obtain the Fokker-Planck equation

$$\frac{\partial\rho}{\partial t} + \nabla \cdot [\rho(\mathbf{u}_a - \mathbf{u}_d)] = \left(\frac{\hbar}{2m}\right) \nabla^2\rho, \quad (25)$$

which corresponds to the entropy equation

$$\frac{\partial s}{\partial t} + \nabla \cdot [(s - \rho)\mathbf{u}_a] = \left(\frac{\hbar}{2m}\right)^{-1} \rho\mathbf{u}_a \cdot \mathbf{u}_d, \quad (26)$$

yielding

$$\frac{\partial}{\partial t}Ent_S = \left(\frac{\hbar}{2m}\right)^{-1} k_B \langle \mathbf{u}_a \cdot \mathbf{u}_d \rangle, \quad (27)$$

thus stating that positive entropy production in the Madelung fluid occurs when the advective and the diffusive velocities are positively correlated within the fluid domain.

5 Summary and Discussion

The Madelung formulation suggests relations between classical hydrodynamic and thermodynamic with quantum mechanics. In Ref. [5], two of us highlighted the role of compressibility in the Madelung fluid, where in the current work we examine further the Shannon entropy production within the Madelung formulation and find that it is proportional to the expectation value of $\nabla \cdot \mathbf{u}_a$. Thus, the expansion of the fluid is equivalent to an entropy increase. Furthermore, we note that interference between plane waves leads to an increase of entropy, but it also renders the Madelung fluid compressible, allowing it to expand. Putting all of the pieces together, we find that a simple link exists between the interference of wave functions, compressibility of the Madelung fluid, and Shannon entropy production.

The Madelung fluid expansion suggests an analogy with diffusive processes such as a free Joule expansion. Ref. [5] related the imaginary part of the quantum velocity to the thermal fluctuations of the Madelung fluid. Following the current analysis, this imaginary part can indeed be interpreted, as a diffusive drift (or osmotic) velocity, since its flux is proportional to the minus sign of the density gradient (as in Fick's first law). Furthermore, this analogy suggests that the diffusion coefficient is $\hbar/2m$, and for the simplest model of diffusion in ideal gas, the relation between the diffusion coefficient, the mean free path, and Brownian momentum provides the lower bound of the Heisenberg uncertainty relation.

The entropy production can be expressed as well in terms of the correlation's expectation value between the advective and diffusive velocities. Moreover, for classical diffusive processes, it was shown that the gradient of the Bohm potential acts as a force to accelerate the diffusion. This appearance of the quantum potential in a classical process may shed light on its role in the Schrödinger equation. It is important to remember however, that in the quantum case the diffusion equation, governed by Fick's second law, cannot be extracted from the Schrödinger equation, i.e., $\frac{\partial \rho}{\partial t} \neq (\hbar/2m)\nabla^2 \rho$, but rather $\frac{\partial \rho}{\partial t} = -\nabla \cdot (\rho \mathbf{u}_a)$. Therefore, processes associated with density variation, such as entropy growth, are due to expansion by the hydrodynamical advective velocity and not by diffusive irreversible processes.

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Appendix

Assuming that the phase space density function, $\rho_{ph}(\mathbf{r}, \mathbf{p}, t)$, in equilibrium can be separated into coordinate and momentum parts, $\rho_{ph}(\mathbf{r}, \mathbf{p}, t) \equiv \rho(\mathbf{r}, t)\chi(\mathbf{p}, t)$, then the Boltzmann entropy becomes

$$Ent_B = -k_B \int \int \rho_{ph} \ln \rho_{ph} d\mathbf{r} d\mathbf{p} = Ent_S - k_B \int \chi \ln \chi d\mathbf{p}. \quad (28)$$

Under the de Broglie-Bohm interpretation, the particle's momentum is $\mathbf{p} = \nabla S(\mathbf{r}, t)$, so that $\chi = \delta(\mathbf{p} - \nabla S)$. As seen from the two terms on the right-hand side of Eq. (28), the Boltzmann entropy is the sum of (i) the entropy Ent_S associated with

the spatial probability distribution (ρ) and (ii) a (formally divergent) entropy associated with the momentum probability distribution χ ,

$$Ent_B = Ent_S - k_B \ln \delta(0). \quad (29)$$

The divergent contribution in the RHS of Eq. (29) results from the (unbounded) singular Dirac's delta distribution for the momentum. In a discrete rendition of χ (i.e., making it a Kronecker delta), this Dirac delta distribution will be replaced by a value of unity when the condition $\mathbf{p} = \nabla S$ is satisfied, i.e., there is no entropic uncertainty associated with the momentum. Consequently, such a discrete probabilistic rendition will lead to no difference between Ent_B and Ent_S . Thus, within the continuum framework that we work in, the singular term in Eq. (29) is an outgrowth of the fact that within the Bohmian interpretation (which indeed differs from the Madelung one [4,7]) the variance of the continuum momentum distribution vanishes, equivalent to an assumption of zero temperature of the Madelung fluid. If, however, one interprets the de Broglie guiding equation ($\mathbf{p} = \nabla S$) only as a mean (hydrodynamic) motion, then the Madelung fluid has a non zero temperature that is proportional to the Fisher information [5], and the Boltzmann entropy in (28) will, generally, not be singular.

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