

Information Dynamics in Quantum Theory

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Received 22 Oct. 2006; Revised 3 Nov. 2006; Accepted 16 Nov. 2006

Shannon entropy and Fisher information functionals are known to quantify certain information-theoretic properties of continuous probability distributions of various origins. We carry out a systematic study of these functionals, while assuming that the pertinent probability density has a quantum mechanical appearance $\rho \doteq |\psi|^2$, with $\psi \in L^2(R)$. Their behavior in time, due to the quantum Schrödinger picture evolution-induced dynamics of $\rho(x, t)$ is investigated as well, with an emphasis on thermodynamical features of quantum motion.

Keywords: Information entropy; Entropy methods; Dynamics of densities; Entropy dynamics; Fisher information; Indeterminacy relations; Entropic inequalities; Laws of thermodynamics; Helmholtz free energy; Quantum motion.

1 Information – is there anything where nobody looks ?

Shannon and von Neumann entropies are typical information theory tools which can be used to quantify the information content and possibly information loss/gain incurred by a quantum system, initially prepared in a specified (macro)state.

The von Neumann entropy is known to vanish on pure states, hence one presumes to have a complete information about such state. An incomplete information concept thus seems to be related only to mixed states.

On the other hand, right in connection with pure states of a quantum mechanical system, the Shannon entropy is known to give an access to another information theory level. Namely, it enables quantifying an information content of continuous probability distributions, that can be inferred from any $\psi \in L^2(R^n)$ vector by means of the Born recipe $\rho \doteq |\psi|^2$.

Since, in physics, the very concept of entropy is typically interpreted as a measure of the degree of randomness and the tendency (trend) of physical systems to become less

organized (disordered), it is quite natural to think of entropy as about the measure of uncertainty or disorder. Notions of information and uncertainty are deeply intertwined. Spectacular examples of this intertwine are provided by information theory measures employed in quantum theory in the description of so-called entropic uncertainty relations that are valid in $L^2(\mathbb{R}^n)$ for Born postulate-induced continuous probability densities, [3].

The term *information*, in the present context, may be literally understood as the *inverse of uncertainty*. As far as the notion of an *organization* is concerned, the Shannon entropy (and a number of other entropic measures) is known to quantify the degree of the probability distribution complexity, [1], and (de)localization, [2], for stationary and non-stationary Schrödinger wave packets.

Let us tentatively accept the casual statement that a (thermodynamically) *isolated* system is represented in quantum mechanics by a state vector which conveys statistic predictions for measurement outcomes. Then, we are tempted to identify and quantify an information content of a state vector, even though we know that the von Neumann entropy (the standard quantum measure of information) identically vanishes on a pure quantum state. The related semantic word-game due to Roger Penrose is worth mentioning: “when a system has a state $|\psi\rangle$ there ought to be some property in the system that corresponds to its $|\psi\rangle$ -ness”, [4].

A more formal issue appears if we pass to the quantum dynamics, when we should in principle address an information theoretic interpretation of quantum evolutions. Clearly, in terms of the von Neumann entropy, nothing illuminating can be said about the quantum motion of pure or mixed states of an isolated system, since the unitary evolution leaves the von Neumann entropy intact. Therefore, the von Neumann entropy behavior in time may become interesting only if we pass from isolated to (thermodynamically) *open* systems.

Quite to the contrary, the Shannon entropy of a continuous probability distribution may show up a non-trivial pattern of temporal behavior which deserves a closer inspection. Even, if our attention is confined to an *isolated* quantum system in its pure state.

2 Information functionals and indeterminacy relations

Given an $L^2(\mathbb{R})$ -normalized function $\psi(x)$. We denote $(\mathcal{F}\psi)(p)$ its Fourier transform. The corresponding probability densities follow: $\rho(x) = |\psi(x)|^2$ and $\tilde{\rho}(p) = |(\mathcal{F}\psi)(p)|^2$. We introduce the related position and momentum information (differential, e.g. Shannon) entropies:

$$\mathcal{S}(\rho) \doteq S_q = -\langle \ln \rho \rangle = - \int \rho(x) \ln \rho(x) dx \quad (2.1)$$

and

$$\mathcal{S}(\tilde{\rho}) \doteq S_p = -\langle \ln \tilde{\rho} \rangle = - \int \tilde{\rho}(p) \ln \tilde{\rho}(p) dp \quad (2.2)$$

where \mathcal{S} denotes the Shannon entropy for a continuous probability distribution. For the sake of clarity, we use dimensionless quantities, see e.g. however [5] for a discussion of how to handle dimensional quantities in the Shannon entropy definition.

We assume both entropies to take finite values. Then, there holds the familiar entropic uncertainty relation [3]:

$$S_q + S_p \geq (1 + \ln \pi). \quad (2.3)$$

If following conventions we define the squared standard deviation value for an observable A in a pure state ψ as $(\Delta A)^2 = (\psi, [A - \langle A \rangle]^2 \psi)$ with $\langle A \rangle = (\psi, A\psi)$, then for the position X and momentum P operators we have the following version of the entropic uncertainty relation (here expressed through so-called entropy powers, see e.g. [6], $\hbar \equiv 1$):

$$\Delta X \cdot \Delta P \geq \frac{1}{2\pi e} \exp[\mathcal{S}(\rho) + \mathcal{S}(\tilde{\rho})] \geq \frac{1}{2} \quad (2.4)$$

which is an alternative version of the entropic uncertainty relation.

An important property of the Shannon entropy $\mathcal{S}(\rho)$ is that for a continuous probability distribution $\rho(x)$ with an arbitrary finite mean $\langle X \rangle$ and a fixed variance $\sigma^2 = \langle (X - \langle X \rangle)^2 \rangle = \Delta X^2$ we would have

$$\mathcal{S}(\rho) \leq \frac{1}{2} \ln(2\pi e \sigma^2). \quad (2.5)$$

$\mathcal{S}(\rho)$ becomes maximized in the set of such densities if and only if ρ is a Gaussian with variance σ^2 . For Gaussian densities, $(2\pi e)\Delta X \cdot \Delta P = \exp[\mathcal{S}(\rho) + \mathcal{S}(\tilde{\rho})]$ holds true, but the minimum $1/2$ on the right-hand-side of Eq. (2.4), is not necessarily reached.

In below, we shall devote some attention to the Fisher information measure [2, 7]:

$$\mathcal{F}(\rho) \doteq \langle (\nabla \ln \rho)^2 \rangle = \int \frac{(\nabla \rho)^2}{\rho} dx \quad (2.6)$$

which stays in a remarkable relationship with the Shannon entropy of the very same continuous probability distribution [7]:

$$\mathcal{F}(\rho) \geq (2\pi e) \exp[-2\mathcal{S}(\rho)] \geq \frac{1}{\sigma^2}. \quad (2.7)$$

Clearly, we have $\mathcal{F}(\rho) \geq (1/\sigma^2)$ with the equality allowed only if ρ is a Gaussian with variance σ^2 .

Let us notice that in view of properties of the Fourier transform, there is a complete symmetry between the inferred information-theory functionals. After the Fourier transformation, the Parseval identity implies that the chain of inequalities Eq. (2.7) can be faithfully reproduced (while replacing ρ by $\tilde{\rho}$) for the ‘‘momentum -space’’ density $\tilde{\rho}$ with the variance $\tilde{\sigma}^2$. As a consequence, taking into account the entropic uncertainty relation Eq. (2.3), we arrive at [3]:

$$4\tilde{\sigma}^2 \geq 2(e\pi)^{-1} \exp[-2\langle \ln \tilde{\rho} \rangle] \geq (2e\pi) \exp[2\langle \ln \rho \rangle] \geq \sigma^{-2} \quad (2.8)$$

Let us consider a momentum operator P that is conjugate to the position operator X in the adopted dimensional convention $\hbar \equiv 1$. Setting $P = -id/dx$ and presuming that all averages are finite, we get:

$$[\langle P^2 \rangle - \langle P \rangle^2] = (\Delta P)^2 = \tilde{\sigma}^2. \quad (2.9)$$

The standard indeterminacy relationship $\sigma \cdot \tilde{\sigma} \geq (1/2)$ follows.

In the above, no explicit time-dependence has been indicated, but all derivations go through with any wave-packet solution $\psi(x, t)$ of the Schrödinger equation. The induced dynamics of probability densities may imply the time-evolution of entropies: $S_q(t), S_p(t)$ and thence the dynamics of quantum uncertainty measures $\Delta X(t) = \sigma(t)$ and $\Delta P(t) = \tilde{\sigma}(t)$.

3 Hydrodynamical velocity fields and their variances

Let us consider the Schrödinger equation:

$$i\partial_t\psi = -D\Delta\psi + \frac{\mathcal{V}}{2mD}\psi. \quad (3.1)$$

where the potential $\mathcal{V} = \mathcal{V}(\vec{x}, t)$ (possibly time-dependent) is a continuous (it is useful, if bounded from below) function with dimensions of energy, $D = \hbar/2m$.

By employing the Madelung decomposition:

$$\psi = \rho^{1/2} \exp(is/2D) \quad (3.2)$$

with the phase function $s = s(x, t)$ defining $v = \nabla s$ we readily arrive at the continuity equation

$$\partial_t\rho = -\nabla(v\rho) \quad (3.3)$$

and the generalized Hamilton-Jacobi equation:

$$\partial_t s + \frac{1}{2}(\nabla s)^2 + (\Omega - Q) = 0 \quad (3.4)$$

where, after introducing an additional velocity field

$$u(x, t) = D\nabla \ln \rho(x, t), \quad (3.5)$$

we have

$$Q = 2D^2 \frac{\Delta\rho^{1/2}}{\rho^{1/2}} = \frac{1}{2}u^2 + D\nabla \cdot u. \quad (3.6)$$

If a quantum mechanical expectation value of the standard Schrödinger Hamiltonian $\hat{H} = -(\hbar^2/2m)\Delta + V$ exists (i.e. is finite [9]),

$$\langle \psi | \hat{H} | \psi \rangle \doteq E < \infty \quad (3.7)$$

then the unitary quantum dynamics warrants that this value is a constant of the Schrödinger picture evolution:

$$\mathcal{H} = \frac{1}{2}[\langle v^2 \rangle + \langle u^2 \rangle] + \langle \Omega \rangle = -\langle \partial_t s \rangle \doteq \mathcal{E} = \frac{E}{m} = \text{const.} \quad (3.8)$$

Let us notice that $\langle u^2 \rangle = -D\langle \nabla u \rangle$ and therefore:

$$\frac{D^2}{2}\mathcal{F} = \frac{D^2}{2} \int \frac{1}{\rho} \left(\frac{\partial \rho}{\partial x} \right)^2 dx = \int \rho \cdot \frac{u^2}{2} dx = -\langle Q \rangle. \quad (3.9)$$

Let us observe that $D^2\mathcal{F}$ stands for the mean square deviation value of a function $u(x, t)$ about its mean value $\langle u \rangle = 0$, whose vanishing is a consequence of the boundary conditions (here, at infinity):

$$(\Delta u)^2 \doteq \sigma_u^2 = \langle [u - \langle u \rangle]^2 \rangle = \langle u^2 \rangle = D^2\mathcal{F}. \quad (3.10)$$

The mean square deviation of $v(x, t)$ about its mean value $\langle v \rangle$ reads:

$$(\Delta v)^2 \doteq \sigma_v^2 = \langle v^2 \rangle - \langle v \rangle^2. \quad (3.11)$$

It is clear, that with the definition $P = -i(2mD)d/dx$, the mean value of the operator P is related to the mean value of a function $v(x, t)$ (we do not discriminate between technically different implementations of the mean): $\langle P \rangle = m\langle v \rangle$. Accordingly,

$$\tilde{\sigma}^2 = (\Delta P)^2 = \langle P^2 \rangle - \langle P \rangle^2 \quad (3.12)$$

Moreover, we can directly check that with $\rho = |\psi|^2$ there holds [8]:

$$\begin{aligned} \mathcal{F}(\rho) &= \frac{1}{D^2}\sigma_u^2 = \int dx |\psi|^2 [\psi'(x)/\psi(x) + \psi^{*'}(x)/\psi^*(x)]^2 = \\ &4 \int dx \psi^{*'}(x)\psi'(x) + \int dx |\psi(x)|^2 [\psi'(x)/\psi(x) - \psi^{*'}(x)/\psi^*(x)]^2 = \\ &\frac{1}{m^2 D^2} [\langle P^2 \rangle - m^2 \langle v^2 \rangle] = \frac{1}{m^2 D^2} [(\Delta P)^2 - m^2 \sigma_v^2] \end{aligned} \quad (3.13)$$

i.e.

$$m^2(\sigma_u^2 + \sigma_v^2) = \tilde{\sigma}^2. \quad (3.14)$$

It is interesting to notice that $\langle (P - mv) \rangle = 0$ and the corresponding mean square deviation reads:

$$\langle (P - mv)^2 \rangle = \langle P^2 \rangle - m^2 \langle v^2 \rangle = m^2 D^2 \mathcal{F}. \quad (3.15)$$

An interesting outcome of this discussion is a definite sharpening of an upper bound in the inequalities Eqs. (2.7). Namely, by passing to dimensionless quantities in Eqs. (3.13) (e.g. $2mD \equiv 1$), and denoting $p_{cl} \doteq (\arg \psi(x, t))'$ we get:

$$\mathcal{F} = 4[\langle P^2 \rangle - \langle p_{cl}^2 \rangle] = 4[(\Delta P)^2 - (\Delta p_{cl})^2] = 4[\tilde{\sigma}^2 - \tilde{\sigma}_{cl}^2] \quad (3.16)$$

and therefore the chain of inequalities Eq. (2.7) gets a sharper form with a manifest upper bound for the Shannon entropy of $\rho = |\psi|^2$ set by:

$$4\tilde{\sigma}^2 \geq 4[\tilde{\sigma}^2 - \tilde{\sigma}_{cl}^2] = \mathcal{F} \geq (2\pi e) \exp[-2\mathcal{S}(\rho)] \geq \frac{1}{\sigma^2}. \quad (3.17)$$

We recall that all ‘‘tilde’’ quantities can be deduced from the once given ψ and its Fourier transform $\tilde{\psi}$.

4 Thermodynamical features of the quantum dynamics

We have emphasized that a pure state of the quantum theory and its Schrödinger picture dynamics are normally attributed to a thermodynamically *isolated* quantum system. We would like to demonstrate that a number of essentially thermodynamical features is encoded in this innocent-looking, apparently non-thermodynamical regime. To this end some basic notions of the non-equilibrium thermodynamics must be introduced.

4.1 Quantum detour - thermodynamics of open systems

We shall give a concise resume of the pertinent framework following [10]. It is taken for granted that in case of an open quantum system, the bath drives a system to an equilibrium state. The state of the system plus reservoir is described by a density matrix. Let ρ_t be the reduced density matrix of a quantum system in a combined weak coupling and adiabatic approximation of the general system-reservoir dynamic problem, $t \geq 0$:

$$\frac{d}{dt}\rho_t = -i[H_{sys}(t), \rho_t] + L_{diss}(t)\rho_t \doteq L(t)\rho_t \quad (4.1)$$

We introduce the following thermodynamical notions: (i) an *internal energy* of the system $E(t) = Tr(\rho_t H_{sys}(t))$, (ii) the *work* performed on the system by external forces $W(t) = \int_0^t Tr[\rho_s(\frac{d}{ds}H_{sys}(s))]ds$. (iii) the *heat* supplied to the system by the reservoir $Q(t) = \int_0^t Tr[(\frac{d}{ds}\rho_s)H_{sys}(s)]ds$.

The laws of thermodynamics, tailored to the manifestly non-equilibrium dynamical regime can now be formulated. The first law of thermodynamics reads:

$$\frac{d}{dt}E(t) = \frac{d}{dt}W(t) + \frac{d}{dt}Q(t). \quad (4.2)$$

Let us introduce the relative entropy $(\rho|\sigma) = Tr(\rho \ln \rho - \rho \ln \sigma)$ and the account for the stationary state input $L(t)\rho_{eq} = 0$, with $\rho_{eq} = Z^{-1} \exp[-\beta H_{sys}(t)]$. Then, the second law of thermodynamics takes the form:

$$\frac{d}{dt}S(\rho_t|\rho_{eq}) = \sigma(\rho_t) + \frac{1}{T} \frac{dQ}{dt} \quad (4.3)$$

where $\sigma(\rho_t) \geq 0$ is called the entropy production, while \dot{Q}/T refers to the entropy/heat exchange with the bath. Obviously, we have $TdS \geq dQ$.

4.2 Back to classical non-equilibrium thermodynamics

For the record, we indicate that the following hierarchy of thermodynamic systems is adopted in the present paper [11,12]: *isolated* with no energy and matter exchange with the environment, *closed* with the energy but *no* matter exchange and *open* where energy-matter exchange is unrestricted.

Our previous discussion was confined to an open quantum system. Accepting the standard text-book wisdom that all isolated systems evolve to the state of equilibrium in which the entropy reaches its maximal value, we shall pay attention to *closed* random systems and their somewhat different asymptotic properties. A concise resume of a non-equilibrium thermodynamics of *closed* systems comprises the I^{st} law of thermodynamics

$$\dot{U} = \dot{Q} + \dot{W} \quad (4.4)$$

and the II^{nd} law of thermodynamics:

$$\dot{S} = \dot{S}_{int} + \dot{S}_{ext}, \quad (4.5)$$

where $\dot{S}_{int} \geq 0$ and $\dot{S}_{ext} = \dot{Q}/T$, c.f. [11, 12]. Let us emphasize that \dot{Q} and \dot{W} are always well defined, but the adopted (time derivative) notation does not imply that one may infer Q and W as legitimate thermodynamic functions, c.f. an issue of “imperfect differentials” in classical thermodynamics.

Thermodynamic extremum principles are usually invoked in connection with the large time behavior of irreversible processes. One looks for direct realizations of the entropy growth paradigm, undoubtedly valid for isolated systems, [13]. Among a number of standard thermodynamic extremum principles, we recall a specific one named the Helmholtz extremum principle. If the temperature T and the available volume V are kept constant, then the minimum of the Helmholtz free energy

$$F = U - TS \quad (4.6)$$

is preferred in the course of the system evolution in time, and there holds [12]

$$\dot{F} = -T\dot{S}_{int} \leq 0 \quad (4.7)$$

In below, we shall analyze the validity of thermodynamic principles and the role played by the direct analog of the Helmholtz free energy, in case of quantum motion, and specifically in the seemingly non-thermodynamical context of the Schrödinger picture evolution.

4.3 Thermodynamical features of the quantum motion - closed systems in action

We come back to the Schrödinger picture evolution of pure states in $L^2(R)$. We impose the natural boundary data on quantum motion and they are implicit (vanishing of various

expressions at integration boundaries) in all averaging procedures in below. One must be aware that we pass-by a number of mathematical subtleties and take for granted that various computational steps are allowed.

The continuity equation is a direct consequence of the Schrödinger equation. It is less obvious that after employing the hydrodynamical velocity fields $u(x, t)$ and $v(x, t)$ the Fokker Planck equation for $\rho = |\psi|^2$ may be deduced. We have:

$$\partial_t \rho = D \Delta \rho - \nabla \cdot (b \rho) \quad (4.8)$$

where $b = v + u = \nabla(s + D \ln \rho)$ where $u = D \nabla \ln \rho$.

The Shannon entropy of a continuous probability distribution $\mathcal{S} = -\langle \ln \rho \rangle$ follows and yields

$$D \dot{\mathcal{S}} = \langle v^2 \rangle - \langle b \cdot v \rangle \doteq D(\dot{\mathcal{S}}_{int} + \dot{\mathcal{S}}_{ext}) \quad (4.9)$$

which is a straightforward analog of the II^{nd} law of thermodynamics in the considered quantum mechanical context:

$$\dot{\mathcal{S}}_{int} = \dot{\mathcal{S}} - \dot{\mathcal{S}}_{ext} = (1/D) \langle v^2 \rangle \geq 0 \Rightarrow \dot{\mathcal{S}} \geq \dot{\mathcal{S}}_{ext}. \quad (4.10)$$

To address an analog of the I^{st} law we need to translate to the present setting the previously discussed thermodynamic notions of U and $F = U - TS$, where the notion of *temperature* is the most serious obstacle. We have no obvious notion of temperature for quantum systems in their pure states (for large molecules, like fullerenes or the likes, the notion of internal temperature makes sense, but we aim to consider any quantum system in a pure state, small or large). Therefore, we shall invoke a dimensional artifice [14].

We formally introduce

$$k_B T_0 \doteq \hbar \omega_0 \doteq m c^2 \quad (4.11)$$

and thence

$$D = \hbar/2m \equiv k_B T_0 / m \beta_0 \quad (4.12)$$

with $\beta_0 \equiv 2\omega_0 = 2m c^2 / \hbar$, and so arrive at

$$k_B T_0 \dot{\mathcal{S}}_{ext} = \dot{Q}. \quad (4.13)$$

In view of

$$\begin{aligned} v &= \nabla s = \nabla(s + D \ln \rho) - D \nabla \ln \rho \doteq \\ &= -\frac{1}{m\beta} \nabla(V + k_B T_0 \ln \rho) \doteq -\frac{1}{m\beta_0} \nabla \Psi, \end{aligned} \quad (4.14)$$

where the time-dependent potential

$$V = V(x, t) \doteq -m\beta_0(s + D \ln \rho) \quad (4.15)$$

is defined to stay in a notational conformity with the standard Smoluchowski process (Brownian motion in a conservative force field [2]) definition $b = -\nabla V/m\beta_0$, we finally get

$$-m\beta\langle s \rangle \equiv \langle \Psi \rangle = \langle V \rangle - TS \implies F = U - TS, \quad (4.16)$$

where $U = \langle V \rangle$ and $F = \langle \Psi \rangle$.

Remembering about an explicit time dependence of $b(x, t) = -(1/m\beta_0)\nabla V(x, t)$, we finally arrive at the I^{st} law of thermodynamics in the present quantum context:

$$\dot{U} = \langle \partial_t V \rangle - m\beta_0 \langle bv \rangle = \dot{W} + \dot{Q}. \quad (4.17)$$

The externally performed work entry reads $\dot{W} = \langle \partial_t V \rangle$. But:

$$V = -m\beta s - k_B T \ln \rho \implies \langle \partial_t V \rangle = -m\beta_0 \langle \partial_t s \rangle = \dot{W}$$

and therefore

$$-\frac{d}{dt}\langle s \rangle = -\langle v^2 \rangle - \langle \partial_t s \rangle \Rightarrow \dot{F} = -T_0 \dot{S}_{int} + \dot{W} \quad (4.18)$$

where $\dot{S}_{int} \geq 0$.

In view of Eq. (3.8), in the thermodynamical description of the quantum motion, we encounter a never vanishing constant work term

$$\dot{W} = m\beta_0 \mathcal{E} = \beta_0 \langle \hat{H} \rangle. \quad (4.19)$$

The associated Helmholtz-type extremum principle reads:

$$\dot{F} - m\beta_0 \mathcal{E} = -T_0 \dot{S}_{int} \leq 0. \quad (4.20)$$

It is instructive to notice that

$$T \dot{S}_{int} = T \dot{S} - \dot{Q} \geq 0 \iff \dot{Q} \leq T \dot{S} \quad (4.21)$$

goes in parallel with

$$\dot{F} \leq \dot{W} = \beta_0 \langle \hat{H} \rangle. \quad (4.22)$$

Let us stress that the non-vanishing external work term is generic to the quantum motion. If a stationary state is considered, our $\langle \hat{H} \rangle$ is equal to a corresponding energy eigenvalue.

For negative eigenvalues, the work term receives an interpretation of the ‘‘work performed by the system’’ (upon its, hitherto hypothetical, surrounding ?). Then \dot{F} is negative and F may possibly have a chance to attain a minimum.

Since bounded from below Hamiltonians can be replaced by positive operators, we may in principle view $m\beta_0 \mathcal{E} = \beta_0 \langle \hat{H} \rangle$ as a positive (constant and non-vanishing) time rate of the ‘‘work externally performed upon the system’’. This observation encompasses the case

of positive energy spectra. Accordingly, \dot{F} may take both negative and positive values. The latter up to an upper bound $m\beta_0\mathcal{E}$.

Basic features of the non-equilibrium thermodynamics of *closed* irreversible systems, somewhat surprisingly have been reproduced in the quantum Schrödinger picture evolution. We have identified direct analogues of the I^{st} and the II^{nd} laws of thermodynamics, together with the involved notions of $\dot{S}_{int} \geq 0$ and $\dot{S}_{ext} = (1/T)\dot{Q}$.

An asymptotic behavior of the quantum motion is controlled by the analog of the II^{nd} law:

$$\dot{F} - \dot{W} = -m\beta_0 \frac{d}{dt} (\langle s \rangle + \mathcal{E}t) = -T_0 \dot{S}_{int} \leq 0. \quad (4.23)$$

where there appears an work (performed *upon* or performed *by* the system) term $\dot{W} = \langle \partial_t V \rangle = m\beta_0\mathcal{E}$ value whose sign is indefinite (either positive or negative).

Let us notice that in classical non-equilibrium thermodynamics the so-called minimum entropy production principle [11] is often invoked in connection with the “speed” with which a minimum of the Helmholtz free energy is approached. For sufficiently large times, when the system is in the vicinity of the stationary (equilibrium) state, one expects that the the entropy production $T\dot{S}_{int} \geq 0$ is a monotonically decaying function of time, i.e. that

$$\frac{d}{dt} \dot{S}_{int} < 0. \quad (4.24)$$

The quantum motion looks different. In that case, \dot{F} may be positive and one cannot exclude transitions (including those of an oscillatory nature) from negative to positive \dot{F} values and back. It may happen that in certain quantum states, the Helmholtz free energy F may have a minimum, a maximum, an infinite number of local minima and maxima, or none at all. There is no reason for the minimum entropy production principle to be valid in quantum theory, except for very special cases.

There is however a “speed” property which is special for the quantum case, with no dissipative counterpart. Namely, since the work term is a constant of quantum motion and $\dot{F} + T_0\dot{S}_{int} = m\beta_0\mathcal{E}$, we have the following *negative feedback* relationship between the speeds of the growth/decay of the entropy production and the Helmholtz free energy time rate:

$$\frac{d}{dt} \dot{F} = -T_0 \frac{d}{dt} \dot{S}_{int}. \quad (4.25)$$

If the Helmholtz free energy time rate drops down, the entropy production time rate needs to increase and in reverse. Therefore a minimum of \dot{F} in principle may be achieved, if a maximum of the entropy production \dot{S}_{int} is attained. In reverse, a maximum of \dot{F} may arise in conjunction with a minimum of \dot{S}_{int} .

Remembering that $T_0\dot{S}_{int} = m\beta_0\langle v^2 \rangle$ and exploiting the total mean energy formula, Eq. (3.8), we can identify the respective “speeds”:

$$\frac{d}{dt} \dot{F} = \beta_0 \frac{d}{dt} (m\langle u^2 \rangle + 2\langle \mathcal{V} \rangle) \quad (4.26)$$

and

$$T_0 \frac{d}{dt} \dot{S}_{int} = m\beta_0 \frac{d}{dt} \langle v^2 \rangle \quad (4.27)$$

that stay in a feedback relationship. By recalling our discussion of Section III, we realize that variances of the hydrodynamical velocity fields decide about the time rate of the entropy production and Helmholtz free energy in the quantum case. They stay in the above mentioned feedback relationship, consult e.g. also [2, 15].

Acknowledgement:

The paper has been supported by the Polish Ministry of Scientific Research and Information Technology under the grant No PBZ-MIN-008/P03/2003.

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