

Information dynamics: temporal behavior of uncertainty measures

Research Article

Piotr Garbaczewski*

Institute of Physics, University of Opole, 45-052 Opole, Poland

Received 21 August 2007; accepted 25 October 2007

Abstract: We carry out a systematic study of uncertainty measures that are generic to dynamical processes of varied origins, provided they induce suitable continuous probability distributions. The major technical tools are the information theory methods and inequalities satisfied by Fisher and Shannon information measures. We focus on the compatibility of these inequalities with the prescribed (deterministic, random or quantum) temporal behavior of pertinent probability densities.

PACS (2008): 03.65.Ta, 02.50.Ey, 05.40.Jc

Keywords: information functionals • information theoretic inequalities • Shannon entropy • Fisher information • dynamics of probability densities • entropy methods • Smoluchowski processes • Schrödinger picture evolution

© Versita Warsaw and Springer-Verlag Berlin Heidelberg.

1. Information and uncertainty

Our primary motivations are an information-theoretic conceptual background and methods of analysis adopted for probability distributions. Such notions like information, uncertainty, indeterminacy and/or information deficit are naturally quantified in terms of information inequalities. The relationship between statistical (informational) and thermodynamic notions of entropy of a physical (model) system, has received some attention as well, [1–6].

The pertinent information measures are seldom considered in the time domain. Our main purpose is to quantify their temporal behavior, while taking for granted that dynamical processes of interest do induce suitable continuous

probability densities (see e.g. [7–10]). Particular attention is paid to the time evolution of information entropies and inferred uncertainty measures [7, 8, 10].

1.1. Entropic functionals

To facilitate further discussion, we shall not attempt a fully fledged space-time formalism, and pass to time-dependent model systems in one space dimension. Let us consider continuous probability densities on the real line, with or without an explicit time-dependence: $\rho \in L^1(\mathbb{R})$; $\int_{\mathbb{R}} \rho(x) dx = 1$. Our minimal demand is that the first and second moments of each density are finite.

Therefore we can introduce a two-parameter family $\rho_{\alpha,\sigma}(x)$, labeled by the mean value $\langle x \rangle = \int x \rho(x) dx = \alpha \in \mathbb{R}$ and the standard deviation (here, square root of the variance) $\sigma \in \mathbb{R}^+$, $\sigma^2 = \langle (x - \langle x \rangle)^2 \rangle$.

For a given probability density ρ we name a function

*E-mail: pgar@uni.opole.pl

$-\ln \rho(x)$ a *surprise level* function and identify its mean value with the familiar notion $S(\rho)$ of the Shannon entropy of a continuous probability distribution, c.f. [8]:

$$S(\rho) = -\langle \ln \rho \rangle = -\int \rho(x) \ln \rho(x) dx. \quad (1)$$

Let us assume $\rho(x)$ to be (weakly) differentiable, so that we can give meaning to its first, second and third derivatives. Besides the obvious information-theoretic notion of the Shannon entropy, we introduce another information-theory functional $\mathcal{F}(\rho)$, often named the Fisher information measure (the name originates from statistical inference theory):

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

The above introduced expressions $\ln \rho(x)$ and $\nabla \ln \rho$ allow us to infer a number of interesting formulas. We assume the natural boundary data at finite or infinite (employed below) integration boundaries. We have:

$$-\nabla \ln \rho = -\frac{\nabla \rho}{\rho} \implies -\left\langle \frac{\nabla \rho}{\rho} \right\rangle = 0 \quad (3)$$

and next

$$\begin{aligned} -\Delta \ln \rho &= -\frac{\Delta \rho}{\rho} + \frac{(\nabla \rho)^2}{\rho^2} \implies \\ -\langle \Delta \ln \rho \rangle &= \left\langle \frac{(\nabla \rho)^2}{\rho^2} \right\rangle = \langle (\nabla \ln \rho)^2 \rangle. \end{aligned} \quad (4)$$

The following identities hold true:

$$\begin{aligned} -\frac{\Delta \rho^{1/2}}{\rho^{1/2}} &= \frac{1}{2} \left[-\frac{\Delta \rho}{\rho} + \frac{1}{2} \frac{(\nabla \rho)^2}{\rho^2} \right] \implies \\ \nabla \left(\frac{\Delta \rho^{1/2}}{\rho^{1/2}} \right) &= \frac{1}{2\rho} \nabla(\rho \Delta \ln \rho) \end{aligned} \quad (5)$$

where we encounter a potential for a “Newton-type force field”. Its functional formula should be compared with Eq. (4). The mean value of the potential function is non-negative

$$-\left\langle \frac{\Delta \rho^{1/2}}{\rho^{1/2}} \right\rangle = \frac{1}{4} \left\langle \frac{(\nabla \rho)^2}{\rho^2} \right\rangle = -\frac{1}{4} \langle \Delta \ln \rho \rangle, \quad (6)$$

while that of the related “force” vanishes:

$$\left\langle \nabla \left(\frac{\Delta \rho^{1/2}}{\rho^{1/2}} \right) \right\rangle = 0. \quad (7)$$

In the above systematics of derivatives there was no indication of a specific physical context. Nonetheless a number of physically interesting quantities can be immediately recognized. They notoriously appear in the local conservation laws for diffusion-type processes and in the hydrodynamical formulation of the Schrödinger picture quantum dynamics [8, 9].

Namely, while keeping in mind (hitherto disregarded) dimensional coefficients, we realize that Eq. (3) introduces a functional expression for an osmotic velocity field. Eqs. (4) and (5) actually set links between the hydrodynamical-type pressure function [9] and the Fisher functional. Eqs. (6) and (7) relate the so-called quantum potential and the pressure. Eq. (8) demonstrates that the mean value of a (known as quantum) potential and the value of the pressure functional coincide, while Eq. (8) tells us that the mean value of the inferred (quantum) force necessarily vanishes.

Let us emphasize that our only input was a *surprise level function* $-\ln \rho(x)$ for a continuous probability density ρ on R , admitting first and second moments, with suitable differentiability properties and with natural boundary data being implicit. No specific physical motivations (e.g. quantum or random dynamics) were spelled out.

1.2. Information inequalities

Let us consider a one-parameter α -family of densities whose mean square deviation value is fixed at σ . We have

$$S(\rho) \leq (1/2) \ln(2\pi e \sigma^2) \quad (8)$$

with a maximum for a Gaussian probability density with the prescribed fixed standard deviation σ . By introducing the mean value:

$$\langle [\sigma^2 \nabla \ln \rho + (x - \langle x \rangle)]^2 \rangle \geq 0 \quad (9)$$

we readily arrive at an inequality

$$\mathcal{F}(\rho) \geq \frac{1}{\sigma^2} \quad (10)$$

in which a minimum of \mathcal{F} is achieved (among all densities with a fixed value of σ) if and only if ρ is a σ -Gaussian, that in parallel with a maximum for S (compare e.g. [5, 11]). We stress that the above information inequalities Eq. (8) and (10) set respectively lower and upper bounds upon Fisher and Shannon functionals, when evaluated with respect to any density in the set of all admissible ones (e.g. with standard deviation value σ fixed once and for all).

Although we have carefully avoided any impact of dimensional quantities, the above Eq. (10) actually associates a primordial “momentum–position” indeterminacy relationship (here, devoid of any quantum connotations) with the probability distributions under consideration. Namely, let D be a positive diffusion constant with dimensions of $\hbar/2m$ or $k_B T/m\beta$ (c.f. [8]). We define an osmotic velocity field $u = u(x) = D\nabla \ln \rho$. There holds:

$$\Delta x \cdot \Delta u \geq D \quad (11)$$

which correlates the position variance $\Delta x = \langle [x - \langle x \rangle]^2 \rangle^{1/2}$ with the osmotic velocity variance $\Delta u = \langle [u - \langle u \rangle]^2 \rangle^{1/2}$. This property extends to time-dependent situations and is known to be respected by diffusion-type processes [12]. Its primary version for free Brownian motion has been found by R. Fürth [11].

Not accidentally, the above formula also closely mimics, and in fact induces (through reasoning based on probabilistic arguments) the fully-fledged quantum mechanical position–momentum relationship $\Delta x \cdot \Delta p \geq \hbar/2$, (tentatively replace u by mu and set $\hbar/2$ instead of D ; see e.g. [13]). We shall come back to this point later.

To conclude this section, let us point out that, given $\rho(x)$ and a suitable function $f(x)$, we can generalize the previous arguments. Let us introduce the notions of variance and covariance (here, directly borrowed from random variable analysis [13]) for x and $f(x)$. By means of the Schwarz inequality, we get:

$$\langle [x - \langle x \rangle]^2 \rangle \cdot \langle [f - \langle f \rangle]^2 \rangle \geq \langle [x - \langle x \rangle] \cdot [f - \langle f \rangle] \rangle^2, \quad (12)$$

hence, accordingly

$$\text{Var}(x) \cdot \text{Var}(f) \geq \text{Cov}^2(x, f). \quad (13)$$

We note that for an osmotic velocity field $u(x)$, we have $\langle u \rangle = 0$ and $\langle x \cdot u \rangle = -D$. Therefore

$$\text{Var}(x) \cdot \text{Var}(u) \geq \text{Cov}^2(x, u) = D^2, \quad (14)$$

as anticipated in Eq. (11).

The casual intuition behind physics-motivated indeterminacy relations is that of the Fourier transform. Indeed, for functions in $L^2(\mathbb{R})$ a non-zero function and its Fourier transform cannot both be sharply localized.

Let us point out notable information-theory inequalities [4, 5]:

$$\mathcal{F}(\rho) \geq (2\pi e) \exp[-2S(\rho)] \geq 1/\sigma^2. \quad (15)$$

and note that an explicit Fourier transformation input allows us to set an upper bound in this chain of inequalities.

The crucial step is to disentangle the $L^2(\mathbb{R})$ ingredients in the $L^1(\mathbb{R})$ functional form of the density ρ . This can be accomplished in many ways. the simplest is either a multiplicative decomposition $\rho(x) = \rho^{1/2}(x) \cdot \rho^{1/2}(x)$, where clearly $\rho^{1/2} \in L^2(\mathbb{R})$. A more general choice involves a complex function $\phi \in L^2(\mathbb{R})$ and its complex conjugate ϕ^* so that $\rho = \phi \cdot \phi^* = |\phi|^2$. (We recall that the Fourier transform of a real function typically is a complex function.) 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:

$$S(\rho) \equiv S_q = -\langle \ln \rho \rangle = - \int \rho(x) \ln \rho(x) dx \quad (16)$$

and

$$S(\tilde{\rho}) \equiv S_p = -\langle \ln \tilde{\rho} \rangle = - \int \tilde{\rho}(p) \ln \tilde{\rho}(p) dp \quad (17)$$

where S denotes the Shannon entropy for a continuous probability distribution. For the sake of clarity, we use dimensionless quantities, although there exists a consistent procedure for handling dimensional quantities in the Shannon entropy definition.

We assume both entropies take finite values. Then, there holds the familiar entropic uncertainty relation which is the sole consequence of the Fourier transform properties in $L^2(\mathbb{R})$ [14]:

$$S_q + S_p \geq (1 + \ln \pi). \quad (18)$$

Let us notice that in view of the 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. (15) 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. (18), we arrive at [14]:

$$4\tilde{\sigma}^2 \geq 2(e\pi)^{-1} \exp[-2\langle \ln \tilde{\rho} \rangle] \geq (2e\pi) \exp[2\langle \ln \rho \rangle] \geq \sigma^{-2} \quad (19)$$

which adds a Fourier transform-inferred upper bound to the previous inequalities Eq. (15)

$$4\tilde{\sigma}^2 \geq \mathcal{F}(\rho) \geq 1/\sigma^2 \quad (20)$$

and sets related upper and lower bounds upon the Shannon entropy as well.

All of this has been considered with no mention of any time evolution. Since the dynamics has a physical provenance, we should carefully investigate the ρ -factorization issue and the impact of a priori dynamical rules for $\rho_0(x) \rightarrow \rho(x, t)$ upon its concrete realisation. We shall focus on the standard random dynamics (Smoluchowski processes and phase-space motion) and the Schrödinger picture quantum dynamics.

2. Quantum indeterminacy in the time domain

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. [4], $\hbar \equiv 1$):

$$\Delta X \cdot \Delta P \geq \frac{1}{2\pi e} \exp [S(\rho) + S(\hat{\rho})] \geq \frac{1}{2} \quad (21)$$

which is an alternative version of the entropic uncertainty relation. For Gaussian densities, $(2\pi e)\Delta X \cdot \Delta P = \exp[S(\rho) + S(\hat{\rho})]$ holds true, but the minimum $1/2$ on the right-hand-side of Eq. (21), is not necessarily reached.

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:

$$[\langle P^2 \rangle - \langle P \rangle^2] = (\Delta P)^2 = \tilde{\sigma}^2. \quad (22)$$

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 $\Delta P(t) = \tilde{\sigma}(t)$.

We consider the Schrödinger equation in the form:

$$i\partial_t \psi = -D\Delta\psi + \frac{\mathcal{V}}{2mD}\psi. \quad (23)$$

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

By employing the Madelung decomposition:

$$\psi = \rho^{1/2} \exp [is/2D], \quad (24)$$

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

$$\partial_t \rho = -\nabla(v\rho) \quad (25)$$

and the generalized Hamilton-Jacobi equation:

$$\partial_t s + \frac{1}{2}(\nabla s)^2 + (\Omega - Q) = 0 \quad (26)$$

where $\Omega = \mathcal{V}/m$. After introducing an osmotic velocity field $u(x, t) = D\nabla \ln \rho(x, t)$, we have (compare e.g., our discussion of Section I):

$$Q = 2D^2 \frac{\Delta \rho^{1/2}}{\rho^{1/2}} = \frac{1}{2}u^2 + D\nabla \cdot u. \quad (27)$$

If a quantum mechanical expectation value of the standard Schrödinger Hamiltonian $\hat{H} = -(\hbar^2/2m)\Delta + V$ exists (i.e. is finite [15]),

$$\langle \psi | \hat{H} | \psi \rangle \equiv E < \infty \quad (28)$$

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

$$\mathcal{H} = \frac{1}{2}[\langle v^2 \rangle + \langle u^2 \rangle] + \langle \Omega \rangle = -\langle \partial_t s \rangle \equiv \mathcal{E} = \frac{E}{m} = const. \quad (29)$$

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

$$\frac{D^2}{2}\mathcal{F} = \frac{D^2}{2} \int \frac{1}{\rho} \left(\frac{\partial \rho}{\partial x} \right)^2 dx = \int \rho \cdot \frac{u^2}{2} dx = -\langle Q \rangle. \quad (30)$$

We 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):

$$(\Delta u)^2 \equiv \sigma_u^2 = \langle [u - \langle u \rangle]^2 \rangle = \langle u^2 \rangle = D^2\mathcal{F}. \quad (31)$$

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

$$(\Delta v)^2 \equiv \sigma_v^2 = \langle v^2 \rangle - \langle v \rangle^2. \quad (32)$$

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,

$$\tilde{\sigma}^2 = (\Delta P)^2 = \langle P^2 \rangle - \langle P \rangle^2 \quad (33)$$

Moreover, we can directly check that with $\rho = |\psi|^2$ there holds [16]:

$$\begin{aligned}\mathcal{F}(\rho) &= \frac{1}{D^2} \sigma_u^2 = \int dx |\psi|^2 [\psi'(x)/\psi(x) + \psi^{*'}(x)/\psi^*(x)]^2 = 4 \int dx \psi^{*'}(x) \psi'(x) + \int dx |\psi(x)|^2 [\psi'(x)/\psi(x) - \psi^{*'}(x)/\psi^*(x)]^2 \\ &= \frac{1}{m^2 D^2} [\langle P^2 \rangle - m^2 \langle v^2 \rangle] = \frac{1}{m^2 D^2} [(\Delta P)^2 - m^2 \sigma_v^2]\end{aligned}\quad (34)$$

i.e.

$$m^2(\sigma_u^2 + \sigma_v^2) = \delta^2. \quad (35)$$

It is interesting to notice that $\langle (P - mv) \rangle = 0$ and the corresponding mean square deviation reads: $\langle (P - mv)^2 \rangle = \langle P^2 \rangle - m^2 \langle v^2 \rangle = m^2 D^2 \mathcal{F}$.

By passing to dimensionless quantities in Eqs. (34) (e.g. $2mD \equiv 1$), and denoting $p_{cl} \equiv (\arg \psi(x, t))'$ we get:

$$\mathcal{F} = 4[\langle P^2 \rangle - \langle p_{cl}^2 \rangle] = 4[(\Delta P)^2 - (\Delta p_{cl})^2] = 4[\tilde{\sigma}^2 - \tilde{\sigma}_{cl}^2] \quad (36)$$

and therefore the chain of inequalities Eq. (15) gets a sharper form:

$$4\tilde{\sigma}^2 \geq 4[\tilde{\sigma}^2 - \tilde{\sigma}_{cl}^2] = \mathcal{F} \geq (2\pi e) \exp[-2\mathcal{S}(\rho)] \geq \frac{1}{\sigma^2}. \quad (37)$$

We recall that all “tilde” quantities can be deduced once given ψ and its Fourier transform $\tilde{\psi}$.

As a side comment, let us add that a direct consequence of the mean energy conservation law Eq. (29) are the identities: $\langle P^2 \rangle / 2m = E - \langle \mathcal{V} \rangle$ and

$$\mathcal{F} = \frac{1}{m^2 D^2} [\langle P^2 \rangle - m^2 \langle v^2 \rangle] = \frac{1}{D^2} [2(\mathcal{E} - \langle \Omega \rangle) - \langle v^2 \rangle] \quad (38)$$

plus a complementary expression for the variance of the momentum observable:

$$(\Delta P)^2 = 2m(E - \langle [\frac{m}{2} \langle v^2 \rangle + \mathcal{V}] \rangle). \quad (39)$$

That combines into the chain of inequalities between various energy characteristics:

$$E - \langle \mathcal{V} \rangle > m \langle v^2 \rangle / 2 \geq m \langle v \rangle^2 / 2 \geq 0. \quad (40)$$

3. Indeterminacy relations for diffusion-type processes

Let us consider spatial random motions—for example, standard Smoluchowski processes and their generalizations. Let us consider $\dot{x} = b(x, t) + A(t)$ with $\langle A(s) \rangle =$

0 , $\langle A(s)A(s') \rangle = \sqrt{2D}\delta(s - s')$ and the corresponding Fokker-Planck equation for the probability density ρ :

$$\partial_t \rho = D \Delta \rho - \nabla \cdot (b\rho) \quad (41)$$

which we analyze under the natural boundary conditions. We assume the gradient form for the forward drift $b = b(x, t)$ and take D as a diffusion constant with dimensions of $k_B T / m\beta$. By introducing $u(x, t) = D \nabla \ln \rho(x, t)$ we define the current velocity of the process $v(x, t) = b(x, t) - u(x, t)$, in terms of which the continuity equation $\partial_t \rho = -\nabla \cdot (v\rho)$ follows. The diffusion current reads $j = v\rho$.

As mentioned before, we have an obvious indeterminacy relationship for the osmotic velocity field $\text{Var}(x) \cdot \text{Var}(u) \geq \text{Cov}^2(x, u) = D^2$. The corresponding relationship for the current velocity field $\text{Var}(x) \cdot \text{Var}(v) \geq \text{Cov}^2(x, v)$, contrary to the previous quantum reasoning, does not naturally yield any analogue of the Heisenberg-type position-momentum uncertainty formulas, c.f. Eq. (35).

The cumulative identity $\text{Var}(x) \cdot [\text{Var}(u) + \text{Var}(v)] \geq \text{Cov}^2(x, v) + D^2$, reproduced in Ref. [13], does not convey any useful message about the diffusion process. It cannot be directly inferred from the Fisher functional $\mathcal{F}(\rho)$ which actually *was* the case in our previous, quantum discussion, e.g. where we have had $\text{Var}P = \text{Var}(mu) + \text{Var}(mv)$. For spatial diffusion processes, the latter identity is plainly nonexistent, since there is no diffusive analogue of the quantum momentum observable.

Let us mention an early attempt [17] to set an uncertainty principle for general diffusion processes. If we adopt our convention (natural boundary data), in view of $\langle u \rangle = 0$ and $v = b - u$, we have $\langle v \rangle = \langle b \rangle$.

For an arbitrary real constant $C \neq 0$, we obviously have: $[C \cdot (v - \langle v \rangle) + (x - \langle x \rangle)]^2 \geq 0$. The mean value of this auxiliary inequality reads:

$$C^2(\Delta v)^2 + 2C \cdot [\text{Cov}(x, b) + D] + (\Delta x)^2 \geq 0. \quad (42)$$

and is non-negative for all C , which enforces a condition

$$[D + \text{Cov}(x, b)]^2 - (\Delta v)^2 \cdot (\Delta x)^2 \leq 0. \quad (43)$$

Note that $Cov(x, v) = D + Cov(x, b)$, so we have in fact an alternative derivation of the previous indeterminacy relationship $Var(x) \cdot Var(v) \geq Cov^2(x, v)$ for the current velocity field.

In case of Smoluchowski processes, forward drifts are proportional to externally imposed force fields, typically through $b = F/m\beta$. Therefore the position-current velocity dispersion correlation is controlled by $Cov(x, F)$. For free Brownian motion (e.g. the Wiener process), we have $b = 0$, and hence $Cov(x, v) = D$.

To get a deeper insight into the "position-momentum indeterminacy issue" for diffusion processes, let us begin from a classic observation that, once we set $b = -2D\nabla\Phi$ with $\Phi = \Phi(x)$, a substitution:

$$\rho(x, t) \equiv \theta_*(x, t) \exp[-\Phi(x)] \quad (44)$$

with θ_* and Φ being real functions, converts the Fokker-Planck equation Eq. (41) into a generalized diffusion equation for θ_* :

$$\partial_t \theta_* = D\Delta\theta_* - \frac{\mathcal{V}(x)}{2mD} \theta_* \quad (45)$$

and its time adjoint

$$\partial_t \theta = -D\Delta\theta + \frac{\mathcal{V}(x)}{2mD} \theta \quad (46)$$

for a real function $\theta(x, t) = \exp[-\Phi(x)]$, where

$$\frac{\mathcal{V}(x)}{2mD} = \frac{1}{2} \left(\frac{b^2}{2D} + \nabla \cdot b \right) = D[(\nabla\Phi)^2 - \Delta\Phi]. \quad (47)$$

Let us note an obvious factorization property for the Fokker-Planck probability density:

$$\rho(x, t) = \theta(x, t) \cdot \theta_*(x, t) \quad (48)$$

which aligns with a quantum mechanical factorization formula $\rho = \psi^* \psi$, albeit presently realized in terms of two real functions θ and θ_* , instead of a complex conjugate pair.

Let us mimic basic steps, outlined in Eq. (34) for the complex factorization of ρ , but in terms of two real functions θ and θ_* . We have:

$$\mathcal{F}(\rho) = \frac{1}{D^2} \sigma_v^2 = \int dx (\theta\theta^*) \left[\frac{\theta'}{\theta} + \frac{\theta_*'}{\theta_*} \right]^2 = \quad (49)$$

$$4 \int dx \theta_*' \theta' + \int dx (\theta\theta_*) \left[\frac{\theta'}{\theta} - \frac{\theta_*'}{\theta_*} \right]^2.$$

Since the continuity equation $\partial_t \rho = -\nabla j$ is identically fulfilled by

$$j(x, t) = \rho(x, t)v(x, t) = D(\theta_* \nabla \theta - \theta \nabla \theta_*) \quad (50)$$

we obviously get:

$$\begin{aligned} \mathcal{F}(\rho) &= \mathcal{F}(\rho = \theta\theta_*) = 4 \int dx (\nabla\theta)(\nabla\theta^*) + \frac{1}{D^2} \langle v^2 \rangle \\ &= -\frac{2}{mD^2} \langle \mathcal{V} \rangle + \frac{1}{D^2} \langle v^2 \rangle, \end{aligned} \quad (51)$$

to be compared with the quantum mechanical result:

$$\begin{aligned} \mathcal{F}(\rho = |\psi|^2) &= 4 \int dx (\nabla\psi)(\nabla\psi^*) - \frac{1}{D^2} \langle v^2 \rangle \\ &= \frac{1}{D^2} [2\langle \mathcal{E} - \langle \Omega \rangle - \langle v^2 \rangle]. \end{aligned} \quad (52)$$

By reintroducing $\Omega = \mathcal{V}/m$ in Eq. (51):

$$\mathcal{F}(\rho = \theta\theta_*) = \frac{1}{D^2} [-2\langle \Omega \rangle + \langle v^2 \rangle] \quad (53)$$

we achieve a notational conformity with Eq. (52).

The major difference between the formulas Eq. (53) and Eq. (52), apart from the presence or absence of an additive term $\mathcal{E} \in \mathbb{R}$, is that a diffusive potential \mathcal{V} has a pre-determined functional form, Eq. (47). Our general restriction on \mathcal{V} , irrespective of whether this potential enters the Schrödinger or the generalized heat equations, is that it should be a continuous and bounded from below function [18]. In the diffusive case this demand guarantees that $\exp(-tH)$ with $H \equiv -D\Delta + (1/2mD)\mathcal{V}$ is a legitimate dynamical semigroup operator.

Let us add that

$$\begin{aligned} \mathcal{F}(\rho = \theta\theta_*) &= \frac{2}{mD^2} \left\langle \frac{mv^2}{2} - \mathcal{V} \right\rangle \\ &\Rightarrow \left\langle \frac{mv^2}{2} - \frac{mu^2}{2} - \mathcal{V} \right\rangle = 0 \end{aligned} \quad (54)$$

while

$$\begin{aligned} \mathcal{F}(\rho = |\psi|^2) &= \frac{2}{mD^2} \left[E - \left\langle \frac{mv^2}{2} + \mathcal{V} \right\rangle \right] \\ &\Rightarrow \left\langle \frac{mv^2}{2} + \frac{mu^2}{2} + \mathcal{V} \right\rangle = E. \end{aligned} \quad (55)$$

The variances of osmotic and current velocity fields are correlated, respectively, as follows

$$\rho = \theta\theta_* \implies m^2[(\Delta u)^2 - (\Delta v)^2] = 2m \left[\frac{m\langle v \rangle^2}{2} - \langle \mathcal{V} \rangle \right] \quad (56)$$

and

$$\begin{aligned}\rho = \psi\psi^* &\implies m^2[(\Delta u)^2 + (\Delta v)^2] \\ &= 2m\left[E - \frac{m\langle v \rangle^2}{2} + \langle \mathcal{V} \rangle\right] = (\Delta P)^2.\end{aligned}\quad (57)$$

Since $(\Delta u)^2 \geq D^2/\sigma^2$, in view of Eqs. (57) and (35) we readily arrive at the standard quantum indeterminacy relation for position and momentum observables $\Delta P \cdot \Delta X \geq mD$.

In case of diffusion-type processes we definitely encounter a non-standard situation. On the left-hand-side of Eq. (56), there appears a difference of variances for the current and osmotic velocity fields, instead of their sum, for example in Eq. (57). This expression is not necessarily positive definite, unless $\langle \mathcal{V} \rangle \leq 0$ for all times.

Let us make a guess that $\Delta u > \Delta v$ at least locally in time (in a finite time interval). Then the resulting expression

$$m^2(\Delta u)^2 = m^2\langle u^2 \rangle = 2m\left\langle \frac{mv^2}{2} - \mathcal{V} \right\rangle \equiv (\Delta p_u)^2 \geq \frac{m^2 D^2}{\sigma^2}, \quad (58)$$

as we already know, yields a dimensionally acceptable position-momentum indeterminacy relationship for diffusion-type processes,

$$\Delta x \cdot \Delta p_u \geq mD, \quad (59)$$

where $\Delta p_u > 0$ may be interpreted as the pertinent ‘‘momentum dispersion’’ measure. For free Brownian motion, we have $\mathcal{V} = 0$ and $v = -u$, hence Eq. (11) is recovered. Upon making an opposite guess (i.e. admit $\Delta v > \Delta u$, again, at least locally in time), in view of $\mathcal{F} \geq 1/\sigma^2$, we would have

$$m^2(\Delta v)^2 = m^2(\Delta u)^2 + 2m\left[\langle \mathcal{V} \rangle - \frac{m\langle v \rangle^2}{2}\right] \equiv (\Delta p_v)^2 \geq \frac{m^2 D^2}{\sigma^2} \quad (60)$$

and thus

$$\Delta x \cdot \Delta p_v \geq mD \quad (61)$$

would ultimately arise.

The above two indeterminacy options (59) and (61) are a consequence of a possibly indefinite sign for a difference $\Delta u - \Delta v$ of standard deviations, in the course of a diffusion process. This sign issue seems to be a local in time property and may not persist in the asymptotic (large time) regime. We shall give an argument towards the non-existence of a fixed positive lower bound for the joint position-current velocity uncertainty measure in the vicinity of an asymptotic stationary solution of the involved Fokker-Planck equation.

In case of Smoluchowski diffusion processes we may take for granted that they asymptotically approach [8, 10] unique stationary solutions, for which the current velocity v identically vanishes. Then $\Delta v = 0$ as well, while $0 < \text{Var}(x) < \infty$ (e.g. Δx stays finite).

In view of Eq. (54), an asymptotic value of the strictly positive Fisher functional \mathcal{F} equals $-(2/mD^2)\langle \mathcal{V} \rangle > 0$. Accordingly, to secure $\mathcal{F} > 0$, an expectation value of \mathcal{V} with respect to the stationary probability density must be negative, even under an assumption that \mathcal{V} is bounded from below.

Consequently, in the large time asymptotic case, we surely have $(\Delta u)^2 > (1/\sigma^2) > (\Delta v)^2$ and $\Delta v \rightarrow 0$, while σ has a finite limiting value (an exception is free Brownian motion when σ diverges). The validity of the above argument can be checked by inspection, after invoking an explicit solution for the Ornstein-Uhlenbeck process [8, 10].

Thus, $\Delta x \cdot \Delta p_v \geq mD$ does not hold true in the vicinity of the asymptotic solution. On the contrary, $\Delta x \cdot \Delta p_u \geq mD$ is universally valid.

4. Entropy methods: Thermodynamical patterns of behaviour in diffusion-type processes

4.1. Thermodynamical hierarchy

Diffusion processes stand for an approximate description of (macro)molecules whose motion is induced by a thermal environment. As such they quantify the dynamics of non-equilibrium thermodynamical systems.

The following hierarchy of thermodynamical systems is adopted below: *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. We keep in mind a standard textbook wisdom that all isolated systems evolve to the state of equilibrium in which the entropy reaches its maximal value. An approach towards equilibrium is here interpreted as an approach towards most disorderly state.

Our further attention will be focused on non-isolated, albeit *closed*, random systems and their somewhat different asymptotic features. Assuming the natural boundary data [10, 21, 22], we shall introduce basic thermodynamical concepts and recall the Helmholtz extremum principle for an intrinsically random motion. Thermodynamic function(al)s like internal energy, Helmholtz free energy and entropy will be inferred, through suitable averaging, from a priori prescribed time-dependent continuous probability densities.

A concise resumé of non-equilibrium thermodynamics of

closed systems comprises the 1st law $\dot{U} = \dot{Q} + \dot{W}$ and the I^{nd} law $\dot{S} = \dot{S}_{int} + \dot{S}_{ext}$, where $\dot{S}_{int} \geq 0$ and $\dot{S}_{ext} = \dot{Q}/T$ (c.f. [19, 20]). We are fully aware that not all objects involved (e.g. Q) can be viewed as legitimate analogues of thermodynamic functions. Nonetheless, in the forthcoming discussion, the heat exchange and work time rates are always well defined and an issue of “imperfect differentials” is consistently bypassed.

Thermodynamical extremum principles are usually invoked in connection with the large time behavior of irreversible processes. Among a number of standard principles, for reference, 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 $F = U - TS$ is preferred in the course of system evolution in time, and there holds $\dot{F} = -T\dot{S}_{int} \leq 0$.

4.2. Thermodynamics of random phase-space motions

Let us consider a phase-space diffusion process governed by the Langevin equation $m\ddot{x} + m\gamma\dot{x} = -\nabla V(x, t) + \xi(t)$, with standard assumptions about the properties of white noise: $\langle \xi(t) \rangle = 0$, $\langle \xi(t)\xi(t') \rangle = \sqrt{2m\gamma k_B T} \delta(t - t')$. Accordingly, the pertinent phase-space density $w = w(x, u, t)$ is a solution of the Fokker-Planck-Kramers equation with suitable initial data:

$$\frac{\partial}{\partial t} w(x, u, t) = \quad (62)$$

$$\left[-\frac{\partial}{\partial x} u + \frac{\partial}{\partial u} \left(\gamma u + \frac{1}{m} \nabla V(x, t) \right) + \frac{\gamma k_B T}{m} \frac{\partial^2}{\partial u^2} \right] w$$

Let us define the Shannon entropy $\mathcal{S} = \mathcal{S}(t)$ of a continuous probability distribution in the phase-space of the system:

$$\mathcal{S}(t) = - \int (w \ln w) dx du = -\langle \ln w \rangle \quad (63)$$

(For dimensional reasons we should insert a factor h with physical dimensions of the action under the logarithm, i.e. use $\ln(hw)$ instead of $\ln w$, but since we shall ultimately work with time derivatives, this step may be safely skipped.)

We define an internal energy U of the diffusion-type stochastic process as follows: $U = \langle E \rangle$, where $E = E(x, u, t) = \frac{mu^2}{2} + V(x, t)$. Then, the 1st law of thermodynamics takes the form

$$\dot{Q} + \dot{W} = \dot{U} \quad (64)$$

where $\dot{W} \equiv \langle \partial_t V \rangle$ is interpreted as the work externally performed upon the system. (For future reference we would like to stress the particular importance of the time-dependent work term in quantum theory.)

Furthermore, let us introduce an obvious analogue of the Helmholtz free energy:

$$F \equiv \langle E + k_B T \ln w \rangle = U - TS \quad (65)$$

so that

$$\dot{F} - \dot{W} = \dot{Q} - T\dot{S} = -T\dot{S}_{int} \leq 0. \quad (66)$$

The above result is a direct consequence of the Kramers equation. Under suitable assumptions concerning the proper behavior of $w(x, u, t)$ at x, u integration boundaries (sufficiently rapid decay at infinities) we have [23] $\dot{Q} = \gamma(k_B T - \langle mu^2 \rangle)$ and $\dot{S} = \gamma \left[\frac{k_B T}{m} \langle \left(\frac{\partial \ln w}{\partial u} \right)^2 \rangle - 1 \right]$.

In view of $(1/T)\dot{Q} = \dot{S}_{ext}$, the I^{nd} law readily follows:

$$\dot{Q} - k_B T \dot{S} = \quad (67)$$

$$-\frac{\gamma}{m} \left\langle \left(k_B T \frac{\partial \ln w}{\partial u} + mu \right)^2 \right\rangle = -T\dot{S}_{int} \leq 0$$

We denote $S \equiv k_B \mathcal{S}$ and so arrive at $\dot{Q} \leq T\dot{S}$. As a byproduct of the discussion we have $\dot{F} \leq \dot{W}$.

For time-independent $V = V(x)$, the extremum principle pertains to minimizing the Helmholtz free energy F in the course of random motion:

$$\dot{F} = \dot{Q} - T\dot{S} \equiv -T\dot{S}_{int} \leq 0 \quad (68)$$

The preceding discussion encompasses both forced and unforced (free) Brownian motion. When $V(x) \equiv 0$, then no asymptotic state of equilibrium (represented by a probability density) is accessible and the motion is sweeping. In the forced case, we realize that $w_*(x, u) = \frac{1}{2} \exp \left[-\frac{E(x, u)}{k_B T} \right]$ is a stationary solution of the Kramer equation. Therefore, we may expect that the dynamics actually relaxes to this, a (unique) stationary state [10] $w \rightarrow w_*$. Obviously, w_* is non-existent in the case of free Brownian motion.

4.3. Thermodynamics of Smoluchowski processes

Analogous thermodynamical features are encountered in spatial random motions like standard Smoluchowski processes and their generalizations. Given a probability density $\rho(x, t)$ solution of a Fokker-Planck equation

$\partial_t \rho = D\Delta\rho - \nabla \cdot (b\rho)$, the related Shannon entropy $\mathcal{S}(t) = -\langle \ln \rho \rangle$ is typically not a conserved quantity and, with boundary restrictions that $\rho, v\rho, b\rho$ vanish at spatial infinities or finite integration interval borders, various equivalent forms of the balance equation follow. We select, [8, 22]:

$$D\dot{\mathcal{S}} = \langle v^2 \rangle - \langle b \cdot v \rangle. \quad (69)$$

A thermodynamic formalism for Smoluchowski processes is straightforward. We pass to time-independent drift fields and set $b = \frac{f}{m\beta}$, adjusting dimensional constants. Exploiting $j \equiv v\rho$, $f = -\nabla V$ and setting $D = k_B T/m\beta$, we give Eq. (69) the conspicuous form of

$$\dot{\mathcal{S}} = \dot{\mathcal{S}}_{int} + \dot{\mathcal{S}}_{ext} \quad (70)$$

where $k_B T \dot{\mathcal{S}}_{int} \equiv m\beta \langle v^2 \rangle \geq 0$ stands for the entropy production, while $k_B T \dot{\mathcal{S}}_{ext} = \dot{Q} = -\int f \cdot j dx = -m\beta \langle b \cdot v \rangle$ (when negative, which is not necessarily the case) may be interpreted as the heat dissipation rate. In view of $\dot{Q} = -\int f \cdot j dx$, there is a definite power release involved. Notice that because of $T\dot{\mathcal{S}} \equiv k_B T \dot{\mathcal{S}}$, we have

$$T\dot{\mathcal{S}}_{int} = T\dot{\mathcal{S}} - \dot{Q} \geq 0 \Rightarrow T\dot{\mathcal{S}} \geq \dot{Q}. \quad (71)$$

In view of $j = \rho v = \frac{\rho}{m\beta} [f - k_B T \nabla \ln \rho] \equiv -\frac{\rho}{m\beta} \nabla \Psi$ i.e. $v = -(1/m\beta) \nabla \Psi$ and $f = -\nabla V$, we can introduce

$$\Psi = V + k_B T \ln \rho \quad (72)$$

whose mean value stands for the Helmholtz free energy of the random motion

$$F \equiv \langle \Psi \rangle = U - TS. \quad (73)$$

Here $S \equiv k_B \mathcal{S}$ and an internal energy is $U = \langle V \rangle$. Assuming that ρ and $\rho V v$ vanish at the integration volume boundaries we get

$$\dot{F} = \dot{Q} - T\dot{\mathcal{S}} = -(m\beta) \langle v^2 \rangle = -k_B T \dot{\mathcal{S}}_{int} \leq 0. \quad (74)$$

As long as there is positive entropy production, the Helmholtz free energy decreases as a function of time towards its minimum. If there is none, the Helmholtz free energy remains constant.

With external forcing reintroduced, the regime $\dot{\mathcal{S}} = 0$ is of particular interest. This occurs necessarily if the diffusion current vanishes and one encounters the state of equilibrium with an invariant density ρ_* . Then, $b = u = D \nabla \ln \rho_*$ and $-(1/k_B T) \nabla V = \nabla \ln \rho_*$ implies $\rho_* = \frac{1}{Z} \exp[-V/k_B T]$. Hence $\Psi_* = V + k_B T \ln \rho_*$ and therefore $\langle \Psi_* \rangle = -k_B T \ln Z \equiv F_*$, with $Z = \int \exp(-V/k_B T) dx$, is a minimum of the Helmholtz free energy F .

For free Brownian motion there is no invariant density and we have $V = 0 = b$, while $v = -D \nabla \ln \rho = -u$, and therefore $\dot{Q} = 0 \Rightarrow \dot{F} = -T\dot{\mathcal{S}} = -m\beta D^2 \int [\frac{(\nabla \rho)^2}{\rho}] dx \leq 0$.

5. Entropy methods in Schrödinger picture quantum dynamics

A pure state of the quantum system and its Schrödinger picture dynamics are normally regarded in conjunction with the notion of a thermodynamically *isolated* quantum system. A standard tool in the thermal context would be the von Neumann entropy notion which is known to vanish on pure states and to be insensitive to the unitary quantum evolution. In the below, we shall pay attention to the Shannon entropy properties in the quantum context [8], to demonstrate that a number of essentially thermodynamical features are encoded in the apparently non-thermodynamical regime of Schrödinger picture quantum dynamics.

We come back to the Schrödinger evolution of pure states in $L^2(\mathbb{R})$. We employ the natural boundary data (actually, the Dirichlet boundary conditions are sufficient) and the vanishing of various expressions at integration boundaries is implicit in all averaging procedures which follow. 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:

$$\partial_t \rho = D\Delta\rho - \nabla \cdot (b\rho) \quad (75)$$

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

$$D\dot{\mathcal{S}} = \langle v^2 \rangle - \langle b \cdot v \rangle \equiv D(\dot{\mathcal{S}}_{int} + \dot{\mathcal{S}}_{ext}) \quad (76)$$

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

$$\dot{\mathcal{S}}_{int} = \dot{\mathcal{S}} - \dot{\mathcal{S}}_{ext} = (1/D) \langle v^2 \rangle \geq 0 \Rightarrow \dot{\mathcal{S}} \geq \dot{\mathcal{S}}_{ext}. \quad (77)$$

To address an analogue 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 (nor physical intuitions about) the temperature for quantum systems in their pure states (for large molecules, like fullerenes or the likes, the notion of an 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 [24].

We formally introduce

$$k_B T_0 \equiv \hbar \omega_0 \equiv m c^2 \quad (78)$$

and thence

$$D = \hbar/2m \equiv k_B T_0/m\beta_0 \quad (79)$$

with $\beta_0 \equiv 2\omega_0 = 2mc^2/\hbar$, and so arrive at the dimensionally acceptable identity

$$k_B T_0 \dot{S}_{ext} = \dot{Q}. \quad (80)$$

In view of:

$$v = \nabla s = b - u = \nabla(s + D \ln \rho) - D \nabla \ln \rho \equiv \quad (81)$$

$$-\frac{1}{m\beta} \nabla(V + k_B T_0 \ln \rho) \equiv -\frac{1}{m\beta_0} \nabla \Psi,$$

where the time-dependent potential

$$V = V(x, t) \equiv -m\beta_0(s + D \ln \rho) \quad (82)$$

is defined to stay in notational conformity with the standard Smoluchowski process (Brownian motion in a conservative force field [8]) definition $b = -\nabla V/m\beta_0$, we finally get

$$-m\beta \langle \dot{s} \rangle \equiv \langle \dot{V} \rangle - T_0 \dot{S} \implies F = U - TS, \quad (83)$$

where $U = \langle V \rangle$ and $F = \langle \dot{V} \rangle$.

Remembering the explicit time dependence of $b(x, t) = -(1/m\beta_0)\nabla V(x, t)$, we arrive at the direct analogue of the 1st law of thermodynamics in the present quantum context:

$$\dot{U} = \langle \partial_t V \rangle - m\beta_0 \langle b v \rangle = \dot{W} + \dot{Q}. \quad (84)$$

The term corresponding to the previous “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

$$-\frac{d}{dt} \langle s \rangle = -\langle v^2 \rangle - \langle \partial_t s \rangle \implies \dot{F} = -T_0 \dot{S}_{int} + \dot{W} \quad (85)$$

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

In view of Eq. (29), in the thermodynamical description of the quantum motion, we encounter a never vanishing constant work term

$$\dot{W} = m\beta_0 \mathcal{E} = \beta_0 \langle \dot{H} \rangle. \quad (86)$$

The quantum version of the Helmholtz-type extremum principle reads:

$$\dot{F} - m\beta_0 \mathcal{E} = -T_0 \dot{S}_{int} \leq 0. \quad (87)$$

It is instructive to notice that

$$T_0 \dot{S}_{int} = T_0 \dot{S} - \dot{Q} \geq 0 \iff \dot{Q} \leq T_0 \dot{S} \quad (88)$$

goes in parallel with

$$\dot{F} \leq \dot{W} = \beta_0 \langle \dot{H} \rangle. \quad (89)$$

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

For negative eigenvalues, the “work” term corresponds to what we might possibly call the “work performed *by* the system” (upon its, here hypothetical, surroundings). Then \dot{F} is negative and F has a chance to attain a minimum.

Since bounded from below Hamiltonians can be replaced by positive operators, we may in principle view $m\beta_0 \mathcal{E} = \beta_0 \langle \dot{H} \rangle$ 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 temporal patterns of behavior, normally associated with the non-equilibrium thermodynamics of *closed* irreversible systems, somewhat surprisingly have been faithfully reproduced in the quantum Schrödinger picture evolution which is known to be time-reversible. Nonetheless, we have identified direct analogues of the 1st and the II^{nd} laws of thermodynamics, together with the involved notions of $\dot{S}_{int} \geq 0$ and $\dot{S}_{ext} = (1/T_0)\dot{Q}$. One should obviously remember about the pre-selected sense of time $t \in \mathbb{R}^+$, that was employed in our discussion.

An asymptotic $t \rightarrow \infty$ behavior of the quantum motion is controlled by the analogue of the II^{nd} law:

$$\dot{F} - \dot{W} = -m\beta_0 \frac{d}{dt} \left(\langle s \rangle + \mathcal{E} t \right) = -T_0 \dot{S}_{int} \leq 0. \quad (90)$$

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

Let us recall that in classical non-equilibrium thermodynamics, the so-called minimum entropy production principle [19] 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

$$\frac{d}{dt} \dot{S}_{int} < 0. \quad (91)$$

The quantum motion obviously 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. 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 in very special cases.

Since the work term is a constant of quantum motion, we have :

$$\dot{F} + T_0 \dot{S}_{int} = m\beta_0 \mathcal{E} \implies \ddot{F} = -T_0 \frac{d}{dt} \dot{S}_{int}, \quad (92)$$

which formally reproduces the temporal behavior characteristic to Smoluchowski diffusion processes, c.f. Eq.(74). There are however “speed” properties which are special to the quantum dynamics and have no dissipative counterpart.

The above time rate formula Eq. (92), which is common to both quantum and diffusive motions scenarios, clearly is consistent with the correlation of a minimum of \dot{F} with a maximum of the \dot{S}_{int} . However, we have as well allowed the reverse scenario—i.e., that a maximum of \dot{F} may arise in conjunction with a minimum of \dot{S}_{int} . More complicated, e.g. oscillating, forms of the entropy production-Helmholtz free energy interplay cannot be a priori excluded in the quantum case.

Remembering that $T_0 \dot{S}_{int} = m\beta_0 \langle v^2 \rangle$ and exploiting the total mean energy formula, Eqs. (29) and (55), we can identify the respective “speeds” in conjunction with the Schrödinger picture quantum motion. In view of Eq. (92), the pertinent time rates stay in a definite *negative feedback* relationship:

$$\ddot{F} = +\beta_0 \frac{d}{dt} \left(m\langle u^2 \rangle + 2\langle \mathcal{V} \rangle \right) = -m\beta_0 \frac{d}{dt} \left\langle v^2 \right\rangle. \quad (93)$$

This observation should be contrasted with the behavior induced by diffusion-type processes, where $Td\dot{S}_{int}/dt = m\beta d\langle v^2 \rangle/dt$. Now, c.f. Eq.(54), we have

$$\ddot{F} = -\beta \frac{d}{dt} \left(m\langle u^2 \rangle + 2\langle \mathcal{V} \rangle \right) = -m\beta \frac{d}{dt} \left\langle v^2 \right\rangle \quad (94)$$

which really makes a difference (in view of the sign inversion in the functional expression for \ddot{F}). There is no feedback anymore.

6. Outlook

We have discussed in detail the uncertainty/indeterminacy measures that can be associated with time-evolving probability distributions of two basic origins. We infer them for diffusion-type processes and Schrödinger picture quantum dynamics.

There are deep analogies between the quantum dynamics in the Madelung representation and the classical Fokker-Planck description of diffusion processes. We have exploited them in two complementary ways.

First, the position-momentum indeterminacy relations for diffusion processes were deduced by a modification of major steps in the quantum procedure (compare, e.g., Eqs. (34) and (49)). Second, we have faithfully reproduced in the quantum setting major thermodynamic relations between heat, work and free energy by adopting to the quantum formalism a number of derivations that were consistently tested in the context of the Smoluchowski diffusion processes.

The minor surprise is that major properties of a non-isolated but *closed* (we use the terminology of Ref. [19]) random system have been directly reproduced for the quantum system, which is normally considered as thermally *isolated*. Our analysis allows us to attribute to the quantum system in a pure state the major properties of a non-isolated but *closed* thermodynamical system. The major difference between the quantum and diffusive behavior, if restricted to thermodynamically motivated quantities, can be read out from the rate formulas Eqs. (93) and (94).

To avoid misunderstandings, let us recall that in the classical situation work, heat and free energy notion have well defined meanings. Work is interpreted as an energy due to macroscopic degrees of freedom which perform an ordered motion and are perceived as a source of work. Heat is perceived as a thermal energy, while free energy is the maximal amount of energy which can be extracted as work. A physical meaning for these three concepts is definitely reliant on a differentiation between the total system, the

investigated physical subsystem and the sources of work and heat (environment).

We cannot propose a clean physical picture for deceptively thermodynamical patterns of behavior associated with quantum dynamics. At the moment, we have no satisfactory explanation of a possible physical meaning for the “work performed upon” and “work performed by” the system, nor for heat, for an isolated quantum system. Albeit we have demonstrated that this system shows patterns of behavior that are characteristic for non-isolated *closed* thermodynamical systems, in parallel with those for diffusion-type processes.

On formal grounds, the present paper exploits properties of $-\langle \ln \rho \rangle$ and of $\langle (\nabla \ln \rho)^2 \rangle$, while admitting the time-dependence of ρ . The functional $\langle (\nabla \ln \rho)^2 \rangle$ plays the major role in all our considerations and is responsible for the emergence of indeterminacy relations, both in the diffusive and quantum motions.

The final outcomes of the discussion heavily rely on the assumed factorization of the probability density ρ . It is accomplished either in terms of two real (time-conjugate) functions $\rho = \theta \cdot \theta_*$, or in terms of two complex conjugate functions $\rho = \psi \cdot \psi^*$.

Appendix

Since the employed thermodynamic formalism may look strange for quantum theory practitioners, let us exemplify the previous observations by invoking simple quantum motion cases.

Case 1: Free evolution

Let us consider the probability density in one space dimension:

$$\rho(x, t) = \frac{\alpha}{[\pi(\alpha^4 + 4D^2t^2)]^{1/2}} \exp\left(-\frac{x^2\alpha^2}{\alpha^4 + 4D^2t^2}\right) \quad (95)$$

and the phase function (we recall that $\psi = \rho^{1/2} \exp(is/2D)$ is adopted):

$$s(x, t) = \frac{2D^2x^2t}{\alpha^4 + 4D^2t^2} - D^2 \arctan\left(-\frac{2Dt}{\alpha^2}\right) \quad (96)$$

which determine a free wave packet solution of the Schrödinger equation with the choice of $\mathcal{V} \equiv 0$ and initial data $\psi(x, 0) = (\pi\alpha^2)^{-1/4} \exp(-x^2/2\alpha^2)$.

One can readily deduce that

$$D\langle \dot{S} \rangle_{int} = \langle v^2 \rangle = \frac{8D^4t^2}{\alpha^2(\alpha^4 + 4D^2t^2)} \quad (97)$$

has an initial value 0 and attains a maximum $2D^2/\alpha^2$ in the large time limit. Moreover, there holds

$$\mathcal{E} = \frac{1}{2}(\langle v^2 \rangle + \langle u^2 \rangle) = \frac{D^2}{\alpha^2}, \quad (98)$$

where $\langle u^2 \rangle = (2D^2\alpha^2)/(\alpha^4 + 4D^2t^2)$. Clearly, an initial value of $\langle u^2 \rangle$ is $2D^2/\alpha^2$, while 0 stands for its asymptotic limit.

The feedback relationship Eq. (92) sets a link between the speed at which the entropy production attains its maximum and the speed at which \dot{F} decreases towards its minimal value $\dot{F}^{min} = m\beta_0\mathcal{E} - T_0\dot{S}_{int}^{max}$, (compare e.g. Eq. (87)).

Case 2: Steady state in a harmonic potential

We choose a harmonic potential $\mathcal{V} = \frac{1}{2}\omega^2x$ in the Schrödinger equation (23) and consider its solution with the probability density:

$$\rho(x, t) = \left(\frac{\omega}{2\pi D}\right)^{1/2} \exp\left[-\frac{\omega}{2D}(x - q(t))^2\right] \quad (99)$$

and the phase function:

$$s(x, t) = (1/m)[xp(t) - (1/2)p(t)q(t) - mD\omega t], \quad (100)$$

where the classical harmonic dynamics with particle mass m and frequency ω is involved such that $q(t) = q_0 \cos(\omega t) + (p_0/m\omega) \sin(\omega t)$ and $p(t) = p_0 \cos(\omega t) - m\omega q_0 \sin(\omega t)$.

We have here $v = \nabla s = p(t)/m$ and therefore:

$$D\langle \dot{S} \rangle_{in} = \frac{p^2(t)}{m^2} \quad (101)$$

so that in view of $E/m = \mathcal{E} = p_0^2/2m^2 + \omega x_0^2/2 + D\omega$ and Eq. (87), remembering that $D = k_B T/m\beta_0 = \hbar/2m$, we get

$$\begin{aligned} \dot{F} &= \omega k_B T_0 + m\beta_0 \left[\frac{p_0^2}{2m^2} + \omega \frac{x_0^2}{2} - \frac{p^2(t)}{m^2} \right] \\ &= \omega k_B T_0 + \beta_0 \left[m\omega \frac{x^2(t)}{2} - \frac{p^2(t)}{2m} \right]. \end{aligned} \quad (102)$$

It is interesting to observe that the actual behavior of $\dot{F}(t)$ depends on a difference of the potential and kinetic energies of the classical oscillator.

Case 3: Stationary state

Let us make a brief comment on the case of stationary states. We take a harmonic oscillator ground state as a reference. The entropy production vanishes since $v = 0$.

We have $\dot{F} = m\beta_0\mathcal{E}_0 = \beta_0 E_0$, where $E_0 = \hbar\omega/2 = mD\omega$. Therefore

$$F(t) = (k_B T_0)\omega t + \text{const} \quad (103)$$

and F is a monotonically growing function.

We recall that presently $\dot{F} = \dot{W} = \beta_0 E_0$. The never ceasing time rate of “work performed upon the surrounding” needs to be kept in memory as a distinguishing feature of the quantum motion.

Because of $-m\beta_0\langle s \rangle = F$ and $\langle s \rangle = s$, we have

$$s(t) = -D\omega t + \text{const}, \quad (104)$$

as should be the case in the exponent of the stationary wave function $\psi = \rho^{1/2} \exp(is/2D)$. Indeed, $-E_0 t/2D = -\omega t/2 = s(t)/2D - \text{const}$.

References

- [1] C.E. Shannon, Bell Syst. Techn. J. 27, 379 (1948)
- [2] C.E. Shannon, Bell Syst. Techn. J. 27, 623 (1948)
- [3] T.M. Cover, J.A. Thomas, Elements of Information Theory (Wiley, New York, 1991)
- [4] M. Ohya, D. Petz, Quantum Entropy and Its use (Springer-Verlag, Berlin, 1993)
- [5] A.J. Stam, Inform. Control 2, 101 (1959)
- [6] A. Dembo, T. Cover, IEEE T. Inform. Theory 37, 1501 (1991)
- [7] K. Sobczyk, Mechanical Systems and Signal Processing 15, 475 (2001)
- [8] P. Garbaczewski, J. Stat. Phys. 123, 315 (2006)
- [9] P. Garbaczewski, Applied Math and Information Science, 1, 1 (2007)
- [10] M.C. Mackey, M. Tyran-Kamińska, Physica A 365, 360 (2006)
- [11] R. Fürth, Z. Phys. 81, 143 (1933)
- [12] F. Illuminati, L. Viola, J. Phys. A 28, 2953 (1995)
- [13] S. Golin, J. Math. Phys. 26, 2781 (1985)
- [14] I. Białyński-Birula, J. Mycielski, Commun. Math. Phys. 44, 129 (1975)
- [15] P. Garbaczewski, Rep. Math. Phys. 56, 153 (2005)
- [16] M.J.W. Hall, Phys. Rev. A 62, 012107 (2000)
- [17] E.I. Verriest, D-R. Shin, Int. J. Theor. Phys. 32, 333 (1993)
- [18] J-C. Zambrini, J. Math. Phys. 27, 2307 (1986)
- [19] P. Glansdorf, I. Prigogine, Thermodynamic Theory of Structure, Stability and Fluctuations (Wiley, New York, 1971)
- [20] D. Kondepudi, I. Prigogine, Modern Thermodynamics (Wiley, New York, 1998)
- [21] H. Hasegawa, Progr. Theor. Phys. 57, 1523 (1977)
- [22] H. Qian, Phys. Rev. E 65, 021111 (2002)
- [23] K. Shizume, Phys. Rev. E 52, 3495 (1995)
- [24] L. de Broglie, La Thermodynamique de la particule isolée (Gauthier-Villars, Paris, 1964)