Modular Schrödinger equation and dual "time arrows"

Piotr Garbaczewski (University of Opole, Poland)

Modular nonlinear Schrödinger equation

$$i\hbar\partial_t\psi = \left[-\frac{\hbar^2}{2m}\Delta + V\right]\psi + \left[\kappa\,\frac{\hbar^2}{2m}\,\frac{\Delta|\psi|}{|\psi|}\right]\psi\,,$$

$\psi(x,t)$ complex, $|\psi| \doteq (\psi^*\psi)^{1/2}$, $V(x)$ real, $\kappa \geq 0$.

(The standard NLS interaction entry would read $[\kappa|\psi|^2]$)

If $\kappa > 0$, the pertinent nonlinear dynamics preserves the $L^2(R^n)$ norm of any initially given ψ, but not the Hilbert space scalar product (ψ, ϕ) of two different, initially given ψ and ϕ. The dynamics is non-unitary in $L^2(R^n)$; unitarity is restored if $\kappa = 0$.

For all $\kappa \geq 0$

$$\partial_t\rho = -\nabla \cdot j$$

where $\rho = \psi^*\psi$ and

$$j = (\hbar/2mi)(\psi^*\nabla\psi - \psi\nabla\psi^*)$$

. We consider normalized solutions only, which sets a standard form of $j \doteq \rho \cdot v$, where

$$v = (\hbar/2mi)[(\nabla\psi/\psi) - (\nabla\psi^*/\psi^*)] \doteq (1/m)\nabla s$$

is regarded as a gradient velocity field and $\rho(x,t) = |\psi|^2(x,t)$ is a probability density on R^n.

Lagrangian formalism

- stationary action principle $\delta I[\psi, \psi^*] = 0$

- functional of ψ-functions, their space and time derivatives, including complex conjugates:

$$I[\psi, \psi^*] = \int_{t_1}^{t_2} L(t) dt$$

where $L(t) = \int \mathcal{L}(x,t)\, dx$, (we leave unspecified, possibly infinite, integration volume).

Pedestrian functional calculus

$$\delta\mathcal{L}/\delta\psi \equiv \partial\mathcal{L}/\partial\psi - \sum_i \nabla_i [\partial\mathcal{L}/\partial(\nabla_i \psi)]$$

One ends up with the Euler-Lagrange equations:

$$\partial_t[\partial\mathcal{L}/\partial(\partial_t\psi^*)] = \delta\mathcal{L}/\delta\psi^*$$

$$\partial_t[\partial\mathcal{L}/\partial(\partial_t\psi)] = \delta\mathcal{L}/\delta\psi$$

If we properly specify the Lagrangian density $\mathcal{L} \doteq \mathcal{L}_\kappa$:

$$\mathcal{L}_\kappa(x,t) = \frac{i\hbar}{2}[\psi^*(\partial_t\psi) - \psi(\partial_t\psi^*)] - \frac{\hbar^2}{2m}\nabla\psi \cdot \nabla\psi^* - V(x)\,\psi\,\psi^* +$$

$$\kappa\,\frac{\hbar^2}{8m}\left[\frac{\nabla\psi^*}{\psi^*} + \frac{\nabla\psi}{\psi}\right]^2 \psi\,\psi^*\,.$$

the stationary action principle yields a **pair** of adjoint modular equations which comprise the previous one in conjunction with its complex conjugate:

$$-i\hbar\partial_t\psi^* = \left[-\frac{\hbar^2}{2m}\Delta + V\right]\psi^* + \left[\kappa\,\frac{\hbar^2}{2m}\,\frac{\Delta|\psi|}{|\psi|}\right]\,\psi^*\,.$$

The gradient assumption

$$v = v(x,t) = (1/m)\nabla s$$

plus the familiar Madelung substitution:

$$\psi = |\psi| \, \exp(is/\hbar)$$

where $|\psi|^2 = \rho$. yield the Lagrangian density

$$\mathcal{L}_\kappa(x,t) = -\rho \left[\partial_t s + \frac{m}{2}(u^2 + v^2) \, + V(x) \, - \kappa \, \frac{m}{2} \, u^2 \right]$$

with

$$u(x,t) \doteq (\hbar/2m) \, \nabla \rho / \rho$$

Here, $\delta I[\rho, s] = 0$ gives rise to

$$\partial_t \rho = -\nabla(\rho \, \cdot v)$$

$$\partial_t s + \frac{1}{2m}(\nabla s)^2 + V + (1-\kappa) \, Q = 0 \, ,$$

where, in view of $|\psi| = \rho^{1/2}$,

$$Q = Q(x,t) \doteq -\frac{\hbar^2}{2m} \, \frac{\Delta \rho^{1/2}}{\rho^{1/2}} = -\frac{\hbar^2}{4m} \, \left[\frac{\Delta \rho}{\rho} - \frac{1}{2} \left(\frac{\nabla \rho}{\rho} \right)^2 \right] \, .$$

The modular Schrödinger equation takes the form:

$$i\hbar \partial_t \psi = [-(\hbar^2/2m)\Delta + V]\psi - \kappa Q \, \psi \, .$$

Hamiltonian formalism

A symplectic structure; given ψ, ψ^* and

$$\pi_\psi = \partial\mathcal{L}/\partial(\partial_t\psi) = (i\hbar/2)\psi^*$$
$$\pi_{\psi^*} = \partial\mathcal{L}/\partial(\partial_t\psi^*) = -(i\hbar/2)\psi$$

The subsequent Legendre-type transformation defines the Hamiltonian density:

$$\mathcal{H}_\kappa = \pi_\psi \cdot \partial_t\psi + \pi_{\psi^*} \cdot \partial_t\psi^* - \mathcal{L}_\kappa =$$

$$\frac{\hbar^2}{2m}\nabla\psi \cdot \nabla\psi^* + \left[V - \kappa\,\frac{\hbar^2}{8m}\left(\frac{\nabla\psi^*}{\psi^*} + \frac{\nabla\psi}{\psi}\right)^2\right]\psi\,\psi^* =$$

$$\rho\left[\frac{m}{2}\,v^2\ + V + (1-\kappa)\,\frac{m}{2}\,u^2\right] = \pi_s\partial_t s - \mathcal{L}_\kappa$$

where, this time with respect to the polar fields $\rho(x,t)$ and $s(x,t)$, we have:

$$\pi_\rho = \partial\mathcal{L}/\partial(\partial_t\rho) = 0$$
$$\pi_s = \partial\mathcal{L}/\partial(\partial_t s) = -\rho$$

$$H_\kappa(t) = \int \mathcal{H}_\kappa(x,t)\,dx$$
$$L(t) = -\langle\partial_t s\rangle - H_\kappa(t)\,,$$

where, in view of $\int \rho\,dx = 1$, we set $\langle\partial_t s\rangle = \int \rho\,\partial_t s\,dx$.

A proper behavior of $\rho \Longrightarrow \langle Q\rangle \doteq \int Q\,\rho\,dx = +(m/2)\langle u^2\rangle > 0$. On dynamically admitted fields $\rho(x,t)$ and $s(x,t)$, we have

$$L(t) \equiv 0 \Leftrightarrow \langle\partial_t s\rangle = -H_\kappa$$

Poisson bracket of $A = \int \mathcal{A}(x,t)\, dx$ and $B = \int \mathcal{B}(x,t)\, dx$.

$$\{A,\, B\} = -\frac{i}{\hbar} \int dx \left(\frac{\delta A}{\delta \psi} \frac{\delta B}{\delta \psi^*} - \frac{\delta A}{\delta \psi^*} \frac{\delta B}{\delta \psi} \,.\right)$$

Identify $A \equiv \psi(x,t)$ and $B \equiv H_\kappa(t) \longrightarrow$

$$\partial_t \psi = \{\psi,\, H_\kappa\}$$

Set $A \equiv \psi^*$

$$\partial_t \psi^* = \{\psi^*,\, H_\kappa\}\,.$$

We recall e. g. that $\dot{\pi}_\psi = -\delta H_\kappa / \delta \psi$ while $\dot{\psi} = \delta H_\kappa / \delta \psi$.

The time dependence of $H_\kappa(t)$ is realized only through the canonical fields, the Hamiltonian surely is a constant of motion. Thence $\langle \partial_t s \rangle$ as well.

The polar decomposition

$$\psi = \rho^{1/2} \exp(is/\hbar)\ ,\ \psi^* = \rho^{1/2} \exp(-is/\hbar)$$

preserves a symplectic structure.

$$\{A, B\} \doteq \{A, B\}_{\psi,\psi^*} = \{A, B\}_{\rho,s}$$

and thence:

$$\partial_t \rho = \{\rho, H_\kappa\} = \frac{\delta H_\kappa}{\delta s} = -\frac{1}{m} \nabla\left(\rho\, \nabla s\right)$$

$$\partial_t s = \{s, H_\kappa\} = -\frac{\delta H_\kappa}{\delta \rho} = -\frac{1}{2m} (\nabla s)^2 - V - (1-\kappa)\, Q\,.$$

The result is valid for all $\kappa \geq 0$. Note that generically

$$G = G(\rho, s) \rightarrow \frac{d\,G}{dt} = \{G, H_\kappa\}\,.$$

Reduction to effective $\kappa = 0$, 1 and 2 self-coupling regimes

(i) $0 \leq \kappa < 1$; if $\psi(x,t) = |\psi| \exp(is/\hbar)$ actually is a solution of modular NLS, then $\psi'(x',t') = |\psi'| \exp(is'/\hbar)$ with

$$x' = x \ , \ t' = (1-\kappa)^{1/2} t$$

$$|\psi'|(x',t') = |\psi|(x, (1-\kappa)^{-1/2} t')$$

$$s'(x',t') = (1-\kappa)^{1/2} s(x,t)$$

automatically solves the linear Schrödinger equation:

$$i\hbar \partial_{t'} \psi' = \left[-\frac{\hbar^2}{2m} \Delta + \frac{1}{1-\kappa} V \right] \psi' \, .$$

(ii) For the borderline value $\kappa = 1$ we encounter the formalism that derives from the wave picture of classical Newtonian mechanics.

Note that (ii) is *not* a naive $\kappa \to 1$ limit of (i).

(iii) In case of $\kappa > 1$, replace $(1-\kappa)^{1/2}$ by $(\kappa - 1)^{1/2}$. Outcome: $\psi'(x',t') = |\psi'| \exp(is'/\hbar)$ is a solution of the nonlinear Schrödinger equation

$$i\hbar \partial'_t \psi' = \left[-\frac{\hbar^2}{2m} \Delta + \frac{V}{\kappa - 1} \right] \psi' + 2 \left[\frac{\hbar^2}{2m} \frac{\Delta |\psi'|}{|\psi'|} \right] \psi'$$

Note that (ii) is *not* a naive $\kappa \to 1$ limit of (iii).

For clarity, consider $\kappa = 2$. If a *complex* function

$$\psi(x,t) = |\psi| \exp(is/\hbar)$$

is a solution of the modular NLS with $\kappa = 2$, then the *real* function

$$\theta_*(x,t) = |\psi| \, \exp(-s/\hbar)$$

is a solution of the generalized (forward) heat equation

$$\hbar \partial_t \theta_* = \left[\frac{\hbar^2}{2m} \Delta + V \right] \theta_*$$

Another real function $\theta(x,t) = |\psi| \, \exp(+s/\hbar)$ is a solution of the time-adjoint (backwards) version of that equation:

$$-\hbar \partial_t \theta = \left[\frac{\hbar^2}{2m} \Delta + V \right] \theta \, .$$

Note that the ill-posed Cauchy problem would possibly become a serious obstacle. That because of the backwards parabolic equation.

Invoke the theory of strongly continuous dynamical semigroups. Choose $V(x)$ to be a continuous function that is bounded from above, so that $V' = -V$ becomes bounded from below. Then the contractive strongly continuous semigroup operator $\exp(-\hat{H}t/\hbar)$ is well defined

$$\hbar \partial_t \theta_* = -\hat{H} \theta_* = \left[\frac{\hbar^2}{2m} \Delta - V' \right] \theta_* \, .$$

together with its time adjoint

$$\hbar \partial_t \theta = \hat{H} \theta = \left[-\frac{\hbar^2}{2m} \Delta + V' \right] \theta$$

Dual Hamiltonians

Consider a product $\mathcal{F}(x,t) \doteq -\rho(x,t)\, s(x,t)$ of conjugate fields s and $\pi_s = -\rho$. The time evolution of

$$F(t) = \int dx\, \mathcal{F}(x,t) \doteq -\langle s \rangle$$

looks quite interesting:

$$\frac{dF}{dt} = \{F,\, H_\kappa\} = -\int dx\, \left[s(x,t)\, \frac{\delta H_\kappa}{\delta s} - \rho(x,t)\, \frac{\delta H_\kappa}{\delta \rho} \right] =$$

$$-\int dx\, \rho\, \left[\frac{m}{2} v^2 - V - (1-\kappa)\frac{m}{2}\, u^2 \right] .$$

A new Hamiltonian-type functional has emerged on the right-hand-side of the above dynamical identity. We denote

$$H_\kappa^\pm = \int dx\, \rho\, \left[\frac{m}{2} v^2 \pm V \pm (1-\kappa)\frac{m}{2}\, u^2 \right] .$$

Note that negative sign has been generated *both* with respect to terms $(m/2)\langle u^2 \rangle$ and $\langle V \rangle$.

The Hamiltonian motion rule rewrites as

$$\frac{dF}{dt} = \{F, H_\kappa^+\} = -H_\kappa^-(t)\,,$$

where $H_\kappa^+ \equiv H$ plays the role of the time evolution generator. H_κ^+ is a constant of motion, while $H_\kappa^-(t)$ is *not.*

A complementary relationship is generated by the *induced* Hamiltonian H_κ^-:

$$\frac{dF}{dt} = \{F, H_\kappa^-\} = -H_\kappa^+(t)\,.$$

Presently, H_κ^+ is a constant of motion, while $H_\kappa^-(t)$ no longer is.

Let $V(x)$ be a continuous function, bounded from below. If the energy operator $\hat{H} = -(\hbar^2/2m)\Delta + V$ is self-adjoint in $L^2(R^n)$, then $\exp(-i\hat{H}t/\hbar)$ is unitary on $L^2(R)$ so that $i\hbar\partial_t\psi = \hat{H}\psi$ ($\kappa = 0$).

In case of $\kappa = 1$ and $\kappa = 2$ we introduce two classes of external potentials $\pm V(x)$, with $+V(x)$ bounded from below.

We discriminate between the confining and scattering regimes (we shall mention the case of periodic potentials later).

In case of $\kappa = 2$, a pair of time-adjoint parabolic equations reads:

$$\hbar\partial_t\theta_* = -\hat{H}\theta_*$$

$$\hbar\partial_t\theta = \hat{H}\theta$$

$\theta_*(x,t) = [\exp(-\hat{H}t/\hbar)\,\theta_*](x,0)$ represents a forward dynamical semigroup evolution, while $\theta(x,T-t) = \exp(+\hat{H}t/\hbar)\,\theta(x,T)$ stands for a backward one.

One should consider the dynamics in a finite time interval $[0,T]$, with suitable end-point data. This restriction is generic, although not always necessary.

The corresponding modular Schrödinger equations (plus their complex conjugate versions) read:

(i) $\kappa = 0 \Longrightarrow i\hbar\partial_t\psi = [-(\hbar^2/2m)\Delta + V]\psi$

(ii) $\kappa = 1 \Longrightarrow i\hbar\partial_t\psi = [-(\hbar^2/2m)\Delta \pm V - Q]\psi$

(iii) $\kappa = 2 \Longrightarrow i\hbar\partial_t\psi = [-(\hbar^2/2m)\Delta - V - 2Q]\psi$.

Induced dynamical rules:

the continuity equation

$$\partial_t \rho = -\nabla(\rho \cdot v)$$

and the Hamilton-Jacobi type equations:

(i) $\kappa = 0$;

$$\mathcal{L} = -\rho \left[\partial_t s + (m/2)(v^2 + u^2) + V \right]$$

$$\Downarrow$$

$$\partial_t s + (1/2m)(\nabla s)^2 + (V + Q) = 0$$

(ii) $\kappa = 1$;

$$\mathcal{L} = -\rho \left[\partial_t s + (m/2)v^2 \pm V \right]$$

$$\Downarrow$$

$$\partial_t s + (1/2m)(\nabla s)^2 \pm V = 0$$

(iii) $\kappa = 2$;

$$\mathcal{L} = -\rho \left[\partial_t s + (m/2)(v^2 - u^2) - V \right]$$

$$\Downarrow$$

$$\partial_t s + (1/2m)(\nabla s)^2 - (V + Q) = 0$$

On dynamically admitted fields $\rho(t)$ and $s(x,t)$, $L(t) \equiv 0$, i. e. $\langle \partial_t s \rangle = -H$. The respective Hamiltonians follow:

$$H^+ \doteq \int dx\, \rho \left[(m/2)v^2 + V + (m/2)u^2 \right]$$

$$H^{\pm}_{cl} \doteq \int dx\, \rho \left[(m/2)v^2 \pm V \right]$$

$$H^- \doteq \int dx\, \rho \left[(m/2)v^2 - V - (m/2)u^2 \right]$$

Comments:

The evolution equations for $F = -\langle s \rangle$, define *dual* pairs:

$$\dot{F} = \{F, H^+\} = -\int dx\, \rho \left[\frac{m}{2}v^2 - V - \frac{m}{2}u^2\right] = -H^-(t)\,,$$

$$\dot{F} = \{F, H^-\} = -\int dx\, \rho \left[\frac{m}{2}v^2 + V + \frac{m}{2}u^2\right] = -H^+(t)$$

and

$$\dot{F} = \{F, H^+_{cl}\} = -\int dx\, \rho \left[\frac{m}{2}v^2 - V\right] = -H^-_{cl}(t)$$

$$\dot{F} = \{F, H^-_{cl}\} = -\int dx\, \rho \left[\frac{m}{2}v^2 + V\right] = -H^+_{cl}(t)\,.$$

The motion rules for $\dot{F}(t)$ can be given more transparent form by reintroducing constants $H^\pm$ of the respective motions.

$$\dot{F}(t) = -m\langle v^2\rangle(t) + H^\pm$$

and

$$\dot{F}(t) = -m\langle v^2\rangle(t) + H^\pm_{cl}\,.$$

The non-negative term $m\langle v^2\rangle(t)$ actually represents the (Shannon) *entropy production* time rate.

Since H^+ and H^- are constants of respective motions,

$$F(t) - t\,H^\pm$$

are monotonically decreasing in time quantities (*Lyapunov functionals*). This property extends to the $H^\pm_{cl}$ generated dynamics as well.

Physics-related implementations of the dual dynamics: An illusion of an "imaginary time"

Harmonic oscillator and its inverted partner

Let us consider a standard classical harmonic oscillator problem, where

$$H \doteq \frac{p^2}{2m} + \frac{1}{2} m\omega^2 q^2 \tag{1}$$

is an obvious constant of motion for the Newtonian system $\dot{p} = m\ddot{q} = -m\omega^2 q$,

$$q(t) = q_0 \cos \omega t + \frac{p_0}{m\omega} \sin \omega t \tag{2}$$

$$p(t) = p_0 \cos \omega t - m\omega q_0 \sin \omega t \, .$$

Clearly $H = p_0^2/2m + (m\omega^2/2)q_0^2$ is a positive constant.

Instead of a trivial mapping $\omega \rightarrow i\omega$ we follow an over-educated route of an analytic continuation in time.

Consider the Wick rotation $t \rightarrow -it$, paralleled by the transformation of initial momentum data $p_0 \rightarrow -ip_0$. We get:

$$H_{-ip_0} = -p_0^2/2m + (m\omega^2/2)q_0^2 \doteq -\overline{H}$$

and

$$q_{-ip_0}(-it) \doteq \overline{q}(t) = q_0 \cosh \omega t - \frac{p_0}{m\omega} \sinh \omega t$$

together with

$$p_{-ip_0}(-it) \doteq +i\overline{p}(t) = -ip_0 \cosh \omega t + im\omega q_0 \sinh \omega t \, ,$$

which simply rewrites as

$$\overline{p}(t) = -p_0 \cosh \omega t + m\omega q_0 \sinh \omega t \, .$$

We observe that

$$\overline{q}(-t) = q_0 \cosh \omega t + \frac{p_0}{m\omega} \sinh \omega t$$

$$-\overline{p}(-t) = p_0 \cosh \omega t + m\omega q_0 \sinh \omega t$$

are the familiar inverted oscillator solutions, generated by $\overline{H}$.

Equations of motion for $\overline{q}(t)$ and $\overline{p}(t)$ directly derive from the Hamiltonian $H_{-ip_0} = -\overline{H}$ with

$$\overline{H} = \frac{\overline{p}^2}{2m} - \frac{1}{2} m\omega^2 \overline{q}^2$$

They give rise to the (inverted, sometimes interpreted as Euclidean) Newton equation $\dot{\overline{p}} = m\ddot{\overline{q}} = +m\omega^2 \overline{q}$.

However ! the dynamics generated by $\overline{H}$ is related to that generated by $-\overline{H}$ by the time reflection: the latter dynamics runs backwards, if the former runs forward.

The Euclidean connection goes beyond the confining vs scattering potential idea of ours and extends to bounded, like e.g. periodic, potentials as well. Examples from the physics of instantons, (all dimensional units are scaled away):

(i) static localized (kink) solutions $\phi(x) = \pm \tanh[(x - x_0)/\sqrt{2}]$ of the ϕ^4 nonlinear field theory in one space dimension $\partial^2\phi/\partial t^2 - \partial^2\phi/\partial x^2 = \phi - \phi^3$ may be interpreted as Euclidean time solutions $q(\tau) = \pm \tanh[(\tau - \tau_0)/\sqrt{2}]$ of the double well potential problem $d^2q/d\tau^2 = q^3 - q$

(ii) the kink solution $\phi(x) = \pm 4 \tan^{-1}[\exp(x - x_0)]$ of the sine-Gordon equation $\partial^2\phi/\partial t^2 - \partial^2\phi/\partial x^2 = -\sin\phi$ may be interpreted as a Euclidean time solution of a plane pendulum problem $d^2q/d\tau^2 = \sin q$, where a "normal" choice $V(q) = 1 - \cos q$ would yield $\ddot{q} = -\sin q$.

Time duality in classical Hamilton-Jacobi evolutions

We have clear hints on how to connect the *dual* classical wave theory evolutions, associated with Hamiltonians $H^{\pm}_{cl}$.

We recall we have the dual Hamilton-Jacobi equations $\partial_t s + (1/2m)(\nabla s)^2 \pm V = 0$ and that there holds $\partial_t \rho = -\nabla \cdot (\rho\, v)$ with $v(x,t) = (1/m)\nabla s(x,t)$.

In the adopted notational convention, we define the initial data $s_0(x) = -\overline{s}_0(x)$ and introduce an "imaginary time" transformation

$$\psi(x,t) = \rho^{1/2} \exp(is/2mD) \longrightarrow \overline{\psi}(x,t) \doteq \psi_{-is_0}(x,-it) =$$
$$\rho^{1/2}_{-is_0}(x,-it) \exp[is_{-is_0}(x,-it)/2mD] \doteq$$
$$\overline{\rho}^{1/2}(x,t) \exp[-\overline{s}(x,t)/2mD]\,.$$

We note that $\lim_{t\downarrow 0}\, is_{-is_0}(x,-it) = i(-is_0)(x,0) = s_0(x)$.

Let us denote $\overline{v} = (1/m)\nabla\overline{s}$. Accordingly, we have replaced

$$H^{+}_{cl} = \int dx\, \rho[(m/2)v^2 + V]$$

by

$$-\overline{H}^{\,-}_{cl} = \int dx\, \overline{\rho}[-(m/2)\overline{v}^2 + V]$$

There holds

$$\partial_t \rho = -\nabla \cdot (\rho v) \longrightarrow \partial_t \overline{\rho} = +\nabla \cdot (\overline{\rho}\, \overline{v})$$

which is the time reflected (backwards) evolution. Analogously

$$\partial_t s + (1/2m)(\nabla s)^2 \pm V = 0 \longrightarrow \partial_t \overline{s} - (1/2m)(\nabla \overline{s})^2 + V = 0$$

where $t \to -t$ induces an expected form of the dual H-J equation:

$$\partial_t \overline{s} + (1/2m)(\nabla \overline{s})^2 - V = 0\,.$$

General notion of time duality

The analytic continuation in time directly extends to the general pair $H^{\pm}$ of dual (quantum vs dissipative) Hamiltonians

$$H^{\pm} = \int dx\, \rho \left[\frac{m}{2} v^2 \pm V \pm \frac{m}{2} u^2\right] .$$

If $\psi(x,t)$ actually is a solution of the Schrödinger equation

$$i(2mD)\partial_t \psi = \hat{H}\psi$$

then

$$\psi_{-is_0}(x,-it) = \overline{\rho}^{1/2}(x,t) \exp[-\overline{s}(x,t)/2mD] \doteq \theta_*(x,t)$$

solves a backwards diffusion-type equation

$$-(2mD)\partial_t \theta_* = \hat{H}\theta_*$$

while

$$\theta(x,t) = \overline{\rho}^{1/2}(x,t) \exp[+\overline{s}(x,t)/2mD]$$

solves the forward equation

$$(2mD)\partial_t \theta = \hat{H}\theta \, .$$

In the above one may obviously identify $D = k_B T/m\beta \rightarrow \hbar/2m$, but the κ scaling possibility should be kept in memory as more natural tool.

The whole procedure can inverted and we can trace back a non-dissipative quantum dynamics pattern which stays in affinity (duality) with a given dissipative dynamics.

Diffusion-type processes: Smoluchowski process

The Hamiltonian appropriate for the description of dissipative processes (strictly speaking, diffusion-type stochastic processes) has the form

$$H^{-} \doteq \int dx\, \rho \left[(m/2)v^2 - V - (m/2)u^2\right]$$

with the a priori chosen, continuous and bounded from below potential $V(x)$. It is the functional form of $V(x)$ which determines local characteristics of the diffusion process.

Once the Fokker-Planck equation is inferred

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

where $\rho_0(x)$ stands for the initial condition, we adopt $b = f/m\gamma$ in the form $f(x) = -\nabla\mathcal{V}$.

Coefficients: γ is a friction (damping) parameter and, instead of $D = \hbar/2m$, we prefer to think in terms of $D = k_B T/m\gamma$ where T stands for an (equilibrium) temperature of the reservoir.

An admissible form of $\mathcal{V} \to f = -\nabla\mathcal{V}$ must be compatible with the Riccatti-type equation, provided the potential function $V(x)$ has been a priori chosen:

$$V(x) = m\left[\frac{1}{2}\left(\frac{f}{m\gamma}\right)^2 + D\nabla \cdot \left(\frac{f}{m\gamma}\right)\right]\,.$$

The Fokker-Planck equation can rewritten as a continuity equation $\partial_t \rho = -\nabla \cdot j$ with the diffusion current j in the form:

$$j = \rho v = \frac{\rho}{m\gamma}[f - k_B T \nabla \ln \rho] \doteq \frac{\rho}{m}\nabla s\,.$$

We recall the general definition of the current velocity $v = (1/m)\nabla s$.

The time-independent $s = s(x)$ is here admissible, hence we have actually determined

$$s = -\frac{1}{\gamma}(\mathcal{V} + k_B T \ln \rho)$$

whose negative mean value $F = -\langle s \rangle$ defines the Helmholtz free energy of the random motion:

$$\Psi \doteq \gamma\, F = U - T\mathcal{S}\,,$$

$\mathcal{S} \doteq k_B\, S$ stands for the Gibbs-Shannon entropy of the continuous probability distribution, $U = \langle \mathcal{V} \rangle$ is an internal energy.

Assuming ρ and $\rho V v$ to vanish at the integration volume boundaries, we get

$$\dot{\Psi} = -(m\gamma) \left\langle v^2 \right\rangle = -k_B T (\dot{\mathcal{S}})_{int} \leq 0\,. \qquad (3)$$

The Helmholtz free energy Ψ decreases as a function of time, or remains constant, hence is a Lyapunov functional in the present case.

$S(t) = -\langle \ln \rho \rangle$ typically is not a conserved quantity. We impose suitable boundary conditions and consider:

$$D\dot{S} = \left\langle v^2 \right\rangle - \langle b \cdot v \rangle\ .$$

which rewrites as follows

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

where

$$k_B T (\dot{S})_{int} \doteq m\gamma \left\langle v^2 \right\rangle \geq 0$$

stands for the entropy production rate, while

$$k_B T (\dot{S})_{ext} = -\int f \cdot j\, dx = -m\gamma\, \langle b \cdot v \rangle$$

(as long as negative) may be interpreted as the heat dissipation rate:$-\int f \cdot j\, dx$.

Let us consider the stationary regime $\dot{S} = 0$ associated with an (a priori assumed to exist) invariant density ρ_*. Then,

$$b = u = D\nabla \ln \rho_*$$

and

$$-(1/k_BT)\nabla\mathcal{V} = \nabla \ln\, \rho_* \Longrightarrow \rho_* = \frac{1}{Z}\exp[-\mathcal{V}/k_BT]\,.$$

Hence

$$-\gamma s_* = \mathcal{V} + k_BT \ln \rho_* \Longrightarrow \Psi_* = -k_BT \ln Z \doteq \gamma F_*$$

with $Z = \int \exp(-\mathcal{V}/k_BT)dx$.

Ψ_* stands for a minimum of the time-dependent Helmholtz free energy Ψ. Because of

$$Z = \exp(-\Psi_*/k_BT)$$

we have

$$\rho_* = \exp[(\Psi_* - V)/k_BT]\,.$$

Therefore, the conditional Kullback-Leibler entropy $\mathcal{H}_c$, of the density ρ relative to an equilibrium (stationary) density ρ_* acquires the form

$$k_BT\mathcal{H}_c \doteq -k_BT \int \rho \ln(\frac{\rho}{\rho_*})dx = \Psi_* - \Psi\,.$$

In view of the concavity property of the function $f(w) = -w\ln w$, $\mathcal{H}_c$ takes only negative values, with a maximum at 0. We have

$$\Psi_* \leq \Psi$$

and

$$k_BT\dot{\mathcal{H}}_c = -\dot{\Psi} \geq 0$$

$\mathcal{H}_c(t)$ is bound to grow monotonically towards 0, while $\Psi(t)$ drops down to its minimum Ψ_* which is reached upon ρ_*.

Note that properties of the free Brownian motion can be easily inferred by setting $b \equiv 0$ in the above discussion. Then, the diffusive dynamics is sweeping and there is no asymptotic invariant density, nor a finite minimum for $\Psi(t)$ which decreases indefinitely.

Reintroducing duality

Once we set $b = -2D\nabla\Phi$ with $\Phi = \Phi(x)$, a substitution:

$$\rho(x,t) \doteq \theta_*(x,t)\exp[-\Phi(x)]$$

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

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

and its (here trivialized in view of the time-independence of Φ) time adjoint

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

A real solution is $\theta(x,t) = \exp[-\Phi(x)]$ and there holds (to be regarded as an identity, not an equation to be solved)

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

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

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

In view of (we restore an explicit "overline" notation):

$$\overline{\rho}^{1/2}(x,t)\,\exp[-\overline{s}(x,t)/2mD] \doteq \theta_*(x,t)$$

we immediately recover

$$\overline{s} = (2mD)[\Phi - (1/2)\ln\overline{\rho}]$$

If there are no external forces, Φ disappears and we are left with the free Brownian motion associated with $\overline{s} = -mD\ln\overline{\rho}$.

Thank you for attention