Nonconservative diffusion processes

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Inspiration (51 pp):

Nonequilibrium diffusion processes via non-Hermitian electromagnetic quantum mechanics with application to the statistics of entropy production in the Brownian gyrator

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Excerpt from the original PRE 107 Abstract

The nonequilibrium Fokker-Planck dynamics in an arbitrary force field $\vec{f}(\vec{x})$ in dimension N is revisited via the correspondence with the non-Hermitian quantum mechanics in a real scalar potential $V(\vec{x})$ and in a purely imaginary vector potential $[-i\vec{A}(\vec{x})]$ of real amplitude $\vec{A}(\vec{x})$.

Meaning for pedestrians in $H^{-}_{quant} = -(1/2)(\vec{\nabla} - i\vec{A})^2$ **replace** $\vec{A}(\vec{x})$ by $[-i\vec{A}(\vec{x})]$ getting $H_{Eucl} = -\frac{1}{2}(\vec{\nabla} - \vec{A})^2$

3 x „non"… nonconservative, non-Hermitian, nonequilibrium

Our focus

Fokker-Planck operators of diffusion processes with nonconservative drift fields, in dimension $N \geq 2$, can be directly related with non-Hermitian electromagnetic-type Hamiltonian generators of motion. The induced nonequilibrium dynamics of probability densities points towards an issue of path integral solutions of the Fokker-Planck equation, and calls for revisiting links between known exact path integral formulas for quantum propagators in real and Euclidean time, with these for Fokker-Planck-induced transition probability density functions.

Non-conservativeness, non-Hermicity and the „magnetic" analogy

Markovian diffusion processes driven by nonconservative (non-gradient) time-independent drift field $\vec{F}(\vec{x})$. For concretness let us consider

$$dX(t) = \vec{F}(\vec{X}(t))dt + \sqrt{2\nu}d\vec{W}(t)$$

N=3: $curl\vec{F} = \vec{\nabla} \times \vec{F} \neq \vec{0}$.

We rescale to ½ the diffusion coefficient

diffusion generator reads $L = \frac{1}{2}\Delta + \vec{F} \cdot \vec{\nabla}$

Fokker-Planck operator $L^* = \frac{1}{2}\Delta - \vec{\nabla} \cdot (\vec{F}\cdot)$ arises as the $L^2(R^N)$ adjoint of L

the inferred Fokker-Planck equation in $N \geq 2$, can be rewritten in the persuasive Euclidean "magnetic" form

$$\partial_t \rho = L^* \rho = -(H_{Eucl} + \mathcal{V})\rho = -H\rho,$$

$$H_{Eucl} = -\frac{1}{2}(\vec{\nabla} - \vec{F})^2,$$

$$\mathcal{V} = \frac{1}{2}[(\vec{\nabla} \cdot \vec{F}) + \vec{F}^2].$$

The transcript of the F-P operator $L^* = -(H_{Eucl} + \mathcal{V}) = -H$ is paralleled by

$$L = -(H^*_{Eucl} + \mathcal{V}) = -H^*$$
$$H^*_{Eucl} = -\frac{1}{2}(\vec{\nabla} + \vec{F})^2,$$

L actually is named a diffusion generator

where H^*_{Eucl} is the $L^2(R^N)$ adjoint of H_{Eucl}

The QM analogy arises by formally setting $\vec{F} \to i\vec{F}$ and t→ it in $e^{(-Ht)}$ (while reintroducing dimensional constants)

There is nothing surprising in connection with **(non-Hermitian) adjoint** „magnetic"-type entries H, H*, since the related non-Hermitian operators L^* and L are intimately related with Markovian diffusion processes.

We recall **that adjoint pairs of parabolic equations** actually rule the evolution in time of transition probability density functions of the diffusion process.

$$\partial_t \rho = L^* \rho \qquad \rho(\vec{x}, t) = \int p(\vec{y}, s, \vec{x}, t)\rho(\vec{y}, s) d^3x$$

$$\boxed{\partial_t p(\vec{y}, s, \vec{x}, t) = L^*_{\vec{x}} p(\vec{y}, s, \vec{x}, t)} \qquad p(\vec{y}, s, \vec{x}, t),\ 0 \le s < t \le T,\ (T \to \infty \text{ is admissible})$$

$$u(\vec{y}, s) = \mathbb{E}[f(\vec{X}_t) | \vec{X}_s = \vec{y}] = \int f(\vec{x}) p(\vec{y}, s, \vec{x}, t) d^N x \qquad s \in [0, t]$$

$$-\partial_s u(\vec{y}, s) = L_{\vec{y}} u(\vec{y}, s)$$

$$\boxed{-\partial_s p(\vec{y}, s, \vec{x}, t) = L_{\vec{y}} p(\vec{y}, s, \vec{x}, t)}$$

Hermitian vs non-Hermitian for conservative diffusion processes : N=1 detour

(Garbaczewski and Żaba, J. Phys. A: Math. Theor. 53 (2020) 315001 (39pp))

given a stationary density $\rho_*(x)$, one can transform the Fokker–Planck dynamics,

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

into an associated Hermitian (Schrödinger-type) dynamical problem in $L^2(R)$, by means of a factorisation

$$\rho(x,t) = \Psi(x,t)\rho_*^{1/2}(x) \quad \Longrightarrow \quad \partial_t\Psi = D\Delta\Psi - \mathcal{V}\Psi = -\hat{H}\Psi$$

We demand that $\hat{H}\,\rho_*^{1/2} = 0$, $\Longrightarrow$ $\mathcal{V}(x) = D\dfrac{\Delta\rho_*^{1/2}}{\rho_*^{1/2}} = \dfrac{1}{2}\left(\dfrac{b^2}{2D} + \nabla b\right)$

Conservativeness: $b(x) = 2D\nabla\ \ln\ \rho_*^{1/2}(x)$

Joint spectral solution for motion generators L, L and Ĥ*

$$\hat{H} = -\rho_*^{1/2} L \rho_*^{-1/2} = -\rho_*^{-1/2} L^* \rho_*^{1/2}. \qquad -L^* = \rho_*^{1/2}\hat{H}\rho_*^{-1/2}$$

Three operators $\hat{H}$, L and L^* are Hermitian (and eventually self-adjoint) in function spaces

$L^2(R)$, $L^2(R,\rho_*)$ and $L^2(R,\rho_*^{-1})$ respectively

Specific meaning of nonequilibrium (existence of steady currents)

The diffusion current notion appears through rewriting the Fokker -Planck equation

$$\partial_t \rho = (1/2)\Delta\rho - \vec{\nabla}\cdot(\vec{F}\cdot\rho)$$

$$\partial_t \rho = -\vec{\nabla}\cdot\vec{j} = -\vec{\nabla}\cdot(\vec{v}\rho),$$
$$\vec{v} = \vec{F} - \vec{\nabla}\ln\rho^{1/2},$$

where $\vec{v}$ is named a current velocity field.

Let us assume that the Fokker-Planck equation admits the stationary pdf $\rho_*(\vec{x})$

In view of $\partial_t \rho_* = 0$, $\vec{j}_* = \rho_* \vec{v}_*$, with $\vec{v_*} = \vec{F} - \vec{\nabla}\ln\rho_*^{1/2}$ needs either to vanish, $\vec{j}_*(\vec{x}) = 0$, or to be divergenceless, $\vec{\nabla}\cdot\vec{j}_* = 0$.

The choice of the drift field in gradient form $\vec{F} = \vec{\nabla}\ln\rho_*^{1/2}$, would secure $\rho(\vec{x},t) \to \rho_*(\vec{x})$, with no steady current at all, since $\vec{j}_* = 0$ identically.

By denoting $\rho_* = \exp(-2\phi)$, (that amounts to $\rho^{1/2} = \exp(-\phi)$, we are left with

$$\partial_t \rho_* = -\vec{\nabla} \cdot [\rho_* (\vec{F} + \vec{\nabla}\phi)] = 0.$$

We shall consider nonconservative drifts in the form

$$\boxed{\vec{F} = \vec{A} - \vec{\nabla}\phi,}$$

comprising $-\phi = \ln \rho_*^{1/2}$, and the non-gradient entry $\vec{A}$

The steady diffusion current $\vec{j} = \vec{A}\rho_*$ must be divergenceless. Accordingly,

$$0 = \vec{\nabla} \cdot (\vec{A}\rho_*) = (\vec{A} \cdot \vec{\nabla})\rho_* + \rho_*(\vec{\nabla} \cdot \vec{A}).$$

This implies that the divergence of the vector field $\vec{A}$ reads $\boxed{\vec{\nabla} \cdot \vec{A} = 2\vec{A} \cdot \vec{\nabla}\phi.}$

An additional assumption that $\vec{A}$ itself is divergenceless, i.e. $\vec{\nabla} \cdot \vec{A} = 0$

would result in the orthogonality relation $\vec{A} \cdot \vec{\nabla}\phi = 0$, valid for all $\vec{x} \in R^N$.

This orthogonality property may be interpreted as a **constraint** on the admissible functional form of the stationary pdf, $\rho_* = \exp(-2\phi)$ **once the non-gradient vector potential has been a priori selected.**

Path integral formulation - hints

The path-wise implementation $d\vec{X}(t) = \vec{F}(\vec{X}(t))dt + \sqrt{2\nu}d\vec{W}(t)$ of the diffusion process in question, motivates our interest in transition probability density functions , which actually are the **integral kernels** (often named propagators) of motion operators $\exp(tL^*) = \exp(-tH)$,

$$[\exp(-tH)\rho_0](\vec{x}) = \rho(\vec{x}, t), \text{ an thence } \partial_t \rho = -H\rho, \text{ with the initial data } \rho_0.$$

The dynamics of the involved transition probability density function

$$p(\vec{y}, s, \vec{x}, t) = [e^{-H(t-s)}](\vec{y}, \vec{x}) \qquad 0 \leq s < t$$

in principle should be amenable to Feyman path integration routines (note the absence of „i"), albeit well beyond the ramifications of the standard Feynman-Kac formula.

Actually, c.f. Wiegel and Ross, (1981), **„Path integral solutions for the Fokker-Planck equation with non-conservative forces",** where the case of N=2 has been studied.

We point out a link (albeit not unrestricted, and demanding some care) with the concept of **density matrices** in statistical mechanics, c.f. **Feynman's „path integral formulation of the density matrix",** 1961-1972, specifically its (unnormalised) version in the position representation. Feynman's (unnormalised) density matrix arises as an integral kernel of $e^{(-\beta H)}$ with $\beta \sim 1/kT$, k being the Boltzmann constant, T labeling the temperature, and the initial condition for $\beta = 0$ (e.g. $T \downarrow \infty$) set in the form of the Dirac delta. Note that $\beta \to \infty$ refers to $T \downarrow 0$. These limiting features get somewhat unexpected „flavour", if a parallelism (e.g. correspondence) with the time label t is kept in memory. One may think about a thermally singular beginning T infnite at t=0, which is followed by the monotonic cooling down to T=0 as t approaches infinity.

The formula for the **„propagator associated with the Langevin system"** (the integral kernel of the operator $\exp(tL^*)$, with $L^* = -H$) reads:

$$p(\vec{y},0,\vec{x},t) = \exp(-Ht)(\vec{y},\vec{x}) = \int_{\vec{x}(\tau=0)=\vec{y}}^{\vec{x}(\tau=t)=\vec{x}} \mathcal{D}\vec{x}(\tau)\, \exp\left[-\int_0^t d\tau \mathcal{L}(\vec{x}(\tau),\dot{\vec{x}}(\tau))\right],$$

$$\mathcal{L}(\vec{x}(\tau),\dot{\vec{x}}(\tau)) = \frac{1}{2}\left[\dot{\vec{x}}(\tau) - \vec{F}(\vec{x}(\tau))\right]^2 + \frac{1}{2}\vec{\nabla}\cdot\vec{F}(\vec{x}(\tau) = \frac{1}{2}\dot{\vec{x}}^2(\tau) - \dot{\vec{x}}(\tau)\cdot\vec{F}(\vec{x}(\tau)) + \mathcal{V}(\vec{x}(\tau).$$

We recall that the "normal" (e.g. **non-Euclidean**) classical Lagrangian would have the form $L = T - V$ with $T = \dot{\vec{x}}^2/2$ and $V(\dot{\vec{x}},\vec{x},t) = \mathcal{V} - \dot{\vec{x}}\cdot\vec{F}$.
Note that actually employed **Euclidean (e.g. diffusion induced)** Lagrangian has the form $L = T + V$. The sign difference has consequences for the functional form of the derived versions of the second Newton law (e.g. the sign of the derived Lorentz force analogue).

Lagrangian dynamics shows an „electromagnetic" affinity

Since we have in hands an explicit Lagrangian , while keeping in memory its relevance for the evaluation of path integrals in the quadratic case, we ask for the dynamical output in terms of the Euler-Lagrange equations, still without specifying detailed properties of the vector field $\vec{F}(\vec{x}(t),t)$, except for tentatively admitting a direct dependence on time.
To compress the resulting formulas we pass to the N=3 notation $\vec{x} = (x_1, x_2, x_3)$, so that $V(x,\dot{x},t) = \mathcal{V}(x,t) - \sum_j \dot{x}_j F_j(x,t)$.

$$\frac{\partial \mathcal{L}}{\partial x_i} - \frac{d}{dt}\frac{\partial \mathcal{L}}{\partial \dot{x}_i} = 0 \Longrightarrow \frac{\partial V}{\partial x_i} - \frac{d}{dt}\left(\frac{\partial \mathcal{T}}{\partial \dot{x}_i} + \frac{\partial V}{\partial \dot{x}_i}\right) = 0$$

The Euler-Lagrange equations are valid for all i=1, 2, 3, (actually for any N) and imply

$$\boxed{\ddot{x}_i = \left(\frac{\partial \mathcal{V}}{\partial x_i} + \frac{\partial F_i}{\partial t}\right) + \sum_j B_{ij}\dot{x}_j,}$$

where

$$\boxed{B_{ij} = \frac{\partial F_i}{\partial x_j} - \frac{\partial F_j}{\partial x_i}}$$

We note that nonvanishing components of the „magnetic matrix” $B = (B_{ij})$ define (for N=3)

$$\vec{\nabla} \times \vec{F} = \vec{B} = (B_1 = B_{32}, B_2 = B_{13}, B_3 = B_{21}) = (\partial_2 F_3 - \partial_3 F_2, \partial_3 F_1 - \partial_1 F_3, \partial_1 F_2 - \partial_2 F_1)$$

and thence $\sum_j B_{ij}\dot{x}_j = F_i^{magn}$ whose vector form looks deceivingly „magnetic”

$$\boxed{\vec{F}^{magn} = -\dot{\vec{x}} \times (\vec{\nabla} \times \vec{F}) = -\dot{\vec{x}} \times \vec{B},}$$

as required (up to a sign, which is opposite to that in the ”classical” case) from the magnetic part of the Lorentz force. The electric analogue of this force reads $\vec{F}^{el} = \vec{\nabla}\mathcal{V} + \partial\vec{F}/\partial t$ and is opposite to that valid in the ”classical” case. For reference, we reproduce the „classic” result

$$\boxed{\ddot{x}_i = -\left[\left(\frac{\partial \mathcal{V}}{\partial x_i} + \frac{\partial F_i}{\partial t}\right) + \sum_j B_{ij}\dot{x}_j\right]}$$

Lagrangian signatures of stationary pdfs

Let us consider $\vec{F} = \vec{A} - \vec{\nabla}\phi,$ comprising $-\phi = \ln \rho_*^{1/2}$, and the non-gradient entry $\vec{A}$

$$\mathcal{L}(\vec{x}(\tau), \dot{\vec{x}}(\tau)) = \frac{1}{2}\dot{\vec{x}}^2(\tau) - \dot{\vec{x}}(\tau) \cdot \vec{F}(\vec{x}(\tau)) + \mathcal{V}(\vec{x}(\tau)$$

The term $\dot{\vec{x}} \cdot \vec{F}$ in the action functional $\left[-\int_0^t d\tau \mathcal{L}(\vec{x}(\tau), \dot{\vec{x}}(\tau))\right]$ contributes

$$\int_0^t \dot{\vec{x}} \cdot [-\vec{\nabla}\phi(\vec{x}(\tau)) + \vec{A}(\vec{x}(\tau)]d\tau = -\int_0^t \frac{d}{d\tau}\phi(\vec{x}(\tau))d\tau + \int_0^t \dot{\vec{x}} \cdot \vec{A}(\vec{x}(\tau)d\tau = \phi(\vec{x}(0)) - \phi(\vec{x}(t)) + \int_0^t \dot{\vec{x}} \cdot \vec{A}(\vec{x}(\tau)d\tau$$

$$p(\vec{y}, 0, \vec{x}, t) = e^{\phi(\vec{y}) - \phi(\vec{x})}\, k(\vec{y}, 0, \vec{x}, t)$$

$$k(\vec{y}, 0, \vec{x}, t) = \int_{\vec{x}(\tau=0)=\vec{y}}^{\vec{x}(\tau=t)=\vec{x}} \mathcal{D}\vec{x}(\tau) \exp\left[-\int_0^t d\tau \mathcal{L}_{magn}(\vec{x}(\tau), \dot{\vec{x}}(\tau))\right]$$

where the new function $k(\vec{y}, 0, \vec{x}, t)$ is no longer a transition probability density but an integral kernel (propagator) $\exp(-tH_{magn})(\vec{y}, \vec{x}) = k(\vec{y}, 0, \vec{x}, t)$ of a new motion generator

$$H_{magn} = e^{\phi} H e^{-\phi} = -\frac{1}{2}(\vec{\nabla} - \vec{A})^2 + \mathcal{V}.$$

$$\mathcal{V} = V + \frac{1}{2}\vec{A}^2 \qquad V(\vec{x}) = \frac{1}{2}[(\vec{\nabla}\phi)^2 - \Delta\phi].$$

$$\mathcal{L}_{magn}(\vec{x}(\tau), \dot{\vec{x}}(\tau)) = \frac{1}{2}\dot{\vec{x}}^2(\tau) - \dot{\vec{x}} \cdot \vec{A}(\vec{x}(\tau) + \mathcal{V}(\vec{x}(\tau)) = \frac{1}{2}\left[\dot{\vec{x}}(\tau) - \vec{A}(\vec{x}(\tau))\right]^2 + V(\vec{x}(\tau))$$

What is it about, if we skip $\vec{A}$ in $\vec{F} = \vec{A} - \vec{\nabla}\phi$, ?

$$\vec{F} = \vec{\nabla} \ln \rho_*^{1/2} = -\vec{\nabla}\phi$$

$$p(\vec{y}, 0, \vec{x}, t) = e^{\phi(\vec{y}) - \phi(\vec{x})}\, k(\vec{y}, 0, \vec{x}, t)$$

$$\mathcal{L} = \mathcal{L}_{st} + \dot{\vec{x}} \cdot \vec{\nabla}\phi$$

$$\mathcal{L}_{st}(\vec{x}(\tau), \dot{\vec{x}}(\tau)) = \frac{1}{2}\dot{\vec{x}}^2(\tau) + V(\vec{x}(\tau)$$

$$V(\vec{x}) = \frac{1}{2}[(\vec{\nabla}\phi)^2 - \Delta\phi] = (1/2)\Delta\rho_*^{1/2}/\rho_*^{1/2}$$

$$k_{st}(\vec{y}, 0, \vec{x}, t) = \int_{\vec{x}(\tau=0)=\vec{y}}^{\vec{x}(\tau=t)=\vec{x}} \mathcal{D}\vec{x}(\tau)\, \exp\left[-\int_0^t d\tau \mathcal{L}_{st}(\vec{x}(\tau), \dot{\vec{x}}(\tau))\right]$$

$$H_{st} = e^{\phi} H e^{-\phi} = -\frac{1}{2}\Delta + V$$

Feynman-Kac framework directly applies

Link with **Schrödinger semigroups** exp(- tH_{st}), and the transformation of the Fokker-Planck equation into the Schrödinger-type equation

A detour: (phase-space) Brownian motion in a magnetic field versus spatial nonconservative processes - explicit N=3 examples

(Czopnik, Garbaczewski: Phys Rev. E 2001, Physica A 2003)

We skip the original phase-space derivations of Phys. Rev. E 63, 0121105, (2001) , and adopt (albeit with suitable adjustments) the arguments of Physica A 317, 448, (2003).

Example 1: curl (.) ≠ 0 drift

$$d\vec{X}(t) = \vec{A}(\vec{X}(t))dt + d\vec{W}(t)$$

where the former drift $\vec{F}(\vec{x})$ is replaced by $\vec{A}(\vec{x}) = (B/2)(-x_2, x_1, 0)$

We infer

$$\partial_t \rho = \frac{1}{2}\Delta\rho - \vec{\nabla}(\vec{A}\rho),$$

$$\vec{A}(\vec{x}(t)) = +\Lambda\vec{x}(t)$$

$$\Lambda = \begin{pmatrix} 0 & -B/2 & 0 \\ B/2 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

The transition probability density function reads

$$p(\vec{y}, s, \vec{x}, t) = \left(\frac{1}{2\pi(t-s)}\right)^{3/2} \exp\left[-\frac{(\vec{x} - U(t-s)\vec{y})^2}{2(t-s)}\right]$$

$$U(t) = \begin{pmatrix} cos(Bt/2) & -sin(Bt/2) & 0 \\ +sin(Bt/2) & cos(Bt/2) & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

Fully compatible with (tedious, technically demanding) N=2 path integration outcome of Wiegel and Ross, (1981)

The above transition pdf solves a pair of adjoint quations

$$\partial_t p(\vec{y}, s, \vec{x}, t) = L^*_{\vec{x}} p(\vec{y}, s, \vec{x}, t)$$

$$-\partial_s p(\vec{y}, s, \vec{x}, t) = L_{\vec{y}} p(\vec{y}, s, \vec{x}, t)$$

where (we note that $\vec{\nabla} \cdot \vec{A} = 0$)

$$L^* = \frac{1}{2}\Delta - \vec{A}\vec{\nabla} = \frac{1}{2}(\vec{\nabla} - \vec{A})^2 - \mathcal{V}$$

$$L = \frac{1}{2}\Delta + \vec{A}\vec{\nabla} = \frac{1}{2}(\vec{\nabla} + \vec{A})^2 - \mathcal{V}$$

with $\mathcal{V} = \vec{A}^2 = (B^2/4)(x^2 + y^2)$.

Accordingly, the **Lagrangian entering the path integral formula for the Fokker-Planck transition pdf, reads**

$$\mathcal{L} = \frac{1}{2}\dot{\vec{x}}^2 - \dot{\vec{x}} \cdot \vec{A} + \frac{1}{2}\vec{A}^2 = \frac{1}{2}\left[\dot{\vec{x}} - \vec{A}(\vec{x}(\tau))\right]^2,$$

while the related Markovian semigroup exp (- Ht) has the (non-Hermitian) generator

$$H = -\frac{1}{2}(\vec{\nabla} - \vec{A})^2 + \frac{1}{2}\vec{A}^2.$$

$$L^* = -H.$$

Example 2: Relaxation with steady current

$\vec{F} = \vec{A} - \vec{x} = \vec{A} - \vec{\nabla}\phi.$

$\vec{A} = (B/2)(-y, x, 0),\ \vec{x} = (x, y, z)$ and $\phi = \vec{x}^2/2.$

$$\mathcal{L}(\vec{x}(\tau), \dot{\vec{x}}(\tau)) = \frac{1}{2}\dot{\vec{x}}^2(\tau) - \dot{\vec{x}}(\tau)\cdot\vec{F}(\vec{x}(\tau)) + \mathcal{V}(\vec{x}(\tau)$$

$$p(\vec{y}, s, \vec{x}, t) = \left[\pi(1 - e^{-2(t-s)})\right]^{-3/2} \exp\left(-\frac{(\vec{x} - e^{-(t-s)}U(t-s)\vec{y})^2}{(1 - e^{-2(t-s)})}\right)$$

The Fokker-Plack operator L^* appears in the functional form $L^* = -H.$

$$L^* = \frac{1}{2}\Delta - \vec{F}\cdot\vec{\nabla} + 3 = \frac{1}{2}(\vec{\nabla} - \vec{F})^2 - \mathcal{V},$$
$$\mathcal{V} = \frac{1}{2}(\vec{F}^2 - 3) = \frac{\vec{A}^2}{2} + \frac{1}{2}(\vec{x}^2 - 3).$$

Since $\vec{A} = (B/2)(-y, x, 0)$, we have $\vec{\nabla}\cdot\vec{A} = 0$, in conjunction with $\phi(\vec{x}) = \vec{x}^2/2$

Hence, we have the stationary pdf : $\rho_*(\vec{x}) = \pi^{-3/2}\exp(-\vec{x}^2)$

and the coexisting divergenceless steady current $j_*(\vec{x}) = \vec{A}(\vec{x})\,\rho_*(\vec{x}).$

Example 3: No $\vec{A}$. $\vec{F} = -\vec{\nabla}\phi = -\vec{x}$ $\mathcal{L} = \frac{1}{2}(\dot{\vec{x}} - \vec{F})^2 + \vec{\nabla}\cdot\vec{F}$

$\phi(\vec{x}) = \vec{x}^2/2$, we can rewrite $\mathcal{L}$ in the form $\mathcal{L} = \frac{1}{2}(\dot{\vec{x}} + \vec{x})^2 - \frac{3}{2}$.

Since now $\vec{F} = -\vec{x}$, we have $\nabla\vec{F} = -3$, and hence $\mathcal{V} = (1/2)\vec{x}^2 - 3/2$

$$L^* = \frac{1}{2}\Delta - \vec{F}\cdot\vec{\nabla} - (\vec{\nabla}\cdot\vec{F}) = \frac{1}{2}(\vec{\nabla} - \vec{F})^2 - \mathcal{V},$$

$$p(\vec{y}, s, \vec{x}, t) = [\pi(t-s)]^{-3/2} \exp\left(-\frac{(\vec{x} - e^{-(t-s)}\vec{y})^2}{(1 - e^{-2(t-s)})}\right)$$

(Ornstein-Uhlenbeck)

This transition pdf is intimately intertwined with the integral kernel of $\exp(-tH)$, where H is (rescaled) quantum harmonic oscillator Hamiltonian

$$p(\vec{y}, s, \vec{x}, t) = e^{3(t-s)/2}\, k(\vec{y}, s, \vec{x}, t)\frac{\phi_1(x)}{\phi_1(y)},$$

where $\Phi_1(\vec{x}) = \pi^{-3/2}\exp(-\vec{x}^2)$, is the ground state function, while the factor $3/2$ in the exponent is the lowest eigenvalue of $H = (1/2)(-\Delta + \vec{x}^2)$.

The function $k(\vec{y}, s, \vec{x}, t)$ is the integral kernel of $\exp[-(t-s)H]$. Setting s=0 we may write

$$k(\vec{y}, \vec{x}, t) = \exp(-3t/2)(\pi[1 - \exp(-2t)])^{-3/2} \exp\left[\frac{1}{2}(\vec{x}^2 - \vec{y}^2) - \frac{(\vec{x} - e^{-t}\vec{y})^2}{(1 - e^{-2t})}\right],$$

$$= (2\pi\sinh t)^{-3/2}\ \exp\left[-\frac{(\vec{x}^2 + \vec{y}^2)\cosh t - 2\vec{x}\cdot\vec{y}}{2\sinh t}\right].$$

In **Example 1,** we have associated the random dynamics $d\vec{X}(t) = \vec{A}(\vec{X}(t))dt + d\vec{W}(t)$

with exp(- tH), where $H = -\frac{1}{2}(\vec{\nabla} - \vec{A})^2 + \frac{1}{2}\vec{A}^2.$ while remembering that $L^* = -H.$

$$H_{Eucl} = -(L^* + \mathcal{V}) = -\frac{1}{2}(\vec{\nabla} - \vec{A})^2 = -\frac{1}{2}\Delta + \vec{A}\cdot\vec{\nabla} - \frac{1}{2}\vec{A}^2,$$
$$H^*_{Eucl} = (L + \mathcal{V}) = -\frac{1}{2}(\vec{\nabla} + \vec{A})^2 = -\frac{1}{2}\Delta - \vec{A}\cdot\vec{\nabla} - \frac{1}{2}\vec{A}^2,$$

non-Hermitian Hamiltonians can be mapped into each other by changing the sign of $\vec{A}$

H_{Eucl} and H^*_{Eucl} are Euclidean analogues of standard Hermitian operators, appropriate for the quantum Schrödinger dynamics with the minimal electromagnetic coupling:

$$H^+_{quant} = -(1/2)(\vec{\nabla} + i\vec{A})^2 \text{ and } H^-_{quant} = -(1/2)(\vec{\nabla} - i\vec{A})^2$$

Note: Formally replacing $\vec{A}$ by $-i\vec{A}$ in the above operators, we arrive (respectively) at

$$H^*_{Eucl} = -\frac{1}{2}(\vec{\nabla} + \vec{A})^2 \qquad H_{Eucl} = -\frac{1}{2}(\vec{\nabla} - \vec{A})^2$$

Both quantum mechanical operators are Hermitian, and actually refer to different QM problems (sign difference of vector potentials can be related to the sign of involved charges). They belong to the functional analytic inventory of **„Schrödinger operators with magnetic fields"** and related operator semigroups, c.f. Avron, Herbst, Simon (1978), with a numer of independent derivations of their integral kernels.
The pertinent semigroup ntegral kernels have been first derived **as (unnormalized) „density matrices"** in the study of the **diamagnetism of free electrons**, c.f. Sonderheimer, Wilson (1951), c.f. also Glasser (1964) for an explicit path integral derivation.

Path integral temptation (handle $H_{Eucl} = -\frac{1}{2}(\vec{\nabla} - \vec{A})^2$), to resist or to give in ?

We are interested in transition probability solutions of Fokker-Planck equations (with Dirac delta initial data). **They need to be positive definite functions.** If interpreted in conjunction with propagators of Markovian semigroups (e.g. with Hamiltonian-type generators), the latter **need to be positive** as well. (The nonnegative case is more intricate and is not considered here.)

Given the quantum mechanical motion operator exp(-iHt) (up to scaled away dimensional constants) . Its „naive" Euclidean version is exp(-Ht). In the thermally-rescaled form exp(-βH) with $\beta \sim 1/kT$, the corresponding propagator is interpreted as an (unnormalized) „density matrix". **Such functions not necessarily are positive, and may even be complex** ! Then, **no link can be established with transition probability densities of the (anticipated as Fokker-Planck related) diffusion process.**

An archival retour – „Diamagnetism of free electrons", 1951- 1964

2·1. The Schrödinger equation for the stationary states E_i of a free electron in a constant magnetic field **H** is

$$\mathscr{H}\psi_i(\mathbf{r}) = \left\{-\frac{h^2}{8\pi^2 m}\nabla^2 + \frac{\epsilon h}{2\pi i m c}\mathbf{A}.\mathrm{grad} + \frac{\epsilon^2\mathbf{A}^2}{2mc^2}\right\}\psi_i(\mathbf{r}) = E_i\psi_i(\mathbf{r}), \qquad (1)$$

where $\mathscr{H}$ is the Hamiltonian operator, $\mathbf{A} = \frac{1}{2}\mathbf{H}\times\mathbf{r}$ is the vector potential, $-\epsilon$ is the charge and m the mass of an electron, and the remaining symbols have their usual meanings.

Consider the expression $e^{-\mathscr{H}/kT}\psi_i$, which is to be interpreted as

$$e^{-\mathscr{H}/kT}\psi_i = \sum_{n=0}^{\infty} \frac{1}{n!}\frac{(-1)^n}{(kT)^n}\mathscr{H}^n\psi_i.$$

Now put $\gamma = 1/kT$, and let

$$\Psi(\mathbf{r}',\mathbf{r},\gamma) = \sum_i \psi_i(\mathbf{r}')^* e^{-\gamma\mathscr{H}}\psi_i(\mathbf{r}),$$

so that

$$Z = \int \Psi(\mathbf{r},\mathbf{r},\gamma)\,d\tau.$$

The calculation of Z is thus reduced to the calculation of the quantity $\Psi(\mathbf{r}',\mathbf{r},\gamma)$, which is known as the density matrix. It satisfies the Schrödinger equation

$$-\partial\Psi/\partial\gamma = \mathscr{H}\Psi, \tag{5}$$

as is obvious by differentiating (3) and noting that $\mathscr{H}$ operates on $\psi_i(\mathbf{r})$ only. Further,

$$\Psi(\mathbf{r}',\mathbf{r},0) = \sum_i \psi_i(\mathbf{r}')^*\psi_i(\mathbf{r}) = \delta(\mathbf{r}-\mathbf{r}'), \tag{6}$$

2·3. If the magnetic field is taken along the z axis, the vector potential is $(-\tfrac{1}{2}Hy, \tfrac{1}{2}Hx, 0)$, and the equation for $\Psi(\mathbf{r}',\mathbf{r},\gamma)$ takes the form

$$\frac{\partial\Psi}{\partial\gamma} = \left\{\frac{h^2}{8\pi^2 m}\nabla^2 - \frac{\epsilon hH}{4\pi imc}\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right) - \frac{\epsilon^2H^2}{8mc^2}(x^2+y^2)\right\}\Psi. \tag{8}$$

When $H = 0$, this equation is formally identical with the differential equation of conduction of heat

$$\frac{\partial v}{\partial t} = \kappa\nabla^2 v$$

$$\Psi(\mathbf{r}',\mathbf{r},\gamma)_{H=0} = \left(\frac{2\pi m}{h^2\gamma}\right)^{\frac{3}{2}} \exp\left[-\frac{2\pi^2 m}{h^2\gamma}\{(x-x')^2+(y-y')^2+(z-z')^2\}\right].$$

The general solution is therefore

$$\Psi(\mathbf{r}',\mathbf{r},\gamma) = \left(\frac{2\pi m}{h^2\gamma}\right)^{\frac{3}{2}} \frac{\mu_0 H\gamma}{\sinh(\mu_0 H\gamma)} \exp\left[-\frac{2\pi^2 m}{h^2\gamma}\{2i\mu_0 H\gamma(x'y-y'x) + \mu_0 H\gamma \coth(\mu_0 H\gamma)((x-x')^2+(y-y')^2)+(z-z')^2\}\right], \quad (12)$$

where $\mu_0 = eh/(4\pi mc)$ is the Bohr magneton. If Z is the partition function per unit volume, it follows that

$$Z = \Psi(\mathbf{r},\mathbf{r},\gamma) = \left(\frac{2\pi m}{h^2\gamma}\right)^{\frac{3}{2}} \frac{\mu_0 H\gamma}{\sinh(\mu_0 H\gamma)}. \quad (13)$$

$$H(\vec{A}) = -\tfrac{1}{2}(\vec{\nabla} - i\vec{A})^2,$$

$$\vec{A} = \{-(B/2)x_2, +(B/2)x_1, 0\}$$

Borrowed from PRE **55** (2), 1401, (1997), P.G. et al.

Explicit complex term !

$$\exp[-tH(\vec{A})](\vec{x},\vec{y}) = \frac{B}{4\pi\sinh(\frac{1}{2}Bt)}\left(\frac{1}{2\pi t}\right)^{1/2} \times \exp\left\{-\frac{1}{2t}(x_3-y_3)^2 - \frac{B}{4}\coth\left(\frac{B}{2}t\right) \times [(x_2-y_2)^2+(x_1-y_1)^2] - i\frac{B}{2}(x_1y_2-x_2y_1)\right\}. \quad (28)$$

We recall: given $H(\vec{A}) = -\frac{1}{2}(\vec{\nabla} - i\vec{A})^2$, **replacing** $\vec{A}(\vec{x})$ by $[-i\vec{A}(\vec{x})]$ one arrives at

$H_{Eucl} = -\frac{1}{2}(\vec{\nabla} - \vec{A})^2$. Since $\vec{A} = \{-(B/2)x_2, +(B/2)x_1, 0\}$, the replacement may be accomplished

by setting – iB instead of B in the previous propagator formula. Accordingly: $\exp[-tH_{Eucl}](\vec{x},\vec{y})$ **formally acquires** the functional form

$$k(\vec{y},s,\vec{x},t) = \frac{B}{4\pi \sin[\frac{1}{2}B(t-s)]}\left(\frac{1}{2\pi(t-s)}\right)^{1/2}$$
$$\times \exp\left\{-\frac{1}{2(t-s)}(x_3-y_3)^2 - \frac{B}{4}\cot\left(\frac{B}{2}(t-s)\right)[(x_2-y_2)^2+(x_1-y_1)^2] - \frac{B}{2}(x_1y_2-x_2y_1)\right\}$$

This function is defective from our point of view (**positive kernel requirement** !) since may take **negative values** beyond the time interval $0 \leq$ t-s $\leq \pi/B$.

For reference:
c. f. Avron Herbst,Simon, (1978)

$$\exp(-tH_{quant})(\vec{y},\vec{x}) = \frac{B}{4\pi\sinh(Bt/2)}\left(\frac{1}{2\pi t}\right)^{1/2} \cdot$$
$$\exp\left\{(iB/2)(-x_1y_2 + x_2y_1) - \frac{B}{4}\left[(y_1-x_1)^2 + (y_2-x_2)^2\right]\coth(Bt/2) - \frac{(y_3-x_3)^2}{2t}\right\}$$

$t \to it$

c. f. Feyman-Hibbs (1965)

$$\exp(-itH_{quant})(\vec{y},\vec{x}) = \left(\frac{1}{2\pi it}\right)^{3/2}\left(\frac{B/2}{\sin(Bt/2)}\right) \cdot$$
$$\exp\left\{(i/2)\left[B(-x_1y_2 + x_2y_1) - [(y_1-x_1)^2 + (y_2-x_2)^2]\frac{B/2}{\tan(Bt/2)} - \frac{(y_3-x_3)^2}{t}\right]\right\}$$

An explicit (detailed) path integral derivation of $\exp[-tH_{Eucl}](\vec{x},\vec{y})$
can be found in in P. Garbaczewski and M. Żaba, **arXiv: 2302.10154**

To evaluate the propagator of $\exp(-H_{Eucl}t)(\vec{y},\vec{x}) = k(\vec{y},0,\vec{x},t)$, with $H_{Eucl} = -\frac{1}{2}(\vec{\nabla} - \vec{A})^2$ we choose $\vec{A} = [-y, x, 0]$, so that $\vec{B} = \frac{1}{2}\left(\nabla \times \vec{A}\right) = (0,0,1)$

$$\mathcal{L}_{Eucl} = \frac{\dot{\vec{x}}^2}{2} - \dot{\vec{x}} \cdot \vec{A}.$$

Path integrals associated with quadratic Lagrangians can be evaluated analytically.

$$k(\vec{y},0,\vec{x},t) = \frac{1}{2\pi|\sin(t)|}\left(\frac{1}{2\pi t}\right)^{1/2} \exp\left\{-x_1y_2 + x_2y_1 - \frac{1}{2}\left[(y_1-x_1)^2 + (y_2-x_2)^2\right]\cot t - \frac{(y_3-x_3)^2}{2t}\right\}$$

$$\int k(\vec{z},0,\vec{y},s)k(\vec{y},s,\vec{x},t)d^3y =$$

$$\frac{1}{(2\pi)^{3/2}}\frac{1}{\sqrt{t}}\frac{\sin s}{|\sin s|}\frac{\sin(t-s)}{|\sin(t-s)|}\frac{1}{\sin t}\exp\left\{-x_1z_2 + x_2z_1 - \frac{1}{2}\left[(z_1-x_1)^2 + (z_2-x_2)^2\right]\cot t - \frac{(z_3-x_3)^2}{2t}\right\}.$$

Obstacles: (i) the kernel is positive, but |sin(t)| and cot t create serious problems, (ii) the semigroup composition rule is valid only when simultaneously sin s and sin(t-s) are positive .

First conclusion:

A consistent path integral analysis of nonconservative diffusion processes cannot be performed for the „bare" generator $(1/2)(\vec{\nabla} \mp \vec{A})^2 : -H_{Eucl}$ (e.g. $L^* - \mathcal{V}$) . We have no link with a legitimate Markovian diffusion scenario valid for all times t $\geq$ 0.

Qiery:

The path integration approach proves to be consistent for

$$H_{magn} = e^{\phi} H e^{-\phi} = -\frac{1}{2}(\vec{\nabla} - \vec{A})^2 + \mathcal{V}.$$

and its adjoint partner. **Is there anything more general in existence ?**

Answer (second conclusion):

Yes, but **it derives** from the general framework of so-called Euclidean Quantum Mechanics due to J.- C. Zambrini (1986 – 2023), specifically Cruzeiro, Zambrini (1991).

More details can be found in: *P. Garbaczewski and M. Żaba,* ***arXiv: 2302.10154***

One more N=1 detour: Schrödinger's two-gate interpolation problem

problem, originally due to Schrödinger : *given two strictly positive (on an open interval) boundary probability distributions $\rho_0(x), \rho_T(x)$ for a process with the time of duration $T \geq 0$. Can we uniquely identify the stochastic process interpolating between them?*

$$m(A,B) = \int_A dx \int_B dy\, m(x,y)$$

$$\int dy\, m(x,y) = \rho_0(x)$$

$$\int dx\, m(x,y) = \rho_T(y)$$

$$m(x,y) = \Theta_*(x,0)\, k(x,0,y,T)\, \Theta(y,T)$$

A Markovian diffusion can be uniquely retrieved from the two-gate formula , if we have at our disposal a bounded strictly positive (semigroup) integral kernel function $k(x,s,y,t)$

$$\Theta_*(x,t) = \int k(0,y,x,t)\Theta_*(y,0)dy$$

$$\Theta(x,s) = \int k(s,x,y,T)\Theta(y,T)dy$$

$$\rho(x,t) = (\Theta_* \Theta)$$

$t \in [0,T]$

Sketchy outline of the more general framework (N=3)

We generalize previous adjoint pairs of equations with non-Hermitian generators

$$\partial_t p(\vec{y}, s, \vec{x}, t) = -H_{\vec{x}} p(\vec{y}, s, \vec{x}, t),$$
$$\partial_s p(\vec{y}, s, \vec{x}, t) = H^*_{\vec{y}} p(\vec{y}, s, \vec{x}, t).$$

Consider perturbations of „bare” Euclidean generators by scalar potentials

$$H_{Eucl} \Longrightarrow H = H_{Eucl} + \mathcal{U},$$
$$H^*_{Eucl} \Longrightarrow H^* = H^*_{Eucl} + \mathcal{U},$$

which might guarrantee, through a suitable choice of $\mathcal{U}$ (encompassing $\mathcal{U} \equiv \mathcal{V}$) that the operator H induces a legitimate (contractive ?) semigroup exp[-(t-s)H] in the time interval [0,T], with s<t . Actually, we presume that $\exp[-(t-s)H](\vec{y}, \vec{x}) = k(s, \vec{y}, s, \vec{x}, t)$ is jointly continuous, strictly positive and obeys the semigroup composition law (the Chapman-Kolmogorov relation analog).

To establish a direct link with Cruzeiro, Zambrini (1991) paper, we must account for their form of the Euclidean mapping : $\vec{A} \rightarrow i\vec{A}$ results in $H_{quant} = -\frac{1}{2}(\vec{\nabla} - i\vec{A})^2 \rightarrow H^*_{Eucl} = -\frac{1}{2}(\vec{\nabla} + \vec{A})^2$, hence **we need to change the sign of** $\vec{A}$, **so that the roles of H-generators do interchange**

$$\theta^*(\vec{x}, t) = \int \theta^*(\vec{y}, 0) k(\vec{y}, 0, \vec{x}, t) d^3y \Longrightarrow \partial_t \theta^*(\vec{x}, t) = -H^* \, \theta^*(\vec{x}, t),$$

$$\theta(\vec{x}, t) = \int k(\vec{x}, t, \vec{y}, T) \theta(\vec{y}, T) d^3y \Longrightarrow \partial_t \theta(\vec{x}, t) = H \, \theta(\vec{x}, t).$$

The **outcome,** actually a **solution of the Schrödinger interpolation and boundary-data problem,** is (reflects the change of sign of the vector potential in the analysis of Cruzeiro, Zambrini,), compare e.g. P. G. et al., Phys. Rev E 55(2), 1401, (1997)):

$$d\vec{X}(t) = \left[\frac{\vec{\nabla}\theta(\vec{X}(t),t)}{\theta(\vec{X}(t),t)} + \vec{A}(\vec{X}(t))\right] dt + d\vec{W}(t)$$

Diffusion pdf $\rho = \theta^* \theta$ $\vec{b}(\vec{x},t) = \vec{\nabla} \ln \theta(\vec{x},t) + \vec{A}(\vec{x}),$ forward drift

$$\partial_t \rho = -\vec{\nabla} \cdot [(\vec{b} - \vec{\nabla} \ln \rho^{1/2})\rho(\vec{x},t)]$$ F-P equation

$$\partial_t \rho = -\vec{\nabla}(\rho \vec{v}),$$
$$\partial_t \vec{v} + (\vec{v} \cdot \vec{\nabla})\vec{v} = -\vec{v} \times \vec{B} + \vec{\nabla}\mathcal{U}.$$

diffusion current

$\vec{B} = \vec{\nabla} \times \vec{A}.$ $\vec{v} = \frac{1}{2}\vec{\nabla} \ln \frac{\theta}{\theta_*} + \vec{A}.$ current velocity

$$p(\vec{y},s,\vec{x},t) = k(\vec{y},s,\vec{x},t)\frac{\theta(\vec{x},t)}{\theta(\vec{y},s)}$$ transition pdf

Appendix on the current non-Hermitian fashions

Review

Non-Hermitian Physics

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A review is given on the foundations and applications of non-Hermitian classical and quantum physics. First, key theorems and central concepts in non-Hermitian linear algebra, including Jordan normal form, biorthogonality, exceptional points, pseudo-Hermiticity and parity-time symmetry, are delineated in a pedagogical and mathematically coherent manner. Building on these, we provide an overview of how diverse classical systems, ranging from photonics, mechanics, electrical circuits, acoustics to active matter, can be used to simulate non-Hermitian wave physics. In particular, we discuss rich and unique phenomena found therein, such as unidirectional invisibility, enhanced sensitivity, topological energy transfer, coherent perfect absorption, single-mode lasing, and robust biological transport. We then explain in detail how non-Hermitian operators emerge as an effective description of open quantum systems on the basis of the Feshbach projection approach and the quantum trajectory approach. We discuss their applications to physical systems relevant to a variety of fields, including atomic, molecular and optical physics, mesoscopic physics, and nuclear physics with emphasis on prominent phenomena/subjects in quantum regimes, such as quantum resonances, superradiance, continuous quantum Zeno effect, quantum critical phenomena, Dirac spectra in quantum chromodynamics, and nonunitary conformal field theories. Finally, we introduce the notion of band topology in complex spectra of non-Hermitian systems and present their classifications by providing the proof, firstly given by this review in a complete manner, as well as a number of instructive examples. Other topics related to non-Hermitian physics, including nonreciprocal transport, speed limits, nonunitary quantum walk, are also reviewed.

Keywords: non-Hermitian systems; nonunitary dynamics; photonics; mechanics; acoustics; electrical circuits; open quantum systems; quantum optics; quantum many-body physics; dissipation; topology; bulk-edge correspondence; topological invariants; edge mode; nonreciprocal transport; quantum walk

Contents

Table 1. A wide variety of classical and quantum systems described by non-Hermitian matrices/operators together with their physical origins of non-Hermiticity, presented in order of appearance in the present review.

Systems / Processes	Physical origin of non-Hermiticity	Theoretical methods
Photonics	Gain and loss of photons	Maxwell equations [12, 13]
Mechanics	Friction	Newton equation [14, 15]
Electrical circuits	Joule heating	Circuit equation [16]
Stochastic processes	Nonreciprocity of state transitions	Fokker-Planck equation [17, 18]
Soft matter and fluid	Nonlinear instability	Linearized hydrodynamics [19–21]
Nuclear reactions	Radiative decays	Projection methods [4–6]
Mesoscopic systems	Finite lifetimes of resonances	Scattering theory [22, 23]
Open quantum systems	Dissipation	Master equation [24, 25]
Quantum measurement	Measurement backaction	Quantum trajectory approach [26–31]

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