Numerical integration of complex SDEs

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In density functional theory from an SDE viewpoint, we want

$$\langle f \rangle = \text{Tr}[f\rho] = \mathbf{E}f = \frac{\int f(x) e^{-S[x]}\, Dx}{\int e^{-S[x]}\, Dx}.$$

$S[x] = H/kT$ is usually $\beta \cdot$ energy, and the $\dim(x)$ is large: $Dx = d^n x$. Yang & Lee (1952) studied properties of

$$Z = \int e^{-S[x]}\, Dx$$

for complex $\beta = 1/kT$. If $\beta = it$ and $S = \int_0^t L[x(s)]ds$, we get Feynman's version of QM. Z is a lot of work and can be awkward. In principle, a simpler procedure (Nelson 1983, Parisi 1981) is

$$\mathbf{E}f = \frac{1}{T} \int_0^T f(X(t))dt$$

for large T. $X(t)$ is a complex process with SDE

$$dX = -\frac{1}{2} \frac{\partial S}{\partial X} dt + d\omega(t).$$

So, what is Brownian motion?

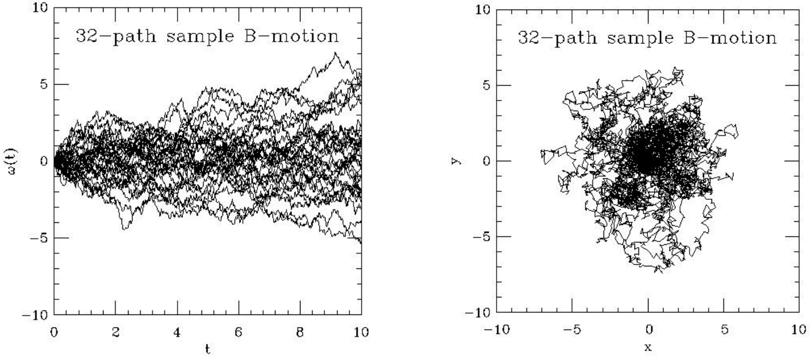

Figure: Left: 1-D Brownian motion, Right: 2-D Brownian motion

The probability density $p(x,t)$ ($\int p\,dx = 1$) for B-motion satisfies heat equation:

$$\frac{\partial p(\omega,t)}{\partial t} = \frac{1}{2}\frac{\partial^2 p(\omega,t)}{\partial \omega^2}.$$

What is $\omega(t)$? It is a sum of increments, each scaling like $(\Delta t)^{1/2}$

$$\omega(t_n) = \sum_{k\le n} \Delta\omega_k,$$

and

$$\mathbf{E}\{\Delta\omega_i \Delta\omega_j\} = \delta_{ij}\Delta t.$$

The infinitesimal version of this is

$$\begin{aligned} \mathbf{E} d\omega(t) &= 0 \\ \mathbf{E}\{d\omega(t)\, d\omega(s)\} &= \delta(t-s)\, dt\, ds. \end{aligned}$$

Example, systems ($m \geq 0$) which become stationary:

$$dx = -x|x|^{m-1}dt + d\omega(t)$$

have solutions whose distribution law satisfies Kolmogorov's forward equation

$$\frac{\partial p(x,t)}{\partial t} = \frac{\partial}{\partial x}\left(\frac{1}{2}\frac{\partial}{\partial x} + x|x|^{m-1}\right) p(x,t) \to 0$$

when $t \to \infty$. Density $p(x, t \to \infty)$, properly normalized, is

$$p(x,\infty) = N_m e^{-\frac{2}{m+1}|x|^{m+1}}.$$

Two examples:

$$\begin{aligned} p(x,\infty) &= e^{-2|x|} && \text{for } m = 0, \\ p(x,\infty) &= \tfrac{1}{\sqrt{\pi}} e^{-|x|^2} && \text{for } m = 1. \end{aligned}$$

In quantum systems, where we are interested in complex processes, R.J. Glauber (1963) suggested the following *coherent states* representation:

$$\rho = \int P_t(\alpha)\Lambda_\alpha d^2\alpha,$$

using the basis

$$\Lambda_\alpha = |\alpha\rangle\langle\alpha|$$

of coherent states

$$|\alpha\rangle = e^{-|\alpha|^2/2} e^{\alpha a^\dagger}|0\rangle.$$

These states are **over complete** - only the diagonal elements needed. The dynamics are from the canonical von Neumann relation ($\hbar = 1$)

$$\dot{\rho} = i[\rho, H].$$

For a single mode BEC situation, the Hamiltonian is

$$H = \frac{1}{2}(a^\dagger a)^2.$$

The idea: take Glauber & Sudarshan's representation (1968), form the dynamical equations, and get a PDE for $P_t(\alpha)$. Using the canonical commutation relation $[a, a^\dagger] = 1$,

$$a^\dagger a \|\alpha\rangle = \alpha \frac{\partial}{\partial \alpha} \|\alpha\rangle$$

where

$$|\alpha\rangle = e^{-|\alpha|^2/2} \|\alpha\rangle$$

in terms of the un-normalized Bargmann states

$$\|\alpha\rangle = e^{\alpha a^\dagger} |0\rangle$$

Integrating by parts, and the notation

$$Q = e^{-|\alpha|^2} P$$

we almost get a Fokker-Planck equation

$$\frac{\partial}{\partial t} Q = \frac{i}{2} \left[(\partial_{\bar{\alpha}} \bar{\alpha})^2 Q - (\partial_\alpha \alpha)^2 Q \right].$$

After some manipulation, and writing α in terms of its real/imaginary parts,

$$\alpha = x_1 + ix_2,$$

we get our Fokker-Planck equation:

$$\frac{\partial}{\partial t}P = (\partial_2 x_1 - \partial_1 x_2)|\alpha|^2 P + \frac{1}{2}(\partial_1 x_2 - \partial_2 x_1)P + \frac{1}{2}\sum_{j,k=1}^{2} \partial_j \partial_k \left[a_{jk} P\right].$$

Notation: $\partial_i = \frac{\partial}{\partial x_i}$, for $i = 1, 2$. The *diffusion* matrix $A = [a_{ij}]$ is

$$\begin{bmatrix} x_1 x_2 & \frac{1}{2}(x_2^2 - x_1^2) \\ \frac{1}{2}(x_2^2 - x_1^2) & -x_1 x_2 \end{bmatrix} = \begin{bmatrix} \frac{1}{2}Im[\alpha^2] & -\frac{1}{2}Re[\alpha^2] \\ -\frac{1}{2}Re[\alpha^2] & -\frac{1}{2}Im[\alpha^2] \end{bmatrix}.$$

Fundamental problem: matrix A is **not** positive definite: eigenvalues of A are $\pm\frac{1}{2}|\alpha|^2$.

Let's go on, pretending we had good sense. First idea: project the flow onto stable directions in the positive eigenspace.

$$\begin{aligned} A &= U \begin{pmatrix} \frac{1}{2}|\alpha|^2 & 0 \\ 0 & -\frac{1}{2}|\alpha|^2 \end{pmatrix} U^T \xrightarrow{P} \frac{1}{2}|\alpha|^2 U \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} U^T \\ &= A'. \end{aligned}$$

To get the term $\sigma d\omega$ in the SDE, with $d\omega = (d\omega_1, d\omega_2)^T$, set $A' = \sigma\sigma^T$ and $\theta = \phi - \pi/4$, $\phi = arg(\alpha)$,

$$\sigma = \frac{|\alpha|}{\sqrt{2}} \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}.$$

This projection is not unique. Any variant of $\sqrt{A'}$ will do.

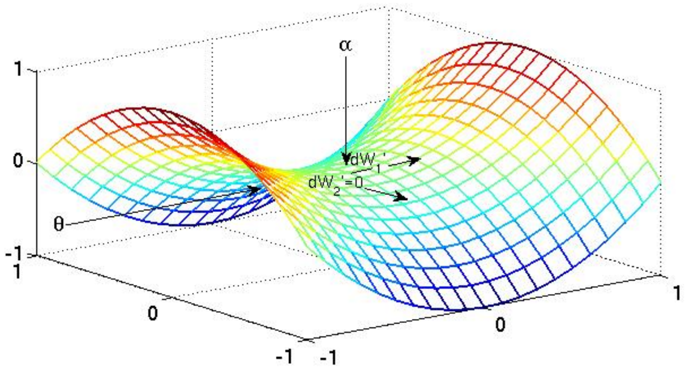

Figure: Stable and unstable fluctuations in the Brownian increment

Where $\phi = \arg(\alpha)$ is the phase of α, choice $\theta = \phi - \pi/4$ keeps $U \in O(2)$ in the subspace of A'. The positive eigenvalue equation is

$$\begin{pmatrix} \sin(2\phi) & -\cos(2\phi) \\ -\cos(2\phi) & -\sin(2\phi) \end{pmatrix} \begin{pmatrix} \cos(\theta) \\ \sin(\theta) \end{pmatrix} = \begin{pmatrix} \cos(\theta) \\ \sin(\theta) \end{pmatrix}.$$

That is,

$$\sin(2\phi - \theta) = \cos(\theta) \qquad \text{and} \qquad \cos(2\phi - \theta) = -\sin(\theta),$$

or $-ie^{2i\phi} = e^{2i\theta}$, with solution $\theta = \phi - \pi/4$. the resulting SDE is

$$d\alpha = -i(|\alpha|^2 + 1/2)\alpha dt + \nu\sqrt{-i/2}\,\alpha\, d\omega_1,$$

where $\nu = \cos(\psi)$ of arbitrary phase ψ. Notice the two singular points: $\alpha = 0$ and $\alpha = \infty$.

Unfortunately, the Brownian increment is not isotropic - it depends on $\phi = \arg\alpha$. All variants of $d\omega' = (d\omega'_1, d\omega'_2)^T$ of the form

$$d\omega' = \begin{pmatrix} \cos(\psi) & -\sin(\psi) \\ \sin(\psi) & \cos(\psi) \end{pmatrix} \begin{pmatrix} d\omega_1 \\ d\omega_2 \end{pmatrix},$$

are equally valid. Thus, we can make any choice $\nu = \cos(\psi)$, $\psi \sim U(0, 2\pi)$ uniformly. Even simpler, $\bar{\nu} = (\langle \cos^2(\psi) \rangle)^{1/2}$, which yields the complex SDE

$$d\alpha = -i(|\alpha|^2 + 1/2)\alpha dt + \frac{1}{2}\sqrt{-i}\,\alpha\, d\omega_1,$$

where $d\omega_1$ is the real component of a complex Brownian increment.

Now we need an integration algorithm, quite generally for the problem

$$dx(t) = b(x(t))dt + \sigma(x(t))d\omega(t),$$

here is a weak 2^{nd} order procedure which is trapezoidal rule stable. It uses 3 stages beginning at x_0:

$$x_{1/2} = x_0 + \frac{h}{4}(b(x_{1/2}) + b(x_0)), \text{ solve for } x_{1/2}, \tag{1a}$$

$$x_1 = x_{1/2} + \int_0^h \sigma(x(s))d\omega(s), \text{ starting at } x_{1/2}, \tag{1b}$$

$$x_h = x_1 + \frac{h}{4}(b(x_h) + b(x_1)), \text{ solve for } x_h. \tag{1c}$$

Another variant is from 1998 (wpp). Martingale step (1b) is described below. Also: see Denis Talay (1986).

$$
\begin{aligned}
x_1 \quad = \quad & x_{1/2} + \frac{1}{2}\{\sigma(x_{1/2} + \sqrt{\frac{1}{2}}\sigma(x_{1/2})\,\xi_0) \\
& \qquad + \sigma(x_{1/2} - \sqrt{\frac{1}{2}}\sigma(x_{1/2})\,\xi_0)\}\,\xi_1 \\
& + (\frac{\partial \sigma}{\partial x})(x_{1/2})\sigma(x_{1/2})\,\Xi.
\end{aligned}
$$

where $\xi_k = \sqrt{h} z_k$ are iid Gaussian RVs with mean zero and variance h. A needed stochastic integral is approximated by

$$
\begin{aligned}
I^{\epsilon\gamma} = \int_t^{t+h} \omega^{\epsilon}(s)\, d\omega^{\gamma}(s) \quad & \approx \quad \Xi^{\epsilon\gamma} \\
& = \quad \frac{h}{2}\,(z_1^{\epsilon} z_1^{\gamma} - \tilde{z}^{\epsilon\gamma}) \qquad \text{if } \epsilon > \gamma, \\
& = \quad \frac{h}{2}\,(z_1^{\epsilon} z_1^{\gamma} + \tilde{z}^{\gamma\epsilon}) \qquad \text{if } \epsilon < \gamma, \\
& = \quad \frac{h}{2}\,((z_1^{\epsilon})^2 - 1) \qquad \text{when } \epsilon = \gamma.
\end{aligned}
$$

Regardless of method, we need metrics to test it. We compared moments. Start with the harmonic oscillator basis

$$|k\rangle = \frac{1}{\sqrt{k!}}(a^\dagger)^k|0\rangle.$$

Completing the square and some algebra

$$\langle\alpha|e^{iHt}a^m e^{-iHt}|\alpha\rangle = \alpha^m \exp\left(|\alpha|^2(e^{-imt}-1) - i\frac{m^2 t}{2}\right).$$

These moments are not physical **observables**.

Here is where we started:

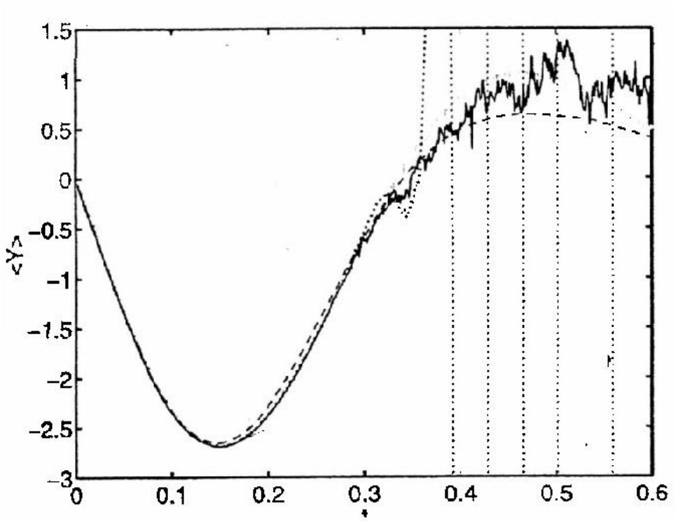

Figure: Im$\mathbf{E}[\alpha]$, Deuar and Drummond, Comp. Phys. Comm., 2001

So, what do these moments actually look like?

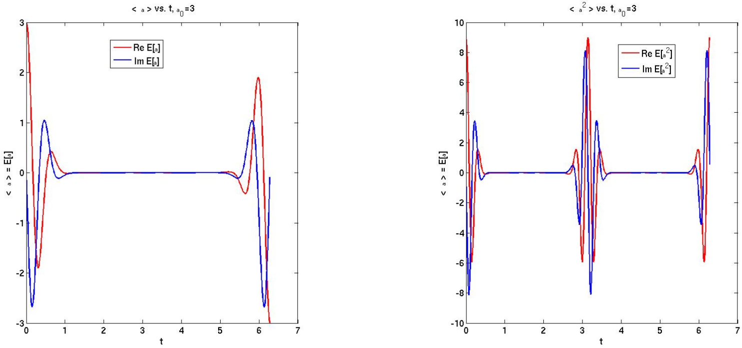

Figure: Left: $\mathbf{E}[\alpha]$, Right: $\mathbf{E}[\alpha^2]$

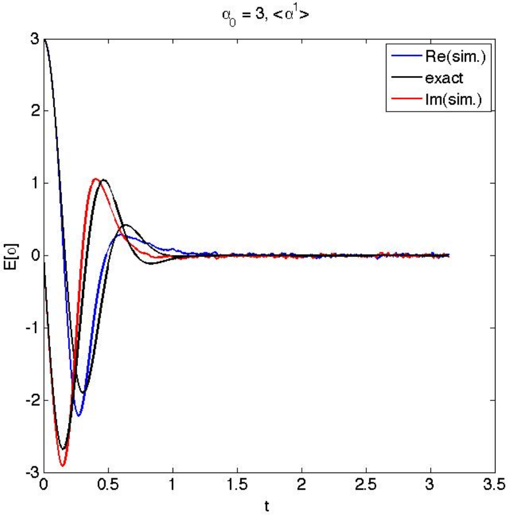

Figure: $\mathbf{E}[\alpha]$ using Glauber-Sudarshan rep. and projection

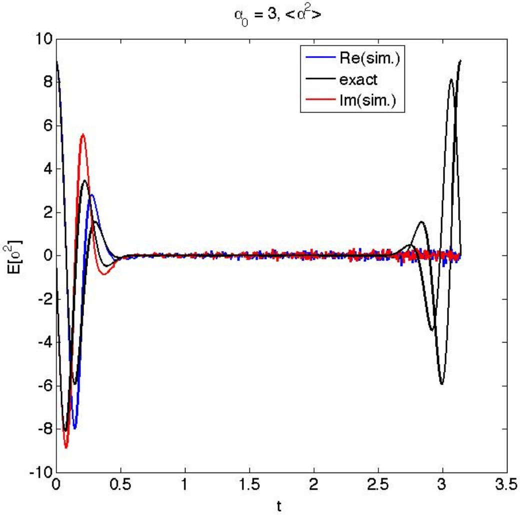

Figure: $\mathbf{E}[\alpha^2]$ using Glauber-Sudarshan rep. and projection

Glauber-Sudarshan results better, but unsatisfactory. Next idea: Deuar and Drummond. Treat α and $\beta = \bar{\alpha}$ separately. SDEs are

$$d\alpha = -i(\bar{\beta}\alpha + 1/2)\alpha dt + \sqrt{-i}\alpha d\omega_1 \tag{2a}$$
$$d\beta = -i(\bar{\alpha}\beta + 1/2)\beta dt + \sqrt{-i}\beta d\omega_2. \tag{2b}$$

Related singular pts. $\alpha = 0$, $\beta = \infty$, and $\beta = 0$, $\alpha = \infty$.

$$\begin{aligned} d\alpha &= -i(\bar{\beta}\alpha + 1/2)\alpha dt \\ d\beta &= -i(\bar{\alpha}\beta + 1/2)\beta dt. \end{aligned}$$

Real α_0, β_0, $d\alpha/\alpha = -d\bar{\beta}/\bar{\beta}$, thus $\bar{\beta}\alpha = n_0$. Solutions

$$\alpha(t) = \alpha_0 e^{-i(n_0+1/2)t} \text{ and } \beta(t) = \beta_0 e^{-i(\bar{n}_0+1/2)t}.$$

Now perturb $n_0 \to n_0 + i\delta$.

$$\alpha(t) \to \alpha(t)e^{\delta t} \text{ and } \beta(t) \to \beta(t)e^{-\delta t}.$$

So, α grows, and $\beta \to 0$.

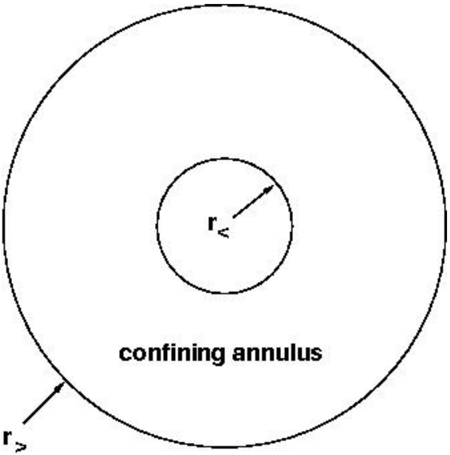

Figure: Annulus regularization: $r_<(\lambda), r_>(\lambda)$.

To control α, β, we need $r_< \leq |\alpha|, |\beta| \leq r_>$ parameterized by λ. A renormalization scheme (also Sidi's GREP)

$$\mathbf{E}[\alpha^m] = \frac{c_{-1}}{\lambda} + c_0 + \sum_{k \geq 1} c_k \lambda^k$$

wasn't very successful, so we settled for optimization: best fit to known $\mathbf{E}[\alpha]$ and compared $\mathbf{E}[\alpha^m]$ for $m > 1$.

$$r_< = \lambda \cdot |\alpha_0| \qquad r_> = \frac{|\alpha_0|}{\lambda^2}.$$

At time step t_k, if α_k is outside annulus:

	toroid	annulus
$\lvert\alpha\rvert > r_>$	$\alpha \to \frac{r_<}{r_>}\alpha$	$\alpha \to (2\frac{r_>}{\lvert\alpha\rvert} - 1)\alpha$
$\lvert\alpha\rvert < r_<$	$\alpha \to \frac{r_>}{r_<}\alpha$	$\alpha \to (2\frac{r_<}{\lvert\alpha\rvert} - 1)\alpha$

Figure: Artificial boundary conditions for $\alpha - \beta$ equations.

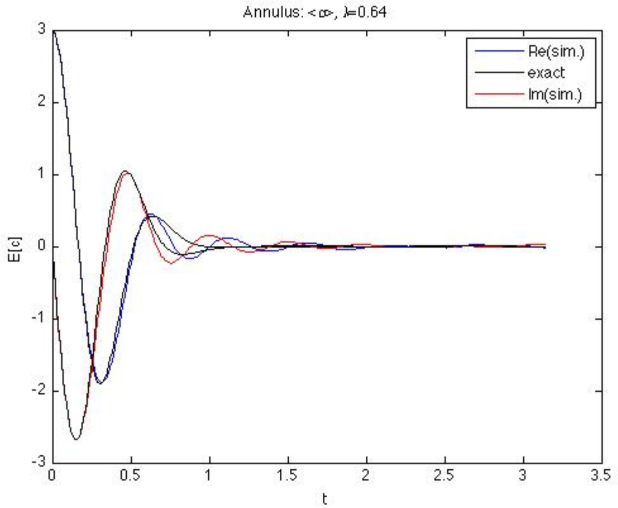

Figure: $\mathbf{E}[\alpha]$ using annulus regularization: $\lambda = 0.64$

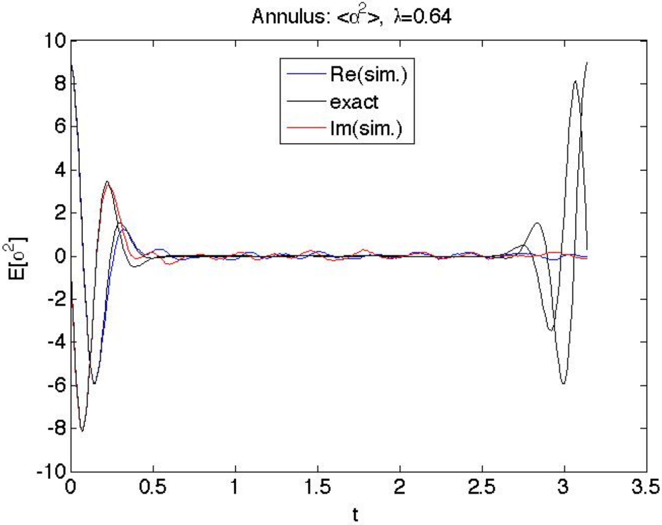

Figure: $\mathbf{E}[\alpha^2]$ using annulus regularization: $\lambda = 0.64$

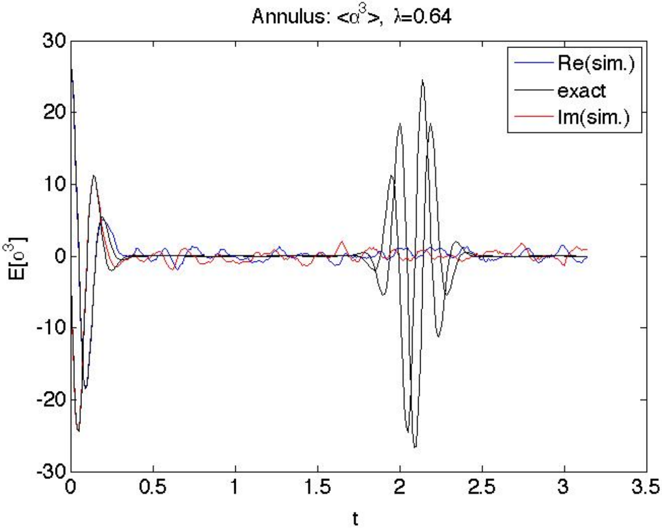

Figure: $\mathbf{E}[\alpha^3]$ using annulus regularization: $\lambda = 0.64$

Conclusions:

- For complex SDEs, instability is not just a problem: it's in the nature of the beasts.
- A good integrator should show growing processes when they are supposed to.
- Regularization is necessary: projections, artificial boundary conditions, **filtrations**.
- Long time functionals are possible if additional Fourier/Laplace information is known.
- Numerical inversion of Laplace transform also needs regularization (Perret, 2010). Likewise, discrete Fourier analysis.
- Wick rotations using formal scaling $\omega(\xi t) = \sqrt{\xi}\tilde{\omega}(t)$ did not work (Perret, 2010).

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