Lecture 10

[Path-integral analysis of fluctuation theorems]

Consider
$$\frac{dx_i}{dt} = F_i(\vec{x};\lambda) + \xi_i(t,\vec{x};\lambda)$$

$i = 1, \ldots, \underset{\uparrow \# \text{DoF}}{N}$ $\qquad \vec{x} = (x_1, \ldots, x_N)$

λ = externally controlled parameter: $\lambda = \lambda(t)$ in general, introducing explicit time dependence.

$$\langle \xi_i(t) \rangle = 0, \quad \langle \xi_i(t)\xi_j(t') \rangle = \underbrace{G_{ij}(\vec{x};\lambda)}_{\substack{\text{elements of a symm.,} \\ \text{pos.-def. matrix } G(\vec{x},\lambda)}} \delta(t-t')$$

This equation corresponds to the following Stratonovich FP eq'n: $\quad$ * not 'standard' Stratonovich form from Gardiner

$$\frac{\partial p}{\partial t} = \underbrace{-\partial^i(F_i p) + \frac{1}{2}\partial^i[G_{ij}(\partial^j p)]}_{\equiv\ \mathcal{J}_\lambda p} . \qquad (*)$$

depends on λ $\to \mathcal{J}_\lambda$

Summation over repeated indices applied

Here, $p = p(\vec{x},t)$ is the probability density

If $\lambda = \text{const}(t)$, $\quad p(\vec{x},t) \to \underbrace{p_s(\vec{x};\lambda)}_{\text{steady state}}$ as $t \nearrow$

Define $$p_s(\vec{x};\lambda) = e^{-\varphi(\vec{x};\lambda)},$$ and note that

$$\mathcal{J}_\lambda e^{-\varphi(\vec{x};\lambda)} = 0 \quad \text{since} \quad \frac{\partial p_s}{\partial t} = 0 .$$

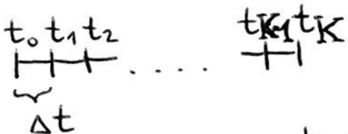
Next, define $\Gamma(\vec{x};\lambda) = G^{-1}(\vec{x};\lambda)$:

$$\Gamma(\vec{x};\lambda)\, G(\vec{x};\lambda) = \mathbb{I}, \quad \text{or}$$

$$\Gamma^{ij} G_{jk} = \delta^i{}_k .$$

We need to justify Eq. (*) as it is of a slightly non-standard form. We will also use this occasion to derive key results leading to path integral formalism.

Define a symmetric time interval $[-\tau, \tau]$:



K subintervals of length $\Delta t = t_{k+1} - t_k$

$k = 0, \ldots, K$ $\qquad$ $K \gg 1$

Focus on 1D case for simplicity:

$$(x(t_k), \lambda(t_k)) \equiv (x_k, \lambda_k)$$

The path is given by $X = \{x_0, \ldots, x_K\}$.

The probability of the path is given by

$$P_\lambda[X|x_0] = \prod_{k=0}^{K-1} \underbrace{W(x_{k+1}|x_k)}_{\text{transition prob.}}, \quad \text{where}$$

$$W(x_{k+1}|x_k) = \underbrace{\tilde{\mathcal{N}}}_{\text{normal'n constant}} e^{-\frac{(x_{k+1}-x_k-F(\bar{x}_k)\Delta t)^2}{2G(\bar{x}_k)\Delta t}} \ominus$$

$$\Gamma(\bar{x}_k) = \frac{1}{G(\bar{x}_k)}$$

$$\begin{cases} \bar{x}_k = \dfrac{x_k + x_{k+1}}{2}, \\ \epsilon_k = x_{k+1} - x_k. \end{cases}$$

$$\ominus \tilde{\mathcal{N}} e^{-\frac{\Delta t^2(\epsilon_k/\Delta t - F(\bar{x}_k))^2}{2G(\bar{x}_k)\Delta t}} =$$

$$= \tilde{\mathcal{N}} e^{-\frac{\Delta t}{2}\left(\frac{\epsilon_k}{\Delta t} - F(\bar{x}_k)\right)^2 \Gamma(\bar{x}_k)}.$$

We need to find $\tilde{\mathcal{N}}$ by insisting on

$$\int dx_{k+1} W(x_{k+1}|x_k) = 1 + \theta(\Delta t^2).$$

Since Δt is small, $\frac{1}{\Delta t}$ is large, making the above integral treatable by Laplace (saddle-point) method.

Recall that to leading order,

$$\int_{-\infty}^{\infty} dx\, e^{-\lambda f(x)} \simeq e^{-\lambda f(x_0)} \sqrt{\frac{2\pi}{\lambda f''(x_0)}},$$ where

x_0 is the solution of $f'(x_0) = 0$.

In our case, $\lambda = \frac{1}{\Delta t}$ and

$$f(x_{k+1}) = \frac{\Gamma\left(\frac{x_{k+1}+x_k}{2}\right)}{2}\left(x_{k+1} - x_k - F\left(\frac{x_{k+1}+x_k}{2}\right)\Delta t\right)^2.$$

1. For simplicity, consider $\Gamma\left(\frac{x_{k+1}+x_k}{2}\right) = \Gamma = \text{const}$ case first:

$$\underbrace{f'(x_{k+1})}_{= \frac{df(x_{k+1})}{dx_{k+1}}} = \Gamma \times \left(x_{k+1} - x_k - F\left(\frac{x_{k+1}+x_k}{2}\right)\Delta t\right) \times \left(1 - \frac{F'\left(\frac{x_{k+1}+x_k}{2}\right)}{2}\Delta t\right).$$

$F'(z) = \frac{dF}{dz}$

$$f'(x^*_{k+1}) = 0 \Rightarrow x^*_{k+1} = x_k + F\left(\frac{x^*_{k+1}+x_k}{2}\right)\Delta t.$$

Note that $f(x^*_{k+1}) = 0$

Likewise,

$$f''(x_{k+1}) = \Gamma \times \left(1 - F'\left(\frac{x_{k+1}+x_k}{2}\right)\frac{\Delta t}{2}\right)^2 +$$

$$+ \Gamma \times (x_{k+1} - x_k - F\Delta t)\left(-\frac{F''}{4}\Delta t\right).$$

Then $$f''(x^*_{k+1}) = \Gamma\left(1 - F'\left(\underbrace{\frac{x^*_{k+1}+x_k}{2}}_{= \bar{x}^*_k}\right)\frac{\Delta t}{2}\right)^2.$$

Finally,

$$\int_{-\infty}^{\infty} dx_{k+1}\, e^{-\frac{f(x_{k+1})}{\Delta t}} \simeq \sqrt{\frac{2\pi\Delta t}{\Gamma\left(1 - \frac{\Delta t}{2}F'(\bar{x}^*_k)\right)^2}} =$$

note that $f(x^*_{k+1}) = 0$ here

$$= \sqrt{\frac{2\pi\Delta t}{\Gamma}}\,\frac{1}{1 - \frac{\Delta t}{2}F'(\bar{x}^*_k)}.$$

This implies that

$$\tilde{\mathcal{N}} = \tilde{\mathcal{N}}(\overline{x}_k^*) = \sqrt{\frac{\Gamma}{2\pi\Delta t}}\left(1 - \underbrace{\frac{\Delta t}{2} F'(\overline{x}_k^*)}_{\mathcal{O}(\Delta t)\text{ correction}}\right).$$

(2.) Now, consider $F\left(\frac{x_{k+1}+x_k}{2}\right) = F = \text{const}$.

Then $f(x_{k+1}) = \dfrac{\Gamma\left(\frac{x_{k+1}+x_k}{2}\right)}{2}(x_{k+1} - x_k - F\Delta t)^2$.

We need a higher-order correction to the usual saddle-point result:

$$\int_{-\infty}^{\infty} dx\, e^{-\lambda f(x)} = e^{-\lambda f(x_0)}\sqrt{\frac{2\pi}{\lambda f''(x_0)}} \times$$

$$\times\left[1 + \frac{1}{\lambda}\left(\frac{5}{24}\frac{f'''(x_0)^2}{f''(x_0)^3} - \frac{1}{8}\frac{f''''(x_0)}{f''(x_0)^2}\right) + \mathcal{O}\left(\frac{1}{\lambda^2}\right)\right].$$

In our case,

$$f'(x_{k+1}) = \frac{\Gamma'}{4}(x_{k+1} - x_k - F\Delta t)^2 +$$

$$+ \Gamma(x_{k+1} - x_k - F\Delta t).$$

Then $f'(x_{k+1}^*) = 0$ yields $x_{k+1}^* = x_k + F\Delta t$, similar to before.

Further,

$$f''(x_{k+1}) = \frac{\Gamma''}{8}(x_{k+1} - x_k - F\Delta t)^2 + \frac{\Gamma'}{2}(x_{k+1} - x_k - F\Delta t) +$$

$$+ \frac{\Gamma'}{2}(x_{k+1} - x_k - F\Delta t) + \Gamma = \frac{\Gamma''}{8}(\dots)^2 + \Gamma'(\dots) + \Gamma.$$

Note that $f''(x_{k+1}^*) = \Gamma(\overline{x}_k^*)$.

Now, $f'''(x_{k+1}) = \frac{\Gamma'''}{16}(\dots)^2 + \frac{\Gamma''}{4}(\dots) +$

$+2\frac{\Gamma''}{4}(\dots) + 2\frac{\Gamma'}{2} + \frac{\Gamma'}{2} = \frac{\Gamma'''}{16}(\dots)^2 +$

$+ \frac{3\Gamma''}{4}(\dots) + \frac{3\Gamma'}{2}.$

Thus, $f'''(x^*_{k+1}) = \frac{3}{2}\Gamma'(\bar{x}^*_k)$.

Finally,

$$f''''(x_{k+1}) = \frac{\Gamma''''}{32}(\dots)^2 + \frac{\Gamma'''}{8}(\dots) + \frac{3\Gamma'''}{8}(\dots) +$$

$$+\frac{3\Gamma''}{4} + \frac{3\Gamma''}{4},$$ such that

$$f''''(x^*_{k+1}) = \frac{3\Gamma''(\bar{x}^*_k)}{2}.$$

Plugging it all in, we obtain:

$$\int_{-\infty}^{\infty} dx_{k+1}\, e^{-\frac{f(x_{k+1})}{\Delta t}} = \sqrt{\frac{2\pi\Delta t}{\Gamma(\bar{x}^*_k)}} \times$$

$$\times\left[1 + \Delta t\left(\frac{5}{24}\,\frac{9}{4}\,\frac{(\Gamma')^2}{\Gamma^3} - \frac{1}{8}\,\frac{3}{2}\,\frac{\Gamma''}{\Gamma^2}\right) + \mathcal{O}(\Delta t^2)\right] =$$

$$= \sqrt{\frac{2\pi\Delta t}{\Gamma}}\left[1 + \frac{\Delta t}{\Gamma}\left(\frac{15}{32}\frac{(\Gamma')^2}{\Gamma^2} - \frac{3}{16}\frac{\Gamma''}{\Gamma}\right) + \mathcal{O}(\Delta t^2)\right].$$

Hence, $$\tilde{\mathcal{N}}(\bar{x}^*_k) \simeq \sqrt{\frac{\Gamma(\bar{x}^*_k)}{2\pi\Delta t}}\left[1 - \frac{\Delta t}{\Gamma(\bar{x}^*_k)}\left(\frac{15}{32}\frac{\Gamma'(\bar{x}^*_k)^2}{\Gamma(\bar{x}^*_k)^2} - \frac{3}{16}\frac{\Gamma''(\bar{x}^*_k)}{\Gamma(\bar{x}^*_k)}\right)\right].$$

It is reasonable to expect (and could be checked directly) that in general,

$$\tilde{\mathcal{N}}(\bar{x}_k^*) \underset{\substack{\uparrow \\ \text{to } \theta(\Delta t)}}{=} \underbrace{\sqrt{\frac{\Gamma(\bar{x}_k^*)}{2\pi\Delta t}}\left\{1-\frac{\Delta t}{\Gamma(\bar{x}_k^*)}\left[\frac{15}{32}\frac{\Gamma'^2}{\Gamma^2}-\frac{3}{16}\frac{\Gamma''}{\Gamma}\right]\right\}}_{''\ \mathcal{N}(\bar{x}_k^*)} \times \left(1-\frac{\Delta t}{2}F'(\bar{x}_k^*)\right)$$

all quantities evaluated at $\bar{x}_k$

saddle point does not work here, we want $\bar{x}_k$, not $\bar{x}_k^*$

Actually, we need $\tilde{\mathcal{N}}(\bar{x}_k) \underset{\theta(\Delta t)}{=} \sqrt{\frac{\Gamma}{2\pi\Delta t}}\left\{1-\frac{\Delta t}{\Gamma}\left[\cancel{\frac{1}{4}}\frac{\Gamma'^2}{\Gamma^2}-\frac{1}{8}\frac{\Gamma''}{\Gamma}\right]\right\}\left(1-\frac{\Delta t}{2}F'\right)$, see S1–S4

Thus, $\tilde{\mathcal{N}}(\bar{x}_k) \simeq \mathcal{N}(\bar{x}_k)\, \underbrace{e^{-\frac{\Delta t}{2}F'(\bar{x}_k)}}_{\text{we do not want F-dependent terms in the prefactor to be able to cancel prefactors more easily}}$.

We can write

$$W(x_{k+1}|x_k) = \mathcal{N}(\bar{x}_k)\, e^{-\frac{\Delta t}{2}\left(\frac{\epsilon_k}{\Delta t}-F(\bar{x}_k)\right)^2\Gamma(\bar{x}_k)} \times e^{-\frac{\Delta t}{2}F'(\bar{x}_k)}$$

~~note the sneaky replacement of $\bar{x}_k^*$ by $\bar{x}_k$ [should be OK in the $\Delta t \to 0$ limit]~~

Finally,

$$P_\lambda[X|x_0] = \prod_{k=0}^{K-1} W(x_{k+1}|x_k) =$$

$$= \underbrace{\mathcal{N}[x]}_{''\ \prod_{k=0}^{K-1}\tilde{\mathcal{N}}(\bar{x}_k)}\, e^{-\frac{\Delta t}{2}\sum_{k=0}^{K-1}\left[\left(\frac{\epsilon_k}{\Delta t}-F(\bar{x}_k)\right)^2\Gamma(\bar{x}_k)+F'(\bar{x}_k)\right]}$$

This will become the path $\int$ in the $K\to\infty$ limit:

in multi-D, one obtains:

$$P_\lambda[X|\underset{\substack{\uparrow\\ \text{initial}\\ \text{microstate}}}{\vec{x}_{-\tau}}] = \mathcal{N}[X]\, e^{-\int_{-\tau}^{\tau} dt\, S_+(\vec{x}_t,\, \dot{\vec{x}}_t;\, \lambda_t)},$$

where $S_+(\vec{x}, \dot{\vec{x}}; \lambda) = \frac{1}{2}(\dot{x}_i - F_i)\Gamma^{ij}(\dot{x}_j - F_j) + \frac{1}{2}\partial^i F_i$.

Now, consider

$$p_{k+1}(x) = \int_{-\infty}^{\infty} dx'\, W(x|x')\, p_k(x') \overset{\substack{\epsilon = x - x';\\ x' = x - \epsilon}}{=}$$

$$= \int_{-\infty}^{\infty} d\epsilon\, W(x|x-\epsilon)\, p_k(x-\epsilon), \quad \text{where}$$

$$W(x|x-\epsilon) = \sqrt{\frac{\Gamma(x-\frac{\epsilon}{2})}{2\pi\Delta t}} \left\{1 - \frac{\Delta t}{\Gamma(x)} \underbrace{\left[\frac{1}{4}\frac{\Gamma'^2}{\Gamma^2} - \frac{1}{8}\frac{\Gamma''}{\Gamma}\right]}_{\substack{\text{all evaluated}\\ \text{at } x \text{ rather}\\ \text{than } \bar{x} = x - \frac{\epsilon}{2}\\ \text{at } O(\Delta t)}}\right\} \otimes$$

$$\bar{x} = \frac{x + x'}{2} = \frac{x + (x-\epsilon)}{2} = x - \frac{\epsilon}{2}$$

$$\otimes \Big(1 - \frac{\Delta t}{2}\underbrace{F'(x)}_{\substack{\text{also evaluated}\\ \text{at } x \text{ to } O(\Delta t)}}\Big)\, e^{-\frac{\Delta t}{2}\big(\underbrace{\epsilon/\Delta t}_{\frac{z}{\sqrt{\Gamma\Delta t}}} - F(x-\frac{\epsilon}{2})\big)^2 \Gamma(x-\frac{\epsilon}{2})}.$$

Now, note that $\epsilon \sim \sqrt{\Delta t} \Rightarrow$ then

$$\Delta t\left(\frac{\epsilon}{\Delta t}\right)^2 \sim \Delta t\,\frac{1}{\Delta t} = O(1), \text{ as expected.}$$

Introduce $\underline{\underline{z = \sqrt{\frac{\Gamma(x)}{\Delta t}}\,\epsilon}} \Rightarrow \int_{-\infty}^{\infty} d\epsilon \to \sqrt{\frac{\Delta t}{\Gamma(x)}}\int_{-\infty}^{\infty} dz$.

One can expand all variables to $\mathcal{O}(\Delta t)$, for example

$$p_k(x - \underbrace{\sqrt{\tfrac{\Delta t}{\Gamma}}\, z}_{=\epsilon}) \simeq p_k(x) - p_k'(x)\sqrt{\frac{\Delta t}{\Gamma}}\, z + \frac{p_k''(x)}{2}\frac{\Delta t}{\Gamma} z^2 .$$

Same for $F(x - \frac{\epsilon}{2})$ and $\Gamma(x - \frac{\epsilon}{2})$.

After expanding to $\mathcal{O}(\Delta t)$ under the $\int_{-\infty}^{\infty} dz$ integral, one is left with

$$\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dz\, e^{-z^2/2} = 1 , \quad \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dz\, z\, e^{-\frac{z^2}{2}} = 0 ,$$

$$\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dz\, z^2 e^{-\frac{z^2}{2}} = 1 , \text{ etc.}$$

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see Mathematica printout, p. S5

Eventually, after much effort, one obtains:

$$p_{k+1}(x) = p_k(x) - \Delta t \Big[F'(x)\, p_k(x) + F(x)\, p_k'(x) + \frac{\Gamma'(x)}{2\Gamma^2(x)}\, p_k'(x) - \frac{1}{2\Gamma(x)}\, p_k''(x) \Big] .$$

In the $\Delta t \to 0$ limit,

$$\frac{\partial p(x,t)}{\partial t} = -\frac{\partial}{\partial x}\big(F(x)\, p(x,t)\big) + \frac{1}{2}\underbrace{\frac{\partial}{\partial x}\Big[\frac{1}{\Gamma(x)}\Big(\frac{\partial p(x,t)}{\partial x}\Big)\Big]}_{\frac{1}{\Gamma}\frac{\partial^2 p}{\partial x^2} - \frac{\Gamma'}{\Gamma^2}\frac{\partial p}{\partial x}}$$

This is the 1D version of the Stratonovich FP equation stated above (Eq. (*)) on p. 1

Consider

$$I = \int dx_{k+1}\, W(x_{k+1}|x_k) \circeq$$

Define

$$\begin{cases} \epsilon_k = x_{k+1} - x_k, \\ \bar{x}_k = \dfrac{x_k + x_{k+1}}{2} = x_k + \dfrac{\epsilon_k}{2} \end{cases}$$

$$\circeq \int_{-\infty}^{\infty} d\epsilon_k\, \overbrace{\tilde{n}\left(x_k + \frac{\epsilon_k}{2}\right) e^{-\frac{\Delta t}{2}\left(\frac{\epsilon_k}{\Delta t} - F\left(x_k + \frac{\epsilon_k}{2}\right)\right)^2 \Gamma\left(x_k + \frac{\epsilon_k}{2}\right)}}^{W(x_k+\epsilon_k|x_k)}.$$

Use $\quad z = \sqrt{\dfrac{\Gamma(x_k)}{\Delta t}}\,\epsilon_k \quad \Rightarrow \int_{-\infty}^{\infty} d\epsilon_k \rightarrow \sqrt{\dfrac{\Delta t}{\Gamma(x_k)}} \int_{-\infty}^{\infty} dz$

We insist that $I = 1 + \Theta(\Delta t^2)$, by normalization.

To the lowest order,

$$I \simeq \sqrt{\frac{\Delta t}{\Gamma}} \int_{-\infty}^{\infty} dz\, \tilde{n}\, e^{-\frac{\Delta t}{2}\left(\sqrt{\frac{\Delta t}{\Gamma}}\frac{z}{\Delta t} - F\right)^2 \Gamma} \circeq$$

Here, $\Gamma, \tilde{n}, F$ are all evaluated at x_k

$$\circeq \tilde{n}\sqrt{\frac{\Delta t}{\Gamma}} \int dz\, e^{-\frac{1}{2}\underbrace{\left(\frac{z}{\sqrt{\Gamma}} - F\sqrt{\Delta t}\right)^2 \Gamma}_{(z - F\sqrt{\Gamma \Delta t})^2}} = \tilde{n}\sqrt{\frac{\Delta t}{\Gamma}}\sqrt{2\pi} = 1,$$

so that

$$\tilde{n}(x_k)_0 = \sqrt{\frac{\Gamma(x_k)}{2\pi \Delta t}}. \qquad (*)$$

lowest order

Now, we need to expand the integrand to $\mathcal{O}(\Delta t)$ and take all $\int_{-\infty}^{\infty} dz$ integrals.

After doing this in Mathematica (see attached), we obtain: ($G \equiv \Gamma$ here)

$$\underset{\substack{\uparrow \\ \text{to } \mathcal{O}(\Delta t)}}{I \simeq} \frac{1}{16}\sqrt{\frac{\pi \Delta t}{2}}\, \frac{1}{G^{7/2}}\,(32 G^3 \tilde{n})\left[\frac{15\,\Delta t\,\tilde{n}\,G'^2}{32\,G^3\,\tilde{n}} + 1 + \right.$$

$$+ \frac{16\cancel{G^3}\,\Delta t\,F'\,\cancel{\tilde{n}}}{32\cancel{G^3}\cancel{\tilde{n}}} + \underbrace{\frac{16\cancel{G^3}\,\tilde{n}'\,\Delta t\,F}{32\cancel{G^3}\,\tilde{n}}}_{a} - \frac{6\,\Delta t\,G \times 2G'\,\tilde{n}'}{32\,G^3\,\tilde{n}} -$$

$$\left. - \frac{6\,\Delta t\,G \times \cancel{\tilde{n}}\,G''}{32\,G^3\,\cancel{\tilde{n}}} - \underbrace{\frac{8\,\Delta t\,G^2\,F\,\cancel{\tilde{n}}\,G'}{32\,G^3\,\cancel{\tilde{n}}}}_{b} + \frac{4\,\Delta t\,G^2\,\tilde{n}''}{32\,G^3\,\tilde{n}}\right] =$$

$$= \underbrace{\sqrt{\frac{2\pi\Delta t}{G}}\,\tilde{n}}_{\text{consistent with Eq. (*)}}\left\{1 + \Delta t\,[\underbrace{\;\ldots\;}]\right\}$$

here, we can replace $\frac{\tilde{n}'}{\tilde{n}}$ and $\frac{\tilde{n}''}{\tilde{n}}$ by $\frac{\tilde{n}'_0}{\tilde{n}_0}$ and $\frac{\tilde{n}''_0}{\tilde{n}_0}$, since all corrections would be higher-order

all quantities: $\tilde{n}$, F, G, G', etc. are evaluated at x_k

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Now,
$$\begin{cases} \tilde{n}'(x_k)_0 = \dfrac{1}{\sqrt{2\pi\Delta t}}\,\dfrac{G'}{2G^{1/2}}, \\[2ex] \tilde{n}''(x_k)_0 = \dfrac{1}{\sqrt{2\pi\Delta t}}\,\dfrac{1}{2}\left[\dfrac{G''}{G^{1/2}} - \dfrac{1}{2}\,\dfrac{(G')^2}{G^{3/2}}\right]. \end{cases}$$

Then $\dfrac{\tilde{n}'_0}{\tilde{n}_0} = \dfrac{G'}{2G}$ and $\dfrac{\tilde{n}''_0}{\tilde{n}_0} = \dfrac{1}{2}\,\dfrac{G''}{G} - \dfrac{1}{4}\,\dfrac{(G')^2}{G^2}$.

Finally,

$$\underset{\uparrow \atop \theta(\Delta t)}{I} = \sqrt{\frac{2\pi\Delta t}{G}}\,\tilde{n}\left\{1+\Delta t\left[\frac{15\,G'^2}{32\,G^3}+\frac{F'}{2}-\frac{6}{16}\frac{G'}{2G}\frac{G'}{G^2}-\frac{6}{32}\frac{G''}{G^2}+\frac{1}{8}\frac{1}{G}\left[\frac{1}{2}\frac{G''}{G}-\frac{1}{4}\frac{G'^2}{G^2}\right]\right]\right\} \Leftrightarrow$$

Note that terms a and b cancel:

$$a:\ \frac{\Delta t\,F}{2}\frac{G'}{2G}=\frac{\Delta t\,F\,G'}{4G}$$

$$b:\ \frac{\Delta t\,F\,G'}{4G}$$

Thus, there is no dependence on F, just on F'

$$\Leftrightarrow \sqrt{\frac{2\pi\Delta t}{G}}\,\tilde{n}\left\{1+\Delta t\,\frac{F'}{2}+\frac{\Delta t}{G}\left[\underline{\frac{15}{32}\frac{G'^2}{G^2}}-\underline{\frac{6}{32}\frac{G'^2}{G^2}}-\frac{6}{32}\frac{G''}{G}+\frac{1}{16}\frac{G''}{G}-\underline{\frac{1}{32}\frac{G'^2}{G^2}}\right]\right\}=$$

$$=\sqrt{\frac{2\pi\Delta t}{G}}\,\tilde{n}\left\{1+\Delta t\,\frac{F'}{2}+\frac{\Delta t}{G}\left[\frac{1}{4}\frac{G'^2}{G^2}-\frac{1}{8}\frac{G''}{G}\right]\right\}.$$

Now, $\tilde{n}(x_k)=\sqrt{\frac{G}{2\pi\Delta t}}\left\{1-\frac{\Delta t}{2}F'-\frac{\Delta t}{G}[\ldots]\right\} \underset{\uparrow \atop \text{to } \theta(\Delta t)}{=}$

recall that $I=1$

$$= \sqrt{\frac{G(x_k)}{2\pi\Delta t}}\left\{1-\frac{\Delta t}{G(x_k)}\left[\frac{1}{4}\frac{G'(x_k)^2}{G^2(x_k)}-\frac{1}{8}\frac{G''(x_k)}{G(x_k)}\right]\right\}\times$$

$$\times\left\{1-\frac{\Delta t}{2}F'(x_k)\right\}.$$

same as (A.3)

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(* This procedure leads to Eq. (A.3) with correct pre-factors *)
ClearAll[eps, z, x]
eps = z * Sqrt[dt / G[x]]
W2[x + eps, x] = Sqrt[dt / G[x]] * nt[x + eps / 2] * Exp[-(G[x + eps / 2] * dt / 2) * (eps / dt - F[x + eps / 2]) ^2]
Ing[z] = Normal[Series[W2[x + eps, x], {dt, 0, 2}, Assumptions → dt > 0]]
Integrate[Ing[z], {z, -Infinity, Infinity}]
```

Out[414]= $z\sqrt{\frac{dt}{G[x]}}$

Out[415]= $e^{-\frac{1}{2}dt\left(-F\left[x+\frac{1}{2}z\sqrt{\frac{dt}{G[x]}}\right]+\frac{z\sqrt{\frac{dt}{G[x]}}}{dt}\right)^2 G\left[x+\frac{1}{2}z\sqrt{\frac{dt}{G[x]}}\right]}\sqrt{\frac{dt}{G[x]}}\,nt\left[x+\frac{1}{2}z\sqrt{\frac{dt}{G[x]}}\right]$

Out[416]= $\sqrt{dt}\,e^{-\frac{z^2}{2}}\sqrt{\frac{1}{G[x]}}\,nt[x]-\frac{dt\,e^{-\frac{z^2}{2}}z\left(-4F[x]G[x]^2nt[x]+z^2nt[x]G'[x]-2G[x]nt'[x]\right)}{4G[x]^2}+$

$\frac{1}{32}dt^{3/2}e^{-\frac{z^2}{2}}\left(\frac{1}{G[x]}\right)^{7/2}\left(-16F[x]^2G[x]^4nt[x]+16z^2F[x]^2G[x]^4nt[x]+\right.$
$16z^2G[x]^3nt[x]F'[x]+16z^2F[x]G[x]^2nt[x]G'[x]-8z^4F[x]G[x]^2nt[x]G'[x]+z^6nt[x]G'[x]^2+$
$\left.16z^2F[x]G[x]^3nt'[x]-4z^4G[x]G'[x]nt'[x]-2z^4G[x]nt[x]G''[x]+4z^2G[x]^2nt''[x]\right)-$

$\frac{1}{384G[x]^5}dt^2e^{-\frac{z^2}{2}}z\left(192F[x]^3G[x]^6nt[x]-64z^2F[x]^3G[x]^6nt[x]+192F[x]G[x]^5nt[x]F'[x]-\right.$
$192z^2F[x]G[x]^5nt[x]F'[x]+96F[x]^2G[x]^4nt[x]G'[x]-240z^2F[x]^2G[x]^4nt[x]G'[x]+$
$48z^4F[x]^2G[x]^4nt[x]G'[x]-96z^2G[x]^3nt[x]F'[x]G'[x]+48z^4G[x]^3nt[x]F'[x]G'[x]+$
$48z^4F[x]G[x]^2nt[x]G'[x]^2-12z^6F[x]G[x]^2nt[x]G'[x]^2+z^8nt[x]G'[x]^3+96F[x]^2G[x]^5nt'[x]-$
$96z^2F[x]^2G[x]^5nt'[x]-96z^2G[x]^4F'[x]nt'[x]-96z^2F[x]G[x]^3G'[x]nt'[x]+$
$48z^4F[x]G[x]^3G'[x]nt'[x]-6z^6G[x]G'[x]^2nt'[x]-48z^2G[x]^4nt[x]F''[x]-48z^2F[x]G[x]^3nt[x]G''[x]+$
$24z^4F[x]G[x]^3nt[x]G''[x]-6z^6G[x]nt[x]G'[x]G''[x]+12z^4G[x]^2nt'[x]G''[x]-$
$\left.48z^2F[x]G[x]^4nt''[x]+12z^4G[x]^2G'[x]nt''[x]+4z^4G[x]^2nt[x]G^{(3)}[x]-8z^2G[x]^3nt^{(3)}[x]\right)$

Out[417]= $\frac{1}{16}\sqrt{dt}\sqrt{\frac{\pi}{2}}\left(\frac{1}{G[x]}\right)^{7/2}\left(15\,dt\,nt[x]G'[x]^2+16G[x]^3\left(nt[x](2+dt\,F'[x])+dt\,F[x]nt'[x]\right)-\right.$
$\left.6\,dt\,G[x]\left(2G'[x]nt'[x]+nt[x]G''[x]\right)+4\,dt\,G[x]^2\left(-2F[x]nt[x]G'[x]+nt''[x]\right)\right)$

$nt \to \tilde{n}$,
$G \to \Gamma$,
$dt \to \Delta t$

This is simplified further by hand

math

```
In[418]:= (* This reproduces Eq. (A.10) (the FP eq'n) with coefficients from Eq. (A.3) but not from the saddle-
           point expansion *)
          a1 = 1 (*15*)
          a2 = 4 (*32*)
          b1 = 1 (*3*)
          b2 = 8 (*16*)
          eps = z * Sqrt[dt / G[x]]
          W[x, x - eps] = Sqrt[G[x - eps / 2] / (2 * Pi * G[x])] *
            (1 - (dt / G[x]) * ((a1 * G'[x]^2 / (a2 * G[x]^2)) - (b1 * G''[x] / (b2 * G[x])))) * (1 - F'[x] dt / 2) *
            Exp[-(G[x - eps / 2] * dt / 2) * (eps / dt - F[x - eps / 2])^2]
          Ing[z] = Normal[Series[W[x, x - eps] * p[x - eps], {dt, 0, 1}, Assumptions -> dt > 0]]
          Integrate[Ing[z], {z, -Infinity, Infinity}]
```

Out[418]= 1

Out[419]= 4

Out[420]= 1

Out[421]= 8

Out[422]= $z\sqrt{\frac{dt}{G[x]}}$

Out[423]= $$\frac{e^{-\frac{1}{2}dt\left(-F\left[x-\frac{1}{2}z\sqrt{\frac{dt}{G[x]}}\right]+\frac{z\sqrt{\frac{dt}{G[x]}}}{dt}\right)^2 G\left[x-\frac{1}{2}z\sqrt{\frac{dt}{G[x]}}\right]}\sqrt{\frac{G\left[x-\frac{1}{2}z\sqrt{\frac{dt}{G[x]}}\right]}{G[x]}}\left(1-\frac{1}{2}dt\,F'[x]\right)\left(1-\frac{dt\left(\frac{G'[x]^2}{4G[x]^2}-\frac{G''[x]}{8G[x]}\right)}{G[x]}\right)}{\sqrt{2\pi}}$$

Out[424]= $$\frac{e^{-\frac{z^2}{2}}p[x]}{\sqrt{2\pi}}+\frac{\sqrt{dt}\,e^{-\frac{z^2}{2}}z\left(\frac{1}{G[x]}\right)^{3/2}\left(4F[x]G[x]^2p[x]-p[x]G'[x]+z^2p[x]G'[x]-4G[x]p'[x]\right)}{4\sqrt{2\pi}}+$$
$$\frac{1}{32\sqrt{2\pi}G[x]^3}dt\,e^{-\frac{z^2}{2}}\Big(-16F[x]^2G[x]^4p[x]+16z^2F[x]^2G[x]^4p[x]-16G[x]^3p[x]F'[x]-$$
$$16z^2G[x]^3p[x]F'[x]-24z^2F[x]G[x]^2p[x]G'[x]+8z^4F[x]G[x]^2p[x]G'[x]-8p[x]G'[x]^2-$$
$$z^2p[x]G'[x]^2-2z^4p[x]G'[x]^2+z^6p[x]G'[x]^2-32z^2F[x]G[x]^3p'[x]+8z^2G[x]G'[x]p'[x]-$$
$$8z^4G[x]G'[x]p'[x]+4G[x]\,p[x]G''[x]+2z^2G[x]\,p[x]G''[x]-2z^4G[x]\,p[x]G''[x]+16z^2G[x]^2p''[x]\Big)$$

Out[425]= $$p[x]\left(1-dt\,F'[x]\right)-\frac{dt\left(2F[x]G[x]^2p'[x]+G'[x]p'[x]-G[x]p''[x]\right)}{2G[x]^2}$$

$p[x] \to p_K(x)$
$G \to \Gamma$, $dt \to \Delta t$

So, $$p_{K+1} = p_K - \Delta t\left[F'p_K + F p_K' + \frac{\Gamma' p_K'}{2\Gamma^2} - \frac{p_K''}{2\Gamma}\right]$$ (A.10) in the paper