A QUANTUM CORRECTION TERM
to
FOKKER-PLANCK EQUATION

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Historic Context

FP to QuantumFP

- Master Equation Form
- Lindblad Theorem
- Modified QFP
  - Motivation (heuristic)
  - Derivations (microscopic)

Summary

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HISTORIC CONTEXT

Newton $F_{frict} = -\eta v$

Einstein $D_{pp} = \eta k_B T$ $\qquad \frac{\eta}{m} = \lambda$

	microscopic	phenomenologic	
classic.	Boltzmann collision bath ⋮	Langevin s.d.e. ⋮	FP p.d.e. ⋮
quantum	Landau harmonic bath ⋮	Gardiner q.s.d.e. ⋮	Agarwal q.p.d.e. ⋮
	QFP : Redfield, Agarwal, Haake-Reibold, Caldeira-Leggett, Zurek, Hu-Paz-Zhao		

Kohen-Marston-Tannor (1997):

A Markovian theory of q-dissipation has been a much sought after goal of at least six communities: NMR, q-optics, condensed matter physicists, mathematical physicists, astrophysicists and condensed phase chemical physicists.

FP $\longrightarrow$ QFP p.d.e.

Classical dissipative motion

$W = W(q,p)$ phase-space density

$$\dot{W} = -\frac{p}{m}\frac{\partial W}{\partial q} + \frac{\partial V}{\partial q}\frac{\partial W}{\partial p} + \lambda \frac{\partial p W}{\partial p} + D_{pp}\frac{\partial^2 W}{\partial p^2}$$

friction

p-diffusion

$$D_{pp} = \lambda m k_B T$$

Let W be Wigner-function of $\hat{\rho}$

$$W(q,p) \Leftrightarrow \hat{\rho}$$

def: $\hat{p}_c, \hat{q}_c$: $\quad \hat{p}_c \hat{O} \equiv \frac{1}{2}\{\hat{p}, \hat{O}\}, \; \hat{q}_c \hat{O} \equiv \frac{1}{2}\{\hat{q}, \hat{O}\}$

$$W(q,p) = \mathrm{tr}\left(\delta(q-\hat{q}_c)\delta(p-\hat{p}_c)\hat{\rho}\right)$$

$$\hat{\rho} = W(\hat{q}_c, \hat{p}_c)$$

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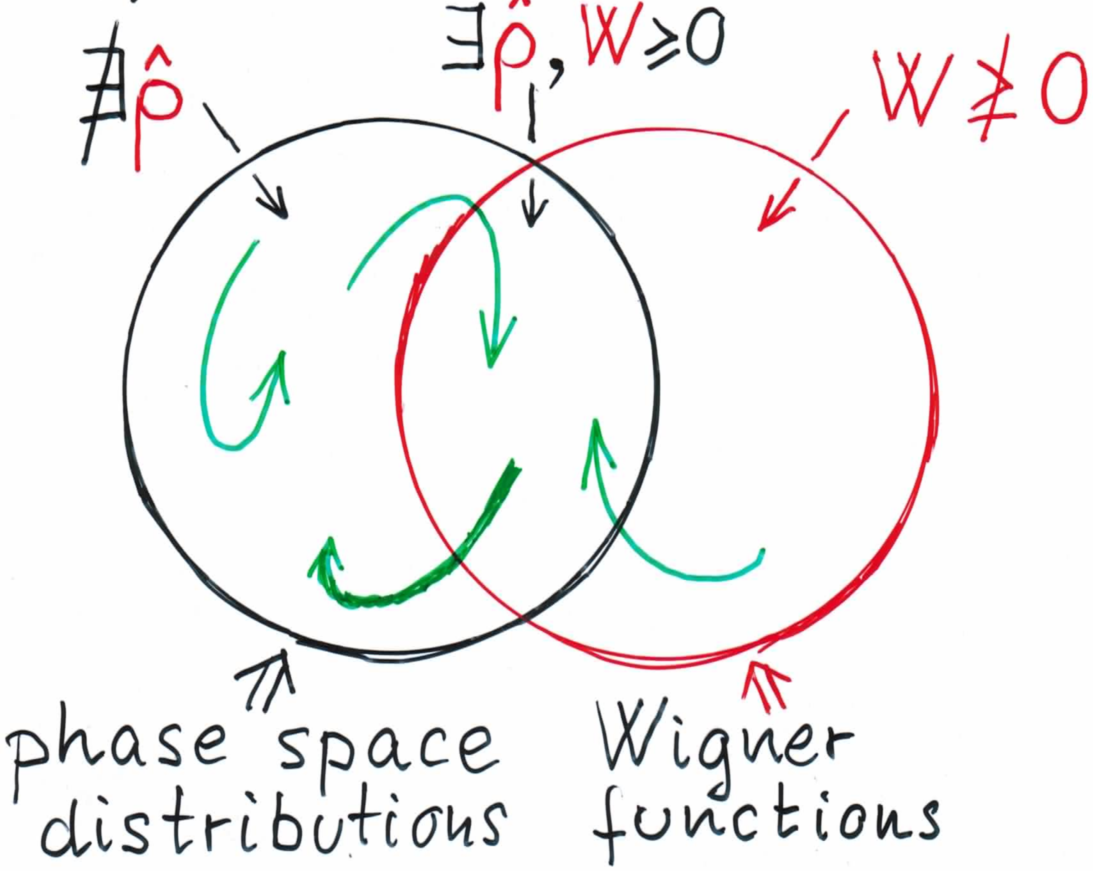
note: $\frac{\partial V}{\partial q}\frac{\partial W}{\partial p} \longrightarrow \frac{2}{\hbar} V\left(q + \frac{i}{2}\hbar\frac{\partial}{\partial p}\right) W$

THE BUG

FP p.d.e. solutions:



QFP MASTER EQ

$$\hat{\rho} = W(\hat{q}_c, \hat{p}_c)$$

$$\dot{\hat{\rho}} = -\frac{i}{\hbar}\left[\frac{\hat{p}^2}{2m} + V(\hat{q}), \hat{\rho}\right] - \frac{i}{2\hbar}\lambda\left[\hat{q}, \{\hat{p}, \hat{\rho}\}\right] -$$

$$-\frac{1}{\hbar^2} D_{pp}\left[\hat{q}, [\hat{q}, \hat{\rho}]\right]$$

Bug: $\hat{\rho}_0 \longrightarrow \hat{\rho}_t \ngeq 0$

example: $\hat{\rho}_0 = |\psi\rangle\langle\psi|$

$\langle\psi|\hat{q}|\psi\rangle = 0$, $\langle\psi|\hat{q}^2|\psi\rangle = \sigma^2$

let $|\varphi\rangle = \sigma^{-1}\hat{q}|\psi\rangle$

$$\langle\varphi|\hat{\rho}_{\Delta t}|\varphi\rangle = \left(-\frac{\lambda}{2} + \frac{2}{\hbar^2}\underset{\substack{\uparrow \\ \lambda m k_B T}}{D_{pp}}\sigma^2\right)\Delta t$$

$\hat{\rho}_{\Delta t} \ngeq 0$ if

$$\sigma < \frac{\hbar}{\sqrt{2}\sqrt{2mk_BT}}$$

LINDBLAD-KOSSAKOWSKI-SUDARSHAN-GORINI- THEOREM ⑥

special case:

$$\dot{\hat{\rho}} = -\frac{i}{\hbar}[\hat{H},\hat{\rho}] - \frac{i}{2\hbar}\lambda[\hat{q},\{\hat{p},\hat{\rho}\}] - \frac{1}{\hbar^2}D_{pp}[\hat{q},[\hat{q},\hat{\rho}]] - \frac{1}{\hbar^2}D_{qq}[\hat{p},[\hat{p},\hat{\rho}]] - \frac{2}{\hbar^2}D_{pq}[\hat{q},[\hat{p},\hat{\rho}]]$$

is mathematically correct eq. iff:

$$\begin{pmatrix} D_{pp} & D_{qp}+\frac{i}{4}\lambda \\ D_{qp}-\frac{i}{4}\lambda & D_{qq} \end{pmatrix} \geq 0$$

In QFP:
$$\begin{pmatrix} \lambda m k_B T & \frac{i}{4}\lambda \\ -\frac{i}{4}\lambda & 0 \end{pmatrix} \ngeq 0$$

$$\uparrow$$
$$D_{qq}$$

Modify QFP!

$$D_{qq} = \kappa \frac{\lambda\hbar^2}{16 m k_B T}$$

$$\kappa \geq 1$$

MOTIVATION (heuristic)

Time coarse-graining of p-diffusion (D_{pp}) yields q-diffusion (D_{qq})

$$-\frac{\lambda m k_B T}{\hbar^2}\left[\hat{q}(\delta t),\left[\hat{q}(\delta t),\,\cdot\,\right]\right]$$

$$\Downarrow$$

$$\left[\hat{q}+\frac{\hat{p}}{m}\delta t,\left[\hat{q}+\frac{\hat{p}}{m}\delta t,\,\cdot\,\right]\right]$$

$$\Downarrow$$

$$\left[\hat{q},\left[\hat{q},\,\cdot\,\right]\right]+\frac{1}{m^2}(\delta t)^2\left[\hat{p},\left[\hat{p},\,\cdot\,\right]\right]$$

$$\delta t \sim \frac{\sqrt{K}}{4}\,\frac{\hbar}{k_B T}$$

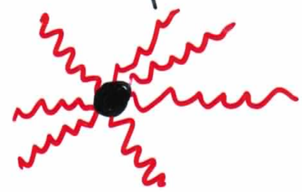
coarse-graining time-scale ~

~ $\hbar$/thermal energy scale

DERIVATION 1 (microscopic à la {Caldeira, Leggett, ...)

Coupling to harmonic bath of temp. T

$$\hat{H}_{S+I} = \frac{\hat{p}^2}{2m} + V(\hat{q}) + \hat{q}\hat{Q}$$



$$\langle \hat{Q}(t) \rangle_B = 0, \quad \langle \hat{Q}(t)\hat{Q}(t') \rangle_B = \frac{1}{\hbar}\alpha(t-t')$$

$$\alpha_I(t) = -\frac{\lambda m}{\pi}\int_0^\Omega \omega \sin(\omega t)\, d\omega$$

$$\alpha_R(t) = \frac{\lambda m}{\pi}\int^\Omega \omega \coth\left(\frac{\hbar\omega}{2k_BT}\right)\cos(\omega t)\, d\omega$$

Markov approximation:

$$\alpha_I(t) \approx \lambda m \dot{\delta}(t) \Rightarrow -\frac{i}{2\hbar}\lambda[\hat{q},\{\hat{p},\hat{\rho}\}]$$

$$\alpha_R(t) \approx \frac{2\lambda m k_B T}{\hbar}\delta(t) - \frac{\lambda m \hbar}{6k_BT}\ddot{\delta}(t) + \dots$$

$$\Downarrow \qquad\qquad \Downarrow$$

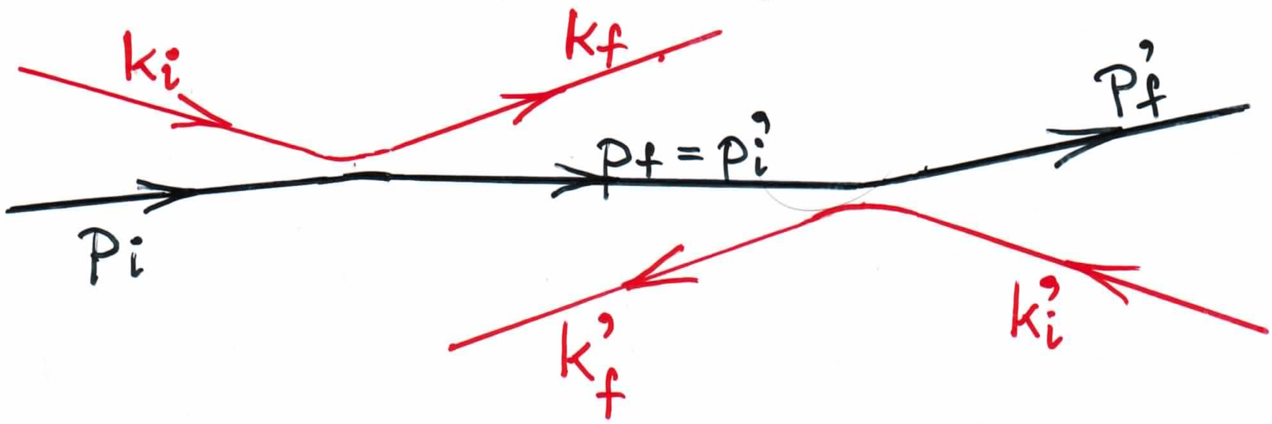
$$-\frac{1}{\hbar^2}\lambda m k_B T[\hat{q},[\hat{q},\hat{\rho}]] - \frac{1}{\hbar^2}\frac{\lambda}{12mk_BT}[\hat{p},[\hat{p},\hat{\rho}]]$$

$(\kappa = 4/3)$

while $D_{qp} \neq 0$

DERIVATION 2 (microscopic à la {Boltzm. ...

Coupling to collision bath of temp. T



Aproximations:

- $m \gg$ mass of bath molecules
- small scattering angles θ
- time coarse-graining over many coll's

$$D_{pp} = \frac{1}{3} \langle \underset{\uparrow \text{ collision rate}}{\nu} (k_f - k_i)^2 \rangle_{av} = \left\{ \begin{array}{l} \text{squared-momentum} \\ \text{transfer rate} \end{array} \right.$$

$$\lambda = \frac{1}{m k_B T} D_{pp}$$

$$D_{qq} = \frac{1}{12} \left(\frac{\hbar}{m k_B T} \right)^2 \langle \nu k^2 \rangle_{av} \sim \left\{ \begin{array}{l} \text{scattered} \\ \text{energy flux} \end{array} \right.$$

$$\kappa = 4 \frac{\langle \nu k^2 \rangle_{av}}{\langle \nu (k_f - k_i)^2 \rangle_{av}} \sim \frac{4}{\langle \theta^2 \rangle_{av}}$$

SUMMARY

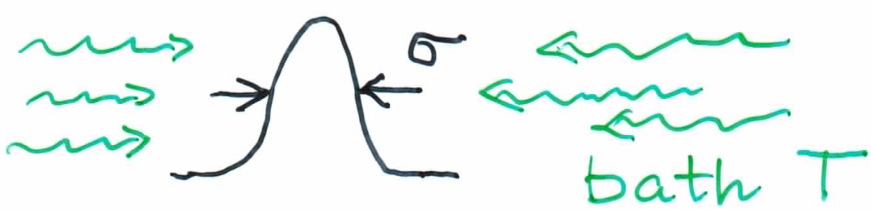
FP & naïve QFP:

$$\dot{W} = -\frac{p}{m}\frac{\partial W}{\partial q} + \frac{\partial V}{\partial q}\frac{\partial W}{\partial p} + \lambda\frac{\partial p W}{\partial p} + \lambda m k_B T \frac{\partial^2 W}{\partial p^2}$$

Modified QFP:

$$\dot{W} = \ldots \text{naïve QFP} \ldots + \kappa\hbar^2 \frac{\lambda}{16 m k_B T}\frac{\partial^2 W}{\partial q^2}$$

- Classical FP thermalizes always to Gibbs
  MQFP thermalizes free particle & harm. osc.
  MQFP $\neq$ universal thermalizing engine
- MQFP is superior in numeric simulations
- Experimental significance?



$$\sigma < \frac{\hbar}{\sqrt{2 m k_B T}}$$