

On the Consistent Theoretical Description of Open (Quantum) Mechanical Systems and its Physical Meaning

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1. Closed vs. open dynamical systems
2. TDSE for closed systems, WP solutions
 - dynamical invariant
 - creation/annihilation operators
 - Wigner function
3. Modifications for open systems
 - effective Hamiltonians via non-canonical transf.
 - NLSEs
 - generalized creation/annihilation operators
 - modified Wigner function
 - GKSL master equation, physical meaning, comparison of different approaches
 - correct friction force in equation of motion
4. Conclusions

1. Closed vs. Open Dynamical Systems

Dynamics of **Closed** Systems

reversible dynamics

conservation of energy

Class:

Newton:

$$\ddot{x} + \frac{1}{m} \frac{\partial}{\partial x} V(x) = 0$$

x : class. **trajectory**

Hamilton: $H = \frac{1}{2m} p^2 + V(x) = T + V$

$$\dot{x} = \frac{\partial H}{\partial p} = \frac{p}{m}, \quad \dot{p} = -\frac{\partial H}{\partial x} = -\frac{\partial V}{\partial x}$$

Gibbs:

$\varrho_\Gamma(x, p)$: phase space **distribution fct.**

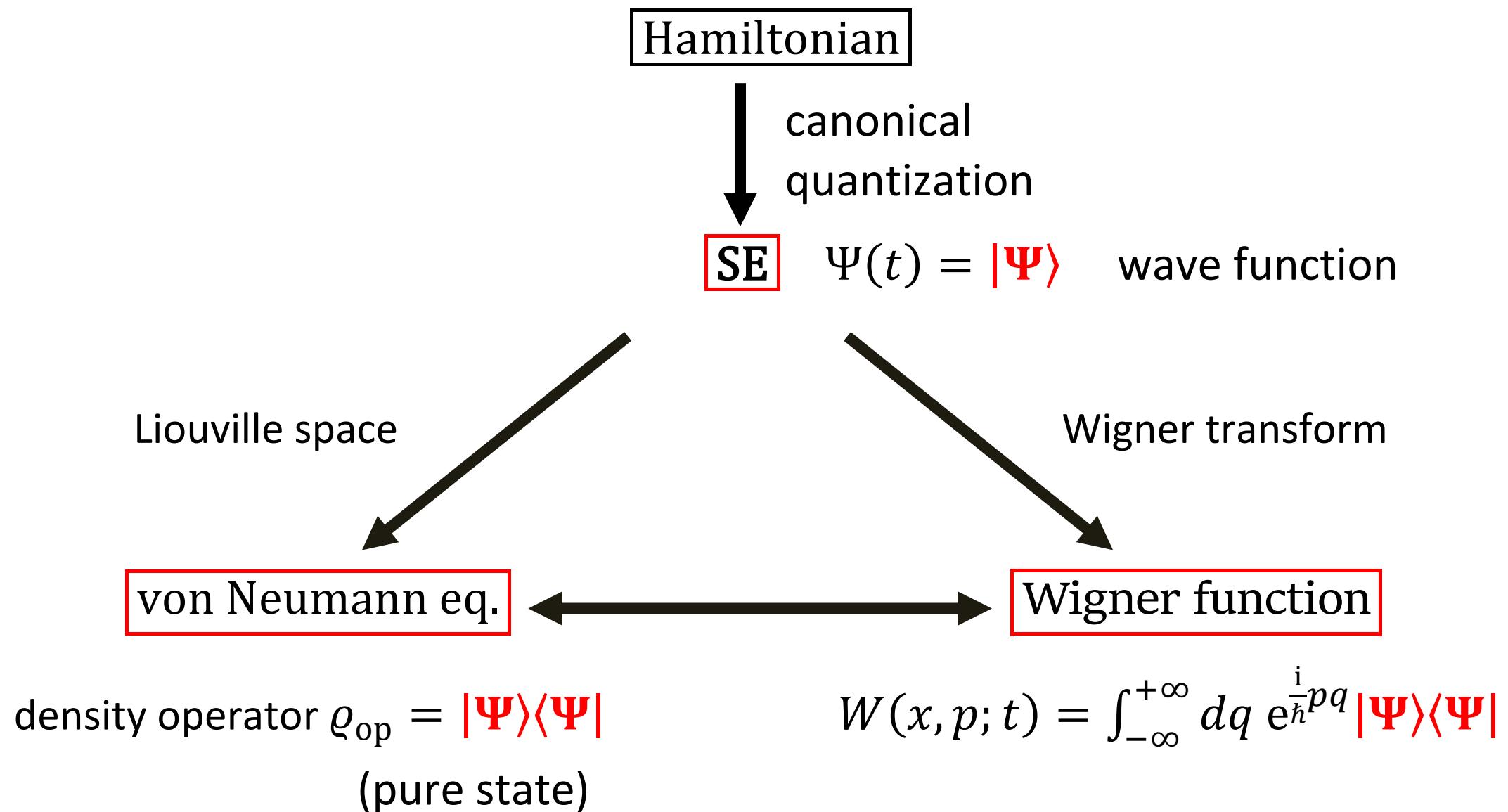
CE:

$$\frac{\partial}{\partial t} \varrho_\Gamma + \frac{\partial}{\partial x} \left(\frac{p}{m} \varrho_\Gamma \right) + \frac{\partial}{\partial p} \left(\left(-\frac{\partial V}{\partial x} \right) \varrho_\Gamma \right) = \frac{\partial}{\partial t} \varrho_\Gamma - \{H, \varrho_\Gamma\}_{\text{PB}} = 0$$

$$\overset{\uparrow}{\dot{x}}$$

$$\overset{\uparrow}{\dot{p}}$$

Closed Quantum Systems



Qm: position space, canon. quantization $x \rightarrow x_{\text{op}} = x$, $p \rightarrow p_{\text{op}} = \frac{\hbar}{i} \frac{\partial}{\partial x}$

$$H \rightarrow H_{\text{op}} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x)$$

Schrödinger:

$$i\hbar \frac{\partial}{\partial t} \Psi(x, t) = H_{\text{op}} \Psi(x, t)$$

Probability density: $\varrho(x, t) = \Psi^*(x, t) \Psi(x, t)$

CE:

$$\frac{\partial}{\partial t} \varrho + \frac{\partial}{\partial x} (v_- \varrho) = 0$$

$$v_- = \frac{\hbar}{2mi} \left(\frac{\frac{\partial \Psi}{\partial x}}{\Psi} - \frac{\frac{\partial \Psi^*}{\partial x}}{\Psi^*} \right) \quad \text{“drift” velocity}$$

$$= \frac{\hbar}{2mi} \frac{\partial}{\partial x} \ln \frac{\Psi}{\Psi^*}$$

real, depending on phase of Ψ

Density operator:

$$\varrho_{\text{op}} = |\Psi\rangle\langle\Psi|$$

pure state

$$\varrho_{\text{op}} = \sum_i w_i |\Psi_i\rangle\langle\Psi_i|$$

mixture, w_i : class. probab.

$$\text{Dirac: } \Psi(x, t) \triangleq |\Psi\rangle, \Psi^*(x, t) \triangleq \langle\Psi|$$

von Neumann:

$$\frac{\partial}{\partial t} \varrho_{\text{op}} + \frac{i}{\hbar} [H_{\text{op}}, \varrho_{\text{op}}]_- = 0$$

$$\text{commutator } \frac{1}{i\hbar} [,]_- \triangleq \{ , \}_{\text{PB}}$$

Wigner:

$$W(x, p, t) = \frac{1}{2\pi\hbar} \int_{-\infty}^{+\infty} dq e^{\frac{i}{\hbar}pq} \underbrace{\left\langle x + \frac{q}{2} \middle| \varrho_{\text{op}} \middle| x - \frac{q}{2} \right\rangle}_{\tilde{\varrho}_{\text{op}}(x, q)}$$

“FT” of ϱ_{op}

pure state:

$$W(x, p, t) = \frac{1}{2\pi\hbar} \int_{-\infty}^{+\infty} dq e^{\frac{i}{\hbar}pq} \Psi^* \left(x + \frac{q}{2} \right) \Psi \left(x - \frac{q}{2} \right)$$

CE:

$$\frac{\partial}{\partial t} W + \frac{\partial}{\partial x} \left(\frac{p}{m} W \right) + \frac{\partial}{\partial p} \left(\left(-\frac{\partial V}{\partial x} \right) W \right) = 0$$

$$\begin{matrix} \uparrow \\ \dot{x} \end{matrix}$$

$$\begin{matrix} \uparrow \\ \dot{p} \end{matrix}$$

Dynamics of Open Systems

irreversible dynamics

dissipation of energy

Class:

Langevin:

$$\ddot{x} + \gamma \dot{x} + \frac{1}{m} \frac{\partial}{\partial x} V = f(t)$$

(phenomenological)

γ : friction coefficient

$mf(t)$: stochastic force, $\langle f \rangle = 0$

Hamilton: ? $H = T + V + W$

$$W = \gamma x p$$

$$\rightarrow \dot{x} = \frac{p}{m} + \gamma x, \quad \dot{p} = -\frac{\partial V}{\partial x} - \gamma p$$

Fokker–Planck:

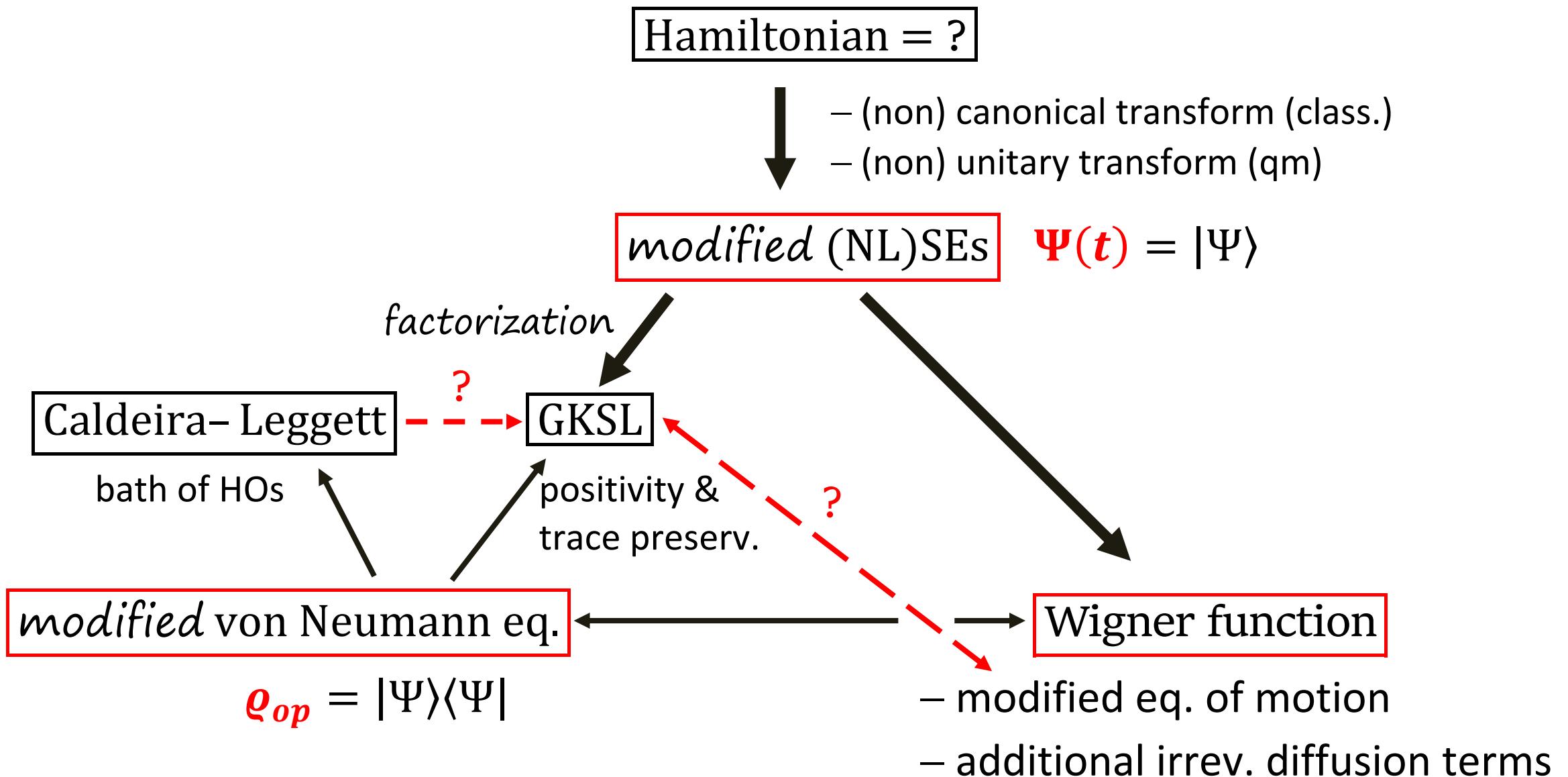
$$\frac{\partial}{\partial t} \varrho_\Gamma + \frac{\partial}{\partial x} \left(\frac{p}{m} \varrho_\Gamma \right) + \frac{\partial}{\partial p} \left(\left(- \frac{\partial V}{\partial x} - \gamma p \right) \varrho_\Gamma \right) - \mathbf{D}_{xx} \frac{\partial^2}{\partial x^2} \varrho_\Gamma - \mathbf{D}_{pp} \frac{\partial^2}{\partial p^2} \varrho_\Gamma = 0$$

↑
 \dot{x}

p

D_{ii} : **diffusion** coefficients, $i = x, p$

Open Quantum Systems



Qm: a) **Modified Schrödinger equations**

- canonical Hamiltonians, e.g., explicitly TD (Caldirola–Kanai)
- NLSEs, also with **non-Hermitian** Hamiltonians
(e.g.: Kostin, Hasse, Gisin, S.C.H., ...)

$$i\hbar \frac{\partial}{\partial t} \Psi(t) = (H_{\text{op}} + \mathbf{W}) \Psi(t)$$

different \mathbf{W}

b) **S+R-approach**

→ generalized **master eq.** for **reduced density op.** ρ_{op} (for **S**)

$$\frac{\partial}{\partial t} \rho_{\text{op}} = \frac{i}{\hbar} [\rho_{\text{op}}, H_{\text{op}}]_- + \mathcal{D}[\rho_{\text{op}}]$$

with **different versions of $\mathcal{D}[\rho_{\text{op}}]$** , representing
the influence of the reservoir **R** on the system **S**
introducing **irreversibility** and, (but not necessarily), **dissipation**
(Caldeira–Leggett, Dekker, Diosi, Sandulescu, **Gao**, **GKSL**, Redfield, ...)

c) **Modified Wigner eq.** (including **diffusion** terms)

Caldeira–Leggett:

$$\mathcal{D}_{\text{CL}}[\varrho] = -\frac{i}{\hbar} \left(\frac{\gamma}{2} [\mathbf{x}, \{\mathbf{p}, \varrho\}_+]_- \right) - \frac{\gamma}{2\hbar} \left(\frac{2mkT}{\hbar} [\mathbf{x}, [\mathbf{x}, \varrho]_-]_- \right) \quad \varrho = \varrho_{\text{op}}$$

Gao:

$$\begin{aligned} \mathcal{D}_{\text{Gao}}[\varrho] = & -i2\mu\nu([\mathbf{x}, \{\mathbf{p}, \varrho\}_+]_- - [xp, \varrho]_-) \\ & - \mu^2 [\mathbf{x}, [\mathbf{x}, \varrho]_-]_- - \nu^2 [\mathbf{p}, [\mathbf{p}, \varrho]_-]_- \end{aligned}$$

Dekker:

$$\begin{aligned} \mathcal{D}_{\text{Dek}}[\varrho] = & -\frac{i}{\hbar} \left(\frac{\gamma}{2} [\mathbf{x}, \{\mathbf{p}, \varrho\}_+]_- \right) + \frac{1}{\hbar^2} (D_{px} + D_{xp}) [\mathbf{p}, [\mathbf{x}, \varrho]_-]_- \\ & - \frac{1}{\hbar^2} D_{pp} [\mathbf{x}, [\mathbf{x}, \varrho]_-]_- - \frac{1}{\hbar^2} D_{xx} [\mathbf{p}, [\mathbf{p}, \varrho]_-]_- \end{aligned}$$

GKSL:

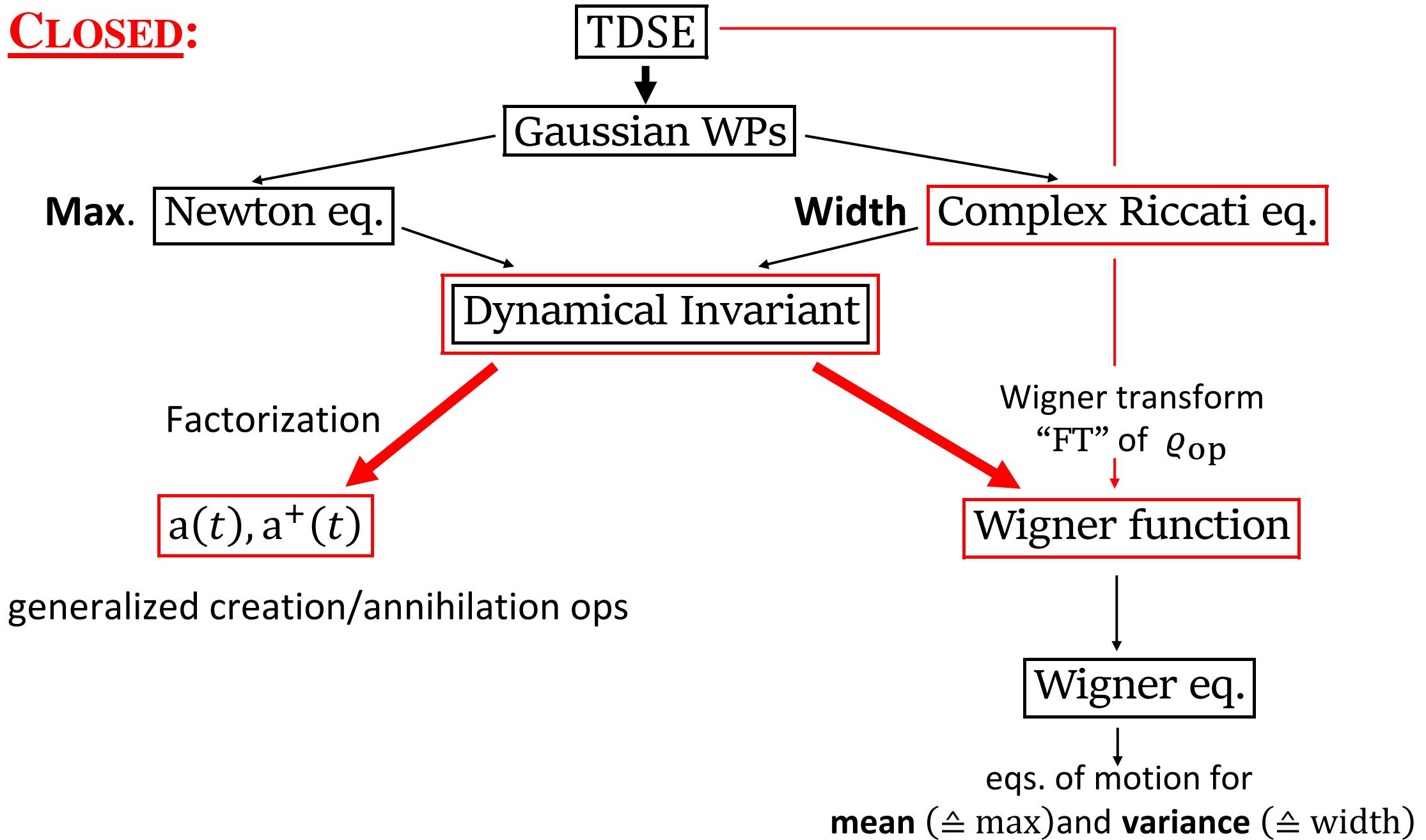
$$\mathcal{D}_{\text{GKSL}}[\varrho] = -\frac{1}{2\hbar} (\{L^+L, \varrho\}_+ - 2L\varrho L^+)$$

Dynamics: **trace-preserving** and **completely positive**

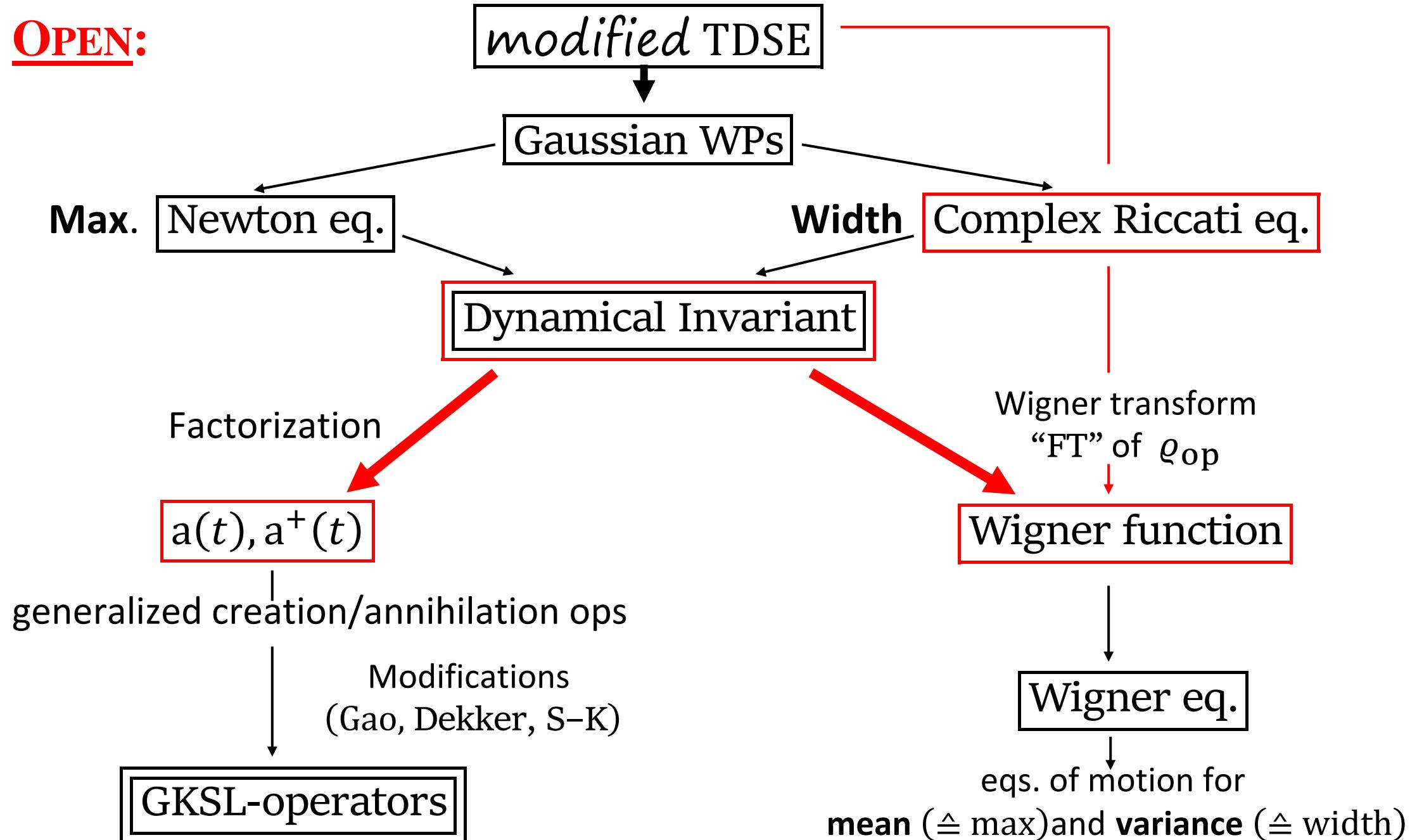
Physical meaning of L^+L ?

Gao, Dekker: L^+L prop.to annihilation/creation operators \mathbf{a}, \mathbf{a}^+ and **modifications**

CLOSED:



OPEN:

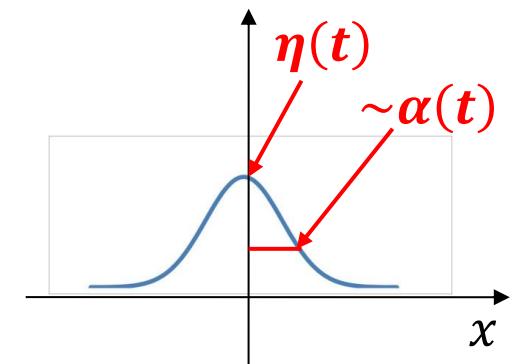


2. TDSE for Closed Systems, WP Solutions

TDSE: $i\hbar \frac{\partial}{\partial t} \Psi(t) = H_{\text{op}} \Psi(t)$ $H_{\text{op}} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + \frac{m}{2} \omega^2 x^2$

Analytical solutions: **Gaussian** WPs

$$\Psi_{\text{WP}}(x, t) = N(t) \exp \left\{ \frac{i}{\hbar} \left[\frac{m}{2} \mathcal{C}(t) \tilde{x}^2 + \langle p \rangle \tilde{x} + K(t) \right] \right\}$$



$$\tilde{x} = x - \langle x \rangle = x - \eta(t)$$

$$\mathcal{C}_I = \frac{\hbar}{2m \langle \tilde{x}^2 \rangle}$$

$$\mathcal{C}(t) = \mathcal{C}_R + i\mathcal{C}_I$$

$$\langle \tilde{x}^2 \rangle = \langle x^2 \rangle - \langle x \rangle^2 = \sigma_{xx}$$

max width

$$\begin{aligned} \ddot{\eta} + \omega^2 \eta &= 0 \\ \dot{\mathcal{C}} + \mathcal{C}^2 + \omega^2 &= 0 \end{aligned}$$

Newton
Complex Riccati

$$\mathcal{C}_I = \frac{1}{\alpha^2}, \mathcal{C}_R = \frac{\dot{\alpha}}{\alpha}$$

⇒

$$\ddot{\alpha} + \omega^2 \alpha = \frac{1}{\alpha^3}$$

Ermakov

$$\Rightarrow I_L = \frac{1}{2} \left[(\dot{\eta} \alpha - \dot{\alpha} \eta)^2 + \left(\frac{\eta}{\alpha} \right)^2 \right] = \text{const}$$

Dynamical invariant

mI_L : **action**

Dynamical (Ermakov) Invariant and generalized Creation/Annihilation Operators

$$H_{\text{op}} = \hbar \omega_0 \left(a^\dagger a + \frac{1}{2} \right) \quad \text{HO}$$

$$a = i \sqrt{\frac{m}{2\hbar\omega_0}} \left(\frac{p_{\text{op}}}{m} - i\omega_0 x \right), \quad a^\dagger = -i \sqrt{\frac{m}{2\hbar\omega_0}} \left(\frac{p_{\text{op}}}{m} + i\omega_0 x \right)$$

Connection with Riccati variable:

$\mathcal{C} = \tilde{\mathcal{C}} + \mathbb{V}(t)$, $\tilde{\mathcal{C}}$: **particular solution**, $\mathbb{V}(t)$: solution of Bernoulli eq.

$$\tilde{\mathcal{C}} = i\tilde{\mathcal{C}}_I = i\omega_0 = i\frac{1}{\alpha_0^2} \quad \text{Generalization: } \mathcal{C}_R = \frac{\dot{\alpha}}{\alpha} \neq 0 \quad \Rightarrow \alpha = \alpha(t), \text{ i.e., TD width}$$

$$a(t) = i \sqrt{\frac{m}{2\hbar}} \alpha(t) \left(\frac{p_{\text{op}}}{m} - \mathcal{C}(t)x \right), \quad a^\dagger(t) = -i \sqrt{\frac{m}{2\hbar}} \alpha(t) \left(\frac{p_{\text{op}}}{m} - \mathcal{C}^*(t)x \right)$$

$$I_{\text{op}} = \frac{\hbar}{m} \left(a^\dagger(t)a(t) + \frac{1}{2} \right) \quad \text{Invariant also for } \omega = \omega(t), \text{ where } H = H(t) \neq \text{const.}$$

Connections between $\mathcal{C}(t)$ and Uncertainties

$$\mathcal{C}_I = \frac{\hbar}{2m\langle\tilde{x}^2\rangle} = \frac{\hbar}{2m\sigma_{xx}} \quad \langle\tilde{x}^2\rangle = \langle x^2\rangle - \langle x\rangle^2 = \sigma_{xx}$$

$$\mathcal{C}_R = \frac{1}{2m} \frac{\langle\{\tilde{x}, \tilde{p}\}_+\rangle}{\langle\tilde{x}^2\rangle} = \frac{1}{2m} \frac{(\sigma_{xp} + \sigma_{px})}{\sigma_{xx}} \quad \sigma_{xp} = \sigma_{px} = \frac{1}{2} \langle\{\tilde{x}, \tilde{p}\}_+\rangle$$

⇒

$$\begin{aligned} a(t) &= \frac{1}{\hbar} \sqrt{\sigma_{xx}} \left[i p_{op} + \left(\frac{\hbar}{2} \frac{1}{\sigma_{xx}} - i \frac{\sigma_{xp}}{\sigma_{xx}} \right) x \right] \\ a^+(t) &= \frac{1}{\hbar} \sqrt{\sigma_{xx}} \left[-i p_{op} + \left(\frac{\hbar}{2} \frac{1}{\sigma_{xx}} + i \frac{\sigma_{xp}}{\sigma_{xx}} \right) x \right] \end{aligned}$$

Coefficients of p_{op} and x **NOT** just “**numbers**” but **TD functions** $\sigma_{ij}(t)$!

⇒ Ermakov invariant rewritten in terms of **uncertainties**:

$$I_L = \frac{1}{m\hbar} [\sigma_{pp}\langle x\rangle^2 - 2\sigma_{xp}\langle x\rangle\langle p\rangle + \sigma_{xx}\langle p\rangle^2] \quad \sigma_{pp} = \langle\tilde{p}^2\rangle$$

Combination of **mean values** and **uncertainties**

Ermakov Invariant, Wigner Function and Equation of Motion (**closed** Systems)

Wigner fct.:

$$\begin{aligned}
 W(x, p, t) &= \frac{1}{\pi\hbar} \exp \left\{ -\frac{2}{\hbar^2} [\sigma_{pp} \tilde{x}^2 - 2\sigma_{xp} \tilde{x}\tilde{p} + \sigma_{xx} \tilde{p}^2] \right\} \\
 &= \frac{1}{\pi\hbar} \exp \left\{ -\frac{m}{\hbar} \left[\left(\dot{\alpha} \tilde{x} - \alpha \frac{\tilde{p}}{m} \right)^2 + \left(\frac{\tilde{x}}{\alpha} \right)^2 \right] \right\} = \frac{1}{\pi\hbar} \exp \left\{ -\frac{2m}{\pi\hbar} \mathbf{I}(\alpha, \tilde{x}) \right\}
 \end{aligned}$$

Wigner eq.:

$$\frac{\partial}{\partial t} W + \frac{\partial}{\partial x} \left(\frac{p}{m} W \right) + \frac{\partial}{\partial p} \left(\left(-\frac{\partial V}{\partial x} \right) W \right) = 0$$

Insert Wigner fct. \Rightarrow

$$\frac{\partial^2}{\partial t^2} \langle x \rangle + \omega^2 \langle x \rangle = 0$$

mean value

$$\dot{\sigma}_{xx} = \frac{2}{m} \sigma_{xp}$$

$$\dot{\sigma}_{pp} = -2m \omega^2 \sigma_{xp}$$

$$\dot{\sigma}_{xp} = \dot{\sigma}_{px} = 2 \left(\frac{1}{2m} \sigma_{pp} - \frac{m}{2} \omega^2 \sigma_{xx} \right)$$

uncertainties

3. Modifications for Open Systems

3.1 Effective Hamiltonians via **non-canonical** transformations

a) **Caldirola/Kanai:** $\hat{L}_{CK} = (T - V)\mathbf{e}^{\gamma t} = \left(\frac{m}{2}\dot{x}^2 - \frac{m}{2}\omega^2x^2\right)\mathbf{e}^{\gamma t}$

$$\hat{p}_{CK} = \frac{\partial \hat{L}_{CK}}{\partial \dot{x}} = m\dot{x}\mathbf{e}^{\gamma t} = p\mathbf{e}^{\gamma t}, \hat{x} = x$$

$$\hat{H}_{CK} = \frac{1}{2m}\hat{p}_{CK}^2 \mathbf{e}^{-\gamma t} + V(x)\mathbf{e}^{\gamma t} \quad \text{NO const. of motion}$$

$$(x, p) \rightarrow (\hat{x} = x, \hat{p}_{CK} = p\mathbf{e}^{\gamma t}) \quad \text{non-canonical}$$

Quantisation: $\hat{p}_{CK} \rightarrow \frac{\hbar}{i}\frac{\partial}{\partial x} \quad \Rightarrow \quad i\hbar\frac{\partial}{\partial t}\hat{\Psi}_{CK}(x, t) = \hat{H}_{CK, \text{op}}\hat{\Psi}_{CK}(x, t)$

Note: **canonical** WF $\hat{\Psi}_{CK}(\mathbf{x}, t) \neq \text{“physical” WF } \Psi(\mathbf{x}, t)$

Connection via **non-unitary** transformation

otherwise: violation of uncertainty relation

b) Expanding CS:

$$(x, p) \rightarrow \left(\hat{Q} = x e^{\frac{\gamma}{2}t}, \hat{P} = m \left(\dot{x} + \frac{\gamma}{2}x \right) e^{\frac{\gamma}{2}t} \right)$$

non-canonical

$$\begin{aligned} \hat{H}_{\text{exp}} &= \frac{1}{2m} \hat{P}^2 + \frac{m}{2} \left(\omega^2 - \frac{\gamma^2}{4} \right) \hat{Q}^2 \\ &\triangleq \left(\frac{1}{2m} p^2 + \frac{\gamma}{2} x p + \frac{m}{2} \omega^2 x^2 \right) e^{\gamma t} \end{aligned}$$

constant of motion

a) and b) both lead to

$$m(\ddot{x} + \gamma \dot{x} + \omega^2 x) = 0$$

(averaged) Langevin eq.

both connected via canonical transformation

$$\hat{Q} = \hat{x} e^{\frac{\gamma}{2}t}, \quad \hat{P} = \hat{p}_{CK} e^{-\frac{\gamma}{2}t} + m \frac{\gamma}{2} \hat{x} e^{\frac{\gamma}{2}t}$$

$$\hat{H}_{\text{exp}} = \hat{H}_{CK} + \underbrace{\frac{\partial}{\partial t} F_2(\hat{x}, \hat{p}, t)}_{\neq 0}$$

Canonical quantization: $\hat{\mathcal{P}} \rightarrow \frac{\hbar}{i} \frac{\partial}{\partial \hat{Q}}, \quad \hat{H}_{\text{exp,op}}(\hat{Q}, \hat{\mathcal{P}}_{\text{op}}), \hat{\Psi}_{\text{exp}}(\hat{Q}, t)$

Canonical WF $\hat{\Psi}_{\text{exp}}$: **Gaussian** WP

Maximum: class. (averaged) **Langevin** eq.

Width complex **Riccati**: $\dot{\hat{\mathcal{C}}}_{\text{exp}} + \hat{\mathcal{C}}_{\text{exp}}^2 + \left(\omega^2 - \frac{\gamma^2}{4} \right) = 0$ like HO, only

Ermakov eq.: $\ddot{\alpha}_{\text{exp}} + \left(\omega^2 - \frac{\gamma^2}{4} \right) \alpha_{\text{exp}} = \frac{1}{\alpha_{\text{exp}}^3}$ $\omega \rightarrow \left(\omega^2 - \frac{\gamma^2}{4} \right)^{\frac{1}{2}} = \Omega$

Ermakov **Invariant**:

$$\begin{aligned} \hat{I}_{\text{exp}} &= \frac{1}{2} \left\{ \left(\left\langle \dot{\hat{Q}} \right\rangle_{\text{exp}} \alpha_{\text{exp}} - \langle \hat{Q} \rangle_{\text{exp}} \dot{\alpha}_{\text{exp}} \right)^2 + \left(\frac{\langle \hat{Q} \rangle_{\text{exp}}}{\alpha_{\text{exp}}} \right)^2 \right\} \\ &\triangleq \frac{1}{2} \mathbf{e}^{\gamma t} \left\{ \left(\dot{\eta} \alpha_{\text{exp}} - \left(\dot{\alpha}_{\text{exp}} - \frac{\gamma}{2} \alpha_{\text{exp}} \right) \eta \right)^2 + \left(\frac{\eta}{\alpha_{\text{exp}}} \right)^2 \right\} \end{aligned}$$

3.2 Nonlinear Modifications of Hamiltonian OPERATOR

By adding “friction potential” W ,

$$H_{\text{NL}} = H_0 + \mathbf{W}$$

based on:

dissipative friction force in EOM (\rightarrow **real** part)

irreversible diffusion terms in CE \rightarrow FPE (\rightarrow **imag.** part)

To include both aspects \rightarrow **complex** addition necessary!

Resulting effective **NLSEs** have analytical **Gaussian WP** solutions

Maximum: classical EOM including friction force

Width: modified Riccati eq.

modified Ermakov eq.

\rightarrow modified Ermakov Invariant I_{NL}

I. Approaches based on **Dissipative Friction Force**

According to Ehrenfest:

$$\frac{\partial}{\partial t} \langle p \rangle + \gamma \langle p \rangle + \langle \frac{\partial}{\partial x} V \rangle = 0$$

Necessary cond. for W

$$\langle \frac{\partial}{\partial x} W \rangle = \gamma \langle p \rangle$$

a) Kostin

$$W_K = \gamma \frac{\hbar}{2i} \left(\ln \frac{\Psi}{\Psi^*} - \langle \ln \frac{\Psi}{\Psi^*} \rangle \right) \quad \text{real}$$

as $\frac{\partial}{\partial x} W_K = \gamma \frac{\hbar}{2i} \frac{\partial}{\partial x} \ln \frac{\Psi}{\Psi^*} = \gamma m v_-$ (see CE for ϱ)

with $\langle v_- \rangle = \langle v \rangle = \frac{1}{m} \langle p \rangle$

Problems:

- 1) unshifted freq. ω instead of $\Omega = \left(\omega^2 - \frac{\gamma^2}{4} \right)^{\frac{1}{2}}$ for damped HO
- 2) solutions of undamped HO (real) solve NLSE
- 3) Eq. for ϱ still **reversible** CE

b) General “friction potential”:

$$W_G = \gamma \langle p \rangle (x - \langle x \rangle) + \frac{\gamma}{2} \mathbf{K} \{ (x - \langle x \rangle), (p - \langle p \rangle) \}_+$$

For **ANY** K ,

$$\left\langle \frac{\partial}{\partial x} W_G \right\rangle = \gamma \langle p \rangle \quad \text{fulfilled}$$

Süssmann

$$K = 1$$

$$W_{\text{Sü}} = \frac{\gamma}{2} \{ (x - \langle x \rangle), p \}_+$$

damped HO: $\Omega_{\text{Sü}} = (\omega_0^2 - \gamma^2)^{1/2}$ **wrong**

Albrecht

$$K = 0$$

$$W_{\text{Al}} = \gamma \langle p \rangle (x - \langle x \rangle)$$

$$\Omega_{\text{Al}} = \omega_0 \quad \text{wrong}$$

General: $\Omega_G = (\omega_0^2 - K^2 \gamma^2)^{1/2} \rightarrow K = \pm \frac{1}{2}$

$$\begin{aligned} W_{\text{Has}} &= \frac{\gamma}{4} \{ (x - \langle x \rangle), (p + \langle p \rangle) \}_+ \\ &= \frac{1}{2} (W_{\text{Sü}} + W_{\text{Al}}) \end{aligned}$$

$$\Omega_{\text{Has}} = \left(\omega_0^2 - \frac{\gamma^2}{4} \right)^{1/2} \quad \text{correct}$$

Hasse

$$K = \frac{1}{2}$$

but $\langle W_{\text{Has}} \rangle \neq 0 \rightarrow \langle H \rangle \neq \langle T \rangle + \langle V \rangle$

II. Approach based on irreversible Diffusion Term

NLSE:

$$i\hbar \frac{\partial}{\partial t} \Psi(x, t) = (H_{op} + \tilde{W}) \Psi(x, t)$$

Breaking time-reversal symmetry via **diffusion term** for probability density:

$$\frac{\partial}{\partial t} \varrho(x, t) + \frac{\partial}{\partial x} (v_- \varrho) - D \frac{\partial^2}{\partial x^2} \varrho = 0$$

Fokker–Planck-type

not separable in general but via **separation condition**

$$-D \frac{\frac{\partial^2}{\partial x^2} \varrho}{\varrho} = \gamma (\ln \varrho - \langle \ln \varrho \rangle)$$

with $D = \frac{\gamma}{2} \langle \tilde{x}^2 \rangle = \frac{\gamma}{2} \sigma_{xx}$

$\Rightarrow \tilde{W} = \gamma \frac{\hbar}{i} (\ln \Psi - \langle \ln \Psi \rangle)$ **complex log NL**

Connection with other NLSEs

$$\begin{aligned}\widetilde{W} &= \gamma \frac{\hbar}{i} (\ln \Psi - \langle \ln \Psi \rangle) \\ &= \underbrace{\gamma \frac{\hbar}{2i} \left(\ln \frac{\Psi}{\Psi^*} - \langle \ln \frac{\Psi}{\Psi^*} \rangle \right)}_{\text{real}} + \underbrace{\gamma \frac{\hbar}{2i} (\ln \varrho - \langle \ln \varrho \rangle)}_{\text{imag.}}\end{aligned}$$

real \triangleq **Kostin**

\Downarrow

$$-\langle \frac{\partial}{\partial x} \widetilde{W} \rangle = -\gamma m \langle v \rangle$$

dissipation

imag. $i \frac{\hbar}{2} D \frac{\partial^2 \varrho}{\partial x^2}$ \triangleq **Doebner–Goldin**

\Downarrow

FPE

irreversibility

$$\widetilde{W} \Psi_{\text{WP}} = (W_{\text{Has}} - \langle W_{\text{Has}} \rangle) \Psi_{\text{WP}} = \widetilde{W}_{\text{Has}} \Psi_{\text{WP}} \quad \text{Hasse}$$

Connection with Canonical Approaches

Hamilton–Jacobi

$$\frac{\partial}{\partial t} S + H \left(x, \frac{\partial}{\partial x} S, t \right) = 0$$

Schrödinger Def.:

$$S_c = \frac{\hbar}{i} \ln \Psi \quad \text{complex!}$$

log NLSE written with S_c :

$$\left(\frac{\partial}{\partial t} + \gamma \right) S_c + H = \gamma \langle S_c \rangle$$

↑ for normalization → neglect

Define:

$$\hat{S}_c = e^{\gamma t} S_c, \quad \hat{H} = e^{\gamma t} H \quad \triangleq \text{Caldirola/Kanai}$$

log NLSE →

$$\frac{\partial}{\partial t} \hat{S}_c + \hat{H} = 0$$

and

$$\ln \hat{\Psi} = e^{\gamma t} \ln \Psi_{\text{NL}}$$

Non-unitary connection between **canonical** WF $\hat{\Psi}(\hat{x}, p)$ and **physical** WF $\Psi_{\text{NL}}(x, p)$!

Properties of the log NLSE

NLSE with **complex logarithmic** nonlinearity:

$$i\hbar \frac{\partial}{\partial t} \Psi = \left\{ H_{\text{op}} + \gamma \frac{\hbar}{i} (\ln \Psi - \langle \ln \Psi \rangle) \right\} \Psi$$

$\underbrace{\phantom{H_{\text{op}} + \gamma \frac{\hbar}{i} (\ln \Psi - \langle \ln \Psi \rangle) \Psi}$ }_{\widetilde{W}_{\text{SCH}}}

Gaussian WP-solutions like for isolated systems ($\gamma = 0$)

modified eqs. of motion:

max width

$$\begin{aligned} \ddot{\eta} + \gamma \dot{\eta} + \omega^2 \eta &= 0 \\ \dot{\mathcal{C}}_{\text{NL}} + \gamma \mathcal{C}_{\text{NL}} + \mathcal{C}_{\text{NL}}^2 + \omega^2 &= 0 \end{aligned}$$

$\eta = \langle x \rangle$
 \mathcal{C}_{NL} : complex

$$\mathcal{C}_{\text{NL,I}} = \frac{1}{\alpha^2}, \quad \mathcal{C}_{\text{NL,R}} = \frac{\dot{\alpha}}{\alpha} - \frac{\gamma}{2} \quad \Rightarrow$$

$$\ddot{\alpha}_{\text{NL}} + \left(\omega^2 - \frac{\gamma^2}{4} \right) \alpha_{\text{NL}} = \frac{1}{\alpha_{\text{NL}}^3}$$

modified **Ermakov invariant**:

$$I_{\text{NL}} = \frac{1}{2} e^{\gamma t} \left[\left(\dot{\eta} \alpha_{\text{NL}} - \left(\dot{\alpha}_{\text{NL}} - \frac{\gamma}{2} \alpha_{\text{NL}} \right) \eta \right)^2 + \left(\frac{\eta}{\alpha_{\text{NL}}} \right)^2 \right] = \text{const}$$

$\triangleq \hat{I}_{\text{exp}}$

Modified Creation/Annihilation Operators

$$\begin{aligned} a_{\text{NL}}(t) &= i \sqrt{\frac{m}{2\hbar}} \alpha_{\text{NL}}(t) \left(\frac{p_{\text{op}}}{m} - \mathcal{C}_{\text{NL}} x \right) e^{\frac{\gamma}{2}t} \\ a_{\text{NL}}^+(t) &= -i \sqrt{\frac{m}{2\hbar}} \alpha_{\text{NL}}(t) \left(\frac{p_{\text{op}}}{m} - \mathcal{C}_{\text{NL}}^* x \right) e^{\frac{\gamma}{2}t} \end{aligned}$$

- Apart from factor $e^{\frac{\gamma}{2}t}$, same form as in isolated system, only $\mathcal{C}(t) \rightarrow \mathcal{C}_{\text{NL}}(t)$, fulfilling Riccati equation with additional **linear term** $\gamma \mathcal{C}_{\text{NL}}$.
- In terms of σ_{ij} , \mathcal{C}_{NL} **same form** as in isolated system,
i.e., $\mathcal{C}_{\text{I}} = \frac{\hbar}{2m} \frac{1}{\sigma_{xx}}$, $\mathcal{C}_{\text{R}} = \frac{1}{m} \frac{\sigma_{xp}}{\sigma_{xx}}$,
only σ_{ij} obey **different eoms** than in isolated system.

Wigner Function

In terms of \tilde{x}, \tilde{p} and σ_{ij} , **same form** as in **isolated** system, **apart from** factor $e^{\gamma t}$,

$$W_{\text{NL}}(x, p, t) = \frac{e^{-\gamma t}}{\pi \hbar} \exp \left\{ -\frac{2}{\hbar^2} e^{\gamma t} [\sigma_{pp} \tilde{x}^2 - 2\sigma_{xp} \tilde{x} \tilde{p} + \sigma_{xx} \tilde{p}^2] \right\}$$

This leads to the modified equation of motion

$$\frac{\partial}{\partial t} W_{\text{NL}} + \frac{\partial}{\partial x} \left(\frac{p}{m} W_{\text{NL}} \right) - \frac{\partial}{\partial p} \left((m\omega^2 x + \gamma p) W_{\text{NL}} \right) + \gamma (\ln W_{\text{NL}} - \langle \ln W_{\text{NL}} \rangle) W_{\text{NL}} = 0$$

with $\dot{p} = -\gamma p - m\omega^2 x$ and $\langle \ln W \rangle = \frac{\hbar^2}{2}$

Inserting W_{NL} leads to an equation of motion for the mean value (from terms linear in \tilde{x}, \tilde{p}):

$$\boxed{\frac{\partial}{\partial t} \langle p \rangle + \gamma \langle p \rangle + m\omega^2 \langle x \rangle = 0}$$

and equations of motion for the σ_{ij}

(from terms quadratic or bilinear in \tilde{x}, \tilde{p}):

$$\boxed{\begin{aligned}\dot{\sigma}_{xx} &= \frac{2}{m} \sigma_{xp} + \gamma \sigma_{xx} \\ \dot{\sigma}_{pp} &= -2m\omega^2 \sigma_{xp} - \gamma \sigma_{pp} \\ \dot{\sigma}_{xp} &= \dot{\sigma}_{px} = 2 \left(\frac{1}{2m} \sigma_{pp} - \frac{m}{2} \omega^2 \sigma_{xx} \right)\end{aligned}}$$

These equations are **consistent** with expressions for $\dot{\sigma}_{ij}$ in terms of $\alpha, \dot{\alpha}$ corresponding to the **log NLSE** and the **respective Ermakov eq.**

Comparison: additional **ln-terms** vs. **diffusion terms**

$$\gamma(\ln W - \langle \ln W \rangle)W = -D_{xx} \frac{\partial^2}{\partial x^2} W - D_{pp} \frac{\partial^2}{\partial p^2} W + (D_{xp} + D_{px}) \frac{\partial^2}{\partial p \partial x} W$$

if $D_{xx} = \frac{\gamma}{2} \sigma_{xx}$, $D_{pp} = \frac{\gamma}{2} \sigma_{pp}$, $D_{xp} = D_{px} = \frac{\gamma}{2} \sigma_{xp} = \frac{\gamma}{2} \sigma_{px}$

In this case, **our Wigner eq.** turns into the one by **Dekker!**

(N.B.: Compare with separation condition leading to our log NLSE)

Mean values: Dekker obtains the same eom including **friction force**.

Dekker Condition for Diffusion Coefficients and Uncertainties

Initially, Dekker used D_{ij} corresponding to particular solution of Riccati eq.,

i.e. without TD of WP width:

$$\sigma_{xx} = \frac{\hbar}{2m\Omega} , \quad \sigma_{pp} = \frac{m\hbar}{2} \frac{\omega^2}{\Omega} , \quad \sigma_{px} = \sigma_{xp} = \frac{-\frac{\gamma}{2}}{\Omega}$$

He obtains a more general form of D_{ij} in terms of σ_{ij} from the Wigner equation, whereby D_{ij} must fulfil a relation corresponding to the

Schrödinger–Robertson uncertainty relation:

$$\sigma_{xx}\sigma_{pp} - \sigma_{xp}^2 \geq \frac{\hbar^2}{4}$$

also valid for the general solution corresponding to the TD σ_{ij} .

The equations of motion for his σ_{ij} are

$$\begin{aligned}\dot{\sigma}_{xx} &= \frac{2}{m} \sigma_{xp} + 2 D_{xx} \\ \dot{\sigma}_{pp} &= -2m\omega^2 \sigma_{xp} - 2\gamma \sigma_{pp} + 2 D_{pp} \\ \dot{\sigma}_{xp} &= \dot{\sigma}_{px} = 2 \left(\frac{1}{2m} \sigma_{pp} - \frac{m}{2} \omega^2 \sigma_{xx} \right) - \gamma \sigma_{px} + D_{px} + D_{xp}\end{aligned}$$

which turn into our equations if D_{ij} is replaced by

$$D_{ij} = \frac{\gamma}{2} \sigma_{ij}$$

Comparison of different GKSL Approaches and Physical Meaning

Connection between L, L^+ and a, a^+

$$a(t) = \frac{1}{\hbar} \sqrt{\sigma_{xx}} \left[i p + \left(\frac{\hbar}{2\sigma_{xx}} - i \frac{\sigma_{xp}}{\sigma_{xx}} \right) x \right]$$

$$C_R = \frac{\dot{\alpha}}{\alpha} - \frac{\gamma}{2}$$

α : WP width \rightarrow

$\dot{\alpha} = 0$, i.e. const. width $\rightarrow \sigma_{xp} = -\frac{\gamma}{2}$ Dekker

$\dot{\alpha} = 0$ and $\gamma = 0 \rightarrow \sigma_{xp} = 0$ Gao

Uncertainty product

$$\sigma_{xx} \sigma_{pp} = \frac{\hbar^2}{4} + \sigma_{xp}^2$$

Minimum uncertainty WP

$$\sigma_{xx} \sigma_{pp} = \frac{\hbar^2}{4}, \quad \text{i.e. } \sigma_{xp} = 0$$

At least for $t = 0$: $\sigma_{xp} = 0$ possible, even for $\dot{\alpha} \neq 0$

Gao

$$\mathcal{C}_R = \frac{\dot{\alpha}}{\alpha} = 0$$

$$a_{Gao} = \frac{1}{\hbar} \sqrt{\sigma_{xx}} \left[i p + \frac{\hbar}{2\sigma_{xx}} x \right]$$

$$L_{Gao} = \mu x + i \nu p$$

μ, ν : **real**, **TI**

$$\begin{aligned} \mu^2 &= \frac{\gamma}{2} \frac{1}{4\sigma_{xx}} = \frac{\gamma}{2} \frac{\sigma_{pp}}{\hbar^2} = \frac{\gamma}{2} \frac{2m\mathbf{kT}}{\hbar^2} \\ \nu^2 &= \frac{\gamma}{2} \frac{\sigma_{xx}}{\hbar^2} = \frac{\gamma}{2} \frac{1}{4\sigma_{pp}} = \frac{\gamma}{2} \frac{1}{8m\mathbf{kT}} \end{aligned}$$

with

$$\frac{\sigma_{pp}}{2m} = \mathbf{kT}$$

Gao: \mathbf{kT} by comparison with C-L

\Rightarrow

$$\mu\nu = \frac{\gamma}{4\hbar}$$

and

$$L_{Gao} = \sqrt{\frac{\gamma}{2}} a_{Gao}$$

$$L_{Gao}^+ L_{Gao} = \frac{\gamma}{2} a_{Gao}^+ a_{Gao}$$

Dekker

$$\mathcal{C}_R = \frac{\dot{\alpha}}{\alpha} - \frac{\gamma}{2} \quad \text{for} \quad \dot{\alpha} = 0 \quad \text{const. width}$$

from **particular** solution $\tilde{\mathcal{C}} = -\frac{\gamma}{2} \pm i\Omega$, $\Omega^2 = \omega^2 - \frac{\gamma^2}{4}$

→ **complex** coeff. of x

$$a_{\text{Dek}} = \frac{1}{\hbar} \sqrt{\sigma_{xx}} \left[i p + \left(\frac{\hbar}{2\sigma_{xx}} + i m \frac{\gamma}{2} \right) x \right]$$

$$D_{ij} = \frac{\gamma}{2} \sigma_{ij} \quad \text{and} \quad L_{\text{Dek}} = \sqrt{\frac{\gamma}{2}} a_{\text{Dek}}$$

TD in σ_{xp} later **via Wigner eq.** and equations of motion for σ_{ij}

S-K

$$\mathcal{C}_R = \frac{\dot{\alpha}}{\alpha} - \frac{\gamma}{2}$$

for $\dot{\alpha} \neq 0$ TD width

from **general** solution $\mathcal{C} = \tilde{\mathcal{C}} + \mathbb{V}(t)$

→ **complex TD** coeff. of x

$$a_{SK}(t) = \frac{1}{\hbar} \sqrt{\sigma_{xx}(t)} \left[i p + \left(\frac{\hbar}{2\sigma_{xx}(t)} - i \frac{\sigma_{xp}(t)}{\sigma_{xx}(t)} \right) x \right]$$

$$L_{SK} = \lambda_x x + i \lambda_p p$$

λ_p : **real** , TD

$\lambda_x = \lambda_x^R + i \lambda_x^I$: **complex** , TD

$$|\lambda_x|^2 = \frac{\gamma}{\hbar} \sigma_{pp} , \quad \lambda_p^2 = \frac{\gamma}{\hbar} \sigma_{xx} , \quad \lambda_p \lambda_x^I = -\frac{\gamma}{\hbar} \sigma_{px} , \quad \lambda_p \lambda_x^R = \gamma$$

$$L_{SK} = \sqrt{\frac{\gamma}{2}} a_{SK}(t)$$

$$L_{SK}^+ L_{SK} = \frac{\gamma}{2} a_{SK}^+ a_{SK} \triangleq \frac{\gamma m}{2 \hbar} e^{-\gamma t} I_{NL}$$

Comparison of $\mathcal{D}[\varrho]$

Gao:

$$\mathcal{D}_{\text{Gao}} = -\frac{\gamma}{2} \left\{ \mathbf{i} \frac{1}{2\hbar} ([x, \{p, \varrho\}_+]_- - [xp, \varrho]_-) \right. \\ \left. + \frac{\tilde{\sigma}_{pp,0}}{\hbar^2} [x, [x, \varrho]_-]_- + \frac{\tilde{\sigma}_{xx,0}}{\hbar^2} [p, [p, \varrho]_-]_- \right\}$$

Dekker:

$$\mathcal{D}_{\text{Dek}} = -\frac{\gamma}{2} \left\{ \mathbf{i} \frac{1}{2\hbar} ([x, \{p, \varrho\}_+]_- - [xp, \varrho]_-) - \frac{1}{\hbar^2} (\tilde{\sigma}_{xp} + \tilde{\sigma}_{px}) [p, [x, \varrho]_-]_- \right. \\ \left. + \frac{\tilde{\sigma}_{pp}}{\hbar^2} [x, [x, \varrho]_-]_- + \frac{\tilde{\sigma}_{xx}}{\hbar^2} [p, [p, \varrho]_-]_- \right\}$$

S-K:

$$\mathcal{D}_{\text{SK}} = -\frac{\gamma}{2} \left\{ \mathbf{i} \frac{1}{2\hbar} ([x, \{p, \varrho\}_+]_- - [xp, \varrho]_-) - \frac{1}{\hbar^2} (\sigma_{xp} [x, [p, \varrho]_-]_- + \sigma_{px} [p, [x, \varrho]_-]_-) \right. \\ \left. + \frac{\sigma_{pp}}{\hbar^2} [x, [x, \varrho]_-]_- + \frac{\sigma_{xx}}{\hbar^2} [p, [p, \varrho]_-]_- \right\}$$

use: a) $[p, [x, \varrho]_-]_- = [x, [p, \varrho]_-]_-$

b) $[x, \{p, \varrho\}_+]_- - [xp, \varrho]_- = \frac{1}{2} ([x, \{p, \varrho\}_+]_- - [p, \{x, \varrho\}_+]_-)$

Solution of the Riccati Equation

$$\mathcal{C}(t) = \tilde{\mathcal{C}} + \mathbb{V}(t)$$

$\tilde{\mathcal{C}}$: **particular** solution

$\mathbb{V}(t)$: solution of (homog.) Bernoulli eq.

Bernoulli eq.

$$\dot{\mathbb{V}} + 2\tilde{\mathcal{C}}\mathbb{V} + \mathbb{V}^2 = 0$$

⇒ **general solution:**

$$\mathcal{C}(t) = \tilde{\mathcal{C}} + \frac{e^{-2\tilde{\mathcal{C}}t}}{\frac{1}{2\tilde{\mathcal{C}}}(1-e^{-2\tilde{\mathcal{C}}t}) + \frac{1}{\mathbb{V}_0}}$$

$$\sigma_{xp} = \frac{\hbar}{2} \alpha^2 \mathcal{C}_R$$

$$\gamma = 0 \quad \mathcal{C}_R = \frac{\dot{\alpha}}{\alpha}, \quad \dot{\alpha} = 0 \rightarrow \mathcal{C}_R = 0 \rightarrow \tilde{\sigma}_{xp,0} = 0$$

$$\gamma \neq 0 \quad \mathcal{C}_R = \frac{\dot{\alpha}}{\alpha} - \frac{\gamma}{2}$$

$$\dot{\alpha} = 0 \rightarrow \tilde{\mathcal{C}}_R = -\frac{\gamma}{2} \rightarrow \tilde{\sigma}_{xp} = -\frac{\gamma}{2} \alpha_0^2 \frac{\hbar}{2} = \text{const.} \neq 0$$

$$\dot{\alpha} \neq 0 \rightarrow \mathcal{C}_R = -\frac{\gamma}{2} + \mathbb{V}_R(t) \rightarrow \sigma_{xp} = \left(-\frac{\gamma}{2} + \frac{\dot{\alpha}}{\alpha} \right) \alpha^2 \frac{\hbar}{2} = \sigma_{xp}(t)$$

Critical comment on Gao's approach:

Wrong Ehrenfest eqs. of motion

$$\frac{\partial}{\partial t} \langle x \rangle = \frac{\langle p \rangle}{m} - \frac{\gamma}{2} \langle x \rangle, \quad \frac{\partial}{\partial t} \langle p \rangle = - \langle \frac{\partial}{\partial x} V \rangle - \frac{\gamma}{2} \langle p \rangle$$

instead of correct dynamics of Brownian motion

$$\frac{\partial}{\partial t} \langle x \rangle = \frac{\langle p \rangle}{m}, \quad \frac{\partial}{\partial t} \langle p \rangle = - \langle \frac{\partial}{\partial x} V \rangle - \gamma \langle p \rangle$$

Similar to “friction potentials”

$$\overline{W_{\text{Has}}} = \frac{1}{2} W_{\text{Sü}} + \frac{1}{2} W_{\text{Al}} = \frac{\gamma}{4} \{(x - \langle x \rangle, p)\}_+ + \frac{\gamma}{2} \langle p \rangle (x - \langle x \rangle)$$

 **complex**  **real**

$$\rightarrow \frac{\gamma}{2} \langle p \rangle \quad \rightarrow \frac{\gamma}{2} \langle p \rangle$$

+ **non-unit.** contrib. + only **unit.** contrib.

General Formalism

$$\frac{\partial}{\partial t} \varrho = \mathcal{L}[\varrho] = -\frac{i}{\hbar} [\mathbf{H}', \varrho]_- + \mathcal{D}[\varrho]$$

unitary contrib. **non-unitary** contrib.

\mathbf{H}' : in general NOT identical with
unperturbed Hamiltonian $H_0 = T_{\text{op}} + V$
of system (due to environment)
→ “renormalization” of energy levels

Gao:	$H' = H_0$	$\left. \begin{array}{l} \mathcal{D}[\varrho] \text{ all fulfill} \\ \text{GKSL-condition,} \\ \text{but different } \sigma_{xp} \end{array} \right\}$
Dekker:	$\mathbf{H}' = H_0 + \frac{\gamma}{4} \{x, p\}_+$	
DS:	$\mathbf{H}' = ?$	

Canonical:

$$\begin{aligned}\hat{H}_{\text{exp}} &= \frac{1}{2m} \hat{\mathcal{P}}^2 + \frac{m}{2} \left(\omega^2 - \frac{\gamma^2}{4} \right) \hat{Q}^2 \\ &\triangleq \left(\frac{p^2}{2m} + \frac{\gamma}{2} \mathbf{x} \mathbf{p} + \frac{m}{2} \omega^2 x^2 \right) \mathbf{e}^{\gamma t} = \text{const}\end{aligned}$$

$$\begin{aligned}\hat{I}_{\text{exp}} &= \frac{1}{2} \left\{ \left(\langle \dot{\hat{Q}} \rangle \hat{\alpha} - \langle \hat{Q} \rangle \dot{\hat{\alpha}} \right)^2 + \left(\frac{\langle \hat{Q} \rangle}{\hat{\alpha}} \right)^2 \right\} \\ &\triangleq \frac{1}{2} \left\{ \left(\dot{\eta} \alpha - \left(\dot{\alpha} - \frac{\gamma}{2} \alpha \right) \eta \right)^2 + \left(\frac{\eta}{\alpha} \right)^2 \right\} \mathbf{e}^{\gamma t} = I_{\text{NL}}\end{aligned}$$

$$\boxed{\hat{H} = H \mathbf{e}^{\gamma t}} \quad \text{non-canonical}$$

$$\boxed{\ln \hat{\Psi} = \mathbf{e}^{\gamma t} \ln \Psi_{\text{NL}}} \quad \text{non-unitary}$$

$$\ln \hat{W} = \mathbf{e}^{\gamma t} \ln W \quad , \quad \ln \hat{W} \sim \hat{I}(\hat{Q}, \hat{\alpha})$$

Physical: Factorization of $\hat{I} \mathbf{e}^{-\gamma t} \rightarrow a(t), a^+(t) \rightarrow \mathcal{D}[\varrho]$

Hamiltonian: $\hat{H}_{\text{exp}} \mathbf{e}^{-\gamma t} \rightarrow \mathbf{H}' = H_0 + \frac{\gamma}{4} \{ \mathbf{x}, \mathbf{p} \}_+ \triangleq \text{Dekker}$

Canonical
level

$$\hat{H}_{\text{CK}}(\hat{x}, \hat{p}, t) = \frac{1}{2m} e^{-\gamma t} \hat{p}^2 + \frac{m}{2} \omega^2 \hat{x}^2 e^{\gamma t} = \hat{H}_{\text{CK}}(t)$$

$$\begin{aligned}\hat{Q} &= \hat{x} e^{\frac{\gamma}{2}t} \\ \hat{P} &= \hat{p} e^{-\frac{\gamma}{2}t} + m \frac{\gamma}{2} \hat{x} e^{\frac{\gamma}{2}t}\end{aligned}$$

canonical
transformation

$$\hat{H}_{\text{exp}}(\hat{Q}, \hat{P}) = \frac{1}{2m} \hat{P}^2 + \frac{m}{2} \left(\omega^2 - \frac{\gamma^2}{4} \right) \hat{Q}^2 = \text{const.}$$

$$\dot{\hat{p}} + m\omega^2 \hat{x} e^{\gamma t} = 0$$

$$\dot{\hat{P}} + m \left(\omega^2 - \frac{\gamma^2}{4} \right) \hat{Q} = 0$$

"conservative"

$$\begin{aligned}\hat{x} &= x \\ \hat{p} &= p e^{\gamma t}\end{aligned}$$

non-canonical
transformation

$$\begin{aligned}\hat{Q} &= x e^{\frac{\gamma}{2}t} \\ \hat{P} &= p e^{-\frac{\gamma}{2}t} + m \frac{\gamma}{2} x e^{\frac{\gamma}{2}t}\end{aligned}$$

non-canonical
transformation

Physical
level

$$H = ?$$

$$\dot{p} + \gamma p + m\omega^2 x = 0$$

$$\begin{aligned}p &= m\dot{x} \\ \dot{E} &= -2\gamma T < 0 : \text{dissipative}\end{aligned}$$

Canonical
level

$$i\hbar \frac{\partial}{\partial t} \widehat{\Psi}_{\text{CK}}(\hat{x}, t) = \widehat{H}_{\text{CK, op}} \widehat{\Psi}_{\text{CK}}(\hat{x}, t)$$

$$\hat{p}_{\text{op}} = \frac{\hbar}{i} \frac{\partial}{\partial \hat{x}}$$

$$\hat{S}_{\text{CK}} = S e^{\gamma t}$$

$$\frac{\hbar}{i} \ln \Psi = e^{-\gamma t} \frac{\hbar}{i} \ln \widehat{\Psi}_{\text{CK}}$$

$$\hat{S}_{\text{exp}} = \hat{S}_{\text{CK}} + m \frac{\gamma}{4} \hat{Q}^2$$

$$\widehat{\Psi}_{\text{CK}} = \exp \left\{ -\frac{im\gamma}{2\hbar} \hat{x}^2 e^{\gamma t} \right\} \widehat{\Psi}_{\text{exp}}$$

$$i\hbar \frac{\partial}{\partial t} \widehat{\Psi}_{\text{exp}}(\hat{Q}, t) = \widehat{H}_{\text{exp, op}} \widehat{\Psi}_{\text{exp}}(\hat{Q}, t)$$

$$\hat{p}_{\text{op}} = \frac{\hbar}{i} \frac{\partial}{\partial \hat{Q}}$$

Schrödinger:

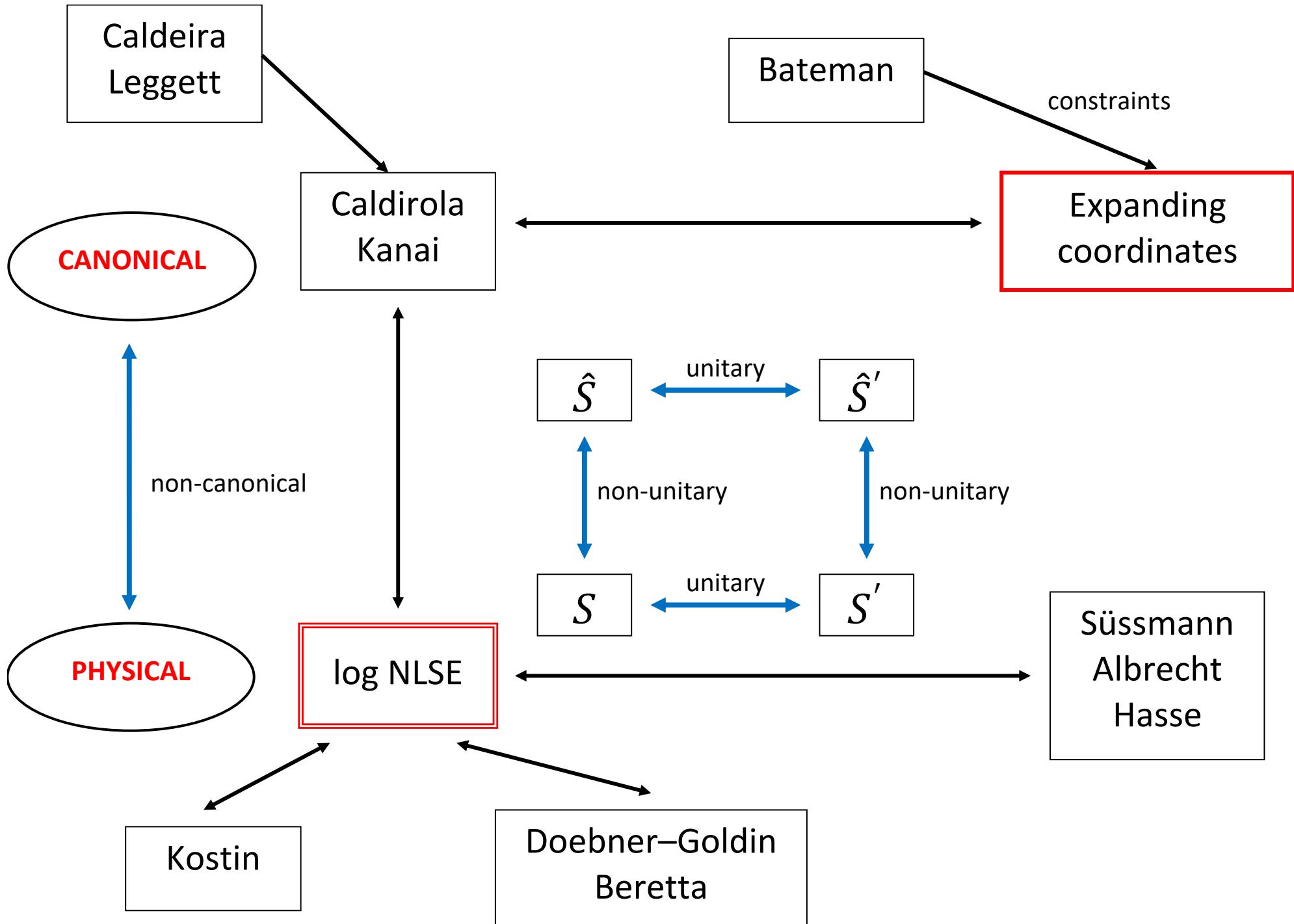
$$S = \frac{\hbar}{i} \ln \Psi$$

$$\hat{S}_{\text{exp}} = S e^{\gamma t} + m \frac{\gamma}{4} \hat{Q}^2$$

Physical
level

$$i\hbar \frac{\partial}{\partial t} \Psi_{\text{NL}}(x, t) = H_{\text{NL, op}} \Psi_{\text{NL}}(x, t) = \{H_{\text{L}} + \tilde{W}_{\text{SCH}}\} \Psi_{\text{NL}}(x, t)$$

$$p_{\text{op}} = \frac{\hbar}{i} \frac{\partial}{\partial x}$$



4. Conclusions

I. **Closed** TD Quantum Systems

TDSE \rightarrow Gaussian WP solutions $|\Psi\rangle$

Dynamics of Maximum: Newton eq. \rightarrow class. trajectory

Width: Riccati/Ermakov eq. \rightarrow position uncertainty

Combined eqs. of motion \rightarrow **Dynamical invariant** (action)

factorization

TD creation/annihilation ops

Liouville eq. for $\varrho_{\text{op}} = |\Psi\rangle\langle\Psi|$

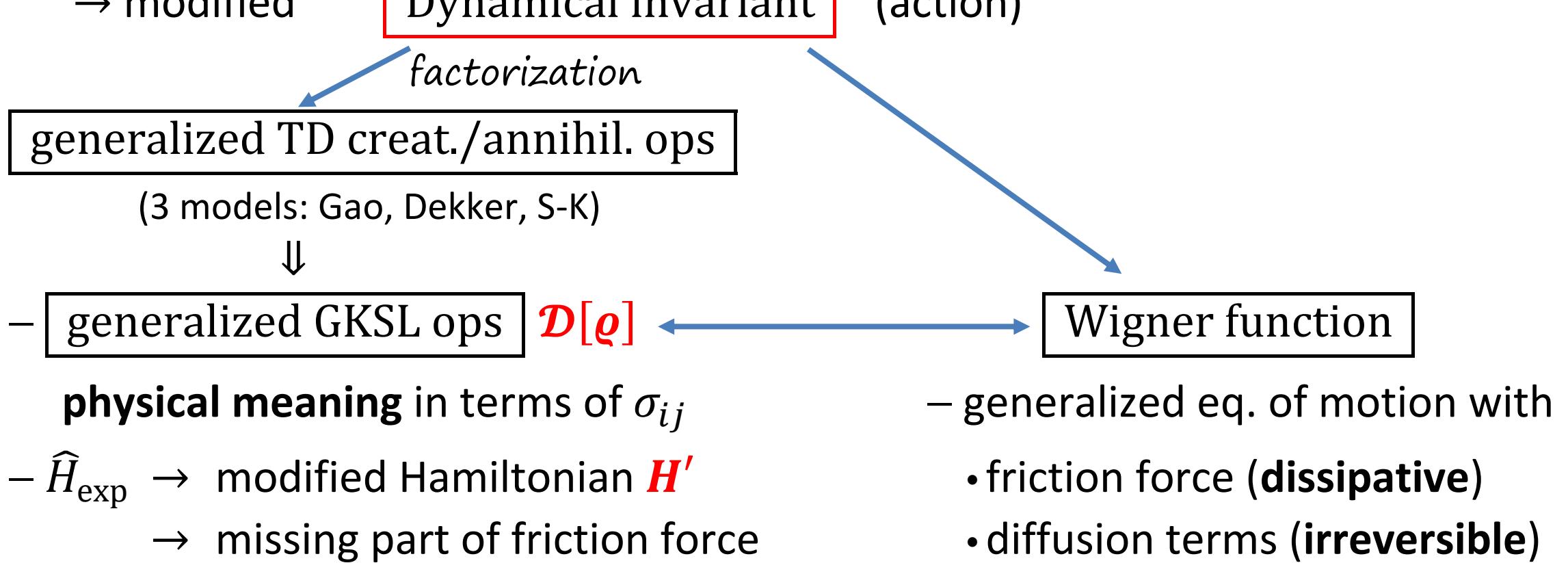
“FT”

Wigner function

II. **Open** TD Quantum Systems

Modified TDSEs – canonical (\hat{H}_{exp})
 \Downarrow non-canonical / non-unitary
 – physical (H_{NL}) , nonlinear

- Gaussian WP solutions $|\Psi\rangle$
- modified eqs. of motion for Maximum (Langevin) and Width
- modified **Dynamical invariant** (action)



combination of coordinate x and momentum p [19],

$$\begin{cases} V = \mu x + i\nu p \\ V^\dagger = \mu x - i\nu p \end{cases} \quad (3)$$

where coefficients μ and ν are arbitrary c numbers that will be determined below. The equation of motion for ρ , $\frac{d\rho}{dt} + \frac{i}{\hbar} [H, \rho] = L_D[\rho]$, can be written out explicitly according to Eqs. (2) and (3),

$$\begin{aligned} \frac{d\rho}{dt} + \frac{i}{\hbar} [H', \rho] &= -\underline{\mu^2[x, [x, \rho]]} - \underline{2i\mu\nu[x, [p, \rho]_+]} \\ &\quad - \underline{\nu^2[p, [p, \rho]]}, \\ H' &= H - 2\mu\nu\hbar xp, \end{aligned} \quad (4)$$

where $[A, B]_+$ represents an anticommutation relation between operators A and B . In obtaining Eq. (4), the identity $[x, p] = i\hbar$ has been used to rearrange the cross terms of x and p . The three terms on the right-hand side and the last one on the left are all traceless (due to the cyclic property of trace), which guarantees $\frac{d}{dt} \text{Tr } \rho = 0$, i.e., the norm conservation of the reduced density matrix. In fact, the general form Eq. (2) is traceless and thus the Lindblad approach is generally norm conserving.

To determine coefficients μ and ν , one easily realizes that the first two terms on the right-hand side of Eq. (4) are essentially the same terms as in the Caldeira-Leggett master equation (1). The latter was exactly derived from a microscopic Hamiltonian in the high-temperature limit, or equivalently the classical limit $\hbar \rightarrow 0$, where the force-force correlation function becomes localized in time. This comparison suggests the following conditions for choosing μ and ν :

$$\begin{cases} \mu^2 = \gamma 2kTm/\hbar^2 \\ 2\mu\nu = \gamma/\hbar, \quad \text{as } T \rightarrow \infty, \\ \nu^2 = 0 \end{cases} \quad (5)$$

which yields straightforwardly $\nu^2 = \gamma/8mkT$ in the high-temperature regime. The latter is different from $D_{qq} = \gamma/6mkT$, a diffusion coefficient that has recently been derived by Diósi by going beyond the lowest order Markovian approximation at high and medium temperatures [11].

To extend the functional to low temperatures, we point out that the two dissipation terms in Eq. (1) have different physical origin. The second term, which is given by the imaginary part of the force-force correlation function $\alpha(t) = \langle F(t)F(0) \rangle$, describes the dissipation effect and is temperature independent [8,10,11]. This indicates that $2\mu\nu = \gamma/\hbar$ is valid at all temperatures. On the contrary, the first term, which is given by the real part of

the same correlation function, results from environment-induced fluctuation (noise) and depends on temperature T as $\alpha_R(t, T) = \int_0^{\Omega_c} I(\omega) \coth(\frac{\hbar\omega}{2kT}) \cos(\omega t) d\omega$. Here $I(\omega) = \eta\omega/\pi$ is the spectral function for the Ohmic environment, and Ω_c is the bandwidth of the spectrum. At low T , $\omega \coth(\frac{\hbar\omega}{2kT})$ is a smooth function of ω while $\cos(\omega t)$ is fast oscillating. This observation leads us to the following approximation:

$$\begin{aligned} \alpha_R(t, T) &\approx \frac{\eta}{\pi} \omega_c \coth\left(\frac{\hbar\omega_c}{2kT}\right) \int_0^{\Omega_c} \cos(\omega t) d\omega \\ &= \eta\omega_c \coth\left(\frac{\hbar\omega_c}{2kT}\right) \tilde{\delta}(t), \end{aligned} \quad (6)$$

where $\tilde{\delta}(t) = \frac{1}{\pi} \int_0^{\Omega_c} \cos(\omega t) d\omega$, and ω_c is a parameter factorizing the noise kernel and has approximately the physical meaning as the center of the $I(\omega)$ band. The Markovian limit is recovered if $\Omega_c \rightarrow \infty$ and thus $\tilde{\delta}(t)$ approaches $\delta(t)$ [20]. This approximation is different from the earlier ones [8,10,11], which are all based on a temperature expansion of the noise kernel. It leads to a replacement of $2kT \rightarrow \hbar\omega_c \coth(\frac{\hbar\omega_c}{2kT})$ in the first diffusion term of Eq. (1) and thus in our choice of μ^2 . In fact, this is a simple replacement from the classical to quantum representation of the fluctuation-dissipation relation in the narrow band approximation. The parameter ω_c can be uniquely determined by a harmonic oscillator approximation at $T = 0$, where the system should essentially occupy its ground state near the potential minimum. The Lindblad operator V then reduces to the annihilation operator of the harmonic oscillator, giving $\mu/\nu = m\Omega$ and in turn $\omega_c = \Omega/2$, i.e., half of the oscillator frequency. The temperature dependence of the two coefficients then reads

$$\mu^2(T) = \frac{\gamma m\Omega}{2\hbar} \coth\left(\frac{\hbar\Omega}{4kT}\right), \quad (7)$$

$$\nu^2(T) = \frac{\gamma}{2\hbar m\Omega} \tanh\left(\frac{\hbar\Omega}{4kT}\right), \quad (8)$$

with the accompanying relation $2\mu\nu = \gamma/\hbar$. Both expressions reduce to Eq. (5) in the high-temperature regime, and have their physical bases on the quantum fluctuation-dissipation theorem. They thus bring the equilibrium behavior into the Lindblad formalism through their temperature dependence.

In coordinate space, the master equation (4) takes the following form:

$$\begin{aligned} \frac{\partial \rho(x, x', t)}{\partial t} + \frac{i}{\hbar} [\tilde{H}(x) - \tilde{H}^*(x')] \rho(x, x', t) &= -\left\{ \mu^2(T) (x - x')^2 + \gamma(x - x') \left(\frac{\partial}{\partial x} - \frac{\partial}{\partial x'} \right) \right. \\ &\quad \left. - \nu^2(T) \hbar^2 \left(\frac{\partial}{\partial x} + \frac{\partial}{\partial x'} \right)^2 \right\} \rho(x, x', t), \end{aligned} \quad (9)$$

$$\tilde{H}(x) = H(x) + i\hbar\gamma x \frac{\partial}{\partial x} + i\frac{\hbar\gamma}{2}. \quad (10)$$

Comment on “Dissipative Quantum Dynamics with a Lindblad Functional”

In a recent Letter [1] Gao addressed the question of master equations “...known to violate the positivity requirement of the density operator....” He began with what we might call a pre-Lindblad equation for a linear oscillator, in a form obtained by many authors, and proposed a modification to put it into Lindblad form [2]. While there have been objections to Gao’s proposal [3], we wish to point out here that the equation with which he began is not unique in the sense that unitarily equivalent microscopic Hamiltonians lead to *different forms* of the pre-Lindblad equation. These different forms describe, of course, the same physi-

cal system, but there is no reason to give any special significance to any one of them. Moreover, there is a *unique* master equation in Lindblad form which is obtained from these various equations by a well-known prescription [4].

For the system of an oscillator coupled to an oscillator heat bath, one can choose a microscopic Hamiltonian with either coordinate or momentum coupling. (The two forms are familiar in electrodynamics as the “ xE ” and the “ pA ” interactions.) The two Hamiltonians are related by a gauge transformation that *does not change the oscillator coordinate* and therefore describe the same system [5]. But the form of the equation for the reduced density matrix one derives from the two microscopic Hamiltonians is different. Thus, if one uses *coordinate coupling* one obtains the equation (ignoring the energy shift)

$$\frac{\partial \rho}{\partial t} = \frac{1}{i\hbar} [H, \rho] - \frac{\gamma(\omega_0)}{2\hbar} \left\{ i[x, p\rho + \rho p] + m\omega_0 \coth \frac{\hbar\omega_0}{2kT} [x, [x, \rho]] \right\}, \quad (1)$$

where $m\gamma(\omega_0)$ is the Newtonian friction constant and H is the free oscillator Hamiltonian. This is the form of the equation obtained in most previous discussions and the high temperature Ohmic case is that with which Gao begins. On the other hand, if one repeats the derivation with the *momentum coupling* model [6], one obtains

$$\frac{\partial \tilde{\rho}}{\partial t} = \frac{1}{i\hbar} [H, \tilde{\rho}] - \frac{\gamma(\omega_0)}{4\hbar} \left\{ -i[p, x\tilde{\rho} + \tilde{\rho}x] + \frac{1}{m\omega_0} \coth \frac{\hbar\omega_0}{2kT} [p, [p, \tilde{\rho}]] \right\}. \quad (2)$$

From either of these equations one obtains the *same master equation* by applying the Wangness-Bloch prescription: go to the *interaction representation*, *discard the terms explicitly oscillating at frequency $2\omega_0$* , and *return to the Schrödinger representation* [4]. The result is

$$\frac{\partial \bar{\rho}}{\partial t} = \frac{1}{i\hbar} [H, \bar{\rho}] - \frac{\gamma(\omega_0)}{4\hbar} \left\{ i([x, p\bar{\rho} + \bar{\rho}p] - [p, x\bar{\rho} + \bar{\rho}x]) + \coth \frac{\hbar\omega_0}{2kT} \left(\frac{1}{m\omega_0} [p, [p, \bar{\rho}]] + m\omega_0 [x, [x, \bar{\rho}]] \right) \right\}. \quad (3)$$

Here we have introduced a bar to indicate that $\bar{\rho}$ is the slowly varying mean. It is a simple matter to verify that *this has the Lindblad form* of the master equation *familiar in quantum optics* [6,7]. This is the equation sought by Gao and other investigators.

We wish to emphasize that *all three of the above equations lead to the same equilibrium state*: $\rho_{eq} = \exp(-H/kT)$; i.e., *detailed balance is obeyed*. The difference is in the *approach to equilibrium*. For the pre-Lindblad equations (1) and (2) this can be through (unphysical) states in which ρ is not positive definite. Note that this form of the equilibrium state holds only if H is the oscillator Hamiltonian.

We are well aware that the Wangness-Bloch prescription requires weak coupling. But Eqs. (1) and (2) as well as master equation (3) are weak coupling results. This is seen in that for all these equations the mean square displacement of the oscillator in the equilibrium state is that of a free oscillator, $\langle x^2 \rangle = \frac{\hbar}{2m\omega_0} \coth \frac{\hbar\omega_0}{2kT}$, while the exact result obtained from the fluctuation-dissipation theorem is [5]

$$\langle x^2 \rangle = \frac{\hbar}{\pi} \operatorname{Im} \int_0^\infty d\omega \frac{\coth \frac{\hbar\omega}{2kT}}{-m\omega^2 - i\omega\tilde{\mu}(\omega) + m\omega_0^2}, \quad (4)$$

where $\operatorname{Re}\{\tilde{\mu}(\omega)\} = m\gamma(\omega)$.

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- Application of **$\mathcal{D}[\rho]$** on pure state $|\Psi\rangle$ and subtracting mean value
 - **NLSE** equivalent to **log NLSE**
 - Same WP solutions, so-called **robust states**
- To avoid possible problems with superluminal info transfer
 - **Classical statistical element** via **Wiener process** etc.
 - **Stochastic SE**

- **Classical statistical element** via inclusion of **heat bath**
using **Wick transform** to **imaginary time** $\tau = i \frac{\hbar}{kT}$

Applying Wick-Transform to General Solution of Riccati Eq.

$$\mathcal{C}(t) \rightarrow \mathcal{C}\left(\frac{\hbar}{kT}\right) \text{ with } \boxed{i\omega_0 t \rightarrow -\frac{\hbar\omega_0}{kT}}$$

$$\boxed{\mathcal{C}\left(\frac{\hbar}{kT}\right) = \frac{\hbar}{2}\omega_0 + \frac{\hbar\omega_0}{e^{\frac{\hbar\omega_0}{kT}} - 1} = \frac{\hbar}{2}\omega_0 \coth\left(\frac{\hbar\omega_0}{2kT}\right)}$$

hyperbolic fct.

$\underbrace{\quad}_{\text{Bose-Einstein distrib. (solution of Bernoulli eq.)}}$

In **momentum space**, essentially the **inverse** quantity
fulfils also a **Riccati eq.** with the **general solution**

$$\boxed{\hat{\mathcal{C}}^{-1}\left(\frac{\hbar}{kT}\right) = \frac{\hbar}{2}\omega_0 - \frac{\hbar\omega_0}{e^{\frac{\hbar\omega_0}{kT}} + 1} = \frac{\hbar}{2}\omega_0 \tanh\left(\frac{\hbar\omega_0}{2kT}\right)}$$

$\underbrace{\quad}_{\text{Fermi-Dirac distrib.}}$

In agreement with Gao's approach.



Thank you for your attention!

Fundamental Theories of Physics 191

Dieter Schuch

Minkowski's explanation of length co

Quantum Theory from a Nonlinear Perspective

Riccati Equations in Fundamental
Physics

Proper length of the identical ball

$$l = \frac{PP'}{OC} = \frac{P'Q}{OC}$$

Springer

Minkowski showed that: