Nonequilibrium thermodynamics for dissipative quantum systems

Hans Christian Öttinger

with thanks to Jérôme Flakowski, Marco Schweizer, Maksym Osmanov

Hermann Grabert, Heinz-Peter Breuer, Sabrina Maniscalco

Department of Materials, ETH Zürich, Switzerland
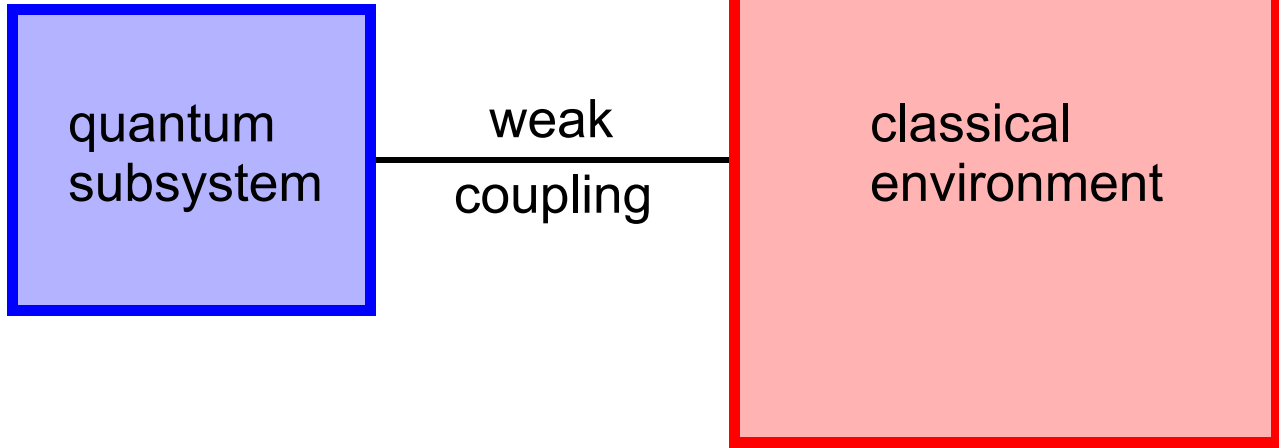
ETH *Polymer Physics*

My story for you

Foundation: The essence of nonequilibrium thermodynamics far beyond equilibrium has been deeply understood from various perspectives; an elegant geometric formulation is available *(energy – Poisson bracket, entropy – dissipation bracket)*.
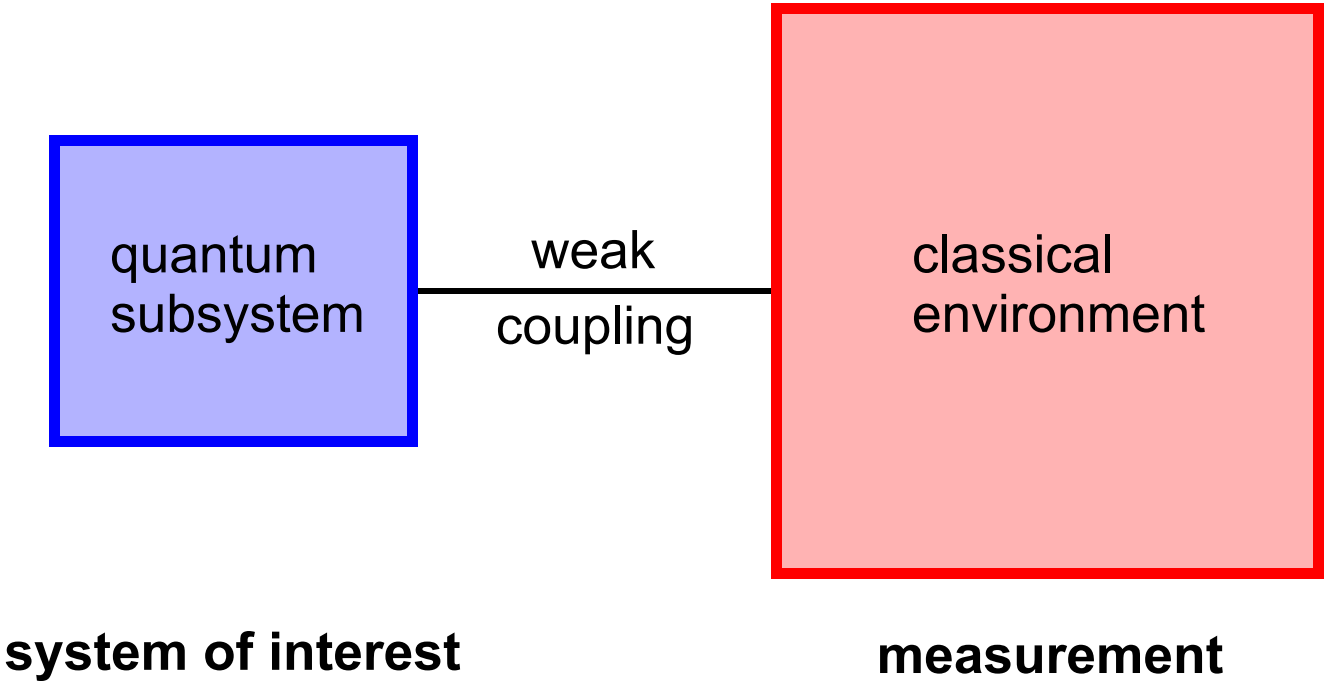
Innovation: **Classical** nonequilibrium thermodynamics is so well-developed and beautifully structured that even a dummy can generalize it to dissipative **quantum** systems.

Provocation: Quantum mechanics of the 1920s is a highly problematic idealization of a truly fundamental "first principles" theory, which is dissipative quantum mechanics *(rule of thumb: a healthy theory should not confuse Einstein)*.
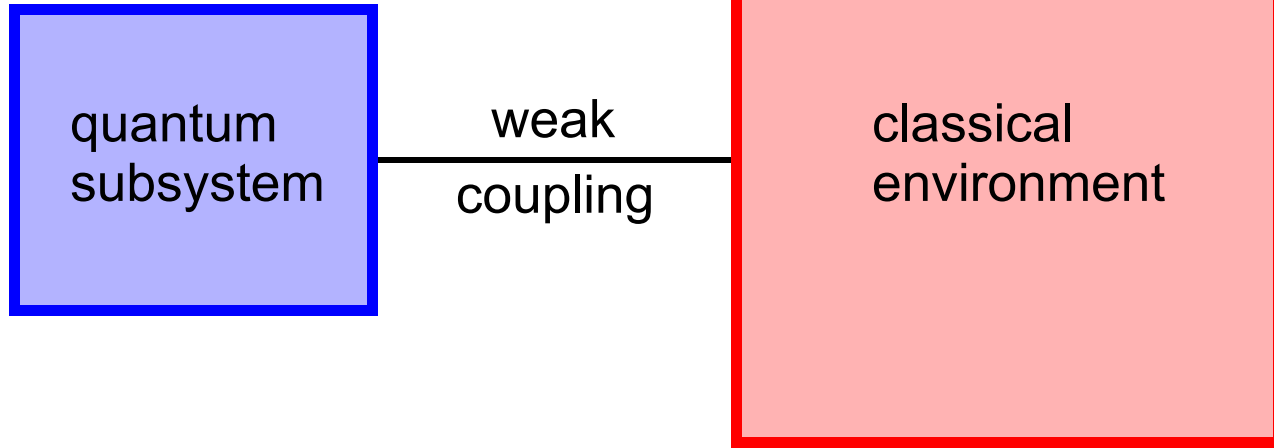
ETH Polymer Physics

Motivation

quantum subsystem

weak coupling

classical environment

GENERIC: Quantum Generalization

Hamiltonian, commutator

von Neumann entropy $\quad -k_{\mathrm{B}} \, \mathrm{Tr}(\rho \ln \rho)$

coupling operator(s)

$$[H_{\mathrm{e}}, H_{\mathrm{e}}]_x^Q \quad \langle [A, Q]; [B, Q] \rangle_\rho$$

strength: coupling bracket(s)

Canonical correlations as new geometric object for quantum dissipation:

$$\langle A; B \rangle_\rho \;=\; \int_0^1 \mathrm{tr}(\rho^\lambda A \rho^{1-\lambda} B)\, d\lambda \;=\; \mathrm{tr}(A_\rho B) \qquad\qquad A_\rho \;=\; \int_0^1 \rho^\lambda A \rho^{1-\lambda}\, d\lambda$$

Hamilton:

$$\frac{d\boldsymbol{r}_i}{dt} = \frac{\boldsymbol{p}_i}{m}$$

$$\frac{d\boldsymbol{p}_i}{dt} = \boldsymbol{F}_i$$

Liouville: $f(\boldsymbol{r}_i, \boldsymbol{p}_i)$

$$\frac{\partial f}{\partial t} = -\frac{\partial}{\partial \boldsymbol{r}_i} \cdot \left(\frac{\boldsymbol{p}_i}{m} f\right) - \frac{\partial}{\partial \boldsymbol{p}_i} \cdot (\boldsymbol{F}_i f)$$

Schrödinger:

$$\frac{\partial \psi}{\partial t} = -\frac{i}{\hbar} H \psi$$

von Neumann:

$$\frac{\partial \rho}{\partial t} = \frac{i}{\hbar} [\rho, H]$$

$$\hbar = 1$$

$$\rho = \sum_n p_n |\psi_n\rangle\langle\psi_n|$$

$$\langle A \rangle = \text{tr}(\rho A)$$

Fokker-Planck:

$$\frac{\partial f}{\partial t} = -\frac{\partial}{\partial x} A(x) f(x) + \underbrace{\frac{1}{2}\frac{\partial}{\partial x} D(x) \frac{\partial}{\partial x} f(x)}$$

$$\frac{-1}{2k_B}\frac{\partial}{\partial x} D(x) f(x) \frac{\partial}{\partial x} [-k_B \ln f(x)]$$

Quantum dissipation:

$$\frac{\partial \rho}{\partial t} = i[\rho, H] - \gamma[Q, [Q, \mu]_\rho]$$

$$\mu = k_B T(\ln \rho - \ln \rho_{eq})$$

$$A_\rho = \int_0^1 \rho^\lambda A \rho^{1-\lambda} d\lambda$$

Hamilton:
$$\frac{d\boldsymbol{r}_i}{dt} = \frac{\boldsymbol{p}_i}{m}$$

$$\frac{d\boldsymbol{p}_i}{dt} = \boldsymbol{F}_i$$

Liouville: $f(\boldsymbol{r}_i, \boldsymbol{p}_i)$

$$\frac{\partial f}{\partial t} = -\frac{\partial}{\partial \boldsymbol{r}_i} \cdot \left(\frac{\boldsymbol{p}_i}{m} f\right) - \frac{\partial}{\partial \boldsymbol{p}_i} \cdot (\boldsymbol{F}_i f)$$

$$\frac{\partial \psi}{\partial t} = -\frac{i}{\hbar} H \psi$$

$$\frac{\partial \rho}{\partial t} = \frac{i}{\hbar} [\rho, H]$$

$$\rho = \sum_n p_n |\psi_n\rangle\langle\psi_n|$$

$$\langle A \rangle = \mathrm{tr}(\rho A)$$

ion:

$$-\gamma[Q, [Q, \mu]_\rho]$$

$$= k_{\mathrm{B}} T (\ln\rho - \ln\rho_{\mathrm{eq}})$$

$$\frac{-1}{2k_{\mathrm{B}}} \frac{\partial}{\partial x} D(x) f(x) \frac{\partial}{\partial x} [-k_{\mathrm{B}} \ln f(x)]$$

$$A_\rho = \int_0^1 \rho^\lambda A \rho^{1-\lambda} d\lambda$$

Hamilton:

$$\frac{d\boldsymbol{r}_i}{dt} = \frac{\boldsymbol{p}_i}{m}$$

$$\frac{d\boldsymbol{p}_i}{dt} = \boldsymbol{F}_i$$

Liouville: $f(\boldsymbol{r}_i, \boldsymbol{p}_i)$

$$\frac{\partial f}{\partial t} = -\frac{\partial}{\partial \boldsymbol{r}_i} \cdot \left(\frac{\boldsymbol{p}_i}{m} f\right) - \frac{\partial}{\partial \boldsymbol{p}_i} \cdot (\boldsymbol{F}$$

Schrödinger:

$$\frac{\partial \psi}{\partial t} = -\frac{i}{\hbar} H \psi$$

von Neumann:

$$\frac{\partial \rho}{\partial t} = \frac{i}{\hbar} [\rho, H]$$

$$\rho = \sum_n p_n |\psi_n\rangle\langle\psi_n|$$

$$\hbar = 1$$

$$\langle A \rangle = \mathrm{tr}(\rho A)$$

Fokker-Planck:

$$\frac{\partial f}{\partial t} = -\frac{\partial}{\partial x} A(x) f(x) + \frac{1}{2}\frac{\partial}{\partial x} D(x)\frac{\partial}{\partial x}$$

$$\underbrace{\frac{-1}{2k_{\mathrm{B}}}\frac{\partial}{\partial x} D(x) f(x) \frac{\partial}{\partial x} [-k_{\mathrm{B}} \ln f(x)]}$$

$$\mu = k_{\mathrm{B}} T (\ln \rho - \ln \rho_{\mathrm{eq}})$$

$$A_\rho = \int_0^1 \rho^\lambda A \rho^{1-\lambda} d\lambda$$

Fokker-Planck:

$$\frac{\partial f}{\partial t} = -\frac{\partial}{\partial x}A(x)f(x) + \underbrace{\frac{1}{2}\frac{\partial}{\partial x}D(x)\frac{\partial}{\partial x}f(x)}$$

$$\underbrace{\frac{-1}{2k_B}\frac{\partial}{\partial x}D(x)f(x)\frac{\partial}{\partial x}\left[-k_B\ln f(x)\right]}$$

$$\frac{-1}{2k_B}\frac{\partial}{\partial x}D(x)f(x)\frac{\partial}{\partial x}\frac{\delta}{\delta f(x)}\left[-k_B\int f(y)\ln f(y)\,dy\right]$$

Hamilton:
$$\frac{d\boldsymbol{r}_i}{dt} = \frac{\boldsymbol{p}_i}{m}$$
$$\frac{d\boldsymbol{p}_i}{dt} = \boldsymbol{F}_i$$

Liouville: $f(\boldsymbol{r}_i, \boldsymbol{p}_i)$

$$\frac{\partial f}{\partial t} = -\frac{\partial}{\partial \boldsymbol{r}_i} \cdot \left(\frac{\boldsymbol{p}_i}{m} f\right) - \frac{\partial}{\partial \boldsymbol{p}_i} \cdot (\boldsymbol{F}_i f)$$

Schrödinger:
$$\frac{\partial \Psi}{\partial t} = -\frac{i}{\hbar} H \Psi$$

von Neumann:
$$\frac{\partial \rho}{\partial t} = \frac{i}{\hbar}[\rho, H]$$

Fokker-Planck:

$$\frac{\partial f}{\partial t} = -\frac{\partial}{\partial x} A(x) f(x) + \underbrace{\frac{1}{2}\frac{\partial}{\partial x} D(x)\frac{\partial}{\partial x} f(x)}$$

$$\frac{-1}{2k_{\mathrm{B}}}\frac{\partial}{\partial x} D(x) f(x) \frac{\partial}{\partial x} \ [-k_{\mathrm{B}}$$

Quantum dissipation:

$$\frac{\partial \rho}{\partial t} = i[\rho, H] - \gamma[Q, [Q, \mu]_\rho]$$

$$\mu = k_{\mathrm{B}} T(\ln\rho - \ln\rho_{\mathrm{eq}})$$

$$A_\rho = \int_0^1 \rho^\lambda A \rho^{1-\lambda} d\lambda$$

A detail:
$$\langle n|A_\rho|m\rangle = \langle n|A|m\rangle \int_0^1 p_n^\lambda p_m^{1-\lambda} d\lambda = \langle n|A|m\rangle \, p_m \int_0^1 e^{(\ln p_n - \ln p_m)\lambda} d\lambda$$

$$= \langle n|A|m\rangle \, \frac{p_n - p_m}{\ln p_n - \ln p_m}$$

$$[A, \ln\rho]_\rho = [A, \rho]$$

Hamilton:

$$\frac{d\boldsymbol{r}_i}{dt} = \frac{\boldsymbol{p}_i}{m}$$

$$\frac{d\boldsymbol{p}_i}{dt} = \boldsymbol{F}_i$$

Liouville: $f(\boldsymbol{r}_i, \boldsymbol{p}_i)$

$$\frac{\partial f}{\partial t} = -\frac{\partial}{\partial \boldsymbol{r}_i} \cdot \left(\frac{\boldsymbol{p}_i}{m} f\right) - \frac{\partial}{\partial \boldsymbol{p}_i} \cdot (\boldsymbol{F}_i f)$$

Schrödinger:

$$\frac{\partial \psi}{\partial t} = -\frac{i}{\hbar} H \psi$$

von Neumann:

$$\frac{\partial \rho}{\partial t} = \frac{i}{\hbar} [\rho, H]$$

$$\hbar = 1$$

$$\rho = \sum_n p_n |\psi_n\rangle\langle\psi_n|$$

$$\langle A \rangle = \mathrm{tr}(\rho A)$$

Fokker-Planck:

$$\frac{\partial f}{\partial t} = -\frac{\partial}{\partial x} A(x) f(x) + \underbrace{\frac{1}{2}\frac{\partial}{\partial x} D(x)\frac{\partial}{\partial x} f(x)}$$

$$\frac{-1}{2k_\mathrm{B}}\frac{\partial}{\partial x} D(x) f(x) \frac{\partial}{\partial x} [-k_\mathrm{B}\ln f(x)]$$

Quantum dissipation:

$$\frac{\partial \rho}{\partial t} = i [\rho, H] - \gamma [Q, [Q, \mu]_\rho]$$

$$\mu = k_\mathrm{B} T (\ln \rho - \ln \rho_\mathrm{eq})$$

$$A_\rho = \int_0^1 \rho^\lambda A \rho^{1-\lambda} d\lambda$$

Nonlinear Thermodynamic Quantum Master Equation

Quantum subsystem:

$$\frac{d\rho}{dt} = \frac{i}{\hbar}[\rho, H] - \frac{1}{k_B}\sum_j [H_e, S_e]_x^j \, [Q_j, [Q_j, H]_\rho] - \sum_j [H_e, H_e]_x^j \, [Q_j, [Q_j, \rho]]$$

Heat bath: *H. Grabert, Z. Phys. B 49 (1982) 161*

$$T_e[H_e, S_e]_{eq}^j = [H_e, H_e]_{eq}^j$$

Canonical equilibrium solution: $\rho \propto \exp\left\{-\dfrac{H}{k_B T_e}\right\}$

Nonlinear Thermodynamic Quantum Master Equation

Quantum subsystem:

$$\frac{d\rho}{dt} = \frac{i}{\hbar}[\rho, H] - \frac{1}{k_B}\sum_j [H_e, S_e]_x^j [Q_j, [Q_j, H]_\rho] - \sum_j [H_e, H_e]_x^j [Q_j, [Q_j, \rho]]$$

Classical environment:

$$\frac{dA_{e,x}}{dt} = \{A_e, H_e\}_x + [A_e, S_e]_x - \frac{1}{k_B}\sum_j [A_e, S_e]_x^j \langle [Q_j, H]; [Q_j, H]\rangle_\rho$$

$$+ \sum_j [A_e, H_e]_x^j \langle [Q_j, [Q_j, H]]\rangle_\rho$$

The geometry and thermodynamics of dissipative quantum systems

HANS CHRISTIAN ÖTTINGER[a]

ETH Zürich, Department of Materials, Polymer Physics, HCI H 543 - CH-8093 Zürich, Switzerland

Abstract – Dirac's method of classical analogy is employed to include quantum degrees of freedom into a geometric framework of nonequilibrium thermodynamics. The proposed formulation of dissipative quantum mechanics builds entirely upon the geometric structures implied by commutators and canonical correlations. A lucid formulation of a nonlinear quantum master equation follows from the thermodynamic structure. The approach is applicable even at very low temperatures and complex classical environments with internal structure can be handled readily.

Polymer Physics

Nonlinear thermodynamic quantum master equation: Properties and examples

Hans Christian Öttinger[*]

ETH Zürich, Department of Materials, Polymer Physics, HCI H 543, CH-8093 Zürich, Switzerland

The quantum master equation obtained from two different thermodynamic arguments is seriously nonlinear. We argue that, for quantum systems, nonlinearity occurs naturally in the step from reversible to irreversible equations and we analyze the nature and consequences of the nonlinear contribution. The thermodynamic nonlinearity naturally leads to canonical equilibrium solutions and extends the range of validity to lower temperatures. We discuss the Markovian character of the thermodynamic quantum master equation and introduce a solution strategy based on coupled evolution equations for the eigenstates and eigenvalues of the density matrix. The general ideas are illustrated for the two-level system and for the damped harmonic oscillator. Several conceptual implications of the nonlinearity of the thermodynamic quantum master equation are pointed out, including the absence of a Heisenberg picture and the resulting difficulties with defining multitime correlations.

Some simple examples!

ETH *Polymer Physics*

Some Nice Features

1. Proper quantum regression theorem

2. Canonical density matrix for equilibrium with a heat bath

3. Positive definite density matrix

Because $\ln\rho$ drives irreversible dynamics!

Some Nice Features

1. Proper quantum regression theorem

2. Canonical density matrix for equilibrium with a heat bath

3. Positive definite density matrix

4. Feedback equation for environment

5. Fulfils Ehrenfest's theorem (consistency with classical mechanics)

6. Environments and couplings of enormous generality can be handled, including open environments

7. "Markovian behavior" of full quantum-classical system

8. Equivalent stochastic simulations in Hilbert space can be performed

My story for you

Foundation: The essence of nonequilibrium thermodynamics far beyond equilibrium has been deeply understood from various perspectives; an elegant geometric formulation is available *(energy – Poisson bracket, entropy – dissipation bracket)*.

Innovation: **Classical** nonequilibrium thermodynamics is so well-developed and beautifully structured that even a dummy can generalize it to dissipative **quantum** systems.

Provocation: Quantum mechanics of the 1920s is a highly problematic idealization of a truly fundamental "first principles" theory, which is dissipative quantum mechanics *(rule of thumb: a healthy theory should not confuse Einstein)*.

Outlook

I will not rest until I can write a short and simple stochastic computer simulation program that

- is based on a thermodynamic quantum master equation

- can be appreciated and reproduced by any motivated third-year student of physics

- can produce high-precison results for the anomalous magnetic dipole moment of the electron

(stochastic particle simulation of quantum electrodynamics)

Dynamic coarse-graining approach to quantum field theory

Hans Christian Öttinger*

ETH Zürich, Department of Materials, Polymer Physics, HCI H 543, CH-8093 Zürich, Switzerland
(Received 11 August 2010; revised manuscript received 11 July 2011; published 6 September 2011)

We build quantum field theory on the thermodynamic master equation for dissipative quantum systems. The vacuum is represented by a thermodynamic equilibrium state in the low-temperature limit. All regularization is consistently provided by a friction mechanism; with decreasing friction parameter, only degrees of freedom on shorter and shorter length scales are damped out of a quantum field theory. No divergent integrals need to be manipulated. Renormalization occurs as a tool to refine perturbation expansions, not to remove divergences. Relativistic covariance is recovered in the final results. We illustrate the proposed thermodynamic approach to quantum fields for the φ^4 theory by calculating the propagator and the β function, and we offer some suggestions on its application to gauge theories.

Basic Ingredients

- Thermodynamic quantum master equation for system dynamics

- Linearization around equilibrium at low temperature

- Friction mechanism for dynamic smoothing of local details

- Renormalization group analysis for refining perturbation theory

- Relativistic covariance (and gauge invariance) only in final results