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Nonequilibrium Statistical Physics

Physics Course Materials

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# 01. Introduction: Maps

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#### Abstract

Part one of course materials for Nonequilibrium Statistical Physics (Physics 626), taught by Gerhard Müller at the University of Rhode Island. Entries listed in the table of contents, but not shown in the document, exist only in handwritten form. Documents will be updated periodically as more entries become presentable.

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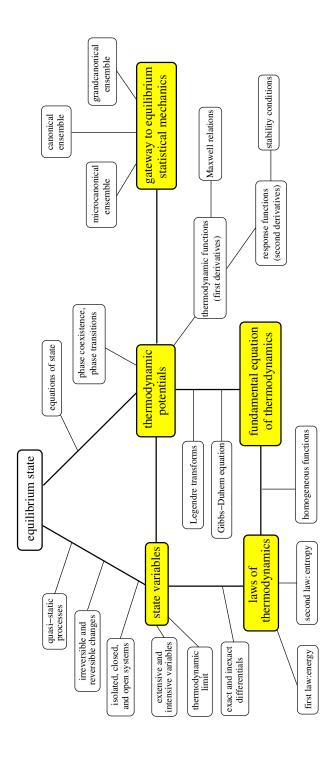
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## Thermal Equilibrium and Nonequilibrium [nln1]

**Equilibrium State Nonequilibrium State** at equilibrium near equilibrium far from equilibrium principle of principle of nonlinear dynamics maximum entropy minimum and fluctuations entropy production quasi-static processes irreversible processes stochastic processes fluctuations at equilibrium linear response to static and dynamic static and dynamic external fields correlation functions (computational probes) (experimental probes) fluctuation-dissipation theorem -

### Distinguish independently between

- equilibrium and nonequilibrium situations,
- time-independent and time-dependent phenomena.

	equilibrium situation	nonequilibrium situation
time-independent phenomena	equal-time correlations	equal-time correlations in steady states
time-dependent phenomena	delayed-time correlations	delayed-time correlations in steady states any correlations in non-steady states

# Levels of Description in Statistical Physics

[nln2]

### microscopic level

N-particle phase space

Liouville equation

generalized

Langevin equation

no contraction

deterministic time evolution

### kinetic level

1-particle phase space

Boltzmann equation Fokker-Planck equation Langevin equation

some contraction

#### thermodynamic level

configuration space

hydrodynamic equations master equation

Fokker-Planck equation

Langevin equation

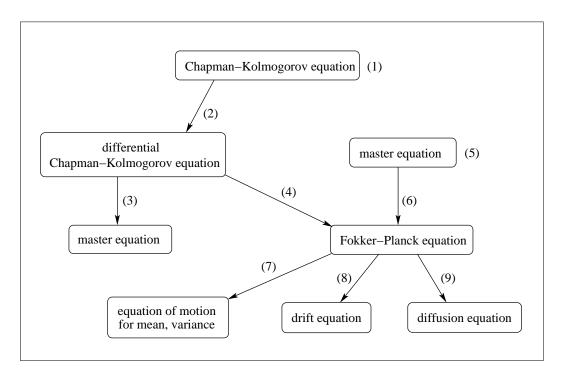
more contraction

probabilistic time evolution

microscopic dynamics	$\Rightarrow$ contraction $\Rightarrow$	stochastic dynamics	
future state determined by present state alone	focus on subset of dynamical variables	future state determined by present and past states	
deterministic time evolution of dynamic variables	#	ignoring memory of past makes dynamics of selected variables probabilistic	
	judicious choice: slow variables and long time scales	deterministic time evolution of probability distributions and mean values	
	$\qquad \qquad \Rightarrow \qquad \qquad \Rightarrow \qquad \qquad$	short memory of fast variables has little impact on dynamics of slow variables at long times	

#### Comments:

- In a classical Hamiltonian system the deterministic time evolution pertains to canonical coordinates and functions thereof.
- The time rate of change of any such variable depends on the instantaneous values of all canonical coordinates.
- On the contracted level of description we seek a way of describing an autonomous time evolution of a subset of variables.
- For that purpose the information contained in the instantaneous values of the variables that do not belong to the subset is transcribed into previous values of the variables that do belong to the subset.
- The autonomous time evolution of the variables belonging to the subset thus includes memory of its previous values.
- Slow variables contribute long memory and fast variables contribute short memory.
- If the subset contains all slow variables then any effects on its autonomous time evolution contributed by the remaining variables involve only short memory.
- Effects of short memory are more easily accounted for than effects of long memory.



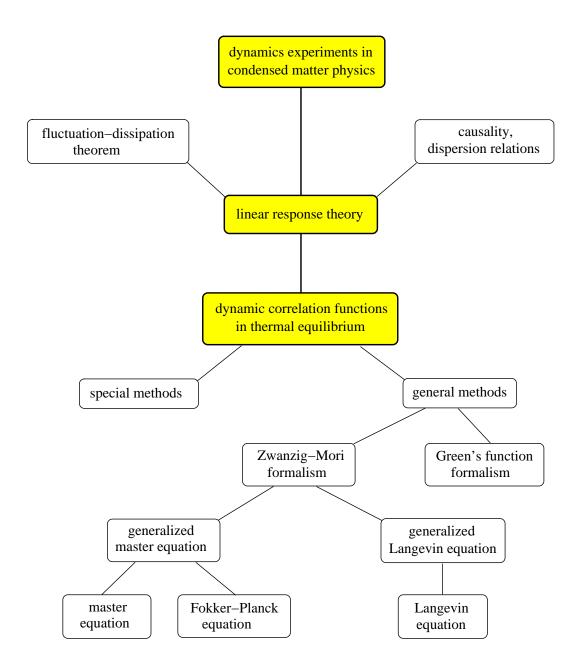
- (1) Chapman-Kolmogorov equation imposes restrictions on permissible functions  $P(x,t|x_0)$  but does not suggest a classification of processes.
- (2) Particular solutions that are specified by
  - -A(x,t) describing drift,
  - -B(x,t) describing diffusion,
  - -W(x|x';t) describing jumps.
- (3) Jump processes exclusively.
- (4) Processes with continuous sample paths, satisfying Lindeberg criterion (drift and diffusion, no jumps).
- (5) Master equation with any W(x|x';t) specifies a Markov process. Natural starting point for processes with discrete stochastic variables.
- (6) Transition rates W(x|x';t) of master equation approximated by two jump moments provided they exist. Approximation captures drift and diffusion parts (on some scale).
- (7) Drift and diffusion determine mean  $\langle \langle x \rangle \rangle$  and variance  $\langle \langle x^2 \rangle \rangle$  via equations of motion for jump moments.
- (8) Deterministic process have no diffusive part: B(x,t) = 0.
- (9) Purely diffusive processes have no drift: A(x,t) = 0.

## Brownian motion: panoramic view [nln23]

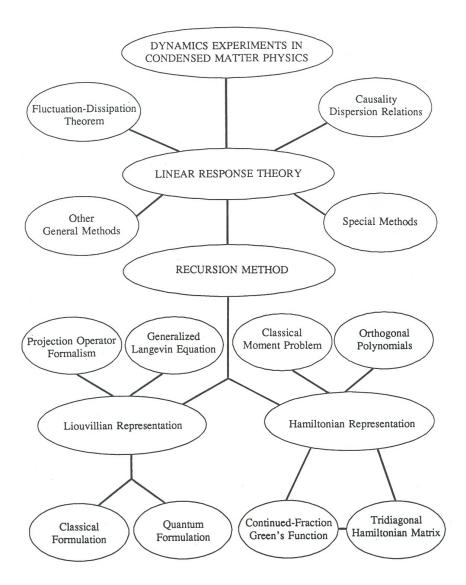
- Levels of contraction (horizontal)
- Modes of description (vertical)

	$\longrightarrow$	contraction $\longrightarrow$	
relevant space	N-particle phase space	1-particle phase space	configuration space
dynamical variables	$\left\{ \mathbf{x}_{i},\mathbf{p}_{i} ight\}$	$\mathbf{x}, \mathbf{p}$	x
theoretical framework	Hamiltonian mechanics	Langevin theory	Einstein theory
for dynamical variables	generalized Langevin equation	Langevin equation (for $dt \ll \tau_R$ )	Langevin equation (for $dt \gg \tau_R$ )
for probability distribution	quant./class. Liouville equation	Fokker-Planck equation (Ornstein- Uhlenbeck process)	Fokker-Planck equation (diffusion process)

- Here dt is the time step used in the theory and  $\tau_R$  is the relaxation time associated with the drag force the Brownian particle experiences.
- The generalized Langevin equation is equivalent to the Hamiltonian equation of motion for a generic classical many-body system and equivalent to the Heisenberg equation of motion for a generic quantum many-body system.

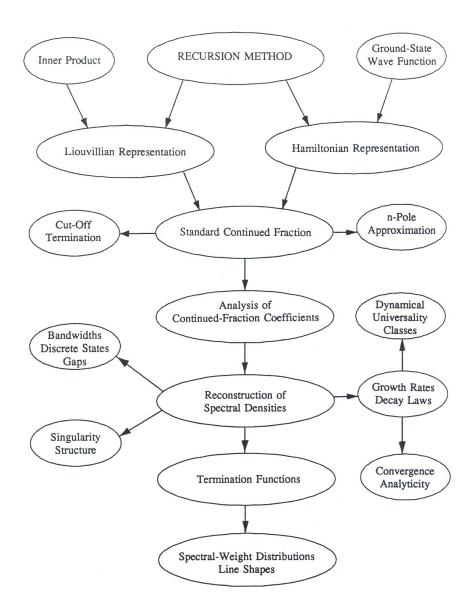


Recursion method as applied to many-body dynamics: backdrop, props, protagonists.



[from Viswanath and Müller 1994]

Recursion method as applied to many-body dynamics: main lines of formal development.



[from Viswanath and Müller 1994]