10-19-2015

01. Introduction: Maps

Gerhard Müller
University of Rhode Island, gmuller@uri.edu

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.
Updated with version 2 on 5/3/2016.

Contents of this Document [ntc1]

Table of Contents [ntc]

- Elements of set theory [nln4]
- Set identities [nex88]
- Elementary probabilities [nln42]
- Probability axioms and simple theorems [nex94]
- Joint probability and conditional probability [nln44] [nex90]
- Elements of probability theory [nln43]
- Statistical independence [nln45]
- Statistical uncertainty and information [nln5], [tex47]
- Event or complement? That is the question [nex9]
- Successive random picks [nex91]
- Heads or tails [nex93]
- Quantity and quality [nex76]
- Diagnosis of a rare disease [nex77]
- Subtlety of statistical independence [nex1]
- Random train connections [nex92]
- Random inkjet printer [nex10]
- Information and the reduction of ignorance [tex48]
- Information of sequenced messages [tex61]

4. Random Variables: Concepts
    - Probability distributions [nln46]
    - Characteristic function, moments, and cumulants [nln47]
    - Cumulants expressed in terms of moments [nex126]
    - Generating function and factorial moments [nln48]
    - Multivariate distributions [nln7]
    - Transformation of random variables [nln49]
    - Sums of independent exponentials [nex127]
    - Propagation of statistical uncertainty [nex24]
    - Chebyshev's inequality [nex6]

- Law of large numbers [nex7]
- Binomial, Poisson, and Gaussian distribution [nln8]
- Binomial to Poisson distribution [nex15]
- De Moivre - Laplace limit theorem [nex21]
- Central limit theorem [nln9]
- Multivariate Gaussian distribution
- Robust probability distributions [nex19]
- Stable probability distributions [nex81]
- Exponential distribution [nln10]
- Waiting time problem [nln11]
- Pascal distribution [nex22]

5. Random Variables: Applications
    - Reconstructing probability distributions [nex14]
    - Probability distribution with no mean value [nex95]
    - Variances and covariances [nex20]
    - Statistically independent or merely uncorrelated? [nex23]
    - Sum and product of uniform distribution [nex96]
    - Exponential integral distribution [nex79]
    - Generating exponential and Lorentzian random numbers [nex80]
    - Random chords (Bertrand's paradox) [nex5]
    - From Gaussian to exponential distribution [nex8]
    - Transforming a pair of random variables [nex78]
    - Gaussian shootist versus Lorentzian shootist [nex3]
    - Moments and cumulants of the Poisson distribution [nex16]
    - Maxwell velocity distribution [nex17]
    - Random bus schedules [nex18]
    - Life expectancy of the young and the old [nex106]
    - Life expectancy of the ever young [nex38]

- Random frequency oscillator [nex35]

6. Stochastic Processes: Concepts
    - Time-dependent probability distributions [nln50]
    - Correlation functions and characteristic functions
    - Degrees of memory [nln51]
    - Markovian or non-Markovian I [nln52]
    - Markovian or non-Markovian II [nln53]
    - Contraction - memory - time scales [nln15]
    - Markov process: general attributes [nln54]
    - Diffusion process and Cauchy process [nln55]
    - Stationarity, normalization, consistency, Markovian nature [nex26]
    - Computer generated sample paths [nsl1]
    - Continuous versus discontinuous processes (Lindeberg condition) [nex97]
    - Differential Chapman-Kolmogorov equation [nln56]
    - Fokker-Planck equation (drift and diffusion processes) [nln57]
    - Drift equation (deterministic processes) [nex29]
    - Master equation (jump processes) [nex28]
    - Non-differentiability of sample paths [nex99]
    - Predominantly small jumps [nln58]
    - Time evolution of mean and variance [nln59]
    - Master equation with finite jump moments [nex32]
    - Equations of motion for mean and variance [nex30]
    - Markov process: map of specifications [nln16]
    - Approach to a stationary state (detailed balance) [nex85]
    - Markov chains [nln61]
    - Master equation with detailed balance (discrete variables, continuous time) [nln12]

- Regression theorem for autocorrelation functions [nex39]
- Birth death processes (specifications, models, levels of description) [nln18]
- Birth and death of single species [nln19]
- Birth-death master equation: stationary state [nln17]
- Nonlinear birth-death process

7. Stochastic Processes: Applications
    - Diffusion process [nex27]
    - Cauchy process [nex98]
    - Random walk in one dimension [nln60]
    - Random walk in one dimension: unit steps at unit times [nex34]
    - Random walk in one dimension: unit steps at random times [nex33]
    - Random walk in one dimension: tiny steps at frequent times [nex100]
    - Random walk in Las Vegas: chance and necessity [nex40]
    - Poisson process [nex25]
    - Free particle with uncertain position and velocity [nex36]
    - Fokker-Planck equation with constant coefficients [nex101]
    - House of the mouse: two-way doors only [nex102]
    - House of the mouse: some one-way doors [nex103]
    - House of the mouse: one-way doors only [nex104]
    - House of the mouse: mouse with inertia [nex105]
    - House of the mouse: mouse with memory [nex43]
    - Mixing marbles red and white [nex42]
    - Random traffic around city block [nex86]
    - Modeling a Markov chain [nex87]
    - Ornstein-Uhlenbeck process [nln62] [nex31] [nex41]
    - Predator-prey system: deterministic, stochastic, observational [nsl3]

- Populations with linear birth and death rates I [nex44]
- Populations with linear birth and death rates II [nex112]
- Populations with linear birth and death rates III [nex130]
- Catalyst-driven chemical reaction: stationary state [nex46]
- Catalyst driven chemical reaction: dynamics [nex107]
- Catalyst driven chemical reaction: total rate of reactions [nex108]
- Air in leaky tank I: generating function [nex48]
- Air in leaky tank II: probability distribution [nex109]
- Air in leaky tank III: detailed balance [nex49]
- Air in leaky tank IV: evolution of mean and variance [nex110]
- Pascal distribution and Planck radiation law [nex50]
- Effects of nonlinear death rate I: Malthus-Verhulst equation [nex111]
- Effects of nonlinear death rate II: stationarity and fluctuations [nex51]
- Modified linear birth rate I: stationarity [nex113]
- Modified linear birth rate II: evolution of mean and variance [nex114]
- Modified linear birth rate III: generating function [nex115]
- Modified linear birth rate IV: probability distribution [nex116]
- Bistable chemical system [nex52]
- Ultracold neutrons in an ideal Steyerl bottle [nex47]
- Random light switch [nex45]

8. Brownian Motion
    - Early Landmarks [nln63]
    - Relevant time scales (collisions, relaxation, observations) [nln64]
    - Einstein's theory [nln65]
    - Diffusion equation analyzed [nln73]
    - Release of Brownian particle from box confinement [nex128]
    - Smoluchowski equation [nln66]

- Einstein's fluctuation-dissipation relation [nln67]
- Smoluchowski vs Fokker-Planck [nln68]
- Fourier's law for heat conduction [nln69]
- Thermal diffusivity [nex117
- Shot noise [nln70]
- Campbell's theorem [nex37]
- Critically damped ballistic galvanometer [nex70]
- Langevin's theory [nln71]
- White noise
- Brownian motion and Gaussian white noise [nln20]
- Wiener process [nsl4]
- Autocorrelation function of Wiener process [nex54]
- Attenuation without memory [nln21]
- Formal solution of Langevin equation [nex53]
- Velocity correlation function of Brownian particle I [nex55]
- Mean-square displacement of Brownian particle [nex56], [nex57], [nex118]
- Ergodicity [nln13]
- Intensity spectrum and spectral density (Wiener-Khintchine theorem) [nln14]
- Fourier analysis of Langevin equation
- Velocity correlation function of Bownian particle II [nex119]
- Generalized Langevin equation [nln72]
- Attenuation with memory [nln22]
- Velocity correlation function of Brownian particle III [nex120]
- Brownian harmonic oscillator [nln75]
- Brownian harmonic oscillator VII: equivalent specifications [nex129]
- Brownian harmonic oscillator I: Fourier analysis [nex121]
- Brownian harmonic oscillator II: position correlation function [nex122]

- Brownian harmonic oscillator III: contour integrals [nex123]
- Brownian harmonic oscillator IV: velocity correlations [nex58]
- Brownian harmonic oscillator V: formal solution for velocity [nex59]
- Brownian harmonic oscillator VI: nonequilibrium correlations [nex60]
- Langevin dynamics from microscopic model [nln74]
- Brownian motion: levels of contraction and modes of description [nln23]

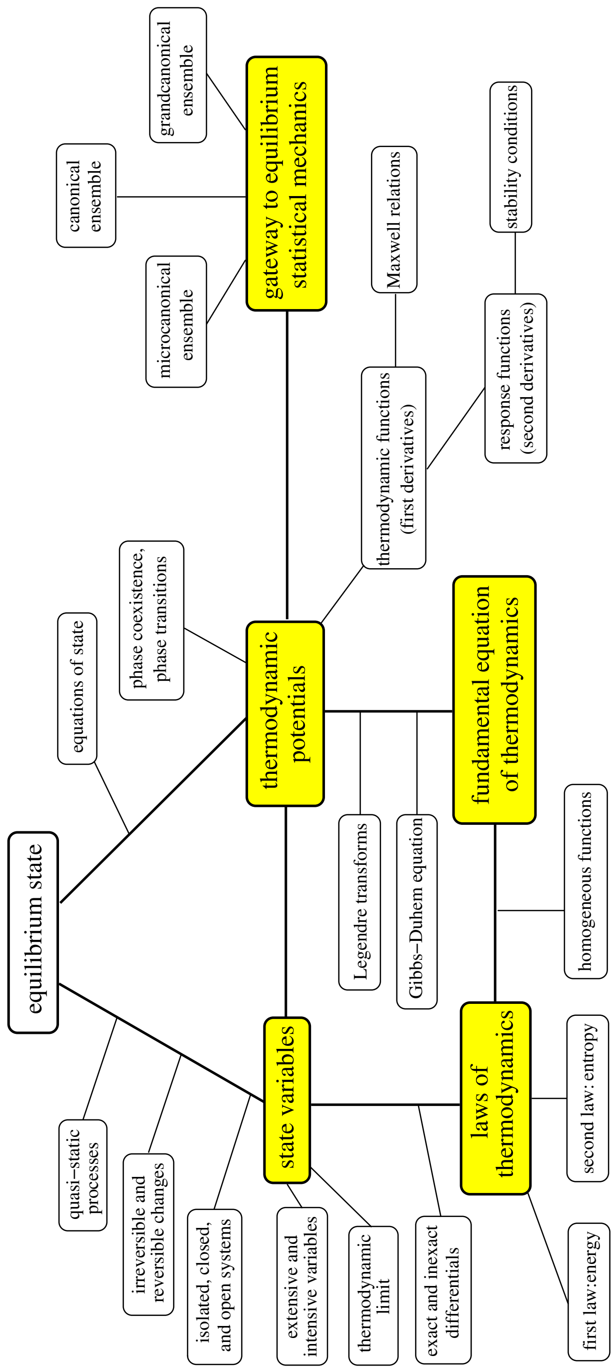
9. Linear Response and Equilibrium Dynamics
   - Overview [nln24]
   - Many-body system perturbed by radiation field [nln25]
   - Response function and generalized susceptibility [nln26]
   - Kubo formula for response function [nln27]
   - Symmetry properties [nln30]
   - Kramers-Kronig dispersion relations [nln37]
   - Causality property of response function [nex63]
   - Energy transfer between system and radiation field [nln38]
   - Reactive and absorptive part of response function [nex64]
   - Fluctuation-dissipation theorem (quantum and classical) [nln39]
   - Moment expansion [nln78]
   - Spectral representations [nex65]
   - Linear response of classical relaxator [nex66]
   - Dielectric relaxation in liquid water [nln76]
   - Linear response of classical oscillator [nex67]
   - Scattering process and dynamic structure factor [nln89]
   - Scattering from free atoms [nln93]
   - Scattering from atoms bound to lattice [nln94]
   - Scattering from a harmonic crystal [nln95]
   - Magnetic resonance or scattering [nln97]

10. Zwanzig-Mori Formalism
    - Introduction [nln28]
    - Time-dependence of expectation values (quantum and classical) [nln77]
    - Zwanzig's kinetic equation: generalized master equation [nln29] [nex68]
    - Projection operator method (Mori formalism) [nln31]
    - Kubo inner product [nln32]
    - Projection operators [nln33]
    - First and second projections [nln34] [nln35]
    - Continued-fraction representation of relaxation function [nln36]
    - n-pole approximation [nln87]
    - Relaxation function with uniform continued-fraction coefficients [nex69]
    - Link to Green's function formalism [nln88]
    - Structure function of harmonic oscillator [nex71], [nex72], [nex73]

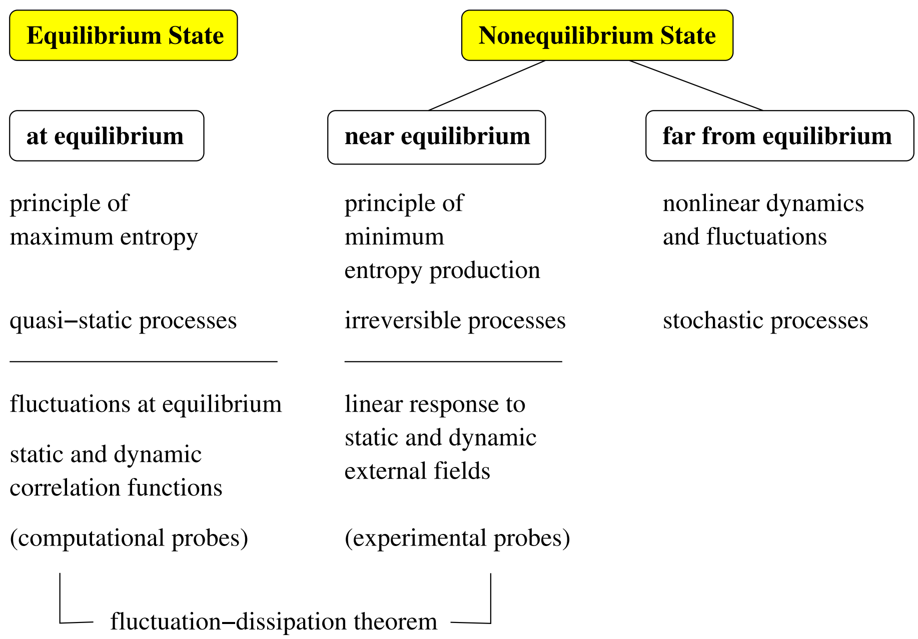
11. Recursion Method: Concepts
    - Stage for recursion method [nln79]
    - Modules of recursion method [nln80]
    - Representations of recursion method [nln81]
    - Orthogonal expansion of dynamical variables [nln82]
    - Gram-Schmidt orthogonalization I [nln83]
    - Relaxation function and spectral density [nln84]
    - Moment expansion vs continued fraction I [nln85]
    - Link to generalized Langevin equation [nln86]
    - Orthogonal expansion of wave functions [nln90]
    - Gram-Schmidt orthogonalization II [nln91]

- Structure function [nln92]
- Moment expansion vs continued fraction II [nln96]
- Genetic code of spectral densities [nln98]
- Spectral Lines from finite sequences of continued-fraction coefficients [nln99]
- Spectral densities with bounded support [nln100]
- Bandwidth and gap in spectral density [nln101]
- Spectral densities with unbounded support [nln102]
- Unbounded support and gap [nln103]

Equilibrium Thermodynamics Overview [nln6]



Thermal Equilibrium and Nonequilibrium [nln1]



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	kinetic level	thermodynamic level
N−particle phase space	1−particle phase space	configuration space
Liouville equation generalized Langevin equation	Boltzmann equation Fokker−Planck equation Langevin equation	hydrodynamic equations master equation Fokker−Planck equation Langevin equation
no contraction	some contraction	more contraction
deterministic time evolution	probabilistic time evolution	

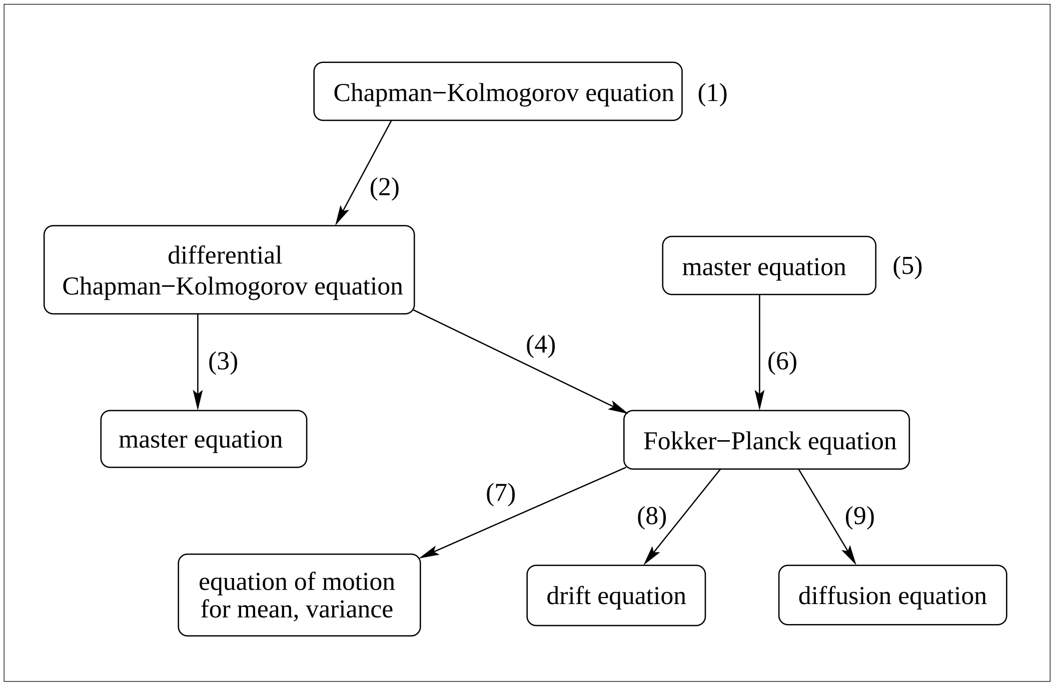
Contraction – memory – time scales [nln15]

microscopic dynamics	**⇒ contraction ⇒**	**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
	⇓ ⇒	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 autononmous 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.

Markov processes: map of specifications [nln16]



(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]

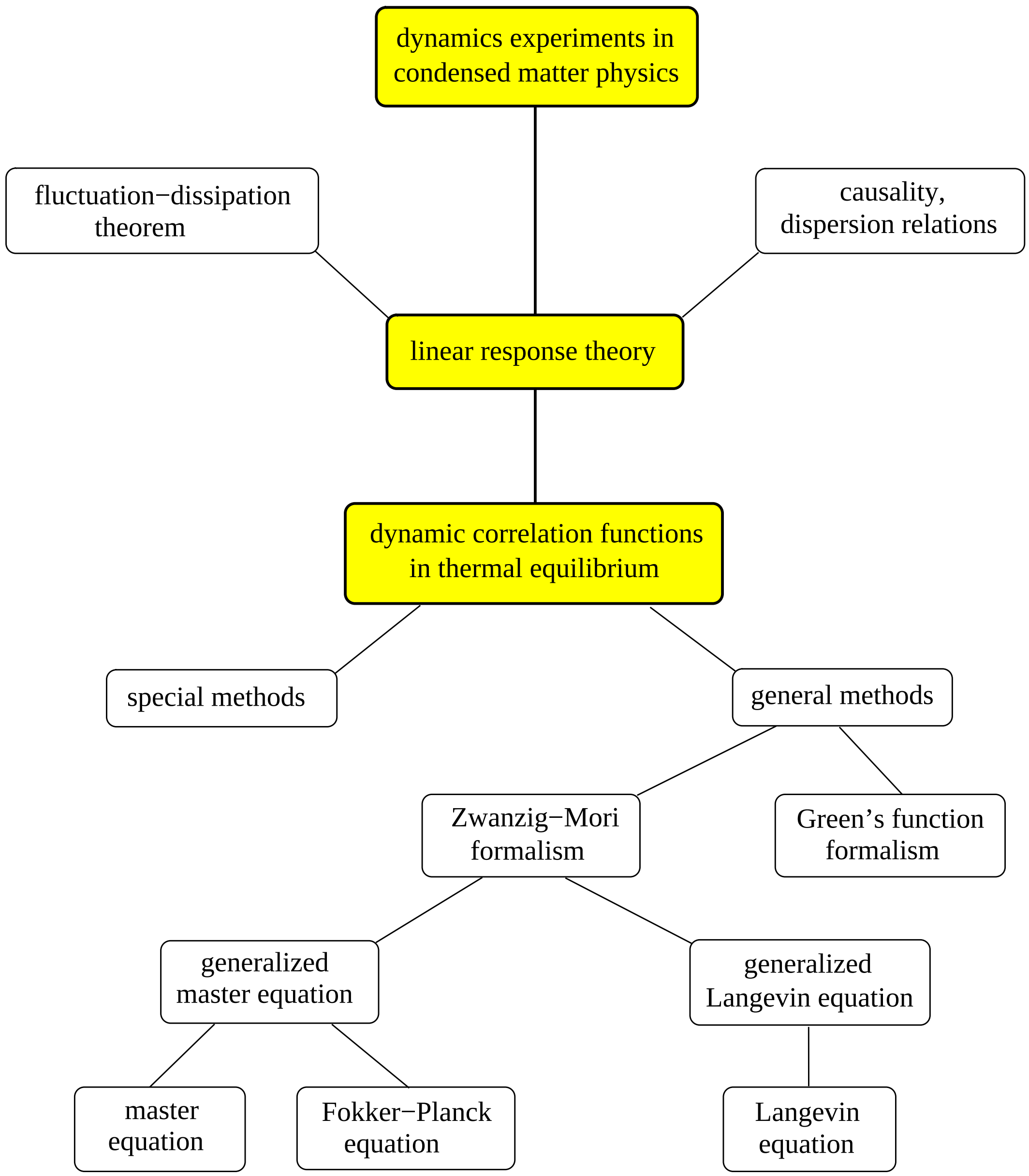
- Levels of contraction (horizontal)
- Modes of description (vertical)

$\longrightarrow$ contraction $\longrightarrow$

relevant space	N-particle phase space	1-particle phase space	configuration space
dynamical variables	$\{\mathbf{x}_i, \mathbf{p}_i\}$	$\mathbf{x}$, $\mathbf{p}$	$\mathbf{x}$
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)

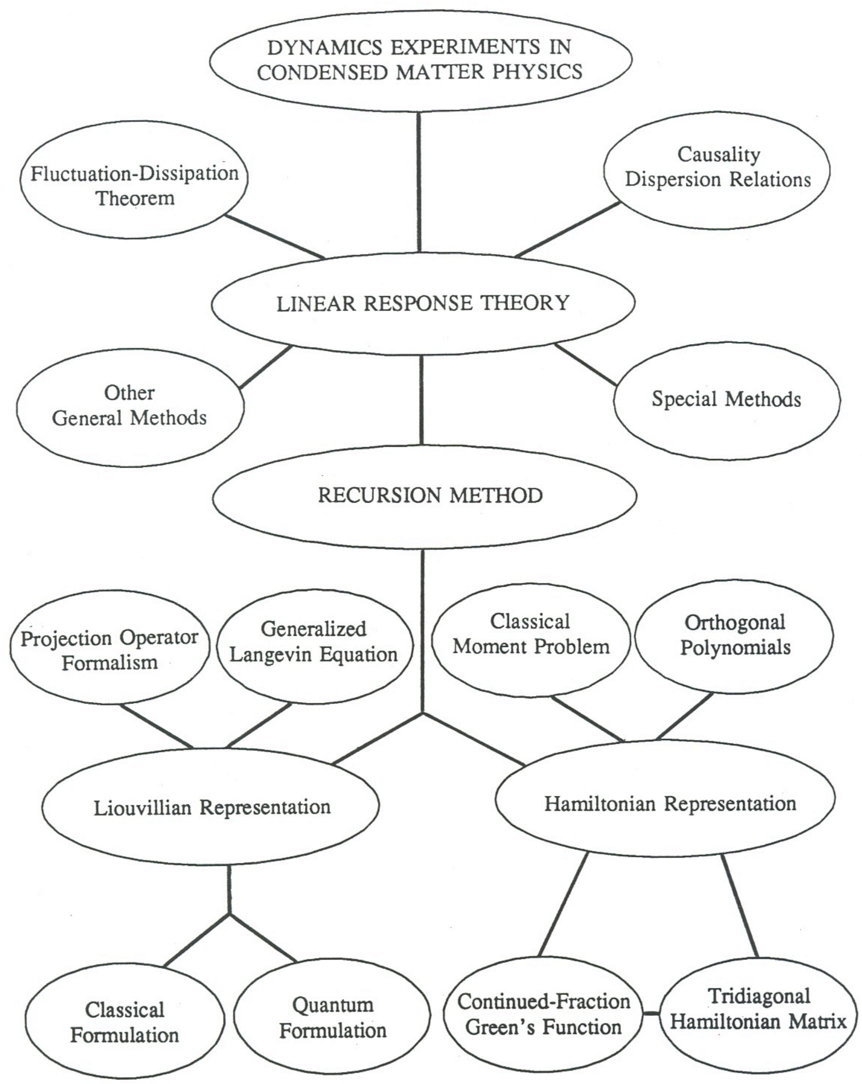
- Here dt is the time step used in the theory and τ_R is the relaxation time associated with the drag force the Brownian particle experiences.
- The generalized Langevin equation is equivalent to the Hamiltonian equation of motion for a generic classical many-body system and equivalent to the Heisenberg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

Linear response and equilibrium dynamics [nln24]



Stage for Recursion Method [nln79]

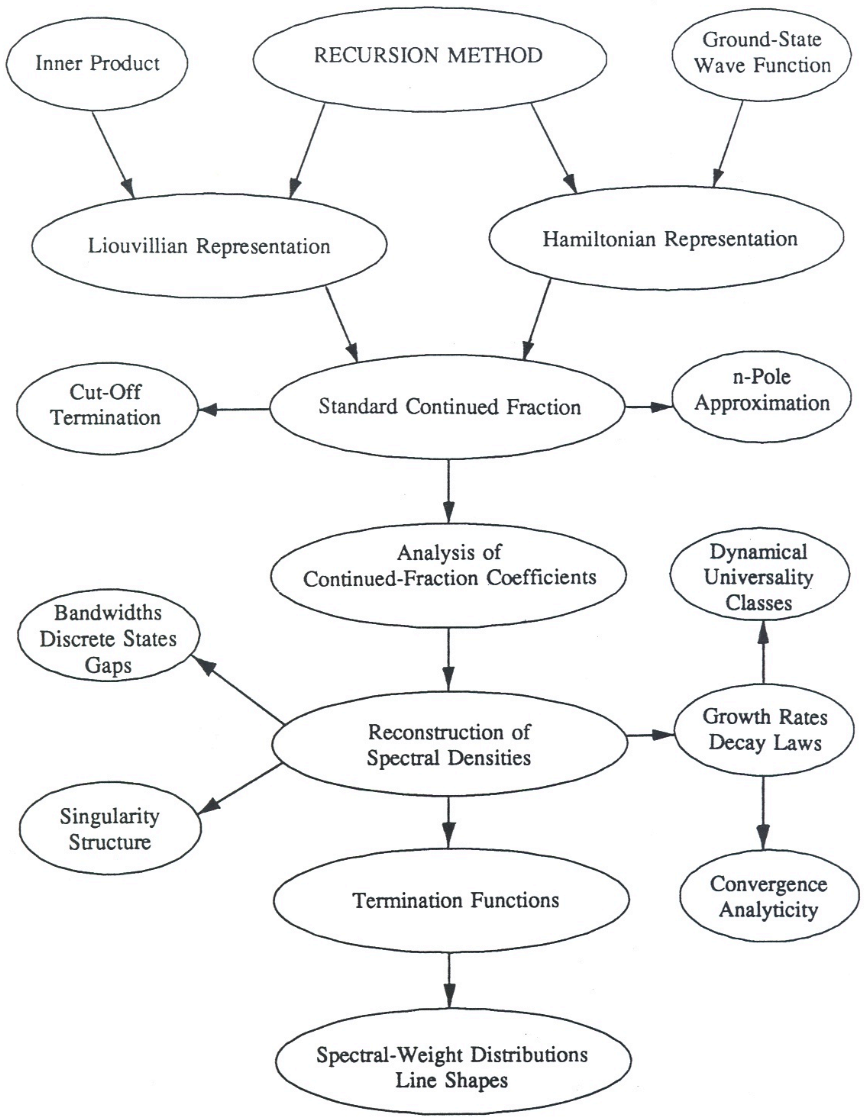
Recursion method as applied to many-body dynamics:
backdrop, props, protagonists.



[from Viswanath and Müller 1994]

Modules of Recursion Method [nln80]

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



[from Viswanath and Müller 1994]