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10. Zwanzig-Mori Formalism

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Abstract

Part ten 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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Contents of this Document [ntc10]

10. Zwanzig-Mori Formalism

- Introduction [nl28]
- Time-dependence of expectation values (quantum and classical)
- Zwanzig's kinetic equation: generalized master equation [nl29] [nex68]
- Projection operator method (Mori formalism) [nl31]
- Kubo inner product [nl32]
- Projection operators [nl33]
- First and second projections [nl34] [nl35]
- Continued-fraction representation of relaxation function [nl36]
- Recursion method (algorithmic implementation of Mori formalism)
- Relaxation function with uniform continued-fraction coefficients [nex69]
- Continued-fraction expansion and moment expansion
- Generalized Langevin equation
- n-pole approximation
- Green's function formalism
- Structure function of harmonic oscillator [nex71], [nex72], [nex73]
- Scattering process and dynamic structure factor
- Electron scattering, neutron scattering, light scattering
- Scattering from a free atom
- Scattering from an atom bound in a harmonic potential
- Scattering from a harmonic crystal

Zwanzig-Mori formalism [nl28]

Beginnings:

Two phenomenological approaches for the dynamics of systems close to or at thermal equilibrium:

- ▷ Phenomenological equations of motion for probability distributions (e.g. master equation, Fokker-Planck equation).
- ▷ Phenomenological equations of motion for dynamical variables (e.g. Langevin equation)

In these approaches, the focus is on selected degrees of freedom. All other degrees of freedom are taken into account summarily in the form of ad-hoc randomness.

Completions:

Microscopic foundations for these phenomenological approaches.

- ▷ Zwanzig (1960): Rigorous derivation of a *generalized master equation* from first principles, i.e. from the Liouville equation.
- ▷ Mori (1965): Rigorous derivation of a *generalized Langevin equation* from first principles, i.e. from the (quantum) Heisenberg equation or the (classical) canonical equations.

The focus is again on selected degrees of freedom but here the effect of the other degrees of freedom are taken into account on a basis that is exact and amenable to systematic approximation.

Variants:

- ▷ Zwanzig's approach leads to a *kinetic equation* of a particular kind. There exist alternative ways to derive kinetic equations from the Liouville equations via systematic approximations (e.g. via BBGKY hierarchy).
- ▷ Mori's approach has been formulated in more than one rendition. The version named *projection operator formalism* is most illuminating regarding the physical meaning of systematic approximations. The version named *recursion method* is most readily amenable to computational applications.

Zwanzig's method [nl29]

Consider classical phase-space density $\rho(t) = \rho(q_1, p_1; q_2, p_2; \dots; q_n, p_n; t)$.

Distinguish system (q_1, p_1) and heat bath $(q_2, p_2; \dots; q_n, p_n)$.

Probability density of system: $\rho_1(t) = \hat{P}\rho(t)$ via projection.

Probability density of heat bath: $\rho_2(t) = \hat{Q}\rho(t)$, where $\hat{Q} = 1 - \hat{P}$.

Implementation of projection:

$$\rho_1 = \hat{P}\rho(q_1, p_1; q_2, p_2; \dots; q_n, p_n; t) = \rho_{eq}(q_2, p_2; \dots; q_n, p_n)\sigma(q_1, p_1; t),$$

where $\partial\rho_{eq}/\partial t = -\imath\hat{L}\rho_{eq} = 0$ and

$$\sigma(q_1, p_1; t) = \int dq_2 dp_2 \dots dq_n dp_n \rho(q_1, p_1; q_2, p_2; \dots; q_n, p_n; t).$$

Idempotency, $\hat{P}\rho_1(t) = \rho_1(t)$, satisfied by construction.

Liouville equation, $\partial\rho(t)/\partial t = -\imath\hat{L}\rho(t)$, split into two coupled equations:

$$\hat{P}\frac{\partial}{\partial t}\rho(t) = \frac{\partial}{\partial t}\rho_1(t) = -\imath\hat{P}\hat{L}[\rho_1(t) + \rho_2(t)], \quad (1)$$

$$\hat{Q}\frac{\partial}{\partial t}\rho(t) = \frac{\partial}{\partial t}\rho_2(t) = -\imath\hat{Q}\hat{L}[\rho_1(t) + \rho_2(t)]. \quad (2)$$

Formal solution of (2) [nex68] to be substituted into (1):

$$\rho_2(t) = e^{-\imath\hat{Q}\hat{L}t}\rho_2(0) - \imath\int_0^t d\tau e^{-\imath\hat{Q}\hat{L}\tau}\hat{Q}\hat{L}\rho_1(t - \tau).$$

Zwanzig's kinetic equation (generalized master equation):

$$\frac{\partial}{\partial t}\rho_1(t) = -\imath\hat{P}\hat{L}\rho_1(t) - \imath\hat{P}\hat{L}e^{-\imath\hat{Q}\hat{L}t}\rho_2(0) - \int_0^t d\tau \hat{P}\hat{L}e^{-\imath\hat{Q}\hat{L}\tau}\hat{Q}\hat{L}\rho_1(t - \tau).$$

#1 Autonomous part of system's time evolution.

#2 Autonomous part of heat bath's time evolution. Instantaneous effect of heat bath on system at time t .

#3 Effect caused by system on heat bath at time $t - \tau$ propagates in heat bath and feeds back into system at time t .

First term often vanishes and second term (inhomogeneity) can be made zero by judicious choice of initial conditions.

Zwanzig's kinetic equation can be used as the starting point for the derivation (via approximations) of a master equation or a Fokker-Planck equation.

[nex68] Zwanzig's kinetic equation

In the derivation of Zwanzig's kinetic equation,

$$\frac{\partial}{\partial t} \rho_1(t) = -i\hat{P}\hat{L}\rho_1(t) - i\hat{P}\hat{L}e^{-i\hat{Q}\hat{L}t}\rho_2(0) - \int_0^t d\tau \hat{P}\hat{L}e^{-i\hat{Q}\hat{L}\tau}\hat{Q}\hat{L}\rho_1(t-\tau),$$

from two projections of the Liouville equation,

$$\hat{P} \frac{\partial \rho}{\partial t} = \frac{\partial \rho_1}{\partial t} = -i\hat{P}\hat{L}[\rho_1 + \rho_2], \quad \hat{Q} \frac{\partial \rho}{\partial t} = \frac{\partial \rho_2}{\partial t} = -i\hat{Q}\hat{L}[\rho_1 + \rho_2], \quad (1)$$

we use the formal solution

$$\rho_2(t) = e^{-i\hat{Q}\hat{L}t}\rho_2(0) - i \int_0^t d\tau e^{-i\hat{Q}\hat{L}\tau}\hat{Q}\hat{L}\rho_1(t-\tau). \quad (2)$$

Verify that (2) is a solution of (1).

Solution:

Projection operator method [nl31]

Goal: Determination of symmetrized time-correlation function (fluctuation function) for a dynamical variable $A(t)$ of a quantum or classical many-body Hamiltonian system \mathcal{H} in thermal equilibrium.

Fluctuation function (real, symmetric, normalized):

$$C_0(t) \doteq \frac{\langle A(t)|A \rangle}{\langle A|A \rangle} = \frac{\langle A|A(-t) \rangle}{\langle A|A \rangle} = \frac{\langle A|e^{-Lt}|A \rangle}{\langle A|A \rangle}.$$

Dirac notation symbolizes inner product of choice as explained in [nl32]. Some properties of dynamic quantities depend on choice of inner product.

Relaxation function (via Laplace transform):¹

$$c_0(z) = \int_0^\infty dt e^{-zt} \frac{\langle A|e^{-Lt}|A \rangle}{\langle A|A \rangle} = \frac{1}{\langle A|A \rangle} \left\langle A \left| \frac{1}{z + \imath L} \right| A \right\rangle.$$

Projection operator method determines relaxation function via systematic approximation.

Inverse Laplace transform,

$$C_0(t) = \frac{1}{2\pi\imath} \int_C dz e^{zt} c_0(z),$$

involves integral along straight path from $\epsilon - \imath\infty$ to $\epsilon + \imath\infty$ for $\epsilon > 0$.

In practical applications, the (real, symmetric) spectral density is inferred from the relaxation function as limit process,

$$\Phi_0(\omega) = 2 \lim_{\epsilon \rightarrow 0} \Re \{ c_0(\epsilon - \imath\omega) \},$$

and the fluctuation function via inverse Fourier transform,

$$C_0(t) = \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} e^{-\imath\omega t} \Phi_0(\omega).$$

¹The last bracket is also known as a Green's function.

Kubo inner product [nl32]

General properties of inner products:

- $\langle A|B \rangle = \langle B|A \rangle^*$,
- $\langle A|A \rangle = ||A||^2 \geq 0$,
- $\langle A|\lambda B \rangle = \lambda \langle A|B \rangle$,
- $\langle A|B + C \rangle = \langle A|B \rangle + \langle A|C \rangle$.

Kubo inner product for quantum system:

$$\langle A|B \rangle \doteq \frac{1}{\beta} \int_0^\beta d\lambda \langle e^{\lambda \mathcal{H}} A^\dagger e^{-\lambda \mathcal{H}} B \rangle,$$

where

$$\langle A \rangle = \frac{1}{Z} \text{Tr}\{e^{-\beta \mathcal{H}} A\}, \quad Z = \text{Tr}\{e^{-\beta \mathcal{H}}\}, \quad \beta = \frac{1}{k_B T}.$$

Alternative inner product for quantum systems:

$$\langle A|B \rangle \doteq \frac{1}{2} \langle A^\dagger B + B A^\dagger \rangle.$$

Both inner products have the same classical limit:¹

$$\langle A|B \rangle \doteq \frac{1}{Z} \int d^n q d^n p e^{-\beta \mathcal{H}(q,p)} A(q,p) B(q,p).$$

Inner products of [nl31] employ...

▷ quantum Liouville operator, $L = \frac{1}{\hbar} [L, \]$,

for time evolution governed by Heisenberg equation of motion,

$$\frac{dA}{dt} = \frac{i}{\hbar} [\mathcal{H}, A] = iLA.$$

▷ classical Liouville operator, $L = i\{\mathcal{H}, \}$ = $i \sum_{j=1}^n \left(\frac{\partial \mathcal{H}}{\partial q_j} \frac{\partial}{\partial p_j} - \frac{\partial \mathcal{H}}{\partial p_j} \frac{\partial}{\partial q_j} \right)$,

for time evolution governed by Hamilton's equation of motion,

$$\frac{dA}{dt} = -\{\mathcal{H}, A\} = iLA$$

¹It is optional to subtract the product of expectation values $\langle A^\dagger \rangle \langle B \rangle$ in all inner products presented here

Projection operators [nl33]

The relaxation function $c_0(z)$ is determined recursively by a succession of subdivisions of the many-body dynamics into components that are treated rigorously and a remainder that is treated phenomenologically. It is expected that the remainder diminishes in importance as the number of rigorous components is increased systematically.

The time evolution of the dynamical variable $A(t)$ can be conceived as a "pirouette" performed by the vector $|A(t)\rangle$ through the Hilbert space.

The subdivisions are implemented by a sequence of projections onto one-dimensional Hilbert subspaces traversed by $|A(t)\rangle$.

Initial condition: $|f_0\rangle \doteq |A(0)\rangle = |A\rangle$.

Projection operators P_n and $Q_n = 1 - P_n$, $n = 0, 1, \dots$.

$$P_0 \doteq |f_0\rangle \frac{1}{\langle f_0|f_0\rangle} \langle f_0|, \quad P_0^2 = P_0, \quad P_0^\dagger = P_0, \quad P_0 Q_0 = Q_0 P_0 = 0.$$

Orthogonal direction:¹

$$|f_1\rangle = \imath L|f_0\rangle, \quad \langle f_0|f_1\rangle = 0, \quad P_0|f_1\rangle = 0, \quad Q_0|f_1\rangle = |f_1\rangle - P_0|f_1\rangle = |f_1\rangle,$$

$$P_1 = |f_1\rangle \frac{1}{\langle f_1|f_1\rangle} \langle f_1|, \quad Q_1 = 1 - P_1.$$

The systematic generation of further orthogonal direction will be discussed in the context of the recursion method.

Successive projections filter out particular aspects of the many-body dynamics. The filters are applied in series. What passes through n filters is the remainder to be treated phenomenologically.

The physical content of this process can be gleaned from the first two projections carried out in detail:

- First projection [nl33],
- Second projection [nl34].

¹Unitary transformation $e^{\imath Lt}$ makes $\imath LA$ orthogonal to A , implying $\langle A|\imath LA\rangle = 0$.

First projection [nl34]

Rewrite relaxation function from [nl31] with projection operators from [nl33] and apply Dyson identity $1/(X + Y) = 1/X - (1/X)Y[1/(X + Y)]$:¹

$$\begin{aligned}\langle f_0|f_0\rangle c_0(z) &= \left\langle f_0 \left| \frac{1}{z + \imath L} \right| f_0 \right\rangle = \left\langle f_0 \left| \frac{1}{z + \imath LP_0 + \imath LQ_0} \right| f_0 \right\rangle \\ &= \left\langle f_0 \left| \frac{1}{z + \imath LQ_0} \right| f_0 \right\rangle + \left\langle f_0 \left| \frac{1}{z + \imath LQ_0} \imath LP_0 \frac{1}{z + \imath L} \right| f_0 \right\rangle.\end{aligned}$$

Simplify both terms:

- $\left\langle f_0 \left| \frac{1}{z} \left[1 + \frac{(-\imath)}{z} LQ_0 + \frac{(-\imath)^2}{z^2} LQ_0 LQ_0 + \dots \right] \right| f_0 \right\rangle = \frac{1}{z} \langle f_0|f_0\rangle.$
- $\left\langle f_0 \left| \frac{1}{z + \imath LQ_0} \imath L \right| f_0 \right\rangle \frac{1}{\langle f_0|f_0\rangle} \left\langle f_0 \left| \frac{1}{z + \imath L} \right| f_0 \right\rangle = \left\langle f_0 \left| \frac{1}{z + \imath LQ_0} \imath L \right| f_0 \right\rangle c_0(z).$

$$\Rightarrow c_0(z) = \frac{1}{z + \frac{1}{\langle f_0|f_0\rangle} \left\langle f_0 \left| \frac{z}{z + \imath LQ_0} \imath L \right| f_0 \right\rangle},$$

$$\begin{aligned}\left\langle f_0 \left| \frac{z}{z + \imath LQ_0} \imath L \right| f_0 \right\rangle &= \left\langle f_0 \left| \left[1 - (z + \imath LQ_0) \frac{1}{z + \imath LQ_0} + \frac{z}{z + \imath LQ_0} \right] \imath L \right| f_0 \right\rangle \\ &= \left\langle f_0 \left| (-\imath) LQ_0 \frac{1}{z + \imath LQ_0} \imath L \right| f_0 \right\rangle = \left\langle f_0 \left| (-\imath) LQ_0 \frac{1}{z + \imath Q_0 LQ_0} Q_0 \imath L \right| f_0 \right\rangle \\ &= \left\langle f_1 \left| \frac{1}{z + \imath L_1} \right| f_1 \right\rangle; \quad |f_1\rangle = Q_0|f_0\rangle = Q_0 \imath L|f_0\rangle, \quad L_1 = Q_0 LQ_0.\end{aligned}$$

Relaxation function after first projection expressed via memory function:

$$c_0(z) = \frac{1}{z + \Sigma_1(z)}, \quad \Sigma_1(z) = \frac{1}{\langle f_0|f_0\rangle} \left\langle f_1 \left| \frac{1}{z + \imath L_1} \right| f_1 \right\rangle.$$

Memory function $\Sigma_1(z)$ of original problem, $\{L, |f_0\rangle\}$, can be reinterpreted as the (as yet non-normalized) relaxation function of a new dynamical problem, $\{L_1, |f_1\rangle\}$.

Projection operator Q_0 acts as filter on the Liouvillian L , absorbing that part of dynamics dealt with explicitly in first projection. Explicit information contained in normalization constant of $\Sigma_1(z)$.

¹Direct consequence of operator identity $(X + Y)/(X + Y) = 1$.

Second projection [nl35]

Rewrite memory function from [nl34] with projection operators from [nl33] and apply Dyson identity:

$$\begin{aligned}
 \langle f_0|f_0\rangle\Sigma_1(z) &= \left\langle f_1 \left| \frac{1}{z + \imath L_1} \right| f_1 \right\rangle = \left\langle f_1 \left| \frac{1}{z + \imath L_1 P_1 + \imath L_1 Q_1} \right| f_1 \right\rangle \\
 &= \left\langle f_1 \left| \frac{1}{z + \imath L_1 Q_1} \right| f_1 \right\rangle - \left\langle f_1 \left| \frac{1}{z + \imath L_1 Q_1} \imath L_1 P_1 \frac{1}{z + \imath L_1} \right| f_1 \right\rangle \\
 &= \frac{1}{z} \langle f_1|f_1\rangle - \left\langle f_1 \left| \frac{1}{z + \imath L_1 Q_1} \imath L_1 \right| f_1 \right\rangle \frac{\langle f_0|f_0\rangle}{\langle f_1|f_1\rangle} \Sigma_1(z),
 \end{aligned}$$

where simplifications analogous to [nl34] are carried out.

$$\Rightarrow \Sigma_1(z) = \frac{\langle f_1|f_1\rangle/\langle f_0|f_0\rangle}{z + \frac{1}{\langle f_1|f_1\rangle} \left\langle f_1 \left| \frac{z}{z + \imath L_1 Q_1} \imath L_1 \right| f_1 \right\rangle},$$

$$\begin{aligned}
 \left\langle f_1 \left| \frac{z}{z + \imath L_1 Q_1} \imath L_1 \right| f_1 \right\rangle &= \dots = \left\langle f_1 \left| (-\imath) L_1 Q_1 \frac{1}{z + \imath Q_1 L_1 Q_1} Q_1 \imath L_1 \right| f_1 \right\rangle \\
 &= \left\langle f_2 \left| \frac{1}{z + \imath L_2} \right| f_2 \right\rangle,
 \end{aligned}$$

with $|f_2\rangle = Q_1 \imath L_1 |f_1\rangle$, $L_2 = Q_1 L_1 Q_1$.

Memory function (first termination function) after second projection expressed via second termination function:

$$\Sigma_1(z) = \frac{\Delta_1}{z + \Sigma_2(z)}, \quad \Sigma_2(z) = \frac{1}{\langle f_1|f_1\rangle} \left\langle f_2 \left| \frac{1}{z + \imath L_2} \right| f_2 \right\rangle$$

with $\Delta_1 = \langle f_1|f_1\rangle/\langle f_0|f_0\rangle$.

The n^{th} projection yields

$$\Sigma_{n-1}(z) = \frac{\Delta_{n-1}}{z + \Sigma_n(z)}, \quad \Sigma_n(z) = \frac{1}{\langle f_{n-1}|f_{n-1}\rangle} \left\langle f_n \left| \frac{1}{z + \imath L_n} \right| f_n \right\rangle$$

with $\Delta_{n-1} = \langle f_{n-1}|f_{n-1}\rangle/\langle f_{n-2}|f_{n-2}\rangle$
and $|f_n\rangle = Q_{n-1} \imath L_{n-1} |f_{n-1}\rangle$, $L_n = Q_{n-1} L_{n-1} Q_{n-1}$.

Continued-fraction representation [nlm36]

Relaxation function after n successive projections:

$$c_0(z) = \frac{1}{z + \frac{\Delta_1}{z + \frac{\Delta_2}{z + \dots + \frac{\Delta_{n-1}}{z + \Sigma_n(z)}}}}$$

The explicit dynamical information extracted from the original many-body system, $\{L, |f_0\rangle\}$, in the first n projections is contained in the continued-fraction coefficients:

$$\Delta_1, \dots, \Delta_n.$$

Each projection adds a layer of projection operators around the original Liouvillian:

$$L_n = Q_{n-1} \cdots Q_0 L Q_0 \cdots Q_{n-1}.$$

Expectation (somewhat naively):

- If n is sufficiently large, all distinctive spectral features of L will have been filtered out and incorporated explicitly into the relaxation function via the Δ_i .
- Whatever features of L still shine through the n filters are adequately represented by a source of white noise.
- The memory function associated with white noise is a constant, commonly represented by a relaxation time:

$$\Sigma_n(z) = \frac{1}{\tau_n} = \text{onst.}$$

- This completion of the continued fraction is known under the name n -pole approximation. The relaxation function is characterized by n poles in the complex frequency plane.

Options used in practical applications:

- A number of continued-fraction coefficients are determined on phenomenological grounds along with a terminating relaxation time τ_n . Examples: classical relaxator (1 pole), classical oscillator (two poles).
- A number of continued-fraction coefficients are calculated from the original many-body system via the recursion method along with a termination function $\Sigma_n(z)$ inferred from an extrapolation scheme.

[nex69] Relaxation function with uniform continued-fraction coefficients.

Find closed-form expressions for the relaxation function $c_0(z)$, the spectral density $\Phi_0(\omega)$, and the fluctuation function $C_0(t)$, of some physical system if we know that the (infinite) sequence of continued-fraction coefficients is

- (a) uniform: $\Delta_1 = \Delta_2 = \dots = \frac{1}{4}\omega_0^2$,
- (b) almost uniform: $\Delta_1 = \frac{1}{2}\omega_0^2$, $\Delta_2 = \Delta_3 \dots = \frac{1}{4}\omega_0^2$.

Solution:

[nex71] Structure function of harmonic oscillator I.

Consider the quantum harmonic oscillator (for $\hbar = 1$),

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega_0^2 q^2 = \omega_0 \left(a^\dagger a + \frac{1}{2} \right),$$

where $q = (a^\dagger + a)/\sqrt{2m\omega_0}$, $p = i\sqrt{m\omega_0/2}(a^\dagger - a)$ relate the position and momentum operators ($[q, p] = i$) to the boson creation and annihilation operators ($[a, a^\dagger] = 1$).

Use the recursion method with inner product $(A, B) = \frac{1}{2}(\langle AB \rangle + \langle BA \rangle)$ to calculate the structure function $S_{qq}(\omega)$ for the position variable at temperature T , where $\langle a^\dagger a \rangle = n_B = (e^{\beta\omega} + 1)^{-1}$, $\beta = 1/k_B T$.

Solution:

[nex72] Structure function of harmonic oscillator II.

Consider the classical harmonic oscillator,

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega_0^2 q^2.$$

Use the recursion method with inner product $(A, B) = \langle AB \rangle$ to calculate the structure function $S_{qq}(\omega)$ for the position variable at temperature T , where $\langle p^2 \rangle / 2m = \frac{1}{2}m\omega_0^2 \langle q^2 \rangle = \frac{1}{2}k_B T$, according to the equipartition theorem.

Solution:

[nex73] Structure function of harmonic oscillator III.

Consider the quantum harmonic oscillator (for $\hbar = 1$),

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega_0^2 q^2 = \omega_0 \left(a^\dagger a + \frac{1}{2} \right),$$

where $q = (a^\dagger + a)/\sqrt{2m\omega_0}$, $p = i\sqrt{m\omega_0/2}(a^\dagger - a)$ relate the position and momentum operators ($[q, p] = i$) to the boson creation and annihilation operators ($[a, a^\dagger] = 1$).

Solve the equation of motion

$$\zeta \langle \langle A; B \rangle \rangle_\zeta^\pm = \langle [A, B]_\pm \rangle + \langle \langle [A, H]; B \rangle \rangle_\zeta^\pm$$

for (a) the Green's function $\langle \langle q; q \rangle \rangle_\zeta^-$ and (b) the Green's function $\langle \langle q; q \rangle \rangle_\zeta^+$. Infer from each Green's function the structure function $S_{qq}(\omega)$ for the position variable at temperature T .

Solution: