Zwanzig's method [nln29]

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

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

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:

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

where $\partial\rho_{eq}/\partial t = 0$ and

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

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:

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

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

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.