

Correlation Functions for Quasi-Linear Response Theory

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Abstract. A “quasi-linear” regression formula is derived by an expansion around quasi-static equilibrium. It relates the relaxation of thermodynamic “forces” to the regression of correlations of thermodynamic “coordinates” in quasi-static equilibrium. Correlation functions and memory kernels can be introduced in almost complete analogy to linear response theory. A non-linear, non-Markovian kinetic equation is derived. The kinetic coefficients are given in terms of correlation functions of stochastic forces in quasi-static equilibrium similar to the linear theory.

1. Introduction

Since the historical work of Langevin (1908) [1] on Brownian motion a vast amount of literature on nonequilibrium statistical mechanics has accumulated in which kinetic coefficients are expressed as limiting values of correlation functions. Let us mention only a small selection of important papers [2–7] and a few review papers and books [8–11] for further references. The aim of nonequilibrium statistical mechanics in general is to study the evolution in time of expectation values

$$Q_k(t) = \overline{q_k(t)} = \text{trace}(q_k(t)q(0)) \quad (1)$$

of a set of operators $q_k(t)$ in an ensemble described by the statistical operator $q(0)$. We are going to use the Heisenberg picture throughout with the equations of motion

$$dq_k(t)/dt = \frac{i}{\hbar} [H, q_k(t)]. \quad (2)$$

The evaluation of the right hand side of (1) for $q_k(t)$ a solution of (2) so far has only been possible in case $q(0)$ is sufficiently close to equilibrium. Usually one considers ensembles in “quasi-static” equilibrium described by the operators

$$q = \exp[-\beta(I(t) - K(t))], \quad (3)$$

where

$$I(t) = H - \sum_k q_k^*(t) f_k(t) \quad (4)$$