Two kinds of mode coupling contributions to transport coefficients

1973 J. Phys. A: Math. Nucl. Gen. 6 L1

(http://iopscience.iop.org/0301-0015/6/1/012)

J. Phys. A: Math., Nucl. Gen., Vol. 6, January 1973. Printed in Great Britain. © 1973

LETTER TO THE EDITOR

Two kinds of mode coupling contributions to transport coefficients

Kyozi Kawasaki

Department of Physics, Temple University, Philadelphia, Pennsylvania 19122, USA

MS received 27 November 1972

Abstract. The two types of mode coupling contributions to transport coefficients are distinguished. The first type arises from drift terms in the starting generalized Langevin equation and gives a positive contribution to transport coefficients whereas the second type comes from dissipative terms and gives a negative contribution.

In recent years nonlinear coupling among hydrodynamic modes was found to play a rather important role in transport phenomena (Kawasaki 1972a, Zwanzig 1972, and the references quoted therein). Such coupling can arise either from (i) streaming terms in hydrodynamic equations or from (ii) dissipative terms through the dependence of 'bare' transport coefficients upon hydrodynamic variables or through nonlinearities in thermodynamic driving forces, which we denote as I and J, respectively. Here we demonstrate that these two types of coupling give contributions of opposite signs to transport coefficients.

We start from the following generalized nonlinear Langevin equation for the gross variables $\{a_i\}$ without memory effects (eg Kawasaki 1972a, and to be published):

$$\frac{\mathrm{d}}{\mathrm{d}t} a_i(t) = (\mathrm{i}\omega_i - \gamma_i)a_i(t) + I_i(t) + J_i(t) + f_i(t), \qquad t > 0 \tag{1}$$

where ω_i is the first moment frequency (eg Mori 1965) and γ_i is the 'bare' damping constant. $I_i(t)$ and $J_i(t)$ are the functions of $\{a_j(t)\}$ representing nonlinear mode coupling for a_i arising from drift and dissipative terms, respectively, and are chosen to be 'orthogonal' to $\{a_j\}$:

$$\langle I_i a_j^* \rangle = \langle J_i a_j^* \rangle = 0 \tag{2}$$

where $\langle \ldots \rangle$ is the equilibrium average. The gross variables are also chosen to be orthonormal: $\langle a_i a_j^* \rangle = \delta_{ij}$. $f_i(t)$ is the random force 'orthogonal' to any function of $\{a\}$;

$$\langle f_i(t) F(\{a(0)\})^* \rangle = 0, \qquad t \gtrless 0. \tag{3}$$

We also need the generalized Langevin equation for negative times where all the dissipative terms must change their signs:

$$\frac{\mathrm{d}}{\mathrm{d}t} a_i(t) = (\mathrm{i}\omega_i + \gamma_i)a_i(t) + I_i(t) - J_i(t) + f_i(t), \qquad t < 0. \tag{4}$$

We now introduce the propagator $G_i(t)$ given by $\langle a_i(t)a_i^*(0) \rangle$ for $t \gtrless 0$. We then find from (1) and (3) the following:

$$\frac{\mathrm{d}}{\mathrm{d}t} G_i(t) = (\mathrm{i}\omega_i - \gamma_i)G_i(t) + \langle I_i(0)a_i^*(-t)\rangle + \langle J_i(0)a_i^*(-t)\rangle \qquad t > 0, \tag{5}$$

where the stationarity condition of time correlation functions has been used also. For $a_i^*(-t)$ in (5) we substitute the integral form of (4) (Kawasaki 1970) which is now written as

$$a_i^*(-t) = G_i^{0*}(-t)a_i^*(0) - \int_0^t \mathrm{d}s G_i^*(-t+s)f_i^*(-s) - \int_0^t \mathrm{d}s G_i^{0*}(-t+s) \times (I_i^*(-s) - J_i^*(-s)) \qquad t > 0 \tag{6}$$

where $G_i^0(t) \equiv \exp(\mathrm{i}\omega_i \mp \gamma_i)t$ for $t \gtrless 0$ is the free propagator. Using (2) and (3) we then obtain

$$\frac{\mathrm{d}}{\mathrm{d}t} G_i(t) = (\mathrm{i}\omega_i - \gamma_i)G_i(t) - \int_0^t \mathrm{d}s \Delta\Gamma_i'(s) G_i^0(t-s) \tag{7}$$

with

$$\Delta\Gamma_i'(t) \equiv \langle (I_i(t) + J_i(t))(I_i^*(0) - J_i^*(0))\rangle. \tag{8}$$

In the language of formal perturbation theory, the 'self-energy' $\Delta\Gamma_i'(t)$ is improper in the sense that it still contains intermediate states with a single mode i excited, which have to be removed to obtain the proper self-energy $\Delta\Gamma_i(t)$. A simple way of achieving this is to remove from I_i and J_i any terms involving a_i, and to replace $G_i^0(t-s)$ by $G_i(t-s)$. The resulting nonlinear coupling terms are again denoted as I_i and J_i. The error committed should vanish in the thermodynamic limit where i is in fact quasi-continuous. Thus, (7) now reduces to

$$\frac{\mathrm{d}}{\mathrm{d}t} G_i(t) = (\mathrm{i}\omega_i - \gamma_i)G_i(t) - \int_0^t \mathrm{d}s \Delta\Gamma_i(s) G_i(t-s) \tag{9}$$

with

$$\Delta\Gamma_i(t) = \Delta\Gamma_i^I(t) - \Delta\Gamma_i^J(t) + \Delta\Gamma_i^{IJ}(t) \tag{10}$$

and

$$\Delta\Gamma_i^I(t) \equiv \langle I_i(t) I_i^*(0)\rangle, \qquad \Delta\Gamma_i^J(t) \equiv \langle J_i(t) J_i^*(0)\rangle, \tag{11}$$

$\Delta\Gamma_i^{IJ}(t)$ being the cross terms involving both I and J. If G_i is replaced by the non-equilibrium average of a_i in (10), it is nothing but the linearized macroscopic equations of motion, and $\Delta\Gamma_i(s)$ contributes to the frequency-dependent complex damping constant (or transport coefficient) $\hat{\Gamma}_i(\omega)$;

$$\hat{\Gamma}_i(\omega) = \gamma_i + \Delta\hat{\Gamma}_i(\omega) \tag{12}$$

with

$$\Delta\hat{\Gamma}_i(\omega) \equiv \int_0^\infty \mathrm{e}^{-\mathrm{i}\omega t} \Delta\Gamma_i(t)\, \mathrm{d}t,$$

etc. Then, it is well known and can be easily shown that

$$\mathrm{Re}\, \Delta\hat{\Gamma}_i^I(\omega) \geqslant 0 \tag{13}$$

$$\mathrm{Re}\, \Delta\hat{\Gamma}_i^J(\omega) \geqslant 0. \tag{14}$$

Thus, we have demonstrated that mode couplings arising from the drift terms and from the dissipative terms in (1) give positive and negative contributions to $\hat{\Gamma}_i(\omega)$, respectively. For the cross term $\hat{\Gamma}_i^{IJ}(\omega)$ no such definite statement can be made. However, one can show that $\Gamma_i^{IJ}(t)$ vanishes for $t = 0$, and its contribution to Re $\hat{\Gamma}_i(\omega)$ is not likely to be important.

The past applications of the mode coupling theory were primarily concerned with $\Delta\hat{\Gamma}_i^I(\omega)$ which was responsible for divergences in transport coefficients near a critical point (Kawasaki 1972a). On the other hand, in the hermitian kinetic Ising model (Kawasaki 1972b) where only dissipative terms are present, mode coupling contributions are shown to decrease the 'bare' damping constant in the second order perturbation theory (Halperin *et al* 1972), which is consistent with our general result (14).

This work was supported by the National Science Foundation.

References

Halperin B I, Hohenberg P C and Ma S 1972 to be published
Kawasaki K 1970 *Ann. Phys., NY* **61** 1–56
——1972a *Statistical Mechanics* ed S A Rice, K F Freed and J C Light (Chicago: University of Chicago Press)
——1972b *Phase Transitions and Critical Phenomena* vol 2 ed C Domb and M S Green (London: Academic Press)
Mori H 1965 *Prog. theor. Phys.* **33** 423–55
Zwanzig R W 1972 *Statistical Mechanics* ed S A Rice, K F Freed and J C Light (Chicago: University of Chicago Press)