New integral equation for mode-coupling problems

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A new integral equation is derived for mode-coupling problems. The equation is identical with the conventional self-consistent equation of Kawasaki in the Markovian limit. In the non-Markovian case the equation predicts very different behavior of frequency-dependent transport coefficients. In particular the vanishing of transport coefficients at low frequencies predicted by Kawasaki's equation for one and two dimensions due to the infrared divergencies of the appropriate kernels may disappear in the present expansion.

The mode-coupling formalism[1–4] plays an important role in our microscopic understanding of critical dynamics. It describes the relaxation of macroscopic modes of a system via nonlinear coupling to other modes. This formalism had remarkable success in calculating the dynamical correlation functions of a variety of systems by properly incorporating our previous knowledge regarding the behavior of static (equal-time) correlation functions (i.e., susceptibilities) which may be obtained from equilibrium thermodynamics. Several nonlinear phenomena such as the long-time tails of hydrodynamic correlation functions and the behavior of transport coefficients near critical points may be quantitatively understood using this formalism.[1–4]

The typical mode-coupling equation focuses on a set of dynamical variables a_k, and the first step in applying it to a physical system is to convert the Liouville equation into the nonlinear Langevin form[1–4]:

$$\frac{da_q}{dt}=(i\omega_q-\gamma_q)a_q(t)-i\lambda\sum_{k<k_c}\mathscr{V}_{q,k,q-k}a_k(t)a_{q-k}(t)+f_q(t)\ . \tag{1}$$

Here ω_q and γ_q are the frequency and damping constant of a_q. The damping arises from nonlinear coupling with large k modes. $\mathscr{V}_{q,k,q-k}$ denotes the nonlinear coupling with small k (long-wavelength) modes with k smaller than a cutoff k_c and $f_q(t)$ is a random force. λ is a dimensionless parameter which characterizes the nonlinear coupling strength and is introduced for bookkeeping purposes.

We shall be interested in calculating the correlation function

$$G_q(t)\equiv\theta(t)\langle a_q(t)a_q^\dagger(0)\rangle/\chi_q\ , \tag{2}$$

where the scalar product $\langle AB\rangle$ may be defined in various ways depending on the problem at hand. The simplest possibility is

$$\langle a_q(t)a_q^\dagger(0)\rangle\equiv\mathrm{Tr}[a_q(t)a_q^\dagger(0)\rho_0]\ , \tag{3a}$$

where ρ_0 is the canonical distribution function. Alternatively, in linear-response problems the scalar product is often defined using the Kubo transform

$$\langle a_q(t)a_q^\dagger(0)\rangle\equiv\mathrm{Tr}\int_0^\beta d\lambda\, e^{\lambda H}a_q(t)e^{-\lambda H}a_q^\dagger(0)\rho_0\ . \tag{3b}$$

$\theta(t)$ is the step function and χ_q is a static susceptibility

$$\chi_q=\langle a_q a_q^\dagger\rangle\ . \tag{4}$$

Equation (1) may be converted into the integral form:

$$a_q(t)=a_q^0(t)-i\lambda\sum_k\int_0^t d\tau\, G_q^0(t-\tau)\mathscr{V}_{q,k,q-k}\times a_k(\tau)a_{q-k}(\tau)\ , \tag{5}$$

where $a_q^0(t)$ is the solution of the linear problem (with $\lambda=0$), i.e.,

$$a_q^0=G_q^0(t)a_q(t=0)+\int_0^t d\tau\, G_q^0(t-\tau)f_q(\tau)\ , \tag{6}$$

and $G_q^0(t)$ is the correlation function of the linear problem

$$G_q^0(t)=\theta(t)\langle a_q^0(t)a_q(0)\rangle/\chi_q$$
$$=\exp(i\omega_q t-\gamma_q t)\,. \qquad (7)$$

The common method to solve Eq. (5) is by iteration to the desired order in λ, multiplying by $a_q^\dagger(0)\rho$, and taking a trace. We then generate a perturbative series for $G_q(t)$:

$$G_q(t)=G_q^0(t)+\lambda^2 G_q^{(2)}(t)+\lambda^4 G_q^{(4)}+\cdots\,, \qquad (8)$$

where we have assumed that $a_q^0(t)$ are Gaussian variables so that only even powers in λ appear.

The next step in the application of the mode-coupling formalism is to find a resummation technique for the series (8) so that a low-order expansion of some quantity will yield an infinite-order approximation for $G_q(t)$. This is usually done using the ansatz

$$G_q(\omega)\equiv -i\int_0^\infty d\tau\exp(i\omega\tau)G_q(\tau)$$
$$=\frac{1}{\omega+\omega_q+i\gamma_q+i\Sigma_q(\omega)}\,, \qquad (9)$$

or alternatively

$$G_q(\omega)=G_q^0(\omega)\frac{1}{1+i\Sigma_q(\omega)G_q^0(\omega)}\,, \qquad (10)$$

where

$$G_q^0(\omega)=\frac{1}{\omega+\omega_q+i\gamma_q}\,. \qquad (11)$$

$\Sigma_q(\omega)$ is the self-energy of the problem and it may be expanded in λ, i.e.,

$$\Sigma_q(\omega)=\lambda^2\Sigma_q^{(2)}(\omega)+\lambda^4\Sigma_q^{(4)}(\omega)+\cdots\,, \qquad (12)$$

where

$$\Sigma_q^{(2)}(\omega)=-\frac{1}{\pi}\int_{-\infty}^{\infty}d\omega'\sum_k \mathscr{V}_{q,k,q-k}$$
$$\times G_{q-k}^0(\omega-\omega')G_k^0(\omega')$$
$$\times\mathscr{V}_{q,k,q-k}\chi_k\chi_{q-k}/\chi_q\,, \qquad (13)$$

etc.

It was suggested[1] to use the following *exact* integral equation as a natural generalization of (13):

$$\Sigma_q(\omega)=-\frac{1}{\pi}\lambda^2\int_{-\infty}^{\infty}d\omega'\sum_k \widetilde{\mathscr{V}}_{q,k,q-k}$$
$$\times G_{q-k}(\omega-\omega')G_k(\omega')$$
$$\times\mathscr{V}_{q,k,q-k}\chi_k\chi_{q-k}/\chi_q\,. \qquad (14)$$

This equation serves as a definition of the vertex function $\widetilde{\mathscr{V}}$. $\widetilde{\mathscr{V}}$ may be expanded in λ and by comparing (14) with (13) it is clear that $\lambda\widetilde{\mathscr{V}}_{q,k,q-k}=\lambda\mathscr{V}_{q,k,q-k}+O(\lambda^2)$. Taking the lowest-order expansion of $\mathscr{V}$ we finally get the *approximate* integral equation:

$$\Sigma_q(\omega)=-\frac{1}{\pi}\lambda^2\int_{-\infty}^{\infty}d\omega'\sum_k|\mathscr{V}_{q,k,q-k}|^2$$
$$\times G_{q-k}(\omega-\omega')$$
$$\times G_k(\omega')\chi_k\chi_{q-k}/\chi_q\,. \qquad (15)$$

This equation, together with Eq. (9) is a closed integral equation for $\Sigma_q(\omega)$ and was extensively used in the literature.[1-4] After solving Eq. (15) for $\Sigma_q(\omega)$, the solution is substituted in Eq. (9) and we get the approximation for $G_q(\omega)$.

We wish to propose here a new ansatz. Instead of (10) we write

$$G_q(t)=G_q^0(t)\exp\left[-\int_0^t d\tau(t-\tau)\phi_q(\tau)\right]. \qquad (16)$$

Upon expanding $\phi_q(\tau)$ in λ,

$$\phi_q(\tau)=\lambda^2\phi_q^{(2)}(\tau)+\lambda^4\phi_q^{(4)}(\tau)+\cdots \qquad (17)$$

and comparing term by term with Eq. (8) we get

$$\phi_q^{(2)}=\sum_{k'}\mathscr{V}_{q,k,q-k}G_{q-k}^0(\tau)$$
$$\times G_k^0(\tau)\mathscr{V}_{q,k,q-k}\chi_{q-k}\chi_k/\chi_q\,. \qquad (18)$$

Proceeding in the same spirit that led from (13) to (14) we postulate now the following *exact* integral equation as a natural generalization of Eq. (18):

$$\phi_q(\tau)=\lambda^2\sum_k\hat{\mathscr{V}}_{q,k,q-k}G_{q-k}(\tau)$$
$$\times G_k(\tau)\mathscr{V}_{q,k,q-k}\chi_k\chi_{q-k}/\chi_q \qquad (19)$$

which is merely the definition of the new vertex function $\hat{\mathscr{V}}$. To lowest order in λ, $\hat{\mathscr{V}}=\mathscr{V}$, and we get the *approximate* integral equation:

$$\phi_q(t)=\lambda^2\sum_k |\mathscr{V}_{q,k,q-k}|^2 \exp\left[-\int_0^t d\tau(t-\tau)\phi_{q-k}(\tau)\right]\exp\left[-\int_0^t d\tau(t-\tau)\phi_k(\tau)\right]G_k^0(t)G_{q-k}^0(t)\frac{\chi_k\chi_{q-k}}{\chi_q} . \tag{20}$$

Equation (20) is the new integral equation; together with Eq. (16) it provides us with a new approximation for $G_q(t)$. We should note the following.

(1) The usual ansatz (9) is based on the exact conventional reduced equation motion (REM) which G_q obeys:

$$\frac{dG_q}{dt}=(i\omega_q-\gamma_q)G_q(t)-\int_0^t d\tau\,\Sigma_q(t-\tau)G_q(\tau) . \tag{21a}$$

The ansatz (16) is based on the alternative REM (Refs. 5–7):

$$\frac{dG_q}{dt}=(i\omega_q-\gamma_q)G_q(t)-\int_0^t d\tau\,\phi_q(\tau)G_q(t) . \tag{21b}$$

Both Σ_q and ϕ_q have closed simple expressions in terms of the total Hamiltonian. Equation (21b) has proved very useful recently for various problems.[7] It was shown that Eqs. (21a) and (21b) are useful for systems with different statistical properties.

(2) In the Markovian limit we assume

$$\Sigma_q(\omega)=\Sigma_q(\omega=0)\equiv\Sigma_q , \tag{22a}$$

$$\phi_q(\tau)=\Sigma_q\delta(\tau) . \tag{22b}$$

In this case both integral equations (15) and (20) assume the form

$$\Sigma_q=\lambda^2\sum_k |\mathscr{V}_{q,k,q-k}|^2\frac{1}{\omega_{q-k}+i\gamma_{q-k}+i\Sigma_{q-k}} \times\frac{1}{\omega_k+i\gamma_k+i\Sigma_k}\frac{\chi_k\chi_{q-k}}{\chi_q} . \tag{23}$$

Various phenomena such as the localization problem are highly non-Markovian[8–10] and the kernel $\Sigma_q(\omega)$ may have infrared divergencies. In such cases the integral equations (15) and (20) have drastically different properties. Let us assume that $\mathscr{V}_{q,k,q-k}$ is independent of q and k. To second order [by putting $\Sigma_q=0$ in the right-hand side of (15) and $\phi_q=0$ in the right-hand side of (20)] we get (taking also $\omega_q=0$)

$$\Sigma_q(\tau)=\phi_q(\tau)\propto\int k^{d-1}dk\,e^{-Dk^2\tau}\sim\tau^{-d/2} , \tag{24}$$

where d is the space dimensionality of the system and where we have put $\gamma_q=Dq^2$ which holds for any conserved variable a_q. Using (24) we have

$$G_q(\omega)=\frac{1}{\omega+i\gamma_q+i\Sigma_q(\omega)} . \tag{25}$$

When $(\omega\to 0)$ we have

$$\Sigma_q(0)\propto\int d\tau\,e^{i\omega\tau}\tau^{-d/2}\sim\begin{cases}\frac{1}{\sqrt{\omega}}, & d=1\\ \ln\omega, & d=2\\ \sqrt{\omega}, & d=3 .\end{cases} \tag{26}$$

We thus see that $G_q(\omega=0)$ vanishes for $d=1,2$. On the other hand, if we use our new Eq. (20) we have

$$G_q(\omega)=-i\int_0^\infty dt\exp(i\omega t-Dq^2t)\exp[-K(t)] , \tag{27}$$

where

$$K(t)\simeq t\int^t\tau^{-d/2}d\tau-\int^t d\tau\,\tau^{1-d/2} . \tag{28}$$

By performing the integration in (28) we note that for $d>2$ the first term in (28) will be dominant at long times and $K(t)$ will be linear in t. For lower dimensionalities however, both terms will contribute and we have

$$K(t)\overset{t\to\infty}{\longrightarrow}\begin{cases}t^{3/2}, & d=1\\ t\ln t-t, & d=2\\ t, & d>2 .\end{cases} \tag{29}$$

More precisely we have for $d>2$ and for long times

$$K(t)\to\left[\int_0^\infty d\tau\,\phi(\tau)\right]t . \tag{30}$$

When substituting Eq. (29) in (27) we see that $G_q(\omega=0)$ does not vanish for any dimensionality d. This is in contrast to the vanishing of $G_q(\omega=0)$ for $d=1$ and 2 predicted by Eq. (26) when substituted in (25). We should note, however, that although this is just the first-order approximation to $G_q(\omega)$ it is sufficient to show how different the ω dependence of $G_q(\omega)$ may be when expanding Eqs. (15) or (20) to a given order in the non-Markovian case. A careful study is needed in order to define the domain of validity of Eqs. (15) and (20).

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