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Exact Transport Parameters for Driving Forces of Arbitrary Magnitude

V. M. Kenkre and M. Dresden
Institute for Theoretical Physics, State University of New York at Stony Brook, Stony Brook, New York 11790
(Received 27 April 1971)

A straightforward analysis of the time-correlation function of interest in response theory involves the entire complicated solution of the dynamical problem. Using projection techniques we derive a simpler equation obeyed by the time-correlation function. Laplace transforms are used to solve this equation for the case when the driving force is a step function of arbitrary magnitude. The results are independent of the near-origin approximation of the Kubo formalism.

The projection techniques of Zwanzig[1] have been used to obtain equations for the distribution functions in nonequilibrium statistical mechanics.[1-3] Recently one of the authors utilized[4] them for deriving an explicit expression for the Laplace transform of the time-correlation function which is the quantity of interest in the Kubo formalism.[5] We shall show how the method may be generalized for the case of the exact time-correlation function appearing in the Peterson formalism[6] which, unlike the Kubo formalism, is not restricted to the near-equilibrium case. We employ Laplace transforms to derive an explicit expression for the exact case where the external stimulus (the additive part in the Hamiltonian) appears as a step function with respect to time. For an arbitrary time dependence our method yields an integro-differential equation for the time-correlation function. However, it cannot be solved by Laplace transforms in as simple a manner.

We treat the step-function case. The time-correlation function of concern is[6]

$$J(t,t') = \mathrm{Tr}\{\rho_0[B(t')A(t)+A(t)B(t')]\}, \qquad (1)$$

where

$$B(t') = U^\dagger(t',0)BU(t',0),$$
$$A(t) = U^\dagger(t,0)AU(t,0), \qquad (1\text{a})$$
$$U(t,0) = \exp[T(-i)\textstyle\int_0^t H_{\mathrm{tot}}(s)ds];$$

T is the time-ordering operator and ρ_0 is the equilibrium density matrix. $H_{\mathrm{tot}}(t)$, which equals $H-\mathfrak{A}f(t)$, where $\mathfrak{A}$ is a time-independent operator and $f(t)$ is a c-number function, becomes for the step-function case

$$H_{\mathrm{tot}}(t) = H - \mathfrak{A}f\theta(t), \qquad (2)$$

where f is a time-independent strength parameter and $\theta(t)$ is the Heaviside step function. Then, the various time-evolution operators take the forms exemplified by

$$U(t,0) = \exp(-itH) \text{ for } t<0,$$
$$= \exp(-it\mathcal{K}) \text{ for } t>0, \qquad (3)$$

where $\mathcal{K} = H - \mathfrak{A}f$.

After permutation of the operators within the trace, Eq. (1) may be cast in the form

$$J(t,t') = \mathrm{Tr}\{AU(t,0) \times[\rho_0B(t')+B(t')\rho_0]U^\dagger(t,0)\}. \qquad (4)$$

We shall write

$$\mathrm{Tr}\{A[\rho_0B(t')+B(t')\rho_0]\} \equiv \chi(t'), \qquad (4\text{a})$$

and define

$$B_1(t') \equiv [1/\chi(t')]B(t'), \qquad (4\text{b})$$
$$J_1(t,t') \equiv [1/\chi(t')]J(t,t'). \qquad (4\text{c})$$

Since for $t>0$, $U^\dagger(t,0)OU(t,0) = e^{it\alpha}O$ for any operator O, where α is defined by $\alpha O \equiv [\mathcal{K}, O]$, we have for $t>0$

$$J_1(t,t') = \mathrm{Tr}\{Ae^{-it\alpha}[\rho_0B_1(t')+B_1(t')\rho_0]\}$$
$$\equiv \mathrm{Tr}[Ae^{-it\alpha}K(0,t')] \qquad (5)$$
$$\equiv \mathrm{Tr}[AK(t,t')].$$

It is the purpose of this note to develop equations for J and J_1 directly. Equation (5) gives J as a trace of a complicated operator. Projections are introduced at this point to select that part of $K(t, t')$ needed in Eq. (5). The hope is to find an equation for J which does not require the full solution of the dynamical problem. We now define an operator P by

$$PO \equiv K(0, t')\mathrm{Tr}(AO) \text{ for any operator } O. \tag{6}$$

We note that (i) P is linear, and (ii) $P^2 = P$. We apply the Zwanzig formulas[1]

$$i\partial PK(t, t')/\partial t = P\alpha PK(t, t') - i\int_0^t ds\, P\alpha G(s)(1-P)\alpha PK(t-s, t'), \tag{7}$$

where the usual initial-condition term is zero since $(1-P)K(0, t') = 0$. Multiplying Eq. (7) from the left by A and taking the trace, there results

$$i\partial J_1(t, t')/\partial t = C(t')J_1(t, t') - i\int_0^t ds\, Q(s, t')J_1(t-s, t'), \tag{8}$$

where $C(t') = \mathrm{Tr}[A\alpha K(p, t')]$ and $Q(s, t') = \mathrm{Tr}[A\alpha G(s)(1-P)\alpha K(0, t')]$ with $G(s) = \exp[-is(1-P)\alpha]$, as is well known.

We have used here the obvious results

$$J_1(0, t') = 1,$$

$$\mathrm{Tr}(APO) = J_1(0, t')\mathrm{Tr}(AO) = \mathrm{Tr}(AO) \text{ for any } O. \tag{9}$$

Taking Laplace transforms, $j(\epsilon) \equiv \int_0^\infty J(t)e^{-t\epsilon}dt$, we find that Eq. (8) yields

$$j_1(\epsilon, t') = [\epsilon + iC + q(\epsilon)]^{-1}. \tag{10}$$

(Lower case letters denote the Laplace transforms.) Multiplying Eq. (10) by $\chi(t')$ we have

$$j(\epsilon, t') = \chi(t')/[\epsilon + iC + q(\epsilon)]. \tag{11}$$

Equation (11) is the principal result of this paper. It gives an exact expression for the Laplace transform of a time-correlation function for any response as long as the stimulus is a step function; it can be of arbitrary size. We thus see that an exact and tractable expression can be obtained independent of the near-origin approximation of Kubo. Equation (11) may be used to calculate $J(t, t')$ through an inversion of the transform. It may also be used directly because under certain conditions the quantity

$$\lim_{\substack{\epsilon \to 0 \\ t' \to \infty}} j(\epsilon, t')$$

can be shown[7] to be equal to a transport coefficient of interest. A result analogous to Eq. (11) has been obtained in Ref. 4 through the explicit use of the commutability of ρ_0, the equilibrium density matrix, and H, the Hamiltonian without the stimulus. This commutability of ρ_0 and the Hamiltonian holds in the Kubo case treated in Ref. 4 but does not hold in the more general Peterson case that we treat because in the latter case one deals with ρ_0 and H_{tot}, the Hamiltonian including the stimulus. Our derivation however, shows that a useful result can be deduced in spite of this difficulty.

The correlation function J depends on *two* times, not on a time difference as in the Kubo case. It can be shown that in the latter case, a change of variables to $t-t'$ can be made to result in the t' disappearing from Eq. (11). One then gets a simpler result but one which is valid only for small stimuli. In this simplified form Eq. (11) can be used[7] as a starting point for several investigations which will, for instance, yield the range of validity of Matthiessen's rule[8] and its refinements.

By using the modified Zwanzig formulas[3] it is possible to obtain the following equation for an arbitrary time dependence:

$$i\partial J_1(t, t')/\partial t = C(t, t')J_1(t, t') - i\int_0^t ds\, Q(s, t, t')J_1(s, t'). \tag{12}$$

However, now the C is dependent on t and the kernel $Q(s, t, t')$ is not $Q(s-t, t')$, and so Laplace transforms do not help in the solution to this equation.

Integro-differential equations like Eq. (10) are not particular to time-correlation functions and have been derived[7] for general response functions.

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Drift-Wave Instabilities of a Compressional Mode in a High-β Plasma

Akira Hasegawa
Bell Telephone Laboratories, Murray Hill, New Jersey 07974
(Received 10 May 1971)

While the ordinary electrostatic drift mode is stabilized by either high-β effects or an admixture of cold plasma, a compressional drift mode is shown to be destabilized under these same circumstances. The condition of the instability is approximately given by $n_h/n_c < \beta\kappa_0^2\rho_i^2/2$, where n_h and n_c are the number densities of the hot and cold components, respectively; κ_0 is a measure of the density, temperature, or magnetic field gradients; and ρ_i is the ion Larmor radius.

The ordinary electrostatic drift-wave instability is known to be stabilized in a high-β plasma ($\beta > 0.13$) by Landau damping of ions drifting as a result of a magnetic field gradient in the same direction as that of electron diamagnetic drift.[1,2] This instability can also be shown to be stabilized by a fractional mixture $[n_c/n_h \gtrsim (m_e/m_i)^{1/2}]$ of cold electrons that short-circuit the parallel (to the ambient magnetic field) electric field which is needed to maintain the drift wave.[3]

On the other hand, drift waves associated with compressional modes (modes which produce changes in the parallel component of the magnetic field) have a tendency to destabilize at a larger value of β because the transit-time damping[4] which is proportional to β plays the role of Landau damping in the electrostatic mode.

Mikhailovskii and Fridman[5] have considered drift waves in magnetosonic modes (coupled modes of an acoustic wave and a compressional wave) and have shown in fact a wider range of unstable regions in the value of β. However, these modes are again strongly modified by an admixture of cold plasma because of the disappearance of the ion acoustic wave. Stabilization of the modes can be shown to occur when $n_c \sim n_h$. Therefore, most of the drift-wave instabilities presented in the past are stabilized in a high-β plasma with an admixture of cold plasma.

We will show here that when the cold-plasma density exceeds a threshold, however, the compressional Alfvén wave is destabilized either by inversed transit-time damping of ions or by inversed Landau damping associated with resonant particles drifting as a result of a magnetic field gradient.

We consider a nonuniform and high-β plasma embedded in a straight magnetic field $B_0(y)\hat{e}_z$. The nonuniformity is taken in the y direction. In the low-frequency ($\omega \ll \omega_{ci}$) and the long-wavelength ($k_\perp v_{Ti} \ll \omega_{ci}$) limit, the dispersion relation for the magnetosonic mode can be written as[5,6]

$$c^2k^2/\omega^2 - (\epsilon_{yy} + \epsilon_{yz}^2/\epsilon_{zz}) = 0. \tag{1}$$

If we consider an admixture of cold electrons with $n_c \sim n_h$, the ϵ_{zz} component becomes very large and the dispersion relation can be reduced to

$$c^2k^2/\omega^2 - \epsilon_{yy} = 0, \tag{1a}$$

where ϵ_{yy} can be derived using the ordinary WKB approximation,[5]

$$\epsilon_{yy} = -\sum_{\text{species}} \frac{\omega_p^2}{\omega} \sum_{n=0,1} \int \frac{v_\perp^2[J_n'(k_\perp v_\perp/\omega_c)]^2}{\omega - n\omega_c - k_\parallel v_\parallel + k_\perp v_d}\left(\frac{m}{T} + \frac{k_\perp}{\omega\omega_c}\frac{\partial}{\partial y}\right) f_0\, dv, \tag{2}$$

where $dv \equiv 2\pi v_\perp dv_\perp dv_\parallel$, $v_d\ [=(v_\perp^2/2\omega_c)(\partial \ln B_0/\partial y)]$ is the ∇B_0 drift speed, and the other notations are standard. We consider the velocity distribution function f_0 to represent an isotropic Maxwellian distribution with both density and temperature being functions of y. Substituting Eq. (2) into Eq. (1a) and expanding the derivatives of the Bessel functions, J_n', to a suitable order, we find the following dis-