A measure of the incompleteness of a statistical description and irreversibility. Fluctuation-dissipation relation (FDR) for multiparticle distribution functions

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The concept of a measure of incompleteness of a statistical description in the presence of irreversible processes is introduced. A generalized FDR, which is valid for nonequilibrium processes, is formulated starting with the density matrix of the macroscopic system. The FDR is obtained on the basis of this relation for a gas, and a fluctuation formulation of the Boltzmann collision integral is proposed.

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We are examining a macroscopic system consisting of N particles with the Hamiltonian H_0. $X(t)$ is a collection of all coordinates and momenta of the particles, while χ is a point in the $6N$-dimensional phase space. We introduce two distribution functions in phase space: a microscopic function $f_N^M(\chi,t) = \delta(\chi - X(t))$, which depends not only on χ but also on $X(t)$, and a distribution function that is averaged over the ensemble $f_N(\chi,t) = \langle f_N^M | (\chi,t) | \rangle$. We define a single-time correlation function $\delta f_N = f_N^M - f_N$

$$< \delta f_N(\chi, t)\delta f_N(\chi,' t)> = \delta(\chi - \chi')f_N(\chi, t) - f_N(\chi, t) f_N(\chi', t). \qquad (1)$$

For a complete mechanical description, when $f_N = f_N^M$, it is equal to zero, while for an incomplete description, it serves as a measure of the incompletenesss of the statistical description.

In quantum theory, we examine two corresponding density matrices: $f_{nm}^M = \Psi_n^+ \Psi_m$ for a pure ensemble (n is the set of quantum numbers of the particles in the system); $f_{nm} = \langle f_{nm}^M \rangle$ for the mixed ensemble. As a measure of the incompleteness of the statistical description, we choose the single-time correlation function $\delta f_{nm} = f_{nm}^M - f_{nm}$, corresponding to (1),

$$\langle \delta f_{nm}(t)\, \delta f_{n_1 m_1}(t) \rangle = \delta_{n m_1} f_{n_1 m} - f_{nm} f_{n_1 m_1} \,. \qquad (2)$$

The correlation functions of the commuting operators for a pure ensemble, determined with the help of (2), are equal to zero. We use appropriate boundary conditions for the two-time correlation function

$$\left(\frac{\partial}{\partial t} + \dot{\Delta} + i\omega_{nm} \right) \langle \delta f_{nm} \delta f^*_{n_1 m_1} \rangle_{t,\, t'} = 0, \qquad t > t'. \qquad (3)$$

For an incomplete description (mixed ensemble), it has, with the initial ($t = t'$) condition (2), a nonvanishing solution. Using this solution, we find an expression for the spectral density. If $f_{nm} = \delta_{nm} f_n$, we have

$$(\delta f_{nm}\delta f_{n_1 m_1})_\omega = \pi\delta(\omega - \omega_{nm})\delta_{nn_1}\delta_{mm_1}(f_m + f_n). \tag{4}$$

This expression can be rewritten in the form of an FDR

$$(\delta f_{nm}\delta f_{n_1 m_1})_\omega = \hbar \operatorname{Im} A_{nmn_1 m_1}(\omega)\frac{f_m + f_n}{f_m - f_n} \; . \tag{5}$$

Here we have introduced the corresponding susceptibility

$$A_{nmn_1 m_1}(\omega) = -\frac{1}{\hbar}\delta_{nn_1}\delta_{mm_1}\frac{f_m - f_n}{\omega + i\Delta - \omega_{nm}} \; . \tag{6}$$

If f_n is the canonical Gibbs distribution, then the most general FDR for fluctuations of a multiparticle density matrix for the equilibrium state of a macroscopic system follows from (5):

$$(\delta f_{nm}\delta f_{n_1 m_1})_\omega = \hbar \operatorname{Im} A_{nmn_1 m_1}(\omega)\operatorname{cth}\frac{\hbar\omega}{2k_B T} \; . \tag{7}$$

With its help, it is possible to obtain the well-known Callen-Welton equation (§ 124 in Ref. 1), as well as a new FDR, for example, for a Boltzmann gas.

It is important that the FDR, expressed in the form (5), can also be used for nonequilibrium states with density matrix $f_{nm}(t) = \delta_{nm} f_n(t)$. The function f_n in this case satisfies a kinetic equation for a multiparticle distribution function $f_n(t)$. This equation describes relaxation to a canonical Gibbs distribution. The kinetic equation for the multiparticle distribution function was first introduced by Leontovich.[2] For the Boltzmann gas, Leontovich's equation describes relaxation to a multidimensional Maxwellian distribution. In Ref. 3, an equation, which describes relaxation to a Gibbs distribution due to a fluctuation electromagnetic interaction, was obtained.

The FDR for a Boltzmann gas follows from Eqs. (5) and (6):

$$(\delta f_{\mathbf{p}_1\mathbf{p}_1'}\delta f_{\mathbf{p}_1\mathbf{p}_1'})_\omega = \hbar \operatorname{Im} A_{\mathbf{p}_1\mathbf{p}_1'}(\omega)\frac{f_1(\mathbf{p}_1') + f_1(\mathbf{p}_1)}{f_1(\mathbf{p}_1') - f_1(\mathbf{p}_1)} \; , \tag{8}$$

$$A_{\mathbf{p}_1\mathbf{p}_1'}(\omega) = -\frac{1}{N}\frac{f_1(\mathbf{p}_1') - f_1(\mathbf{p}_1)}{\hbar(\omega + i\Delta) - (E_{\mathbf{p}_1} - E_{\mathbf{p}_1'})}, \quad E_{\mathbf{p}} = \mathbf{p}^2/2m \tag{9}$$

The distribution function $f_1(\mathbf{p}_1, t)$ satisfies the Boltzmann equation. Substituting a Maxwell distribution into (8) and (9), we obtain the FDR for an equilibrium gas.

If the FDR (5) and (8) are used for nonequilibrium states, the quantity Δ, which determines the width of the functions $\delta(\omega - \omega_{nm})$, and $\delta(\omega - (E_{\mathbf{p}} - E_{\mathbf{p}_1'})/\hbar)$, satisfies the collisionless approximation condition $\Delta\tau_{\mathrm{rel}} \gg 1$, in which τ_{rel} is the corresponding time for relaxation to equilibrium.

Starting from the FDR (8) and (9), we can introduce a fluctuation representation for the Boltzmann collision integral

$$I(\mathbf{p}_1, t) = \frac{1}{(2\pi)^3\hbar} \int d\omega\, d\mathbf{k}\, d\mathbf{p}_1'\, \delta(\hbar\mathbf{k} - (\mathbf{p}_1 - \mathbf{p}_1'))\delta(\hbar\omega - (E_{\mathbf{p}_1} - E_{\mathbf{p}_1'})).$$

(10)

$$[(\delta U \delta U)_{\omega, \mathbf{k}, \mathbf{p}_1 + \mathbf{p}_1'} (f_1(\mathbf{p}_1') - f_1(\mathbf{p}_1)) - \hbar \mathrm{Im}\, D(\omega, \mathbf{k}, \mathbf{p}_1 + \mathbf{p}_1')(f_1(\mathbf{p}_1') + f_1(\mathbf{p}_1))]$$

This equation contains an expression for the spectral density of fluctuations in the potential, corresponding to the scattering problem

$$\delta U_{\mathbf{p}_1 \mathbf{p}_1'}(\omega) = N \int T(\mathbf{p}_1 \mathbf{p}_2, \mathbf{p}_1' \mathbf{p}_2') \delta(\mathbf{p}_1 + \mathbf{p}_2 - \mathbf{p}_1' - \mathbf{p}_2') \delta f_{\mathbf{p}_2' \mathbf{p}_2}(\omega) \frac{V}{(2\pi\hbar)^3} d\mathbf{p}_2 d\mathbf{p}_2' . \tag{11}$$

Equations for the spectral density of fluctuations δU and the imaginary part of the corresponding susceptibility $\mathrm{Im}D(\omega,\mathbf{p}_1,\mathbf{p}_1')$ follow from (8) and (11). These functions depend not only on ω and $k = (\mathbf{p}_1 - \mathbf{p}_1')/\hbar$, but also on $\mathbf{p}_1 + \mathbf{p}_1'$. The later dependence disappears only in the approximation of perturbation theory, when the T matrix is related to the Fourier component of the interaction potential by the equality

$$T(\mathbf{p}_1 \mathbf{p}_2, \mathbf{p}_1' \mathbf{p}_2') = \frac{1}{V} \nu\left(\frac{|\mathbf{p}_1 - \mathbf{p}_1'|}{\hbar}\right) \frac{(2\pi\hbar)^3}{V} \delta(\mathbf{p}_1 + \mathbf{p}_2 - \mathbf{p}_1' - \mathbf{p}_2'). \tag{12}$$

Using the fluctuation representation of the Boltzmann collision integral, it is possible to obtain an expression for the collision integral, which incorporates simultaneously both the strong pair collisions at small distances and weak, collective interactions at large distances. To accomplish this, we define the corresponding dielectric permittivity

$$\epsilon(\omega, \mathbf{p}_1, \mathbf{p}_1') = 1 + \frac{N}{V} \int \frac{V}{(2\pi\hbar)^3} d\mathbf{p}_2 d\mathbf{p}_2' ,$$

$$\frac{|T(\mathbf{p}_1 \mathbf{p}_2, \mathbf{p}_1' \mathbf{p}_2')|^2}{\nu\left(\frac{|\mathbf{p}_1 - \mathbf{p}_1')}{\hbar}\right)} \frac{\delta(\mathbf{p}_1 + \mathbf{p}_2 - \mathbf{p}_1' - \mathbf{p}_2')(f(\mathbf{p}_2') - f(\mathbf{p}_2))}{\hbar(\omega + i\Delta) - (E_{\mathbf{p}_2'} - E_{\mathbf{p}_2})} . \tag{13}$$

Polarization can be incorporated into the Boltzmann collision integral (using the usual representation) by introducing into the integrand an expression for the symmetrized polarization factor

$$\frac{1}{2}[|\epsilon(\omega, \mathbf{p}_1, \mathbf{p}_1')|^{-2} + |\epsilon(\omega, \mathbf{p}_2, \mathbf{p}_2')|^{-2}] . \tag{14}$$

The generalized expression obtained in this manner for the collision integral unifies the Boltzmann approximation and the polarization approximation, which for a Coulomb system corresponds to the Balescu-Lenard collision integral.[4,5] Of the number of possible solutions, the solution of this problem (§ 46 in Ref. 4 and § 56 in Ref. 5) proposed by us is internally most consistent. This consistency is necessary, in particular, when nonideality effects are taken into account in kinetic equations.[5]

Strong and weak collective interactions must be taken into account simultaneously in many cases: in the kinetic theory of spectral-line broadening, in the kinetic theory of partially ionized plasma, and so on.[6,3]

The measure of incompleteness of the statistical description introduced above is important not only in the statistical theory of many particles but also in quantum-mechanical problems such as those in the theory of quantum transitions.

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