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A LINEAR SYSTEM IN THE FIELD OF THERMAL FORCES

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The response of a system to a weak thermal perturbation that varies arbitrarily in space and time is considered. A rigorous proof of the fluctuation-dissipation theorem is presented for the corresponding generalized susceptibility, which plays the role of the heat capacity of the system and is "complex and dependent on ω and $\mathbf{k}$."

INTRODUCTION

THE response of a linear dissipative system to thermal perturbation was considered in a number of papers [1,2] under the assumptions that the period of the perturbation is much shorter than the relaxation time of the system and that the spatial inhomogeneity is weak. In this case, the response of the system does not contain temporal or spatial dispersion, the phenomenological equations are valid in the usual form, and the problem reduces to finding statistical transport coefficients such as the thermal conductivity.

Cases are encountered, however, when the thermal perturbation, while still small, does not satisfy the foregoing properties of weak temporal and spatial inhomogeneity. In such cases it is necessary to take into account the dependence of the response of the system on the temporal and spatial variations of the external field. The generalized susceptibility of the system is in this case a function of ω and $\mathbf{k}$.

Let us consider an equilibrium system in contact with a large reservoir at a temperature T_0. The interaction between them causes the statistical properties of the system to be described by a density matrix. We assume further that the temperature of the reservoir changes in arbitrary fashion in space and in time, but so that $\delta T(\mathbf{r}, t) = T(\mathbf{r}, t) - T_0 \ll T_0$, where $T(\mathbf{r}, t)$ is the temperature of the reservoir at the point $\mathbf{r}$ and at the instant t. The interaction with the reservoir unbalances the system and the macroscopic quantities characterizing the system deviate from their equilibrium values. The smallness of the deviation of the parameters of the reservoir from the equilibrium values and the weakness of its interaction with the system make it possible to assume that the response of the system to the violation of the equilibrium of the system with the reservoir is a linear function of the change in the reservoir parameters.

Let the system be such that the particle and momentum fluxes due to the influence of the external field, as well as the possible thermal expansion, can be neglected. In this case the deviation of the energy density from the equilibrium value $\delta\epsilon(\mathbf{r}, t) = \langle \hat{h}(\mathbf{r}) \rangle - \langle \hat{h}(\mathbf{r}) \rangle_0$ ($\langle \ldots \rangle_0$ represents averaging over the equilibrium density matrix corresponding to the temperature T_0, and $\langle \ldots \rangle$ averaging over the nonequilibrium density matrix describing the state of the system at the instant t) is a linear function of the variation of the temperature of the reservoir:

$$\delta\varepsilon = \hat{C}(\mathbf{r}, t)\,\delta T,$$

$\hat{C}(\mathbf{r}, t)$ is a certain linear integral operator.

If the temperature of the reservoir changes infinitely slowly in space and in time, then the system can keep up with the reservoir and its susceptibility is the specific heat of the system C_V. In the general case, the behavior of the system is described by a generalized susceptibility $C_V(\omega, \mathbf{k})$, which can be called the "complex and dependent on ω and $\mathbf{k}$" heat capacity of the system. The purpose of the present paper is to derive an expression for this susceptibility. We shall show rigorously that $C_V(\omega, \mathbf{k})$ is determined by the autocorrelation function for the fluctuation of the energy density of a canonical system.

Let us present examples in which the kinetic and the relaxation properties of the system are determined by the complex heat capacity. Consider a complicated system that can be subdivided in the equilibrium state into two weakly-interacting subsystems I and II. In other words, the Hamiltonian $\hat{H}'$ of the interaction is small compared with the Hamiltonians $\hat{H}_I$ and $\hat{H}_{II}$, of the subsystems I and II. We also assume that the heat capacity of system I is large compared with the heat capacity of system II. We place such a system in a weakly-alternating homogeneous field that changes the energy of subsystem I. Let the period of the external field T exceed the relaxation time τ_I of subsystem I. Then subsystem I is at any instant of time in a state of local equilibrium, which can be described by the local temperature $T(\mathbf{r}, t)$. The energy of this system is a single-valued function of the temperature. With respect to subsystem II, we assume either that the external perturbation does not act on it directly, or that its relaxation time is $\tau_{II} \gg T$.

The interaction between the subsystems causes the change $\delta\epsilon_{II}(\mathbf{r}, t)$ of the energy density of subsystem II to be determined completely by the change $\delta\epsilon_I(\mathbf{r}, t)$ in the density of the energy of subsystem I. For the chosen field $\delta\epsilon_{II}$ lags $\delta\epsilon_I$ that is, it lags also

$$\delta T(\mathbf{r}, t) = T(\mathbf{r}, t) - T_0,$$

where T_0 is the equilibrium temperature of the entire system. In view of the inhomogeneity of the external field, the connection between $\delta\epsilon_{II}$ and δT has in general a nonlocal character. Therefore $\delta\epsilon_{II}$ is a general linear function of δT. The generalized susceptibility of subsystem II in the external field under consideration is $C_V(\omega, \mathbf{k})$ $(\omega < 1/\tau_I)$. In accordance with the assumptions made concerning subsystems I and II, we neglect the dependence of $\delta\epsilon_I$ on $\delta\epsilon_{II}$.

When considering the propagation of sound in a system consisting of polyatomic molecules, the subsystem of translational and rotational degrees of freedom and the subsystem of vibrational degrees of freedom play the roles of subsystems I and II at low temperatures. $C_V(\omega, \mathbf{k})$ is in this case the complex heat capacity of the vibrational subsystem and describes Kneser processes in the system.

In a paramagnetic spin-lattice system in a weak alternating and inhomogeneous magnetic field, the spin and lattice subsystems satisfy at low temperature the conditions imposed on subsystems I and II. In this case $C_V(\omega, \mathbf{k})$ is the lattice specific heat and describes the magnetocaloric effect.

1. DETERMINATION AND PROPERTIES OF THE COMPLEX HEAT CAPACITY

The change in the energy density of a spatially-homogeneous and isotropic system in the field of a thermal force can be represented in the form

$$\delta\varepsilon(\mathbf{r}, t) = \int_0^\infty d\tau \int d\mathbf{r}' L(\tau, \mathbf{r}') \delta T(\mathbf{r} - \mathbf{r}', t - \tau). \quad (1.1)$$

Here $L(\tau, \mathbf{r})$ is the response function of the system. This function vanishes when τ is much larger than the relaxation times of the system, making it possible to use infinity as the upper limit in (1.1). We shall assume that $L(\tau, \mathbf{r})$ does not contain any singularities in τ. For an unbounded system we get, taking the Fourier transform of (1.1),

$$\delta\varepsilon(\omega, \mathbf{k}) = C_v(\omega, \mathbf{k}) \delta T(\omega, \mathbf{k}), \quad (1.2)$$

where

$$C_v(\omega, \mathbf{k}) = \int_0^\infty d\tau \int d\mathbf{r} \, L(\tau, \mathbf{r}) e^{i(\omega\tau - \mathbf{k}\mathbf{r})} \quad (1.3)$$

is the generalized susceptibility of the system and was called by us the complex heat capacity. The response function can be related to the imaginary part of the heat capacity. By assumption, $L(0, \mathbf{r}) = 0$, and on this basis the response function can be continued into the region of negative τ, putting

$$L(\tau, \mathbf{r}) = -L(-\tau, \mathbf{r}). \quad (1.4)$$

Then

$$L(\tau, \mathbf{r}) = \frac{i}{\pi} \int d\omega \int \frac{d\mathbf{k}}{(2\pi)^3} \exp\{i(\mathbf{k}\mathbf{r} - \omega t)\} C_v''(\omega, \mathbf{k}). \quad (1.5)$$

A complex $C_V(\omega, \mathbf{k})$ means that the states $\delta\epsilon$ and δT are shifted in phase and that the entropy production in the system differs from zero. The corresponding calculation can be carried out without difficulty for small ω and $\mathbf{k}$, when the thermodynamic relations are valid. Thus, the production of entropy can be represented in the form

$$\sigma = -T^{-2} \delta\varepsilon \delta\dot{T}. \quad (1.6)$$

Putting

$$\delta T(\mathbf{r}, t) = \frac{1}{2} \{\delta T_0 e^{-i(\omega t - \mathbf{k}\mathbf{r})} + \delta T_0^* e^{i(\omega t - \mathbf{k}\mathbf{r})}\}, \quad (1.7)$$

we get from (1.1)—(1.3) and (1.6), averaging over the space-time period of the perturbation (1.7),

$$\sigma(\omega, \mathbf{k}) = \frac{\omega}{2T^2} C_v''(\omega, \mathbf{k}) |\delta T_0|^2. \quad (1.8)$$

It follows therefore that the imaginary part of the heat capacity determines the production of entropy in the system.

If the temperature varies infinitely slowly, then

$$\delta\varepsilon(\mathbf{k}) = C_v(0, \mathbf{k}) \delta T(\mathbf{k}). \quad (1.9)$$

In the latter expression the quantity $C_V(0, \mathbf{k})$ describes the response to an adiabatically applied inhomogeneous perturbation and can be called the "equilibrium wave-number-dependent" heat capacity of the system:

$$C_v(0,\mathbf{k}) \equiv C_v(\mathbf{k}).$$

When ω and $\mathbf{k}$ tends to zero, $C_V(\omega, \mathbf{k})$ goes over into the equilibrium specific heat, for which we have the Gibbs distribution

$$C_v = \frac{1}{k_B T_0^2 V} \langle (\hat{H} - E)^2 \rangle_0. \qquad (1.10)$$

It is easy to determine $C_V(\mathbf{k})$ from the last equation.

The spectrum of the equilibrium fluctuations of the energy density is described by the correlation function

$$\varphi_h(\mathbf{r},\tau) = \frac{1}{2} \langle \{ \delta\hat{h}(\mathbf{r}',t),\ \delta\hat{h}(\mathbf{r}'-\mathbf{r}, t-\tau) \} \rangle, \qquad (1.11)$$

where $\delta\hat{h}(\mathbf{r}, t) = \hat{h}(\mathbf{r}, t) - \langle \hat{h}(\mathbf{r}) \rangle_0$, $\hat{h}(\mathbf{r}, t)$ is the operator in the Heisenberg representation, and $\{\ldots\}$ is the anticommutator. From (1.3) we get

$$C_v(\mathbf{k}) = \int d\mathbf{r} K(\mathbf{r}) e^{-i\mathbf{k}\mathbf{r}}, \qquad (1.12)$$

where

$$K(\mathbf{r}) = \int_0^\infty d\tau L(\tau, \mathbf{r}).$$

Using (1.11) and (1.12), we represent (1.10) in the form

$$\frac{1}{k_B T_0^2} \int \varphi_h(\mathbf{r}, 0)\, d\mathbf{r} = \int K(\mathbf{r})\, d\mathbf{r}. \qquad (1.13)$$

The latter take place for any V, and therefore the integrands are equal. For $C_V(\mathbf{k})$ we get

$$C_v(\mathbf{k}) = \frac{1}{2 k_B T_0^2} \langle \{ \delta\hat{h}(\mathbf{r}',t),\ \delta\hat{h}(\mathbf{r}'-\mathbf{r}, t) \} \rangle_{\mathbf{k}}. \qquad (1.14)$$

From the dispersion relation for the real and imaginary parts of the complex heat capacity we can relate $C_V(\mathbf{k})$ with $C_V''(\omega, \mathbf{k})$:

$$C_v(\mathbf{k}) = \int_{-\infty}^{\infty} \frac{d\omega}{\pi} \frac{C_v''(\omega, \mathbf{k})}{\omega}. \qquad (1.15)$$

2. FLUCTUATION-DISSIPATION THEOREM FOR THE HEAT CAPACITY

Our purpose is to find a dynamically justified expression for the complex heat capacity $C_V(\omega, \mathbf{k})$.

Inasmuch as a thermal perturbation cannot be uniquely represented in the Hamiltonian of the system, it is impossible to apply the usual methods [3,4] directly to the problem under consideration. To get around this difficulty, we shall show that the problem (1.1) can be reduced to a dynamic problem that admits of a simple treatment.

We introduce the $\mathbf{k}$-component of the response function

$$L(\tau, \mathbf{k}) = \int d\mathbf{r}\, e^{-i\mathbf{k}\mathbf{r}} L(\tau, \mathbf{r}) \qquad (2.1)$$

and represent (1.1) in the form

$$\delta\varepsilon(\mathbf{k}, t) = \int_0^\infty L(\tau, \mathbf{k}) \delta T(\mathbf{k}, t - \tau)\, d\tau. \qquad (2.2)$$

Let $\delta T(\mathbf{k}, t)$ vary as follows:

$$\delta T(\mathbf{k}, t) = \begin{cases} \delta T(\mathbf{k}) e^{\varepsilon t} & t \leqslant 0 \\ 0 & t > 0. \end{cases} \qquad (2.3)$$

Such a character of the variation of the parameters of the reservoir denotes that when $t = -\infty$ the system and the reservoir are in equilibrium at a temperature T_0, when $t \in (-\infty, 0)$ the temperature of the reservoir changes adiabatically from T_0 to $T_0 + \delta T(\mathbf{r}) e^{\epsilon t}$, and when $t \geq 0$ the system is placed in a thermostat whose temperatures is T_0. For $t \geq 0$ we find from (2.2) that the energy density varies as follows:

$$\delta\varepsilon(\mathbf{k}, t) = \int_t^\infty L(\tau, \mathbf{k})\, d\tau \cdot \delta T(\mathbf{k}). \qquad (2.4)$$

The relaxation properties of the system are described by the function

$$\Phi(\mathbf{k}, t) = \int_t^\infty L(\tau, \mathbf{k})\, d\tau. \qquad (2.5)$$

The introduced relaxation function can be connected with the complex heat capacity of the system by using (1.5)

$$\Phi(\mathbf{k}, t) = \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{C_v''(\omega, \mathbf{k})}{\omega} e^{-i\omega t} d\omega. \qquad (2.6)$$

We get therefore for $t = 0$

$$\Phi(\mathbf{k}, 0) = C_v(\mathbf{k}) \qquad (2.7)$$

and for $t = \infty$

$$\Phi(\mathbf{k}, \infty) = 0. \qquad (2.8)$$

The function $\Phi(\mathbf{k}, t)$ describes the relaxation of the energy of the system from

$$\delta\varepsilon(\mathbf{k}, 0) = C_v(\mathbf{k}) \delta T(\mathbf{k}) \qquad (2.9)$$

at $t = 0$ to 0 at $t = \infty$. We can then use (2.4), (2.5), and (2.9) to reduce the problem (2.2) to the following form:

$$\delta\varepsilon(\mathbf{k}, t) = \frac{\Phi(\mathbf{k}, t)}{C_v(\mathbf{k})} \delta\varepsilon(\mathbf{k}, 0). \qquad (2.10)$$

Formula (2.10) describes the relaxation from a specified value $\delta\epsilon(\mathbf{k}, 0)$, of the energy of a system situated in the reservoir having a temperature T_0.

For the system and reservoir under consideration, the relaxation law is determined only by the magnitude of the initial deviation of the energy density from the equilibrium, and does not depend on how the indicated deviation is produced. This means that if a deviation $\delta\epsilon(\mathbf{k}, 0)$ from $\langle\hat{h}(\mathbf{r})\rangle_0$ is produced in our system by any suitable external field before the instant $t = 0$, but there no longer any field when $t > 0$, then the relaxation of $\delta\epsilon(\mathbf{k}, 0)$ occurs in accordance with (2.10).

In our system the external fields do not produce particle fluxes, so that the only mechanism producing $\delta\epsilon(\mathbf{k}, 0)$ can be an external field that leads to a direct energy effect. Such a field is the gravitational field proposed by Luttinger[2]. If the potential of the field is denoted by $c^2\psi(\mathbf{r}, t)$, then its contribution to the Hamiltonian of the system is equal to

$$\delta\hat{H}(t) = -\int d\mathbf{r}\hat{h}(\mathbf{r})\psi(\mathbf{r}, t). \tag{2.11}$$

Let us place the system and the thermostat, which are in equilibrium at the temperature T_0, in a gravitational field which had been turned on adiabatically at $t = -\infty$ and was turned off at $t = 0$. Assume that the field is such that prior to $t = 0$ the deviation of the energy density of the system from the initial value is $\delta\epsilon(\mathbf{k}, 0)$. The field is turned on adiabatically, the system is in equilibrium with the thermostat if $t \in (-\infty, 0)$, and the energy varies isothermally. The response of the system at $t = 0$ is the response to a constant perturbation

$$\delta\hat{H} = -\int d\mathbf{r}\hat{h}(\mathbf{r})\psi(\mathbf{r}) \tag{2.12}$$

and

$$\delta\varepsilon(\mathbf{r}, 0) = \frac{\mathrm{Sp}\, e^{-\beta_0(\hat{H}+\delta\hat{H})}\hat{h}(\mathbf{r})}{\mathrm{Sp}\, e^{-\beta_0(\hat{H}+\delta\hat{H})}} - \frac{\mathrm{Sp}\, e^{-\beta_0\hat{H}}\hat{h}(\mathbf{r})}{\mathrm{Sp}\, e^{-\beta_0\hat{H}}} \tag{2.13}$$

($\beta_0 = 1/k_B T_0$). In the approximation linear in $\delta\hat{H}$ we have

$$\delta\varepsilon(\mathbf{k}, 0) = \chi_T(\mathbf{k})\psi(\mathbf{k}), \tag{2.14}$$

where

$$\chi_T(\mathbf{k}) = \frac{1}{2k_{\text{Б}}T_0}\langle\{\delta\hat{h}(\mathbf{r}, t), \delta\hat{h}(\mathbf{r}-\mathbf{r}', t)\}\rangle_{\mathbf{k}} \tag{2.15}$$

is the "wave-number-dependent" isothermal susceptibility of the system in the gravitational field. Comparing with (1.14), we get

$$T_0 C_v(\mathbf{k}) = \chi_T(\mathbf{k}). \tag{2.16}$$

When $t > 0$, the value of $\delta\epsilon(\mathbf{k}, t)$ is determined by the relaxation function of the system, which we obtain for the gravitational field in accordance with the usual procedure[3]:

$$\delta\varepsilon(\mathbf{k}, t) = \Phi_\psi(\mathbf{k}, t)\psi(\mathbf{k}),$$

$$\Phi_\psi(\mathbf{k}, t) = \frac{i}{\hbar}\int_t^\infty \langle[\hat{h}(\mathbf{k}, t), \hat{h}(-\mathbf{k}, t'-\tau)]\rangle_0 d\tau. \tag{2.17}$$

The presence of a thermostat having a temperature T_0 causes the averaging to be carried out with respect to the canonical distribution function at the temperature T_0. Using (2.15), we get

$$\delta\varepsilon(\mathbf{k}, t) = \frac{\Phi_\psi(\mathbf{k}, t)}{T_0 C_v(\mathbf{k})}\delta\varepsilon(\mathbf{k}, 0). \tag{2.18}$$

From the equality of (2.10) and (2.18) it follows that

$$T_0\Phi(\mathbf{k}, t) = \Phi_\psi(\mathbf{k}, t). \tag{2.19}$$

Taking into account the connection between the Fourier transforms of the relaxation and correlation functions[3] and using (2.6), we get

$$C_v''(\omega, \mathbf{k}) = \frac{\pi}{\hbar T_0}\langle\{\delta\hat{h}(\mathbf{r}', t), \delta\hat{h}(\mathbf{r}'-\mathbf{r}, t-\tau)\}\rangle_{\omega,\mathbf{k}} \,\mathrm{th}\, \frac{\hbar\omega}{2k_B T_0}. \tag{2.20}$$

The last relation is the analog of the fluctuation-dissipation theorem for the heat capacity, and coincides, accurate to $1/T_0$, with the formulation of the theorem for the dynamic susceptibilities[4].

3. SOME EXAMPLES

In the case of slow space-time variations of physical quantities, the equations of hydrodynamics are valid and the properties of the system are described by the transport coefficients and by the relaxation times. Knowledge of the exact expression for $C_V(\omega, k)$ makes it possible to obtain for these quantities dynamically justified expressions.

In analogy with[5], we have proceeded as follows. Using different hydrodynamic models, we get an expression for $C_V(\omega, k)$ with ω and k tending to zero, and compare the results with the exact expression (2.20).

Let us consider a closed system in which there is a temperature gradient. In the case of slow space-time variations of the temperature gradient, the heat flux can be represented in the form

$$\mathbf{j}^Q(\mathbf{r}, t) = -\frac{\varkappa}{C_v}\nabla\varepsilon(\mathbf{r}, t). \tag{3.1}$$

Here κ is the thermal conductivity coefficient and C_V the specific heat of the system. Since, by assumption, there are no particle fluxes in the system, the energy flux in the system coincides with the flux (3.1). Since the system is closed, we can, using the conservation law, represent the time variation of the energy in the form

$$\delta\varepsilon(\mathbf{k},t)+k^2\frac{\varkappa}{C_v}\delta\varepsilon(\mathbf{k},t)=0. \tag{3.2}$$

We multiply the last equation by $e^{i\omega t}$ and integrate with respect to time from zero to infinity; then

$$\left(-i\omega+k^2\frac{\varkappa}{C_v}\right)\int_0^\infty dt\, e^{i\omega t}\delta\varepsilon(\mathbf{k},t)=\delta\varepsilon(\mathbf{k},0). \tag{3.3}$$

We assume that the temperature varies like (2.3), and get, in accord with (2.9) and (2.4),

$$\delta\varepsilon(\mathbf{k},t)=\begin{cases}C_v(\mathbf{k})\,\delta T(\mathbf{k})\,e^{\varepsilon t} & t\leqslant 0,\\ \Phi(\mathbf{k},t)\,\delta T(\mathbf{k}) & t\geqslant 0\end{cases} \tag{3.4}$$

where $\Phi(\mathbf{k}, t)$ is given by (2.6). Then we get from (3.3)

$$\frac{C_v''(\omega,\mathbf{k})}{\omega}+\frac{i}{\pi}\int\frac{C_v''(\omega',\mathbf{k})}{\omega'(\omega-\omega')}d\omega'=\frac{C_v(\mathbf{k})}{-i\omega+k^2\varkappa/C_v}. \tag{3.5}$$

Equating the real quantities on the left and on the right, we get

$$C_v''(\omega,\mathbf{k})=\frac{C_v(\mathbf{k})\,k^2\omega\varkappa/C_v}{\omega^2+(k^2\varkappa/C_v)^2}. \tag{3.6}$$

Thus, at small values of ω and k the values of $C_V''(\omega, \mathbf{k})$ depend essentially on the relative values of ω and k^2. In the limit when ω and k tend to zero, we obtain for $C_V''(\omega, \mathbf{k})$ two different limits at $\omega \ll k^2\kappa/C_V$ and $k^2\kappa/C_V \ll \omega$. In the "fast case" with $k^2\kappa/C_V \ll \omega$ (k approaches 0 more rapidly than ω) we have

$$C_v''(\omega,\mathbf{k})\approx\frac{k^2}{\omega}\varkappa. \tag{3.7}$$

Therefore

$$\varkappa=\lim_{\omega\to 0}\lim_{\mathbf{k}\to 0}\frac{\omega}{k^2}C_v''(\omega,\mathbf{k}). \tag{3.8}$$

Using (2.20) we obtain a dynamically-justified expression for the thermal conductivity coefficient

$$\varkappa=\frac{\pi}{\hbar T_0}\lim_{\omega\to 0}\lim_{\mathbf{k}\to 0}\frac{\omega}{k^2}\langle\{\delta\hat{h}(\mathbf{r}',t),\delta\hat{h}(\mathbf{r}'-\mathbf{r},t-\tau)\}\rangle_{\omega,\mathbf{k}}\times\ \mathrm{th}\frac{\hbar\omega}{2k_\mathrm{B}T_0}. \tag{3.9}$$

From the continuity equation we get

$$\delta\hat{h}(\omega,\mathbf{k})=\frac{1}{\omega}\mathbf{k}\mathbf{j}^\varepsilon(\omega,\mathbf{k}) \tag{3.10}$$

and

$$\varkappa=\frac{\pi}{2k_\mathrm{E}T_0^2}\lim_{\omega\to 0}\lim_{\mathbf{k}\to 0}\langle\{\hat{\mathbf{j}}_x^\varepsilon(\mathbf{r}',t),\hat{\mathbf{j}}_x^\varepsilon(\mathbf{r}'-\mathbf{r},t-\tau)\}\rangle_{\omega,\,\mathbf{k}}, \tag{3.11}$$

which agrees with the result of Luttinger[2].

In the foregoing derivation it was assumed that the establishment of the equilibrium in the system is determined by transport processes, and that no energy leaks out of the system. In the case when $C_V(\omega, \mathbf{k})$ describes a slow subsystem, if one can neglect the energy exchange between the slow and fast subsystems, then (3.11) determines the contribution of the slow subsystem to the total thermal conductivity of the system.

Thus, when considering the thermal conductivity of a system of polyatomic molecules, where the transformation of energy from the vibrational subsystem into translational energy can be neglected, Eq. (3.11) describes the thermal conductivity of the vibrational subsystem. Such a subdivision of the thermal conductivity system into parts corresponding to the conductivities of the vibrational and translational subsystems is in agreement with Euker's calculations[6].

Similarly, (3.11) determines the lattice thermal conductivity for the case of a spin-lattice system at low temperatures, if energy exchange between the spins and the lattice can be neglected.

Let us consider now the opposite limiting case, when exchange of energy between the fast and slow subsystems plays the principal role in the establishment of equilibrium between the subsystems. In this case the time variation of the energy of the slow subsystem can be represented in the form

$$\dot{\delta\varepsilon}(\mathbf{k},t)=-\frac{1}{\tau(\mathbf{k})}\delta\varepsilon(\mathbf{k},t). \tag{3.12}$$

Here $\tau(\mathbf{k})$ is the relaxation time of the k-component of the energy density. Just as in the preceding case, we get

$$C_v''(\omega,\mathbf{k})=\frac{\omega\tau(\mathbf{k})C_v(\mathbf{k})}{\omega^2\tau^2+1}. \tag{3.13}$$

When k = 0, such an expression for the imaginary part of the vibrational thermal conductivity is obtained in the theory of Kneser relaxation. From (3.13) we get in the "slow case" (ω tends to zero more rapidly than k)

$$C_v''(\omega,\mathbf{k})\approx\omega\tau(\mathbf{k})C_v(\mathbf{k}) \tag{3.14}$$

and

$$\tau=\lim_{\mathbf{k}\to 0}\lim_{\omega\to 0}\frac{C_v''(\omega,\mathbf{k})}{\omega C_v(\mathbf{k})}. \tag{3.15}$$

Using (2.20) and (1.14), we obtain a dynamically-justified expression for the relaxation time of the slow subsystem:

$$\tau=\frac{2k_\mathrm{B}\pi T_0}{\hbar}\lim_{\mathbf{k}\to 0}\lim_{\omega\to 0}\times\frac{\langle\{\delta\hat{h}(\mathbf{r}',t),\delta\hat{h}(\mathbf{r}'-\mathbf{r},t-\tau)\}\rangle_{\omega,\mathbf{k}}\,\mathrm{th}(\hbar\omega/2k_\mathrm{B}T_0)}{\omega\langle\{\delta\hat{h}(\mathbf{r}',t),\delta\hat{h}(\mathbf{r}'-\mathbf{r},t)\}\rangle_\mathbf{k}}. \tag{3.16}$$

In the examples indicated above, the last expression provides an estimate of the spin-lattice relaxation time and of the time of relaxation of the excitation in a system of polyatomic molecules.

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