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SOME TYPES OF KINETIC EQUATIONS REDUCIBLE TO PARTIAL DIFFERENTIAL EQUATIONS

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The possibility of passing from the kinetic equation to a partial differential equations is rigorously mathematically proved for the case of nearly elastic scattering processes. Some examples are considered.

Key words: *diffusion, quasi-elastic scattering, Boltzmann equation, Green function, laws of conservation of energy and momentum, photon, electron, phonon.*

The Boltzmann integrodifferential kinetic equation describing the spatial–temporal dynamics of the distribution function appears in modeling nonequilibrium phenomena in solids [1, 2]. The corresponding kinetic processes have been well studied; nevertheless, there is one issue that has not been considered earlier (see below) and it is studied in the present paper.

We consider a scattering process that involves two fast particles and one slow particle, in particular: 1) two photons and one phonon; 2) two electrons and one phonon; 3) two photons and one nonrelativistic electron (moving, for example, on a Fermi surface), etc. A common feature of the large number of such processes is that all of them are quasi-elastic ones.

Let us consider a process of the first type. Because the phase velocity of light in matter $v = c/\sqrt{\varepsilon\mu}$ (ε and μ are the dielectric and magnetic permeabilities, respectively) considerably exceeds the sound velocity c_s, it can be assumed that, in the energy conservation law $v(k_1 - k_2) - c_s k_3 = 0$, the last term $c_s k_3$ is always small and, hence, $k_1 \approx k_2$ (k_1 and k_2 are the photon wave vectors before and after scattering, respectively, and k_3 is the phonon wave vector). The same is valid for processes of the second and third types.

The question arises: What for should the nonlocal and evolution concentrations of photons and electrons be introduced into consideration? According to the definition of the extinction (attenuation) coefficient given in [3], it can be written as

$$h = \frac{\langle \delta\varepsilon^2 \rangle}{18\pi c} V q^4,$$

where V is the volume of the macroparticle on which there is scattering of a photon of wavelength $\lambda = 2\pi/q \gg V^{1/3}$, $\langle \delta\varepsilon^2 \rangle$ are the dielectric permeability fluctuations due to the incidence of the electromagnetic wave on the body, and q is the wave vector of the incident photon. Since the fluctuation can be represented as

$$\delta\varepsilon = \frac{\partial\varepsilon}{\partial\rho}\,\delta\rho,$$

where $\delta\rho$ is the density fluctuation, we obtain

$$h = \langle \delta\rho^2 \rangle \Big(\frac{\partial\varepsilon}{\partial\rho}\Big)^2 q^4 V.$$

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However,

$$\langle \delta\rho^2 \rangle = \Big(\frac{\partial\rho}{\partial V}\Big)^2 \langle \delta V^2 \rangle = \frac{M^2}{V^2 C_V} = \frac{\rho^2}{C_V}$$

(C_V is the isochoric heat capacity and M is the mass); therefore,

$$h \sim \frac{M^2}{V C_V}\Big(\frac{\partial\varepsilon}{\partial\rho}\Big)^2 q^4.$$

Because the photon concentration is defined as $n = 1/V$, the extinction coefficient

$$h \sim n\,\frac{M^2}{C_V}\Big(\frac{\partial\varepsilon}{\partial\rho}\Big)^2 q^4,$$

and, hence, it depends greatly on the photon concentration.

In the above definition, the concentration n is a stationary homogeneous function of the coordinates and time, but its distribution $n(\boldsymbol{r}, t)$ should be determined from the diffusion approximation, which is discussed in the present work.

For electrons, the conductivity is defined [4] as $\sigma = e^2 n\tau/m$ (e is the electron charge, m is its mass, τ is the relaxation time, and n is the electron concentration); therefore, all inferences on the homogeneity and stationarity of the function $n(\boldsymbol{r}, t)$ are the same as for photons.

Thus, if the diffusion time in the $\boldsymbol{r}$-space is $\Delta t = L^2/D$ ($L \sim V^{1/3}$ is the characteristic size and D is the diffusion coefficient), which is much larger than the electron diffusion time in the momentum $\boldsymbol{p}$-space ($\Delta t^* = p_{\mathrm{F}}^2/D_p = (p_{\mathrm{F}}/\delta p)^2\tau \sim p_{\mathrm{F}}^2\tau/(mT)$, where p_{F} is the Fermi momentum, T is the temperature, and the Boltzmann constant is set equal to unity), the establishment of the equilibrium electron concentration is determined by the time $\Delta t = L^2/D$. If the experiment is terminated before this time, the electrons are a nonequilibrium system, and, hence, any experimental measurements of metal conductivity can be called into question. The same is true for the extinction coefficient h.

Let us show that in the approximation of quasi-elastic particle scattering (quasi-particles), the right side of the Boltzmann kinetic equation for the distribution function $f(\boldsymbol{r}, \boldsymbol{p}, t)$: $\dot f = L\{f\}$ ($L\{f\}$ is the collision integral), after being integrated over all momenta $\boldsymbol{p}$ can always be represented as

$$\int L\{f\}\,\frac{d^3p}{(2\pi\hbar)^3} = D_1\,\Delta n - D_2\,\Delta^2 n + D_3\,\Delta^3 n - \ldots = \sum_{i=1}^{k} (-1)^{i+1} D_i\,\Delta^i n, \tag{1}$$

where Δ is the Laplace operator, D_i are the diffusion coefficients of the corresponding dimension ($D_1 = D_3 = \ldots = 0$ and $D_2 \neq 0$ for photons, and $D_1 \neq 0$ and $D_2 = D_3 = \ldots = 0$ for electrons), and $\hbar$ is Planck's constant.

The left side of the Boltzmann kinetic equation becomes

$$\frac{\partial n}{\partial t} = \int \frac{\partial f}{\partial t}\,\frac{d^3p}{(2\pi\hbar)^3}.$$

Let us prove formula (1). We write the photon–phonon collision integral as

$$L\{f\} = \frac{2\pi V^3}{\hbar(2\pi\hbar)^3}\int d^3p' \int |\psi_1|^2 \{[(1+f_p) f_{p'} \bar N_k - f_p (1+f_{p'})(1+\bar N_k)]\delta(\varepsilon_p - \varepsilon_{p'} - \hbar\omega_k)\delta(\boldsymbol{q} - \boldsymbol{q}' - \boldsymbol{k})$$

$$+ [(1+f_p) f_{p'}(1+\bar N_k) - f_p (1+f_{p'})\bar N_k]\delta(\varepsilon_p - \varepsilon_{p'} + \hbar\omega_k)\delta(\boldsymbol{q} - \boldsymbol{q}' + \boldsymbol{k})\}\,d^3k, \tag{2}$$

where $\bar N_k$ is the equilibrium distribution function for phonons, which are considered a thermostat and δ are delta-functions that take into account the conservation laws for the energy and momentum of the particles (quasi-particles) participating in the scattering processes. The remaining notation is the same as in [2].

As is known, the scattering amplitude for the photon–phonon mechanism is given by the formula

$$\psi_1 = i\,\frac{8\pi\hbar g}{V}\Big(\frac{\hbar k \omega_q \omega_{q'}}{2\rho V c_s}\Big)^{1/2}, \tag{3}$$

where $\omega_q = cq/\sqrt{\varepsilon\mu}$ is the photon oscillation frequency and g is the photon–phonon interaction constant [5].

Because the ambient temperature is considered fairly high: $T \gg \hbar\omega_k$, it can be assumed that $1 + N_k \approx N_k \approx T/(\hbar\omega_k)$. Then, the nonlinear collision integral (2) becomes linear in the photon distribution function:

$$L\{f\} = \frac{(2\pi)^2 V^3 T}{\hbar^2 (2\pi\hbar)^3} \int d^3p' \int |\psi_1|^2 \{(f_{p'} - f_p)[\delta(\varepsilon_p - \varepsilon_{p'} - \hbar\omega_k)\delta(\boldsymbol{q} - \boldsymbol{q}' - \boldsymbol{k})$$

$$+ \delta(\varepsilon_p - \varepsilon_{p'} + \hbar\omega_k)\delta(\boldsymbol{q} - \boldsymbol{q}' + \boldsymbol{k})]\} \frac{d^3k}{\omega_k}. \tag{4}$$

Since $p' = p + \delta p$, where $\delta p = \hbar k$ and $\delta p \ll p$, in (4), according to (3), we can set

$$|\psi_1|^2 = g^2 \frac{(8\pi)^2}{2} \frac{\hbar^3 q q' k c^2}{V^3 c_s \varepsilon \mu} \approx 32\pi^2 g^2 \frac{\hbar^3 q^2 k c^2}{V^3 c_s \varepsilon \mu}. \tag{5}$$

We integrate the collision integral (4) over all $\boldsymbol{q}$. After transformation to spherical coordinates with allowance for (5), we have

$$\int L\{f_p\} \frac{d^3p}{(2\pi\hbar)^3} = \int L\{f_q\} \frac{q^2\, dq}{(2\pi)^3} 4\pi. \tag{6}$$

We expand the photon distribution function in a Fourier integral using the well-known representation

$$f_q = \int f_x \, \mathrm{e}^{i\boldsymbol{q}\boldsymbol{x}} \, d^3x.$$

Because expression (6) is linear in f_q, it follows that

$$\int q^4 \, dq(\,\cdot\,) \, \mathrm{e}^{i\boldsymbol{q}\boldsymbol{x}} \, d^3x = -\Delta^2 \int dq \, d^3x (\,\cdot\,) \, \mathrm{e}^{i\boldsymbol{q}\boldsymbol{R}}, \tag{7}$$

where $\boldsymbol{R} = \boldsymbol{x} - \boldsymbol{r}$ and the differentiation is performed over $\boldsymbol{R}$.

After simple mathematical calculations, we obtain the following diffusion equation for the photon concentration $n(\boldsymbol{r}, t)$:

$$\frac{\partial n}{\partial t} = -D_2 \, \Delta^2 n. \tag{8}$$

It can be shown that the diffusion coefficient is given by the relation

$$D_2 = 1024\pi^3 T c g^2 \xi / (\rho c_s^2 \varepsilon \mu), \tag{9}$$

where

$$\xi = \int\limits_{-1}^{1} dx \int\limits_{-1}^{1} dy \left[\frac{x^2y^2 + (1-x^2)(1-y^2)}{|x|} \Big(\frac{1}{\sqrt{4(1-x^2)(1-y^2) - 1}} - \frac{1}{4\sqrt{1 - x^2 - y^2 + xy}} - \frac{1}{4\sqrt{1 - x^2 - y^2 + xy}} \Big) \right.$$

$$\left. + \frac{1}{4|x|} \left(\sqrt{4(1-x^2)(1-y^2) - 1} - \sqrt{1 - x^2 - y^2 + xy} - \sqrt{1 - x^2 - y^2 - xy} \right) \right]. \tag{10}$$

The principal Cauchy value of integral (10) is approximately 6.34.

Equation (8) can be solved by setting concrete boundary and initial conditions. Indeed, at the initial time, let the photon concentration be equal to $n(\boldsymbol{r}, t)\Big|_{t=0} = \varphi(\boldsymbol{r})$. The function $\varphi(\boldsymbol{r})$ can be measured, for example, by gauges inserted into the structure at some distance from the boundary and spaced from each other at certain intervals in the direction of the Pointing vector. This allows one to determine the spatial behavior of $n(\boldsymbol{r}, 0)$. The second condition can be obtained by measuring the rate of decrease in the concentration or, more precisely, its derivative:

$$\frac{\partial n(\boldsymbol{r}, t)}{\partial t}\Big|_{t=0} = \psi(\boldsymbol{r}).$$

As regards the boundary conditions, the concentration value on the surface of the structure can be specified, for example, in the form $n(\boldsymbol{r}, t)\Big|_{\Sigma_V} = n_0(t)$, where Σ_V is the boundary of the solid scatterer. Since the concentration can be a decreasing function, one more boundary condition can be specified by requiring that the concentration $n(\boldsymbol{r}, t)$ also decrease with increasing distance d into the depth of the material. This condition can be supplemented

by the requirement of a negative derivative of the function $n(\boldsymbol{r},t)$ in the direction perpendicular to the boundary of the solid. In addition, the concentration gradient should be oriented strictly along the Pointing vector.

It should be noted that the boundary (and initial) conditions should be specified on the basis of a particular experiment.

Generally, it can only be stated that for the initial concentration distribution there are two possibilities: a reduction in the concentration with increasing depth (i.e., for $\boldsymbol{r} \to \infty$) or a weak dependence on the distance $n(\boldsymbol{r},t)$. The weak dependence $n(\boldsymbol{r},t)$ follows from the solution of Eq. (8) and is easily checked in the one-dimensional case for the radial concentration distribution.

The aforesaid refers to the case of nearly elastic scattering of photons by phonons.

Let us consider nearly elastic scattering of conductivity electrons in a metal by density fluctuations. In this case,

$$\psi_2 = -ig\Big(\frac{\hbar k}{2\rho V c_s}\Big)^{1/2}\frac{1}{V} \tag{11}$$

and, similarly to (4) (considering phonons a thermostat), we have

$$L\{f\} = \frac{(2\pi)^2 V^3 T}{\hbar^2(2\pi\hbar)^3}\int d^3p' \int |\psi_2|^2\{(f_{p'}-f_p)[\delta(\varepsilon_p-\varepsilon_{p'}-\hbar\omega_k)\delta(\boldsymbol{q}-\boldsymbol{q}'-\boldsymbol{k})+\delta(\varepsilon_p-\varepsilon_{p'}+\hbar\omega_k)\delta(\boldsymbol{q}-\boldsymbol{q}'+\boldsymbol{k})]\}\,\frac{d^3k}{\omega_k}.$$

The expression for the scattering amplitude (11) does not include the multiplier $qq' \approx q^2$; therefore, by analogy with (7)–(10), we obtain the equation

$$\frac{\partial n}{\partial t} = D_1\,\Delta n,$$

where D_1 is the electron diffusion coefficient:

$$D_1 \approx 512\pi^3 T v_{\mathrm{F}} g^2/(\rho c_s^2 a^2) \tag{12}$$

(a is the interatomic distance).

The difficulty in estimating by formula (12) is due to arbitrariness in the definition of the electron–phonon interaction constant g. However, for the estimates, it is sufficient to set, for example, $g = 10^{-4}$.

For room temperature (density $\rho = 7.8$ g/cm^3, Fermi velocity $v_{\mathrm{F}} = 10^8$ cm/sec, sound velocity $c_s = 10^5$ cm/sec, interatomic distance $a = 3\cdot 10^{-8}$ cm) from (12) we obtain the electron diffusion coefficient in the coordinate space $D \approx 10^{-6}$ cm^2/sec. Therefore, the diffusion time (assuming that the process proceeds in the interval $L = 10^{-6}$ cm) is $\delta t = L^2/D_1 \approx 10^{-6}$ sec. Since the electron relaxation time τ is much smaller than δt, the above numerical estimate is fairly accurate.

Thus, formula (1) can be considered proved.

Thus, it was shown that in the approximation of nearly elastic scattering of particles or quasi-particles, the integrodifferential kinetic equation always reduces to the diffusion equation, whose right side contains the operator Δ^m ($m = 1, 2, 3, \dots$).

Depending on the type of particles participating in the scattering process, the particle differential equation changes significantly: its right side contains the term $D_1\,\Delta n$ or the term $-D_2\,\Delta^2 n$, $D_3\,\Delta^3 n$, … (see examples of solution of similar problems in [5]).

Solution of the diffusion equation (8) subject to the corresponding initial and boundary conditions allows one to describe the nontrivial spatial–temporal distribution of the photon concentration over the volume of the material.

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