SOVIET PHYSICS JETP VOLUME 26, NUMBER 4 APRIL, 1968

CONTRIBUTION TO THE QUANTUM THEORY OF KINETIC AND RELAXATION PROCESSES

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Submitted February 23, 1967

Zh. Eksp. Teor. Fiz. 53, 1327–1339 (October, 1967)

It is assumed that during a relatively short time τ_0 a simplification occurs in the description of a system described by a Hamiltonian $\mathscr{H} = \mathscr{H}_0 + V$. The time dependence of the density matrix ρ when $t \gg \tau_0$ is determined only by the time dependence of some parameters γ_k. In most cases the simplification of the description of the system as well as the form of the parameters γ_k themselves is due to separation, from the total Hamiltonian of the system $\mathscr{H}$, of relatively strong interactions $\mathscr{H}_0$ which, however, possess certain symmetry properties. These symmetry properties of the strong interaction define the set of parameters γ_k which describe the state of the system when $t \gg \tau_0$. An integral equation is derived for the density matrix $\rho(\gamma)$, in which the boundary conditions for $t \to +\infty$ are taken into account. Likewise, equations are derived for the time dependence of the parameters γ_k. As an illustration of the application of the general scheme, kinetic equations are obtained for γ_k in the second approximation of perturbation theory with respect to the weak interaction V, and a derivation of the quantum kinetic equation in the low-density approximation is presented.

1. INTRODUCTION

If a physical system has several distinct relaxation times τ_j, then its relaxation to the equilibrium state can occur in a number of steps. This means that during the course of the evolution of the system there takes place a successive reduction (in relatively large time intervals) of the number of parameters necessary to describe the state of the system. For example, if τ_0 is the smallest of the relaxation times, then when $t \gg \tau_0$ the first reduction in the description of the system takes place when all the correlation functions (or, which is the same, the density matrix of the system) are defined by a certain set of parameters γ_k. Thus, when $t \gg \tau_0$, the system forgets some of its earlier correlations, with the exception of those which determine the parameters γ_k. The set of the parameters γ_k itself, as well as the first correlation time τ_0, is determined by the properties of the system, i.e., by its Hamiltonian and to a lesser degree by the initial state of the system. If the next relaxation time τ_1 is much larger than τ_0, then when $t \gg \tau_1$ there can occur a further reduction in the number of the parameters characterizing the state of the system. The set of parameters γ_k becomes redundantly full and we can confine ourselves to a narrower choice of parameters γ'_k. Thus, when $t \gg \tau_1$ the system forgets all its correlations connected with the initial values of the parameters γ_k, with the exception of those correlations which determine the parameters γ'_k. The set of parameters γ'_k and the time τ_1 are determined by the concrete properties of the system.

If we denote by ρ the density matrix of the system, then when $t \gg \tau_0$ the operator ρ should schematically have the following structure:

$$\rho(t) = \rho(\gamma) + \rho'\{\rho(0)\}e^{-t/\tau_0}, \tag{1}$$

where $\rho(\gamma)$ depends on the time only via the time dependence of the parameters γ, for which it is necessary to formulate equations of the kinetic type. On the other hand, the operator $\rho'\{\rho(0)\}$ depends on all the initial correlations in the system. Thus, when $t \gg \tau_0$ the density matrix $\rho(\gamma)$ describes asymptotically exactly the state of the system. Similarily, it is possible to visualize schematically further reduction in a number of the parameters characterizing the state of the system when $t \gg \tau_1$, when the density matrix becomes a functional of the parameters γ'_k.

The very fact that the number of the parameters necessary to describe the state of the system is reduced, together with the form of the parameters γ_k themselves, is connected in most cases with the separation, from the total Hamiltonian of the system, of relatively strong interactions, which, however, have certain symmetry properties. These symmetry properties of the strong interactions determine the reduced set of parameters γ_k describing the state of the system when $t \gg \tau_j$.

The foregoing scheme for the description of nonequilibrium processes was first formulated and applied to the relaxation of not too dense gases during the kinetic stage (the kinetic equations) and during the hydrodynamic stage (the hydrodynamic equations) in the classical case by Bogolyubov[1] and in the quantum case by Bogolyubov and Gurov[2].

The purpose of the present paper is to formulate the foregoing problem for a somewhat more general case, intended for use not only for low-density gases but also for systems in which the parameters γ_k comprise not the single-particle density matrix, but a physically entirely different set of parameters (for example, the problems of paramagnetic and ferromagnetic relaxation), wherein the strongest interactions (which cannot be considered by perturbation theory) that lead to the possibility of describing the system with the aid of the parameters γ_k can be isolated from the very beginning in a rather simple fashion in the boundary conditions for the density matrix. Thus, our problem consists of finding the correct expression for the density matrix $\rho(\gamma)$ in formula (1) and finding the equations describing the time variation of the parameters γ_k.

By way of an application of the general scheme, we present the derivation of the quantum kinetic equation in the low-density approximation.

2. FORMULATION OF PROBLEM

We start from the equation for the density matrix ρ in the Schrödinger representation:

$$\partial\rho / \partial t - i[\rho, \mathcal{H}] = 0, \tag{2}$$

where $\mathcal{H}$ is the Hamiltonian of the system under the assumption that the Hamiltonian $\mathcal{H}$ can be broken up into two parts:

$$\mathcal{H} = \mathcal{H}_0 + V, \tag{3}$$

where $\mathcal{H}_0$ is the "main" Hamiltonian and V is the relatively weak "interaction" Hamiltonian. Owing to the "main" Hamiltonian $\mathcal{H}_0$, there will occur, after a relatively short time interval τ_0, a reduction in the number of the parameters necessary to describe the state of the system. This reduced set of parameters will be denoted by γ_k. The operators corresponding to the parameters γ_k will be denoted by $\hat{\gamma}_k$.

We shall henceforth confine ourselves only to systems for which

$$[\mathcal{H}_0, \hat{\gamma}_k] = a_{kl}\hat{\gamma}_l, \tag{4}$$

where a_{kl} are certain c-numbers[1].

Formula (4) indeed expresses that symmetry property of the Hamiltonian $\mathcal{H}_0$, which was referred to in the introduction. Condition (4) is satisfied by a large number of physical systems. This condition is arrived at in problems connected with the determination of the kinetic equations for the single-particle density matrix, problems involving ferromagnetic and paramagnetic relaxation of the density of the magnetic moment, etc. In the case of the kinetic equations, the role of $\mathcal{H}_0$ is played by the free-particle Hamiltonian $\mathcal{H}_0 = \sum_p \epsilon_p a_p + a_p$, and it is necessary to choose the operators $\hat{\gamma}_k$ in the form $\hat{\gamma}_k = a_p + a_p$ (a_p and a_p^+ are the operators of annihilation and creation of a particle with momentum **p** and energy ϵ_p). In this case V describes the usual interaction between the particles.

In the case of problems connected with ferromagnetic relaxation, the role of $\mathcal{H}_0$ is played by the exchange-interaction Hamiltonian

$$\mathcal{H}_0 = -\sum_{lm} I(\mathbf{R}_{lm})\mathbf{s}_l\mathbf{s}_m - \mu\mathbf{H}_0\sum_l \mathbf{s}_l,$$

and the operators $\hat{\gamma}_k$ must be chosen in the form $\hat{\gamma}_k = \Sigma\mathbf{s}_l$ ($\mathbf{s}_l$—spin operator in l-th site, $I(\mathbf{R}_{lm})$ is the exchange interval between the l-th and m-th sites, and $\mathbf{H}_0$ is the external magnetic field). A strong exchange interaction makes it possible to describe the system with the aid of the parameters $\sum_l \mathbf{s}_l$. The relaxation of the latter to the equilibrium values is the result of the relatively weak relativistic interactions V (the magnetic-anisotropy energy, the energy of the magnetic dipole interaction, etc.). The equations of motion for the parameters $\sum_l \mathbf{s}_l$ represent the equations of motion of the magnetic moment, which are obtained in the present method directly, bypassing the kinetic equations for the spin waves. Similarly, in problems connected with paramagnetic relaxation, the role of $\mathcal{H}_0$ is played by the Hamiltonian of the system, neglecting the magnetic interactions (but with allowance for all the remaining stronger interactions). The operator V describes in this case relatively weak magnetic interactions.

It follows from (2) and (4) that when V = 0 the parameters γ_k satisfy the equation

$$\dot{\gamma}_k = i a_{kl}\gamma_l. \tag{5}$$

thus, the Hamiltonian $\mathcal{H}_0$ does not lead the system to a stationary state if $a_{kl} \neq 0$. Owing to the "interaction" V, the parameters γ_k which determine the state of the physical system when $t \gg \tau_0$ will also satisfy a certain differential equation that differs from (5). The structure of this equation should be such that when $t \to +\infty$ it leads to equilibrium values of the parameters γ_k. To find this equation it is necessary to know the density matrix when $t \gg \tau_0$. According to the foregoing, when $t \gg \tau_0$ the density matrix $\rho(t)$ depends on the time only via the time dependence of the quantities γ_k, which define the density matrix ρ:

$$\rho(t) \equiv \rho(\gamma), \quad \gamma_k = \gamma_k(t).$$

According to (2), the equation for the parameter γ_k is

$$\gamma_k = L_k(\gamma), \tag{6}$$

where

$$L_k(\gamma) = i\,\mathrm{Sp}\,\rho(\gamma)[\mathcal{H}, \hat{\gamma}_k].$$

the density matrix $\rho(\gamma)$ satisfies in this case the equation

$$L_k(\gamma)\frac{\partial\rho(\gamma)}{\partial\gamma_k} - i[\rho(\gamma), \mathcal{H}] = 0. \tag{7}$$

Thus, our problem consists in simultaneously solving the system of Eqs. (6) and (7). For a unique solution of this system of equations we need certain boundary conditions, which lead to an irreversible character of the variation of the parameters γ_k. Let us proceed to establish these boundary conditions. To this end, we consider the operator

$$e^{-i\mathcal{H}_0\tau}\rho(\gamma)e^{i\mathcal{H}_0\tau}, \tag{8}$$

which represents, when V = 0, the density matrix of the system at the instant of time τ, provided its value at the initial instant of time was $\rho(\gamma)$.

According to our assumption, for sufficiently large τ the density matrix (8) will depend on τ only via the τ-dependence of the parameters $\gamma_k(\tau)$, which now obey Eq. (5):

$$d\gamma_k(\tau)/d\tau = L_k^{(0)}(\gamma(\tau)), \quad L_k^{(0)}(\gamma) = i a_{kl}\gamma_l \tag{9}$$

and the initial condition

$$\gamma_k(\tau)\,|_{\tau=0} = \gamma_k,$$

where γ_k are the values of the operators $\hat{\gamma}_k$ in the state $\rho(\gamma)$:

$$\gamma_k = \mathrm{Sp}\,\hat{\gamma}_k\rho(\gamma). \tag{10}$$

The solution of (9) is

$$\gamma(\tau) = S_\tau^{(0)}\gamma, \tag{11}$$

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[1] It is necessary to sum over repeated indices connected with the parameters γ.

or

$$\gamma_k(\tau) = (S_\tau^{(0)})_{kl}\gamma_l, \tag{12}$$

where

$$S_\tau^{(0)} = e^{ia\tau}$$

and a is a matrix with w elements equal to a_{kl}. Thus, when $\tau \to \infty$ we have

$$e^{-i\mathcal{H}_0\tau}\rho(\gamma)e^{i\mathcal{H}_0\tau} \to \rho^{(0)}(S_\tau^{(0)}\gamma),$$

where $\rho^{(0)}(\gamma)$ satisfies the equation

$$L_k^{(0)}(\gamma)\frac{\partial\rho^{(0)}(\gamma)}{\partial\gamma_k} - i[\rho^{(0)}(\gamma), \mathcal{H}_0] = 0. \tag{13}$$

Therefore

$$\lim_{\tau\to-\infty} e^{i\mathcal{H}_0\tau}\rho(S_\tau^{(0)}\gamma)e^{-i\mathcal{H}_0\tau} = \rho^{(0)}(\gamma). \tag{14}$$

We should choose as the density matrix $\rho^{(0)}(\gamma)$ that solution of (13) which is obtained as a result of mixing with the aid of the Hamiltonian $\mathcal{H}_0$. Such a density matrix corresponds to a Gibbs distribution with specified parameters γ_k:

$$\rho^{(0)}(\gamma) = \exp\Big(-\sum_k \hat{\gamma}_k X_k(\gamma)\Big), \tag{15}$$

Where the quantities $X_k(\gamma)$ are determined from the conditions

$$\gamma_l = \mathrm{Sp}\,\hat{\gamma}_l \exp\Big(-\sum_k \hat{\gamma}_k X_k(\gamma)\Big) = \mathrm{Sp}\,\hat{\gamma}_l\rho^{(0)}(\gamma) \tag{16}$$

(the number of parameters $\hat{\gamma}_k$ should obviously include also the Hamiltonian $\mathcal{H}_0$ itself, which satisfies relations of the type (4)).

It is easy to verify that owing to (4) the operator $\rho^{(0)}(\gamma)$, which is determined by (15), actually satisfies (13), and as a consequence of (4) we have

$$\begin{gathered} e^{-i\mathcal{H}_0\tau}\rho^{(0)}(\gamma)e^{i\mathcal{H}_0\tau} = \rho^{(0)}(S_\tau^{(0)}\gamma), \\ X(\gamma) = X(S_\tau^{(0)}\gamma)S_\tau^{(0)}. \end{gathered} \tag{17}$$

Relations (14) and (15) are the sought boundary conditions for the system of equations (6) and (7).

3. SOLUTION OF EQUATIONS

Our next task is to replace (6) and (7) by an integral equation which automatically satisfies the boundary condition (14) and makes it possible to develop a perturbation theory in terms of the "interaction" V.

To this end we represent (7) in the form

$$L_k^{(0)}(\gamma)\frac{\partial\rho(\gamma)}{\partial\gamma_k} - i[\rho(\gamma), \mathcal{H}_0] = f(\gamma), \tag{18}$$

where

$$f(\gamma) = i[\rho(\gamma), V] - \frac{\partial\rho(\gamma)}{\partial\gamma_k}(L_k(\gamma) - L_k^{(0)}(\gamma)).$$

Noting that

$$L^{(0)}(S_\tau^{(0)}\gamma) = \frac{\partial}{\partial\tau}S_\tau^{(0)}\gamma,$$

we represent (18) in the form

$$\frac{\partial}{\partial\tau}\rho(S_\tau^{(0)}\gamma) - i[\rho(S_\tau^{(0)}\gamma), \mathcal{H}_0] = f(S_\tau^{(0)}\gamma).$$

Introducing the operator

$$\tilde{\rho}(\tau) = e^{i\mathcal{H}_0\tau}\rho(S_\tau^{(0)}\gamma)e^{-i\mathcal{H}_0\tau}$$

we obtain

$$\frac{\partial\tilde{\rho}(\tau)}{\partial\tau} = e^{i\mathcal{H}_0\tau}f(S_\tau^{(0)}\gamma)e^{-i\mathcal{H}_0\tau}.$$

Since, according to the boundary condition (14), $\tilde{\rho}(-\infty) = \rho^{(0)}(\gamma)$, we get

$$\tilde{\rho}(\tau) = \rho^{(0)}(\gamma) + \int_{-\infty}^{\tau} d\tau' e^{i\mathcal{H}_0\tau'}f(S_{\tau'}^{(0)}\gamma)e^{-i\mathcal{H}_0\tau'},$$

or

$$\rho(S_\tau^{(0)}\gamma) = e^{-i\mathcal{H}_0\tau}\rho^{(0)}(\gamma)e^{i\mathcal{H}_0\tau} + \int_{-\infty}^{0} d\tau' e^{i\mathcal{H}_0\tau'}f(S_{\tau+\tau'}^{(0)}\gamma)e^{-i\mathcal{H}_0\tau'}.$$

Recognizing that $\exp(-i\mathcal{H}_0\tau)\rho^{(0)}(\gamma)\exp(i\mathcal{H}_0\tau) = \rho^{(0)}(S_\tau^{(0)}\gamma)$ (see (17)) and replacing γ by $S_{-\tau}^{(0)}\gamma$, we obtain

$$\rho(\gamma) = \rho^{(0)}(\gamma) + \int_{-\infty}^{0} d\tau e^{\eta\tau}e^{i\mathcal{H}_0\tau}f(S_\tau^{(0)}\gamma)e^{-i\mathcal{H}_0\tau}, \quad \eta \to +0. \tag{19}$$

This equation is the sought integral equation for the density matrix $\rho(\gamma)$.

Let us now verify the compatibility of relations (10) and (16), i.e., let us show that

$$\mathrm{Sp}\,\hat{\gamma}_k\rho(\gamma) = \mathrm{Sp}\,\hat{\gamma}_k\rho^{(0)}(\gamma). \tag{20}$$

Since, according to (4),

$$e^{-i\mathcal{H}_0\tau}\hat{\gamma}e^{i\mathcal{H}_0\tau} \equiv \hat{\gamma}(-\tau) = e^{-ia\tau}\hat{\gamma},$$

it follows that

$$\mathrm{Sp}\,\hat{\gamma}\rho(\gamma) - \mathrm{Sp}\,\hat{\gamma}\rho^{(0)}(\gamma) = \int_{-\infty}^{0} d\tau e^{\eta\tau}e^{-ia\tau}\,\mathrm{Sp}\,\hat{\gamma}f(S_\tau^{(0)}\gamma)$$

and consequently to prove (20) it is sufficient to verify that $\mathrm{Tr}\,\hat{\gamma}f(\gamma) \equiv 0$. We shall show that the latter relation does indeed hold.

Using the definition of $f(\gamma)$, we have

$$\mathrm{Sp}\,\hat{\gamma}_k f(\gamma) = i\,\mathrm{Sp}\,\hat{\gamma}_k[\rho(\gamma), V] - (L_i(\gamma) - L_i^{(0)}(\gamma))\,\mathrm{Sp}\,\gamma_k\frac{\partial\rho(\gamma)}{\partial\gamma_i}.$$

since $\mathrm{Tr}\,\hat{\gamma}_k\rho(\gamma) = \gamma_k$, we have

$$\mathrm{Sp}\,\hat{\gamma}_k f(\gamma) = i\,\mathrm{Sp}\,\rho(\gamma)[V, \hat{\gamma}_k] - L_k(\gamma) + L_k^{(0)}(\gamma) = i\,\mathrm{Sp}\,\rho(\gamma)[\mathcal{H}, \hat{\gamma}_k] - L_k(\gamma)$$

and consequently, $\mathrm{Tr}\,\hat{\gamma}_k f(\gamma) = 0$ by virtue of the definition (6) of the quantity $L(\gamma)$.

Thus, the equations

$$\begin{gathered} \rho(\gamma) = \rho^{(0)}(\gamma) + \int_{-\infty}^{0} d\tau e^{\eta\tau}e^{i\mathcal{H}_0\tau}f(S_\tau^{(0)}\gamma)e^{-i\mathcal{H}_0\tau}, \quad \eta \to +0, \\ L_k(\gamma) - L_k^{(0)}(\gamma) = i\,\mathrm{Sp}\,\rho^{(0)}(\gamma)[V, \hat{\gamma}_k] \\ + i\int_{-\infty}^{0} d\tau e^{\eta\tau}\,\mathrm{Sp}\,[V, \hat{\gamma}_k]e^{i\mathcal{H}_0\tau}f(S_\tau^{(0)}\gamma)e^{-i\mathcal{H}_0\tau} \end{gathered} \tag{21}$$

are compatible with the definition (18) of the operator $f(\gamma)$ and constitute the sought system of equations for the density matrix $\rho(\gamma)$ and for the quantity $L_k(\gamma)$, which determines the time variation of the parameters γ_k.

The simplest method of solving the obtained system is to use perturbation theory in powers of the interaction V. From the second equation of the system (21) we see that the first approximation of $L(\gamma)$ in terms of V is

$$L_k^{(1)}(\gamma) = i\,\mathrm{Sp}\,\rho^{(0)}(\gamma)[V, \hat{\gamma}_k] \tag{22}$$

and consequently, in the approximation linear in V, the operator $f(\gamma)$ is equal to

$$f^{(1)}(\gamma) = i[\rho^{(0)}(\gamma), V] - L_k^{(1)}(\gamma)\frac{\partial\rho^{(0)}(\gamma)}{\partial\gamma_k}.$$

This expression for $f^{(1)}(\gamma)$ makes it possible to find the density matrix $\rho(\gamma)$ in an approximation linear in V:

$$\rho^{(1)}(\gamma) = \int_{-\infty}^{0} d\tau e^{\eta\tau} e^{i\mathscr{H}_0\tau} f^{(1)}(S_\tau^{(0)}\gamma) e^{-i\mathscr{H}_0\tau}.$$

Knowing $\rho^{(1)}(\gamma)$ from the second equation of (21), we can easily find the value of $L(\gamma)$ in the second approximation in V:

$$L_k^{(2)}(\gamma) = i \operatorname{Sp} \rho^{(1)}(\gamma)[V, \hat{\gamma}_k] = L_k^{(2)\prime}(\gamma) + L_k^{(2)\prime\prime}(\gamma),$$

where

$$L_k^{(2)\prime}(\gamma) = -\int_{-\infty}^{0} d\tau e^{\eta\tau} \operatorname{Sp} e^{i\mathscr{H}_0\tau} [\rho^{(0)}(S_\tau^{(0)}\gamma), V] e^{-i\mathscr{H}_0\tau} [V, \hat{\gamma}_k]$$

$$L_k^{(2)\prime\prime}(\gamma) = -i \int_{-\infty}^{0} d\tau e^{\eta\tau} L_l^{(1)}(S_\tau^{(0)}\gamma) \operatorname{Sp} e^{i\mathscr{H}_0\tau} \frac{\partial\rho^{(0)}(S_\tau^{(0)}\gamma)}{\partial(S_\tau^{(0)}\gamma)_l} e^{-i\mathscr{H}_0\tau} [V, \hat{\gamma}_k].$$

Using the first relation of (17) we can transform $L_k^{(2)\prime}(\gamma)$ into

$$L_k^{(2)\prime}(\gamma) = -\int_{-\infty}^{0} d\tau e^{\eta\tau} \operatorname{Sp} \rho^{(0)}(\gamma)[V(\tau), [V, \hat{\gamma}_k]],$$

where

$$V(\tau) = e^{i\mathscr{H}_0\tau} V e^{-i\mathscr{H}_0\tau}.$$

We now simplify the expression for $L_k^{(2)\prime\prime}(\gamma)$. Again, using the first relation of (17), we get

$$L_i^{(1)}(S_\tau^{(0)}\gamma) e^{i\mathscr{H}_0\tau} \frac{\partial\rho^{(0)}(S_\tau^{(0)}\gamma)}{\partial(S_\tau^{(0)}\gamma)_i} e^{-i\mathscr{H}_0\tau} = L_i^{(1)}(S_\tau^{(0)}\gamma) \frac{\partial\gamma_j}{\partial(S_\tau^{(0)}\gamma)_i} \frac{\partial\rho^{(0)}(\gamma)}{\partial\gamma_j}.$$

Since $\gamma = S_{-\tau}^{(0)} S_\tau^{(0)}(\gamma)$, we have

$$\partial\gamma_j / \partial(S_\tau^{(0)}\gamma)_i = (S_{-\tau}^{(0)})_{ji}$$

and consequently, in accordance with (17) and (22):

$$L_i^{(1)}(S_\tau^{(0)}\gamma) \frac{\partial\gamma_j}{\partial(S_\tau^{(0)}\gamma)_i} = (S_{-\tau}^{(0)})_{ji} L_i^{(1)}(S_\tau^{(0)}\gamma)$$
$$= i \operatorname{Sp} \rho^{(0)}(\gamma) e^{i\mathscr{H}_0\tau} [V, (S_{-\tau}^{(0)})_{ji} \hat{\gamma}_i] e^{-i\mathscr{H}_0\tau}.$$

Noting that

$$(S_{-\tau}^{(0)})_{ji} \hat{\gamma}_i = e^{-i\mathscr{H}_0\tau} \hat{\gamma}_j e^{i\mathscr{H}_0\tau} = \hat{\gamma}_j(-\tau),$$

we obtain

$$L_i^{(1)}(S_\tau^{(0)}\gamma) \frac{\partial\gamma_j}{\partial(S_\tau^{(0)}\gamma)_i} = i \operatorname{Sp} \rho^{(0)}(\gamma)[V(\tau), \hat{\gamma}_j].$$

Thus,

$$L_k^{(2)\prime\prime}(\gamma) = -i \frac{\partial L_k^{(1)}(\gamma)}{\partial\gamma_j} \int_{-\infty}^{0} d\tau e^{\eta\tau} \operatorname{Sp} \rho^{(0)}(\gamma)[V(\tau), \hat{\gamma}_j]$$

and consequently

$$L_k^{(2)}(\gamma) = -\int_{-\infty}^{0} d\tau e^{\eta\tau} \operatorname{Sp} \rho^{(0)}(\gamma) \left[V(\tau), [V, \hat{\gamma}_k] + i\hat{\gamma}_j \frac{\partial L_k^{(1)}(\gamma)}{\partial\gamma_j} \right]. \quad (23)$$

Formulas (9), (22), and (23) determine the value of $L_k(\gamma)$ accurate to V^2:

$$L_k(\gamma) = L_k^{(0)}(\gamma) + L_k^{(1)}(\gamma) + L_k^{(2)}(\gamma).$$

4. INCREASE OF ENTROPY AND KINETIC COEFFICIENTS

We now assume that the operators $\hat{\gamma}_k$ are such that

$$[\mathscr{H}_0, \hat{\gamma}_k] = 0, \quad [\hat{\gamma}_k, \hat{\gamma}_l] = 0.$$

In this case

$$L_k^{(0)}(\gamma) = L_k^{(1)}(\gamma) = 0,$$

$$L_k^{(2)}(\gamma) = -\int_{-\infty}^{0} d\tau \operatorname{Sp} \rho^{(0)}(\gamma)[V(\tau), [V, \hat{\gamma}_k]].$$

Replacing the variable τ by $-\tau$ and noting that

$$[V(\tau), [V, \hat{\gamma}_k]] = [V, [(\tau), \hat{\gamma}_k]] + [\hat{\gamma}_k, [V, V(\tau)]]$$

and

$$[\hat{\gamma}_k, \rho^{(0)}(\gamma)] = 0,$$

we obtain

$$L_k^{(2)}(\gamma) = -\frac{1}{2} \int_{-\infty}^{\infty} d\tau \operatorname{Sp} \rho^{(0)}[V(\tau), [V, \hat{\gamma}_k]]. \quad (24)$$

Calculating the trace in the system of common eigenvectors of the operators $\mathscr{H}_0$ and $\hat{\gamma}_k$, we get

$$L_k^{(2)}(\gamma) = 2\pi \sum_{nm} \rho_n^{(0)}(\gamma) |V_{nm}|^2 (\gamma_{k,m} - \gamma_{k,n}) \delta(\varepsilon_n - \varepsilon_m), \quad (25)$$

where ϵ_n and $\gamma_{k,n}$ are the eigenvalues of the operators $\mathscr{H}_0$ and $\hat{\gamma}_k$.

We define the entropy of the system by the formula

$$\sigma = -\operatorname{Sp} \rho^{(0)} \ln \rho^{(0)}, \quad (26)$$

where

$$\rho^{(0)} = \exp(\Omega - \hat{\gamma}_i X_i), \quad \Omega = -\ln \operatorname{Sp} \exp(-\hat{\gamma}_i X_i).$$

it is easy to see that $\gamma_i = -\partial\Omega/\partial X_i$ and, consequently,

$$\frac{\partial\sigma}{\partial\gamma_j} = \frac{\partial}{\partial\gamma_j}(\gamma_i X_i - \Omega) = X_j. \quad (27)$$

therefore $\dot{\sigma} = X_i L_i^{(2)}(\gamma)$. Introducing the symbol $Q_n = X_i \gamma_{i,n}$, we get

$$\sigma = \pi \sum_{nm} |V_{nm}|^2 \delta(\varepsilon_n - \varepsilon_m)(Q_m - Q_n)(1 - e^{Q_n - Q_m}) e^{\Omega - Q_n}.$$

since $(Q_n - Q_m)(1 - \exp[Q_n - Q_m]) \leq 0$ for all $Q_n - Q_m$, we get $\dot{\sigma} \geq 0$.

If we regard the quantities γ_i as generalized coordinates of the system, then, in accordance with (27), the quantities X_i are generalized forces. The equilibrium values of the generalized forces are determined by the equation

$$X_i^{(0)} \left[\hat{\gamma}_i, \int_{-\infty}^{\infty} V(\tau) d\tau \right] = 0,$$

or

$$\sum_i X_i^{(0)} V_{nm}(\gamma_{i,n} - \gamma_{i,m}) \delta(\varepsilon_n - \varepsilon_m) = 0.$$

from this and from (24) it follows that

$$L_i^{(2)}(\gamma) X_i^{(0)} = 0 \quad (28)$$

for arbitrary γ. Equations (28) are the integrals of motion of the system of equations $\hat{\gamma}_i = L_i^{(2)}(\gamma)$.

For states close to equilibrium, the quantities $L_i^{(2)}(\gamma)$ can be represented in the form

$$L_i^{(2)}(\gamma) = g_{ij} \delta X_j,$$

where

$$g_{ij} = -\frac{1}{2} \int_{-\infty}^{\infty} d\tau \operatorname{Sp} \rho_0 [V(\tau), \hat{\gamma}_j][V, \hat{\gamma}_i], \quad \delta X_j = X_j - X_j^{(0)} \quad (29)$$

and ρ_0 is the equilibrium density matrix

$$\rho_0 = \exp(\Omega - \hat{\gamma}_j X_j^{(0)}).$$

Therefore the equations for the generalized coordinates of the system take the form

$$\dot{\gamma}_i = g_{ij}\delta X_j. \tag{30}$$

Thus, the quantities g_{ij} defined by formula (29) are the kinetic coefficients.

Using the invariance of the equations of motion of quantum mechanics against time reversal we can easily prove the symmetry of the kinetic coefficients (29).

The rate of entropy production $\dot{\sigma}$ can obviously be determined by the formula

$$\dot{\sigma} = g_{ij}X_iX_j. \tag{31}$$

5. KINETIC EQUATIONS IN THE LOW-DENSITY APPROXIMATION

We have seen in Sec. 3 that it is easy to obtain a solution of the system (21) under the assumption that the interaction is weak. In particular, formulas (9), (22), and (23) make it possible to obtain quite simply the kinetic equations for the particles or elementary excitations if a weak interaction exists between them.

Now, however, we shall consider the derivation of the kinetic equation for another limiting case, when the interaction is not assumed weak but the particle density is sufficiently small. In this case we can no longer use the ready-made formulas (22) and (23), but must find another method of solving the system (21).

The Hamiltonian $\mathscr{H}_0$ can be represented in the form

$$\mathscr{H}_0 = \sum_{\mathbf{p}} \varepsilon_{\mathbf{p}} a_{\mathbf{p}}^+ a_{\mathbf{p}},$$

where ϵ_p is the energy of a particle with momentum p. We shall henceforth assume, for concreteness, that the particles obey Bose statistics, i.e.,

$$[a_{\mathbf{p}}, a_{\mathbf{p}'}^+] = \delta_{\mathbf{p}\mathbf{p}'}.$$

The interaction between the particles will be written in the form

$$\hat{V} = \frac{1}{4}\sum_{1234} V(12;\ 34)\, a_1^+a_2^+a_3a_4,$$

where we put, to abbreviate the notation, $1 \equiv p_1$, $2 \equiv p_2$, ... The quantity V(12; 34) characterizes, obviously, the interaction between the particles, and without loss of generality we can put

$$V(12;34) = V(21;34) = V^*(34;12).$$

When $t \gg \tau_0 \equiv r_0/v$, where r_0 is the radius of the initial correlations and v is the average particle velocity, the state of the system can be described in the spatially homogeneous case with the aid of the single-particle distribution function $f_p = \mathrm{Tr}\, \rho a_p^+ a_p$.

The role of the operators $\hat{\gamma}_i$ in this problem is played by the operators $a_p^+a_p$, which obviously satisfy the relations (4), and the density matrix $\rho^{(0)}$ equals, in accordance with (15),

$$\rho^{(0)} = \exp\Big(\Omega - \sum_{\varkappa} X_\varkappa(f)\, a_\varkappa^+ a_\varkappa\Big),$$

where Ω and $X_\kappa(f)$ are defined by the equations

$$\mathrm{Sp}\, \rho^{(0)} = 1, \qquad \mathrm{Sp}\, \rho^{(0)} a_\varkappa^+ a_\varkappa = f_\varkappa.$$

It is easy to see that $L^{(0)} = 0$ and $L^{(1)} = 0$.

Obviously, to find mean values of the type $\mathrm{Tr}\, \rho^{(0)} a_1^+ a_2^+ \ldots$ we can use the ordinary Wick rules. For example,

$$\mathrm{Sp}\, \rho^{(0)} a_1^+a_2^+a_3a_4 = f_1f_2\delta_{14}\delta_{23} + f_1f_2\delta_{13}\delta_{24},$$

$$\mathrm{Sp}\, \rho^{(0)} a_1^+a_2^+a_3^+a_4a_5a_6 = f_1f_2f_3(\delta_{14}\delta_{25}\delta_{36} + \delta_{14}\delta_{26}\delta_{35} + \delta_{15}\delta_{24}\delta_{36} + \delta_{15}\delta_{26}\delta_{34} + \delta_{16}\delta_{24}\delta_{35} + \delta_{16}\delta_{25}\delta_{34}).$$

we introduce the notation $f_{34,12} = \mathrm{Tr}\, \rho(\gamma) a_1^+ a_2^+ a_3 a_4$. Then, noting that

$$[\hat{V}, a_\varkappa^+ a_\varkappa] = -\frac{1}{2}\sum_{1234} V(12;\ 34)\,(a_1^+a_2^+a_3a_\varkappa\delta_{\varkappa 4} - a_\varkappa^+a_1^+a_3a_4\delta_{\varkappa 2}),$$

we get

$$L_k = \frac{i}{2}\sum_{1234} V(12;\ 34)\,(f_{3k,\,12}\delta_{4k} - f_{34,\,k1}\delta_{2k}).$$

Regarding $f_{12,34}$ and $V(12;\ 34) \equiv V_{12,34}$ as matrix elements of the operators f and V between the two-particle states (3, 4) and (1, 2), we can rewrite the last formula in the form

$$L_k = i\sum_{1} [f, V]_{1k;\,1k}.$$

We took account here of the fact that the states (1, 2) and (2, 1) are identical.

According to formulas (21)

$$\begin{aligned} f_{34;\,12} = f_{34;\,12}^{(0)} + i\int_{-\infty}^{0} d\tau e^{\eta\tau} \Big\{ &\mathrm{Sp}\, \rho(\gamma)\, [\hat{V}, e^{-i\mathscr{H}_0\tau} a_1^+a_2^+a_3a_4 e^{i\mathscr{H}_0\tau}] \\ &+ i\sum_{\mathbf{p}} L_{\mathbf{p}} \frac{\partial}{\partial f_{\mathbf{p}}} \mathrm{Sp}\, \rho(\gamma)\, e^{-i\mathscr{H}_0\tau} a_1^+a_2^+a_3a_4 e^{i\mathscr{H}_0\tau} \Big\}, \end{aligned} \tag{32}$$

where $f_{34;12}^{(0)} = f_1f_2(\delta_{13}\delta_{24} + \delta_{14}\delta_{23})$. Since $f_p \ll 1$ and $f_{34;12} \sim f_p^2$ at low density, we have

$$L_{\mathbf{p}} \frac{\partial}{\partial f_{\mathbf{p}}} \mathrm{Sp}\, \rho(\gamma)\, a_1^+a_2^+a_3a_4 \sim f^3$$

and consequently, in the region $f_p \ll 1$, we can neglect the second term under the integral sign in formula (32). Noting that

$$e^{-i\mathscr{H}_{\gamma}\tau} a_1^+ e^{i\mathscr{H}_{\iota}\tau} = a_1^+ e^{-i\varepsilon_1\tau},$$

we have

$$f_{34;\,12} = f_{34;\,12}^{(0)} + i\int_{-\infty} d\tau e^{\eta\tau + i\tau(\varepsilon_3+\varepsilon_4-\varepsilon_1-\varepsilon_2)}\, \mathrm{Sp}\, \rho(\gamma)[\hat{V}, a_1^+a_2^+a_3a_4] \tag{33}$$

Let us find now $\mathrm{Tr}\, \rho(\gamma)\, [V,\ a_1^+a_2^+a_3a_4]$ in the low-density approximation. To this end we note that

$$\begin{aligned} [a_{1'}^+a_{2'}^+a_{3'}a_{4'}, a_1^+a_2^+a_3a_4] = {} & a_{1'}^+a_{2'}^+a_3a_4(\delta_{14'}\delta_{23'} + \delta_{13'}\delta_{24'}) \\ & - a_1^+a_2^+a_{3'}a_{4'}(\delta_{1'4}\delta_{2'3} + \delta_{1'3}\delta_{2'4}) + a_{1'}^+a_{2'}^+(a_1^+a_{3'}\delta_{24'} \\ & + a_1^+a_{4'}\delta_{23'} + a_2^+a_{3'}\delta_{14'} + a_2^+a_{4'}\delta_{13'})\, a_3a_4 \\ & - a_1^+a_2^+(a_{1'}^+a_3\delta_{2'4} + a_{1'}^+a_4\delta_{2'3} + a_{2'}^+a_3\delta_{1'4} \\ & + a_{2'}^+a_4\delta_{1'3})\, a_{3'}a_{4'}. \end{aligned}$$

Since the mean value in the state $\rho(\gamma)$ of an N-ordered system of six operators a^+ and a, namely $\mathrm{Tr}\, \rho(\gamma) a_1^+a_2^+a_3^+a_4a_5a_6$ is proportional, at most, to f_p^3 we get in the low-density approximation,

$$\mathrm{Sp}\, \rho(\gamma)[\hat{V}, a_1^+a_2^+a_3a_4] = \frac{1}{2}\sum_{1'2'} V(1'2';\ 12)\, f_{34;\,1'2'} - \frac{1}{2}\sum_{3'4'} V(34;\ 3'4')\, f_{3'4';\,12},$$

or in other words

$$\mathrm{Sp}\, \rho(\gamma)\, [\hat{V}, a_1^+a_2^+a_3a_4] = [f, V]_{34;\,12}.$$

Taking this relation into account, we can rewrite (33) in the form

$$(\varepsilon_1 + \varepsilon_2 - \varepsilon_3 - \varepsilon_4 + i\eta)\, f_{34;\,12} + [f, V]_{34;12} = i\eta f_{34;\,12}^{(0)},$$

or in the operator form

$$[f, \mathscr{H}] + i\eta f = i\eta f^{(0)},$$

where $\mathscr{H} = \mathscr{H}_0 + V$ is the Hamiltonian of a system of two particles with allowance for their paired interaction.

It is easy to verify that the solution of the last equation is

$$f = \frac{\eta}{2\pi}\int_{-\infty}^{\infty} dE R_+(E) f^{(0)} R_-(E), \qquad (34)$$

where

$$R_\pm(E) = (E - \mathscr{H} \pm {}^1\!/_2 i\eta)^{-1}.$$

Noting that

$$[f, V]_{1k;\,1k} = [f, \mathscr{H}]_{1k;\,1k} \text{ and } [f^{(0)}, \mathscr{H}_0] = 0,$$

we have

$$[f, V]_{1k;\,1k} = \frac{\eta}{2\pi}\int_{-\infty}^{\infty} dE\, \{R_+(E)[f^{(0)}, V]R_-(E)\}_{1k;\,1k}.$$

Thus, according to (33),

$$L_k = \frac{i\eta}{2\pi}\int_{-\infty}^{\infty} dE \sum_1 \{R_+(E)[f^{(0)}, V]R_-(E)\}_{1k;\,1k}.$$

We continue the transformation, now already formal, of the quantity L_k by following the paper of Luttinger and Kohn[3]. To this end we introduce the scattering operators $T_\pm(E)$:

$$T_\pm(E) = V + T_\pm(E) R_\pm{}^0(E) V,$$

where

$$R_\pm{}^0(E) = (E - \mathscr{H}_0 \pm {}^1\!/_2 i\eta)^{-1}.$$

Noting that $R_\pm = R^0_\pm + R^0_\pm T_\pm R^0_\pm$, we can easily transform the integrand of (33)

$$\begin{aligned} R_+(E)[f^{(0)}, V]R_-(E) = R_+{}^0(E)\{f^{(0)}T_-(E) - T_+(E)f^{(0)} \\ + T_+(E)f^{(0)}(R_+{}^0(E) - R_-{}^0(E))T_-(E)\}R_-{}^0(E). \end{aligned} \qquad (35)$$

Recognizing that $T_+(E)$ has no singularities in the upper half plane of E, and $T_-(E)$ has no singularities in the lower half plane of E, we get

$$\int_{-\infty}^{\infty} dE R_+{}^0(E) R_+{}^0(E) T_+(E) = \int_{-\infty}^{\infty} dE R_-{}^0(E) R_-{}^0(E) T_-(E) = 0. \qquad (36)$$

With the aid of (35) and (36) we can represent L_k in the form

$$\begin{aligned} L_k = -\frac{i\eta}{2\pi}\int_{-\infty}^{\infty} dE \sum_1 i\eta R^0_{+\varkappa\varkappa} R^0_{-\varkappa\varkappa}\{(T_+ f^{(0)} R_+{}^0 R_-{}^0 T_-)_{\varkappa\varkappa} \\ + f^{(0)}_{\varkappa\varkappa} T_{+\varkappa\varkappa} R^0_{+\varkappa\varkappa} + f^{(0)}_{\varkappa\varkappa} T_{-\varkappa\varkappa} R^0_{-\varkappa\varkappa}\}, \end{aligned}$$

where κ are the quantum numbers of the two-particle states, $\kappa \equiv (1, k)$.

Let us transform the last two terms of this formula. According to the definition of $R_\pm(E)$

$$\frac{\eta}{2\pi}\int_{-\infty}^{\infty} R_+(E) R_-(E) dE = 1.$$

From this we get with the aid of the formula $R_\pm = R^0_\pm + R^0_\pm T_\pm R^0_\pm$

$$\int_{-\infty}^{\infty} dE R_+{}^0 \{R_-{}^0 T_- + T_+ R_+{}^0 + T_+ R_+{}^0 R_-{}^0 T_-\} R_-{}^0 = 0.$$

The last equation allows us to reduce L_k to the form

$$L_k = \frac{\eta^2}{2\pi}\int_{-\infty}^{\infty} dE \sum_1 R^0_{+\varkappa\varkappa} R^0_{-\varkappa\varkappa}\{T_+ f^{(0)} R_+{}^0 R_-{}^0 T_- - f^{(0)} T_+ R_+{}^0 R_-{}^0 T_-\}_{\varkappa\varkappa}.$$

Noting that

$$\eta R^0_{+\varkappa\varkappa} R^0_{-\varkappa\varkappa} \longrightarrow 2\pi\delta(E - \mathscr{E}_\varkappa),$$

where $\mathscr{E}_k$ are the energy of the two-particle states in the absence of interaction, we represent L_k in the form

$$L_k = 2\pi \sum_{1\varkappa'} \delta(\mathscr{E}_\varkappa - \mathscr{E}_{\varkappa'}) \,|T_{+\varkappa\varkappa'}(\mathscr{E}_\varkappa)|^2 (f^{(0)}_{\varkappa'\varkappa'} - f^{(0)}_{\varkappa\varkappa}), \qquad \varkappa \equiv (1, k)$$

Recalling the definition (32) of the quantity $f^{(0)}_{12;34}$ we obtain finally

$$L_k = \pi \sum_{134} \delta(\varepsilon_1 + \varepsilon_k - \varepsilon_3 - \varepsilon_4)\,|T_{+1k;\,34}(\varepsilon_1 + \varepsilon_k)|^2 (f_3 f_4 - f_1 f_k). \qquad (37)$$

The expression for L_k was obtained accurate to terms of order f_p^2. Therefore, the identity of the particles is not taken into account in this approximation. If we expand not in powers of the density but in powers of the interaction, we get an expression similar to (37) for the collision integral. In this expression, however, the quantity $f_3 f_4 - f_1 f_k$ is replaced by $f_3 f_4(1 + f_1)(1 + f_k) - f_1 f_k(1 + f_3)(1 + f_4)$ (allowance for the identity of the particles), but the scattering amplitude T_+ is taken only in the first Born approximation.

In conclusion, the authors are deeply grateful to V. Bar'yakhtar for a constant discussion of the results.

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Translated by J. G. Adashko
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