DERIVATION OF GENERALIZED KINETIC EQUATIONS BY MEANS OF THE NONEQUILIBRIUM STATISTICAL OPERATOR

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Abstract

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DERIVATION OF GENERALIZED KINETIC EQUATIONS BY MEANS OF THE NONEQUILIBRIUM STATISTICAL OPERATOR

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Recently, in the work of S. V. Peletminskii and A. A. Yatsenko ([1]), a quantum theory of kinetic and relaxation processes was developed, based on a generalization of N. N. Bogolyubov' s ideas on the existence of different relaxation-time scales ([2], [3]) to quantum systems of a definite, but fairly general, type. On the other hand, there exists a general theory of irreversible processes, developed most consistently in the works of D. N. Zubarev with the use of local integrals of motion ([4]) and in the works of MacLennan, in which nonconservative forces are introduced to describe the influence of a thermostat ([5]). These works lead to identical results, although they differ methodologically. The general theory of irreversible processes has been successfully applied to the solution of a number of problems ([4], [6]-[11]). In the present work we shall obtain generalized kinetic equations for quantum systems by the methods of the general theory of irreversible processes ([4], [5]) and show that it leads to the same results as ([1]).

Consider a quantum system with Hamiltonian $H = H_0 + V$, where V is an interaction assumed to be small. Suppose that there are two time scales τ_1 and τ_2, $\tau_1 \ll \tau_2$, and that during the time τ_1 a reduction occurs in the number of parameters necessary to describe the state of the system, while at times $\tau_1 < t < \tau_2$ the macroscopic state is determined by specifying the mean values of some set of dynamical quantities P_i. We shall seek kinetic equations describing the time evolution of the mean values of these dynamical quantities:

$$d\langle P_k\rangle/dt = L_k(\dots\langle P_i\rangle\dots), \tag{1}$$

where L_k are the functions to be found.

For this purpose, following ([4]), we write the nonequilibrium statistical operator which, in the limit $\varepsilon \to 0$, satisfies the Liouville equation,

$$\rho = Q^{-1} \exp \left\{ - \sum_k F_k(t) P_k + \right.$$

$$\left. + \int_{-\infty}^{0} dt_1 e^{\varepsilon t_1} \sum_k \left[F_k(t+t_1) \dot{P}_k(t_1) + \frac{dF_k(t+t_1)}{dt} P_k(t_1) \right] \right\}, \tag{2}$$

where $F_k(t)$ are certain parameters; Q is the statistical sum; the time argument of the operators denotes the Heisenberg representation. The statistical operator (2) satisfies the Liouville equation for any dependence of the parameters F_k on t. Therefore we define this dependence by means of the additional conditions

$$\langle P_k \rangle = \mathrm{sp}\, P_k \rho = \langle P_k \rangle_0 = \mathrm{sp}\, P_k \rho_0, \tag{3}$$

where ρ_0 is the quasiequilibrium statistical operator

$$\rho_0 = Q^{-1} \exp \left\{ - \sum_k F_k(t) P_k \right\}, \qquad Q_0 = \mathrm{sp} \exp \left\{ - \sum_k F_k(t) P_k \right\}. \tag{4}$$

Next we can write

$$\frac{d\langle P_k \rangle}{dt} = \langle \dot{P}_k \rangle = (i\hbar)^{-1} \langle [P_k, H] \rangle, \tag{5}$$

where $\langle ... \rangle$ is averaging over the ensemble (2). It follows from (5) that $d\langle P_k \rangle / dt$ depends on the ensemble parameters $F_k(t)$, which in turn, by virtue of (3), are determined through $\langle P_k \rangle$. Thus, relations (2), (3), and (5) already determine, although in implicit form, the desired kinetic equations (1). We shall seek an expansion of the right-hand side of (1) in powers of the interaction

$$L_k(... \langle P_i \rangle ...) = L_k^{(0)} + L_k^{(1)} + L_k^{(2)} + ... \tag{6}$$

For this purpose we write

$$\dot{P}_k = (i\hbar)^{-1} [P_k, H] = -(i\hbar)^{-1} a_{kl} P_l + (i\hbar)^{-1} [P_k, V], \tag{7}$$

where, as in (1), we assume that $[H_0, P_k] = a_{kl} P_l$; a_{kl} are certain coefficients (summation over repeated indices is implied). This condition is satisfied in most of the problems considered. With the aid of conditions (3) one can eliminate the derivatives $dF_k(t+t_1)/dt$ in (2). We have

$$\frac{dF_k(t)}{dt} = \frac{\partial F_k}{\partial \langle P_l \rangle} \langle \dot{P}_l \rangle = - \frac{1}{i\hbar} \frac{\partial F_k}{\partial \langle P_l \rangle} a_{lm} \langle P_m \rangle + \frac{1}{i\hbar} \frac{\partial F_k}{\partial \langle P_l \rangle} \langle [P_l, V] \rangle. \tag{8}$$

Next note that

$$F_k a_{kl}\langle P_l\rangle = \langle [H_0, F_{kP} k]\rangle_0 \equiv 0. \tag{9}$$

Hence, differentiating with respect to F_k, we obtain

$$a_{km}\langle P_m\rangle + F_m a_{ml}\frac{\partial\langle P_l\rangle}{\partial F_k} = 0. \tag{10}$$

Taking into account that

$$\frac{\partial\langle P_l\rangle}{\partial F_k} = -\frac{\partial^2 \ln Q_0}{\partial F_k \partial F_l} = \frac{\partial\langle P_k\rangle}{\partial F_l}, \tag{11}$$

we multiply (10) by $\partial F_i/\partial\langle P_k\rangle$ and sum over k. As a result we obtain

$$\frac{\partial F_i}{\partial\langle P_k\rangle} a_{kl}\langle P_l\rangle + F_m a_{mi} = 0. \tag{12}$$

With the aid of (12) we bring (8) to the form

$$\frac{dF_k(t)}{dt} = \frac{1}{i\hbar} a_{lk} F_l(t) + \frac{1}{i\hbar}\frac{\partial F_k}{\partial\langle P_l\rangle}\langle [P_l, V]\rangle. \tag{13}$$

Substituting (7) and (13) into (2), we obtain the nonequilibrium statistical operator in the form

$$\rho = Q^{-1}\exp\left\{-\sum_k F_k(t)P_k + \int_{-\infty}^{0} dt_1 e^{\varepsilon t_1}(i\hbar)^{-1}\left([V(t_1), P_k(t_1)]F_k(t+t_1) + \frac{\partial F_k(t+t_1)}{\partial\langle P_l\rangle}\langle [P_l, V]\rangle_{t+t_1} P_k(t_1)\right)\right\} \tag{14}$$

where the index $t+t_1$ on the averaging sign means that the averaging is performed with the statistical operator (2) taken at the time $t+t_1$. It is seen from (14) that the integral term in the exponent is of first order of smallness in the interaction.

Substituting (7) into (5) and expanding the statistical operator (14) in the interaction, we obtain the expansion (6), in which

$$L_k^{(0)} = -(i\hbar)^{-1} a_{kl}\langle P_l\rangle, \tag{15}$$

$$L_k^{(1)} = -(i\hbar)^{-1}\langle [V, P_k]\rangle_0, \tag{16}$$

$$L_k^{(2)} = L_k^{\prime(2)} + L_k^{\prime\prime(2)}, \tag{17}$$

$$L_k^{\prime(2)} = -\frac{1}{\hbar^2}\int_{-\infty}^{0} dt_1 e^{\varepsilon t_1} \int_0^1 d\lambda \, \left\langle [V, P_k] e^{-\lambda A} \left\{ [V(t_1), P_l(t_1)] - \right.\right.$$
$$\left.\left. -\langle [V(t_1), P_l(t_1)] \rangle_0 \right\} e^{\lambda A} \right\rangle F_l(t + t_1), \tag{18}$$

$$L_k^{\prime\prime(2)} = -\frac{1}{\hbar^2}\int_{-\infty}^{0} dt_1 e^{\varepsilon t_1} \int_0^1 d\lambda \, \langle [V, P_k] \times$$
$$\times e^{-\lambda A} \frac{\partial F_l(t+t_1)}{\partial \langle P_m \rangle} \langle [V(t_1), P_m(t_1)] \rangle_0 (P_l(t_1) - \langle P_l(t_1) \rangle) e^{\lambda A} \rangle_0, \tag{19}$$

$$A = \sum_k F_k(t) P_k,$$

where, in the Heisenberg representation, one may omit the interaction in the evolution operators and, when calculating $F_l(t + t_1)$ and the analogous term in (19) that depends on two times, the evolution may be regarded as free. Therefore in (18) one may put

$$\sum_l F_l(t + t_1) P_l(t_1) = \sum_l F_l(t) P_l, \tag{20}$$

since, when the interaction is neglected, this sum is an integral of motion. Noting also that

$$\sum_l e^{-\lambda A} [V(t_1), P_{lF} l(t)] e^{\lambda A} = \frac{d}{d\lambda} e^{-\lambda A} V(t_1) e^{\lambda A}, \tag{21}$$

we obtain

$$L^{\prime(2)} = -\frac{1}{\hbar^2}\int_{-\infty}^{0} dt_1 e^{\varepsilon t_1} \langle [V(t_1), [V, P_k]] \rangle_0. \tag{22}$$

Having calculated, with the interaction neglected, the time derivative of the matrix

$$\frac{\partial \langle P_k \rangle}{\partial F_l} = \int_0^1 d\lambda \, \langle P_k e^{-\lambda A} (P_l - \langle P_l \rangle_0) e^{\lambda A} \rangle_0, \tag{23}$$

which, by virtue of (13) and (9), is equal to

$$\frac{d}{dt}\frac{\partial\langle P_k\rangle}{\partial F_l} = -\frac{1}{i\hbar}\left(a_{km}\frac{\partial\langle P_m\rangle}{\partial F_l} + a_{lm}\frac{\partial\langle P_k\rangle}{\partial F_m}\right), \tag{24}$$

one can show that

$$\frac{d}{dt_1}\frac{\partial F_l(t+t_1)}{\partial\langle P_m\rangle}\langle[V(t_1), P_m(t_1)]\rangle_0(P_l(t_1) - \langle P_l(t_1)\rangle) = 0. \tag{25}$$

Therefore in (19) we may omit t_1 everywhere except in $V(t_1)$. Noting also that

$$\int_0^1 d\lambda\,\langle[V, P_k]e^{-\lambda A}(P_l - \langle P_l\rangle)e^{\lambda A}\rangle_0 = i\hbar\,\frac{\partial L_k^{(1)}}{\partial F_l}, \tag{26}$$

we can write (19) in the form

$$L_k^{\prime\prime(2)} = -\frac{i}{\hbar}\int_{-\infty}^0 dt_1 e^{\varepsilon t_1}\left\langle\left[V(t_1), P_m\frac{\partial L_k^{(1)}}{\partial\langle P_m\rangle}\right]\right\rangle_0, \tag{27}$$

or, combining (22) and (27), we obtain

$$L_k^{(2)} = -\frac{1}{\hbar^2}\int_{-\infty}^0 dt_1 e^{\varepsilon t_1}\left\langle\left[V(t_1), [V, P_k] + i\hbar P_m\frac{\partial L^{(1)}}{\partial\langle P_m\rangle}\right]\right\rangle_0. \tag{28}$$

Relations (15), (16), and (28) give the desired expansion of the right-hand side of the generalized kinetic equation (1) in powers of the interaction. They coincide entirely with the results of [1]. This proves the equivalence of the Peletminskii-Yatsenko method to the Zubarev-McLennan method, accurate up to terms of second order in the interaction.

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Note: Figure translations are in progress. See original paper for figures.