ON THE IRREVERSIBLE EVOLUTION OF A DYNAMICAL SYSTEM INTERACTING WITH A STATISTICAL ENSEMBLE

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Abstract

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ON THE IRREVERSIBLE EVOLUTION OF A DYNAMICAL SYSTEM INTERACTING WITH A STATISTICAL ENSEMBLE

(Presented by Academician N. N. Bogolyubov, May 24, 1966)

1. In paper ([1]), by the method of N. N. Bogolyubov ([2], [3]), an approximate equation was obtained describing the evolution of the density matrix of the probability distribution ρ_S of a certain small system S interacting with a thermostat Σ, and the exact solution of this approximate equation was found for a simple model with a quadratic Hamiltonian. Here by a small system S one should understand a dynamical system with a fixed finite number of degrees of freedom, whereas the thermostat Σ is a system the number of whose degrees of freedom tends to infinity. In the present paper we shall not use the aforementioned approximate equation, and shall find the probability density of the distribution of the small system S by exact methods for the same model. This will make it possible to judge the degree of accuracy of the previously obtained approximate equation for the density matrix.

2. Consider a model whose Hamiltonian has the form

$$H(t) = H_S(t) + H_\Sigma(t) + H_{\text{int}}(t) = \omega b^+(t)b(t) + \sum_{(k)} \omega_k a_k^+(t)a_k(t) + \\ + \frac{\varepsilon}{\sqrt{V}} \sum_{(k)} A_k\{b(t)a_k^+(t) + a_k(t)b^+(t)\}, \tag{1}$$

where H_S, H_Σ, and H_{int} are, respectively, the Hamiltonians of the systems S and Σ and the interaction Hamiltonian (the interaction will be regarded as small, ε being an infinitely small quantity); the operators $b(t)$, $b^+(t)$, $a(t)$, $a^+(t)$ are fermion creation and annihilation operators; V is the volume of the system; K is a quasidiscrete spectrum, which in the limit $V \to \infty$ becomes continuous.

We assume that at the initial instant of time ($t = 0$) the interaction is absent and the systems ρ and Σ are independent. Then the initial conditions can be represented in the form

$$U(0) = \rho_S(0)\rho_\Sigma(0), \tag{2}$$

where U is the probability density of the distribution of the whole system $(S+\Sigma)$, ρ_Σ is the probability density of the distribution of the thermostat Σ, and

$$\rho_\Sigma(0) = ke^{-H_\Sigma/\theta}, \tag{3}$$

$$\operatorname*{Sp}_{\Sigma}\{\rho_\Sigma(0)\} = 1. \tag{4}$$

The density matrix $\rho_S(t)$ for this model can be represented in the form

$$\rho_S(t) = bb^+\rho^s_{00}(t) + b^+b\rho^s_{11}(t) + b\rho^s_{10}(t) + b^+\rho^s_{01}(t), \tag{5}$$

where

$$b = \begin{vmatrix} 0 & 1 \\ 0 & 0 \end{vmatrix}, \quad b^+ = \begin{vmatrix} 0 & 0 \\ 1 & 0 \end{vmatrix},$$

$$\rho_S(t) = \operatorname*{Sp}_{(\Sigma)}\{U(t)\}. \tag{6}$$

Then, using the property of operators:

$$\mathrm{Sp}\{A(0)\cdot U(t)\} = \mathrm{Sp}\{A(t)\cdot U(0)\}, \tag{7}$$

we obtain

$$\begin{aligned}
\rho^s_{01}(t) &= \mathrm{Sp}_{(S\Sigma)}\{b^+(t)\cdot U(0)\} = \langle b^+(t)\rangle, \\
\rho^s_{10}(t) &= \mathrm{Sp}_{(S\Sigma)}\{b(t)\cdot U(0)\} = \langle b(t)\rangle, \\
\rho^s_{11}(t) &= \mathrm{Sp}_{(S\Sigma)}\{b^+(t)b(t)\cdot U(0)\} = \langle b^+(t)b(t)\rangle, \\
\rho^s_{00}(t) &= \mathrm{Sp}_{(S\Sigma)}\{b(t)b^+(t)\cdot U(0)\} = \langle b(t)b^+(t)\rangle,
\end{aligned} \tag{8}$$

where the symbol $\langle\ \rangle$ denotes the quantum-mechanical average.
The operators $b(t)$ and $b^+(t)$ are found from the equation of motion

$$i\,dA(t)/dt = [A(t)\cdot H(t)]. \tag{9}$$

Taking (8) into account, we obtain:

$$i\,\frac{d\rho_{10}^s(t)}{dt} = \omega\rho_{10}^s(t) + \frac{\varepsilon^2}{i}\int_0^t K(t-\tau)\rho_{10}^s(\tau)\,d\tau; \tag{10}$$

here

$$K(t-\tau) = K(z) = \frac{1}{V}\sum_{(k)}|A_k|^2 e^{-i\omega_k z} = \frac{1}{(2\pi)^3}\int |A_k|^2 e^{-i\omega_k z}\,d\mathbf{k}. \tag{11}$$

Performing the Laplace transform of equation (10), we obtain

$$\rho_{10}^s(p) = \frac{\rho_{10}^s(0)}{p + i\omega + \varepsilon^2 K(p)} = \frac{\rho_{10}^s(0)}{p + i\omega + \frac{1}{2}\varepsilon^2 I(E) - i\varepsilon^2 J(E)}, \tag{12}$$

where $J(E) > 0,\ I(E) > 0,\ E = \mathrm{Re}(ip)$.
The inverse Laplace transform gives

$$\rho_{10}^s(t) = \rho_{10}^s(0)e^{-i\{\omega-\varepsilon^2 J(\omega)\}t}e^{-\frac{1}{2}\varepsilon^2 I(\omega)t}. \tag{13}$$

Thus, as $t \to \infty$ $(t \gg 1/\varepsilon^2)$, $\rho_{10}^s(t)$ decays as $e^{-\frac{1}{2}\varepsilon^2 I(\omega)t}$.

3. To find the diagonal elements of the density matrix, we use the equations for the retarded and advanced Green functions

$$G^{+}_{\substack{\mathrm{ret}\\ \mathrm{adv}}} = \pm i[\pm\theta(t-t')]\langle[b(t)b^+(t')]_+\rangle = \langle\langle b(t), b^+(t)\rangle\rangle_{\substack{\mathrm{ret}\\ \mathrm{adv}}}, \tag{14}$$

$$\begin{aligned} i\,\frac{d}{dt}G_{\substack{\mathrm{ret}\\ \mathrm{adv}}}(t-t',t') &= \mp\delta(t-t') + \omega G_{\substack{\mathrm{ret}\\ \mathrm{adv}}}(t-t',t') \\ &\quad + \frac{\varepsilon^2}{i}\int_0^t K(t-\tau)G_{\substack{\mathrm{ret}\\ \mathrm{adv}}}(\tau-t',t')\,d\tau + \langle\langle f(t)b^+(t')\rangle\rangle_{\substack{\mathrm{ret}\\ \mathrm{adv}}}, \end{aligned} \tag{15}$$

where

$$f(t) = \frac{\varepsilon}{\sqrt{V}}\sum_{(k)}A_k a_k^0 e^{-i\omega_k t} = \frac{\varepsilon}{(2\pi)^{3/2}}\int A_k a_k^0 e^{-i\omega_k t}\,d\mathbf{k}, \tag{16}$$

$$b^+(t') = \frac{1}{2\pi i}\int_{\tau_0 - i\infty}^{\tau_0 + i\infty}\frac{b^+(0) + if^+(p)}{p - i\omega + \varepsilon^2 K^+(p)}e^{pt'}\,dp, \tag{17}$$

$$f^+(p) = \int_0^\infty e^{-pt''}\frac{\varepsilon}{(2\pi)^{3/2}}\int d\mathbf{k}\,A_k a_k^+(0)e^{i\omega_k t''}\,dt''. \tag{18}$$

The Fourier transform of equation (15) is written in the form

$$G_{\substack{\text{ret}\\ \text{adv}}} = \frac{1/2\pi + \psi^{\text{adv}}_{\text{ret}}(\widetilde{E}, t')}{\widetilde{E} - \omega + i\varepsilon^2 k_e(-i\widetilde{E})}, \tag{19}$$

where

$$\psi_{\text{ret}}(\widetilde{E}, t') = \frac{1}{2\pi}\int_{-\infty}^{\infty} \langle\langle f(t) b^+(t')\rangle\rangle_{\text{ret}}\, e^{i\widetilde{E}(t-t')}\, d(t-t') =$$

$$= \frac{\varepsilon^2}{(2\pi)^4}\int \frac{dk\, |A_k|^2 e^{-i\omega_k t'}}{(\omega_k - A - i\delta)(\omega_k - \widetilde{E} - i\varepsilon)} e^{-\delta t'} e^{iAt'}. \tag{20}$$

As $t' \to \infty$, this expression decays as $e^{-\delta t'}$ $(\delta = I(E)/2)$. Thus, in formula (19) the quantity $\psi(\widetilde{E}, t')$ may be neglected.

We now write the expressions for the matrix elements of the density matrix

$$\rho_{00}(t - t', t') = \langle b(t) b^+(t')\rangle = \frac{1}{i}\int_{-\infty}^{\infty} \frac{G(E + i\varepsilon, t') - G(E - i\varepsilon, t')}{1 - e^{-\beta E}} e^{-iE(t-t')}\, dt;$$

$$(21)$$

$$\rho_{11}(t - t', t') = \langle b^+(t) b(t')\rangle =$$

$$= \frac{1}{i}\int_{-\infty}^{\infty} \frac{e^{-\beta E}\{G(E + i\varepsilon, t') - G(E - i\varepsilon, t')\}}{1 + e^{-\beta E}} e^{-iE(t-t')}\, dt.$$

Taking the above into account and putting $t = t'$, we obtain

$$\rho_{00}(t) \underset{t\to\infty}{\longrightarrow} \frac{1}{1 + e^{-\beta\omega}}, \qquad \rho_{11}(t) \underset{t\to\infty}{\longrightarrow} \frac{e^{-\beta\omega}}{1 - e^{-\beta\omega}}.$$

Thus, as a result of the weak interaction of the small system with a thermostat which, before the interaction, was in a state of thermodynamic equilibrium, the density matrix $\rho^s(t)$ of the small system tends to its equilibrium value for a sufficiently long interaction time $(t \to \infty)$. The result obtained coincides with that obtained for this model by using approximate equations of general form.

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