SCHRÖDINGER-TYPE EQUATION WITH DAMPING FOR A DYNAMICAL SYSTEM IN A THERMAL BATH

K. Valyasek, D. N. Zubarev,
and A. L. Kuzemskii

A study is made of a dynamical system that interacts weakly with a thermal bath. The nonequilibrium statistical operator method is used to establish a Schrödinger-type equation with damping for this system. In the case of Bose statistics, a system of coupled nonlinear equations of Schrödinger and kinetic types is obtained.

1. Introduction

In the present paper we consider the behavior of a small dynamical system interacting with a thermal bath, i.e., with a system that has effectively an infinite number of degrees of freedom. Examples of such systems are an atomic (or molecular) system interacting with the electromagnetic field it generates and with a thermal bath; a system of nuclear spins interacting with the lattice; an exciton or electron system interacting with the phonon field, etc. A similar problem has been considered in quantum field theory [1], the Dirac equation with radiative corrections being obtained for the nonquantized wave function from the second-quantized theory.

The aim of the present paper is to obtain a Schrödinger-type equation with damping for the mean values of the amplitudes of a second-quantized field of Bose or Fermi particles weakly coupled to a thermal bath. We shall assume that the system of particles is a long way from equilibrium with the thermal bath and cannot, in general, be characterized by a temperature. As a result of the interaction with the thermal bath, such a system will acquire some statistical characteristics but will remain essentially a mechanical system. The basic idea behind the solution is to eliminate the thermal bath, this influence then being manifested as an effect of friction of the particles in a medium. The presence of friction leads to dissipation and, thus, to irreversible processes. We shall therefore use the general method of description of irreversible processes by constructing a nonequilibrium statistical operator [2-4].

The basic idea behind this method is as follows. If a set of mean values of certain operators P_m or their conjugate parameters $F_m(t)$ is sufficient to describe the nonequilibrium state of the system, then one can find a special solution of the Liouville equation

$$\frac{\partial \rho}{\partial t}+\frac{1}{i\hbar}[\rho(t,0),H]=0,$$

which depends on the time only through $F_m(t)$. The first argument of the nonequilibrium statistical operator $\rho(t, 0)$ indicates its implicit dependence on the time and the second its dependence through the Heisenberg representation.

The boundary conditions for the Liouville equation for $\rho(t, 0)$ can be formulated by the introduction of an infinitesimally small source that violates the symmetry under time reflection. Similar boundary conditions based on the introduction of infinitesimally small sources that violate the symmetry under time reflection are used in the formal theory of scattering in the Gell-Mann–Goldberger form [5]. We introduce an infinitesimally small source into the Liouville equation for $\ln\rho(t, 0)$ as follows [4]:

$$\frac{\partial \ln\rho(t,0)}{\partial t}+\frac{1}{i\hbar}[\ln\rho(t,0),H]=-\varepsilon(\ln\rho(t,0)-\ln\rho_q(t,0)), \tag{1}$$

Joint Institute of Nuclear Research. Translated from Teoreticheskaya i Matematicheskaya Fizika, Vol. 5, No. 2, pp. 281-292, November, 1970. Original article submitted April 10, 1970.

where

$$\rho_q(t,0) = \exp\left\{-\Phi - \sum_m F_m(t) P_m(0)\right\} \equiv \exp\{-S(t,0)\} \qquad (2)$$

is the quasiequilibrium statistical operator and

$$\Phi = \ln \operatorname{Sp} \exp\left\{-\sum_m P_m F_m(t)\right\}. \qquad (3)$$

Now S(t, 0) can be called the entropy operator since $S = \langle S(t,0)\rangle_q$ is the entropy. Here $\langle \ldots \rangle_q = \operatorname{Sp}(\rho_q \ldots)$. In the calculation of the mean values the passage to the limit $\varepsilon \to +0$ is made after the thermodynamic limiting process.

It is readily seen that the source on the right-hand side of Eq. (1) indeed violates the symmetry of the Liouville equation under time reflection and tends to zero as $\varepsilon \to +0$. Integrating Eq. (1) from $-\infty$ to 0, we obtain the nonequilibrium statistical operator in the form

$$\rho(t,0) = \exp\left\{\varepsilon \int_{-\infty}^{0} dt_1 e^{\varepsilon t_1} \ln \rho_q(t+t_1, t_1)\right\} \equiv \exp\{-\widetilde{S(t,0)}\}. \qquad (4)$$

The wavy bar denotes the operation of taking the quasi-invariant part with respect to evolution with the total Hamiltonian H. The average value of any dynamical variable A is

$$\langle A\rangle = \lim_{\varepsilon \to +0} \operatorname{Sp}(A\rho(t,0)), \qquad (5)$$

i.e., it is in fact a quasiaverage in the sense of N. N. Bogolyubov [6, 7].

2. Averaged Equations for the Amplitudes of the Second-Quantized Field

Let us consider the behavior of a small sybsystem with Hamiltonian H_1 interacting with a thermal bath with Hamiltonian H_2. The Hamiltonian of the complete system has the form

$$H = H_1 + H_2 + V, \qquad (6)$$

where V is the interaction Hamiltonian.

For simplicity we shall consider a system of noninteracting Bose or Fermi particles with Hamiltonian

$$H_1 = \sum_\alpha E_\alpha a_\alpha^+ a_\alpha. \qquad (7)$$

We take the interaction Hamiltonian in the form

$$V = \sum_{\alpha\beta} \varphi_{\alpha\beta} a_\alpha^+ a_\beta, \qquad \varphi_{\beta\alpha}^+ = \varphi_{\alpha\beta}, \qquad (8)$$

where $\varphi_{\alpha\beta}$ are operators that act only on the variables of the medium, i.e., of the thermal bath, whose Hamiltonian we shall not write down explicitly.

As operators P_m determining the nonequilibrium state of the small subsystem, we take a_α, a_α^+, and $n_\alpha = a_\alpha^+ a_\alpha$. We shall describe the thermal bath by its Hamiltonian H_2. The choice of only the operators n_α and H_2 would lead to kinetic equations for the system in the thermal bath [8]. The inclusion of the operators a_α and a_α^+ in the set of operators P_m corresponds to our intention to give a dynamical description of the system.

The quasiequilibrium statistical operator (2) is determined from the extremum of the information entropy:

$$S = -\operatorname{Sp}(\rho \ln \rho), \qquad (9)$$

subject to the additional conditions that the quantities

$$\mathrm{Sp}\,(\rho a_\alpha) = \langle a_\alpha \rangle; \;\; \mathrm{Sp}\,(\rho a_\alpha^+) = \langle a_\alpha^+ \rangle; \;\; \mathrm{Sp}\,(\rho n_\alpha) = \langle n_\alpha \rangle \tag{10}$$

remain constant during the variation and the normalization $\mathrm{Sp}\,\rho = 1$ is preserved. The operator has the form

$$\rho_q = \exp\left\{-\Phi - \sum_\alpha (f_\alpha(t)a_\alpha + f_\alpha^*(t)a_\alpha^+ + F_\alpha(t)n_\alpha) - \beta H_2\right\} \equiv \exp\{-S(t, 0)\}, \tag{11}$$

where

$$\Phi = \ln \mathrm{Sp}\exp\left\{-\sum_\alpha (f_\alpha(t)a_\alpha + f_\alpha\;\;(t)a_\alpha^+ + F_\alpha(t)n_\alpha) - \beta H_2\right\}.$$

Here, f_α, f_α^*, and F_α are Lagrangian multipliers determined by the conditions (10). They are the parameters conjugate to $\langle a_\alpha \rangle_q$, $\langle a_\alpha^+ \rangle_q$, and $\langle n_\alpha \rangle_q$:

$$\langle a_\alpha \rangle_q = -\frac{\delta\Phi}{\delta f_\alpha(t)}; \quad \langle n_\alpha \rangle_q = -\frac{\delta\Phi}{\delta F_\alpha(t)},$$

$$f_\alpha(t) = \frac{\delta S}{\delta\langle a_\alpha \rangle_q}; \quad F_\alpha(t) = \frac{\delta S}{\delta\langle n_\alpha \rangle_q}. \tag{12}$$

For what follows, it is convenient to write the quasiequilibrium statistical operator (11) in the form

$$\rho_q = \rho_1\rho_2, \tag{13}$$

where

$$\rho_1 = Q_1^{-1}\exp\left\{-\sum_\alpha (f_\alpha(t)a_\alpha + f_\alpha^*(t)a_\alpha^+ + F_\alpha(t)n_\alpha)\right\},$$

$$Q_1 = \mathrm{Sp}\exp\left\{-\sum_\alpha (f_\alpha(t)a_\alpha + f_\alpha^*(t)a_\alpha^+ + F_\alpha(t)n_\alpha)\right\} \tag{13a}$$

and

$$\rho_2 = Q_2^{-1}\exp\{-\beta H_2\}; \quad Q_2 = \mathrm{Sp}\exp\{-\beta H_2\}. \tag{13b}$$

We now write the nonequilibrium statistical operator (4) in the explicit form

$$\rho = \exp\{-\widetilde{S(t, 0)}\}, \tag{14}$$

where

$$\widetilde{S(t, 0)} = \tilde{\Phi} + \varepsilon\int_{-\infty}^{0} dt_1 e^{\varepsilon t_1}\left\{\sum_\alpha (f_\alpha(t+t_1)a_\alpha(t_1) + f_\alpha^*(t+t_1)a_\alpha^+(t_1) + n_\alpha(t_1)F_\alpha(t+t_1)) + \beta H_2(t_1)\right\},$$

$\tilde{\Phi} = \varepsilon\int_{-\infty}^{0}\Phi(t + t_1)e^{\varepsilon t_1}dt_1$ and $\exp\{-\tilde{\Phi}\}$ is a normalizing factor. The normalization is preserved after the quasi-invariant part is taken if the following conditions are satisfied [2-4]:

$$\langle a_\alpha \rangle_q = \langle a_\alpha \rangle, \;\; \langle a_\alpha^+ \rangle_q = \langle a_\alpha^+ \rangle, \;\; \langle n_\alpha \rangle_q = \langle n_\alpha \rangle. \tag{15}$$

We shall take as our starting point the equations of motion for the operators averaged with the nonequilibrium statistical operator (14):

$$i\hbar\frac{d\langle a_\alpha \rangle}{dt} = \langle [a_\alpha, H] \rangle = \langle [a_\alpha, H_1] \rangle + \langle [a_\alpha, V] \rangle, \tag{16}$$

$$i\hbar\frac{d\langle n_\alpha \rangle}{dt} = \langle [n_\alpha, H] \rangle = \langle [n_\alpha, H_1] \rangle + \langle [n_\alpha, V] \rangle. \tag{17}$$

The equation for $\langle a_\alpha^+ \rangle$ can be obtained by taking the conjugate of (16). We shall use the nonequilibrium statistical operator (14) to calculate the right-hand side of Eqs. (16) and (17). Restricting ourselves to the second order in the interaction V, we obtain, as in [8], the following equations:

$$i\hbar\frac{d\langle a_\alpha\rangle}{dt}=E_\alpha\langle a_\alpha\rangle+\frac{1}{i\hbar}\int_{-\infty}^{0}\langle[[a_\alpha,V]V(t_1)]\rangle_q e^{\varepsilon t_1}\,dt_1, \tag{18}$$

$$i\hbar\frac{d\langle n_\alpha\rangle}{dt}=\frac{1}{i\hbar}\int_{-\infty}^{0}\langle[[n_\alpha,V]V(t_1)]\rangle_q e^{\varepsilon t_1}\,dt_1. \tag{19}$$

Here, $V(t_1)$ denotes the interaction representation of the operator V.

Expanding the double commutator in Eq. (18), we obtain

$$i\hbar\frac{d\langle a_\alpha\rangle}{dt}=E_\alpha\langle a_\alpha\rangle+\frac{1}{i\hbar}\int_{-\infty}^{0}dt_1e^{\varepsilon t_1}\Big\{\sum_{\alpha_1,\beta_1,\beta}\langle\varphi_{\alpha\beta}\tilde{\varphi}_{\alpha_1\beta_1}(t_1)\rangle_q\langle a_\beta\overset{+}{a}_{\alpha_1}a_{\beta_1}\rangle_q-\langle\tilde{\varphi}_{\alpha_1\beta_1}(t_1)\varphi_{\alpha\beta}\rangle_q\langle\overset{+}{a}_{\alpha_1}a_{\beta_1}a_\beta\rangle_q\Big\}, \tag{20}$$

where

$$\tilde{\varphi}_{\alpha\beta}(t)=\varphi_{\alpha\beta}(t)\,e^{\frac{i}{\hbar}(E_\alpha-E_\beta)t}.$$

We transform Eq. (20) to the form

$$i\hbar\frac{d\langle a_\alpha\rangle}{dt}=E_\alpha\langle a_\alpha\rangle+\frac{1}{i\hbar}\sum_{\alpha_1,\beta}\int_{-\infty}^{0}dt_1e^{\varepsilon t_1}\langle\varphi_{\alpha\alpha_1}\tilde{\varphi}_{\alpha_1\beta}(t_1)\rangle_q\langle a_\beta\rangle+\frac{1}{i\hbar}\sum_{\alpha_1,\beta_1,\beta}\int_{-\infty}^{0}dt_1e^{\varepsilon t_1}\langle[\varphi_{\alpha\beta_1},\tilde{\varphi}_{\alpha_1\beta_1}(t_1)]\rangle_q\langle\overset{+}{a}_{\alpha_1}a_{\beta_1}a_\beta\rangle_q.$$

We shall assume that the terms of higher order than linear can be ignored in (20a) (below, we shall formulate conditions when this is possible). Then

$$i\hbar\frac{d\langle a_\alpha\rangle}{dt}=E_\alpha\langle a_\alpha\rangle+\frac{1}{i\hbar}\sum_{\alpha_1,\beta}\int_{-\infty}^{0}dt_1e^{\varepsilon t_1}\langle\varphi_{\alpha\alpha_1}\tilde{\varphi}_{\alpha_1\beta}(t_1)\rangle_q\langle a_\beta\rangle. \tag{21}$$

The form of the linear equation (21) is the same for Bose and Fermi statistics. We now introduce the spectral intensities of the correlation functions of the medium:

$$\langle\tilde{\varphi}_{\alpha_1\beta}(t_1)\varphi_{\alpha\alpha_1}\rangle_q=\frac{1}{2\pi}\int_{-\infty}^{\infty}J_{\alpha_1\beta,\,\alpha\alpha_1}(\omega)\,e^{i\left(\omega+\frac{E_{\alpha_1}-E_\beta}{\hbar}\right)t_1}\,d\omega,$$

$$\langle\varphi_{\alpha\alpha_1}\tilde{\varphi}_{\alpha_1\beta}(t_1)\rangle_q=\frac{1}{2\pi}\int_{-\infty}^{\infty}J_{\alpha\alpha_1,\,\alpha_1\beta}(\omega)\,e^{-i\left(\omega+\frac{E_\beta-E_{\alpha_1}}{\hbar}\right)t_1}\,d\omega \tag{22}$$

and transform Eq. (21), using (22), to

$$i\hbar\frac{d\langle a_\alpha\rangle}{dt}=E_\alpha\langle a_\alpha\rangle+\sum_\beta K_{\alpha\beta}\langle a_\beta\rangle, \tag{23}$$

where

$$K_{\alpha\beta}=\frac{1}{i\hbar}\sum_{\alpha_1}\int_{-\infty}^{0}dt_1e^{\varepsilon t_1}\langle\varphi_{\alpha\alpha_1}\tilde{\varphi}_{\alpha_1\beta}(t_1)\rangle_q=\frac{1}{2\pi}\sum_{\alpha_1}\int_{-\infty}^{\infty}d\omega\frac{J_{\alpha\alpha_1,\,\alpha_1\beta}(\omega)}{\hbar\omega+E_\beta-E_{\alpha_1}+i\varepsilon}. \tag{24}$$

Thus, we have obtained the Eq. (23) of Schrödinger type for $\langle a_\alpha\rangle$; this equation describes the energy shift and the damping due to the interaction of the particles with the medium.

To conclude this section we shall show how, in the case of Bose statistics, we can take into account the nonlinear terms which lead to a coupled system of equations for $\langle a_\alpha\rangle$ and $\langle n_\alpha\rangle$. Consider the quantity $\langle a_{\alpha_1}^{+}a_{\beta_1}a_\beta\rangle_q$. After the canonical transformation

$$a_\alpha=b_\alpha+\langle a_\alpha\rangle;\quad a_\alpha^+=b_\alpha^++\langle a_\alpha^+\rangle$$

the operator ρ_1 in (13a) can be written in the form

$$\rho_1 = Q_1^{-1}\exp\Big\{-\sum_\alpha F_\alpha b_\alpha^+ b_\alpha\Big\}, \quad \langle a_\alpha\rangle = -f_\alpha^*/F_\alpha. \tag{25}$$

Note that Q_1 in (25) is not, in general, equal to Q_1 in (13a). Using Wick's theorem for the operators b_α and b_α^+ and returning to the original operators a_α and a_α^+, we obtain

$$\langle a_{\alpha_1}^+ a_{\beta_1} a_\beta\rangle_q \approx (\langle n_{\alpha_1}\rangle - |\langle a_{\alpha_1}\rangle|^2)\langle a_{\beta_1}\rangle \delta_{\alpha_1\beta} + (\langle n_{\alpha_1}\rangle - |\langle a_{\alpha_1}\rangle|^2)\langle a_\beta\rangle\delta_{\alpha_1\beta_1}. \tag{26}$$

Using (26), we can rewrite Eq. (20a) in the form

$$i\hbar\frac{d\langle a_\alpha\rangle}{dt} = E_\alpha\langle a_\alpha\rangle + \frac{1}{i\hbar}\sum_{\alpha_1\beta}\int_{-\infty}^{0} dt_1 e^{\varepsilon t_1}\langle \varphi_{\alpha\alpha_1}\tilde{\varphi}_{\alpha_1\beta}(t_1)\rangle_q\langle a_\beta\rangle$$

$$+ i\hbar\sum_{\alpha_1\beta}\int_{-\infty}^{0} dt_1 e^{\varepsilon t_1}\{\langle[\varphi_{\alpha\alpha_1}, \tilde{\varphi}_{\alpha_1\beta}(t_1)]\rangle_q + \langle[\varphi_{\alpha\beta}, \tilde{\varphi}_{\alpha_1\alpha_1}(t_1)]\rangle_q\} \times (\langle n_{\alpha_1}\rangle + |\langle a_{\alpha_1}\rangle|^2)\langle a_\beta\rangle.$$

Now consider Eq. (19). Expand the double commutator and, in the same way as the threefold terms were neglected in the derivation of Eq. (21), ignore the fourfold terms in (19) (see also [8]). Then

$$\frac{d\langle n_\alpha\rangle}{dt} = \sum_\beta W_{\beta\to\alpha}(\langle n_\beta\rangle - |\langle a_\beta\rangle|^2) - \sum_\beta W_{\alpha\to\beta}(\langle n_\alpha\rangle - |\langle a_\alpha\rangle|^2)$$

$$+ \frac{1}{i\hbar}\sum_\beta K_{\alpha\beta}\langle a_\alpha^+\rangle\langle a_\beta\rangle + \frac{1}{i\hbar}\sum_\beta K_{\alpha\beta}^*\langle a_\alpha\rangle\langle a_\beta^+\rangle + \sum_{\alpha_1\beta_1} R_{\alpha\alpha,\alpha_1\beta_1}\langle a_{\alpha_1}^+\rangle\langle a_{\beta_1}\rangle, \tag{27}$$

where

$$W_{\beta\to\alpha} = \frac{1}{\hbar^2}J_{\beta\alpha,\alpha\beta}\left(\frac{E_\alpha - E_\beta}{\hbar}\right),$$

$$W_{\alpha\to\beta} = \frac{1}{\hbar^2}J_{\alpha\beta,\beta\alpha}\left(\frac{E_\beta - E_\alpha}{\hbar}\right)$$

are the transition probabilities expressed in terms of the spectral intensities of the correlation functions of the operators of the medium, and

$$R_{\alpha\alpha,\alpha_1\beta_1} = \frac{1}{\hbar^2}\int_{-\infty}^{0}\{\langle \varphi_{\alpha_1\alpha}\tilde{\varphi}_{\alpha\beta_1}(t_1)\rangle_q + \langle\tilde{\varphi}_{\alpha_1\alpha}(t_1)\varphi_{\alpha\beta_1}\rangle_q\} e^{\varepsilon t_1}\, dt_1.$$

Note that

$$R_{\alpha\alpha,\beta\beta} = W_{\beta\to\alpha} \text{ и } \frac{1}{i\hbar}(K_{\alpha\alpha} + K_{\alpha\alpha}^*) = \sum_\beta W_{\alpha\to\beta}.$$

Thus, in the general case Eqs. (18) and (19) form a coupled system of nonlinear equations of Schrödinger and kinetic types. The nonlinear equation (20a) of Schrödinger type is an auxiliary equation and, in conjunction with the equation of kinetic type (27), determines the parameters of the nonequilibrium statistical operator since in the case of Bose statistics

$$\langle a_\alpha\rangle = -\frac{f_\alpha^*(t)}{F_\alpha(t)}; \quad \langle n_\alpha\rangle = (e^{F_\alpha(t)} - 1)^{-1} + \frac{|f_\alpha(t)|^2}{F_\alpha(t)^2}.$$

Therefore, the linear Schrödinger equation is a fairly good approximation if

$$\langle n_\alpha\rangle - |\langle a_\alpha\rangle|^2 = (e^{F_\alpha(t)} - 1)^{-1} \ll 1,$$

a condition that, essentially, corresponds to $\langle b_\alpha^+ b_\alpha\rangle \ll 1$. This corresponds to allowance for only the weakly excited states in the system of quasiparticles corresponding to the operators b_α and b_α^+.

In the case of Fermi statistics, one cannot eliminate the linear terms by a shift of the operators by a c-number since this is not a canonical transformation. In quantum field theory [9] the sources linear in the Fermi operators are introduced by means of classical spinor fields that anticommute with one another and with the original fields. We shall not consider this more complicated case.

3. Schrödinger-Type Equation with Damping

In the foregoing section we obtained an equation for the mean values of the amplitudes in the form (23). It is now expedient to go over to the coordinate representation

$$\psi(\mathbf{r})=\sum_{\alpha}\chi_\alpha(\mathbf{r})\langle a_\alpha\rangle, \tag{28}$$

where $\{\chi_\alpha(\mathbf{r})\}$ is a complete orthonormalized system of single-particle functions of the operator $\{-(\hbar^2/2m)\nabla^2+v(\mathbf{r})\}$, where $v(\mathbf{r})$ is the potential energy, and

$$\left\{-\frac{\hbar^2}{2m}\nabla^2+v(\mathbf{r})\right\}\chi_\alpha(\mathbf{r})=E_\alpha\chi_\alpha(\mathbf{r}).$$

In a certain sense, the quantity $\psi(\mathbf{r})$ plays the role of the wave function of a classical Schrödinger field. Using (28), we transform Eq. (23) to the form

$$i\hbar\frac{\partial\psi(\mathbf{r})}{\partial t}=\left\{-\frac{\hbar^2}{2m}\nabla^2+v(\mathbf{r})\right\}\psi(\mathbf{r})+\int K(\mathbf{r},\mathbf{r}')\psi(\mathbf{r}')\,d\mathbf{r}'. \tag{29}$$

The kernel $K(\mathbf{r},\mathbf{r}')$ of the integral equation (29) has the form

$$K(\mathbf{r},\mathbf{r}')=\sum_{\alpha\beta}K_{\alpha\beta}\chi_\alpha(\mathbf{r})\chi_\beta^*(\mathbf{r}')=\frac{1}{i\hbar}\sum_{\alpha,\beta,\alpha_1}\int_{-\infty}^{0}dt_1e^{\varepsilon t_1}\langle\varphi_{\alpha\alpha_1}\tilde{\varphi}_{\alpha_1\beta}(t_1)\rangle_q\chi_\alpha(\mathbf{r})\chi_\beta^*(\mathbf{r}'). \tag{30}$$

Equation (29) can be called a Schrödinger-type equation with damping for a dynamical system in a thermal bath. It is interesting to note that similar Schrödinger equations with a nonlocal interaction are used in scattering theory [10] to describe interaction with many scattering centers.

For the remainder of the investigation of Eq. (29), it is convenient to introduce the shift operator $e^{i\mathbf{r}_1\mathbf{p}/\hbar}$, where $\mathbf{r}_1=\mathbf{r}'-\mathbf{r}$; $\mathbf{p}=-i\hbar\nabla_\mathbf{r}$. We rewrite Eq. (29) in the form

$$i\hbar\frac{\partial\psi(\mathbf{r})}{\partial t}=\left\{-\frac{\hbar^2}{2m}\nabla^2+v(\mathbf{r})\right\}\psi(\mathbf{r})+D(\mathbf{r},\mathbf{p})\psi(\mathbf{r}). \tag{31}$$

Here

$$D(\mathbf{r},\mathbf{p})=\int d^3r_1K(\mathbf{r},\mathbf{r}+\mathbf{r}_1)e^{\frac{i}{\hbar}\mathbf{r}_1\mathbf{p}}. \tag{32}$$

We shall assume that $\psi(\mathbf{r})$ varies little over the correlation length characteristic for the kernel $K(\mathbf{r},\mathbf{r}')$. Then, expanding $\exp\{i\mathbf{r}_1\mathbf{p}/\hbar\}$ in a series, we obtain the following equation in the zeroth order:

$$i\hbar\frac{\partial\psi(\mathbf{r})}{\partial t}=\left\{-\frac{\hbar^2}{2m}\nabla^2+v(\mathbf{r})+\operatorname{Re}U(\mathbf{r})\right\}\psi(\mathbf{r})+i\operatorname{Im}U(\mathbf{r})\psi(\mathbf{r}), \tag{33}$$

where

$$U(\mathbf{r})=\operatorname{Re}U(\mathbf{r})+i\operatorname{Im}U(\mathbf{r})=\int d^3r_1K(\mathbf{r},\mathbf{r}+\mathbf{r}_1).$$

The expression (33) has the form of a Schrödinger equation with a complex potential. Equations of this form are well known in collision theory [10], in which one introduces an interaction describing absorption ($\operatorname{Im}U(\mathbf{r})<0$). Further, expanding $\exp\{i\mathbf{r}_1\mathbf{p}/\hbar\}$ in a series up to second order inclusively, we can represent Eq. (29) in the form (see also [10])

$$i\hbar\frac{\partial\psi(\mathbf{r})}{\partial t}=\left\{\left(-\frac{\hbar^2}{2m}\nabla^2+v(\mathbf{r})\right)+U(\mathbf{r})-\frac{1}{i\hbar}\int d^3r_1K(\mathbf{r},\mathbf{r}+\mathbf{r}_1)\mathbf{r}_1\mathbf{p}\right. \tag{34}$$
$$\left.+\frac{1}{2}\int d^3r_1K(\mathbf{r},\mathbf{r}+\mathbf{r}_1)\sum_{i,k=1}^{3}r_1^ir_1^k\nabla_i\nabla_k\right\}\psi(\mathbf{r}).$$

Introducing the function

$$A(\mathbf{r})=\frac{mc}{i\hbar e}\int d^3r_1K(\mathbf{r},\mathbf{r}+\mathbf{r}_1)\mathbf{r}_1, \tag{35}$$

which, in a certain sense, is the analog of the complex vector potential of an electromagnetic field, and the tensor of the reciprocal effective masses

$$\left\{\frac{1}{M(\mathbf{r})}\right\}_{ik}=\frac{1}{m}\delta_{ik}-\int d^3r_1\,\mathrm{Re}\,K(\mathbf{r},\mathbf{r}+\mathbf{r}_1)r_1^i r_1^k, \tag{36}$$

we can express Eq. (34) in the form

$$i\hbar\frac{\partial\psi(\mathbf{r})}{\partial t}=\left\{-\frac{\hbar^2}{2}\sum_{ik}\left(\frac{1}{M(\mathbf{r})}\right)_{ik}\nabla_i\nabla_k+v(\mathbf{r})+U(\mathbf{r})+\frac{ie\hbar}{mc}A(\mathbf{r})\nabla+iT(\mathbf{r})\right\}\psi(\mathbf{r}), \tag{37}$$

where

$$T(\mathbf{r})=\frac{1}{2}\int d^3r_1\,\mathrm{Im}\,K(\mathbf{r},\mathbf{r}+\mathbf{r}_1)\sum_{ik}r_1^i r_1^k\nabla_i\nabla_k.$$

In an isotropic medium the tensor $\{1/M(\mathbf{r})\}_{ik}$ is diagonal and $A(\mathbf{r})=0$.

Finally, note that the introduction of $\psi(\mathbf{r})$ does not mean that the state of the small dynamical subsystem is pure. It remains mixed since it is described by the statistical operator (14), the evolution of the parameters $f_\alpha(t)$, $f_\alpha^*(t)$, and $F_\alpha(t)$ of the latter being governed by a coupled system of equations of Schrödinger and kinetic types.

4. Examples. Interaction of Excitons (or Electrons) with a Phonon Field

In the present section we shall consider examples that illustrate the general method. We shall take a system of excitons (or electrons) interacting with lattice phonons and show how the damping and energy shift for such systems are obtained.

First, consider a system of excitons in a lattice described by the Hamiltonian [11]:

$$H=\sum_{\mathbf{k}}E(\mathbf{k})b_{\mathbf{k}}^+b_{\mathbf{k}}+\sum_{\sigma,\mathbf{q}}\hbar\omega_{\sigma,\mathbf{q}}a_{\sigma,\mathbf{q}}^+a_{\sigma,\mathbf{q}}+\frac{1}{\sqrt{N}}\sum_{\mathbf{k}_1,\mathbf{k},\sigma}G_\sigma(\mathbf{k},\mathbf{k}_1)Q_{\sigma,\mathbf{k}-\mathbf{k}_1}b_{\mathbf{k}}^+b_{\mathbf{k}}, \tag{38}$$

where $\hbar\omega_{\sigma,\mathbf{q}}$ is the phonon energy; $b_{\mathbf{k}}^+$, $b_{\mathbf{k}}$, $a_{\sigma,\mathbf{q}}^+$, and $a_{\sigma,\mathbf{q}}$ are the Bose operators of creation and annihilation of excitons and phonons, respectively. The function $G_\sigma(\mathbf{k},\mathbf{k}_1)$ determines the coupling of the excitons to the phonon medium [11], $G_\sigma^*(\mathbf{k},\mathbf{k}_1)=G_\sigma(\mathbf{k}_1,\mathbf{k})$, and

$$Q_{\sigma,\mathbf{q}}=\left(\frac{\hbar}{2\omega_{\sigma,\mathbf{q}}}\right)^{1/2}(a_{\sigma,\mathbf{q}}+a_{\sigma,-\mathbf{q}}^+)$$

is the operator of the normal coordinates of the phonon system. Here, N is the number of molecules in the crystal. In accordance with (8), we write the interaction Hamiltonian in the form

$$V=\sum_{\mathbf{k}_1\mathbf{k}}\varphi(\mathbf{k},\mathbf{k}_1)b_{\mathbf{k}}^+b_{\mathbf{k}_1}, \tag{39}$$

where

$$\varphi(\mathbf{k},\mathbf{k}_1)=\frac{1}{\sqrt{N}}\sum_\sigma G_\sigma(\mathbf{k},\mathbf{k}_1)\left(\frac{\hbar}{2\omega_{\sigma,\mathbf{k}-\mathbf{k}_1}}\right)^{1/2}(a_{\sigma,\mathbf{k}-\mathbf{k}_1}+a_{\sigma,\mathbf{k}_1-\mathbf{k}}^+). \tag{40}$$

We write the Schrödinger-type equation (23) for $\langle b_{\mathbf{k}}\rangle$ with allowance for (38)-(40) in the form

$$i\hbar\frac{d\langle b_{\mathbf{k}}\rangle}{dt}=E(\mathbf{k})\langle b_{\mathbf{k}}\rangle+\sum_{\mathbf{k}_1}K(\mathbf{k},\mathbf{k}_1)\langle b_{\mathbf{k}_1}\rangle, \tag{41}$$

where

$$K(\mathbf{k},\mathbf{k}_1)=\frac{1}{i\hbar}\sum_{\mathbf{k}_2}\int_{-\infty}^{0}dt_1e^{\varepsilon t_1}\langle\varphi(\mathbf{k},\mathbf{k}_2)\tilde{\varphi}(\mathbf{k}_2,\mathbf{k}_1,t_1)\rangle_q \tag{42}$$

$$=\delta(\mathbf{k}-\mathbf{k}_1)\frac{\Omega}{(2\pi)^3}\int d^3k_2\sum_\sigma\frac{\hbar|G_\sigma(\mathbf{k},\mathbf{k}_2)|^2}{2\omega_{\sigma,\mathbf{k}-\mathbf{k}_2}}\left\{\frac{\langle n_{\sigma,\mathbf{k}-\mathbf{k}_2}\rangle}{E(\mathbf{k})-E(\mathbf{k}_2)+\hbar\omega_{\sigma,\mathbf{k}-\mathbf{k}_2}+i\varepsilon}+\frac{\langle n_{\sigma,\mathbf{k}-\mathbf{k}_2}\rangle+1}{E(\mathbf{k})-E(\mathbf{k}_2)-\hbar\omega_{\sigma,\mathbf{k}-\mathbf{k}_2}+i\varepsilon}\right\}.$$

The integration is extended over the first Brillouin zone; Ω is the volume of the unit cell; and

$$\langle n_{\sigma,\,\mathbf{q}}\rangle = (e^{\beta\omega_{\sigma,\,\mathbf{q}}} - 1)^{-1}.$$

Separating the real and the imaginary parts in (42), we obtain

$$i\hbar\frac{d\langle b_{\mathbf{k}}\rangle}{dt} = E(\mathbf{k})\langle b_{\mathbf{k}}\rangle + \Delta E(\mathbf{k})\langle b_{\mathbf{k}}\rangle - \frac{i\hbar}{2}\Gamma(\mathbf{k})\langle b_{\mathbf{k}}\rangle,$$

where

$$\Delta E(\mathbf{k}) = -\frac{\Omega}{(2\pi)^3}P\int d^3k_1\sum_{\sigma}\frac{\hbar|G_\sigma(\mathbf{k},\mathbf{k}_1)|^2}{2\omega_{\sigma,\,\mathbf{k}-\mathbf{k}_1}}\times\left\{\frac{\langle n_{\sigma,\,\mathbf{k}-\mathbf{k}_1}\rangle}{E(\mathbf{k})-E(\mathbf{k}_1)-\hbar\omega_{\sigma,\,\mathbf{k}-\mathbf{k}_1}} + \frac{(\langle n_{\sigma,\,\mathbf{k}-\mathbf{k}_1}\rangle + 1)}{E(\mathbf{k}_1)-E(\mathbf{k})+\hbar\omega_{\sigma,\,\mathbf{k}-\mathbf{k}_1}}\right\} \tag{43}$$

is the energy shift of an exciton, and

$$\Gamma(\mathbf{k}) = \frac{2\pi}{\hbar}\frac{\Omega}{(2\pi)^3}\int d^3k_1\sum_{\sigma}\frac{\hbar|G_\sigma(\mathbf{k},\mathbf{k}_1)|^2}{2\omega_{\sigma,\,\mathbf{k}-\mathbf{k}_1}}$$

$$\times\ \{\langle n_{\sigma,\,\mathbf{k}-\mathbf{k}_1}\rangle\,\delta[E(\mathbf{k})-E(\mathbf{k}_1)+\hbar\omega_{\sigma,\,\mathbf{k}-\mathbf{k}_1}] + (\langle n_{\sigma,\,\mathbf{k}-\mathbf{k}_1}\rangle + 1)\,\delta[E(\mathbf{k})-E(\mathbf{k}_1)-\hbar\omega_{\sigma,\,\mathbf{k}-\mathbf{k}_1}]\} \tag{44}$$

is the damping of the exciton. Equations (43) and (44) show we have obtained the well-known results [11] and we shall therefore omit a discussion of these equations.

As the second example, let us consider briefly a system of electrons in a lattice described by the Hamiltonian [12]

$$H = \sum_{\mathbf{k},\sigma}T(\mathbf{k})a_{\mathbf{k}\sigma}^+a_{\mathbf{k}\sigma} + \sum_{\mathbf{q}}\hbar\omega_{\mathbf{q}}b_{\mathbf{q}}^+b_{\mathbf{q}} + \frac{1}{\sqrt{\Omega}}\sum_{\mathbf{k}_1,\,\mathbf{k}_2,\,\sigma}A(\mathbf{k}_1-\mathbf{k}_2)$$

$$\times\ a^+_{\mathbf{k}_1\sigma}a_{\mathbf{k}_2\sigma}(b_{\mathbf{k}_1-\mathbf{k}_2} + b^+_{\mathbf{k}_2-\mathbf{k}_1}),$$

where $\hbar\omega_{\mathbf{q}}$ is the phonon energy; $a_{\mathbf{k}\sigma}^+$, $a_{\mathbf{k}\sigma}$, $b_{\mathbf{q}}^+$, and $b_{\mathbf{q}}$ are the operators of creation and annihilation of electrons and phonons, respectively; $T(k) = (\hbar^2k^2/2m) - \mu$; and $A(\mathbf{q})$ determines the electron–phonon coupling:

$$A(\mathbf{q}) = g(\mathbf{q})\left(\frac{\omega_{\mathbf{q}}}{2}\right)^{1/2}.$$

As in the exciton example, the Schrödinger-type equation for $\langle a_{\mathbf{k},\,\sigma}\rangle$ can be represented in the form

$$i\hbar\frac{d\langle a_{\mathbf{k},\,\sigma}\rangle}{dt} = (T(k) + \Delta E(\mathbf{k}))\langle a_{\mathbf{k},\,\sigma}\rangle - \frac{i\hbar}{2}\Gamma(\mathbf{k})\langle a_{\mathbf{k},\,\sigma}\rangle,$$

where

$$\Delta E(\mathbf{k}) = P\sum_{k_1}|A(\mathbf{k}-\mathbf{k}_1)|^2\left\{\frac{\langle n_{\mathbf{k}_1-\mathbf{k}_2}\rangle + 1}{T(\mathbf{k})-T(\mathbf{k}_1)-\hbar\omega_{\mathbf{k}-\mathbf{k}_1}} + \frac{\langle n_{\mathbf{k}-\mathbf{k}_1}\rangle}{T(\mathbf{k})-T(\mathbf{k}_1)+\hbar\omega_{\mathbf{k}-\mathbf{k}_1}}\right\} \tag{45}$$

is the energy shift of an electron, and

$$\Gamma(\mathbf{k}) = \frac{2\pi}{\hbar}\sum_{\mathbf{k}_1}|A(\mathbf{k}-\mathbf{k}_1)|^2\{(\langle n_{\mathbf{k}-\mathbf{k}_1}\rangle + 1)\,\delta(T(\mathbf{k})-T(\mathbf{k}_1)-\hbar\omega_{\mathbf{k}-\mathbf{k}_1})$$

$$+\langle n_{\mathbf{k}-\mathbf{k}_1}\rangle\delta(T(\mathbf{k})-T(\mathbf{k}_1)+\hbar\omega_{\mathbf{k}-\mathbf{k}_1})\} \tag{46}$$

is the electron damping. The expressions (45) and (46) are the same as those obtained by the Green's functions method [12] if one sets $\langle a_{\mathbf{k}\sigma}^+a_{\mathbf{k}\sigma}\rangle \approx 0$ in the latter. This is natural since the linear equation of Schrödinger type was obtained in the approximation of small occupation numbers.

Note that the equation for the single-particle Green's functions is very similar to the Schrödinger-type equation but does not contain an inhomogeneity on the right-hand side [13-14].

We should like to express our gratitude to N. M. Plakida and Yu. A. Tserkovnikov for helpful discussions.

LITERATURE CITED

1. N. N. Bogolyubov and D. V. Shirkov, Introduction to the Theory of Quantized Fields, Interscience, New York (1959), § 38.

2. D. N. Zubarev, Dokl. Akad. Nauk SSSR, 140, 92 (1961); 162, 532 (1965); 162, 1794 (1965); 164, 537 (1965); Institute of Theoretical Physics [in Russian], Preprint ITF-69-6, Kiev (1969).
3. D. N. Zubarev and V. P. Kalashnikov, Teor. Mat. Fiz., 1, 137 (1969).
4. D. N. Zubarev, Preprint R4-4886 [in Russian], JINR, Dubna (1970); P4-4920 [in Russian], JINR, Dubna (1970); Teor. Mat. Fiz., 3, 126 (1970).
5. M. Gell-Mann and M. L. Goldberger, Phys. Rev., 91, 398 (1953).
6. N. N. Bogolyubov, Preprint D-788 [in Russian], JINR, Dubna (1961).
7. N. N. Bogolyubov, Physica, Suppl., 26, 1 (1960).
8. K. Walasek and A. L. Kuzemsky, Preprint E4-4862, JINR, Dubna (1970).
9. N. N. Bogolyubov and D. V. Shirkov, Introduction to the Theory of Quantized Fields, Interscience, New York (1959), § 36.
10. N. F. Mott and H. S. W. Massey, The Theory of Atomic Collisons, Oxford (1965).
11. R. S. Noakes, Theory of Excitons, Supplement 5 to Solid State Physics, Academic Press, New York (1963).
12. D. N. Zubarev, Uspekhi Fiz. Nauk, 71, 71 (1960).
13. J. Schwinger, Proc. Nat. Acad. Sci., 37, 452, 455 (1951).
14. V. L. Bonch-Bruevich and S. V. Tyablikov, The Green Function Method in Statistical Mechanics, North-Holland Publishing Co., Amsterdam (1962).