Journal of Statistical Physics, Vol. 16, No. 4, 1977

Invariants and Nonequilibrium Density Matrices

V. V. Dodonov,[1] I. A. Malkin,[1] and V. I. Man'ko[1]

Received October 26, 1976

A new method of calculating nonequilibrium density matrices with the aid of the quantum integrals of motion is proposed. The method is shown to be very effective in the case of systems described by means of quadratic Hamiltonians. The possibility of constructing phenomenological nonstationary Hamiltonians for a wide class of dissipative systems is discussed. The exact formulas for nonequilibrium density matrices of arbitrary quadratic systems are obtained. The quantum problem of the motion of a charged particle in uniform electric and magnetic fields in the presence of a frictional force proportional to the velocity is solved exactly by means of introducing the new phenomenological Hamiltonian.

KEY WORDS: Density matrices; integrals of the motion; nonequilibrium processes; quadratic Hamiltonians; phenomenological Hamiltonians; Hall's effect.

1. INTRODUCTION

In Refs. 1 and 2 a new method of calculating Green's functions and equilibrium density matrices of quantum systems with the aid of quantum integrals of the motion was developed. The aim of the present paper is to derive similar equations relating the time evolution of a density matrix to the integrals of the motion of the quantum system under study. We use these equations to obtain the exact formulas describing the time evolution of the density matrices of the most general quadratic quantum systems and some special examples of such systems.

For simplicity we consider in the present paper only nondegenerate systems obeying Maxwell–Boltzmann statistics.

We consider a new general approach which enables us to give a phenomenological description of nonequilibrium processes in the framework of quantum mechanics.

[1] P. N. Lebedev Institute of Physics, Moscow, USSR.

The main problem in studying nonequilibrium systems is to describe dissipative processes in the framework of quantum mechanics. The most correct way to do this is to place the system considered in a large heat reservoir and to calculate the evolution of the enlarged system. After this the density matrix of the system under study can be obtained by means of integrating over the variables of the reservoir.[3] This method was used, e.g., in a recent paper[4] for calculating the exact nonequilibrium density matrix of a particle in a uniform electric field. However, the calculations in the framework of this scheme can be made exactly only in few cases. Therefore, although there are several elegant and effective methods which enable one to obtain the approximate expressions for the nonequilibrium density matrices for arbitrary Hamiltonians and arbitrary weak external fields, such as Kubo's method and others,[3,5,6] the elaboration of simple and effective methods in the theory of nonequilibrium processes is still a topical problem.

Besides microscopic methods, many authors have considered other methods which can be called phenomenological. Although phenomenological approaches are not strictly well-founded, they are simpler from the viewpoint of calculations, and they yield rather reasonable results in many cases. For example, one can consider non-Hermitian Hamiltonians with complex coefficients leading to damping.[7] Another approach is to consider various nonlinear generalizations of the Schrödinger equation (see Refs. 8–10 and references therein). The second method is usually applied to obtain a satisfactory explanation of the experimental results on nuclear collisions.

Many authors have considered nonstationary Hamiltonians to describe phenomenologically friction in quantum mechanics. (See, e.g., the earlier references 11–13 and the more recent references 14–18 and references therein.) All such Hamiltonians had the form

$$\hat{H} = \epsilon(\hat{p}_1, \hat{p}_2, \ldots, \hat{p}_N)e^{-\Gamma t} + \varphi(\hat{x}_1, \hat{x}_2, \ldots, \hat{x}_N)e^{\Gamma t} \tag{1}$$

The Hamiltonian (1) leads to the following classical equations of the motion:

$$\ddot{x}_k = -\Gamma\dot{x}_k - \sum_{j=1}^{N} \frac{\partial^2\epsilon}{\partial p_k\,\partial p_j}\frac{\partial\varphi}{\partial x_j}, \qquad k = 1, 2, \ldots, N \tag{2}$$

Therefore Γ is the friction coefficient. However, the Hamiltonian (1) only describes systems with potential forces (besides frictional ones). It is of interest to find such Hamiltonians that describe damping in systems with nonpotential forces, e.g., for a particle in an external magnetic field. This problem was not considered earlier, but it can be easily solved if one takes into account Havas' results.[19] Havas has shown that for a wide class of systems of ordinary differential equations one can always find an equivalent system of equations that are Euler's equations for certain Lagrangians.

Using his method, we show how to construct the nonstationary Hamiltonians describing arbitrary systems with forces depending linearly on the velocities and coordinates. To illustrate the general scheme, we consider the Hall effect by means of the new approach.

2. THE APPLICATION OF INTEGRALS OF MOTION FOR CALCULATING DENSITY MATRICES OF QUANTUM SYSTEMS

Let us consider an arbitrary quantum system with N degrees of freedom. The set of generalized coordinates $(x_1,..., x_N)$ will be designated by the vector $\mathbf{x}$, and the set of generalized momenta $(p_1, p_2,..., p_N)$ by the vector $\mathbf{p}$. An operator $\hat{I}(t)$ is called the integral of the motion if it satisfies the equation [$\hat{H}(t)$ is the Hamiltonian of the system]

$$[i\hbar\,\partial/\partial t - \hat{H}(t), \hat{I}(t)]\psi = 0 \tag{3}$$

in the space of functions ψ satisfying the Schrödinger equation and necessary boundary conditions.

If the evolution operator $\hat{U}(t)$ satisfying the equation

$$i\hbar\,\partial\hat{U}/\partial t = \hat{H}\hat{U}, \quad t > 0; \qquad \hat{U}(0) = \hat{E} \tag{4}$$

($\hat{E}$ is the unit operator; the initial moment always will be chosen to be equal to zero for convenience) were known, the statistical operator $\hat{\rho}(t)$ (the density matrix is the kernel of this operator) at the moment $t > 0$ could be calculated by means of the formula[3] (provided the Hamiltonian is Hermitian)

$$\hat{\rho}(t) = \hat{U}(t)\hat{\rho}_0\hat{U}^{-1}(t); \qquad \hat{\rho}_0 \equiv \hat{\rho}(0) \tag{5}$$

However, if a sufficient number of integrals of the motion is known, the evolution of the density matrix in time can be determined with the aid of a more direct method which does not require the preliminary calculation of the evolution operator.

Let us consider an arbitrary system of $2N$ operators $\hat{f}_j, j = 1, 2,..., 2N$. Let us introduce another set of operators $\varphi_j, j = 1, 2,..., 2N$, related to $\hat{f}_j$ and the initial statistical operator $\hat{\rho}_0$ as follows:

$$\hat{\mathbf{f}}\hat{\rho}_0 = \hat{\rho}_0\hat{\boldsymbol{\varphi}}; \qquad \hat{\mathbf{f}} = (\hat{f}_1, \hat{f}_2,..., \hat{f}_{2N}), \qquad \hat{\boldsymbol{\varphi}} = (\hat{\varphi}_1, \hat{\varphi}_2,..., \hat{\varphi}_{2N}) \tag{6}$$

The operators $\hat{\varphi}_j$ always exist provided the operator $\hat{\rho}_0^{-1}$ exists: $\hat{\boldsymbol{\varphi}} = \hat{\rho}_0^{-1}\hat{\mathbf{f}}\hat{\rho}_0$. In particular, if the initial density matrix can be expressed in the form

$$\hat{\rho}_0 = \exp(-\beta\hat{H}_0) \tag{6a}$$

where β is a certain parameter (in the equilibrium case β^{-1} is the temperature) and $\hat{H}_0$ is a formal "initial Hamiltonian," the operator $\hat{\boldsymbol{\varphi}}$ always exists.

Moreover, it can be considered as the integral of the motion corresponding to the Hamiltonian $\hat{H}_0$ and depending on "time" β. At the initial "moment" $\beta = 0$ this integral of the motion coincides with the operator $\hat{\mathbf{f}}$:

$$\hat{\boldsymbol{\varphi}} = \exp(\beta\hat{H}_0)\hat{\mathbf{f}}\exp(-\beta\hat{H}_0) \tag{6b}$$

Let us designate the integrals of the motion that coincide at the initial moment of real time t with the operators $\hat{\mathbf{f}}$ and $\hat{\boldsymbol{\varphi}}$ by the symbols $\hat{\mathbf{F}}$ and $\hat{\boldsymbol{\Phi}}$, respectively.

One can easily check that the operators $\hat{\mathbf{F}}$, $\hat{\mathbf{f}}$, and $\hat{U}(t)$ are related as follows:

$$\hat{\mathbf{F}} = \hat{U}(t)\hat{\mathbf{f}}\hat{U}^{-1}(t) \tag{7}$$

Therefore the following relations hold:

$$\hat{\mathbf{F}}\hat{\rho}(t) = \hat{U}\hat{\mathbf{f}}\hat{U}^{-1}\hat{U}\hat{\rho}_0\hat{U}^{-1} = \hat{U}\hat{\mathbf{f}}\hat{\rho}_0\hat{U}^{-1} = \hat{U}\hat{\rho}_0\hat{\boldsymbol{\varphi}}\hat{U}^{-1} = \hat{\rho}(t)\hat{\boldsymbol{\Phi}} \tag{8}$$

Proceeding to the kernel of the operator $\hat{\rho}(t)$ [the density matrix $\rho(\mathbf{x}_1; \mathbf{x}_2; t)$], one obtains the following vector equation (or the system of $2N$ scalar equations):

$$\hat{\mathbf{F}}_{(1)}\rho(\mathbf{x}_1; \mathbf{x}_2; t) = \hat{\boldsymbol{\Phi}}^T_{(2)}\rho(\mathbf{x}_1; \mathbf{x}_2; t) \tag{9}$$

The symbol $\hat{\mathbf{F}}_{(j)}\rho(\mathbf{x}_1;\ldots; \mathbf{x}_j;\ldots)$ means that the operator $\hat{\mathbf{F}}$ acts on the function ρ as the function of the jth argument only, while the other arguments are considered as parameters; for example,

$$\hat{\mathbf{F}}_{(2)}\rho(\mathbf{x}; \mathbf{y}) = \int \mathbf{F}(\mathbf{y}; \mathbf{x}')\rho(\mathbf{x}; \mathbf{x}')\, d\mathbf{x}'$$

[$\hat{\mathbf{F}}(\mathbf{y}; \mathbf{x}')$ is the kernel of the operator $\hat{\mathbf{F}}$]. The symbol $\hat{\boldsymbol{\Phi}}^T$ means the transposed operator with the kernel $\boldsymbol{\Phi}(\mathbf{y}; \mathbf{x})$, $\boldsymbol{\Phi}(\mathbf{x}; \mathbf{y})$ being the kernel of the operator $\hat{\boldsymbol{\Phi}}$. The advantage of Eq. (9) consists in the following. In some cases the integrals of the motion of the quantum system can be simply obtained, e.g., proceeding from the correspondence between classical and quantum mechanics or by means of some approximate methods. Then, solving Eq. (9) is the simplest and most direct way to calculate the density matrix, because no extra information such as the Green's function is needed in this approach. Note that, unlike the problem of calculating the Green's function with the aid of equations similar to Eq. (9),[1,2] when one has to know $2N$ integrals of the motion, in the case under study one has to know in general $6N$ integrals of the motion: $4N$ of them correspond to the evolution Hamiltonian $\hat{H}(t)$ and other $2N$ correspond to the initial formal Hamiltonian $\hat{H}_0$. However, in many cases the operators $\hat{\boldsymbol{\Phi}}_j$ can be expressed in terms of $\hat{F}_j$, so that the required number of integrals of the motion is again $2N$.

Equation (9) determines the density matrix up to an arbitrary factor depending only on time (the variable t in these equations is a parameter). To calculate this factor one should take into account the equation for the evolution of the density matrix

$$i\hbar(\partial/\partial t)\rho(\mathbf{x}_1; \mathbf{x}_2; t) = [\hat{H}_{(1)} - \hat{H}^T_{(2)}]\rho(\mathbf{x}_1; \mathbf{x}_2; t) \tag{10}$$

(which becomes an ordinary differential equation since the dependence of the function ρ on $\mathbf{x}_1$ and $\mathbf{x}_2$ is already known) and the initial condition $\rho(0) = \rho_0$.

If one chooses as the operators $\hat{f}_j$ the operators $\hat{\mathbf{x}}$ and $\hat{\mathbf{p}}$ and designates the operators corresponding to them $\hat{\varphi}_j$ as $\hat{\mathbf{y}}$ and $\hat{\boldsymbol{\pi}}$, respectively, then Eq. (9) can be rewritten as follows (capital letters designate the integrals of the motion corresponding to the operators $\hat{\mathbf{x}}$, $\hat{\mathbf{p}}$, $\hat{\mathbf{y}}$, and $\hat{\boldsymbol{\pi}}$),

$$\begin{pmatrix} \hat{\mathbf{X}}_{(1)} - \hat{\mathbf{Y}}^T_{(2)} \\ \hat{\mathbf{P}}_{(1)} - \hat{\boldsymbol{\Pi}}^T_{(2)} \end{pmatrix} \rho(\mathbf{x}_1; \mathbf{x}_2; t) = 0 \tag{11}$$

These equations were first used in Ref. 20.

Let us consider an example. Suppose that the initial density matrix ρ_0 is given by

$$\rho_0 = \exp[-\tfrac{1}{2}a(\mathbf{x}_1 - \mathbf{x}_2)^2] \tag{12}$$

Using the identity

$$\mathbf{x}_1 \exp\left[-\frac{a}{2}(\mathbf{x}_1 - \mathbf{x}_2)^2\right] = \left(\mathbf{x}_2 + \frac{1}{a}\frac{\partial}{\partial \mathbf{x}_2}\right) \exp\left[-\frac{a}{2}(\mathbf{x}_1 - \mathbf{x}_2)^2\right]$$

one obtains $\hat{\mathbf{y}}^T = \hat{\mathbf{x}} + i\hat{\mathbf{p}}/\hbar a$; therefore $\hat{\mathbf{y}} = \hat{\mathbf{x}} - i\hat{\mathbf{p}}/\hbar a$. Analogously, since $(\partial/\partial \mathbf{x}_1 + \partial/\partial \mathbf{x}_2)\rho_0 = 0$, one obtains $\hat{\boldsymbol{\pi}} = \hat{\mathbf{p}}$. Consequently, Eq. (11) in the case under study has the following form:

$$\begin{pmatrix} \hat{\mathbf{X}}_{(1)} - [\hat{\mathbf{X}}^T - (i/\hbar a)\hat{\mathbf{P}}^T]_{(2)} \\ \hat{\mathbf{P}}_{(1)} - \hat{\mathbf{P}}^T_{(2)} \end{pmatrix} \rho(\mathbf{x}_1; \mathbf{x}_2; t) = 0 \tag{13}$$

Let us turn on at the moment $t = 0$ the uniform constant field $\mathscr{E}$. The quantum integrals of the motion $\hat{\mathbf{X}}$ and $\hat{\mathbf{P}}$ in this case coincide with the classical ones:

$$\hat{\mathbf{P}} = \hat{\mathbf{p}} - \mathscr{E}t; \qquad \hat{\mathbf{X}} = \hat{\mathbf{x}} - \hat{\mathbf{p}}\frac{t}{m} + \frac{\mathscr{E}t^2}{2m} \tag{14}$$

(m is the mass of a particle). Assuming $a = m/\beta\hbar^2$ (this means that the initial state was an equilibrium state at the temperature β^{-1}) and substituting the operators (14) into Eq. (13), one obtains the following equations:

$$\begin{gathered} \left(\mathbf{x}_1 - \mathbf{x}_2 + \frac{i\hbar t}{m}\frac{\partial}{\partial \mathbf{x}_1} + \frac{i\hbar}{m}(t + i\beta\hbar)\frac{\partial}{\partial \mathbf{x}_2} - \frac{i\beta\hbar}{m}\mathscr{E}t\right)\rho(\mathbf{x}_1; \mathbf{x}_2; t) = 0 \\ \left(\frac{\partial}{\partial \mathbf{x}_1} + \frac{\partial}{\partial \mathbf{x}_2}\right)\rho(\mathbf{x}_1; \mathbf{x}_2; t) = 0 \end{gathered} \tag{15}$$

The second of these equations means that $\rho = \rho(\mathbf{x}_1 - \mathbf{x}_2)$. Then the first equation immediately leads to the result

$$\rho(\mathbf{x}_1; \mathbf{x}_2; t) = \exp\left[-\frac{m(\mathbf{x}_1 - \mathbf{x}_2)^2}{2\beta\hbar^2} + \frac{i\mathscr{E}t}{\hbar}(\mathbf{x}_1 - \mathbf{x}_2)\right] \tag{16}$$

[In the case considered Eq. (10) is reduced to the form $\partial\rho/\partial t = 0$.] Evidently, the calculations in this example are much easier and more elegant than the tedious integration by means of the formula (5).

3. NONEQUILIBRIUM DENSITY MATRICES OF QUADRATIC SYSTEMS

The most general quadratic N-dimensional Hamiltonian can be written as follows:

$$\hat{H} = \tfrac{1}{2}\hat{\mathbf{q}}B(t)\hat{\mathbf{q}} + \mathbf{C}(t)\hat{\mathbf{q}}$$
$$\mathbf{q} = \begin{pmatrix}\mathbf{p}\\ \mathbf{x}\end{pmatrix}; \qquad \mathbf{C} = \begin{pmatrix}\mathbf{c}_1\\ \mathbf{c}_2\end{pmatrix}; \qquad B = \begin{pmatrix}b_1 & b_2\\ b_3 & b_4\end{pmatrix}; \qquad b_3 = \tilde{b}_2 \tag{17}$$

B is a symmetric block $2N \times 2N$ matrix (the matrices $B_j, j = 1, 2, 3, 4$, have the dimension $N \times N$); $\mathbf{c}_1$ and $\mathbf{c}_2$ are N-dimensional vectors. We consider Hermitian Hamiltonians; therefore B and $\mathbf{C}$ consist of real elements.

The integrals of the motion $\hat{\mathbf{X}}$ and $\hat{\mathbf{P}}$ for quadratic systems are linear functions of the operators $\hat{\mathbf{x}}$ and $\hat{\mathbf{p}}$:

$$\begin{pmatrix}\hat{\mathbf{P}}\\ \hat{\mathbf{X}}\end{pmatrix} = \Lambda(t)\begin{pmatrix}\hat{\mathbf{p}}\\ \hat{\mathbf{x}}\end{pmatrix} + \boldsymbol{\Delta}(t); \qquad \Lambda = \begin{pmatrix}\lambda_1 & \lambda_2\\ \lambda_3 & \lambda_4\end{pmatrix}; \qquad \boldsymbol{\Delta} = \begin{pmatrix}\boldsymbol{\delta}_1\\ \boldsymbol{\delta}_2\end{pmatrix} \tag{18}$$

Substituting (18) into Eq. (3), one obtains the following system of ordinary differential equations for the $2N \times 2N$ matrix $\Lambda(t)$ and the $2N$-dimensional vector $\boldsymbol{\Delta}(t)$:

$$(d/dt)\Lambda(t) = \Lambda\Sigma B; \qquad \Lambda(0) = E_{2N}; \qquad \Sigma = \begin{pmatrix}0 & E_N\\ -E_N & 0\end{pmatrix}$$
$$(d/dt)\boldsymbol{\Delta}(t) = \Lambda\Sigma\mathbf{C}; \qquad \boldsymbol{\Delta}(0) = 0 \tag{19}$$

E_N is the $N \times N$ unit matrix. The properties of the solutions to these equations were discussed in Refs. 1 and 2.

The aim of the present section is to obtain the exact formula describing the time evolution of the density matrix of the quadratic system with the Hamiltonian (17) for $t > 0$ that was in the equilibrium state for $t < 0$. As was shown in Ref. 1, the equilibrium density matrix of a quadratic system is the exponential of a certain quadratic form (provided the system is steady, i.e., the matrix B is nonnegative definite).

In addition, $\rho(\mathbf{x}_1; \mathbf{x}_2) = \rho^*(\mathbf{x}_2; \mathbf{x}_1)$ due to the Hermiticity of the statistical operator. Consequently, the initial density matrix can be expressed as follows:

$$\rho_0(\mathbf{x}_1; \mathbf{x}_2) = K \exp(-\tfrac{1}{2}\mathbf{x}_1 a \mathbf{x}_1 - \mathbf{x}_1 g \mathbf{x}_2 - \tfrac{1}{2}\mathbf{x}_2 a^* \mathbf{x}_2 + \mathbf{d}\mathbf{x}_1 + \mathbf{d}^* \mathbf{x}_2) \qquad a = \tilde{a}; \quad g = g^\dagger \tag{20}$$

a and g are $N \times N$ matrices; d is an N-dimensional vector (the tilde means transposition; the asterisk denotes complex conjugation; the dagger denotes Hermitian conjugation).

One can check that the operators $\hat{\mathbf{Y}}^T$ and $\hat{\mathbf{\Pi}}^T$ introduced in the previous section can be expressed in the case of the matrix ρ_0 given by Eq. (20) in terms of the operators $\hat{\mathbf{X}}$ and $\hat{\mathbf{P}}$:

$$\begin{aligned} \hat{\mathbf{Y}}^T &= \tilde{g}^{-1}[(i/\hbar)\hat{\mathbf{P}}^T - a^* \hat{\mathbf{X}}^T + \mathbf{d}^*] \\ \hat{\mathbf{\Pi}}^T &= i\hbar(g - a\tilde{g}^{-1}a^*)\hat{\mathbf{X}}^T - a\tilde{g}^{-1}\hat{\mathbf{P}}^T + i\hbar(a\tilde{g}^{-1}\mathbf{d}^* - \mathbf{d}) \end{aligned} \tag{21}$$

Substituting these operators into Eq. (11), one obtains a system of linear differential equations in partial derivatives of the first order. The solution to this system has the same form as (20) but with new coefficients a', g', and $\mathbf{d}'$. To find these coefficients it is sufficient to obtain the dependence of $\rho(\mathbf{x}_1; \mathbf{x}_2)$ on only one argument ($\mathbf{x}_1$ or $\mathbf{x}_2$), due to the relation $\rho(\mathbf{x}_1; \mathbf{x}_2) = \rho^*(\mathbf{x}_2; \mathbf{x}_1)$. The calculations lead to the following formulas [to obtain these formulas one should take into account that the elements of the matrix $\Lambda(t)$ satisfy several identities following from the relation $\Lambda\Sigma\tilde{\Lambda} = \Sigma$][1,2]:

$$a' = (i/\hbar)\lambda_3^{-1}[\lambda_4 - (i/\hbar)\chi\psi^* g^{-1}\tilde{\lambda}_3^{-1}] \tag{22}$$

$$g' = (1/\hbar^2)\lambda_3^{-1}\chi\tilde{\lambda}_3^{-1} \tag{23}$$

$$\mathbf{d}' = (i/\hbar)\lambda_3^{-1}(\chi\gamma - \delta_2) \tag{24}$$

We have introduced the following notation:

$$\begin{aligned} \psi &= a + (i/\hbar)\lambda_1\lambda_3^{-1} = \tilde{\psi} \\ \chi &= (\psi^* g^{-1}\psi - g^*)^{-1} = \chi^\dagger \\ \gamma &= \psi^* g^{-1}\mu - \mu^*; \qquad \mu = \mathbf{d} - (i/\hbar)(\delta_1 - \lambda_1\lambda_3^{-1}\delta_2) \end{aligned} \tag{25}$$

The preexponential factor K' can be obtained from Eq. (10):

$$K' = K \exp\left\{\int_0^t [\hbar^{-1} \operatorname{Im}(\operatorname{Tr}(b_1 a') - \mathbf{d}' b_1 \mathbf{d}') - 2\mathbf{c}_1 \operatorname{Re} \mathbf{d}']\, d\tau\right\} \tag{26a}$$

$$= K[\det(\hbar^2\lambda_3^2 g\chi^{-1})]^{-1/2} \exp(\tfrac{1}{2}\mu\psi^{-1}\mu + \tfrac{1}{2}\gamma^*\psi^{-1}g\chi^*\gamma^*) \tag{26b}$$

The formulas (22)–(26) were obtained (in other notations) in Ref. 20. If the initial matrix ρ_0 has the form (12), i.e., $\mathbf{d} = 0$, $a = -g = \alpha E_N$, then the formulas (22)–(26) can be simplified:

$$\begin{aligned} a' &= \alpha\lambda_1^{-1}\tilde{\lambda}_1^{-1} + (i/\hbar)\lambda_1^{-1}\lambda_2 \\ g' &= -\alpha\lambda_1^{-1}\tilde{\lambda}_1^{-1}; \qquad \mathbf{d}' = -(i/\hbar)\lambda_1^{-1}\boldsymbol{\delta}_1; \qquad K' = K(\det \lambda_1)^{-1} \end{aligned} \tag{27}$$

Therefore in this important special case one only has to calculate the matrices λ_1 and λ_2 and the vector $\boldsymbol{\delta}_1$. Physically the result (27) means that if the system was in the spatially uniform state [$\rho_0(\mathbf{x}; \mathbf{x}) = \text{const}$] at the initial moment, it will stay in the spatially uniform state at all subsequent moments [with the space density $K' = K(\det \lambda_1)^{-1}$].

4. PHENOMENOLOGICAL HAMILTONIANS FOR DISSIPATIVE SYSTEMS

The essence of the phenomenological approach to nonequilibrium processes consists in the following. Starting from the known classical equations of motion of the dissipative system, one tries to describe this system in the language of Hamiltonian mechanics. If this is possible, then replacing the canonically conjugate coordinates and moments by the operators one obtains the quantum phenomenological model of the nonequilibrium system under study. In the present section we consider dissipative systems that can be described by quadratic Hamiltonians.

Let us consider a classical system described by equations of motion of the type

$$G_i(\ddot{\mathbf{x}}; \dot{\mathbf{x}}; \mathbf{x}; t) = 0, \quad i = 1, 2, \ldots, N; \qquad \mathbf{G} \equiv (G_1, G_2, \ldots, G_N) \tag{28}$$

In the general case these equations cannot be derived from any Lagrangian. However, one can try to construct an equivalent system of equations

$$G_i' = \sum_{k=1}^{N} F_{ik}(\dot{\mathbf{x}}; \mathbf{x}; t) G_k(\ddot{\mathbf{x}}; \dot{\mathbf{x}}; \mathbf{x}; t) = 0, \qquad \det\|F_{ik}\| \neq 0. \tag{29}$$

such that the solutions to Eq. (29) are the solutions to Eq. (28) and vice versa, but the functions G_i' can be obtained from a certain Lagrangian $L(\dot{\mathbf{x}}; \mathbf{x}; t)$:

$$G_i' = \frac{\partial}{dt}\frac{\partial L}{\partial \dot{x}_j} - \frac{\partial L}{\partial x_j} \tag{30}$$

Havas[19] proved that such equivalent Lagrangians can be found for a wide class of functions $G_i(\ddot{\mathbf{x}}; \dot{\mathbf{x}}; \mathbf{x}; t)$. Let us apply Havas' idea to find the equiva-

lent Lagrangian for the general system of linear differential equations, which can be written in the matrix form as follows:

$$\mathbf{G} \equiv \ddot{\mathbf{x}} + A(t)\dot{\mathbf{x}} + D(t)\mathbf{x} + \mathbf{J}(t) = 0 \tag{31}$$

A and D are arbitrary real $N \times N$ matrices, and $\mathbf{J}(t)$ is an arbitrary N-dimensional real vector. It is natural to look for the equivalent Lagrangian in the form of a quadratic form of $\mathbf{x}$ and $\dot{\mathbf{x}}$:

$$L = \tfrac{1}{2}\dot{\mathbf{x}}M(t)\dot{\mathbf{x}} + \tfrac{1}{2}\mathbf{x}W(t)\mathbf{x} + \dot{\mathbf{x}}V(t)\mathbf{x} + \mathbf{R}\mathbf{x} + \mathbf{S}\dot{\mathbf{x}}; \qquad M = \tilde{M}; \quad W = \tilde{W} \tag{32}$$

Therefore the matrix $F = \|F_{ik}\|$ must depend only on time. Substituting the expressions (29), (31), and (32) into Eq. (30), one obtains the following system of equations:

$$F = M = \tilde{F} \tag{33a}$$

$$FA = \dot{F} + V - \tilde{V} \tag{33b}$$

$$FD = \dot{V} - W \tag{33c}$$

$$F\mathbf{J} = \dot{\mathbf{S}} - \mathbf{R} \tag{33d}$$

If Eq. (31) has the Lagrange form, then $F = E_N$; in this case Eqs. (33a)–(33d) lead to the following restrictions for the matrices A and D:

$$A = -\tilde{A}; \qquad D - \tilde{D} = \dot{A} \tag{34}$$

To consider the general case it is convenient to rewrite Eqs. (33a)–(33d) (excluding the matrices V and W from them) as follows:

$$2\dot{F} = FA + \tilde{A}F \tag{35}$$

$$F(D - \tfrac{1}{4}A^2 - \tfrac{1}{2}\dot{A}) = (\tilde{D} - \tfrac{1}{4}\tilde{A}^2 - \tfrac{1}{2}\dot{\tilde{A}})F \tag{36}$$

Therefore the problem is reduced to finding the symmetric matrix $F(t)$ satisfying both Eqs. (35) and (36). Let us consider for simplicity the case $\dot{A} = 0$. Then the solution to Eq. (35) can be expressed as follows[3]:

$$F(t) = \exp(\tfrac{1}{2}\tilde{A}t)\, F_0 \exp(\tfrac{1}{2}At) \tag{37}$$

Evidently, if the initial matrix F_0 is symmetric, the matrix $F(t)$ is also symmetric. Equation (36) imposes the following restrictions on F_0:

$$F_0[\exp(\tfrac{1}{2}At)](D - \tfrac{1}{4}A^2)\exp(-\tfrac{1}{2}At) = [\exp(-\tfrac{1}{2}\tilde{A}t)](\tilde{D} - \tfrac{1}{4}\tilde{A}^2)[\exp(\tfrac{1}{2}\tilde{A}t)]F_0 \tag{38}$$

Equation (38) is equivalent to the following set of equations:

$$F_0(D - \tfrac{1}{4}A^2) = (\tilde{D} - \tfrac{1}{4}\tilde{A}^2)F_0 \tag{38a}$$

$$F_0[A, D] = \widetilde{[A, D]}F_0; \qquad [A, D] \equiv AD - DA \tag{38b}$$

$$F_0[A, D]_n = \widetilde{[A, D]}_n F_0; \qquad [A, D]_n \equiv [A, [A, D]_{n-1}]; \qquad n \geqslant 2 \tag{38c}$$

Each of these equations independently has nonsingular symmetric solutions for arbitrary matrices A and D. Indeed, since the matrices D and $\tilde{D}$ have the same normal Jordan form,[21] $\tilde{D} = fDf^{-1}$, where f is a nonsingular matrix. Then the matrix $F = f + \tilde{f}$ is the required symmetric solution to the equation $FD = \tilde{D}F$. However, the system of equations (38a)–(38c) in the general case is incompatible. For example, if the two-dimensional matrices A and $D' = D - \frac{1}{4}A^2$ are given by

$$A = \begin{pmatrix} a_1 & 0 \\ a_{21} & a_2 \end{pmatrix}; \qquad D' = \begin{pmatrix} d_1 & 0 \\ 0 & d_2 \end{pmatrix}; \qquad a_{21} \neq 0; \quad d_1 \neq d_2$$
$$[A, D] = \begin{pmatrix} 0 & 0 \\ a_{21}(d_1 - d_2) & 0 \end{pmatrix} \tag{39}$$

then any matrix F satisfying both Eqs. (38a) and (38b) has the only nonzero element F_{11}; therefore it is singular.

Consequently, we arrive at the conclusion that in the general case the system (31) cannot be replaced by an equivalent system with quadratic Lagrangian.

We have no intention of deriving in the present paper all the necessary and sufficient conditions for the compatibility of Eqs. (38a)–(38c). Instead we consider some simple sufficient conditions. One such condition is

$$[A, D] = \lambda E_N \tag{40}$$

(note that this is not a necessary condition) or its simpler variant $[A, D] = 0$. A more general condition is

$$[A, D]_n = f_n(D - \tfrac{1}{4}A^2) \tag{41}$$

where the f_n are arbitrary functions.

If F satisfies the equations

$$FA = -\tilde{A}F; \qquad FD = \tilde{D}F \tag{42}$$

then the system (31) can be reduced to the Lagrange form by means of a time-independent transformation. Physically this means that Eq. (31) are simply written in coordinate-free form: For example, the equations $\ddot{x} = \dot{y}\mathcal{H}/m_x$ and $\ddot{y} = -\dot{x}\mathcal{H}/m_y$ have no Lagrangian, while equivalent equations $m_x\ddot{x} = \dot{y}\mathcal{H}$ and $m_y\ddot{y} = -\dot{x}\mathcal{H}$ can be obtained from the usual Lagrangian $L = \frac{1}{2}(m_x\dot{x}^2 + m_y\dot{y}^2) + \mathcal{H}x\dot{y}$. One of the necessary conditions for the compatibility of Eqs. (42) is the equality of all elementary divisors of the matrices A and $-\tilde{A}$.[21]

The choice of the other parameters determining the quadratic form (32) —the matrices W and V, and the vectors $\mathbf{R}$ and $\mathbf{S}$—is not unique. The simplest and most symmetric expressions for them are as follows:

$$V = -\tilde{V} = \tfrac{1}{4}(FA - \tilde{A}F), \qquad W = \tfrac{1}{8}(FA^2 - \tilde{A}^2F) - FD$$
$$\mathbf{R} = -F\mathbf{J}, \qquad \mathbf{S} = 0 \tag{43}$$

The Hamiltonian can be constructed as usual: $H = \mathbf{p}\dot{\mathbf{x}} - L$, $\mathbf{p} = \partial L/\partial \dot{\mathbf{x}}$:

$$H = \tfrac{1}{2}\mathbf{p}F^{-1}\mathbf{p} - \mathbf{p}F^{-1}V\mathbf{x} + \tfrac{1}{2}\mathbf{x}(\tilde{V}F^{-1}V - W)\mathbf{x} - \mathbf{R}\mathbf{x} \tag{44}$$

For example, in the important special case of a spatially uniform system, when $D = 0$, the equivalent Hamiltonian always exists and can be written in the following simple form:

$$H = \tfrac{1}{2}\mathbf{p}[\exp(-At)]M_0\mathbf{p} + \mathbf{x}M_0^{-1}[\exp(At)]\mathbf{J} \tag{45}$$

with the symmetric nonsingular matrix M_0 satisfying the equation

$$M_0\tilde{A} = AM_0$$

Considering $\mathbf{x}$ and $\mathbf{p}$ in Eq. (44) as operators, we arrive at the phenomenological quantum model of the classical dissipative system (31).

5. EXAMPLES

The simplest example is the case where the matrix A is proportional to the unit matrix: $A = \Gamma E_N$. Then the equivalent Hamiltonian has the form (1). Since such Hamiltonians have been considered in many papers,[11–18] let us consider here another interesting example, which has not been studied previously: the motion of a charged particle under the action of uniform electric and magnetic fields and a frictional force proportional to the velocity. The classical equations of motion are as follows (evidently, it is sufficient to consider only the two-dimensional problem):

$$\begin{aligned} G_1 &\equiv \ddot{x} - \mathscr{H}\dot{y} + \Gamma\dot{x} - \mathscr{E}_1(t) = 0 \\ G_2 &\equiv \ddot{y} + \mathscr{H}\dot{x} + \Gamma\dot{y} - \mathscr{E}_2(t) = 0 \\ m &= e = c = 1; \qquad \mathscr{H} = \text{const} \end{aligned} \tag{46}$$

In this case the matrix D is equal to zero, so that the equivalent Hamiltonian is given by Eq. (45). The matrices A and $\exp(-At)$ are given by

$$A = \begin{pmatrix} \Gamma & -\mathscr{H} \\ \mathscr{H} & \Gamma \end{pmatrix}; \qquad \exp(-At) = \begin{pmatrix} \cos(\mathscr{H}t) & \sin(\mathscr{H}t) \\ -\sin(\mathscr{H}t) & \cos(\mathscr{H}t) \end{pmatrix} \tag{47}$$

The matrix M_0 can be chosen as follows:

$$M_0 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{48}$$

Therefore the Hamiltonian is given by

$$\begin{aligned} H = e^{-\Gamma t}\{&\tfrac{1}{2}[\cos(\mathscr{H}t)](p_x^2 - p_y^2) - [\sin(\mathscr{H}t)]p_xp_y\} \\ &+ e^{\Gamma t}\{[\cos(\mathscr{H}t)][\mathscr{E}_2(t)y - \mathscr{E}_1(t)x] \\ &+ [\sin(\mathscr{H}t)][\mathscr{E}_2(t)x + \mathscr{E}_1(t)y]\} \end{aligned} \tag{49}$$

Let us consider the simplest case, when the initial matrix ρ_0 has the form (12). This means that for $t < 0$ the external field is absent, and the system is in the equilibrium state. Since the matrices b_2 and b_4 in the Hamiltonian (49) are equal to zero, then $\lambda_1 = E_2$, $\lambda_2 = 0$ (the sense of these matrices was explained in Section 3).

Furthermore, since the Hamiltonian (49) is only a crude model of the real physical system, the density matrix $\rho(t)$ may have a physical significance only for large t, such that $\exp(-\Gamma t) \ll 1$, when the nonsteady-state process caused by the sudden switching on of the external fields will end. Therefore one only has to calculate the asymptotic formula for the vector $\boldsymbol{\delta}_1(t)$ for $t \gg \Gamma^{-1}$. This formula has the following form:

$$\boldsymbol{\delta}_1(t) = \int_{-\infty}^{t} e^{\Gamma\tau} \begin{pmatrix} \mathscr{E}_2(\tau)\sin(\mathscr{H}\tau) - \mathscr{E}_1(\tau)\cos(\mathscr{H}\tau) \\ \mathscr{E}_2(\tau)\cos(\mathscr{H}\tau) + \mathscr{E}_1(\tau)\sin(\mathscr{H}\tau) \end{pmatrix} d\tau + O(e^{-\Gamma t}) \tag{50}$$

Using the formulas (27), one can obtain the following asymptotic expression for $\rho(t)$ [for simplicity we give the result only in the simplest case $\mathscr{E} = \text{const}$; $r = (x, y)$]:

$$\begin{aligned} \rho(\mathbf{r}_1; \mathbf{r}_2; t) &= \rho_0 \exp\left[\frac{i}{\hbar}\boldsymbol{\delta}_1(t)(\mathbf{r}_2 - \mathbf{r}_1)\right] \\ &= \rho_0 \exp\Bigg(-\frac{i}{\hbar}\frac{e^{\Gamma t}}{\Gamma^2 + \mathscr{H}^2}\{[\Gamma\sin(\mathscr{H}t) - \mathscr{H}\cos(\mathscr{H}t)] \\ &\quad \times [\mathscr{E}_2(x_1 - x_2) + \mathscr{E}_1(y_1 - y_2)] \\ &\quad + [\Gamma\cos(\mathscr{H}t) + \mathscr{H}\sin(\mathscr{H}t)][\mathscr{E}_2(y_1 - y_2) - \mathscr{E}_1(x_1 - x_2)]\}\Bigg) \end{aligned} \qquad t \gg \Gamma^{-1} \tag{51}$$

The current density operator is

$$\begin{pmatrix} \hat{j}_x \\ \hat{j}_y \end{pmatrix} = \frac{i}{\hbar}\left[\hat{H}, \begin{pmatrix} \hat{x} \\ \hat{y} \end{pmatrix}\right] = e^{-\Gamma t}\begin{pmatrix} \hat{p}_x\cos(\mathscr{H}t) - \hat{p}_y\sin(\mathscr{H}t) \\ -\hat{p}_y\cos(\mathscr{H}t) - \hat{p}_x\sin(\mathscr{H}t) \end{pmatrix} \tag{52}$$

Consequently, the current density is

$$\begin{aligned} \mathbf{j} &= \tfrac{1}{2}[\hat{\mathbf{j}}_{(1)}\rho(r_1; r_2) + \hat{\mathbf{j}}^{T}_{(2)}\rho(r_1; r_2)]|_{\mathbf{r}_1 = \mathbf{r}_2} \\ &= \frac{\rho_0(\mathbf{r}; \mathbf{r})}{\Gamma^2 + \mathscr{H}^2}\begin{pmatrix} \mathscr{H}\mathscr{E}_2 + \Gamma\mathscr{E}_1 \\ -\mathscr{H}\mathscr{E}_1 + \Gamma\mathscr{E}_2 \end{pmatrix} \end{aligned} \tag{53}$$

One can easily see that Eq. (53) describes the Hall effect. This means that the Hamiltonian (49), in spite of its very exotic form, leads to quite reasonable results.

In the special case $\mathscr{H} = 0$ the density matrix (51) becomes

$$\rho(r_1; r_2; t) = \rho_0 \exp\left\{-\frac{ie^{\Gamma t}}{\hbar\Gamma}\left[\mathscr{E}_2(y_1 - y_2) - \mathscr{E}_1(x_1 - x_2)\right]\right\}, \qquad t \gg \Gamma^{-1} \quad (54)$$

and formula (53) gives Ohm's law $\mathbf{j} = \rho(\mathbf{x}; \mathbf{x})\Gamma^{-1}\mathscr{E}$.

6. CONCLUSION

The examples considered above show that both the method using the integrals of the motion and the method using phenomenological Hamiltonians are useful tools for investigating a sufficiently wide class of nonequilibrium quantum systems. These methods have many obvious defects, but they also have evident advantages, the most important of which is the simplicity of the calculations. Therefore these methods can be used for solving many interesting physical problems—for example, for investigating galvanomagnetic properties of thin films (provided the film is approximated by a harmonic potential). In addition, the exact formulas for the density matrices of quadratic systems obtained in Section 3 enable one to study in detail nonequilibrium quadratic systems from the microscopic point of view and to compare the results with the results of the phenomenological approach and various known approximate methods.

ACKNOWLEDGMENT

The authors thank E. S. Fradkin and M. A. Markov for discussions and the referees for useful remarks and recommendations.

REFERENCES

1. V. V. Dodonov, I. A. Malkin, and V. I. Man'ko, *J. Phys. A* **8**:L19 (1975).
2. V. V. Dodonov, I. A. Malkin, and V. I. Man'ko, *Teor. Mat. Fiz.* **24**:164 (1975); *Int. J. Theor. Phys.* **14**:37 (1975).
3. D. ter Haar, *Elements of Statistical Mechanics*, Holt, Rinehart and Winston, New York (1961); *Rep. Prog. Phys.* **24**:304 (1961).
4. G. J. Papadopoulos, *Physica* **74**:529 (1974).
5. R. Kubo, *J. Phys. Soc. Japan* **12**:570 (1957).
6. A. Isihara, *Statistical Physics*, Academic Press, New York (1971).
7. M. Pardy, *Int. J. Theor. Phys.* **8**:31 (1973).
8. M. D. Kostin, *J. Chem. Phys.* **57**:3589 (1973); *J. Stat. Phys.* **12**:145 (1975).
9. K. Albrecht, *Phys. Lett.* **56B**:127 (1975).
10. B. K. Skagerstam, *Phys. Lett.* **58B**:21 (1975).
11. P. Caldirola, *Nuovo Cimento* **18**:393 (1941); **46B**:172 (1966).
12. E. Kanai, *Progr. Theor. Phys.* **3**:440 (1948).
13. W. E. Brittin, *Phys. Rev.* **77**:396 (1950).

14. G. J. Papadopoulos, *J. Phys. A* **7**:209 (1974).
15. L. H. Buch and H. H. Denman, *Am. J. Phys.* **42**:304 (1974).
16. H. Dekker, *Z. Physik* **B21**:295 (1975).
17. R. W. Hasse, *J. Math. Phys.* **16**:2005 (1975).
18. I. R. Svin'in, *Teor. Mat. Fiz.* **22**:97 (1975); **27**:270 (1976).
19. P. Havas, *Nuovo Cimento Suppl.* **5**:363 (1957).
20. V. V. Dodonov, I. A. Malkin, and V. I. Man'ko, P. N. Lebedev Institute of Physics, Preprint No. 42 (1976).
21. F. R. Gantmaher, *Teoriya Matritz*, Nauka, Moscow (1967).