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LETTER TO THE EDITOR

Dissipation in quantum systems

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Abstract. The quantum dynamics of a mechanical subsystem interacting with a thermal bath is studied. A new approach to dissipated quantum mechanics is proposed which is based on the thermodynamic treatment of the energy balance. Simple application of the theory to ideal gases is considered and equations for the evolution of the main average quantities are derived.

The dynamics of systems of many quantum particles attracted attention many years ago. It is as important for pure theoretical investigation as it is practically. Much of the contemporary technological progress is due to collective phenomena such as phonon–electron interactions [1], quasiparticle excitations [2], etc. In this sense, it is interesting to develop a theory to describe the irreversible mechanics of complex quantum systems. In the literature, some authors have introduced dissipative Schrödinger equations [3, 4], while others have incorporated stochastic sources in the wavefunction Hilbert space [5, 6]. A very useful idea is to divide the whole system into a subsystem under observation and thermal bath [7, 8]. In this manner either quantum stochastic equations [9–11] or reduced density matrix [2] and master [12] equations have been derived. Finally, the problem of quantum chaos has also been discussed [13, 14].

The goal of the present letter is to apply the method of subsystem–bath separation to justify a new heuristic approach to dissipative quantum mechanics developed by the present author [15]. Let us consider a mechanical system consisting of a constant number of particles situated in a box with constant volume V . Macroscopically, the system is at thermodynamic equilibrium. In the framework of the quantum mechanics, the dynamics of microscopic processes occurring in the system is described by the Schrödinger equation

$$i\hbar \frac{\partial \Psi}{\partial t} = \hat{\mathcal{H}}\Psi \quad (1)$$

where Ψ is the wavefunction and $\hat{\mathcal{H}}$ is the Hamiltonian of the system. At a given moment accepted as initial, N system particles are chosen and called the subsystem S, while the excluded part of the system is called bath B. The aim of the present consideration is to describe the evolution of the subsystem interchanging energy with the bath. The Hamiltonian of the whole system can be presented as a sum of the subsystem and bath Hamiltonians plus a potential accounting for the SB interaction [8]

$$\hat{\mathcal{H}} = \hat{\mathcal{H}}_S + \hat{\mathcal{H}}_B + U_{SB}. \quad (2)$$

Due to the last term the subsystem and bath are coupled and in this way the processes occurring in S depend on B and *vice versa*. Let us consider the weak SB interaction limit.

In this case the correlation part of the wavefunction which is due to the subsystem–bath interaction does not contribute in the frame of a linear analysis. Hence, Ψ can be presented as a product of the wavefunctions Φ and Θ of the subsystem and bath, respectively,

$$\Psi = \Phi(r, t)\Theta(R, t). \quad (3)$$

Here r is the $3N$ -dimensional vector of the subsystem particles coordinates and R is the corresponding vector of the bath. Equation (3) implies the statistical independence of S and B. The factorization of the wavefunction is a very popular approach for modelling processes in many-particle quantum systems [7].

Introducing expressions (2) and (3) in equation (1), multiplying the result by the complex conjugated wavefunction of the bath or subsystem and integrating over R or r one obtains the following two equations describing the evolution of the subsystem and bath wavefunctions

$$i\hbar \frac{\partial \Phi}{\partial t} = \hat{H}_S \Phi + (E_B - \bar{E}_B) \Phi \quad (4)$$

$$i\hbar \frac{\partial \Theta}{\partial t} = \hat{H}_B \Theta + (E_S - \bar{E}_S) \Theta. \quad (5)$$

The constrained and average energies of the bath and subsystem are introduced here by the relations

$$E_B(r, t) = \int \Theta^* (\hat{H}_B + U_{SB}) \Theta dR \quad \bar{E}_B(t) = i\hbar \int \Theta^* \frac{\partial \Theta}{\partial t} dR$$

$$E_S(R, t) = \int \Phi^* (\hat{H}_S + U_{SB}) \Phi dr \quad \bar{E}_S(t) = i\hbar \int \Phi^* \frac{\partial \Phi}{\partial t} dr.$$

Due to these expressions, equations (4) and (5) are coupled and a method to obtain rigorously their solution is the well known iterative procedure. However, these equations are still many-particle ones and the application of this method is practically impossible. In the present study an alternative approach is proposed which is based on a statistical thermodynamic treatment of the problem [15]. The basic idea is that instead of solving the coupled equations (4) and (5) one can express the unknown quantities in equation (4) in terms of the wavefunction Φ to obtain a mean field self-consistent equation.

The possibility of completing such a program is provided by combination of statistical and non-equilibrium thermodynamics of irreversible processes. Due to conservation of the system energy, the conditional energy of the subsystem can be calculated by

$$\bar{E}_S(r, t) = \bar{E}_S + \bar{E}_B - \bar{E}_B(r, t). \quad (6)$$

However, neither S nor B are isolated parts and usage of the energy as a function of state is not appropriate. As mentioned before, the whole system is at thermodynamic equilibrium. This means that during the evolution of the considered microscopic processes no change in the macroscopic state takes place. For this reason, all thermodynamic parameters of the system like its volume V , temperature T , etc, remain constant. According to the thermodynamics, the characteristic function of the subsystem at constant N , V and T is the free energy F which can be related to the subsystem energy via the Gibbs–Helmholtz equation

$$E = \frac{\partial(\beta F)}{\partial \beta}$$

where $\beta = (kT)^{-1}$ and k is the Boltzmann constant. Using this relation and equation (6), equation (4) can be rewritten as

$$i\hbar \frac{\partial \Phi}{\partial t} = \hat{H}_S \Phi + \frac{\partial(\beta \delta F)}{\partial \beta} \Phi \quad (7)$$

where $\delta F = \bar{F} - \tilde{F}$ is the difference between the mean and conditional free energies of the subsystem. This equation is a Schrödinger one for a subsystem interacting weakly with an equilibrium bath having temperature T .

Let us consider first the case of the quasistatic evolution of the microscopic processes. In the framework of the theory of equilibrium thermodynamic fluctuations [16], the probability density of finding the subsystem at a given state is exponentially proportional to the derivation of the subsystem's free energy from its equilibrium value, i.e.

$$\delta F_e \propto kT \ln |\Phi|^2.$$

Therefore, equation (7) takes the form

$$i\hbar \frac{\partial \Phi}{\partial t} = \hat{\mathcal{H}}_S \Phi + \frac{\partial \ln |\Phi|^2}{\partial \beta} \Phi. \quad (8)$$

Equation (8) is a mean-field Schrödinger equation describing the quasistatic fluctuations of the particles configuration in the subsystem. Its solution is

$$\Phi_n = \exp \left[\frac{\bar{F} - E_n}{2kT} - \frac{it\bar{E}_S}{\hbar} \right] \varphi_n(\mathbf{r}) \quad (9)$$

where $\{E_n(N, V), \varphi_n(\mathbf{r}, N, V)\}$ is the set of eigenvalues and normalized eigenfunctions of the subsystem Hamiltonian satisfying the ordinary stationary Schrödinger equation

$$\hat{\mathcal{H}}_S \varphi_n = E_n \varphi_n.$$

One can calculate from equation (9) the probability density of finding the subsystem at a given configuration if the number of particles N , volume V and temperature T are constant:

$$|\Phi_n|^2 = \exp \left[\frac{\bar{F} - E_n}{kT} \right] |\varphi_n|^2. \quad (10)$$

As seen, this is the well known quantum canonical Gibbs distribution. The average free energy of the subsystem can be obtained by the normalization of equation (10) and the result

$$\bar{F}(N, V, T) = -kT \ln \sum_n \exp(-E_n/kT)$$

coincides with the equilibrium statistical thermodynamics expression [16].

The fact that the probability density provided by equation (8) is time independent is not surprising because it was derived in a quasistatic approximation. To take into account the relaxation processes one should complete equation (8) by the irreversible part δF_i of the free energy changes to obtain

$$i\hbar \frac{\partial \Phi}{\partial t} = -\frac{\hbar^2}{2} \nabla \cdot \mathbf{M}^{-1} \cdot \nabla \Phi + U \Phi + \frac{\partial \ln |\Phi|^2}{\partial \beta} \Phi + \frac{\partial (\beta \delta F_i)}{\partial \beta} \Phi. \quad (11)$$

For the sake of further considerations, the exact form of the subsystem Hamiltonian is introduced in equation (11). Here $\nabla \equiv (\partial/\partial \mathbf{r})$ is a $3N$ dimensional nabla operator, \mathbf{M} is the $3N \times 3N$ diagonal mass matrix and U is the subsystem potential energy. Equation (11) requires an expression for δF_i . As has been demonstrated [15], the probabilistic presentation of the quantum mechanics is more appropriate for doing this. In general, the complex wavefunction Φ can be presented by two real functions, ρ and Ω , as

$$\Phi = \sqrt{\rho} \exp(i\Omega). \quad (12)$$

It is clear that $\rho \equiv |\Phi|^2$ is the probability density. Substituting expression (12) in equation (11) the latter splits into two new equations corresponding to the real and imaginary parts:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0 \quad (13)$$

$$\frac{\partial(\mathbf{M} \cdot \mathbf{v})}{\partial t} + \mathbf{v} \cdot \nabla(\mathbf{M} \cdot \mathbf{v}) = -\nabla \left[\frac{1}{\sqrt{\rho}} \hat{H}_S \sqrt{\rho} + \frac{\partial \ln \rho}{\partial \beta} + \frac{\partial(\beta \delta F_i)}{\partial \beta} \right]. \quad (14)$$

The velocity $3N$ dimensional vector \mathbf{v} is introduced here via the relation

$$\mathbf{M} \cdot \mathbf{v} = \hbar \nabla \Omega. \quad (15)$$

Equation (13) is the continuity equation in the probability space while equation (14) is the 'momentum balance' there.

The introduction of ρ and \mathbf{v} instead of Φ by relations (12) and (15) helps to model the irreversible part of the free energy production. According to the linear non-equilibrium thermodynamics [16], a linear relationship between the gradient of δF_i and velocity \mathbf{v} exists

$$\nabla \delta F_i = \mathbf{B} \cdot \mathbf{v} \quad (16)$$

where \mathbf{B} is the $3N \times 3N$ friction matrix being positively defined. In general, \mathbf{B} is a function of the particle coordinate \mathbf{r} and in the nonlinear case of the velocity \mathbf{v} . Introducing equation (16) in equation (14), the following equation is obtained:

$$\frac{\partial(\mathbf{M} \cdot \mathbf{v})}{\partial t} + \mathbf{v} \cdot \nabla(\mathbf{M} \cdot \mathbf{v}) + \frac{\partial(\beta \mathbf{B} \cdot \mathbf{v})}{\partial \beta} = -\nabla \left(-\frac{\hbar^2}{2\sqrt{\rho}} \nabla \cdot \mathbf{M}^{-1} \cdot \nabla \sqrt{\rho} + U + \frac{\partial \ln \rho}{\partial \beta} \right). \quad (17)$$

Equations (13) and (17) are a self-consistent system of differential equations providing the probability density evolution in the subsystem configuration space. Once the solution for ρ and \mathbf{v} has been obtained, one can reconstruct the wavefunction Φ by means of equations (12) and (15). Since at equilibrium $\mathbf{v} = 0$, according to equation (17) the equilibrium probability density is given by the canonical Gibbs distribution (10) again. In the case of high friction limit the first two inertial terms of equation (17) can be neglected compared to the third one and after integration of the result over β one gets the following expression for the velocity:

$$\mathbf{v} = -kT \mathbf{B}^{-1} \cdot \nabla \int_0^\beta \left(-\frac{\hbar^2}{2\sqrt{\rho}} \nabla \cdot \mathbf{M}^{-1} \cdot \nabla \sqrt{\rho} + U + \frac{\partial \ln \rho}{\partial \beta} \right) d\beta.$$

Introducing this into the continuity equation (13) the latter acquires the form

$$\frac{\partial \rho}{\partial t} = \nabla \cdot \mathbf{B}^{-1} \cdot \left[\rho \nabla U + kT \rho \nabla \int_0^\beta \left(\frac{\partial \ln \rho}{\partial \beta} - \frac{\hbar^2}{2\sqrt{\rho}} \nabla \cdot \mathbf{M}^{-1} \cdot \nabla \sqrt{\rho} \right) d\beta \right]. \quad (18)$$

Note that this equation is self-consistent only if \mathbf{B} is independent of the velocity \mathbf{v} . The last term in the small brackets of equation (18) is the so-called 'quantum potential' which disappears in the classical limit $\hbar \rightarrow 0$. In this case, equation (18) reduces to a Fokker-Planck equation

$$\frac{\partial \rho}{\partial t} = \nabla \cdot \mathbf{B}^{-1} \cdot (\rho \nabla U + kT \nabla \rho)$$

which is a basic result of the theory of classical Markov diffusion processes and provides as equilibrium solution the Gibbs-Boltzmann configuration distribution.

Finally, let us apply our theory to the simplest model of a subsystem, i.e. an ideal gas. In this case all subsystem particles are identical and not interacting with each other. The mass

and friction matrices are given by $\mathbf{M} = m\mathbf{I}$ and $\mathbf{B} = b\mathbf{I}$ where \mathbf{I} is the $3N \times 3N$ dimensional unit matrix, m and b are the mass and friction coefficient of a particle, respectively. The potential energy U is due only to external fields and is modelled in the present study by

$$U = \frac{1}{2}m\omega^2 r^2 - f \cdot r.$$

In this harmonic presentation f is a constant force. It is well known that the quantum equilibrium distribution of a harmonic oscillator being the sum over the quantum states of the expression (10) is Gaussian. For this reason we are looking for a solution of equation (18) in the form of a normal distribution function

$$\rho(r, t) = \frac{1}{\sqrt{(2\pi\sigma^2)^{3N}}} \exp\left[-\frac{(r - \bar{r})^2}{2\sigma^2}\right].$$

Substituting the above expressions in equation (18), the following two equations describing the evolution of the average configuration \bar{r} and dispersion σ^2 are derived:

$$b \frac{\partial \bar{r}}{\partial t} + \left[m\omega^2 - \frac{\hbar^2 kT}{4m} \int_0^\beta \frac{1}{\sigma^4} d\beta \right] \bar{r} + \frac{\hbar^2 kT}{4m} \int_0^\beta \frac{\bar{r}}{\sigma^4} d\beta = f \quad (19)$$

$$\frac{b}{2} \frac{\partial \sigma^2}{\partial t} + \left[m\omega^2 - \frac{\hbar^2 kT}{4m} \int_0^\beta \frac{1}{\sigma^4} d\beta \right] \sigma^2 = kT. \quad (20)$$

As seen, both equations are affected by quantum effects. In the classical limit these equations reduce to well known results. While equation (19) describes the average response against a constant external force, equation (20) is relevant to quantum Brownian motion and diffusion. The quantum terms complicate finding the solutions of these equations. The only simple results we have obtained are the equilibrium expressions

$$\bar{r}_e = \frac{f}{m\omega^2}$$

$$\sigma_e^2 = \frac{\hbar}{2m\omega} \coth\left(\frac{\hbar\omega}{2kT}\right)$$

which coincide with the expressions provided by the equilibrium statistical mechanics [8].

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