Chapter 3

Nonequilibrium Thermodynamic and Quantum Model of a Damped Oscillator

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Additional information is available at the end of the chapter

http://dx.doi.org/10.5772/61010

Abstract

We describe the linearly damped harmonic quantum oscillator in Heisenberg’s interpretation by Onsager’s thermodynamic equations. Ehrenfest’s theorem is also discussed in this framework. We have also shown that the quantum mechanics of the dissipative processes exponentially decay to classical statistical theory.

Keywords: quantum oscillator, damping, Onsager’s theory, Ehrenfest’s theory, classic limit

1. Introduction

Dissipation is essential for the evolution of a quantum-damped oscillator. It is responsible for the decay of quantum states, the broadening of the spectral line, and the shifting the resonance frequency. This has been a persistent challenge for a long time since dissipation causes difficulties in the quantization of the damped oscillator [1, 2, 3]. This problem has remained under intensive investigation [4, 5]. There are some widely accepted Hamilton-like variation theories about the treatment of a linearly damped classic or quantum-damped oscillator. One of these theories is Bateman’s mirror-image model [1], which consists of two different damped oscillators, where one of them represents the main linearly damped oscillator. The energy dissipated by the main oscillator will be absorbed by the other amplified oscillator, and thus the energy of the total system will be conserved. The fundamental commutation relations of this model are time independent; however, the time-dependent uncertainty products, obtained in this way, vanish as time tends to infinity [6]. The Caldirola–Kanai theory with an explicit
time-dependent Hamiltonian is another kind of variation theory [7, 8, 9]. In the quantum version of this theory, both the canonical commutation rules and the uncertainty products tend to zero as time tends to infinity. The system-plus-reservoir model [10, 11] is another damped oscillator model. It is coupled linearly to a fluctuating bath. If the bath is weakly perturbed by the system, then it can be modeled with a continuous bath of the harmonic oscillator. A quantum Langevin equation in the form of a Heisenberg operator differential equation can be deduced in this model. However, this equation in general does not obey Onsager’s regression hypothesis [12], i.e., only in case when $\hbar \to 0$ [13]. A direct consequence of this fact is that the expected value of the fundamental observable does not satisfy the equation of the classic linearly damped oscillator. Another consequence is that no spontaneous dissipative process exists in this theory. The above models are based on the Heisenberg’s mechanical reinterpretation model [14].

A possible reinterpretation model based on irreversible thermodynamics was recently published [15]. This model started from the Rosen–Chambers restricted variation principle of the nonequilibrium thermodynamics [16, 17, 18] and used a Hamilton-like variation approach to the linearly damped oscillator. The usual formalisms of classical mechanics, such as the Lagrangian, Hamiltonian, and Poisson brackets, were also covered by this variational principle. By means of canonical quantization, the quantum mechanical equations of the linearly damped oscillator are given. The resulting Heisenberg operator differential equations of the damped oscillator are consistent with the classical equations of motion and can be solved by using ladder operators, which are time dependent. By this theory, the exponential decay of quantum states, the natural width of the spectral line, and the shifts in the resonance frequency can be explained. This work describes the quantum theory of a linearly damped oscillator, which could be reinterpreted in terms of a classical model based on Onsager’s nonequilibrium thermodynamic theory, corresponding to the Heisenberg reinterpretation principle. The first chapters are devoted to Onsager’s thermodynamic theory and the quantum theory of a damped oscillator. The dissipative quantum theory given in the Heisenberg picture is deduced from the general evolution equation of a Hermitian observable by means of two system-specific constitutive equations. The first of the constitutive equations belongs to unitary dynamics, while the second belongs to the dissipative dynamics of the observable. The fundamental commutators, which are a consequence of the constitutive equations, are time dependent. The quantum mechanical equations of motion of the oscillator in the Heisenberg picture, the Ehrenfest theorem, and the uncertainty principle of that oscillator are given. A significant part of the work deals with applications such as the expected value of the main operators of the damped oscillator, the probability description of the wave packet motion belonging to the damped oscillator, the calculation of the wave function by matrix calculus, the spectral density of the energy dissipation, and the natural width of the spectral line. Another significant part of this work deals the quantum statistics of the damped oscillator. By a generalization of the Liouville–von Neumann equation, the statistical thermodynamic theory of the ensemble of the damped oscillators in contact with a thermal bath is given. By introducing the quantum entropy of the ensemble, it is shown that the entropy of the ensemble grows in a dissipative process and in thermal equilibrium for the probability distribution of the quantum states, such that Gibbs’ canonical distribution is valid. Finally, a wave equation of the linearly damped oscillator is given.
2. Nonequilibrium thermodynamic theory of the linearly damped oscillator

Meixner was the first to propose a nonequilibrium thermodynamic theory for linear dissipative networks [19, 20]; for a general overview on network thermodynamics, see [21]. In this theory, it can be shown that, for example, electrical networks are thermodynamic systems, and it is possible to derive the network equations (Kirchhoff equations) by application of the principles of nonequilibrium thermodynamics. In what follows, we give an Onsagerian thermodynamic theory of the linearly damped harmonic oscillator. A damped oscillator, as a primitive network, is considered under the isotherm condition, which is maintained by removing the irreversible heat as it developed in damping resistance, or in other words, by placing the damping resistance of the oscillator in a temperature bath. In this case, it is possible to speak not only of the entropy of the damped oscillator but also of the free energy, and not of entropy production but of energy dissipation instead. To show these, we give the actual form of the first law of thermodynamics in the case of a damped oscillator. To do this, let us introduce from the energy conservation law of the oscillator + thermal bath system (Figure 1), such that we obtain the following:

\[
\frac{d}{dt}(U + U_{\text{bath}}) = 0 \rightarrow \frac{dU}{dt} = -\frac{dU_{\text{bath}}}{dt}
\]  

(1)

where \( U \) and \( U_{\text{bath}} \) are the internal energies of the oscillator and the thermal bath. Since the oscillator is isolated by a rigid diathermal wall, the energy exchange between the oscillator and the bath must be heat transfer only. Thus, the first law of thermodynamics of the oscillator and the thermal bath has the following forms

\[
\frac{dU}{dt} = \frac{dQ}{dt} - \frac{dU_{\text{bath}}}{dt} = \frac{dQ}{dt}
\]  

(2)

where \( \frac{dQ}{dt} \) is the power of exchanged heat on the rigid diathermal wall.

Figure 1. Mechanical equivalent circuit of a linearly damped oscillator.
Assume that the entropy $S$ of the oscillator exists, and it is a state function of the variables $U, q$. By the second law of nonequilibrium thermodynamics, the entropy $S(U, q)$ satisfies the balanced equation:

$$\frac{dS}{dt} = \frac{dS_r}{dt} + \frac{dS_i}{dt}, \quad \frac{dS}{dt} \geq 0$$

(3)

where $\frac{dS_r}{dt}$ is the reversible rate of change of the entropy or entropy flux on the rigid diathermal wall and $\frac{dS_i}{dt}$ is the so-called entropy production. From the second law of the thermodynamics follows the well-known expression for entropy flux:

$$\frac{dS_r}{dt} = \frac{1}{T} \frac{dQ}{dt}$$

(4)

On the other hand, the rate of change in the entropy of the oscillator can be written as

$$\frac{dS}{dt} = \frac{\partial S}{\partial U} \frac{dU}{dt} + \frac{\partial S}{\partial q} \frac{dq}{dt}$$

(5)

From this equation and Equations (2) and (4), the following relations can result:

$$\frac{\partial S}{\partial U} \frac{1}{T'} \frac{dS_i}{dt} = \frac{\partial S}{\partial q} \frac{dq}{dt} \geq 0$$

(6)

Thus, the entropy balance equation has the form

$$\frac{dS}{dt} = \frac{1}{T} \frac{dQ}{dt} + \frac{\partial S}{\partial q} \frac{dq}{dt}$$

(7)

Because the temperature of the oscillator is constant, we could introduce

$$F = U - TS$$

(8)

i.e., the free energy of the oscillator, and from Equations (2) and (7), we can obtain the simple balanced equation for free energy

$$\frac{dF}{dt} = -T \frac{\partial S}{\partial q} \frac{dq}{dt} \leq 0$$

(9)
Also, entropy production and the so-called rate of energy dissipation

\[ R = T \frac{dS}{dt} = T \frac{\partial S}{\partial q} \frac{dq}{dt} \geq 0 \]  

(10)

decrease the free energy of the oscillator. In what follows, we shall give the actual form of the rate of energy dissipation. Next, we see from Equation (10) that the rate of energy dissipation must be some explicit function of \( \frac{dq}{dt} \) and may depend implicitly on \( U, q \) and the following equation

\[ R = R(\frac{dq}{dt}; U, q) \geq 0 \]  

(11)

such that

\[ R(0; U, q) = 0 \]  

(12)

is therefore quite general. We now expand the energy dissipation Equation (11) in a Taylor series, i.e.,

\[ R = A_0 + A_1 \frac{dq}{dt} + \frac{1}{2} A_2 \left( \frac{dq}{dt} \right)^2 + \ldots \]  

(13)

The sufficient condition of nonnegativity of entropy production, which will always be satisfied, is the complete exclusion of all odd terms in \( \frac{dq}{dt} \) in Equation (13), and \( A_0 \) must be zero to exclude entropy production in an equilibrium state. Thus, one need only neglect the fourth-order term in the Taylor series (Equation (13)) to obtain the Rayleigh dissipation function

\[ R = c \left( \frac{dq}{dt} \right)^2, \quad c = \frac{1}{2} A_2 \]  

(14)

In addition, the so-called damping constant of oscillator \( c \) must be positive to satisfy the nonnegativity condition in Equation (13). If we assume that the nondissipative elements of the damped oscillator are linear, then the free energy in Equation (8) can be identified with the energy stored in the mass \( m \) and the spring of the oscillator (Figure 1.). Also, the free energy is equal to the Hamiltonian of the oscillator, i.e.,
where $q$ is the displacement of the mass from its equilibrium position, $p$ is the momentum of the mass of the oscillator, and $k$ is the constant of the spring. A direct consequence of the above results is that $R$ can be constructed as a bilinear form, namely,

$$
R = -\frac{dH}{dt} = \frac{dq}{dt} \left( -\frac{\partial H}{\partial q} \right) + \frac{dp}{dt} \left( -\frac{\partial H}{\partial p} \right) \geq 0
$$

Here we now interpret, in the usual nonequilibrium thermodynamic fashion, the quantities $\left(\frac{dq}{dt}, \frac{dp}{dt}\right)$ in terms of thermodynamic fluxes and the quantities $\left(-\frac{\partial H}{\partial q}, -\frac{\partial H}{\partial p}\right)$ in terms of thermodynamic forces. Since we now have Equation (14) of the rate of energy dissipation of the damped oscillator, Equation (16) can be written in the form

$$
\frac{dq}{dt} \left( -\frac{\partial H}{\partial q} \right) + \frac{dp}{dt} \left( -\frac{\partial H}{\partial p} \right) = \epsilon \left( \frac{dq}{dt} \right)^2 \geq 0
$$

In Onsagerian thermodynamics, the constitutive (kinetic) equations between fluxes and forces are linear

$$
\begin{bmatrix}
\frac{dq}{dt} \\
\frac{dp}{dt}
\end{bmatrix} =
\begin{bmatrix}
L_{qq} & L_{qp} \\
L_{pq} & L_{pp}
\end{bmatrix}
\begin{bmatrix}
-\frac{\partial H}{\partial q} \\
-\frac{\partial H}{\partial p}
\end{bmatrix}
$$

where the kinetic matrix

$$
L =
\begin{bmatrix}
L_{qq} & L_{qp} \\
L_{pq} & L_{pp}
\end{bmatrix}
$$

can be split into nondissipative (so-called reactive) and dissipative parts. To do this, take these kinetic equations into Equation (17), and using Equation (15), with a simple calculation, we obtain for these kinetic matrices
Here, $a$ is an arbitrary constant. Now, we see that the dissipative part of the kinetic matrix satisfies the Onsager symmetry relation and the positivity of the damping constant $c$ trivially. The constant $a$ can be evaluated as follows. In the case of zero for the dissipative part of the kinetic matrix, these equations must be transformed into Hamilton equations of a simple harmonic oscillator. From this fact, it follows that $a$ is a universal constant and $a=1$. Also, the final form of the Onsagerian constitutive (kinetic) equation of damped oscillator is

$$
\begin{bmatrix}
\frac{dq}{dt} \\
\frac{dp}{dt}
\end{bmatrix} = \left(\begin{bmatrix}
0 & -a \\
a & 0
\end{bmatrix} + \begin{bmatrix}
0 & 0 \\
0 & c
\end{bmatrix} \right) \begin{bmatrix}
-\frac{\partial H}{\partial q} \\
-\frac{\partial H}{\partial p}
\end{bmatrix}
$$

Here, $a$ is an arbitrary constant. Now, we see that the dissipative part of the kinetic matrix satisfies the Onsager symmetry relation and the positivity of the damping constant $c$ trivially. The constant $a$ can be evaluated as follows. In the case of zero for the dissipative part of the kinetic matrix, these equations must be transformed into Hamilton equations of a simple harmonic oscillator. From this fact, it follows that $a$ is a universal constant and $a=1$. Also, the final form of the Onsagerian constitutive (kinetic) equation of damped oscillator is

$$
\begin{bmatrix}
\frac{dq}{dt} \\
\frac{dp}{dt}
\end{bmatrix} = \left(\begin{bmatrix}
0 & -1 \\
1 & 0
\end{bmatrix} + \begin{bmatrix}
0 & 0 \\
0 & c
\end{bmatrix} \right) \begin{bmatrix}
-\frac{\partial H}{\partial q} \\
-\frac{\partial H}{\partial p}
\end{bmatrix}
$$

It is easy to show that these kinetic equations are equivalent to the Newtonian equations of motion of the linearly damped oscillator, namely,

$$
\frac{dq}{dt} = \frac{\partial H}{\partial p} = \frac{p}{m}, \quad \frac{dp}{dt} = -\frac{\partial H}{\partial q} - c \frac{\partial H}{\partial p} = -kq - c \frac{p}{m}
$$

From this equivalence, it follows that the velocity of oscillator as a generalized thermodynamic flux has only a reactive part, while the rate of momentum, as another thermodynamic flux, has both reactive and dissipative constituents. The presented thermodynamic deduction of equations of a linearly damped oscillator enables us to build a stochastic force $F_s$ into equations of motion (Equation (22)). This stochastic force and the thermodynamic forces introduced above are statistically independent and take into account the effect of the temperature bath. In this case, the thermodynamic fluxes are fluctuations, which obey another type of equation (Equation (22)). The correct form of these equations follows from the regression hypothesis of Onsager [22], which states that “the average regression of fluctuations will obey the same laws as the corresponding macroscopic irreversible process.” From this, we give the Langevin-type equations for a linearly damped oscillator,

$$
\frac{dq}{dt} = \frac{\partial H}{\partial p}, \quad \frac{dp}{dt} = -\frac{\partial H}{\partial q} - c \frac{\partial H}{\partial p} + F_s
$$
A consequence of these equations is that the dissipative kinetic coefficient $c$ can be related to the correlation coefficient $\langle p(t), p(t + t') \rangle$ via the fluctuation dissipation theorem [23, 24]. According to Equation (22), we can conclude that the fluctuations of thermodynamic fluxes are similar to an impressed macroscopic deviation, except they appear spontaneously.

**2.1. Bohlin’s first integral**

By means of Equation (21) or (22), we can deduce the time rate of change of any observable defined in the phase space of the damped oscillator. Let $O(q, p, t)$ be an observable, such that its time rate of change can be expressed as

$$
\frac{dO}{dt} = \frac{\partial O}{\partial t} + \frac{\partial O}{\partial q} \frac{dq}{dt} + \frac{\partial O}{\partial p} \frac{dp}{dt} = \frac{\partial O}{\partial q} \frac{dq}{dt} - \frac{\partial O}{\partial p} \frac{dp}{dt} - \frac{\partial O}{\partial H} \frac{dH}{dt} - c \frac{\partial O}{\partial p} \frac{\partial O}{\partial q} \frac{dq}{dt} - c \frac{\partial O}{\partial p} \frac{\partial O}{\partial q} \frac{dp}{dt} \tag{24}
$$

where we take into account the Onsagerian equations (Equation (22)). An observable $O(q, p, t)$ is the first integral of the (Onsagerian equation (Equation (21)) of the damped oscillator if

$$
\frac{dO}{dt} = 0 \tag{25}
$$

and if it is a constant of the motion. Now, let us give the constant of the motion of the linearly damped harmonic oscillator. It was Bohlin [25] who first dealt with the problem of the constants of motion for a damped linear oscillator. It is easy to prove that Bolin’s observable, defined as

$$
B(q, p, t) = \frac{m}{2} e^{2\beta t} \left( \frac{dq}{dt} - \gamma q \right) - \frac{\gamma^* q}{\gamma q - \gamma^* q} \tag{26}
$$

where

$$
\beta = \frac{c}{2m}, \omega_0 = \sqrt{\frac{k}{m}}, \gamma = -\beta + i\omega, \quad \gamma^* = -\beta - i\omega, \quad \omega = \sqrt{\omega_0^2 - \beta^2} \tag{27}
$$

is the first integral of the damped oscillator. Now, we may see that the Bolin’s observable in the case of the undamped oscillator is equal to the Hamiltonian of the oscillator.
3. Quantum theory of linearly damped oscillator

In the standard theory of quantum mechanics, two kinds of evolution processes are introduced, which are qualitatively different from each other. One is the spontaneous process, which is a reactive (unitary) dynamical process and is described by the Heisenberg or Schrödinger equation in an equivalent manner. The other is the measurement process, which is irreversible and described by the von Neumann projection postulate [26], which is the rigorous mathematical form of the reduction of the wave packet principle. The former process is deterministic and is uniquely described, while the latter process is essentially probabilistic and implies the statistical nature of quantum mechanics.

3.1. The general evolution equation of the Hermitian operator

Unlike classical quantum mechanics, the spontaneous processes of the damped oscillator are irreversible, so its quantum mechanical description needs changes to some instruments of classical quantum mechanics. To do this, we use the Heisenberg picture of quantum processes. In this picture, the observables are time-dependent linear Hermitian operators, and the state vector of the system is time independent. Using the terminology introduced in the first part, the infinitesimal time transformation of the Hermitian operator could happen in two ways:

• By reactive transformation, when the orthonormal eigenvectors of the Hermitian observable turn in time, keeping the orthonormal system with unchanged eigenvalues. The eigenvectors belonging to the different moments are connected with unitary transformation, as in classic quantum mechanics. Dynamics belonging to this transformation are so-called unitary dynamics.

• By dissipative transformation, when the real eigenvalues of the Hermitian operator change irreversibly in time.

Let us study the general evolution equation of the Hermitian operator, considering both the above time-dependent processes. For simplicity in demonstrating the derivation, we suppose a discrete eigenvalue spectrum of the Hermitian operator, although the spectra of the displacement and momentum operators could be continuous. In this case, the orthonormal eigenvectors \( |\Psi_{\lambda_i}(t)\rangle \) and eigenvalues \( \lambda_{\lambda_i}(t) \) are solutions of the eigenvalue equation

\[
O(t)|\Psi_{\lambda_i}(t)\rangle = \lambda_{\lambda_i}(t)|\Psi_{\lambda_i}(t)\rangle, \quad (i = 1, 2, 3,...)
\]

and the eigenvectors form a complete orthonormal basis in a Hilbert space, when the eigenvalue spectrum is nondegenerate. Thus, the spectral representation of the operator would be

\[
O(t) = \sum_{\lambda_{\lambda_i}} |\Psi_{\lambda_i}(t)\rangle \langle \Psi_{\lambda_i}(t)|, \quad \delta = \sum_{\lambda_{\lambda_i}} |\Psi_{\lambda_i}(t)\rangle \langle \Psi_{\lambda_i}(t)|
\]
where $\delta$ is the unity operator and $\langle \Psi_{O_i}(t) \rangle$ is the dual of $|\Psi_{O_i}(t)\rangle$, so $\langle \Psi_{O_i}(t) \rangle|\Psi_{O_i}(t)\rangle = 1$.

Since the observable is Hermitian, the transformation of the eigenvector $|\Psi_{O_i}(0)\rangle$ at $t=0$ to the eigenvector $|\Psi_{O_i}(t)\rangle$ at time $t$ will be represented by a unitary operator $U(t)$. Hence,

$$|\Psi_{O_i}(t)\rangle = U(t)|\Psi_{O_i}(0)\rangle, \quad \langle \Psi_{O_i}(t) | = U^*(t)\langle \Psi_{O_i}(0) |, \quad U(t)U^*(t) = \delta$$

Let us substitute Equation (30) into Equation (29), then we obtain

$$O(t) = \sum_{i>0} \lambda_{O_i}(t)U(t)|\Psi_{O_i}(0)\rangle\langle \Psi_{O_i}(0) |U^*(t)$$

The time derivative of the operator is

$$\dot{O}(t) = \sum_{i>0} \lambda_{O_i}(t)U(t)|\Psi_{O_i}(0)\rangle\langle \Psi_{O_i}(0) |U^*(t) +$$

$$+ \sum_{i>0} \lambda_{O_i}(t)\dot{U}(t)|\Psi_{O_i}(0)\rangle\langle \Psi_{O_i}(0) |U^*(t) +$$

$$+ \sum_{i>0} \lambda_{O_i}(t)U(t)|\Psi_{O_i}(0)\rangle\langle \Psi_{O_i}(0) |\dot{U}^* +$$

or by using the instantaneous eigenvectors, $|\Psi_{O_i}(t)\rangle$ can be written as

$$\dot{O}(t) = \sum_{i>0} \lambda_{O_i}(t)U(t)|\Psi_{O_i}(0)\rangle\langle \Psi_{O_i}(0) |U^*(t) +$$

$$+ \sum_{i>0} \lambda_{O_i}(t)\dot{U}(t)|\Psi_{O_i}(0)\rangle\langle \Psi_{O_i}(0) |U^*(t) +$$

$$+ \sum_{i>0} \lambda_{O_i}(t)U(t)|\Psi_{O_i}(0)\rangle\langle \Psi_{O_i}(0) |\dot{U}^* +$$

$$= \sum_{i>0} \lambda_{O_i}(t)|\Psi_{O_i}(t)\rangle\langle \Psi_{O_i}(t) | + \dot{U}(t)U^*(t)\left(\sum_{i>0} \lambda_{O_i}(t)|\Psi_{O_i}(t)\rangle\langle \Psi_{O_i}(t) |\right) +$$

$$+ \left(\sum_{i>0} \lambda_{O_i}(t)|\Psi_{O_i}(t)\rangle\langle \Psi_{O_i}(t) |\right)U(t)\dot{U}^* +$$

$$\dot{U}(t)U^*(t)O(t) + O(t)U(t)\dot{U}^*$$

Using the identity $\dot{U}(t)U^* = -U(t)U$, which is a consequence of unitarity, the general evolution equation of the Hermitian operator results
\[ \dot{O}(t) = \frac{\partial O(t)}{\partial t} + \left[ \dot{U}(t) U^*(t), O(t) \right], \quad (34) \]

\[ \frac{\partial O(t)}{\partial t} := \sum_{j=0}^\lambda \omega_j (t) \left| \Psi_j (t) \right\rangle \left\langle \Psi_j (t) \right| \]

where [ , ] is Dirac’s symbol of a quantum mechanical commutator and \( \frac{\partial O(t)}{\partial t} \) is the local time rate of change of the operator in the coordinate system of the instantaneous eigenvectors. This equation is universal in the meaning of its independence of the constitutive behavior of the quantum system.

### 3.2. The Heisenberg equation of motion of the linearly damped oscillator

The actual form of Heisenberg’s dynamic equation can be constructed when the expression

\[ U(t) U^*(t) \]

is formed from the unitary operator and the local rate of change of the operator \( \frac{\partial O(t)}{\partial t} \) can be connected to the constitutive properties of the studied physical system. The first term will be ordered to the unitary/reactive and the second to the dissipative dynamics. To do this, we accept Heisenberg’s reinterpretation principle [14] (for the philosophical details of this principle, see [27]), which states the possibility of constructing a quantum mechanical description of a physical system whose classical description is known. In our case, the physical system is a linearly damped oscillator, for which we know its Onsagerian thermodynamic description. This description uses the Hamiltonian and the rate of energy dissipation of the system represented by the Rayleigh potential. Since the Hamiltonian is not the first integral of the motion, Bohlin’s first integral could be used for the unitary dynamics. In classical quantum theory, the Hamiltonian belongs to the unitary dynamics as a constitutive property, i.e.,

\[ \frac{i}{\hbar} H = \dot{U}(t) U^*(t) \]

(35)

where the Hamilton operator \( H \) is a first integral of the system. In a closed physical system, the local time derivative of the observables is zero since the system is reactive. On this basis, the constitutive equations of classical quantum mechanics are

\[ \frac{i}{\hbar} H = \dot{U}(t) U^*(t), \quad \frac{\partial O(t)}{\partial t} = 0 \]

(36)

With these constitutive equations from Equation (34), the general evolution equation we give to Heisenberg’s equation of the observable is

\[ \dot{O} = \frac{i}{\hbar} [H, O] \]

(37)
Also, the all constitutive properties of the quantum system are contained in the Hamilton operator only, which could have originated from the Hamilton function of the classical model by means of Heisenberg’s reinterpretation principle. Figure 2 shows the above-presented scheme of the deduction of Heisenberg’s equation of motion.

![Figure 2](image)

**Figure 2.** The schema of the deduction of Heisenberg’s equation of motion of a Hermitian operator and the role of Heisenberg’s reinterpretation principle.

The Hamiltonian $H$ is a trivial nullifier of Dirac’s commutator in this approach, so $H$ is a conserved observable of motion, as was requested. To summarize, we get Heisenberg’s classical Equation (37) from the general evolution Equation (34), if the $\frac{\partial O(t)}{\partial t}$ local rate of change of the operator in the coordinate system of the instantaneous eigenvectors is zero. In the case of the Heisenberg’s equation (Equation (37)), the entropy of the system is constant in time, as proven by von Neumann [26]. However, the entropy cannot remain constant in dissipative processes. Consequently, in a correct description of the dissipative system, it is possible to take into account the local rate of change of the operator. In the case of a damped oscillator, this means that for the time rate of change $\frac{\partial q(t)}{\partial t}, \frac{\partial p(t)}{\partial t}$ of two fundamental observables of a linearly damped oscillator must be given constitutive equations. In this way, we assume that the constitutive equations of the linearly damped oscillator are

$$\frac{\partial q(t)}{\partial t} = -\beta q(t), \quad \frac{\partial p(t)}{\partial t} = -\beta p(t), \quad \frac{i}{\hbar} B = \dot{U}(t)U^\dagger(t)$$

(38)

where the Hermitian operator $B$ belonging to unitary/reactive dynamics is the quantum mechanical equivalent of Bohlin’s constant in Equation (26). Following Equation (26), this could be written as

$$B = e^{2\beta t} \left( \frac{p^2}{2m} + \frac{\beta}{2} pq + \frac{\beta}{2} qP + \frac{m\omega_b^2}{2} q^2 \right)$$

(39)
Note, the third constitutive equation of (38) is the direct consequence of Stone’s theorem [28]. If we take into account these constitutive equations in the general evolution Equation (34) of the Hermitian operators, then we obtain Heisenberg’s equations of motion of a quantum-damped oscillator

$$\dot{q}(t) = -\beta q(t) + \frac{i}{\hbar} [B, q(t)], \quad = -\beta p(t) + \frac{i}{\hbar} [B, p(t)]$$

(40)

According to Heisenberg’s reinterpretation principle, these equations could be interpreted by means of the Onsagerian equations of the oscillator. To do this, split the Bohlin operator (Equation (39)) into two parts. The first part contains the Hamilton operator $H$ of the oscillator and the second part $D$ belongs to the dissipation. We then obtain

$$q(t) = -\beta q(t) + \frac{i}{\hbar} [B, q(t)] = \left[ \frac{\partial q(t)}{\partial t} + \frac{i}{\hbar} e^{2\beta t} [D, q(t)] \right] + \frac{i}{\hbar} e^{2\beta t} [H, q(t)]$$

$$p(t) = -\beta p(t) + \frac{i}{\hbar} [B, p(t)] = \left[ \frac{\partial p(t)}{\partial t} + \frac{i}{\hbar} e^{2\beta t} [D, p(t)] \right] + \frac{i}{\hbar} e^{2\beta t} [H, p(t)]$$

$$H = \left( \frac{p^2}{2m} + \frac{ma^2}{2} q^2 \right), \quad D = \frac{\beta}{2} (qp + pq)$$

(41)

The expression in $\{\}$ is connected to dissipative thermodynamic current by analogy, while the currents outside the bracket are analogous to reactive currents. This interpretation, analogous to Equation (22), is supported by

$$\frac{\partial q(t)}{\partial t} + \frac{i}{\hbar} e^{2\beta t} [D, q(t)] = 0, \quad \frac{\partial p(t)}{\partial t} + \frac{i}{\hbar} e^{2\beta t} [D, p(t)] = 2 \frac{\partial p(t)}{\partial t} = -2\beta p(t)$$

(42)

where the two first equations of Equation (38) were used. In detail, we could write

$$\frac{\partial q}{\partial t} + \frac{i}{\hbar} e^{2\beta} [D, q] = -\beta q + \frac{\beta}{2} \left( \frac{i}{\hbar} e^{2\beta} [p, q] \right) u + \frac{\beta}{2} q \left( \frac{i}{\hbar} e^{2\beta} [p, q] \right) = 0$$

$$\frac{\partial p}{\partial t} + \frac{i}{\hbar} e^{2\beta} [D, p] = -\beta p - \frac{\beta}{2} p \left( \frac{i}{\hbar} e^{2\beta} [p, q] \right) + \frac{\beta}{2} \left( \frac{i}{\hbar} e^{2\beta} [p, q] \right) = -2\beta p$$

(43)

Now, we could see the desired interpretation analogy could be applied when the commutator relation $e^{2\beta t} [p, q] = \frac{\hbar}{\imath} \delta$ is valid. Since every operator commutes with itself, we also have the fundamental brackets of our quantum theory
\[ \{p, q\} = \frac{i}{\hbar} \delta_{ij}, \quad \{q, p\} = 0, \quad \{p, p\} = 0, \quad \{\cdot, \cdot\} := e^{2i\theta t} \left[ \cdot, \cdot \right] \]  

(44)

Consequently, the first fundamental bracket in Equation (44) ensures that the dissipative part \( \frac{\beta}{2} q p + \frac{\beta}{2} p q \) of the Bohlinian adds \( \beta q(t) \) term to the first equation and the \( -\beta q(t) \) term to the second equation in Equation (41). This allows to us change our attention from Bohlinian to Hamiltonian in Equation (41), obtaining

\[
\begin{align*}
\dot{q}(t) &= \frac{i}{\hbar} e^{2i\theta t} [H(t), q(t)] = \frac{i}{\hbar} \{H(t), q(t)\}, \\
\dot{p}(t) &= -2\beta p(t) + \frac{i}{\hbar} e^{2i\theta t} [H(t), p(t)] = -2\beta p(t) + \frac{i}{\hbar} \{H(t), p(t)\}
\end{align*}
\]

(45)

which are equivalent with the equations

\[
\begin{align*}
\dot{q}(t) &= \frac{i}{\hbar} \{H(t), q(t)\}, \\
\dot{p}(t) &= \frac{i}{\hbar} \{H(t), p(t)\} - c \frac{i}{\hbar} \{H(t), q(t)\}
\end{align*}
\]

(46)

The quantum mechanical equations of a damped oscillator with the fundamental brackets in Equation (44), applying the rules of Lie algebra, are as follows

\[
\begin{align*}
\dot{q}(t) &= \frac{i}{\hbar} \{H(t), q(t)\} = \frac{p(t)}{m}, \\
\dot{p}(t) &= \frac{i}{\hbar} \{H(t), p(t)\} - c \frac{i}{\hbar} \{H(t), q(t)\} = -2\beta p(t) - m\omega_0^2 q(t)
\end{align*}
\]

(47)

which are the operator differential equations version of Onsager’s equations in Equation (22).

To use the Lie algebraic method in an evaluation of the above-introduced time-dependent commutators, it is assumed that the scalar time functions must necessarily be considered as ordinary numbers (for details, see [15]). In summary, according to the Onsagerian equations of the damped oscillator by application of Heisenberg’s reinterpretation principle, the quantum mechanical equation of a damped oscillator in the Heisenberg picture can be obtained.

### 3.3. Ehrenfest theorem of a linearly damped oscillator

It is easy to show, similar to classical quantum mechanics, that the following operator analytics relations are valid [29]

\[
\begin{align*}
\frac{i}{\hbar} \{H, q\} &= \frac{\partial H}{\partial p}, \\
\frac{i}{\hbar} \{H, p\} &= -\frac{\partial H}{\partial q}
\end{align*}
\]

(48)
As a consequence of Equation (48), Equation (47), the quantum mechanical equations of the oscillator, could be written in the form

\[
\dot{\mathbf{q}}(t) = \frac{\partial \mathbf{H}}{\partial \mathbf{p}} = \frac{m}{\hbar} \mathbf{p}(t), \quad \dot{\mathbf{p}}(t) = \frac{\partial \mathbf{H}}{\partial \mathbf{q}} - \frac{c}{\hbar} \frac{\partial \mathbf{H}}{\partial \mathbf{p}} = -2\beta \mathbf{p}(t) - m\omega_0^2 \mathbf{q}(t)
\]

(49)

where the formal equivalence with Onsager’s equations Equation (22) is obvious.

It is well-known in the Heisenberg picture that the expectation value of an operator is defined as

\[
\langle \mathbf{O}(t) \rangle = \langle \Psi | \mathbf{O}(t) | \Psi \rangle
\]

(50)

where \(| \Psi \rangle\) is the time-independent state vector of the oscillator. Thus, from Equation (49), the expectation values of the time rate of change of displacement and momentum can be evaluated as

\[
\begin{align*}
\frac{d\langle \mathbf{q}(t) \rangle}{dt} := & \langle \Psi | \dot{\mathbf{q}} | \Psi \rangle = \frac{i}{\hbar} \langle \Psi | [\mathbf{H}, \mathbf{q}] | \Psi \rangle = \langle \Psi | \frac{\partial \mathbf{H}}{\partial \mathbf{p}} | \Psi \rangle = \frac{1}{m} \langle \Psi | \mathbf{p} | \Psi \rangle = \frac{\langle \mathbf{p}(t) \rangle}{m}, \\
\frac{d\langle \mathbf{p}(t) \rangle}{dt} := & \langle \Psi | \dot{\mathbf{p}} | \Psi \rangle = \frac{i}{\hbar} \langle \Psi | [\mathbf{H}, \mathbf{p}] | \Psi \rangle - c \frac{i}{\hbar} \langle \Psi | [\mathbf{H}, \mathbf{q}] | \Psi \rangle = -\langle \Psi | \frac{\partial \mathbf{H}}{\partial \mathbf{q}} | \Psi \rangle - c \langle \Psi | \frac{\partial \mathbf{H}}{\partial \mathbf{p}} | \Psi \rangle = -m\omega_0^2 \langle \mathbf{q} | \mathbf{q} \rangle - \frac{c}{m} \langle \mathbf{p} | \mathbf{p} \rangle = \\
& = -\frac{c}{m} \langle \mathbf{p}(t) \rangle - m\omega_0^2 \langle \mathbf{q}(t) \rangle
\end{align*}
\]

(51)

where we take into account Equation (49). Also, the expectation values of displacement and momentum of the linearly damped oscillator obey time evolution equations, which are exactly equivalent to those of Onsager’s equations (Equations (21) and (22)). This result is Ehrenfest’s theorem.

4. Evaluation of the equations of the quantum linearly damped oscillator

The solutions of the operator differential equations (Equation (49)) are

\[
\mathbf{q} = \sqrt{\frac{\hbar}{2m\omega_0}} \left( \mathbf{A} e^{\imath \omega t} + \mathbf{A}^* e^{\imath \omega^* t} \right), \quad \mathbf{p} = \sqrt{\frac{\hbar m}{2\omega_0}} \left( \gamma \mathbf{A} e^{\imath \omega t} + \gamma^* \mathbf{A}^* e^{\imath \omega^* t} \right), \quad \mathbf{A} = \mathbf{A} e^{-\beta t}
\]

(52)
By substituting the above two expressions into the first fundamental commutation relation of Equation (44), the time-dependent and time-independent amplitude operators are used to obtain the following commutation relations

\[ \{ A, A^\dagger \} = e^{-2\beta t} \delta \rightarrow [ a, a^\dagger ] = \delta \]  

(53)

To solve the damped oscillator problem, we have to determine the operator A because this should be known for the specification of displacement, momentum, and the energy of the oscillator. In the case of a nondamped oscillator, the amplitude operator can be determined from the Hamilton operator of the oscillator, which is a constant of the motion. This is, however, not true for our case; thus, we will use the Bohlin operator introduced earlier. By substituting Equation (52) into the Bohlinian Equation (39), we get

\[ B = e^{2\beta t}\left( \frac{P^2}{2m} + \frac{\beta}{2} pq + \frac{\beta}{2} q^2 + \frac{m\omega^2}{2} - q^2 \right) = \frac{\hbar \omega_m}{2} e^{2\beta t} \left( AA^\dagger + A^\dagger A \right) = \]  

\[ = \hbar \omega_m e^{2\beta t} \left( A^\dagger A + \frac{1}{2} e^{2\beta t} \right) = \hbar \omega_m \left( a^\dagger a + \frac{1}{2} \right), \quad \omega_m = \omega^2 \omega_0^1 \]  

(54)

where the commutation relations (Equation (44)) were used. Pursuant to the above two relations, it is easy to show that the time-independent amplitude operators fulfill the equations

\[ [ B, a^\dagger ] = \hbar \omega_m a^\dagger, [ a, B ] = \hbar \omega_m a \]  

(55)

Now, we see that if we replace the operator B by the Hamiltonian H of a simple oscillator, these equations are identical to the corresponding equations of the simple quantum oscillator [30, 31]. According to this strong analogy, we are able to determine the amplitude matrix and the matrices of the Bohlin operator B, the displacement operator and the momentum operator. The results are as follows:

- The operators a, a\(^\dagger\), B and the occupation number operator N: = a\(^\dagger\)a have the same eigenvectors and different eigenvalues. Since N: = a\(^\dagger\)a is positive definite, B can possess no negative eigenvalue. The lowest eigenvalue of B belongs to the eigenket \( |0\rangle \) of the operator a for which the relation \( a |0\rangle = 0 \) holds. From Equation (54), this so-called vacuum state belongs to the \( \frac{1}{2} \hbar \omega_m \) zero-point Bohlinian eigenvalue and zero occupation number eigenvalue. The Bohlinian eigenvalue belonging to the eigenket \( |n\rangle \) (where the occupation number is \( n \)) can be calculated in the form of \( |n\rangle = \frac{a^\dagger n}{\sqrt{n!}} |0\rangle \) is \( (\frac{1}{2} + n) \hbar \omega_m \), while the occupation number eigenvalue is \( n \).
• For the actions of the eigenket \( |n\rangle \) of the ladder operators, \( a \) and \( a^+ \) can be written as
\[
a|n\rangle = (n-1)|n-1\rangle, \quad a^+|n\rangle = (n+1)|n+1\rangle,
\]
from which it follows for the occupation number operator that \( N|n\rangle = n|n\rangle \).

• The matrices of the above-introduced operators are
\[
a = \begin{bmatrix}
0 & \sqrt{1} & 0 \\
0 & 0 & \sqrt{2} \\
0 & 0 & 0 \\
\vdots & \vdots & \ddots
\end{bmatrix}, \quad (56)
\]
\[
N = aa^+ = \begin{bmatrix}
1 & 0 & 0 \\
0 & 2 & 0 \\
0 & 0 & 3 \\
\vdots & \vdots & \ddots
\end{bmatrix}.
\]

on the basis of which is formed the orthonormal eigenkets
\[
|0\rangle = \begin{bmatrix} 1 \\ 0 \\ \cdots \end{bmatrix}, \quad |1\rangle = \begin{bmatrix} 0 \\ 1 \\ \cdots \end{bmatrix}, \quad |2\rangle = \begin{bmatrix} 0 \\ 0 \\ 1 \\ \cdots \end{bmatrix}, \text{etc.,} \quad (58)
\]

It is easy to see that the matrices that belong to \( aa \) and \( a^+a^+ \) are not diagonal. From the above equations, it follows that the rules for the time-dependent ladder and occupation number operators are
\[
A^+(t)|n\rangle = e^{-\beta t} \sqrt{n+1}|n\rangle, \quad A(t)|n\rangle = e^{-\beta t} \sqrt{n-1}|n-1\rangle,
\]
\[
N(t)|n\rangle = e^{-2\beta t}|n\rangle.
\]

5. Applications

5.1. Expected values of the main operators of a linearly damped oscillator

Moreover, the expected value of the occupation number in the \( n \)th energy eigenstate at time \( t \) is
\[ \langle N \rangle(t) := \langle n|N(t)|n \rangle = N_0 e^{-2\beta t}, \] (60)

where \( N_0 \) is the occupation number at \( t=0 \). This result agrees well with the corresponding result derived from the system-plus-reservoir model [32]. In the energy representation, since the matrices of the operators \( a, a^+, a^2, a^{*2} \) have zero diagonal elements, the expected values of the operators \( A, A^+, A^2, A^{*2} \) are zero in every energy eigenstate, i.e.,

\[ \langle A \rangle = 0, \quad \langle A^+ \rangle = 0, \quad \langle A^2 \rangle = 0, \quad \langle A^{*2} \rangle = 0 \] (61)

According to these equations, the expected values \( \langle q \rangle = \langle n | q | n \rangle, \langle p \rangle = \langle n | p | n \rangle \) of the displacement and the momentum operator

\[ q = \sqrt{\frac{\hbar}{2m\omega_0}} (A e^{-i\omega t} + A^* e^{i\omega t}), \quad p = \sqrt{\frac{\hbar m}{2\omega_0}} (\gamma A e^{-i\omega t} + \gamma^* A^* e^{i\omega t}) \] (62)

in the \( n \)th energy eigenstate are zero. The variance \( \langle q^2 \rangle = \langle n | q^2 | n \rangle, \langle p^2 \rangle = \langle n | p^2 | n \rangle \) of the displacement and momentum operator in the \( n \)th energy eigenstate can be evaluated as

\[ \langle q^2 \rangle = \frac{\hbar}{2m\omega_0} \langle AA^* + A^*A \rangle = \frac{\hbar}{2m\omega_0} \langle \delta e^{-2\beta t} + 2AA^* \rangle = \frac{\hbar}{2m\omega_0} e^{-2\beta t} (1 + 2n) \] (63)

and

\[ \langle p^2 \rangle = \frac{\hbar m}{2\omega_0} \langle \gamma^* (A e^{i\omega t}) (A^* e^{-i\omega t}) + \gamma (A^* e^{-i\omega t}) (A e^{i\omega t}) \rangle = \frac{m\hbar \omega_0}{2} (\delta e^{-2\beta t} + 2(A e^{i\omega t}) (A^* e^{-i\omega t})) = \frac{m\hbar \omega_0}{2} e^{-2\beta t} (1 + n) \] (64)

where we considered the commutation relation (Equation (53)). According to these results, we obtain the expected value of the energy of the damped oscillator

\[ \langle H \rangle(t) = \frac{\langle p^2 \rangle}{2m} + m\omega_0^2 \frac{\langle q^2 \rangle}{2} = \hbar \omega_0 \langle \delta e^{-2\beta t} + 2AA^* \rangle = \hbar \omega_0 e^{-2\beta t} \left( n + \frac{1}{2} \right) \] (65)
and the uncertainty relation
\[
(\Delta q)(\Delta p) = \frac{\hbar}{2} e^{-2\beta t} (2n + 1), \quad \Rightarrow \quad (\Delta q)(\Delta p) \geq \frac{\hbar}{2} e^{-2\beta t} \tag{66}
\]
\[
(\Delta q)^2 := \left( q - \delta \langle q \rangle \right)^2 = \langle q^2 \rangle, \quad (\Delta p)^2 := \left( p - \delta \langle p \rangle \right)^2 = \langle p^2 \rangle
\]

where we considered that \(\langle q \rangle = 0, \quad \langle p \rangle = 0\). Now, we can see Heisenberg’s uncertainty relation is not fulfilled and, in the case of the simple oscillator and also when \(\epsilon = 0\), this relation transforms into Heisenberg’s relation.

5.2. Probability description of the wave packet motion of the damped oscillator

To learn something about the time dependence of our system in a certain state \(|\psi\rangle\), we will calculate \(\langle q | \psi(t) \rangle \) and \(\langle q | \psi(t) |^2 \rangle\), which represent the probability amplitude and probability of finding the damped oscillator at \(q\) at time \(t\) in that state. In particular, it is useful to study the so-called coherent state \(|\alpha\rangle\), which is an eigenstate of the non-Hermitian time-dependent operator \(A\), i.e.,

\[
A e^{i\omega t} |\alpha\rangle = \sqrt{m_o \omega} e^{-\beta t} e^{i\omega t} |\alpha\rangle \tag{67}
\]

We shall also calculate the probability amplitude \(\Psi_s(q) = \langle q | a \rangle\) of the wave packet \(|a\rangle\) at \(q\). To do this, we shall start the following fact of bracket calculus

\[
\langle q | A e^{i\omega t} | q \rangle = \int \langle q | A e^{i\omega t} | q' \rangle \langle q' | q \rangle dq' = \int \langle q | A e^{i\omega t} | q' \rangle \Psi_s(q') dq' = \sqrt{m_o \omega} e^{-\beta t} e^{i\omega t} \Psi_s(q) \tag{68}
\]

Now, we are going to express the operator \(A\) by using the displacement and the momentum operator (52), so we get

\[
A e^{i\omega t} = \sqrt{\frac{2m}{\omega_0}} \frac{p - my'q}{i\omega} \tag{69}
\]

Taking this expression into (68), we obtain

\[
\int \langle q | A e^{i\omega t} | q \rangle \Psi_s(q') dq' = m_o A_o e^{-\beta t} e^{i\omega t} \Psi_s(q) \tag{70}
\]
According to the following

\[ \langle q | p | q' \rangle = e^{-2i\beta t} \frac{\hbar}{i} d\delta(q-q') + f(q), \quad \langle q | q' \rangle = q\delta(q-q') \tag{71} \]

coordinate representation of the operators originating from the commutation relation Equation (44) (for details, see [15]), we get

\[ \left( \omega q + \hbar \frac{d}{dp} e^{-2\beta t} \right) \Psi_d(q) = \omega A q e^{-\beta t} e^{i\omega t} \Psi_d(q) \tag{72} \]

an ordinary differential equation, where \(-c q\) is chosen for the arbitrary function \(f(q)\). The solution of this equation in a normalized form is

\[ \Psi_d(q) = g(t) \left( \frac{\hbar \omega}{\pi} \right)^{\frac{1}{4}} e^{\frac{-q^2}{2\hbar} \left( \frac{e^{i\omega t} + e^{-i\omega t}}{2} \right)} \tag{73} \]

where the function \(g(t)\) is evaluated in follows. From which the probability will be

\[ \left| \Psi_d(q) \right|^2 = \left( \frac{m \omega}{2\hbar} \right)^{\frac{1}{2}} \frac{1}{2} e^\beta e^{\frac{\hbar}{\omega} \left( q - A q e^{-\beta t} \right)^2} \tag{74} \]

Now, we might see that this is the Gaussian distribution with the

\[ \left| \Psi_d(q) \right|^2 = \frac{1}{\sqrt{2\pi}} \left( \frac{\hbar}{m \omega} e^{-\beta t} \right)^{\frac{1}{2}} e^{-\left( q - A q e^{-\beta t} \right)^2} \tag{75} \]

probability density function. Therefore, the motion of the center of the wave packet \( |a\rangle \) is a damped oscillation, and its uncertainty width decreases exponentially from the initial value of \( \sqrt{\frac{\hbar}{m \omega}} \) to zero (see Figure 3).
Figure 3. The evolution of the wave packet $|a\rangle$. The motion of the center of packet and its uncertainty width $\Delta q$ are represented.

Now, we see that the initial uncertainty of the packet $|a\rangle$ keeps getting smaller with the progression of time and becomes negligible as $t \to \infty$. Also, the evolution of the wave packet continually proceeds toward the motion of a classic damped oscillator with the progression of time.

5.3. Calculation of wave function by matrix calculus

Resulting from Equation (52) using Equation (56), the matrix of the displacement operator in energy representation has the form

\[
\begin{bmatrix}
0 & 1 & 0 & 0 & 0 \\
1 & 0 & \sqrt{2} & 0 & 0 \\
0 & \sqrt{2} & 0 & \sqrt{3} & 0 \\
0 & 0 & \sqrt{3} & 0 & \sqrt{4} \\
0 & 0 & 0 & \sqrt{4} & 0 \\
\end{bmatrix}
\]

Here, the displacement operator was used in a narrow sense. Next, we are going to solve the eigenvalue problem in terms of the $d_n = \langle n | a \rangle$ probability amplitudes. To do this, we rewrite the above eigenvalue equation in matrix form

\[
\sum_{n \geq 0} \langle n | q | n' \rangle \langle n' | q \rangle = q \langle n | q \rangle, (n = 0, 1, 2, \ldots) \]

where we take into account the $\sum_{n \geq 0} | n \rangle \langle n | = \delta$ closure relation. In explicit form, this looks like
\[
\begin{bmatrix}
0 & 1 & 0 & 0 & 0 \\
1 & 0 & \sqrt{2} & 0 & 0 \\
0 & \sqrt{2} & 0 & \sqrt{3} & 0 \\
0 & 0 & \sqrt{3} & 0 & \sqrt{4} \\
0 & 0 & 0 & \sqrt{4} & 0
\end{bmatrix}
\]

\[e^{-\beta t} = \begin{bmatrix} d_0 \\ d_1 \\ d_2 \\ d_3 \\ \vdots \end{bmatrix} = \begin{bmatrix} \sqrt{\frac{2m\omega_0}{\hbar}} q \\ d_1 \\ \sqrt{\frac{2m\omega_0}{\hbar}} q \\ d_3 \\ \vdots \end{bmatrix}.
\]

From this, we get the difference schema

\[
d_1 = \frac{q^0}{\sqrt{1}} d_1, \quad d_2 = \frac{q^0}{\sqrt{2}} d_1 - \frac{1}{\sqrt{2}} d_0, \ldots,
\]
\[
d_n = \frac{q^0}{\sqrt{n}} d_{n-1} - \frac{\sqrt{n-1}}{\sqrt{n}} d_{n-2}
\]
\[
q^0 = \sqrt{\frac{2m\omega_0}{\hbar}} e^{\beta t} q
\]

After some algebra, we obtain another form

\[
d_n' = 2 \frac{q^0}{\sqrt{2}} d_{n-1}' - 2(n-1)d_{n-2}', \quad d_n := \sqrt{2^n n!} d_n
\]

By introducing a new coordinate variable, we have the difference equation

\[
d_n' = 2q d_{n-1}' - 2(n-1)d_{n-2}', \quad q := \frac{q^0}{\sqrt{2}}
\]

This difference equation is satisfied by the Hermitian polynomials. Thus, we obtain

\[
\langle n | q \rangle = d_n = c_0 \left( e^{\beta t} \sqrt{\frac{m\omega_0}{\hbar}} q \right) \frac{1}{\sqrt{2^n n!}} H_n \left( e^{\beta t} \sqrt{\frac{m\omega_0}{\hbar}} q \right),
\]

where \( c_0 \left( e^{\beta t} \sqrt{\frac{m\omega_0}{\hbar}} q \right) \) is a function to be determined. Starting from the fact that \( \langle q' | q'' \rangle = \delta(q' - q'') \), we get
By using the

\[
\sum_n \frac{1}{2^n n!} H_n \left( e^{\beta t} \sqrt{\frac{m \omega_0}{\hbar}} q \right) \times H_n \left( e^{\beta t} \sqrt{\frac{m \omega_0}{\hbar}} q'' \right) = \\
= \sqrt{\pi} e^{\frac{1}{2} \left( \frac{m \omega_0}{\hbar} \right)^2} \delta \left( e^{\beta t} \sqrt{\frac{m \omega_0}{\hbar}} q' - e^{\beta t} \sqrt{\frac{m \omega_0}{\hbar}} q'' \right) = \\
= \sqrt{\frac{\pi m \omega_0}{\hbar}} e^{\frac{1}{2} \left( \frac{m \omega_0}{\hbar} \right)^2} e^{-\beta t} \delta (q'' - q')
\]

relationship, the final form of Equation (83) is given by

\[
\Psi_n(q) := \langle n | q \rangle = d_n = e^{\frac{1}{2} \beta t} \left( \frac{m \omega_0}{\hbar \pi} \right)^{\frac{1}{2}} e^{-\frac{1}{2} \frac{m \omega_0 q^2}{\hbar}} \frac{1}{2^n n!} H_n \left( e^{\beta t} \sqrt{\frac{m \omega_0}{\hbar}} q \right)
\]

The physical meaning of the strange variable in the Hermit polynomials is that the distance of the nodes of these functions keeps getting smaller with the progression of time by the exponential law $e^{-\beta t}$. According to this result, the probability density of the $n$th energy state with displacement $q$ is

\[
\left| \Psi_n(q) \right|^2 = \left| \langle n | q \rangle \right|^2 = \frac{1}{2^n n!} e^{\beta n} \left( \frac{m \omega_0}{\hbar \pi} \right)^{\frac{1}{2}} e^{-\frac{1}{2} \frac{m \omega_0 q^2}{\hbar}} \frac{1}{2^n n!} H_n \left( e^{\beta t} \sqrt{\frac{m \omega_0}{\hbar}} q \right)
\]

\[
= \frac{1}{\sqrt{2\pi}} \left( \frac{\hbar}{2m \omega_0} e^{-\beta t} \right)^{\frac{1}{2}} e^{-\frac{1}{2} \frac{m \omega_0 q^2}{\hbar}} \left[ \frac{1}{2^n n!} H_n \left( e^{\beta t} \sqrt{\frac{m \omega_0}{\hbar}} q \right) \right]
\]
This result is exactly identical to the equation given by Kim and Page [33] on the basis of another theory. Now, we might see that this is the density function of a modulated Gaussian distribution, where the modulating term has finite amplitude which runs over in time, while the Gaussian distribution sharpens toward to a Dirac delta distribution. This means that the particle will get closer and closer to the equilibrium point as \( t \to \infty \). From last result, we can conclude that in the case of \( \beta \to 0 \) we get back to the well-known wave function of the simple oscillator.

5.4. Spectrum of the energy dissipation of the linearly damped oscillator

We are going to give the frequency spectrum of radiation and explain the natural width of the spectrum line. As an atom emits photons, its energy drops and the amplitude of transition decreases over time. Therefore, the emission is not harmonic, and a spectrum occurs. We shall see that the natural width of the spectral line can be connected to the attenuation coefficient of the damped oscillator. Inversely, from the width of the spectral line, we might determine the attenuation coefficient of the oscillator.

5.4.1. Spectral density of the energy dissipation

In the first section, the time rate of energy dissipation for a damped oscillator is introduced by the Rayleigh dissipation potential. The quantum version of this quantity, i.e., the time rate of the energy dissipation operator, can be originated from Equation (14) as

\[
\mathbf{R} := \frac{\hbar}{2m} \mathbf{p}^2 = \frac{2\beta}{m} \mathbf{p}^2
\]  

(88)

From this, it follows that the expected value of the operator of energy dissipation is

\[
\bar{w}_{\text{diss}} = \frac{\hbar}{\omega_0} \int_0^\infty \left( \mathbf{A} \mathbf{e}^{i\omega t} \right) \left( \mathbf{A}^\dagger \mathbf{e}^{-i\omega t} \right) dt = \frac{\hbar \omega_0}{2} + 2\beta \omega_0 \int_0^\infty \left( \mathbf{a} \mathbf{a}^\dagger \right) e^{i\gamma t} e^{i\gamma^*} dt
\]  

(89)

Substituting the expression of the momentum operator (Equation (64)) into this equation, then the above equation has the form

\[
\bar{w}_{\text{diss}} = \beta \hbar \omega_0 \int_0^\infty \left( \gamma \left( \mathbf{A} \mathbf{e}^{i\omega t} \right) \left( \mathbf{A}^\dagger \mathbf{e}^{-i\omega t} \right) + \gamma^* \left( \mathbf{A} \mathbf{e}^{-i\omega t} \right) \left( \mathbf{A}^\dagger \mathbf{e}^{i\omega t} \right) \right) dt = \\
= \beta \hbar \omega_0 \int_0^\infty \left( \mathbf{e}^{-2\gamma t} \mathbf{A} \mathbf{e}^{-i\omega t} \right) \left( \mathbf{A}^\dagger \mathbf{e}^{-i\omega t} \right) dt = \frac{\hbar \omega_0}{2} + 2\beta \omega_0 \int_0^\infty \left( \mathbf{a} \mathbf{a}^\dagger \right) e^{i\gamma t} e^{i\gamma^*} dt
\]  

(90)

In this case, we have \( \gamma = \beta + i\omega \).
where we assume that the occupation number is \( n \), i.e., \( n = \langle a^a \rangle \). Evidently, the first term of this expression belongs to the vacuum fluctuation, and the second term belongs to the essential dissipative process of the damped oscillator in which the occupation number could change. We will evaluate the second term of this energy dissipation formula. According to the Parseval theorem of the Fourier transformation theory, this term of energy dissipation may be written as

\[
\Delta w_{\text{diss}}(n) = 2 \beta \hbar \omega_0 \int_0^\infty e^{\gamma t} e^{i\omega t} dt = n 2\beta \hbar \omega_0 \left[ F\left[ e^{\gamma t} \right] F\left[ e^{\gamma t} \right] \right] d\omega =
\]

\[
= n 2\beta \hbar \omega_0 \int_0^\infty \frac{d\omega'}{(\omega - \omega')^2 + \beta^2}
\]

where \( F\left[ e^{\gamma t} \right] \) is the Fourier transform of \( e^{\gamma t} \). Also, the spectral density of the dissipated energy is

\[
\Delta \omega = \beta
\]

where \( \Delta \omega \) is the Fourier transform of \( e^{\gamma t} \). Also, the spectral density of the dissipated energy is

\[
\frac{2 \beta \hbar \omega_0}{(\omega - \omega')^2 + \beta^2}
\]

i.e., a Lorentz distribution about the shifted circular frequency \( \omega \) of the damped oscillator. This result agrees well with corresponding result derived from the two-state atom model of Wigner and Weisskopf [34, 35] and the system-plus-reservoir model [10, 32, 36]. It is well known that the half value width \( \Delta \omega \) of this distribution is

\[
\Delta \omega = \beta
\]

Now, we can see the transition from the \( n \)th occupation number state to the vacuum state, in which the oscillator will emit \( n \hbar \omega_0 \) energy. Indeed, from Equation (91) it follows that

\[
\Delta w_{\text{diss}}(n) = n 2\beta \hbar \omega_0 \int_0^\infty \frac{d\omega'}{(\omega - \omega')^2 + \beta^2} = n \hbar \omega_0
\]

5.4.2. Natural width of the spectral line

The natural line width of the spectral line is a significant result of the dissipative quantum process which accompanies the spontaneous emission of an atom. We will treat this emission process in a dissipative two-state model. We consider the two states of the atom as the zeroth and the first occupation number state of a linearly damped oscillator. In this case, the spontaneous emission of a photon is the consequence of the transition from the first occupations number state to the equilibrium state of the damped oscillator. In this model, the spectrum density of the emitted photon follows from Equation (92)
The width of this frequency spectrum of a spontaneous emission of the atom is a direct consequence of the dissipative self-force on the atom due to the back-reaction of the emitted photon. This back-reaction of the emitted photon can be characterized by two physical quantities, namely, the frequency shift $\omega_0 \rightarrow \omega$ and the half value width $\Delta \omega = \beta$ of the spectrum.

If we consider $\hbar \frac{\Delta \omega}{2}$ as the energy uncertainty $\Delta E$ of the emitted wave packet and the time constant of the emission process $\Delta t = \beta^{-1}$ as the time uncertainty, we obtain an uncertainty relation

$$\Delta E \Delta t \geq \frac{\hbar \beta}{2} = \frac{\hbar}{2}\beta$$

(96)

The quantum mechanical interpretation of the width of the natural spectral line should be based on this relation, in which the physical quantities $\Delta E$ and $\Delta t = \beta^{-1}$ have a precise meaning. In our model, the natural line width occurs at wavelength $\lambda$ and can be calculated as

$$\Delta \lambda = \Delta \frac{2 \pi c}{\omega} = \frac{2 \pi c}{\omega^2} \Delta \omega = \frac{2 \pi c}{\omega^2} \beta$$

(97)

where Equation (93) was used and $c$ is the vacuum velocity of light. It is well known that in the classical dipole model of light emission, the natural line width can be calculated as

$$\Delta \lambda = \frac{4 \pi \epsilon_0}{3mc^2}$$

(98)

where $\epsilon_0$ is the vacuum permittivity and $r_e = \frac{\epsilon_0}{3mc^2} = 2.818 \times 10^{-15} m$ is the so-called classical electron radius. From the above two equations, it follows that

$$\beta = \frac{2}{3} \frac{\omega^2}{c} \frac{r_e}{\lambda} = \frac{4 \pi}{3} \frac{r_e}{\lambda} \omega$$

(99)

in the dipole radiation model.
6. Uncertainty relation of the linearly damped oscillator

The standard derivation of Heisenberg’s uncertainty relation neglects the possibility that two operators $A$ and $B$, say $q$ and $p$, which fulfill the commutator relation

$$\{A, B\} = i\hbar$$

(100)

could have a compatible component which is the first part of the trivial identity

$$AB = \frac{AB + BA}{2} + \frac{AB - BA}{2}$$

(101)

This observation has importance when we take into account the irreversibility. Due to irreversibility, the damped oscillator proceeds to thermal equilibrium with the thermal bath. This thermal equilibrium can be characterized in terms of classical statistic theory. However, in classical statistics, random variables have a joint distribution function, which could exist in the case of quantum theory if the operators are compatible. The commutator relation (Equation (100)) is compatible this physical picture, but from Equations (100) and (101), we obtain

$$AB = \frac{AB + BA}{2} + \frac{i\hbar}{2} e^{-2\beta t}$$

(102)

From this relation, in the case of $t \to \infty$, the compatibility of the operators follows, i.e.,

$$AB = \frac{AB + BA}{2} \rightarrow AB = BA$$

(103)

In what follows, we will show that the above-mentioned arguments appear in the uncertainty relation. The variance of the Hermitian operators $A$ and $B$ can be calculated by the norm of the following vectors

$$f = (A - \delta\langle A \rangle)\Psi(0), g = (B - \delta\langle B \rangle)\Psi(0)$$

(104)

Indeed, we can write

$$\begin{align*}
(\Delta A)^2 &= \|f\|^2 = \langle \Psi(0) | (A - \delta\langle A \rangle)^2 | \Psi(0) \rangle \\
(\Delta B)^2 &= \|g\|^2 = \langle \Psi(0) | (B - \delta\langle B \rangle)^2 | \Psi(0) \rangle
\end{align*}$$

(105)
where $\Psi(0)$ is the state vector of the system, $\langle A \rangle$ and $\langle B \rangle$ are the expected value of the operators defined as

$$\langle A \rangle = \langle \Psi(0) | A | \Psi(0) \rangle, \langle B \rangle = \langle \Psi(0) | B | \Psi(0) \rangle$$

(106)

Thus, the $\| f \| \| g \| \geq |\langle f, g \rangle|^2$ Schwarz inequality implies

$$\left( \Delta A \right)^2 \left( \Delta B \right)^2 \geq \left| \langle \Psi(0) | (A - \delta A)(B - \delta B) | \Psi(0) \rangle \right|^2 = \left| \langle AB \rangle - \langle A \rangle \langle B \rangle \right|^2$$

(107)

By substituting into this expression the identity (Equation (101)), then we get

$$\left( \Delta A \right)^2 \left( \Delta B \right)^2 \geq \left| \frac{\langle AB \rangle + \langle BA \rangle}{2} + \frac{\langle AB - BA \rangle}{2} - \langle A \rangle \langle B \rangle \right|^2 = \left| \frac{\langle AB \rangle + \langle BA \rangle}{2} + \frac{\langle AB \rangle - \langle BA \rangle}{2} - \langle A \rangle \langle B \rangle \right|^2$$

(108)

where we take into account that the square of the absolute value of a complex number is equally the sum of the square of its real and imaginary parts. From the above expression, in the case of $t \to \infty$, it follows that

$$\Delta A \Delta B \geq \frac{\langle AB \rangle + \langle BA \rangle}{2} - \langle A \rangle \langle B \rangle, \quad \Delta A := +\sqrt{\left( \Delta A \right)^2}, \quad \Delta B := +\sqrt{\left( \Delta B \right)^2}$$

(109)

On the another hand, in this case, the commutating relation (Equation (103)) is valid; thus, we can conclude that

$$\left( \Delta A \right) \left( \Delta B \right) \geq \left( \langle AB \rangle - \langle A \rangle \langle B \rangle \right) \to 0 \leq \frac{\langle AB \rangle - \langle A \rangle \langle B \rangle}{\langle \Delta A \rangle \langle \Delta B \rangle} \leq 1$$

(110)

which is the most primitive “uncertainty relation” of classical statistic theory in which the random variables have a joint distribution function. It states the simple fact that the regression coefficient is smaller than one if the random variables are not statistically independent.

In summary, we can provide a speculative interpretation of irreversibility in quantum mechanics, namely, in an irreversible quantum process. The incompatible operators proceed to compatible ones, which are submitted to the laws of classical statistic theory.
7. Quantum statistics of the linearly damped oscillator

It was von Neumann [26] who first dealt with the problem of the quantum statistical ensemble. The density operator is the statistical operator of a quantum statistical ensemble. In our case, the statistical ensemble is a set of linearly damped oscillators of several quantum states in contact with a heat bath with temperature \( T \). The density operator is an operator whose eigenvalues are the classical statistical probability of the chosen microstates denoted by \( p_i \). If the chosen microstates are denoted by \( \mid i \rangle \), which are eigenstates of a Hermitian operator but not necessarily the eigenstate of a Bohlinian or Hamiltonian, the general density operator is written as

\[
\rho := \rho \delta = \sum_{i \in \Omega} \rho \mid i \rangle \langle i \mid = \sum_{i \in \Omega} p_i \mid i \rangle \langle i \mid, \quad \delta = \sum_{i \in \Omega} \mid i \rangle \langle i \mid
\]  

From this definition, it follows that \( \rho \) is Hermitian and normalized

\[
\rho = \rho^*, \quad Tr \rho = 1
\]

In the Heisenberg picture, the density operator is time independent and is written as

\[
\rho_H = \sum_{i \in \Omega} \rho_i \mid i(0) \rangle \langle i(0) \mid
\]

The ensemble average of an operator in the Heisenberg picture \( A_H(t) \) is defined as

\[
\langle A \rangle(t) = Tr \left( \rho_H A_H(t) \right) = \sum_{i \in \Omega} p_i \mid i(0) \rangle \langle i(0) \mid A_H(t) \mid i(0) \rangle
\]

Ensemble averages of time rate of change of the displacement and the momentum of the linearly damped oscillator can be evaluated from Equation (51) as follows

\[
\frac{d}{dt} \langle q \rangle = \frac{i}{\hbar} Tr \left( \rho_H \frac{\partial}{\partial q} \right) = \frac{i}{\hbar} Tr \left( \rho_H \left( H, q \right) \right) = \frac{i}{\hbar} \frac{\partial}{\partial q} \langle H \rangle = - \frac{\partial}{\partial q} \langle q \rangle - c \langle \frac{\partial}{\partial p} \rangle = - m \omega_o^2 \langle q \rangle - \frac{\partial}{\partial q} \langle p \rangle - \frac{\partial}{\partial q} \langle p \rangle
\]

\[
\frac{d}{dt} \langle p \rangle = \frac{i}{\hbar} Tr \left( \rho_H \frac{\partial}{\partial p} \right) = \frac{i}{\hbar} Tr \left( \rho_H \left( H, p \right) \right) - c \frac{i}{\hbar} Tr \left( \rho_H \left( H, q \right) \right) = - \frac{i}{\hbar} \frac{\partial}{\partial p} \langle H \rangle = - \frac{i}{\hbar} \frac{\partial}{\partial p} \langle H \rangle = \frac{c}{m} \langle p \rangle
\]

\[
= - \frac{c}{m} \langle p \rangle(t) - m \omega_o^2 \langle q \rangle(t)
\]
Here, Equation (50) was used. Now, we see that these equations are equivalent to those of the macroscopic Onsagerian equations (Equation (21) or (22)). In the Schrödinger picture, the density operator is time dependent, but the observables of the oscillator are time independent. We define this density operator as

$$\rho(t) = \sum_{i \in \Omega} p_i(t) |i(t)\rangle \langle i(t)|$$  \hspace{1cm} (116)$$

where we allowed a time-dependent probability $p_i(t)$ to microstate $i(t)$. Also in this picture, the occupation of microstates is not conserved. The ensemble average of an operator $A_S$ in the Schrödinger picture is defined as

$$\langle A \rangle(t) = Tr(\rho(t)A_S) = \sum_{i \in \Omega} p_i(t) |i(t)\rangle \langle A_S | i(t)\rangle$$  \hspace{1cm} (117)$$

Two ensemble averages of an observable $A$ must be equal, i.e.,

$$Tr(\rho(t)A_S) = Tr(\rho(t)A_S)$$  \hspace{1cm} (118)$$

from which, in the case of pure unitary dynamics, follows the well-known transformation

$$\rho(t) = U^*(t)\rho(t)U(t)$$  \hspace{1cm} (119)$$

where the unitary operator $U(t)$ belongs to time evolution [37]. Since, as we have seen in the case of dissipative processes, this cannot be written by unitary dynamics only, we will use this requirement in a weaker form. We require that the basic ensemble averaged equations of the damped oscillator have the same forms in each picture, i.e.,

$$\frac{d}{dt} \langle q \rangle(t) = Tr\left(\rho(t) \dot{q} \right) = Tr\left( \rho_{\varepsilon} \dot{q} \right) = \frac{\langle p(t) \rangle}{m}$$

$$\frac{d}{dt} \langle p \rangle(t) = Tr\left(\rho(t) \dot{p} \right) = Tr\left( \rho_{\varepsilon} \dot{p} \right) = -\frac{c}{m} \langle p(t) \rangle - m\omega_0^2 \langle q(t) \rangle$$  \hspace{1cm} (120)$$

According to this requirement, we could give the actual form of the equation of motion for the density operator in the Schrödinger picture. We will see that this equation corresponds to the Liouville–von Neumann equation in the case of dissipative processes. From Equations (113) and (119), it follows that the density operator in the Schrödinger picture could be written by a Hermitian operator in the form
\[ \rho_s(t) = \sum_{i=0}^{n} p_i(t) U^*(t) |i(0)\rangle \langle i(0)| U(t) \] (121)

From the general evolution equation (Equation (34)) of the Hermitian operator, the equation of motion of the density operator in Schrödinger picture could be derived as follows:

\[
\frac{\partial \rho_s(t)}{\partial t} = -\frac{i}{\hbar} [\hat{H}, \rho_s(t)] + \sum_{i=0}^{n} \frac{dp_i(t)}{dt} \left[ U^*(t) |i(0)\rangle \langle i(0)| U(t) \right]
\] (122)

where in the case of a damped oscillator, the unitary transformation belongs to the Bohlin operator of Equation (38), i.e.,

\[
\hat{U}^*(t) U(t) = -\frac{i}{\hbar} \hat{B}
\] (123)

Thus, the equation of motion of Schrödinger’s density operator is

\[
\frac{\partial \rho_s(t)}{\partial t} = \frac{\partial \rho_s(t)}{\partial t} + \frac{i}{\hbar} [\hat{B}, \rho_s(t)] + \frac{i}{\hbar} [\hat{H}, \rho_s(t)] + \frac{i}{\hbar} [\hat{D}, \rho_s(t)]
\] (124)

Here, similar to the Heisenberg equations (Equation (41)), we introduced the Hamiltonian and the dissipation operator, by means of the commutator \([\ , \ ] = e^{2\pi i [\ , \ ]}\). To construct a constitutive equation for the local change in the density operator, one must take into account the consequences of the commutation relation (Equation (44)) and the facts (Equations (102) and (103)) by which the incompatibility of the operators show strict fading over time. A consequence of this fading property could be increasing uncertainty in the distinction of the quantum states of the oscillators. On the other hand, in a canonical ensemble, the oscillators weakly interact with each other. By this means, the occupation of the states could change in the ensemble. Thus, we can assume that the occupation of states is not conserved in the time evolution of the ensemble. As a consequence, the statistical ensemble of the oscillators could proceed to a final state in which the classical probabilities of the microstates correspond to a classical thermal equilibrium distribution. Denoted by the density operator \(\rho_s\) in the instantaneous and \(\rho_{seq}\) in the equilibrium final state, then the suggested linear constitutive equation is

\[
\frac{\partial \rho_s}{\partial t} = -\beta \left( \rho_s - \rho_{seq} \right), \quad Tr \left( \rho_s \right) = Tr \left( \rho_{seq} \right)
\] (125)
Thus, the final form of the Liouville–von Neumann Equation (124) is

\[
\dot{\rho_s} = \frac{d\rho_s(t)}{dt} = -\beta (\rho_s - \rho_{eq}) + \frac{i}{\hbar} [B, \rho_s] = -\beta (\rho_s - \rho_{eq}) + \frac{i}{\hbar} \{H, \rho_s\} + \frac{i}{\hbar} \{D, \rho_s\}
\]  

(126)

We will show that this evolution equation guarantees that the equivalence relation (Equation (120)) is fulfilled, the density matrix proceeds to an equilibrium state and that the entropy of the ensemble of the damped oscillator proceeds the maximum value over time, which corresponds to thermal equilibrium. Indeed, the proof of the relations in Equation (120) proceeds as follows

\[
\frac{d\langle q \rangle(t)}{dt} = Tr(\dot{\rho}_s q) = -\beta Tr((\rho_s - \rho_{eq})q) + \frac{i}{\hbar} Tr(\{H, \rho_s\} q) + \frac{i}{\hbar} Tr(\{D, \rho_s\} q) = -\beta \langle q \rangle(t - \beta \langle q \rangle_{eq} + \frac{i}{\hbar} Tr(\rho_s \{H, q\}) + \frac{i}{\hbar} Tr(\rho_s \{D, q\}) = -\beta \langle q \rangle(t) - \beta \langle q \rangle_{eq} + Tr(\rho_s \frac{\partial H}{\partial p}) + \beta Tr(\rho_s q) = -\beta \langle q \rangle + \frac{\langle p \rangle(t)}{m}
\]

\[
\frac{d\langle p \rangle(t)}{dt} = Tr(\dot{\rho}_s p) = -\beta Tr((\rho_s - \rho_{eq})p) + \frac{i}{\hbar} Tr(\{H, \rho_s\} p) + \frac{i}{\hbar} Tr(\{D, \rho_s\} p) = -\beta \langle p \rangle(t) - \beta \langle p \rangle_{eq} + \frac{i}{\hbar} Tr(\rho_s \{H, p\}) + \frac{i}{\hbar} Tr(\rho_s \{D, p\}) = -\beta \langle p \rangle(t) - \beta \langle p \rangle_{eq} - Tr(\rho_s \frac{\partial H}{\partial q}) - \beta Tr(\rho_s p) = -\beta \langle p \rangle_{eq} - \frac{c}{m} \langle p \rangle(t) - mao_q^2 \langle q \rangle(t)
\]  

(127)

where we take into account the cyclic invariance of the trace and the facts in Equation (42).

Now we see that if we choose an ensemble of a damped oscillator in which $$\langle q \rangle_{eq} = 0$$, $$\langle q \rangle_{eq} = 0$$, the required equivalence of the ensemble averages is fulfilled. To prove the increase in entropy, first we introduce quantum entropy. The $$k_B\rho_s \ln \rho_s$$ operator is an operator whose eigenvalues are the terms of Shannon entropy $$k_B \rho_i(t) \ln \rho_i(t)$$. Thus, the Shannon entropy is the minus trace of that operator [26]

\[
S(t) := -k_B \sum_{i=0} p_i(t) \ln p_i(t) = -k_B Tr(\rho_s \ln \rho_s)
\]  

(128)

Here, $$k_B$$ is the Boltzmann constant. According to this definition, the excess entropy of an ensemble, as suggested by Bedeaux and Mazur [38], is given by
The time rate of change of the entropy in that approximation is

\[
\frac{dS(t)}{dt} = -\frac{1}{2} k_B \text{Tr} \left( \left( \Delta \rho_{\text{seq}}^{-1} + \rho_{\text{seq}}^{-1} \Delta \rho_s \right) \frac{d\rho_s}{dt} \right)
\]

(130)

Entropy production results by substituting the Liouville–von Neumann equation into this equation

\[
\frac{dS(t)}{dt} = -\frac{1}{2} k_B \text{Tr} \left( \left( \Delta \rho_{\text{seq}}^{-1} + \rho_{\text{seq}}^{-1} \Delta \rho_s \right) \frac{d\rho_s}{dt} \right) = -\frac{1}{2} k_B \text{Tr} \left( \left( \Delta \rho_{\text{seq}}^{-1} + \rho_{\text{seq}}^{-1} \Delta \rho_s \right) \left( -\beta \Delta \rho_s + i\hbar \{B, \rho_s\} \right) \right) = \frac{\beta}{2} k_B \text{Tr} \left( \left( \Delta \rho_{\text{seq}}^{-1} + \rho_{\text{seq}}^{-1} \Delta \rho_s \right) \left( i\hbar \{B, \rho_s\} \right) \right) = \frac{\beta}{2} k_B \text{Tr} \left( \rho_{\text{seq}}^{-1} \left( \Delta \rho_s \right)^2 \right) \geq 0
\]

(131)

where the cyclic invariance of the trace and the fact that the Bohlin operator and the $\rho_{\text{seq}}^{-1}$ commutator were used. The positivity of entropy production follows from the fact that the matrices of both operators $\rho_{\text{seq}}^{-1}$ and $(\Delta \rho_s)^2$ have nonnegative elements only. Thus, the increase in entropy is demonstrated. It can be seen from the above deduction of entropy production that pure unitary dynamics (in the case of an undamped oscillator) is isentropic and that the entropy production is a direct consequence of the unconserved property of the occupation of states. In the thermal equilibrium, from Equation (126), it follows that $B$ and $\rho_{\text{seq}}$ commute, i.e.,

\[
\frac{d\rho_s(t)}{dt} = 0, \quad \rho_s = \rho_{\text{seq}}, \quad \left[ B, \rho_{\text{seq}} \right] = 0
\]

(132)

So the equilibrium density operator $\rho_{\text{seq}}$ is a function of the Bohlinian $B$. At equilibrium, the entropy is at maximum. Now, we maximize $S = -k_B \sum_{n \geq 0} p_n \ln p_n$ under the conditions

\[
\text{Tr}(\rho_s) = \sum_{n \geq 0} p_n = 1, \quad \langle B \rangle = \text{Tr}(\rho_s B) = \sum_{n \geq 0} p_n B_n = \text{const}, \quad B_n = \langle n | B | n \rangle = \hbar \omega_n \left( \frac{1}{2} + n \right)
\]

(133)
where we use Equation (54). The necessary condition of that maximum is

\[-k_B \sum_{n \geq 0} \delta p_n (\ln p_n + 1) = 0\]  

(134)

where the variations \(\delta p_n\) are restricted by the conditions

\[\sum_{n \geq 0} \delta p_n = 0, \quad \sum_{n \geq 0} \delta p_n B_n = 0\]  

(135)

Applying the method of Lagrange multipliers, we get

\[\sum_{n \geq 0} \delta p_n [\ln p_n + 1 + \beta B_n + \gamma] = 0\]  

(136)

So

\[p_n = e^{-\beta B_n - \gamma - 1}\]  

(137)

From the first equation of the conditions (133), the normalized version of the probability distribution is obtained

\[p_n = \frac{e^{-\beta B_n}}{\sum_{i \geq 0} e^{-\beta B_i}}\]  

(138)

Choosing \(\beta = \frac{1}{k_B T}\) as usual, then we get Gibbs’ canonical distribution for the occupation probabilities

\[p_n = \frac{e^{-\beta B_n}}{\sum_{i \geq 0} e^{-\beta B_i}}\]  

(139)

Introducing the partition function by definition

\[Z := Tr(e^{-\beta B}) = \sum_{i \geq 0} e^{-\beta B_i}\]  

(140)
then we get the equilibrium density operator

\[ \rho_{\text{equ}} = \frac{e^{-\beta B}}{Z} \]  

(141)

Thus, the equilibrium ensemble average of an operator \( A \) can be written as

\[ \langle A \rangle = \text{Tr}\left( \rho_{\text{equ}} A \right) = \frac{\text{Tr}\left( e^{-\beta B} A \right)}{Z} = \frac{\sum_{n \geq 0} \langle n | A | n \rangle e^{-\beta E_n}}{\sum_{i \geq 0} e^{-\beta E_i}} \]  

(142)

In particular, for the ensemble average of the Bohlinian, this is

\[ \langle B \rangle = \frac{\sum_{n \geq 0} B_n e^{-\beta E_n}}{\sum_{n \geq 0} e^{-\beta E_n}} = -\frac{\partial \ln Z}{\partial \beta} = \hbar \omega_m \left( \frac{1}{2} + \frac{e^{-\hbar \omega_m / k_B T}}{1 - e^{-\hbar \omega_m / k_B T}} \right) = \frac{\hbar \omega_m}{2} \coth \frac{\hbar \omega_m}{k_B T} \]  

(143)

Introducing the free energy by definition \( F = -k_B T \ln Z \), then in terms of free energy, the Gibbs distribution is written as usual

\[ p_n = e^{\frac{T-B}{k_B T}} \]  

(144)

Substituting this into the definition equation of entropy (128), then we get

\[ S = \frac{\langle B \rangle - F}{T} \rightarrow F = \langle B \rangle - TS \]  

(145)

Thus, the ensemble average of the Bohlinian is the equilibrium internal energy. It is evident that the actual choice of the angular frequency \( \omega_m \) in the Bohlinian is a convention. It depends on the normalization of Bohlin’s constant (Equation (26)). What is the correct angular frequency? It seems from the physical aspect that the correct choice is that the angular frequency is \( \omega_0 \). In this case, Bohlin’s constant of motion corresponds to the maximum free energy of the linearly damped oscillator measured at time \( t=0 \), so it is the exergy of the linearly damped oscillator.
8. Wave equation of the linearly damped oscillator

From the above-presented theory, we can conclude that an ensemble from a pure state always proceeds to a mixed state a consequence of irreversibility. Thus, it is impossible to describe the evolution of the pure state of a damped oscillator in the Schrödinger picture. Consequently, it is impossible to construct a linear Schrödinger equation in which the position and the momentum operator are time independent.

However, when the operators are time dependent, the model could show similarities to Schrödinger’s interpretation, which we show below.

In the case of a linearly damped oscillator, the transformation of the Heisenberg picture into the Schrödinger picture by the method applied in classical quantum theory is impossible because the operator has a time-dependent part due to the dissipative process. Thus, a new way must be found to construct the wave equation of the oscillator. Kostin introduced a supplementary dissipation potential into his wave equation and constructed this dissipation potential by an assumption that the energy eigenvalues of the oscillator decay exponentially over time [39]. In Kostin’s version of the wave equation, the operators are time independent, but the dissipation potential is nonlinear with respect to the wave function. In our theory, it is assumed that the abstract wave equation of the linearly damped oscillator has the form

\[
\frac{d}{dt} \Psi(t) = (H - D) \Psi
\]

(146)

where the Hamiltonian \( H \) and the dissipative term \( D \) has the same mathematical form as in the Bohlinian, i.e.,

\[
H \left( \hat{p}, \hat{q} \right) = \frac{\hat{p}^2}{2m} + \frac{m \omega_0^2 \hat{q}^2}{2}, \quad D \left( \hat{p}, \hat{q} \right) = \frac{\beta}{2} \left( \hat{p} \hat{q} + \hat{q} \hat{p} \right),
\]

(147)

The operators \( \hat{p}, \hat{q} \) in this picture are time dependent and satisfy the classical fundamental commutators

\[
\left[ \hat{p}, \hat{q} \right] = \frac{\hbar}{i} \delta, \quad \left[ \hat{p}, \hat{p} \right] = \left[ \hat{q}, \hat{q} \right] = 0
\]

(148)

The time derivative in Equation (146) is “material” (in the sense of continuum mechanics) because of the time dependence of the observable \( \hat{q} \). To construct a wave equation, first we rewrite this abstract wave equation in the eigenbase \( |q\rangle \) of the position operator. To do this, consider the following one-dimensional eigenvalue problem
which could constitute a continuous spectrum. Thus, we must write the orthonormality condition and completeness relation for the eigenvectors as follows

\[ \langle q | q' \rangle = \delta(q - q'), \quad \int |q' \rangle \langle q'| dq' = \delta \]

(150)

where \( \delta(q - q') \) is Dirac’s distribution and \( \delta \) is the unity operator. The wave function is the probability amplitude that a position measurement on the damped oscillator in state \( |\Psi(t)\rangle \) will yield an eigenvalue \( q \), mathematically

\[ \Psi(q, t) = \langle q | \Psi(t) \rangle \]

(151)

Inserting Equation (150) of the unity operator in the abstract wave Equation (146) and projecting from the left with \( q | \), then we obtain

\[ i\hbar \langle q | \frac{d}{dt} |\Psi(t)\rangle = \frac{d}{dt} \langle q | \Psi(t) \rangle = \langle q | H \langle \hat{\mathbf{p}}, \hat{\mathbf{q}} \rangle \int |q' \rangle \langle q'| |\Psi(t)\rangle dq' + \]

\[ -\langle q | D \left( \hat{\mathbf{p}}, \hat{\mathbf{q}} \right) \int |q' \rangle \langle q'| |\Psi(t)\rangle dq' \]

(152)

We chose the differential operator representation for the time-dependent operators in the eigenbase \( |q\rangle \) of the position operator in the form

\[ \hat{\mathbf{p}} = \frac{\hbar}{i} \frac{\partial}{\partial \mathbf{e}^{\beta t} q}, \quad \hat{\mathbf{q}} = \mathbf{e}^{\beta t} \]

(153)

which resulted in the following wave equation

\[ i\hbar \frac{d}{dt} |\Psi(e^{\beta t} q, t)\rangle = (H - D) |\Psi(e^{\beta t} q, t)\rangle, \]

\[ H = -\frac{\hbar^2}{2m} \frac{d^2}{d(e^{\beta t} q)^2} + \frac{m\omega_0^2}{2} \left( e^{\beta t} q \right)^2, \quad D = -i \hbar \left( \frac{\beta}{2} + \beta \left( e^{\beta t} q \right)^2 \frac{d}{d(e^{\beta t} q)} \right) \]

(154)
which is a linear partial differential equation. To construct the eigenvalue problem that belongs to this wave equation, we chose the wave function as

$$\Psi_n = e^{i\frac{E_n}{\hbar}t} \Phi_n(e^{\beta t}q)$$

(155)

With this wave function, the eigenvalue equation

$$-\frac{\hbar^2}{2m} \frac{d^2\Phi_n}{d(e^{\beta t}q)^2} + \frac{m\omega_0^2}{2}(e^{\beta t}q)^2 \Phi_n = E_n \Phi_n$$

(156)

is obtained from the wave equation because the equation

$$-D(e^{\frac{\beta t}{2}}\Phi_n) = i\hbar\beta\left(\frac{1}{2} + \frac{qe^{\beta t}}{\hbar}\right)\frac{d}{d(qe^{\beta t})}\left(e^{\frac{\beta t}{2}}\Phi_n\right) = i\hbar\frac{d}{dt}e^{\frac{\beta t}{2}}\Phi_n =$$

(157)

$$= i\hbar\frac{\beta}{2}e^{\frac{\beta t}{2}}\Phi_n + i\hbar e^{\frac{\beta t}{2}}\Phi_n + i\hbar e^{\frac{\beta t}{2}}$$

is satisfied identically for every eigenfunction $\Phi_n$. By introducing a new variable into the eigenvalue Equation (156) defined as $\xi = \sqrt{\frac{m\omega_0}{\hbar}}e^{\beta t}q$, then we get

$$\frac{d^2\Phi_n}{d\xi^2} + \left(\frac{2E_n}{\hbar\omega_0} - \xi^2\right)\Phi_n = 0$$

(158)

We chose the eigenfunction $\Phi_n$ in the form

$$\Phi_n = e^{-\frac{\xi^2}{2}} \psi_n$$

(159)

then we obtained the differential equation

$$\frac{d^2\psi_n}{d\xi^2} - 2\xi \psi_n + \left(\frac{2E_n}{\hbar\omega_0} - 1\right)\psi_n = 0$$

(160)
which has a solution in terms of Hermitian polynomials if the

$$\frac{2E_n}{\hbar \omega_0} - 1 = 2n \rightarrow E_n = \left(n + \frac{1}{2}\right) \hbar \omega_0, \quad n = 1, 2, 3... \quad (161)$$

relation is fulfilled. With these, the solution of the wave equation is obtained as follows:

$$\Psi_n(\xi, t) = e^{\left(\frac{E_n}{\hbar \omega_0} - \frac{\beta t}{2}\right)} \Phi_n(e^{\beta t} q) \times e^{-\left(\frac{\omega_0}{2}\right) t} e^{\frac{\beta t}{2}} e^{-\frac{q^2}{2}} H_n(\xi), \quad \xi = \sqrt{\frac{m \omega_0}{\hbar}} e^{\beta t} q \quad (162)$$

from which the probability density function of the oscillator has the form

$$\left|\Psi_n(q)\right|^2 = \frac{1}{2n! \sqrt{2\pi}} \frac{1}{\sqrt{\frac{\hbar}{2m \omega_0}} e^{\beta t}} e^{-\frac{q^2}{2\left(\frac{\hbar}{2m \omega_0} e^{\beta t}\right)}} e^{2\left(\frac{\hbar}{2m \omega_0} e^{\beta t}\right)} \left[H_n^2\left(e^{\beta t} \sqrt{\frac{m \omega_0}{\hbar}} q\right)\right] \quad (163)$$

which is exactly identical to Equation (87) resulting from the Heisenberg picture of the damped oscillator and the equation given by Kim and Page [33] using another theory. Due to this correspondence, the quantum decoherence of linearly damped oscillators could be described in the same way as done in the publication by Kim et al. [40].

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References

[1] Bateman, H. (1931). On dissipative systems and related variational principles. Phys. Rev. 38:815.

[2] Feynman, R.P., Vernon, F.L. (1963). The theory of a general quantum system interacting with a linear dissipative system. Ann. Phys. 24:118–173.
[3] Weiss, U. (2008). Quantum Dissipative Systems, 3rd edition. Singapore: World Scientific.

[4] Ingold, G.L. (2012). Thermodynamic anomaly of the free damped quantum particle: the bath perspective. Eur. Phys. J. B. 85:30.

[5] Philbin, T.G. (2012). Quantum dynamics of the damped harmonic oscillator. New J. Phys. 14:083043.

[6] Chung-In, Um et al. (2002). The quantum damped harmonic oscillator. Physics Report.362:63–192.

[7] Caldirola, P. (1941). Forze non conservative nellameccanicaquantistica. NuovoCimento. 18:393.

[8] Kanai, E. (1948). On the quantization of the dissipative systems. Prog. Theor. Phys. 3:440.

[9] Cadirola, P. (1983). Quantum theory of nonconservative systems. NuovoCimento B. 77(2):241–262.

[10] Ullersma, P. (1966). An exactly solvable model for Brownian motion. Physica. 23, 27, 56, 74, 90.

[11] Caldeira, A. O., Leggett, A. J. (1981). Influence of dissipation on quantum tunneling in macroscopic systems. Phys. Rev. Lett. 46:211–214.

[12] Ford, G. W., O’Connell R. F. (1996). There is no quantum regression theorem. Phys. Rev. Lett. 77(5):798–801.

[13] Onsager, L. (1931). Reciprocal relations in irreversible processes. II. Phys. Rev. 38:2265.

[14] Heisenberg, W. (1925). Über die quantentheoretische Umdeutung kinematischer und mechanischer Beziehungen. Z. Phys. 33:879–893.

[15] Vincze, Gy., Szász, A. (2014). Rosen–Chambers variational theory of linearly-damped oscillator. J. Adv. Phys. 4(1):404.

[16] Rosen, P. (1954). Use of restricted variational principles for the solution of differential equations. J. Appl. Phys. 25(3):336.

[17] Rosen, P. (1953). On variational principles for irreversible processes. J. Chem. Phys. 21:1220–1221.

[18] Chambers, L. (1956). A variational principle for the conduction of heat. Quart. J. Mech. Appl. Math. 9:234.

[19] Meixner, J. (1963). Thermodynamics of electrical networks and the Onsager–Casmir reciprocal relations. J. Math. Phys. 4:154.
[20] Meixner, J. (1966). Network theory and its relation to thermodynamics. In: Proceedings of the Symposium on Generalized Networks. Polytechnic Press of the Polytechnic Institute of Brooklyn, New York. pp.13–25.

[21] Perelson, A. (1975). Network Thermodynamics an Overview. Biophys. J. Jul 1975; 15(7):667–685.

[22] Onsager, L. (1931). Reciprocal relations in irreversible processes. II. Phys. Rev. 38:2265.

[23] Callen, H. and Welton, T. (1951). Irreversibility and generalized noise. Phys. Rev. 83:34–40.

[24] Kubo, R. (1966). The fluctuation-dissipation theorem. Rep. Prog. Phys. 29:225.

[25] Bohlin K. (1911). Note sur le problème des deux corps et sur une intégration nouvelle dans le problème des trois corps, Bull. Astr. 28:144.

[26] von Neumann, J. (1932). Mathematische Grundlagen der Quantenmechanik. Berlin: Springer, 1932; von Neumann, J. (1955). Mathematical Foundations of Quantum Mechanics. Princeton University Press.

[27] Landsman, N.P. (2005). Between classical and quantum. arXiv: quant-ph/0506082v2, 25 Jul.

[28] Stone, M. H. (1930). Linear transformations in Hilbert space. III. operational methods and group theory. ProcNatl AcadSciUSA. 16:172–175.

[29] Pauli, W. (1958). Die Allgemeine Prinzipien der Wellenmechanik. In: Handbuch der Physik, Band 5., Teil 1. (pp. 1–168). Berlin: Springer-Verlag; Pauli, W. (1980). General principles of quantum mechanics (translated by P. Achuthan and K. Venkatesan). Berlin: Springer Verlag (1980).

[30] Liboff, R. (2002). Introductory Quantum Mechanics, 4th edition. Addison-Wesley.

[31] Griffiths, D. (2004). Introduction to Quantum Mechanics, 2nd ed. Prentice Hall.

[32] Van Kampen, N.G. (2004). Stochastic Processes in Physics and Chemistry. Elsevier.

[33] Kim, S.P., Page, D.N. (2001). Classical and quantum action-phase variables for time-dependent oscillators. Phys. Rev. A. 64:012104.

[34] Weisskopf, V., Wigner, E. (1930). Berechnungen der Natürlichen Linienbreite auf Grund der Diracschen Lichttheorie. Z. Phys. 63:54–73.

[35] Heitler, W. (1954). The Quantum Theory of Radiations. Oxford: Clarendon Press.

[36] Dekker, H. (1981). Classical and quantum mechanics of the damped harmonic oscillator. Physics Report. 80:1.

[37] Merzbacher, E. (1980). Quantum Mechanics. Wiley International.
[38] Bedeaux, D., Mazur, P. (2001). Mesoscopic non-equilibrium thermodynamics for quantum systems. Physica A. 298:81–100.

[39] Kostin, M.D. (1972). On the Schrödinger–Langevin equation. J. Chem. Phys. 57:3589.

[40] Kim, S.P. et al. (2002). Decoherence of Quantum Damped Oscillators. arXiv:quant-ph/0202089v1 15 Feb.