



Onsagerian Quantum Mechanics

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ABSTRACT

We describe the basic quantum-mechanical categories and properties of the thermodynamical basis of Onsager's theorem. 3 basic principles are used: 1. energy dissipation; 2. Hamiltonian formalism; 3. Onsager's linearity. We obtain the 2 characteristic values of the observables, their main-value and the deviation, the first and second momentums of the probability distribution function, which we also derived also from the same principles.

Keywords

energy-dissipation, Hamiltonian, Onsager's theorem, probability distribution-function, measurability

Academic Discipline And Sub-Disciplines

Thermodynamics, quantum mechanics

INTRODUCTION

We describe the basic quantum-mechanical categories and properties of the thermodynamical basis of Onsager's theorem. 3 basic principles are used: 1. energy dissipation; 2. Hamiltonian formalism; 3. Onsager's linearity. We obtain the 2 characteristic values of the observables, their main-value and the deviation, the first and second momentums of the probability distribution function, which we also derived also from the same principles.

In developing the principles of quantum-mechanics, the Hamiltonian formalism had a central role [1].

Onsager's principles drive the description of non-equilibrium thermodynamics near equilibrium, which is a linear theory [2], [3]. The principle is based on the entropy-production in general or on the energy-dissipation in isothermal systems in special cases. Onsager's reciprocal principle cannot be derived from mechanical roots like the Liouville or Hamilton dynamical equations, and it is also not possible to derive it from any of the basic quantum-mechanical principles of Schrodinger, Heisenberg or von Neumann. The main problem is the so-called irreversibility paradox [4], centered on time reversibility, which is complete in mechanics but, due to entropy production, is not valid in non-equilibrium thermodynamical systems. The dispersion-dissipation theorem cannot be derived from the theorems of traditional mechanics alone [5]. Consequently, it is hardly surprising that the understanding of quantum-mechanics on the basis of thermodynamics has been debated over a long time [6], [7], [8], [9].

A non-linear equation of motion was proposed to solve this problem [10], [11], [12], [13], the new description being called quantum-thermodynamics. Another approach has been mesoscopic non-equilibrium thermodynamics for quantum mechanics [14], recognizing the differences between macro- and micro-relaxation phenomena.

METHODS

Consider an isothermal system. We use the energy-dissipation following Onsager's original meaning. The actual energy of the system is described by the $H(q_i, p_i)$ Hamiltonian. We suppose the time dependence of the Hamiltonian is included solely through the actual state of the system. The dissipated energy when the system does not interact with its environment would be the product of the generalized forces and currents:

$$\begin{aligned}
 D &:= \frac{dH}{dt} = \sum_{i=1}^n \frac{\partial H}{\partial q_i} \frac{dq_i}{dt} + \sum_{i=1}^n \frac{\partial H}{\partial p_i} \frac{dp_i}{dt} = \langle \bar{x}, \bar{j} \rangle, \\
 \bar{x} &:= \bar{\nabla}H = \left(\frac{\partial H}{\partial q_1}, \dots, \frac{\partial H}{\partial q_i}, \dots, \frac{\partial H}{\partial q_n}, \dots, \frac{\partial H}{\partial p_1}, \dots, \frac{\partial H}{\partial p_i}, \dots, \frac{\partial H}{\partial p_n} \right), \\
 \bar{j} &:= \left(\frac{dq_i}{dt}, \dots, \frac{dq_i}{dt}, \dots, \frac{dq_n}{dt}, \frac{dp_1}{dt}, \dots, \frac{dp_i}{dt}, \dots, \frac{dp_n}{dt} \right)
 \end{aligned} \tag{1}$$

According to the Onsager's principle, the thermodynamic forces and currents have a linear constitutive relationship:



$$\bar{j} = \bar{L}x \quad (2)$$

where \bar{L} is the conduction-matrix.

The participation of the vectors of forces and current is as follows:

$$\begin{aligned} \bar{j} &:= \begin{bmatrix} \bar{j}_q \\ \bar{j}_p \end{bmatrix}, \quad \bar{j}_q := \left(\frac{dq_i}{dt}, \dots, \frac{dq_i}{dt}, \dots, \frac{dq_n}{dt} \right), \quad \bar{j}_p := \left(\frac{dp_1}{dt}, \dots, \frac{dp_i}{dt}, \dots, \frac{dp_n}{dt} \right) \\ \bar{x} &:= \begin{bmatrix} \bar{x}_q \\ \bar{x}_p \end{bmatrix}, \quad \bar{x}_q := \left(\frac{\partial H}{\partial q_1}, \dots, \frac{\partial H}{\partial q_i}, \dots, \frac{\partial H}{\partial q_n} \right), \quad \bar{x}_p := \left(\frac{\partial H}{\partial p_1}, \dots, \frac{\partial H}{\partial p_i}, \dots, \frac{\partial H}{\partial p_n} \right) \\ \begin{bmatrix} \bar{j}_q \\ \bar{j}_p \end{bmatrix} &= \begin{bmatrix} \bar{L}_{qq} & \bar{L}_{qp} \\ \bar{L}_{pq} & \bar{L}_{pp} \end{bmatrix} \begin{bmatrix} \bar{x}_q \\ \bar{x}_p \end{bmatrix} \end{aligned} \quad (3)$$

Interference could happen in isotropic systems only between the forces and currents having identical tensor-rank and tensor-characters (i.e. the Curie Principle).

Time reversal shows that:

$$\begin{aligned} t &\mapsto -t \\ \bar{j}_q &:= \left(\frac{dq_i}{dt}, \dots, \frac{dq_i}{dt}, \dots, \frac{dq_n}{dt} \right) \text{ reversed} \\ \bar{j}_p &:= \left(\frac{dp_1}{dt}, \dots, \frac{dp_i}{dt}, \dots, \frac{dp_n}{dt} \right) \text{ un-reversed} \\ \bar{x}_q &:= \left(\frac{\partial H}{\partial q_1}, \dots, \frac{\partial H}{\partial q_i}, \dots, \frac{\partial H}{\partial q_n} \right) \text{ un-reversed} \\ \bar{x}_p &:= \left(\frac{\partial H}{\partial p_1}, \dots, \frac{\partial H}{\partial p_i}, \dots, \frac{\partial H}{\partial p_n} \right) \text{ reversed} \end{aligned} \quad (4)$$

Applying Equation (4) to the Curie Principle in reversible systems gives:

$$\bar{L} = \begin{bmatrix} 0 & \bar{L}_{qp} \\ \bar{L}_{pq} & 0 \end{bmatrix} \quad (5)$$

With no dissipation, when the system is conservative:

$$\bar{L}_{pq} = -\bar{L}_{qp} \quad (6)$$



Damped linear oscillator

The energetic description of the damped linear oscillator characterized by the Hamiltonian function:

$$H(q, p) = \frac{p^2}{2m} + \frac{kq^2}{2} \quad (7)$$

As well as the dissipative function:

$$D = -c \left(\frac{dq}{dt} \right)^2 \quad (8)$$

These 2 functions are connected with the energy-balance:

$$\begin{aligned} \frac{dH(q, p)}{dt} &= \frac{\partial H}{\partial q} \frac{dq}{dt} + \frac{\partial H}{\partial p} \frac{dp}{dt} = \\ &= kq \frac{dq}{dt} + \frac{p}{m} \frac{dp}{dt} = -c \left(\frac{dq}{dt} \right)^2 \end{aligned} \quad (9)$$

Equation (9) could be solved for currents such as:

$$\begin{bmatrix} \frac{dq}{dt} \\ \frac{dp}{dt} \end{bmatrix} = \begin{bmatrix} 0 & a \\ -a & -c \end{bmatrix} \begin{bmatrix} \frac{\partial H}{\partial q} \\ \frac{\partial H}{\partial p} \end{bmatrix} \quad (10)$$

where a is arbitrary. This is a set of equations for an oscillator in Onsagerian frame of reference. When $a = 1$, the dynamic equation of the oscillator is as follows:

$$\begin{bmatrix} \frac{dq}{dt} \\ \frac{dp}{dt} \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ -1 & -c \end{bmatrix} \begin{bmatrix} \frac{\partial H}{\partial q} \\ \frac{\partial H}{\partial p} \end{bmatrix} \quad (11)$$

In the case of $c = 0$ we receive the Hamilton function of the non-damped oscillator.

These equations could be formulated with Poisson brackets as well, because

$$\frac{\partial H}{\partial p} = [q, H], \quad \frac{\partial H}{\partial q} = -[p, H] \quad (12)$$

where we used the classical Poisson bracket:



$$[f, g] = \frac{\partial f}{\partial q} \frac{\partial g}{\partial p} - \frac{\partial f}{\partial p} \frac{\partial g}{\partial q} \quad (13)$$

Consequently,

$$\frac{dq}{dt} = \frac{\partial H}{\partial p} = [q, H], \quad \frac{dp}{dt} = -\frac{\partial H}{\partial q} - c \frac{\partial H}{\partial p} = [p, H] - c[q, H] \quad (14)$$

With these equations, the changing dynamism of any actual A physical value could be determined. When $A = A(t, p, q)$, then we obtain from Equation (14):

$$\begin{aligned} \frac{dA}{dt} &= \frac{\partial A}{\partial t} + \frac{\partial A}{\partial q} \frac{dq}{dt} + \frac{\partial A}{\partial p} \frac{dp}{dt} = \frac{\partial A}{\partial t} + \frac{\partial A}{\partial q} \frac{\partial H}{\partial p} - \frac{\partial A}{\partial p} \frac{\partial H}{\partial q} - c \frac{\partial A}{\partial p} \frac{\partial H}{\partial p} = \\ &= \frac{\partial A}{\partial t} + [A, H] - c[q, A][q, H] \end{aligned} \quad (15)$$

Applying Equation (15) to the Hamilton-function:

$$\frac{dH}{dt} = \frac{\partial H}{\partial t} + [A, H] - c[q, H][q, H] = 0 + 0 - c[q, H]^2 = -c \left(\frac{\partial H}{\partial p} \right)^2 = -c \left(\frac{p}{m} \right)^2 \quad (16)$$

Evaluation of the equations with Poisson brackets could be performed using algebra, knowing the following relations for all the thermodynamic state functions:

$$[p, q] = 1, \quad [q, q] = [p, p] = 0 \quad (17)$$

The identical transformations that could be used for the algebraic formulation are then:

$$\begin{aligned} (f, g) &= -(g, f), \\ (f, f) &= (g, g) = 0, \\ (f, const) &= 0, \\ (f_1 f_2, g) &= (f_1, g) f_2 + f_1 (f_2, g), \\ (f, g_1 g_2) &= (f, g_1) g_2 + g_1 (f, g_2), \\ \frac{\partial}{\partial t} (f, g) &= \left(\frac{\partial f}{\partial t}, g \right) + \left(f, \frac{\partial g}{\partial t} \right), \\ (f, (g, h)) + (g, (h, f)) + (h, (f, g)) &= 0 \end{aligned} \quad (18)$$

In this way the Poisson brackets in Equation (14) are:



$$\begin{aligned}
 [q, H] &= \frac{1}{2m} [q, p^2] + \frac{k}{2} [q, q^2] = & (19) \\
 &= \frac{1}{2m} [q, p]p + \frac{1}{2m} p[q, p] + \frac{k}{2} [q, q]q + \frac{k}{2} q[q, q] = \\
 &= \frac{p}{m}, \\
 [p, H] &= \frac{1}{2m} [p, p^2] + \frac{k}{2} [p, q^2] = \\
 &= \frac{1}{2m} [q, p]p + \frac{1}{2m} p[p, p] + \frac{k}{2} [p, q]q + \frac{k}{2} q[p, q] = -kq
 \end{aligned}$$

From the Onsagerian Equation (14), the canonic dynamic equations of the damped oscillator are obtained:

$$\frac{dq}{dt} = [q, H] = \frac{p}{m}, \quad \frac{dp}{dt} = [p, H] - c[q, H] = -kq - c\frac{p}{m} \quad (20)$$

Dirac's approach to Onsagerian quantum-mechanics

The classical equations formulated by Poisson brackets are identical to the quantum-mechanical ones in non-dissipative systems. However, according to Dirac, the Poisson brackets have to be defined differently, keeping the identical transformations shown in Equation (18), valid. The observable values in these equations must be the operators of the Hilbert-space.

Dirac's proposal for the quantum-mechanical interpretation of the Poisson bracket in non-dissipative systems was as follows:

$$[\mathbf{u}, \mathbf{v}] = \frac{1}{i\hbar} (\mathbf{u}\mathbf{v} - \mathbf{v}\mathbf{u}) = \frac{1}{i\hbar} (\mathbf{u}, \mathbf{v}) \quad (21)$$

So the consequent commutative rules are:

$$(\mathbf{p}, \mathbf{q}) = i\hbar, \quad (\mathbf{p}, \mathbf{p}) = (\mathbf{q}, \mathbf{q}) = 0 \quad (22)$$

The equation for a non-dissipative quantum-mechanical systems is:

$$\frac{d\mathbf{q}}{dt} = \frac{1}{i\hbar} (\mathbf{q}, \mathbf{H}), \quad \frac{d\mathbf{p}}{dt} = \frac{1}{i\hbar} (\mathbf{p}, \mathbf{H}) \quad (23)$$

where the bold letters are operators. We would like to transfer Dirac's method for the dissipative systems too, and rewrite the Equation (12) as follows:



$$\frac{d\mathbf{q}}{dt} = [\mathbf{q}, \mathbf{H}], \quad \frac{d\mathbf{p}}{dt} = [\mathbf{p}, \mathbf{H}] - c[\mathbf{q}, \mathbf{H}], \quad (24)$$

$$\mathbf{H} = \frac{\mathbf{p}^2}{2m} + \frac{k}{2}\mathbf{q}^2$$

where the definition of the Poisson bracket has a new, time-dependent equation due to the dissipative processes:

$$[\mathbf{u}, \mathbf{v}] = g(t) \frac{1}{i\hbar} (\mathbf{u}\mathbf{v} - \mathbf{v}\mathbf{u}) = g(t) \frac{1}{i\hbar} (\mathbf{u}, \mathbf{v}) \quad (25)$$

where $g(t)$ is a time-dependent function, which we define later on.

This definition fulfils the identities in Equation (17), and the observable values have commutative rules like:

$$(\mathbf{q}, \mathbf{p}) = \frac{i\hbar}{g(t)}, \quad (\mathbf{p}, \mathbf{p}) = (\mathbf{q}, \mathbf{q}) = 0 \quad (26)$$

Applying this definition, we obtain from Equation (23):

$$\frac{d\mathbf{q}}{dt} = \frac{g(t)}{i\hbar} (\mathbf{q}, \mathbf{H}) = \frac{\mathbf{p}}{m}, \quad \frac{d\mathbf{p}}{dt} = \frac{g(t)}{i\hbar} (\mathbf{p}, \mathbf{H}) - c \frac{g(t)}{i\hbar} (\mathbf{q}, \mathbf{H}) = -k\mathbf{q} - c \frac{\mathbf{p}}{m} \quad (27)$$

which describes the quantum-mechanical damped oscillator well:

$$m \frac{d^2\mathbf{q}}{dt^2} + c \frac{d\mathbf{q}}{dt} + k\mathbf{q} = 0, \quad (28)$$

This is an operator differential equation having a formal identity with the classical equation of the damped oscillator, only it uses an operator instead of a simple variable. The solution to this equation is also formally identical to the classical solution:

$$\mathbf{q} = \mathbf{a} e^{-\frac{c}{2m}t} e^{i\omega t} + \mathbf{b} e^{-\frac{c}{2m}t} e^{-i\omega t}, \quad (29)$$

$$\omega = \sqrt{\left(\frac{k}{m}\right)^2 - \left(\frac{c}{2m}\right)^2}$$

Requesting the Hermitian observables (i.e. the real eigenvalues), then from the condition of $\mathbf{q} = \mathbf{q}^+$ we obtain:

$$\mathbf{q} = \mathbf{b} e^{-\frac{c}{2m}t} e^{-i\omega t} + \mathbf{b}^+ e^{-\frac{c}{2m}t} e^{i\omega t}, \quad (30)$$



where the cross is a sign of the same time transposition and conjugation. For a better similarity of Equation (30) to the non-damped oscillator, we will use the equivalent form:

$$\mathbf{q} = \sqrt{\frac{\hbar}{2m\omega}} (\mathbf{A}e^{-i\omega t} + \mathbf{A}^+ e^{i\omega t}), \quad \mathbf{A} = \mathbf{a}e^{-\frac{c}{2m}t} \quad (31)$$

The operator of the momentum according to Equation (26) is expressed as:

$$\mathbf{p} = \sqrt{\frac{\hbar m}{2\omega}} (\gamma \mathbf{A}e^{-i\omega t} + \gamma^* \mathbf{A}^+ e^{i\omega t}), \quad (32)$$

$$\gamma = -\frac{c}{2m} - i\omega$$

Putting the expressions of Equations (32) and (28) together, the exchange relationship of the amplitudes will be:

$$(\mathbf{A}, \mathbf{A}^+) = \frac{1}{g(t)}, \quad (33)$$

The damped oscillator is determined when we calculate the operator \mathbf{A} , due to the amplitude, momentum and energy becoming calculable. In the non-damped case, the amplitude A is calculable from the energy of the oscillator, which is a conserved value. However, it is not possible in the damped case, so we will use the conserved value introduced by Blochin [15]. Using the quantum-mechanical formulation, the matrices belonging to the constant must be Hermitian due to the real eigenvalues. It is expected that the constants are free from deviations, consequently (as later we prove) the matrix has to be diagonal. This diagonal condition is enough to determine the matrix \mathbf{A} . The Blochin-constant (i.e. the energy) is calculated using:

$$\mathbf{F} = \frac{m}{4} e^{\left(\frac{c}{m}\right)t} \left\{ \left(\frac{d\mathbf{q}}{dt} - \gamma \mathbf{q} \right) \left(\frac{d\mathbf{q}}{dt} - \gamma^* \mathbf{q} \right) + \left(\frac{d\mathbf{q}}{dt} - \gamma^* \mathbf{q} \right) \left(\frac{d\mathbf{q}}{dt} - \gamma \mathbf{q} \right) \right\} = \quad (34)$$

$$= \frac{\hbar\omega}{2} e^{\left(\frac{c}{m}\right)t} (\mathbf{A}\mathbf{A}^+ + \mathbf{A}^+\mathbf{A}) = \hbar\omega e^{\left(\frac{c}{m}\right)t} \left(\mathbf{A}^+\mathbf{A} + \frac{1}{2g(t)} \right)$$

Due to the correspondence-principle, this value has to be constant; consequently:

$$g(t) = e^{\left(\frac{c}{m}\right)t}$$

And therefore:

$$\mathbf{F} = \hbar\omega \left(\mathbf{a}^+ \mathbf{a} + \frac{1}{2} \right), \quad (35)$$



where $\mathbf{a} = \mathbf{A}(t = 0)$ is the initial amplitude that satisfies the commutative relationship:

$$(\mathbf{a}^+, \mathbf{a}) = 1, \quad (36)$$

Based on these equations,

$$\begin{aligned} (\mathbf{F}, \mathbf{a}^+) &= \hbar\omega\mathbf{a}^+ \\ (\mathbf{a}, \mathbf{F}) &= \hbar\omega\mathbf{a} \end{aligned}, \quad (37)$$

Consequently, these conditions are valid for the \mathbf{A} and \mathbf{A}^+ operators too:

$$\begin{aligned} (\mathbf{F}, \mathbf{A}^+) &= \hbar\omega\mathbf{A}^+ \\ (\mathbf{A}, \mathbf{F}) &= \hbar\omega\mathbf{A} \end{aligned}, \quad (38)$$

Consequently, the amplitude matrices, the eigenvalues of the conserved value (energy) and so we obtain the matrices of amplitudes, velocities and momentums. The results show that:

- The smallest eigenvalue of energy is zero, connected to the eigenvector $\mathbf{a}\psi_{F0} = 0$
- The vacuum-state has $\frac{1}{2}\hbar\omega$ zero-point energy,
- The eigenvector belonging to the n-th state is $\psi_{Fn} = \frac{\mathbf{a}^{+n}}{n!}\psi_{F0}$. Having energy eigenvalue $(\frac{1}{2} + n)\hbar\omega$
- The matrices

$$\mathbf{a} = [a_{ik} = \delta_{ni, nk-1}\sqrt{n_k}] = \begin{bmatrix} 0 & \sqrt{1} & 0 & 0 \\ 0 & 0 & \sqrt{2} & 0 \\ 0 & 0 & 0 & \sqrt{3} \\ 0 & 0 & 0 & 0 \end{bmatrix}, \quad (39)$$

$$\mathbf{a}\mathbf{a}^+ = [a_{ik} = \delta_{ni, nk}n_k] = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & 3 & 0 \\ 0 & 0 & 0 & 4 \end{bmatrix}, \quad (40)$$

$$\mathbf{a}^+\mathbf{a} = [a_{ik} = \delta_{ni, nk}n_k - 1] = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 3 \end{bmatrix}, \quad (41)$$

- And the vectors:



$$\psi_{F0} = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}, \quad \psi_{F1} = \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}, \quad \psi_{F2} = \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix},$$

From here we see that the \mathbf{aa} and $\mathbf{a}^+ \mathbf{a}^+$ matrices are not diagonal.

Mean value of the amplitude and the momentum

The mean values of the observables are determined by the values of the main diagonal of the corresponding matrix. Consequently, the mean value of the amplitude and the momentum is zero. The standard deviation could be calculated putting zeros into the main diagonal and making the prepared matrix square. The values in the main diagonal of this squared matrix are the corresponding standard deviations. Consequently:

$$\overline{\Delta q^2}_n = \left[\frac{\hbar}{2m\omega} (\mathbf{A}^+ \mathbf{A} + \mathbf{A} \mathbf{A}^+) \right]_{nn} = \frac{\hbar}{2m\omega} e^{-\frac{c}{m}t} (2n+1), \quad (43)$$

$$\overline{\Delta p^2}_n = \left[\frac{\hbar m}{2\omega} \gamma \gamma^+ (\mathbf{A}^+ \mathbf{A} + \mathbf{A} \mathbf{A}^+) \right]_{nn} = \quad (44)$$

$$= \frac{\hbar m}{2\omega} \omega_0^2 e^{-\frac{c}{m}t} (2n+1),$$

$$\omega_0 = \sqrt{\frac{k}{m}}$$

The product of the deviation will give the Heisenberg's uncertainty condition in the form of:

$$\sqrt{\overline{\Delta p_n^2} \overline{\Delta q_n^2}} = \frac{\hbar}{2\omega} \omega_0 e^{-\frac{c}{m}t} (2n+1), \quad (45)$$

Equation (45) shows that the product of deviations tends to zero by time. This contradicts the conventional uncertainty principle.

The mean value of the energy would be:

$$E_n = \left[\frac{1}{2} m \left(\frac{d\mathbf{q}}{dt} \right)^2 + \frac{1}{2} m \omega_0^2 \mathbf{q}^2 \right]_{nn} = \frac{\hbar}{\omega} \omega_0^2 e^{-\frac{c}{m}t} \left(n + \frac{1}{2} \right), \quad (46)$$

The amplitude is, by the classical theory:

$$E = m \omega_0^2 A^2, \quad (47)$$



Consequently, from Equations (46) and (47), the amplitude of the n-th state is:

$$A = \sqrt{\frac{\hbar}{\omega m}} e^{-\frac{c}{2m}t} \sqrt{2n+1}, \quad (48)$$

So the initial amplitude of the fluctuation at the zero-point is proportional to $1/\sqrt{\omega}$. These initial amplitudes are quantised but continuously decrease with time.

The probability description of wave-packet motion of the wave-function

Let us now study the probability amplitude of the eigenvalue of the oscillator-amplitude in the eigenstate of the creation operator, calculating the time-dependence of the function:

$$\Psi_d(q) = \langle \mathbf{q} | \mathbf{d} \rangle \quad (49)$$

We express the creation operator with the operators of actual position:

$$\mathbf{q} = \sqrt{\frac{\hbar}{2m\omega}} (\mathbf{A}e^{-i\omega t} + \mathbf{A}^+ e^{i\omega t}) \quad (50)$$

and momentum:

$$\mathbf{p} = \sqrt{\frac{\hbar m}{2\omega}} (\gamma \mathbf{A}e^{-i\omega t} + \gamma^* \mathbf{A}^+ e^{i\omega t}), \quad (51)$$

$$\gamma = -\frac{c}{2m} - i\omega$$

In this case the creation operator would be:

$$\mathbf{A}e^{-i\omega t} = \sqrt{\frac{m}{2\hbar\omega}} \left(\frac{i\mathbf{p}}{m} + \frac{\gamma^*}{i} \mathbf{q} \right) \quad (52)$$

The eigenvalue equation for the creation operator is:

$$\mathbf{a} | \mathbf{d} \rangle = \sqrt{\frac{\omega m}{2\hbar}} d | \mathbf{d} \rangle \quad (53)$$

from where



$$\langle \mathbf{q} | \mathbf{a} | \mathbf{q} \rangle = \int \langle \mathbf{q} | \mathbf{a} | \mathbf{q}' \rangle \langle \mathbf{q}' | \mathbf{d} \rangle d\mathbf{q}' = \int \langle \mathbf{q} | \mathbf{a} | \mathbf{q}' \rangle \Psi_d(\mathbf{q}') d\mathbf{q}' = \sqrt{\frac{\omega m}{2\hbar}} d \Psi_d(\mathbf{q}') \quad (54)$$

and the time-dependence is:

$$\int \langle \mathbf{q} | \sqrt{\frac{m}{2\hbar\omega}} \left(i \frac{\mathbf{p}}{m} + \frac{\gamma^*}{i} \mathbf{q} \right) | \mathbf{q}' \rangle \Psi_d(\mathbf{q}') d\mathbf{q}' = \sqrt{\frac{\omega m}{2\hbar}} d e^{-\beta t} e^{-i\omega t} \Psi_d(\mathbf{q}) \quad (55)$$

Substituting the values:

$$\langle \mathbf{q} | \mathbf{p} | \mathbf{q}' \rangle = e^{-2\beta t} \hbar \delta'(q - q') + A(q) \delta(q - q'), \quad \langle \mathbf{q} | \mathbf{q} | \mathbf{q}' \rangle = q \delta(q - q') \quad (56)$$

We obtain:

$$\left(\left[\frac{\gamma^*}{i} + A(q) \right] q + \frac{\hbar}{m} \frac{d}{dq} e^{-2\beta t} \right) \Psi_d(q) = \omega d e^{-\beta t} e^{-i\omega t} \Psi_d(q) \quad (57)$$

Choosing the A(q) arbitrary function in the rectangular bracket we have. Then, the solution to the differential equation after normalizing will be:

$$\Psi_d(q) = \left(\frac{m\omega}{\hbar\pi} \right)^{\frac{1}{4}} e^{\frac{1}{2}\beta t} e^{-\frac{m\omega}{2\hbar} e^{2\beta t} (q - d e^{-\beta t} e^{-i\omega t})^2} \quad (58)$$

The questioned probability would be:

$$|\Psi_d(q)|^2 = \left(\frac{m\omega}{\hbar\pi} \right)^{\frac{1}{2}} e^{\beta t} e^{-\frac{m\omega}{\hbar} e^{2\beta t} (q - d e^{-\beta t} \cos(\omega t))^2} \quad (59)$$

It is a Gaussian distribution with the function of probability density:

$$|\Psi_d(q)|^2 = \frac{1}{\sqrt{\pi} \left(\sqrt{\frac{\hbar}{m\omega}} e^{-\beta t} \right)} e^{-\frac{(q - d e^{-\beta t} \cos(\omega t))^2}{2 \left(\sqrt{\frac{\hbar}{m\omega}} e^{-\beta t} \right)^2}} \quad (60)$$

Consequently, the movement of the weight-centre of the wave-packet $|\mathbf{d}\rangle$ is a damped oscillation, with an exponentially decreasing spreading (deviation) from the $\sqrt{\frac{\hbar}{m\omega}}$ initial value to zero (see Figure 1).

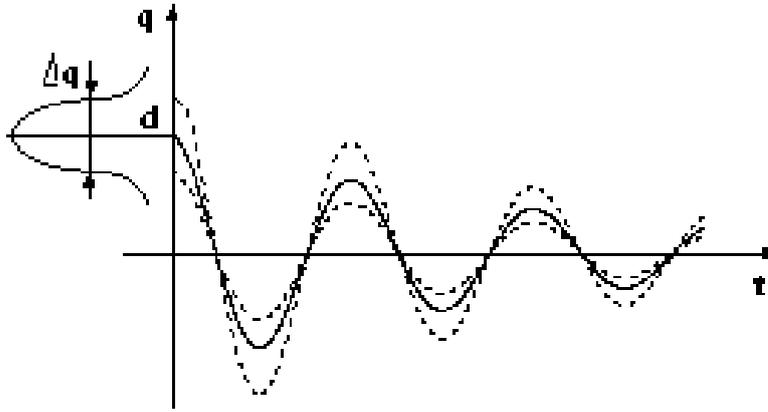


Figure 1. Representation of the motion of packet $|\mathbf{d}\rangle$. The motion of the centre of the packet with Δq are represented. The initial distribution of the packet is also shown as an insert on the vertical axis.

Mean values of the observables

The physical quantities (observables) are $\mathbf{O}(t)$ operators acting on the element's time-dependent complex Hilbert-space in the Heisenberg's description, while the status of the system is described by a time-independent $\Psi(t=0)$ element of this field. The state is dimensionless, while the observables have dimensions.

The operator of the given observable connect the state-vector of the system to a vector in Hilbert-space:

$$f_O(t) = \mathbf{O}(t)\Psi(0) \quad (61)$$

which also has dimensions. This is the state-parameter of the system belonging to the actual observable in the actual time. This is the reason why we could describe the actual place, momentum, energy, and the angular-momentum of the system. Knowing the actual state-vector of the observable, we can follow the state of the system:

$$\mathbf{O}^{-1}(t)f_O(t) = \Psi(0) \quad (62)$$

In the case where the state of the system is the eigenstate of one observable, then the actual state of the observable is:

$$f_O(t) = \lambda_O(t)\Psi(0) = \mathbf{O}(t)\Psi(0) \quad (63)$$

In this case, the system is in the eigenstate by the actual physical quantity time momentum, energy, angular-momentum, etc. In this case, the system could have a number, which we consider the quantity of the given physical parameter in the actual time moment. These values must be real, so the operators of the physical systems must be Hermitian-type. The system of the eigenvalues and eigenvectors has an important role in the measurability of the real situation. These values and vectors are the solutions of the following equation:



$$\mathbf{O}(t)\Psi_i(t) = \lambda_{O_i}(t)\Psi_i(t) \quad (64)$$

When we make any measurement on the system at the t -time-point for the physical quantity represented by the \mathbf{O} operator, the state of the system will be one of the eigenvectors of Equation (4) at the given t time-point. Consequently, the following change of the state happens:

$$\Psi(0) \rightarrow \Psi_i(t) \quad (65)$$

Equation (65) is the so-called reduction of the wave-packet. The value of the physical quantity will be the eigenvalue belonging to the same eigenvector:

$$\lambda_{O_i}(t) \quad (66)$$

The meaning of the value of the physical quantity in one eigenstate is definite this way, but it is completely probabilistic which eigenvector will be the new state of the system after the actual measurement. This fact emphasises the meaninglessness of individual measurements, due to the results of the subsequent measurements being probably different. In summary, the measurement in an eigenstate gives a numerical value, and also a distribution of values as the complete result. Consequently, the correct measurement is statistical, i.e. make a large number of measurements of the identical state of the system with identical observables, and evaluate using the rules of probability theory. Then, the results of the measurements are the mean and standard deviation of the physical quantity, which both need the probability distribution function.

When the probability of a measurement in the i -th eigenstate at t -time is $w_{O_i}(t)$, then the mean value at this time-point is:

$$\bar{\mathbf{O}}(t) = \sum_i w_{O_i}(t)\lambda_{O_i}(t) \quad (67)$$

The same result is obtained when evaluating the expression

$$\bar{\mathbf{O}}(t) = \sum_i w_{O_i}(t)\lambda_{O_i}(t) = \langle \Psi(0)\mathbf{O}(t)\Psi(0) \rangle \quad (68)$$

Let us now construct the state of the system by the superposition of the eigenstates of the given observable:

$$\Psi(0) = \sum_i \langle \Psi_i(t)\Psi(0) \rangle \Psi_i(t) \quad (69)$$

Substituting Equation (69) into (68) we obtain:

$$\begin{aligned} \bar{\mathbf{O}}(t) &= \langle \Psi(0)\mathbf{O}(t)\Psi(0) \rangle = \sum_i \langle \Psi(0)\mathbf{O}(t)\Psi_i(t) \rangle \langle \Psi_i(t)\Psi(0) \rangle = \\ &= \sum_i \langle \Psi(0)\Psi_i(t) \rangle \langle \Psi_i(t)\Psi(0) \rangle \lambda_{O_i}(t) \end{aligned} \quad (70)$$

Comparing Equations (67) and (70), the distribution function is obtained:



$$w_{O_i}(t) = |\langle \Psi(0) \Psi_i(t) \rangle|^2 \quad (71)$$

We constructed a closed theory in this way, because, knowing the state of the system and the eigenfunctions of the observables, we constructed the statistical probability distribution function of the measurements. Consequently the first and second moments of the distribution (i.e. the mean and standard deviation) are determined, and the exact measurement of the observable is complete. The probability amplitude is a complex value:

$$\langle \Psi(0) \Psi_i(t) \rangle \quad (72)$$

Result of the measurement on the matrix-basis

An operator could be represented by its matrix, which is definitive on the base-function system like:

$$O_{mn}(t) = \langle \Phi_m \mathbf{O}(t) \Phi_n \rangle \quad (73)$$

The diagonal elements are the mean values of the O operator in Φ_n state:

$$O_{nn}(t) = \langle \Phi_n \mathbf{O}(t) \Phi_n \rangle \quad (74)$$

The task is to determine the matrix of the operator. Its main diagonal shows the mean values of the states corresponding to the various eigenstates of the operator:

$$\bar{O}(t) = [O_{mn}(t) \delta_{mn}] = [\langle \Phi_m \mathbf{O}(t) \Phi_n \rangle \delta_{mn}] \quad (75)$$

This diagonal matrix is the matrix of the measured values of the actual observable.

The general definition of the deviation:

$$(\Delta O)^2 = \overline{(O(t) - \bar{O}(t))^2} = \overline{O^2(t)} - \bar{O}^2(t) \quad (76)$$

Consequently, the deviation of the measured value of a system in Φ_n state is:

$$\sum_m O_{nm}(t) O_{mn}(t) - (O_{nn}(t))^2 \quad (77)$$

Due to the result it could be time-dependent, the mean in time would be also important. This mean can be calculated as:



$$\begin{aligned} \bar{\mathbf{O}} &= \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T \sum_i w_{O_i}(t') \lambda_{O_i}(t') dt' = \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T \sum_i \langle \Psi(0) \mathbf{O}(t') \Psi(0) \rangle dt' = \\ &= \left\langle \Psi(0) \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T \mathbf{O}(t') dt' \Psi(0) \right\rangle \end{aligned} \quad (78)$$

This means in operator matrix representation:

$$\bar{O}_{mn} = \left\langle \Psi_m \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T \mathbf{O}(t') dt' \Psi_n \right\rangle \quad (79)$$

We studied the clean ensembles, turning now to the mixed ones. Let the measured mixed ensembles in which the mean of the given observable has to be determined to contain N-numbers of the clean ensembles. When the measurement ensemble is the existing probability of the k-th clean ensembles p_k , then the mean of the operator is:

$$\bar{\mathbf{O}}(t) = \sum_k p_k \langle \Psi_k(0) \mathbf{O}(t) \Psi_k(0) \rangle \quad (80)$$

The matrices of the operators $\mathbf{a}, \mathbf{a}^+, \mathbf{a}^2, \mathbf{a}^{+2}$ have zero values, so:

$$\bar{\mathbf{a}} = 0, \bar{\mathbf{a}}^+ = 0, \bar{\mathbf{a}}^2 = 0, \bar{\mathbf{a}}^{+2} = 0 \quad (81)$$

And the mean of the number of particles operator is:

$$\bar{\mathbf{N}} = \overline{\mathbf{A}^+ \mathbf{A}} = ne^{-\frac{c}{m}t} \quad (82)$$

The Hamilton operator could be interpreted as:

$$\mathbf{H} = \mathbf{A}^+ \mathbf{A} + \overline{\mathbf{A}^+ \mathbf{A}} = ne^{-\frac{c}{m}t} \quad (83)$$

and

$$\mathbf{q} = \sqrt{\frac{\hbar}{2m\omega}} \left(\mathbf{A} e^{-i\omega t} + \mathbf{A}^+ e^{i\omega t} \right) \quad (84)$$



$$\mathbf{p} = \sqrt{\frac{\hbar m}{2\omega}} (\gamma \mathbf{A} e^{-i\omega t} + \gamma^* \mathbf{A}^+ e^{i\omega t}), \quad (85)$$

$$\gamma = -\frac{c}{2m} - i\omega$$

Hence the mean values of these equations are zero. Consequently, the mean value of the deviations could be calculated as:

$$\overline{\mathbf{q}^2} = \frac{\hbar}{2m\omega} (\overline{\mathbf{A}\mathbf{A}^+ + \mathbf{A}^+\mathbf{A}}) = \frac{\hbar}{2m\omega} \left(\overline{\delta e^{-\frac{c}{m}t} + 2\mathbf{A}\mathbf{A}^+} \right) = \quad (86)$$

$$= \frac{\hbar}{2m\omega} e^{-\frac{c}{m}t} (1 + 2n)$$

$$\overline{\mathbf{p}^2} = \frac{\hbar m}{2\omega} (\overline{\gamma\gamma^* \mathbf{A}\mathbf{A}^+ + \gamma\gamma^* \mathbf{A}^+\mathbf{A}}) = \frac{\hbar m\omega_0^2}{2\omega} \left(\overline{\delta e^{-\frac{c}{m}t} + 2\mathbf{A}\mathbf{A}^+} \right) = \quad (87)$$

$$= \frac{\hbar m\omega_0^2}{\omega} e^{-\frac{c}{m}t} \left(\frac{1}{2} + n \right),$$

$$\omega_0^2 = \frac{k}{m}$$

And so the mean value of the Hamiltonian is:

$$\overline{\mathbf{H}} = \frac{\overline{\mathbf{p}^2}}{2m} + m\omega_0^2 \frac{\overline{\mathbf{q}^2}}{2} = \frac{\hbar\omega_0^2}{\omega} \left(\overline{\delta e^{-\frac{c}{m}t} + 2\mathbf{A}\mathbf{A}^+} \right) = \quad (88)$$

$$= \frac{\hbar\omega_0^2}{\omega} e^{-\frac{c}{m}t} \left(n + \frac{1}{2} \right)$$

The matrix of the velocity operator

The operator of acceleration is obtained by differentiation of the displacement operator twice:

$$\frac{d\mathbf{q}}{dt} = \sqrt{\frac{\hbar}{2m\omega}} (\gamma \mathbf{a} e^{\gamma t} + \gamma \mathbf{a}^+ e^{\gamma^* t}) \quad (89)$$

The matrix elements of Equation (89) are:

$$\left(\frac{d\mathbf{q}}{dt} \right)_{mn} = \sqrt{\frac{\hbar}{2m\omega}} (\gamma \langle \Psi_{Fm} | \mathbf{a} | \Psi_{Fn} \rangle e^{\gamma t} + \gamma \langle \Psi_{Fm} | \mathbf{a}^+ | \Psi_{Fn} \rangle e^{\gamma^* t}) \quad (90)$$



Using the absorption-emission operators we obtain:

$$\left(\frac{d\mathbf{q}}{dt}\right)_{mn} = \sqrt{\frac{\hbar}{2m\omega}} \left(\gamma\sqrt{n}\delta_{mn-1}e^{\gamma t} + \gamma\sqrt{n+1}\delta_{mn+1}e^{\gamma^*t} \right) \quad (91)$$

It seems that the matrix of the operator of acceleration contains non-zero terms only in the neighbouring diagonals of the main one. Consequently, we have non-zero terms of the matrix of acceleration in the emission process, when $n = m - 1$ ($m > n$). Hence

$$\left(\frac{d\mathbf{q}}{dt}\right)_{mm-1} = \sqrt{\frac{\hbar}{2m\omega}} \gamma^* \sqrt{m} e^{\gamma^*t} \quad (92)$$

Natural line-width of the spectrum

The spectrum of emission in the instance of $m = 1$ is:

$$\left(\frac{d\mathbf{q}}{dt}\right)_{10} = \sqrt{\frac{\hbar}{2m\omega}} \gamma^* e^{\gamma^*t} \quad (93)$$

Supposing a damped oscillator model of the emission process interacts with an electromagnetic field, then the current induced by the changes of the electric dipole-momentums is:

$$\left(\frac{d\mathbf{q}}{dt}\right)_{10} Q_e = Q_e \sqrt{\frac{\hbar}{2m\omega}} \gamma^* e^{\gamma^*t} \quad (94)$$

On the other hand, the velocity of the transition probability is proportional to the velocity of the dipole-momentums in the dipole approximation [16]:

$$\left(\frac{w}{dt}\right)_{10} \propto \left|\left(\frac{d\mathbf{q}}{dt}\right)_{10} Q_e\right|^2 = |\gamma^*|^2 |e^{\gamma^*t}|^2 = \omega_0^2 |e^{\gamma^*t}|^2 \quad (95)$$

Hence the probability of one photon-emission until the t-time point is:

$$w(t) = A \int_0^t |e^{\gamma^*t'}|^2 dt' \quad (96)$$

where A is a normalization constant.



$$w(t = \infty) = 1 = A \int_0^{\infty} \left| e^{\gamma^* t} \right|^2 dt' \quad (97)$$

Using the Parseval theorem [17], we obtain the form:

$$w(t = \infty) = A \int_0^{\infty} \left| e^{\gamma^* t} \right|^2 dt' = A \int_0^{\infty} F \left[e^{\gamma^* t} \right]^2 d\omega' = A \int_0^{\infty} \frac{d\omega'}{(\omega - \omega')^2 + \left(\frac{c}{2m} \right)^2} \quad (98)$$

The spectral term is the Wiegner-Weiskopf formula [18]:

$$A \frac{d\omega'}{(\omega - \omega')^2 + \left(\frac{c}{2m} \right)^2} \quad (99)$$

This formula is the probability of the event when the frequency of the emitted photon is in the interval $(\omega', \omega' + d\omega')$. Note the original formula of Wiegner-Weiskopf was ω_0 instead of ω . This is a small deviation of the present calculation from the classical one, but on the other hand the model of a harmonic oscillator bath of quantum-dissipative systems [19] is in complete harmony, giving an identical result to the one presented here.

On this basis the intensity of the radiation in interval $(\omega', \omega' + d\omega')$ will be:

$$I(\omega') d\omega' = A \frac{\hbar \omega'}{(\omega - \omega')^2 + \left(\frac{c}{2m} \right)^2} d\omega' \quad (100)$$

Representation of the momentum operator in q space

We follow the method of Fong [20], [21], starting with the commutative relationship:

$$(\mathbf{q}, \mathbf{p}) = \frac{i\hbar}{g(t)} \delta \quad (101)$$

The set of polynomials in the space of the square-integrable function is dense, so the functions:

$$1, q, q^2, \dots, q^n \quad (102)$$

form a basis, and with them every function in the Hilbert-space could be constructed.



From Equation (101) we obtain, for an arbitrary $\Psi(q)$ wave-function, that:

$$\mathbf{p}(q\Psi(q)) = q\mathbf{p}(\Psi(q)) - \frac{i\hbar}{g(t)}\Psi(q) \quad (103)$$

Using this into the first term of Equation (102), we obtain:

$$\mathbf{p}(q) = q\mathbf{p}(1) - \frac{i\hbar}{g(t)} \quad (104)$$

Supposing the following relationship holds:

$$\mathbf{p}(q^{n-1}) = q^{n-1}\mathbf{p}(1) - \frac{i\hbar}{g(t)}(n-1)q^{n-2} \quad (105)$$

Then, by the method of complete induction, we obtain from Equation (103):

$$\mathbf{p}(q^n) = \mathbf{p}(qq^{n-1}) = q\mathbf{p}(q^{n-1}) - \frac{i\hbar}{g(t)}q^{n-1} = q^n\mathbf{p}(1) - n\frac{i\hbar}{g(t)}q^{n-1} \quad (106)$$

Introducing $A(q) = \mathbf{p}(1)$ we obtain from the above:

$$\mathbf{p} = -\frac{i\hbar}{g(t)}\frac{d}{dq} + A(q) \quad (14)$$

CONCLUSION

We derived fundamental quantum-mechanical categories and properties from the thermodynamical basis. Hamiltonian formalism was applied for energy dissipation in the frame of Onsager's linearity. We formulated the main-value and deviation-value of observables.

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