Quantum and classical approaches in statistical physics: some basic inequalities

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Abstract

We present some basic inequalities between the classical and quantum values of free energy, entropy and mean energy. We investigate the transition from the deterministic case (classical mechanics) to the probabilistic case (quantum mechanics). In the first part of the paper, we assume that the reduced Planck constant $\hbar$, the absolute temperature $T$, the frequency of an oscillator $\omega$, and the degree of freedom of a system $N$ are fixed. This approach to the problem of comparing quantum and classical mechanics is new (see [35]–[37]).

In the second part of the paper, we simultaneously derive the semiclassical limits for four cases, that is, for $\hbar \to 0$, $T \to \infty$, $\omega \to 0$, and $N \to \infty$. We note that only the case $\hbar \to 0$ is usually considered in quantum mechanics (see [21]). The cases $T \to \infty$ and $\omega \to 0$ in quantum mechanics were initially studied by M. Planck and by A. Einstein, respectively.

Keywords Quantum mechanics, classical mechanics, free energy, entropy, mean energy, semiclassical limit.

1 Introduction

1. Let us consider some system A in classical mechanics and the same system A in quantum mechanics. The absolute temperature $T$ and the reduced

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Planck constant $\hbar$ are fixed. There is a general natural tendency to achieve a minimum of the free energy: $F_c(T)$ in classical case and $F_q(T, \hbar)$ in quantum case. We note that

$$F_c(T) = E_c(T) - TS_c(T), \quad F_q(T, \hbar) = E_q(T, \hbar) - TS_q(T, \hbar). \quad (1.1)$$

Here, $E_c(T)$ and $E_q(T, \hbar)$ are mean energies of the system A in classical and in quantum mechanics, respectively, and $S_c(T)$ and $S_q(T, \hbar)$ are entropies of the system A in classical and in quantum mechanics, respectively. The important topic of the classical-quantum duality is discussed (and various references are given) in the interesting works [24, 25].

Recall that the regularized statistical sum $Z_r(T, \hbar)$ is connected with the quantum statistical sum $Z_q(T, \hbar)$ by the relation

$$Z_r(T, \hbar) = (2\pi \hbar)^N Z_q(T, \hbar), \quad (1.2)$$

where $N$ is the dimension of the corresponding coordinate space. It is well known that

$$\lim_{\hbar \to 0} Z_r(T, \hbar) = Z_c(T), \quad (1.3)$$

The regularized free energy $\mathcal{F}_r(T)$ can be written in the form [13, 22]:

$$\mathcal{F}_r(T, \hbar) = -T \log Z_r(T, \hbar). \quad (1.4)$$

We introduce the regularized entropy and mean energy $S_r$ and $E_r$:

$$S_r(T, \hbar) = S_q(T, \hbar) + N \log(2\pi \hbar), \quad (1.5)$$

$$E_r(T, \hbar) = E_q(T, \hbar). \quad (1.6)$$

It is easy to see that

$$\mathcal{F}_r(T, \hbar) = E_r(T, \hbar) - TS_r(T, \hbar). \quad (1.7)$$

The choice of such regularization is explained in section 7.

**Remark 1.1** Values $F_c(T)$ and $\mathcal{F}_r(T, \hbar)$ are also minimal solutions of the corresponding extremal problems (see sections 2 and 3).

In the first part of the paper, we study the signs of the physical values

$$\mathcal{F}_r(T, \hbar) - F_c(T), \quad E_r(T, \hbar) - E_c(T), \quad S_r(T, \hbar) - S_c(T). \quad (1.8)$$
In all the examples, which we investigate in the present paper, the following inequalities hold:

\[ F_r(T, \hbar) - F_c(T) > 0, \quad \mathcal{E}_r(T, \hbar) - E_c(T) > 0. \]  \quad (1.9)

The expression for entropy satisfies the inequality

\[ S_r(T, \hbar) - S_c(T) < 0 \]  \quad (1.10)

in the case of a potential well and

\[ S_r(T, \hbar) - S_c(T) > 0 \]  \quad (1.11)

in all other cases, which we considered. It follows from (1.7) that

\[ \text{sgn } S_r(T, \hbar) = \text{sgn } [\mathcal{E}_r(T, \hbar) - F_r(T, \hbar)]. \]  \quad (1.12)

We note that harmonic oscillators and potential wells being classical objects of research are also of great current interest (see, e.g., recent papers [1, 2, 3, 14, 18, 26] and references therein), and the inequalities we deal with are basic for those cases.

2. There are a number of studies comparing classical and quantum mechanics (see some discussions and references in the recent works [5, 16, 17, 19, 30, 43]). This comparison is made according to different criteria. Our approach is based on a comparison of average values. We believe that such approach is both natural and important. In this way, we erase the probability barrier which separates classical and quantum mechanics. (However, classical mechanics remains deterministic and quantum mechanics is probabilistic.) Well-known limit theorems (e.g., by H. Weyl, A. Pleijel, M. Kac and Kirkwood–Wigner) are also based on the comparison of average values.

The extremal principles, for instance, the Fermat’s principle of least time [6] and the principle of least action [23, Ch. 1] remain central in modern physics (see some further references in [9, 28, 33, 39, 40, 41]). The named above extremal principles are formulated in terms of one physical value.

**Remark 1.2** Here, we investigate the interaction of three physical values: mean energy \( E \), entropy \( S \) and free energy \( F \). The corresponding extremal principle (see sections 2 and 3) may be considered as a cooperative game. In a cooperative game, all players have the same goal.
Let’s describe the content of the article in more detail. At first, we consider the classical case, the quantum case, and the minimal points $F_c(T)$ and $F_q(T, \hbar)$ of the corresponding extremal problems. In the next step, we compare the results of the two cases (classical and quantum).

From this point of view, we consider the connection between classical mechanics (deterministic strategy) and quantum mechanics (probabilistic strategy). We note that such comparison of the quantum and classical approaches without the requirement for Planck constant $\hbar$ being small or for absolute temperature $T$ being large is of essential scientific and methodological interest.

In order to understand the situation, we study in detail two following examples: the potential well (polyhedron) and the harmonic oscillator. In the present paper, we (in particular) improve, develop and generalize our previous results [35, 36] and [37, Ch. 6 and 9].

Using relation (1.9), we formulate our hypothesis. **Hypothesis.** The members $F_r(T, \hbar)$ and $E_r(T, \hbar)$ of the cooperative game satisfy the equality

$$\text{sgn} \ [F_r(T, \hbar) - F_c(T)] = \text{sgn} \ [E_r(T, \hbar) - E_c(T)].$$

(1.13)

3. In the second part of the paper, we study the semiclassical limits, which is an actively developed domain of research (see some recent references in [4, 7, 8, 44]). We consider the following four cases.

Case 1: $\hbar \to 0$,  Case 2: $T \to \infty$,  Case 3: $\omega \to 0$,  Case 4: $N \to \infty$.

Here, $\omega$ is the frequency of the oscillator and $N$ is the degree of freedom of a system. Usually, the cases 1-3 are investigated by semiclassical analysis [27] and micro-local analysis [24], and the case 4 involves the methods of C*-algebras [24, 38]. Our method is based on the fact that we know the eigenvalues of the corresponding boundary problems. This knowledge allows us to study all the cases 1–4 from one point of view and obtain the corresponding explicit formulas.

**Remark 1.3** The semiclassical approach in quantum mechanics deals usually with the case $\hbar \to 0$ (see [27]). The first works dedicated to the semiclassical approach were written by A. Einstein ([10], case $\omega \to 0$) and by M. Planck ([32], case $T \to \infty$).
4. As mentioned above, the free energy (in classical mechanics and quantum mechanics, respectively) is considered in sections 2 and 3. In section 4, we consider in detail two simple but important examples: one-dimensional potential well and one-dimensional harmonic oscillator. These two examples differ greatly. However, they have also some common properties. In particular, the following inequalities

\[ E_r(T, \hbar) > E_c(T), \quad F_r(T, \hbar) > F_c(T) \]  

are fulfilled in both examples (for all \( T \) and for \( \hbar > 0 \)). The \( N \)-dimensional potential well in the domain

\[ Q_N = \{ x : x = (x_1, \ldots, x_N), \quad 0 \leq x_k \leq a_k \quad (1 \leq k \leq N) \} \]  

is studied in section 5. We introduce the corresponding boundary value problem

\[ -\frac{\hbar^2}{2m} \sum_{k=1}^{N} \frac{\partial^2}{\partial x_k^2} \psi(x_1, x_2, \ldots, x_N) - E\psi(x_1, x_2, \ldots, x_N) = 0, \]

\[ \psi|_{\Gamma} = 0. \]  

Here, \( \Gamma \) stands for the boundary of the domain \( Q_N \). The inequalities (1.14) are valid in this case too.

Section 6 is dedicated to the \( N \)-dimensional oscillator, that is, we consider the differential operator

\[ \mathcal{L}\psi = -\frac{\hbar^2}{2m} \sum_{k=1}^{N} \frac{\partial^2}{\partial x_k^2} \psi(x) + V(x)\psi(x), \quad x \in \mathbb{R}^N, \]  

where

\[ V(x) = \sum_{k=1}^{N} \frac{m\omega_k x_k^2}{2}, \quad \omega_k > 0. \]  

We prove the inequalities (1.14) in the case of the \( N \)-dimensional oscillator as well. In section 7, we explain the notions of the regularized statistical sum, mean energy, free energy, and entropy. We note that the regularized values have the following important properties:

\[ Z_r(T, \hbar) \to Z_c(T), \quad F_r(T, \hbar) \to F_c(T), \quad h \to +0, \]

\[ E_r(T, h) \to E_c(T), \quad S_r(T, h) \to S_c(T), \quad h \to +0. \]  

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Remark 1.4 The following facts are essential for our theory (see section 4).

1. The quotients $Z_r(T, h)/Z_c(T)$ and $E_r(T, h)/E_c(T)$ depend, in the case of the 1-dimensional potential well $0 \leq x \leq a$, on only one variable:

$$\mu = h\sqrt{\frac{2\pi}{ma^2T}}.$$  \hspace{1cm} (1.22)

Thus, we have

$$Z_r(T, h, a)/Z_c(T, a) = f_1(\mu), \quad E_r(T, h)/E_c(T) = g_1(\mu).$$  \hspace{1cm} (1.23)

2. The quotients $Z_r(T, h, \omega)/Z_c(T, \omega)$ and $E_r(T, h)/E_c(T)$ depend, in the case of the 1-dimensional oscillator (with frequency $\omega$), on only one variable:

$$\tau = \frac{h\omega}{2T}.$$  \hspace{1cm} (1.24)

Hence, we have

$$Z_r(T, h, \omega)/Z_c(T, \omega) = f_2(\tau), \quad E_r(T, h, \omega)/E_c(T, \omega) = g_2(\tau).$$  \hspace{1cm} (1.25)

3. The functions $f_1(\mu), g_1(\mu)$ and $f_2(\tau), g_2(\tau)$ are presented in this paper in an explicit form.

In section 8, we study the $N$-dimensional potential well (1.15) and derive the following asymptotic formulas for the statistical sum

$$Z_r(T, h)/Z_c(T) = V_N^{-1}[V_N - \rho\frac{V_{N-1}}{2} + \ldots + (-1)^N \rho^N \frac{V_0}{2^NV_N}] + O(\rho^{N+1}),$$  \hspace{1cm} (1.26)

and for the mean energy

$$E_r(T, h)/E_c(T, h) = 1 + \rho\frac{V_{N-1}}{2NV_N} + O(\rho^2),$$  \hspace{1cm} (1.27)

where

$$\rho = h\sqrt{\frac{\pi}{2mT}}.$$  \hspace{1cm} (1.28)

Here, $V_N$ is the Lebesgue measure of the domain $Q_N$, $V_{N-1}$ is Lebesgue measure of the boundary $\Gamma$, $V_{N-2}$ is the Lebesgue measure of the domain $\Gamma_1$ formed by the intersection of the faces of the domain $\Gamma$, \ldots, and, finally, $V_0$ is the number of the vertices of the polyhedron.
Example 1.5 Let $N = 3$. Then, $V_3$ is the volume of the polyhedron (5.1), $V_2$ is the area of the boundary, $V_1$ is the sum of the lengths of the edges, and $V_0$ is the number of the vertices of the polyhedron (1.15).

In section 9, we consider an $N$-dimensional potential well in a sufficiently general domain and formulate the well-known results (by H. Weyl, A. Pleijel, and M. Kac) dedicated to this case.

In section 10, we consider the general-type potential $V(x)$ without assuming that the potential $V(x)$ has the form (1.19). We formulate the well-known Kirkwood–Wigner result (see [20]) dedicated to the general-type potential $V(x)$. This result implies the assertions

1. The inequality
   \[ F_r(T, \hbar) > F_c(T) \]  
   (1.29)
holds for small $\hbar$ in the general case.

2. The following semiclassical result
   \[ \lim_{\hbar \to 0} F_r(T, \hbar) = F_c(T) \]  
   (1.30)
is valid.

We consider the Quantum-Classical correspondence at the level of the inequalities (see (1.9), (1.11), (1.14) and (1.29)). The traditional semiclassical approach [21] is to consider the limit relations when $\hbar \to 0$ (see (1.20), (1.21), and (1.30)).

Remark 1.6 We applied our approach to Boltzmann equation [37, Ch. 10] and (jointly with A. Sakhnovich) to Fokker-Planck equation [34].

2 Free energy (classical case)

Let us introduce the classical Hamiltonian $H(p, q)$, where $p$ are the corresponding generalized momenta, $q$ are the corresponding generalized coordinates. In this case the mean energy $E_c$ and the entropy $S_c$ are defined by the formulas

\[ E_c = \int \int H(p, q)P(p, q)dpdq, \]  
(2.1)

\[ S_c = -\int \int P(p, q) \log P(p, q)dpdq, \]  
(2.2)
\[P(p,q) \geq 0, \quad \int \int P(p,q)dpdq = 1. \quad (2.3)\]

Free energy \(F_c\) is defined by the formula

\[F_c = E_c - TS_c, \quad (2.4)\]

where \(T\) is the absolute temperature, \(P(p,q)\) is the probability density. In order to find the equilibrium state (\(T\) is fixed) we use the calculus of variations. The corresponding Euler equation has the form

\[
\frac{\delta}{\delta P} [H(p,q)P(p,q)] + TP(p,q) \log P(p,q) + \mu P(p,q) = 0. \quad (2.5)
\]

Here, \(\frac{\delta}{\delta P}\) stands for the functional derivation and \(\mu\) is the Lagrange multiplier. We note that our extremal problem is conditional (see (2.3)). Formula (2.5) yields

\[H(p,q) + T + T \log P(p,q) + \mu = 0. \quad (2.6)\]

From (2.6) we obtain

\[P(p,q) = Ce^{-\lambda H(p,q)}, \quad \lambda = 1/T. \quad (2.7)\]

Formulas (2.3) and (2.7) imply that

\[P(p,q) = e^{-\lambda H(p,q)}/Z_c, \quad (2.8)\]

where

\[Z_c = \int \int e^{-\lambda H(p,q)}dpdq \quad (2.9)\]

is the statistical sum.

**Remark 2.1** We deduced above the well-known formulas (2.8) and (2.9). These formulas define the equilibrium state.

**Remark 2.2** The inequality

\[
\frac{\delta^2}{\delta P^2} F_c(p,q) = T/P(p,q) > 0 \quad (2.10)
\]

shows that the free energy \(F_c\) has its minimum in the equilibrium state which is defined by formulas (2.8), (2.9).
The strategy of free entropy $S_c$ and mean energy $E_c$ is common and is defined by formulas (2.1)-(2.3) and (2.8),(2.9).

**Definition 2.3** This strategy defined by formulas (2.1)-(2.3) and (2.8),(2.9) is optimal. Only by this strategy of all players free energy obtained the minimum.

Hence the following statement is valid:

**Proposition 2.4** The entropy $S_c$ and the mean energy $E_c$ are cooperating members of the game with common goal (minimize free energy)

We can write the following relation:

$$F_c = \min F,$$

(2.11)

where the value $F$ is defined by formulas (2.1)-(2.4) and the free energy $F_c$ is defined by formulas (2.1)–(2.4) and (2.7)–(2.9). The free energy $F_c(T)$ can be written in the form (see [22, 13]):

$$F_c(T) = -T \log Z_c(T).$$

(2.12)

### 3 Free energy (quantum case)

Let eigenvalues $E_n$ of the energy operator be given. Consider the mean quantum energy

$$E_q = \sum_n P_n E_n$$

(3.1)

and the quantum entropy

$$S_q = -\sum_n P_n \log P_n,$$

(3.2)

where $P_n$ are the corresponding probabilities. Hence we have

$$P_n \geq 0, \quad \sum_{n=1}^{\infty} P_n = 1$$

(3.3)

Free energy $F_c$ is defined by the formula

$$F_q = E_q - TS_q,$$

(3.4)
where $T > 0$ is the absolute temperature.

In order to find the stationary point $P_{st}$ we calculate

$$
\frac{\partial}{\partial P_k}(F_q - \mu \sum_{n=1}^{\infty} P_n),
$$

(3.5)

where $T$ is fixed and $\mu$ is Lagrange multiplier. We note that our extremal problem is conditional (see (3.3)). According to (3.5) we have

$$
E_n + T + T \log P_n - \mu = 0.
$$

(3.6)

It follows from (3.6) that

$$
P_n = Ce^{-\lambda E_n}, \quad \lambda = 1/T,
$$

(3.7)

where $C$ is a constant. Relations (3.3) imply that

$$
C = 1/Z_q, \quad Z_q = \sum_{n=1}^{\infty} e^{-\lambda E_n},
$$

(3.8)

where $Z_q$ is the statistical sum.

**Corollary 3.1** The equilibrium position $P_{st}$ is unique and is defined by the formulas (3.7) and (3.8).

By direct calculation we obtain the equalities:

$$
\frac{\partial^2}{\partial P_n^2} F_q = \frac{T}{P_n} > 0, \quad \frac{\partial^2}{\partial P_n \partial P_k} F_q = 0, \quad (n \neq k).
$$

(3.9)

Relations (3.9) imply the following assertion.

**Corollary 3.2** The equilibrium state $P_{st}$ is a minimum state of the free energy $F_q$.

The strategy $P_n$ is common for entropy $S_q$ and mean energy $E_q$. Hence, the following statement is valid.

**Proposition 3.3** The mean energy $E_q$ and the entropy $S_q$ are cooperating members of the game with common goal (minimize the free energy).
The strategy $P_n$ is optimal (see Definition 2.3).

Using Proposition 3.3, Corollary 3.3 and relations (1.4)-(1.6) we obtain the statements:

**Corollary 3.4** The equilibrium state $P_{st}$ is a minimum state of the regularized free energy $F_r$.

**Proposition 3.5** The regularized free energy $F_r$, the regularized mean energy $E_r$ and the regularized entropy $S_r$ are cooperating members of the game.

### 4 Examples

In the present section we consider in detail two simple but typical examples.

**Example 4.1** Harmonic oscillator.

In the classical case, the Hamiltonian for the harmonic oscillator has the form:

$$H(p, q) = \frac{p^2}{2m} + \frac{m\omega^2 q^2}{2}.$$  \hfill (4.1)

In the quantum case, the harmonic oscillator is described (see [21, Ch.3] and [13, Ch. 1]) by the equation:

$$-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} y - (E - \frac{m\omega^2 x^2}{2}) y = 0, \quad -\infty < x < \infty.$$  \hfill (4.2)

The spectrum $E_n$ of the boundary problem (4.1) is defined by the formula:

$$E_n = \hbar \omega (n - 1/2), \quad n = 1, 2, ...$$  \hfill (4.3)

Let us consider $Z_c(T)$ and $Z_r(T, \hbar)$. It follows from (2.9) and (4.3) that

$$Z_c(T) = \frac{2\pi T}{\omega}. \hfill (4.4)$$

Taking into account relations (1.2), (3.8), and (4.1), we have

$$Z_q(T, \hbar) = \frac{1}{2 \sinh(\tau)}, \quad Z_r(T, \hbar) = 2T \frac{\pi \tau}{\omega \sinh(\tau)}, \quad \tau = \frac{\hbar \omega}{2T}. \hfill (4.5)$$

Hence, the inequality

$$\frac{d}{d\tau} [Z_r(T, \hbar)/Z_c(T)] = \frac{\sinh(\tau) - \tau \cosh(\tau)}{\sinh^2(\tau)} < 0 \hfill (4.6)$$

is valid. Using relation (4.6) we obtain the assertion.
Proposition 4.2 For harmonic oscillator, the expression $Z_r(T, h)/Z_c(T)$ monotonically decreases with respect to $\tau$ and its limit is given by the formula

$$\lim_{\tau \to 0} [Z_r(T, h)/Z_c(T)] = 1. \quad (4.7)$$

Now, consider the regularized mean energy $\mathcal{E}_r(T, h)$. It follows from (2.1) and (4.3) that

$$E_c(T) = T. \quad (4.8)$$

Taking into account relations (3.1), (3.8), (4.2), and the formula

$$\sum_{n=1}^{\infty} e^{-an}n = \frac{e^{-a}}{(1 - e^{-a})^2}, \quad a > 0, \quad (4.9)$$

we obtain

$$\mathcal{E}_r(T, h) = T \frac{\tau}{\tanh(\tau)}, \quad \tau(T, h) = \hbar \omega/(2T). \quad (4.10)$$

The last formula implies that

$$\frac{d}{d\tau} [\mathcal{E}_r(T, h)/E_c(T)] = \frac{[\sinh(2\tau) - 2\tau]/(2 \sinh^2(\tau)) > 0, \quad (4.11)$$

Relation (4.11) yields the next assertion.

Proposition 4.3 For harmonic oscillator, the expression $\mathcal{E}_r(T, h)/\mathcal{E}_c(T)$ monotonically increases with respect to $\tau$ and

$$\lim_{\tau \to 0} [\mathcal{E}(T, h)/E_c(T)] = 1. \quad (4.12)$$

Let us turn to the regularized free energy $F_r(T, h)$. It follows from (2.12) that

$$F_r(T, h) = F_c(T) - T \log[Z_r(T, h)/Z_c(T)]. \quad (4.13)$$

Taking into account (3.4), we have

$$S_r(T, h) = S_c(T) + \frac{\tau}{\tanh(\tau)} - 1 + \log[Z_r(T, h)/Z_c(T)]. \quad (4.14)$$

Using relations (4.5), (4.10) and (4.11), (4.14) we calculate the derivative:

$$\frac{d}{d\tau} S_r(T, \tau) = [\sinh^2(\tau) - 2\tau^2]/(2\tau \sinh^2(\tau)) > 0. \quad (4.15)$$
We note that

\[ F_c(T) = -T \log Z_c(T), \quad S_c(T) = 1 + \log Z_c(T), \quad (4.16) \]

where \( Z_c(T) \) is defined by \( (4.4) \). In view of \( (4.14) \), we have the proposition below.

**Proposition 4.4** For harmonic oscillator, the expression \( S_r(T, \hbar) \) monotonically increases with respect to \( \tau \) and

\[ S_r(T, \hbar) > \lim_{\tau \to 0} S_r(T, \hbar) = S_c(T). \quad (4.17) \]

In view of Propositions 4.2–4.4, and relation \((4.13)\), the following corollary is valid.

**Corollary 4.5** Consider the harmonic oscillator and let the parameters \( T \) and \( \omega \) be fixed. By transition from deterministic strategy (classical mechanics) to probabilistic strategy (quantum mechanics), all members of the game (i.e., the regularized free energy, the regularized mean energy and the regularized entropy) increase when \( \tau \) increases.

We think that the comparison of the deterministic and probabilistic strategies has a practical and methodological interest. Formulas \((4.7)\), \((4.12)\), \((4.13)\) and \((4.17)\) imply the following semiclassical limits.

**Case 1.** Let the parameters \( T \) and \( \omega \) be fixed. If \( \hbar \to 0 \) then

\[
Z_r(T, \hbar) \to Z_c(T), \quad \mathcal{E}_r(T, \hbar) \to E_c(T), \\
F_r(T, \hbar) \to F_c(T), \quad S_r(T, \hbar) \to S_c(T).
\]

**Case 2.** Let the parameters \( \hbar \) and \( \omega \) be fixed. If \( T \to \infty \) then

\[
Z_r(T, \hbar) \sim Z_c(T), \quad \mathcal{E}_r(T, \hbar) \sim E_c(T), \quad S_r(T, \hbar) \sim S_c(T).
\]

**Case 3.** Let the parameters \( T \) and \( \hbar \) be fixed. If \( \omega \to 0 \) then

\[
Z_r(T, \hbar, \omega) \sim Z_c(T, \omega), \quad \mathcal{E}_r(T, \hbar, \omega) \sim E_c(T, \omega), \\
F_r(T, \hbar, \omega) \sim F_c(T, \omega), \quad S_r(T, \hbar, \omega) \sim S_c(T).
\]

For brevity, we omit \( \omega \) in some notations above (when \( \omega \) is fixed).
Remark 4.6  Recall that the semiclassical approach in quantum mechanics deals usually with the case ($\hbar \rightarrow 0$) (see [21]).

We need the following result for analytic functions. The functions $\frac{z}{\sinh(z)}$ and $\frac{z}{\tanh(z)}$ have Loran series expansions which converge for all values $0 < |z| < \pi$:

\[
\frac{z}{\sinh(z)} = 1 + \sum_{n=1}^{\infty} \frac{2(1 - 2^{2n-1})B_{2n}z^{2n}}{(2n)!},
\]

(4.18)

\[
\frac{z}{\tanh(z)} = 1 + \sum_{n=1}^{\infty} \frac{2^n B_{2n}z^{2n}}{(2n)!},
\]

(4.19)

where $B_{2n}$ are Bernoulli numbers.

Corollary 4.7  The functions

\[
f(\tau) = Z_r(T, \hbar)/Z_c(T, \hbar) = \frac{\tau}{\sinh(\tau)},
\]

(4.20)

and

\[
g(\tau) = E_r(T, \hbar)/E_c(T, \hbar) = \frac{\tau}{\tanh(\tau)},
\]

(4.21)

are analytic in the domain $|\tau| < \pi$, and the coefficients of the corresponding Loran series may be written down explicitly.

In particular, we have partial expansions:

\[
f(\tau) = 1 - B_2 \tau^2 + O(\tau^4), \quad B_2 = 1/6,
\]

(4.22)

\[
g(\tau) = 1 + B_2 \tau^2 + O(\tau^4), \quad B_2 = 1/6.
\]

(4.23)

Example 4.8 Potential well

In the classical case the Hamiltonian for the potential well has the form:

\[
H(p, q) = \begin{cases} 
\frac{p^2}{2m}, & q \in [0, a] ; \\
\infty, & \text{otherwise}.
\end{cases}
\]

(4.24)
In the quantum case the potential well is described \cite[Ch. 3]{22} by the equation

\[-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} y - Ey = 0, \quad y(0) = y(a) = 0.\] \hspace{1cm} (4.25)

The spectrum $E_n$ of the boundary problem (4.25) is given by the formula:

\[E_n = \frac{\hbar^2 \pi^2}{2ma^2} n^2, \quad n = 1, 2, \ldots \] \hspace{1cm} (4.26)

It follows from (2.9) and (4.24) that

\[Z_c(T) = a \int_{-\infty}^{+\infty} \exp\left(-\frac{p^2}{2mT}\right) dp = a\sqrt{2mT\pi}.\] \hspace{1cm} (4.27)

From (2.1) and (4.27) we have

\[E_c(T) = a \int_{-\infty}^{+\infty} \frac{p^2}{2m} \exp\left(-\frac{p^2}{2mT}\right) dp / Z_c(T) = T/2.\] \hspace{1cm} (4.28)

Next, let us consider $Z_r(T, \hbar)$. Using (1.2), (3.8), and (4.26), we derive

\[Z_r(T, \hbar) = 2\pi \hbar \sum_{n=1}^{\infty} e^{-\left(\frac{\pi}{4}\right)n^2 \mu^2},\] \hspace{1cm} (4.29)

where

\[\mu = \hbar \sqrt{\frac{2\pi}{ma^2 T}}.\] \hspace{1cm} (4.30)

It follows from (4.27), (4.29), and (4.30) that

\[Z_r(T, \hbar)/Z_c(T) = \mu \sum_{n=1}^{\infty} e^{-\left(\frac{\pi}{4}\right)n^2 \mu^2}.\] \hspace{1cm} (4.31)

Hence, we have

\[\frac{d}{d\mu}[Z_r(T, \hbar)/Z_c(T)] = \sum_{n=1}^{\infty} e^{-\left(\frac{\pi}{4}\right)n^2 \mu^2} (1 - (\pi/2)n^2 \mu).\] \hspace{1cm} (4.32)

Relation (4.32) implies the following assertion.
Lemma 4.9 If the inequality

\[ \mu \geq 2/\pi \]  

holds, then

\[ \frac{d}{d\mu} \left[ \frac{Z_r(T, \hbar)}{Z_c(T)} \right] < 0. \]  

(4.34)

Now, let us consider a more difficult case, where

\[ 0 < \mu \leq 2/\pi. \]  

(4.35)

Lemma 4.10 If the inequality (4.35) holds, then

\[ \frac{d}{d\mu} \left[ \frac{Z_r(T, \hbar)}{Z_c(T)} \right] < 0. \]  

(4.36)

Proof. Recall the Poisson formula (see, e.g., [11]):

\[ \sum_{n=0}^{\infty} F(n) = \frac{1}{2} F(0) + \int_{0}^{\infty} F(x) dx + 2 \sum_{n=1}^{\infty} \int_{0}^{\infty} F(x) \cos(2\pi nx) dx. \]  

(4.37)

Let us consider the case \( F(x) = e^{-x^2/(\pi/4)\mu^2} \). Since

\[ \int_{0}^{\infty} \exp(-x^2/\nu) \cos(2\pi nx) dx = \frac{\sqrt{\nu \pi}}{2} \exp(-n^2\nu \pi^2), \quad n = 0, 1, 2, \ldots \]  

(4.38)

we have

\[ Z_r(T, \hbar)/Z_c(T) = \mu \left\{ -\frac{1}{2} + \frac{\sqrt{\lambda \pi}}{2} + \sqrt{\lambda \pi} \sum_{n=1}^{\infty} \exp[-(n\pi)^2\lambda] \right\}, \]  

(4.39)

where

\[ \lambda = \frac{4}{\pi \mu^2}. \]  

(4.40)

Let us calculate the derivative:

\[ \frac{d}{d\mu} \left[ Z_r(T, \hbar)/Z_c(T) \right] = -1/2 + [16/(\mu^3 \pi)] \sum_{n=1}^{\infty} \exp[-(n\pi)^2\lambda](n\pi)^2. \]  

(4.41)
We need also the following derivative:
\[
\frac{d}{d\mu}\{\mu^{-3}\exp[-(n\pi)^2\lambda]\} = (8\pi n^2 \mu^{-6} - 3\mu^{-4}) \exp[-(n\pi)^2\lambda].
\]

(4.42)

Taking into account (4.35), we have
\[
8\pi n^2 - 3\mu^2 \geq 8\pi - 3\mu^2 > 0.
\]

(4.43)

It follows from (4.41)–(4.43) that the function \(\frac{d}{d\mu}[\mathcal{Z}_r(T, h)/\mathcal{Z}_c(T)]\) monotonically increases and that
\[
\frac{d}{d\mu}[\mathcal{Z}_r(T, h, \mu)/\mathcal{Z}_c(T)] \leq \frac{d}{d\mu}[\mathcal{Z}_r(T, h, 2/\pi)/\mathcal{Z}_c(T)] =: G.
\]

(4.44)

Earlier we omitted for brevity the dependence of the function \(\mathcal{Z}_r\) on the variable \(\mu\). Formulas (4.40) and (4.41) imply
\[
G = -1/2 + 2(\pi)^4 \sum_{n=1}^{\infty} n^2 e^{-n^2\pi^3}.
\]

(4.45)

In order to estimate \(G\), we study the integral
\[
\int_0^{\infty} x^2 e^{-x^2/\eta} dx = \frac{\eta \sqrt{\eta \pi}}{4}.
\]

(4.46)

We note that
\[
\frac{d}{dx}[x^2 e^{-x^2/\eta}] = 2x e^{-x^2/\eta}(1 - x^2/\eta).
\]

(4.47)

Hence, the function
\[
U(x, \eta) = x^2 e^{-x^2/\eta}
\]

is monotonically decreasing if \(x > \sqrt{\eta}\). In the case under consideration (see (4.45)), we have
\[
\eta = \pi^{-3} < 1.
\]

(4.49)

Thus, we proved that
\[
\int_1^{\infty} U(x, \eta) dx > \sum_{n=2}^{\infty} U(n, \eta), \quad \eta = \pi^{-3}.
\]

(4.50)
Using numerical calculation, we obtain
\[ \int_0^1 U(x, \eta)dx = 0, 0025665 > U(1, \eta) = 3, 420(10)^{-14}, \quad \eta = \pi^{-3}. \] (4.51)

Then, we have
\[ \int_0^\infty U(x, \eta)dx > \sum_1^\infty U(n, \eta), \quad \eta = \pi^{-3}. \] (4.52)

According to (4.46) the equality
\[ 2\pi^4 \int_0^\infty U(x, \eta)dx = 1/2, \quad \eta = \pi^{-3} \] (4.53)
holds. The assertion of the lemma follows from (4.45), (4.52) and (4.53).

Using Lemmas 4.8 and 4.9, we obtain the proposition below.

**Proposition 4.11** For the potential well case the expression \( Z_r(T, \hbar)/Z_c(T) \) monotonically decreases with respect to \( \mu \) and
\[ Z_r(T, \hbar)/Z_c(T) < \lim_{\mu \to 0}[Z_r(T, \hbar)/Z_c(T)] = 1. \] (4.54)

Let us consider the mean energy \( E_r(T, \hbar) \). Introduce
\[ V(T, \hbar) := T \sum_{n=1}^\infty e^{-(\pi/4)\mu^2n^2} (\pi/4)\mu^2n^2 = T \sum_{n=1}^\infty e^{-n^2/\lambda}(n^2/\lambda), \] (4.55)
where \( \mu \) and \( \lambda \) are defined by the relations (4.30) and (4.40), respectively. The mean energy \( E_r(T, \hbar) \) may be written in the form
\[ E_r(T, \hbar) = V(T, \hbar)/Z_q(T, \hbar), \] (4.56)
where \( Z_q(T, \hbar) \) is defined by the relation
\[ Z_q(T, \hbar) = \sum_{n=1}^\infty e^{-(\pi/4)\mu^2n^2} = \sum_{n=1}^\infty e^{-(n^2/\lambda)}. \] (4.57)

**Remark 4.12** The expression \( E_r(T, \hbar)/E_c(T) \) depends on only one variable, namely, on \( \mu \) (see (1.55) – (1.57)).
Using relations (4.55)-(4.57) we obtain the assertion.

**Proposition 4.13** If the inequality

\[ \mu \geq \frac{2}{\pi} \]  

holds, then (in the case of the potential well) we have

\[ \mathcal{E}_r(T, \hbar)/E_c(T) > 1. \]  

(4.59)

Let us proceed with a further study of the case

\[ \mu \leq \frac{2}{\pi}. \]  

(4.60)

Using formula (4.39) and equality

\[ Z_q(T, \hbar) = \left[Z_r(T, \hbar)/Z_c(T)\right]/\mu, \]  

(4.61)

we have

\[ Z_q(T, \hbar) = -\frac{1}{2} + \frac{\sqrt{\lambda \pi}}{2} + \sqrt{\lambda \pi} \sum_{n=1}^{\infty} \exp[-(n\pi)^2\lambda]. \]  

(4.62)

Differentiating (4.62) with respect to \( \lambda \), we derive

\[ \frac{d}{d\lambda} Z_q(T, \hbar) = \frac{1}{4} \sqrt{\frac{\pi}{\lambda}} + \frac{1}{2} \sqrt{\frac{\pi}{\lambda}} \sum_{n=1}^{\infty} e^{-(n\pi)^2\lambda} - \sqrt{\lambda \pi} \sum_{n=1}^{\infty} (n\pi)^2 e^{-(n\pi)^2\lambda} \]  

(4.63)

On the other hand, (4.57) yields

\[ \frac{d}{d\lambda} Z_q(T, \hbar) = \sum_{n=1}^{\infty} e^{-n^2/\lambda} (n^2/\lambda^2). \]  

(4.64)

It follows from (4.55) and (4.64) that

\[ V(T, \hbar) = T\lambda \frac{d}{d\lambda} Z_q(T, \hbar). \]  

(4.65)

Let us introduce the functions

\[ W_0(T, \hbar) = 1 - (\lambda \pi)^{-1/2} + 2 \sum_{n=1}^{\infty} e^{-\frac{(n\pi)^2}{\lambda}}, \]  

(4.66)

\[ W_1(T, \hbar) = 1 + 2 \sum_{n=1}^{\infty} e^{-\frac{(n\pi)^2}{\lambda}} - 4\lambda \sum_{n=1}^{\infty} (n\pi)^2 e^{-\frac{(n\pi)^2}{\lambda}}. \]  

(4.67)
Relations (4.62), (4.63), and (4.65)–(4.67) imply that
\[
\frac{d}{d\lambda} Z_q(T, h) = \frac{1}{4} \sqrt{\frac{\pi}{\lambda}} W_1(T, h), \quad Z_q(T, h) = \frac{\sqrt{\lambda\pi}}{2} W_0(T, h). \tag{4.68}
\]

It follows from, (4.56), (4.65) and (4.68) that
\[
\mathcal{E}_r(T, h) = (T/2)W_1(T, h)/W_0(T, h). \tag{4.69}
\]

**Lemma 4.14** If condition (4.60) is fulfilled, then
\[
W_1(T, h) > W_0(T, h). \tag{4.70}
\]

**Proof.** Inequality (4.70) may be rewritten in the equivalent form
\[
1 > 4\lambda^{3/2}\pi^{5/2}\sum_{n=1}^{\infty} n^2 e^{-(n\pi)^2\lambda}. \tag{4.71}
\]

It is easy to see that
\[
x^2 e^{-\lambda x^2\pi^2} \leq e^{-\lambda x\pi^2}, \quad x \geq 1, \quad \lambda \geq 1. \tag{4.72}
\]

It follows from (4.72) that
\[
\sum_{n=1}^{\infty} n^2 e^{-(n\pi)^2\lambda} \leq e^{-\lambda\pi^2}/(1 - e^{-\lambda\pi^2}). \tag{4.73}
\]

Taking into account relations (4.40) and (4.60), we have
\[
\lambda \geq \pi. \tag{4.74}
\]

The function \(\lambda^{3/2}e^{-\lambda\pi^2}\) is monotonically decreasing for \(\lambda \geq \pi\). Hence, the inequality
\[
\lambda^{3/2}e^{-\lambda\pi^2} \leq 2\pi^{3/2} e^{-\pi^3}, \quad \lambda \geq \pi \tag{4.75}
\]
holds. Since \(e^{-\pi^3} = 3, 420(10)^{-14}\) (see (4.51)) the following relation is valid:
\[
4\lambda^{3/2}\pi^{5/2} e^{-\lambda\pi^2}/(1 - e^{-\lambda\pi^2}) < 1 \tag{4.76}
\]

The inequality (4.70) follows from (4.73) and (4.76). The lemma is proved.
Proposition 4.15 The following inequality is valid for the potential well in the case $\mu \leq 2/\pi$:
\[ \frac{E_r(T, \hbar)}{E_c(T)} > 1. \] (4.77)

Formulas (4.65)–(4.67) immediately imply the asymptotic relation
\[ \frac{E_r(T, \hbar)}{E_c(T)} = \frac{1}{1 - \mu/2} + O(e^{-4\pi/\mu^2}), \quad \mu \to +0. \] (4.78)

From propositions 4.2–4.4 and relation (4.77) we obtain the following theorem.

Theorem 4.16 In the case of the potential well, we have
\[ \frac{E_r(T, \hbar)}{E_c(T)} > \lim_{\mu \to +0} [\frac{E_r(T, \hbar)}{E_c(T)}] = 1. \] (4.79)

Let us consider the regularized entropy $S_r(T, \hbar)$ in the case of the potential well. It follows from (1.7) that
\[ S_r(T, \hbar) = \frac{[E_r(T, \hbar) - F_r(T, \hbar)]}{T}. \] (4.80)

According to (4.61) and (4.62) the asymptotic equality
\[ \frac{Z_r(T, \hbar)}{Z_c(T, \hbar)} = (1 - \mu/2) + O(e^{-4\pi/\mu^2}), \quad \mu \to +0 \] (4.81)
holds. In view of (4.78), (4.80), and (4.81), we have
\[ S_r(T, \hbar) = S_c(T) - \mu/4 + O(\mu^2), \quad \mu \to +0, \] (4.82)
where
\[ S_c(T) = \frac{1}{2} + \log(a \sqrt{2mT\pi}). \] (4.83)

Remark 4.17 The following assertion is valid for the potential well. By transition from the deterministic strategy (classical mechanics) to the probabilistic strategy (quantum mechanics) two members of the game (i.e., the regularized free energy and the regularized mean energy) increase.

We can estimate the regularized entropy for potential well only for small $\mu$.

Remark 4.18 Formula (4.81) implies: if $\mu$ is small, then by transition from the deterministic strategy (classical mechanics) to the probabilistic strategy (quantum mechanics) the regularized entropy for the potential well decreases.
Relations (4.30), (4.54), (4.14), (4.79) and (4.82) yield the following semiclassical limits:

**Case 1.** Let the parameters $T$, $a$ and $m$ be fixed. If $\hbar \to 0$, then

\begin{align*}
Z_r(T, \hbar) &\to Z_c(T), \quad \mathcal{E}_r(T, \hbar) \to E_c(T), \\
F_r(T, \hbar) &\to F_c(T), \quad S_r(T, \hbar) \to S_c(T).
\end{align*}

**Case 2.** Let the parameters $m$, $a$ and $\hbar$ be fixed. If $T \to \infty$, then

\begin{align*}
Z_r(T, \hbar) &\sim Z_c(T), \quad \mathcal{E}_r(T, \hbar) \sim E_c(T), \\
F_r(T, \hbar) &\sim F_c(T), \quad S_r(T, \hbar) \sim S_c(T).
\end{align*}

**Case 3.** Let the parameters $\hbar$, $T$ and $m$ be fixed. If $a \to \infty$, then

\begin{align*}
Z_r(T, \hbar, a) &\sim Z_c(T, a), \quad \mathcal{E}_r(T, \hbar, a) \sim E_c(T, a), \quad S_r(T, \hbar) \sim S_c(T, a).
\end{align*}

**Case 4.** Let the parameters $\hbar$, $T$ and $a$ be fixed. If $m \to \infty$, then

\begin{align*}
Z_r(T, \hbar, m) &\sim Z_c(T, m), \quad \mathcal{E}_r(T, \hbar, m) \sim E_c(T, m), \quad S_r(T, \hbar, m) \sim S_c(T, m).
\end{align*}

When the parameters $a$ and $m$ are constant, we omit them for brevity.

## 5 $N$-Dimensional Potential Well

Let us consider the $N$-dimensional potential well $Q_N$:

\begin{equation}
0 \leq x_k \leq a_k, \quad 1 \leq k \leq N. \tag{5.1}
\end{equation}

We introduce the corresponding boundary problem

\begin{align*}
\frac{\hbar^2}{2m} \sum_{k=1}^{N} \frac{\partial^2}{\partial x_k^2} \psi(x_1, x_2, ..., x_N) + E \psi(x_1, x_2, ..., x_N) &= 0, \tag{5.2} \\
\psi|_\Gamma &= 0. \tag{5.3}
\end{align*}

Here, $\Gamma$ stands for the boundary of the domain $Q_N$. The spectrum of the boundary problem (5.1)-(5.3) is given by the formula:

\begin{equation}
E_{n_1, ..., n_N} = \frac{\hbar^2 \pi^2}{2m} \sum_{k=1}^{N} \frac{n_k^2}{a_k} \quad (n_k = 1, 2, ...). \tag{5.4}
\end{equation}
We need the relation (see (3.8)):

$$-\left[ \frac{\partial}{\partial \beta} Z_{q,k}(T, \hbar) \right] / Z_{q,k}(T, \hbar) = E_{q,k}(T, \hbar), \quad \beta = 1/T. \quad (5.5)$$

It follows from (5.4) and (5.5) that

$$Z_q(T, \hbar) = \prod_{k=1}^{N} Z_{q,k}(T, \hbar), \quad E_q(T, \hbar) = \sum_{k=1}^{N} E_{q,k}(T, \hbar), \quad (5.6)$$

where $Z_{q,k}(T, \hbar)$ and $E_{q,k}(T, \hbar)$ are defined by the relations

$$Z_{q,k}(T, \hbar) = \sum_{n=1}^{\infty} \exp\left(-\frac{\pi}{4} n^2 \mu_k^2\right), \quad (5.7)$$

$$E_{q,k}(T, \hbar) = T \sum_{n=1}^{\infty} \left(\frac{\pi}{4}\right) n^2 \mu_k^2 \exp\left(-\frac{\pi}{4} n^2 \mu_k^2\right) / Z_{q,k}(T, \hbar), \quad (5.8)$$

and

$$\mu = \hbar \sqrt{\frac{2\pi}{ma_k^2 T}}. \quad (5.9)$$

Let us introduce the regularized statistical sum $Z_r(T, \hbar)$ and the mean energy $E_r(T, \hbar)$ in the $N$-dimensional case:

$$Z_r(T, \hbar) = (2\pi \hbar)^N Z_q(T, \hbar), \quad E_r(T, \hbar) = E_q(T, \hbar). \quad (5.10)$$

In the $N$-dimensional case, according to (4.27) and (4.28) we have

$$Z_c(T) = (2mT\pi)^{N/2} \prod_{k=1}^{N} a_k, \quad E_c(T) = N(T/2). \quad (5.11)$$

In view of (4.13) and (5.6), the following asymptotic equality holds:

$$Z_r(T, \hbar) / Z_c(T) = \prod_{k=1}^{N} (1 - \mu_k/2) + O(e^{-1/\varepsilon^2}), \quad \varepsilon \to 0. \quad (5.12)$$

Here,

$$\varepsilon^2 = (4/\pi) \max[\mu_1^2, \mu_2^2, ..., \mu_N^2]. \quad (5.13)$$
Taking into account (4.78) and (5.6), we write:

$$E_r(T, \hbar) = \frac{T}{2} \left[ \sum_{n=1}^{N} (1 - \mu_k/2)^{-1} + O(e^{-1/\varepsilon^2}) \right], \quad \varepsilon \to +0. \quad (5.14)$$

It follows from (4.82) and (4.83) that in case of the $N$-dimensional potential well (5.1) we have

$$S_r(T, \hbar) = S_c(T) - \sum_{k} \mu_k/4 + O(\varepsilon^2), \quad \varepsilon \to +0, \quad (5.15)$$

where

$$S_c(T) = \frac{N}{2} + \sum_{k} \log(a_k \sqrt{2mT\pi}). \quad (5.16)$$

**Remark 5.1** By transition from the deterministic strategy (classical mechanics) to the probabilistic strategy (quantum mechanics), the regularized entropy decreases for the $N$-dimensional potential well in the case of small values of $\varepsilon$.

We note that $\varepsilon$ is defined by relation (5.13).

**Theorem 5.2** The following results are valid for the boundary problem (5.1) – (5.3).

1. The regularized statistical sum $Z_r(T, \hbar)$ of a quantum equilibrium system monotonically decreases with respect to $\mu_k$ and

$$Z_r(T, \hbar) < \lim_{\varepsilon \to 0} Z_r(T, \hbar) = Z_c(T) \quad (5.17)$$

2. We have

$$E_r(T, \hbar) > \lim_{\varepsilon \to +0} E_r(T, \hbar) = E_c(T) = NT/2, \quad (5.18)$$

3. The regularized free energy $F_r(T, \hbar) = -T \log Z_r(T, \hbar)$ of a quantum equilibrium system monotonically increases with respect to $\mu_k$ and

$$F_r(T, \hbar) > \lim_{\varepsilon \to 0} F_r(T, \hbar) = F_c(T) = -T \log[Z_c(T)]. \quad (5.19)$$
Remark 5.3 The following assertion is valid for the potential well \((N \geq 1)\). By transition from deterministic strategy (classical mechanics) to probabilistic strategy (quantum mechanics) two members of the game (the regularized free energy and the regularized mean energy) increase.

Remark 5.4 By transition from the deterministic strategy (classical mechanics) to the probabilistic strategy (quantum mechanics), the regularized entropy for the potential well \((N \geq 1)\) decreases with respect to \(\mu_k\), if \(\varepsilon\) is small.

Formulas (5.12)-(5.15) imply the following semiclassical limits.

Case 1. Let parameters \(T\), \(a_k\) and \(m\) be fixed. If \(\hbar \to 0\), then
\[
\mathcal{Z}_r(T, \hbar) \to \mathcal{Z}_c(T), \quad \mathcal{E}_r(T, \hbar) \to \mathcal{E}_c(T),
\]
\[
\mathcal{F}_r(T, \hbar) \to \mathcal{F}_c(T), \quad \mathcal{S}_r(T, \hbar) \to \mathcal{S}_c(T).
\]

Case 2. Let parameters \(m\), \(a_k\) and \(\hbar\) be fixed. If \(T \to \infty\), then
\[
\mathcal{Z}_r(T, \hbar) \sim \mathcal{Z}_c(T), \quad \mathcal{E}_r(T, \hbar) \sim \mathcal{E}_c(T),
\]
\[
\mathcal{F}_r(T, \hbar) \sim \mathcal{F}_c(T), \quad \mathcal{S}_r(T, \hbar) \sim \mathcal{S}_c(T).
\]

Case 3. Let parameters \(\hbar\), \(T\) and \(m\) be fixed. If \(a_k \to \infty\) \((1 \leq k \leq N)\), then
\[
\mathcal{Z}_r(T, \hbar, a) \sim \mathcal{Z}_c(T, a), \quad \mathcal{E}_r(T, \hbar, a) \sim \mathcal{E}_c(T, a), \quad \mathcal{S}_r(T, \hbar) \sim \mathcal{S}_c(T, a).
\]

Case 4. Let parameters \(\hbar\), \(T\) and \(a_k\) be fixed. If \(m \to \infty\), then
\[
\mathcal{Z}_r(T, \hbar, m) \sim \mathcal{Z}_c(T, m), \quad \mathcal{E}_r(T, \hbar, m) \sim \mathcal{E}_c(T, m), \quad \mathcal{S}_r(T, \hbar, m) \sim \mathcal{S}_c(T, m).
\]

When the parameters \(a_k\) and \(m\) are constant, we omit them for brevity.

6 \(N\)-dimensional oscillator

Schrödinger differential operator (quantum case) has the form
\[
L\psi = -\frac{\hbar^2}{2m} \sum_{k=1}^{N} \frac{\partial^2}{\partial x_k^2} \psi(x) + V(x)\psi(x), \quad x = [x_1, x_2, ..., x_N], \quad (6.1)
\]
and the corresponding Hamiltonian (classical case) is given by

$$H(p, x) = \frac{1}{2m} \sum_{j=1}^{N} p_j^2 + V(x). \quad (6.2)$$

The $N$-dimensional oscillator is determined by the operator $\mathcal{L} = L$ such that

$$V(x) = \sum_{k=1}^{N} \frac{m\omega_k^2 x_k^2}{2}, \quad \omega_k > 0. \quad (6.3)$$

The operator $\mathcal{L}$ has the following spectrum:

$$E_{n_1, n_2, \ldots, n_N}(\hbar) = \sum_{k=1}^{N} \hbar \omega_k (n_k - 1/2). \quad (6.4)$$

Using (4.6) we obtain:

$$Z_r(T, \hbar) = \prod_{k=1}^{N} \left[ 2T \pi \frac{\tau_k}{\omega_k \sinh(\tau_k)} \right], \quad (6.5)$$

where

$$\tau_k = \frac{\hbar \omega_k}{2T}. \quad (6.6)$$

Relation (4.11) implies that

$$E_r(T, \hbar) = T \sum_{k=1}^{N} \frac{\tau_k}{\tanh(\tau_k)}. \quad (6.7)$$

The following corollary is valid.

**Corollary 6.1** The functions

$$f(\tau_1, \ldots, \tau_N) = Z_r(T, \hbar)/Z_c(T, \hbar) = \prod_{k=1}^{N} \left[ \frac{\tau_k}{\sinh(\tau_k)} \right] \quad (6.8)$$

and

$$g(\tau_1, \ldots, \tau_N) = E_r(T, \hbar)/E_c(T, \hbar^*) = \sum_{k=1}^{N} \frac{\tau_k}{\tanh(\tau_k)} \quad (6.9)$$

are analytic in the domain $|\tau_k| < \pi$ $(1 \leq k \leq N)$, and the coefficients of the corresponding Loran series expansions may be written in explicit forms (see (4.18) and (4.19)).
Example 6.2 Partial expansions of \( f \) and \( g \) are given by the formulas

\[
 f(\tau_1, \ldots, \tau_N) = 1 - B_2 \sum_{k=1}^{N} \tau_k^2 + O(\delta^4), \quad B_2 = 1/6; \quad (6.10)
\]

\[
 g(\tau_1, \ldots, \tau_N) = 1 + B_2 \sum_{k=1}^{N} \tau_k^2 + O(\delta^4), \quad B_2 = 1/6, \quad (6.11)
\]

where

\[
 \delta = \max\{\tau_1, \tau_2, \ldots, \tau_N\}. \quad (6.12)
\]

A number of the results, which we have proved for the case \( N = 1 \) (see section 4, Example 4.1), are valid for the case \( N \geq 1 \) as well. Indeed, taking into account formulas \( (6.5) \), \( (6.7) \) and \( (6.12) \) we obtain the next theorem.

**Theorem 6.3** The following results are valid for the system \( (6.1) \)–\( (6.3) \).

1. The regularized statistical sum \( Z_r(T, \hbar) \) of the corresponding quantum equilibrium system monotonically decreases with respect to \( \tau_k \) and

\[
 Z_r(T, \hbar) \sim Z_c(T) = \prod_{k=1}^{N} \frac{2T\pi}{\omega_k} \quad \text{for} \quad \delta \to 0. \quad (6.13)
\]

2. The regularized mean energy \( E_r(T, \hbar) \) of the quantum equilibrium system monotonically increases with respect to \( \tau_k \) and

\[
 E_r(T, \hbar) \sim E_c(T) = TN/2 \quad \text{for} \quad \delta \to 0. \quad (6.14)
\]

3. The regularized free energy \( F_r(T, \hbar) \) of the quantum equilibrium system monotonically increases with respect to \( \tau_k \) and

\[
 F_r(T, \hbar) \sim F_c(T) = -T \log[\prod_{k=1}^{N} \frac{2T\pi}{\omega_k}] \quad \text{for} \quad \delta \to 0. \quad (6.15)
\]

4. The regularized entropy \( S_r(T, \hbar) \) of the quantum equilibrium system monotonically increases with respect to \( \tau_k \) and

\[
 S_r(T, \hbar) \sim S_c(T) \quad \text{for} \quad \delta \to 0. \quad (6.16)
\]
Remark 6.4 The following assertion is valid for the $N$-dimensional harmonic oscillator ($N \geq 1$). By transition from the deterministic strategy (classical mechanics) to the probabilistic strategy (quantum mechanics) all three members of the game (the regularized free energy, the regularized mean energy, and the regularized entropy) increase.

Formulas (6.10)–(6.12) imply the following semiclassical limits.

**Case 1.** Let parameters $T$ and $\omega_k$ be fixed. If $\hbar \to 0$, then

\[ Z_r(T, \hbar) \to Z_c(T), \quad \mathcal{E}_r(T, \hbar) \to \mathcal{E}_c(T), \]

\[ \mathcal{F}_r(T, \hbar) \to \mathcal{F}_c(T), \quad \mathcal{S}_r(T, \hbar) \to \mathcal{S}_c(T). \]

**Case 2.** Let parameters $\hbar$ and $T$ be fixed. If $\delta \to 0$, then

\[ Z_r(T, \hbar) \sim Z_c(T), \quad \mathcal{E}_r(T, \hbar) \sim \mathcal{E}_c(T), \]

\[ \mathcal{F}_r(T, \hbar) \sim \mathcal{F}_c(T) \quad \mathcal{S}_r(T, \hbar) \sim \mathcal{S}_c(T). \]

**Case 3.** Let parameters $\hbar$ and $\omega_k$ be fixed. If $T \to \infty$, then

\[ Z_r(T, \hbar, a) \sim Z_c(T, a), \quad \mathcal{E}_r(T, \hbar, a) \sim \mathcal{E}_c(T, a), \quad \mathcal{S}_r(T, \hbar) \sim \mathcal{S}_c(T, a). \]

When the parameters $\omega_k$ are constant, we omit them for brevity.

7 Regularization

Let us recall the notion of the regularization. The volume $V$ of the phase space is defined (see, e.g., [22]) by the relation

\[ dV = \frac{dpdq}{(2\hbar\pi)^N}. \]  

(7.1)

Hence, in view of (2.9) we have

\[ Z_r(T, \hbar) = (2\hbar\pi)^N Z_q(T, \hbar). \]  

(7.2)

Using (2.12) we write

\[ \mathcal{F}_r(T, \hbar) = -T \log[Z_r(T, \hbar)]. \]  

(7.3)
According to (2.1) and (2.3), the following equality is valid:

$$\mathcal{E}_c(T) = \int \int H(p, q)\tilde{P}(p, q)dpdq \bigg/ \int \int \tilde{P}(p, q)dpdq,$$

(7.4)

where $\tilde{P}(p, q) \geq 0$. It follows from (7.1) and (7.4) that

$$\mathcal{E}_r(T, \hbar) = \mathcal{E}_q(T, \hbar).$$

(7.5)

Relations (2.4) and (3.4) imply that

$$\mathcal{S}_r(T, \hbar) = [\mathcal{E}_r(T, \hbar) - \mathcal{F}_r(T, \hbar)]/T.$$

(7.6)

## 8 Geometrical interpretation

Formula (5.12) may be rewritten as

$$Z_r(T, \hbar)/Z_c(T) = U_N^{-1}[U_N - U_{N-1}\rho + \ldots + (-1)^N \rho^N U_0] + O(e^{-1/\varepsilon^2}), \quad (8.1)$$

where $\varepsilon \to 0$,

$$\rho = \hbar \sqrt{\frac{\pi}{2mT}}, \quad (8.2)$$

and

$$U_k = \sum a_{i_1} \ldots a_{i_k}, \quad 1 \leq i_1 < i_2 < \ldots < i_k = N, \quad U_0 = 1.$$  

(8.3)

In view of (8.3), the coefficients $U_k$ have clear geometrical interpretation, namely

$$U_k = V_k/2^{N-k}, \quad 1 \leq k \leq N.$$  

(8.4)

Here, $V_N$ is Lebesgue measure of the domain $Q_N$, $V_{N-1}$ is Lebesgue measure of its boundary $\Gamma$, $V_{N-2}$ is Lebesgue measure of the domain $\Gamma_1$ formed by the intersection of the faces of the domain $\Gamma$, \ldots, and, finally, $V_0$ is the number of the vertices of the polyhedron.

**Example 8.1** Let $N = 3$. Then, $V_3$ is the volume of the polyhedron (5.1), $V_2$ is the area of the boundary, $V_1$ is the sum of the lengths of the edges and $V_0$ is the number of the vertices of the polyhedron (5.1).
Relations (8.1) and (8.4) imply (see [36]) that

\[ Z_r(T, h)/Z_c(T) = V_N^{-1}[V_N - \rho \frac{V_{N-1}}{2} + ... + (-1)^N \rho^N \frac{V_0}{2^N}] + O(e^{-1/\varepsilon^2}), \]  

(8.5)

where \( \varepsilon \to 0 \). Formula (5.11) yields

\[ Z_c(T) = (2mT\pi)^{N/2} V_N. \]  

(8.6)

It follows from (5.14) and (5.18) that the mean energy \( E_r(T, \hbar) \) satisfies the relation

\[ E_r(T, \hbar)/E_c(T, \hbar) = 1 + \rho \frac{V_{N-1}}{2N V_N} + O(\rho^2). \]  

(8.7)

**Corollary 8.2** Let the potential well \( Q_N \) be defined by (5.1). According to (5.13) and (8.2), formulas (8.5) and (8.7) are valid in the following cases:

Case 1. Parameters \( T \) and \( m \) are fixed, \( \hbar \to 0 \).

Case 2. Parameters \( m \) and \( \hbar \) are fixed, \( T \to \infty \).

Case 3. Parameters \( T \) and \( \hbar \) are fixed, \( m \to \infty \).

**Hypothesis.** For a bounded convex non-degenerate \( N \)-dimensional polyhedron \( Q_N \), \( N \geq 2 \) we have

\[ Z_q(T, 1) = (4\pi t)^{-N/2}[V_N - \rho \frac{V_{N-1}}{2} + \sum_{k=2}^{N} (-1)^k (\rho/2)^k A_k + O(\rho^{N+1})], \]  

(8.8)

where \( \rho = \sqrt{\pi t} \to 0 \), \( \hbar = 1 \), \( m = 1/2 \), \( t = 1/T \) and

\[ A_k = \sum_{j=1}^{M_{N-k}} \frac{[\pi/\omega_{N-k}(j) - \omega_{N-k}(j)/\pi]}{V_{N-k}(j)}(3/2)V_{N-k}(j). \]  

(8.9)

Here, \( V_N \) is the volume of \( Q_N \) and \( V_{N-1} \) is the measure of its boundary (similar to the case (5.1)), \( M_{N-k} \) is the number of the \( (N-k) \)-dimensional faces \( F_{N-k}(j) \) of \( Q_N \), \( V_{N-k}(j) \) is the \( (N-k) \)-dimensional measure of the face \( F_{N-k}(j) \), and \( \omega_{N-k}(j) \) is the mean magnitude of the \( (N-k+1) \)-dimensional dihedral angles at the face \( F_{N-k}(j) \).

**Remark 8.3** The vertices of the polyhedron (in the hypothesis above) have the dimension 0 and the measure 1.
Support of the hypothesis.
1. If \( Q_N \) is given by (5.1), then \( \omega_{N-k}(j) = \pi/2 \). In this case, the formulas (8.8) and (8.9) are valid (compare with (8.5) and (8.6)).
2. If \( N = 2 \), then the formulas (8.8) and (8.9) are valid as well (see the result of M. Kac in [20] and the work [29]).
3. If \( N \geq 3 \), then the coefficient \( A_2 \) in (8.8) has the form (8.9) (see the papers [12, 15] by B.V. Fedosov and by A. Goldman and P. Calka).

\section{N-dimensional potential well, historical remarks}

Consider the Schrödinger differential operator

\[
L\psi = -\frac{\hbar^2}{2m} \sum_{k=1}^{N} \frac{\partial^2}{\partial x_k^2} \psi(x), \quad x \in Q_N,
\]

where \( Q_N \) is a bounded domain with a piecewise-smooth boundary \( \Gamma \). Introduce the following boundary condition:

\[
\psi|_{\Gamma} = 0.
\]

H. Weyl proved in 1911 [42] that

\[
Z_r(T, \hbar) \sim (2mT\pi)^{N/2} V_N, \quad \rho \to +0,
\]

where \( V_N \) is Lebesgue measure of the domain \( Q_N \). For the case \( N = 2 \), A. Pleijel proved [31] the relation:

\[
Z_r(T, \hbar) \sim (2mT\pi)^{1/2} (V_2 - \rho \frac{V_1}{2}), \quad \rho \to +0,
\]

where \( V_2 \) is the area of the region \( Q_2 \), \( V_1 \) is the length of the boundary \( \Gamma \), and \( \rho \) is defined by the relation (8.2). The case \( N \geq 2 \) was investigated in the papers [20, 29, 42]. For a smooth boundary \( \Gamma \), the following result was obtained:

\[
Z_r(T, \hbar) \sim (2mT\pi)^{N/2} (V_N - \rho \frac{V_{N-1}}{2}), \quad \rho \to +0.
\]
10 Semiclassical limit, Kirkwood-Wigner expansion

In the present section, we study the case when \( h \) is small (\( h \to 0 \)). Let us consider again the Schrödinger differential operator (quantum case)

\[
L\psi = -\frac{\hbar^2}{2m} \sum_{k=1}^{N} \frac{\partial^2}{\partial x_k^2} \psi(x) + V(x)\psi(x), \quad x \in \mathbb{R}^N,
\]

and the corresponding Hamiltonian (classical case)

\[
H(p, x) = \frac{1}{2m} \sum_{k=1}^{N} p_k^2 + V(x).
\]

J.G. Kirkwood and E. Wigner obtained the following result:

**Theorem 10.1** Let the inequalities

\[
Z_0(T) = \int e^{-V(x)/T} dx < \infty,
\]

\[
Z_2(T) = \frac{1}{24mT^3} \int e^{-V(x)/T} \|\nabla [V(x)]\|^2 dx < \infty
\]

be valid. Then, the relations

\[
Z_r(T, \hbar) = (2\pi)^N Z_q(T, \hbar) = (2\pi mT)^{N/2} [Z_0(T) - \hbar^2 Z_2(T) + O(\hbar^4)],
\]

\[
Z_c(T) = (2\pi mT)^{N/2} Z_0(T)
\]

hold.

From Theorem 10.1 and relation (7.3) we obtain:

**Corollary 10.2** Let the conditions (10.3) and (10.4) be fulfilled. Then,

\[
\mathcal{F}_r(T, \hbar) = F_c(T) + \hbar^2 T Z_2(T)/Z_0(T) + O(\hbar^4), \quad (10.5)
\]

where

\[
F_c(T) = -T \log Z_c(T).
\]

Formula (10.5) is derived in the book [22, Ch 3, section 33].
Corollary 10.3 Let the conditions of Theorem 10.1 be fulfilled. Then, the regularized free energy $F_r(T, \hbar)$ of the quantum equilibrium system satisfies the relation

$$F_r(T, \hbar) > \lim_{\hbar \to 0} F_r(T, \hbar) = F_c(T). \quad (10.7)$$

Let us compare Theorem 10.1 and Corollary 10.2 with the results of section 6 for the $N$-dimensional oscillator. It follows from (6.9)–(6.11) that in the case of the $N$-dimensional oscillator we have

$$Z_r(T, \hbar) = \prod_{k=1}^{N} [(2T\pi)/\omega_k][1 - \sum_{k=1}^{N} (\hbar \omega_k)^2/24T^2 + O(\hbar^4)], \quad (10.8)$$

$$\mathcal{E}_r(T, \hbar) = T \sum_{k=1}^{N} [1 + (\hbar \omega_k)^2/12T^2 + O(\hbar^4)]. \quad (10.9)$$

Using (7.3), (7.6) and (10.8), (10.9), we derive

$$F_r(T, \hbar) = F_c(T) + \hbar^2 T \sum_{k=1}^{N} (\hbar \omega_k)^2/24T^2 + O(\hbar^4)], \quad (10.10)$$

$$S_r(T, \hbar) = S_c + \sum_{k=1}^{N} (\hbar \omega_k)^2/24T^2 + O(\hbar^4)]. \quad (10.11)$$

By comparing relations (10.8) and (10.10) we obtain the following assertion.

**Corollary 10.4** In the case of the $N$-dimensional oscillator, we have:

$$Z_2(T)/Z_0(T) = \sum_{k=1}^{N} (\omega_k)^2/24T^2. \quad (10.12)$$

**Corollary 10.5** In the case of the $N$-dimensional oscillator, formulas (10.9) and (10.11) may be rewritten in the form:

$$\mathcal{E}_r(T, \hbar) = E_c(T) + 2\hbar^2 T Z_2(T)/Z_0(T) + O(\hbar^4), \quad (10.13)$$

$$S_r(T, \hbar) = S_c(T) + \hbar^2 Z_2(T)/Z_0(T) + O(\hbar^4). \quad (10.14)$$
11 Appendix. The limit $N \to \infty$

The general situation in the case $N \to \infty$ is discussed in the interesting work \cite{24} by N.P. Landsman. Numerous useful references on this topic are given in \cite{24} as well. In this section, we consider two simple examples: the $N$-dimensional potential well and the $N$-dimensional oscillator. For these examples we obtain concrete formulas, which show the interconnections between quantum and classical results.

We assume that $N \to \infty$ together with $\varepsilon_N \to 0$ in (11.3) and (11.4). Similarly, we assume that $N \to \infty$ together with $\delta_N \to 0$ in (11.8) and (11.9).

**Example 11.1** The $N$-dimensional potential well.

Let the relations (5.1)–(5.3) be fulfilled. Introduce $\varepsilon_N > 0$ and $\nu_N > 0$ by the equalities

$$\varepsilon_N^2 = \max\{\mu_1^2, \mu_2^2, \ldots, \mu_N^2\}$$  \hspace{1cm} (11.1)

and

$$\nu_N^2 = \min\{\mu_1^2, \mu_2^2, \ldots, \mu_N^2\}.$$  \hspace{1cm} (11.2)

Using (5.12), we derive:

$$\mathcal{E}_r(T, h, N)/\mathcal{E}_c(T, N) = 1 + \frac{1}{N} \sum_{k=1}^{N} \mu_k + O(\varepsilon_N^2), \quad \varepsilon_N \to 0,$$  \hspace{1cm} (11.3)

$$\mathcal{Z}_r(T, h, N)/\mathcal{Z}_c(T, N) = 1 - \frac{1}{N} \sum_{k=1}^{N} \mu_k + O(\varepsilon_N^2), \quad \varepsilon_N \to 0.$$  \hspace{1cm} (11.4)

The parameters $\mu_k$ are defined by (5.9) and the following inequalities hold:

$$\nu_N \leq \frac{1}{N} \sum_{k=1}^{N} \mu_k \leq \varepsilon_N.$$  \hspace{1cm} (11.5)

**Example 11.2** The $N$-dimensional oscillator.

We assume that the relations (6.1) and (6.3) are valid. We introduce $\delta_N$ and $\kappa_N$ by the equalities

$$\delta_N = \max\{\tau_1, \tau_2, \ldots, \tau_N\}$$  \hspace{1cm} (11.6)
\[ \kappa_N = \min\{\tau_1, \tau_2, \ldots, \tau_N\}. \] 

Using (6.8) and (6.9), we obtain:

\[ \mathcal{E}_r(T, \hbar, N)/E_c(T, N) = 1 + \frac{1}{6N} \sum_{k=1}^{N} \tau_k^2 + O(\delta_N^4), \quad \delta_N \to 0, \] 

(11.8)

\[ \mathcal{Z}_r(T, h, N)/Z_c(T, N) = 1 - \frac{1}{6N} \sum_{k=1}^{N} \tau_k^2 + O(\delta_N^4), \quad \delta_N \to 0. \] 

(11.9)

Here, the parameters \( \tau_k \) are defined in (6.6). We note that

\[ \kappa_N^2 \leq \frac{1}{N} \sum_{k=1}^{N} \tau_k^2 \leq \delta_N^2. \] 

(11.10)

**Remark 11.3** Formulas (11.3), (11.4), (11.8), and (11.9) are also valid for the case of the fixed \( N \).

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