Partial thermalization in the quantum chain of harmonic oscillators

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Abstract

This preprint contains the English translation of the paper "Relaxation dynamics of a quantum chain of harmonic oscillators", which was published by the author in 1980 in the Ukrainian Physical Journal. Comments describing its motivations, background ideas and results are presented as well. This paper addressed to the problem of approach to the thermal equilibrium in an isolated macroscopic quantum system, which was studied on the example of the quantum chain of weakly interacting harmonic oscillators. In the initial state, macroscopic energy was supplied to one oscillator (atom) in the chain. Subsequent evolution of the quantum state of the whole chain was determined due to the model integrability. The main subject of interest was the time evolution of the reduced density operators characterizing the quantum state of a particular atom. On the short time-scale, the energy perturbation expands along the chain with the velocity of the fastest phonon mode. On the long-time scale, the single-atom density operators display strong fluctuations around the canonical Gibbs distribution. These fluctuations are caused by the degeneracy of the energy level differences (presence of resonances) in the model of coupled harmonic oscillators. After lifting this degeneracy, fluctuations are suppressed providing, that the reduced density operator of each atom in the chain becomes very close to the Gibbs distribution at almost any time moment.

Introduction

The claim that an isolated (closed) macroscopic system evolves to the thermal equilibrium state lies in the very basis of the statistical mechanics. The question about the precise meaning of this statement for classical and quantum systems arises for every student studying the university course of statistical mechanics. With me this happens in Kharkov University in 1978. Two years later, I published two papers [1, 2] in Russian-language journals, in which relaxation of the isolated macroscopic quantum system to the thermal equilibrium was studied on the example of the chain of harmonic oscillators. It turns out, that the set of problems considered in these papers and underlying ideas became the subject of considerable theoretical interest in subsequent years, to much extent, due to experiments on quantum dynamics in the ultracold atomic gases [3, 4, 5]. This relates, in particular, to the quantum quench problem [6, 7, 8, 9, 10, 11, 12], and to the

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equilibration scenario in quantum systems based on the *Eigenstate Thermalization Hypothesis* (ETH) \cite{13, 14} and on the idea of canonical typicality \cite{15, 16, 17, 18, 19, 20}.

While the second paper \cite{2} was later translated into English, the first one \cite{1} remained without translation. The aim of the present retrospective publication is to present the English translation of paper \cite{1}, complemented with comments relating to its motivations and results.

In the both papers \cite{1, 2}, the isolated linear chain of $N \gg 1$ weakly coupled quantum harmonic oscillators (‘the atoms’) was considered. The model Hamiltonian reads as

$$ H = \sum_{k=0}^{N-1} \frac{1}{2} \left[ p_k^2 + \Omega_k^2 (q_k - q_{k+1})^2 + \Omega_0^2 q_k^2 \right], \quad \Omega \ll \Omega_0. $$

(1)

Here index $k = 0, \ldots, N - 1$, $N$ enumerates the atoms in the chain, $q_k$ and $p_k$ denote the special coordinate and momentum of the $k$-th atom, periodical boundary conditions are implied. At $t = 0$, the chain was taken in the inhomogeneous pure state $|\psi(0)\rangle$, in which the macroscopic energy $E = \mathfrak{H} \Omega_0$, with $\bar{n} = \mathfrak{H} / N \sim 1$ was supplied to one atom with $k = 0$. At $t > 0$, the chain evolved into the state $|\psi(t)\rangle$, which was determined due to exact integrability of the model \cite{1}.

In the first paper \cite{1}, the time evolution of the reduced density operator $\rho(k, t)$ of the atom located at the $k$-th site of the chain was calculated and studied,

$$ \rho(k, t) = \text{Tr}(r) \rho(t), $$

(2)

where $k = 0, \ldots, N - 1$, $\rho(t) = |\psi(t)\rangle\langle\psi(t)|$ is the projector-type density operator of the whole chain, and $\text{Tr}(r)$ denotes the trace over the space corresponding to the rest $N - 1$ atoms.

On the short-time scale, the slow spreading of the energy from the initially excited atom along the chain with the velocity $\Omega^2 / \Omega_0$ was found. On the other hand, the time average of the reduced density operators $\rho(k, t)$ of each atom in the chain over the infinite time interval was found to approach to the Gibbs distribution in the thermodynamic limit $N \to \infty$. It turns out, however, that the time-fluctuations of the single-atom reduced density operators $\rho(k, t)$ remain considerable on the long-time scale. Such atypical behavior was associated with the strong degeneracy of the energy level differences $(E_n - E_{n'})$ in model \cite{1}. It was shown in \cite{1}, that lifting this degeneracy by arbitrary weak nonlinear interaction provides suppression of these fluctuations and guaranties approach of the single-atom density operators $\rho(k, t)$ to the Gibbs distribution at large $t$. Though this result was proved only for the case $\bar{n} < 1$, it is very likely, that it holds also for $\bar{n} \geq 1$.

It was shown in \cite{1} as well, that for a huge majority of eigenstates $|n\rangle$ of the total Hamiltonian \cite{1}, the reduced density operators $\rho(k, n) = \text{Tr}(r) |n\rangle\langle n|$ corresponding to each individual $k$-th atom in the chain are equal to the Gibbs distribution in the thermodynamic limit. In other words, a typical exact pure stationary state $|n\rangle$ of the chain Hamiltonian would be perceived as the thermal equilibrium state by the observer, which can see just one atom in the chain. This result agrees with the ETH, which was put forward later by Deutsch \cite{13} and Srednicki \cite{14}.

In paper \cite{2} the results of \cite{1} were partly extended to the subsystems consisting of $N'$ neighbouring atoms in the chain, $1 \ll N' \ll N$. Starting from the same initial pure state $|\psi(0)\rangle$, the time evolution of the reduced density operator $\rho^{(s)}(t)$ of the subsystem containing $N'$ atoms was calculated. Qualitative behavior of $\rho^{(s)}(t)$ at large $t$ was shown to be similar to that of the single-atom reduced density operator $\rho(k, t)$ described in \cite{1}. It should be noted, however, that calculation of the time-average in \cite{2} was not completely rigorous, but applied a certain reasonable conjecture, see equation (10) in \cite{2}.
The following note is in order here. The quantum chain of harmonic oscillators determined by Hamiltonian \( H \) has the complete set of \( N \) commuting integrals of motion \( \{n_l\}_{l=1}^N \) which characterize the number of phonons with given quasimomenta \( \tau_l = 2\pi l/N, \ l = 1, \ldots, N \). Integrability of model \( H \) is the direct consequence of existence of these integrals of motion. The other side of the coin is that conservation of \( N \) integrals of motion makes impossible the complete thermalization of a typical initial state in this model. However:

(a) An observer, which can see just one atom in the chain, can not distinguish phonon modes with different quasimomenta \( \tau_l \). By this reason, conservation of the phonon numbers \( \{n_l\}_{l=1}^N \) in the whole quantum chain does not conflict with the chain partial thermalization, which is registered by the observer watching at a single atom.

(b) Anyway, complete thermalization in model \( H \) could be still possible for some particular initial states of the chain.

The rest of this preprint is organized as follows. Section 1 describes in detail the background ideas on thermalization in quantum systems, which stimulated me to do the model calculations described in [1, 2]. In a very brief form, these ideas were present already in the introductory parts of these two papers. Section 2 contains comments on the results and some calculation details of paper [1], which English translation is given in the Appendix. Section 3 contains new results illustrating the effect of the nonlinear interaction on the thermalization of the atom energies in the chain.

1 Thermalization in isolated macroscopic quantum system

The fundamental question about the meaning and the mechanism of thermalization in a macroscopic isolated dynamical system can be divided into two parts:

(i) What is the precise meaning (microscopic definition) of the term 'the thermal equilibrium state' for the isolated macroscopic system?

(ii) In what sense the isolated macroscopic system approaches to the equilibrium state due to its dynamical evolution?

Though for classical systems, at least, partial answers to these questions could be found in the ergodic theory, the situation with the quantum systems was much less certain. In the statistical mechanics textbooks (for example, see [21]), the equilibrium state of an isolated quantum system with the Hamiltonian \( H \) and the energy lying in the interval between \( E \) and \( E + \Delta, (\Delta \ll E) \) is usually defined through the equal a priori probability postulate, leading to the microcanonical density operator \( \rho_\Delta(E, H) \),

\[
\rho_\Delta(E, H) = \frac{g_\Delta(E, H)}{\text{Tr} g_\Delta(E, H)},
\]

\[
g_\Delta(E, H) = \theta(H - E - \Delta) - \theta(H - E),
\]

where \( \text{Tr} A \) denotes the trace of the operator \( A \), and \( \theta(x) \) is the Heaviside step function.

However, it is not easy to answer to the question (ii) with this conventional definition of the thermal equilibrium state. Really, the matrix elements of the density operator \( \rho(t) \) of the isolated
system calculated in the basis of its stationary states only change their phases with time and do not approach to the matrix elements of the microcanonical distribution \( \rho(0) \). Furthermore, evolution of the isolated system from some non-equilibrium pure state \( |\psi(0)\rangle \) is described by the unitary operator \( U(t) = \exp(-iHt) \), \( |\psi(t)\rangle = U(t)|\psi(0)\rangle \). Corresponding density operator \( \rho(t) = U(t) \rho(0) U^{-1}(t) \) being the orthogonal projector operator at \( t = 0 \),

\[
\rho(0) = |\psi(0)\rangle \langle \psi(0)|,
\]

remains, of course, to be the orthogonal projector operator at all \( t \neq 0 \),

\[
\rho(t) = |\psi(t)\rangle \langle \psi(t)|.
\]

Since the microcanonical density operator \( \rho(0) \) is not a projector operator, the projector-type density operator \( \rho(t) \) can not approach to it in some simple sense, say, in the strong or weak operator topology.

The common way used in the textbooks to avoid this problem, is to remind that the notion of the isolated system is a physical idealization, and in reality, all systems interact with their surrounding. However, though this statement is undoubtedly correct, one could hardly believe, that it is the true origin of thermalization, and that the latter can not be understood within the concept of the isolated quantum system.

If only isolated systems are concerned, the possible way to answer question (ii) is to restrict the set 'physically observable' operators \( A_i \), to some family \( \mathcal{A} \) and to claim, that only for these operators \( A_i \in \mathcal{A} \) one should expect approaching of the quantum expectation values \( \langle A(t) \rangle \) to the their (microcanonical) equilibrium values:

\[
\langle A(t) \rangle = \text{Tr} \left[ A_i \cdot \rho(t) \right] \rightarrow \text{Tr} \left[ A_i \cdot \rho_\Delta(E, H) \right],
\]

with subsequent fluctuations. This idea was realized by von Neumann in his Quantum Ergodic Theorem \([22, 23]\). In this theorem, operators \( A_i \) were treated by von Neumann as operators of 'the macroscopic observables', and were assumed to commute with each other,

\[
[A_i, A_j] = 0, \text{ for } A_i, A_j \in \mathcal{A}.
\]

A deep analysis of foundations of the statistical mechanics was given by Landau and Lifshitz in their Course of Theoretical Physics. They define the thermal equilibrium in the following way (see Pages 6 and 2 in \([24]\)):

**Definition 1.1.** If a closed macroscopic system is in a state such that in any macroscopic subsystem the macroscopic physical quantities are to a high degree of accuracy equal to their mean values, the system is said to be in a state of statistical equilibrium (or thermodynamic or thermal equilibrium).

The subsystems here are implied to be small compared with the whole system and weakly interacting with surrounding. Such subsystems will be called as 'allowed subsystems' in the sequel.

In the above definition, thermalization behavior is required for the reduced family of 'the macroscopic observables', which relate to the macroscopic subsystems of the isolated system.

Taking definition [11] as a starting point, one could arrive to a nice physical scenario, in which thermalization in the isolated macroscopic quantum system could result solely from its quantum

\footnote{Notation \( f(t) \sim C \) will be used to indicate that the value of the time-dependent quantity \( f(t) \) is close (equals in the thermodynamic limit) to \( C \) at almost any moment \( t \).}
mechanical evolution. The first step was to drop two underlined words ‘macroscopic’ in the above definition. This extended the family $\mathcal{A}$ of ‘thermalizable’ physical observable to all physical observables, which characterize the state of allowed subsystems, either macroscopic or not. Then, definition 1.1 becomes equivalent to the following one:

**Definition 1.2** $[$2$]$. A closed macroscopic system with Hamiltonian $H$ at the time moment $t$ is in the state of equilibrium if any sufficiently small, possibly macroscopic subsystem of it that is weakly coupled to the surroundings has the Gibbs distribution. Let us denote by $\alpha$ some subdivision of our isolated macroscopic quantum system into the allowed subsystem $\{s, \alpha\}$ with the Hamiltonian $H_{s, \alpha}$, and the rest of the system $\{r, \alpha\}$, which plays the role of the thermal bath. The Hilbert space $\mathcal{L}$ of the whole system can be decomposed into the tensor product $\mathcal{L} = \mathcal{L}_{s, \alpha} \otimes \mathcal{L}_{r, \alpha}$ of the Hilbert spaces $\mathcal{L}_{s, \alpha}$ and $\mathcal{L}_{r, \alpha}$ corresponding to the subsystem, and its surrounding, respectively.

**Definition 1.3** An isolated macroscopic quantum system will be called to be in the (partial) thermal equilibrium with respect to the allowed subsystem $\{s, \alpha\}$, if the reduced density operators $\rho_{s, \alpha}(t)$ of this subsystem is to a high accuracy equal to the canonical density operators $\rho_{G}^{(s, \alpha)}$ given by the Gibbs formula

$$\rho_{G}^{(s, \alpha)} = Z_{s, \alpha}^{-1} \exp[-\beta(\alpha)H_{s, \alpha}],$$

$$Z_{s, \alpha} = \text{Tr}^{(s, \alpha)} \exp[-\beta(\alpha)H_{s, \alpha}],$$

where $\text{Tr}^{(s, \alpha)}$ denotes the trace over the Hilbert space corresponding to the quantum states of the subsystem $\{s, \alpha\}$, and $\beta(\alpha)$ is the inverse temperature which could depend on the subsystem $\{s, \alpha\}$. Note, that the reduced density operator of the subsystem $\rho^{(s, \alpha)}(t)$ is related with the density operator $\rho(t)$ of the whole system as

$$\rho^{(s, \alpha)}(t) = \text{Tr}^{(r, \alpha)} \rho(t),$$

where $\text{Tr}^{(r, \alpha)}$ denotes the trace over the thermal bath space $\mathcal{L}_{r, \alpha}$.

It is clear, that the macroscopic quantum system stays in the global thermal equilibrium in the sense of definition 1.2 if and only if it is in the partial thermal equilibrium with respect to all its allowed subsystems $\{s, \alpha\}$ with the same inverse temperature $\beta$.

Definition 1.2 has several important advantages. First, it does not refer to the notion of the microcanonical ensemble and to the equal a priori probability postulate. Second, with definition 1.2, the answer to the question (ii) becomes straightforward and leads to the natural treatment of the thermalization phenomenon in quantum systems.

**Proposition 1.4** Thermalization in the macroscopic isolated quantum system means, that after the relaxation time, the matrix elements of the reduced density operators $\rho^{(s, \alpha)}(t)$ of all its allowed subsystems $\{s, \alpha\}$ in the basis of their stationary states $|\Phi_{n}^{(s, \alpha)}\rangle$ should approach (up to further fluctuations) to those of the canonical density operators (7).

$$\langle \Phi_{n}^{(s, \alpha)} | \rho^{(s, \alpha)}(t) | \Phi_{n'}^{(s, \alpha)} \rangle \sim Z_{s, \alpha}^{-1} \exp(-\beta \mathcal{E}_{n}^{(s, \alpha)}) \delta_{n,n'},$$

where $Z_{s, \alpha} = \sum_{n} \exp(-\beta \mathcal{E}_{n}^{(s, \alpha)})$, $\mathcal{E}_{n}^{(s, \alpha)} = \langle \Phi_{n}^{(s, \alpha)} | H^{(s, \alpha)} | \Phi_{n}^{(s, \alpha)} \rangle$. 

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and $\mathcal{E}_n^{(s,\alpha)}$, $n = 1, 2, \ldots$ is the energy spectrum of the subsystem \{s, \alpha\}.

Third, one can easily see, that the problem mentioned in the beginning of this Section does not arise with definition 1.4. Really, if the whole system is in a pure state described by some projector density operator (6), the subsystem reduced density operator (8) can correspond to a mixed state due to the quantum entanglement, and this mixed state can approach to the equilibrium Gibbs state (7).

If a macroscopic isolated quantum system possesses the property of thermalization, one should expect, that a typical initial state $|\psi(0)\rangle$ having macroscopically well determined total energy would approach in its unitary evolution to the equilibrium state, understood according to definition 1.2 and then remain in this state almost at any time.

It is tempting to take the initial state $|\psi(0)\rangle$ of the whole system as a single stationary state $|n\rangle$ of its Hamiltonian, $H|n\rangle = E_n|n\rangle$. Then, the previous statement naturally leads to the ETH [13, 14], which can be formulated as follows:

**Proposition 1.5** In a thermalizable isolated quantum system, the huge majority of individual stationary states $|n\rangle$ of the whole system represent the thermal equilibrium state. This means, that

$$\text{Tr}_{r,\alpha}|n\rangle\langle n| = Z_{r,\alpha}^{-1} \exp(-\beta H_{r,\alpha}),$$

(10)

for all allowed subsystems \{s, \alpha\}, and almost all stationary states $|n\rangle$.

Though the described above heuristic scenario of thermalization looked rather reasonable and attractive for me in 1979, I had no idea how to put it on a more firm basis for a generic isolated quantum system. So, it was natural to try to test this scenario on some simple model of interacting particles. Such a test was partly realized in [1, 2] for the model of the quantum chain of harmonic oscillators.

It should be noted, that definition 1.2 provided the basis of the described above treatment of thermalization. It implies that the family $\mathcal{A}$ of thermalizable observables can be associated with all observables which characterize the states of allowed subsystems. Approach to the thermalization problem emphasizing the role of the canonical ensemble for the subsystem state as the main indication of thermal equilibrium in quantum systems was developed later by several groups. Important results along this direction were obtained by Tasaki [20], Popescu, Short, and Winter [15], Linden et al. [16], and by Goldstein et al. [17, 18].

## 2 Comments on the results of paper [1]

In the normal mode representation, the quantum chain of harmonic oscillators reduces to the free phonon gas. As it was mentioned in the Introduction, conservation of phonon numbers $\{n_r\}_{r=1}^{2\pi/N}$ makes impossible complete thermalization of a typical initial state $|\psi(0)\rangle$ in this model. However, the quantum measurements performed on one atom in the chain does not allow one to distinguish different phonon modes. So, it is natural to expect, that for model [1], the weak versions of the thermalization property (proposition 1.4) and of the ETH (proposition 1.5) are still valid, in which Equations (7) and (9) are required only for the subsystems \{s, k\} consisting of one $k$-th atom in the chain. Paper [1], which English translation is given in Appendix, was dedicated to verification of this statement.

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2 The origin of this approach comes back to Erwin Schrödinger [25], see discussion in [17].

3 Note, that due to the requirement $\Omega \ll \Omega_0$, each atom in the chain weakly interacts with its surrounding and, therefore, represents an allowed subsystem by itself.
2.1 Eigenstate thermalization for free bosons

The Eigenstate Thermalization Hypothesis (see proposition [1.5]) was the important part of the described above heuristic scenario of thermalization, which provided motivation for [1] [2]. Note, that the ETH was not formulated explicitly in [1] [2], this has been done later by Deutsch [13] and Srednicki [14]. However, a weak form of the ETH for model [1] was proved in [1]. Namely, equation (A.8) validates the ETH (proposition 1.5) in model (1) for the single-atom subsystems. It was conjectured also in [1], that, "perhaps, this result holds to some extent in other dynamical systems".

Parameter $\bar{n} = \mathfrak{R}/N$ in (A.8) is related with the inverse temperature $\beta$ by the Plank's formula

$$\bar{n} = \frac{1}{\exp(\beta \Omega_0) - 1}$$

and $\mathfrak{R} = \sum_{l=1}^{N} n_l$. In the case $\bar{n} < 1$, equation (A.8) can be easily obtained from (A.7) which, in turn, follows from the results of Appendix 1 of paper [2].

To prove (A.8), let us rewrite (A.7) for $n = n'$ in the explicit form

$$\text{Tr}(r) |n\rangle \langle n| = \sum_{J=0}^{\mathfrak{R}} |J\rangle \langle J| \sum_{P=J}^{\mathfrak{R}} \sum_{l=0}^{P} \frac{P!(\bar{n})_{P-l}}{(P-l)!} \sum_{m_l=P}^{N} \frac{n_l!}{\prod_{l=1}^{m_l} (n_l - m_l)! m_l!^2},$$

where $m$ denotes the set of integer numbers $\{m_l\}_{l=1}^{N}$, which lie in the interval $0 \leq m_l \leq n_l$. Denote by $N_1$ the number of nonzero integers in the set $\{n_l\}_{l=1}^{N}$. For fixed $P > 0$ and macroscopic $N_1$, the leading contribution to the sum

$$S_2(n_1, \ldots, n_N; P) = \sum_{\sum_{l=1}^{m_l=P}} \frac{n_l!}{\prod_{l=1}^{m_l} (n_l - m_l)! m_l!^2}$$

comes from configurations $\{m_l\}_{l=1}^{N}$, in which $m_l$ takes values either 0, or 1. Contribution of all the rest terms is smaller by the factor $N_1^{-1}$. The same is valid also for the sum

$$S_1(n_1, \ldots, n_N; P) = \sum_{\sum_{l=1}^{m_l=P}} \frac{n_l!}{\prod_{l=1}^{m_l} (n_l - m_l)! m_l!} = \frac{1}{P!} (\partial_z)^P I_{z=0} \prod_{l=1}^{N_1} (1 + z)^{n_l} = \frac{\mathfrak{R}!}{P!(\mathfrak{R} - P)!}$$

Therefore,

$$S_2(n_1, \ldots, n_N; P) = S_1(n_1, \ldots, n_N; P)[1 + O(N_1^{-1})] = \frac{\mathfrak{R}!}{P!(\mathfrak{R} - P)!}[1 + O(N_1^{-1})] = \frac{\mathfrak{R}!}{P!} [1 + O(N_1^{-1})],$$

at fixed $P$ and $\mathfrak{R} \sim N_1 \sim N \rightarrow \infty$. Formal substitution of (15) into (12) yields

$$\text{Tr}(r) |n\rangle \langle n| = \sum_{J=0}^{\infty} |J\rangle \langle J| \sum_{P=J}^{\infty} \frac{P!(\bar{n})_{P-J}}{J!(P-J)!} [1 + O(N_1^{-1})] = \sum_{J=0}^{\infty} \frac{\bar{n}^J}{(1 + \bar{n})^{J+1}} |J\rangle \langle J|.$$
in agreement with (A.8). If $\bar{n} < 1$, the above formal manipulations can be justified, since the infinite series in $P$ in (10) converges uniformly in $N \to \infty$.

At $\bar{n} \geq 1$, the series in $P$ in (16) diverges. Nevertheless, it is also possible to prove (A.8) at $\bar{n} \geq 1$ directly from (A.7), though the proof is more complicated, than at $\bar{n} < 1$. On the other hand, a much easier indirect way to confirm (A.8) exists, which is suitable for all positive $\bar{n}$. Namely, one can check that the quantum expectation values of the operator $b_0^{I_1} b_0^{I_2}$ calculated with the both sides of this equation lead to the same results for any integer $J_1, J_2 \geq 0$.

**Proposition 2.1** Let $\{a_1\}^N_{i=1}$ and $\{b_1\}^N_{k=1}$ are the two sets of $N$ bosonic annihilation operators, which are related by the linear transformation

$$b_k = \sum_{l=1}^{N} A_{kl}(N) a_l,$$  \hspace{1cm} (17)

with the unitary $N$-dependent matrix $A_{kl}(N)$, and

$$|n_1, \ldots, n_N\rangle = (n_1! \ldots n_N!)^{-1/2} (a_1^{\dagger})^{n_1} \ldots (a_N^{\dagger})^{n_N} |0\rangle,$$  \hspace{1cm} (18)

denotes the basis associated with the first set of the bosonic operators. For each $N$, let us choose a basis vector $|n_1(N), \ldots, n_N(N)\rangle$ in such a way, that

$$|A_{kl}(N)|^2 n_l(N) < C/N \text{ for all } k, l \in \{1, N\}, \text{ with some fixed } C > 0,$$  \hspace{1cm} (19)

and the limits

$$\bar{n}(k) = \lim_{N \to \infty} \sum_{l=1}^{N} |A_{kl}(N)|^2 n_l(N),$$  \hspace{1cm} (20)

exist for given $k$. Then

$$\lim_{N \to \infty} \langle n_1(N), \ldots, n_N(N) | b_k^{M_1} b_k^{M_2} | n_1(N), \ldots, n_N(N) \rangle = M_1! [\bar{n}(k)]^{M_1} \delta_{M_1, M_2}.$$  \hspace{1cm} (21)

**Proof** First, it is clear, that operator $b_k^{M_1} b_k^{M_2}$ with $M_1 \neq M_2$ has zero diagonal matrix elements in the basis (15), since this operator changes the number of bosons. So, it is sufficient to put $M_1 = M_2 = M$ in (21). Then, substitution of (17) into the matrix element in the left-hand side of this equation followed by straightforward calculations yields

$$\langle n_1, \ldots, n_N | b_k^{M_1} b_k^{M_2} | n_1, \ldots, n_N \rangle =$$

$$\sum_{t_1 + \ldots + t_N = M} \frac{M!^2}{t_1!^2 \ldots t_N!^2} |A_{kl_1} \ldots A_{kl_N}|^2 \langle n_1, \ldots, n_N | a_{l_1}^{\dagger N} \ldots a_{l_1}^{\dagger N} a_{l_2}^{\dagger N} \ldots a_{l_2}^{\dagger N} | n_1, \ldots, n_N \rangle =$$

$$\sum_{t_1 + \ldots + t_N = M} \frac{M!^2}{t_1!^2 \ldots t_N!^2} |A_{kl_1} \ldots A_{kl_N}|^2 \frac{n_1! \ldots n_N!}{(n_1 - l_1)! \ldots (n_N - l_N)!} =$$

$$M! \left. \frac{\partial^M}{\partial t^M} \right|_{t=0} \prod_{l=1}^{N} L_{n_l}(-t |A_{kl}|^2),$$  \hspace{1cm} (22)
where $L_n(z)$ is the Laguerre polynomial,

$$L_n(z) = \sum_{l=0}^{n} \frac{n!(-z)^l}{l!^2(n-l)!}.$$  

The explicit form of (22) read as

$$\langle n_N, \ldots, n_1 | b^\dagger_k b_k | n_1, \ldots, n_N \rangle = \sum_{l=1}^{N} |A_{kl}|^2 n_l,$$

$$\langle n_N, \ldots, n_1 | b^\dagger_k b^2_k | n_1, \ldots, n_N \rangle = 2 \left[ \sum_{l=1}^{N} |A_{kl}|^2 n_l \right]^2 - \sum_{l=1}^{N} |A_{kl}|^4 (n_l + n_l^2),$$

$$\langle n_N, \ldots, n_1 | b^\dagger_k b^3_k | n_1, \ldots, n_N \rangle = 3! \left[ \sum_{l=1}^{N} |A_{kl}|^2 n_l \right]^3 + \sum_{l=1}^{N} |A_{kl}|^6 (2n_l + 6n_l^2 + 4n_l^3) -$$

$$9 \sum_{l=1}^{N} |A_{kl}|^4 \sum_{m=1}^{N} (n_l n_m + n_l^2),$$

$$\langle n_N, \ldots, n_1 | b^\dagger_k M b_k^M | n_1, \ldots, n_N \rangle = M! \left[ \sum_{l=1}^{N} |A_{kl}|^2 n_l \right]^M + \ldots$$

It is easy to understand, that only the first term in the right-hand side of the above relations survives in the thermodynamic limit $N \to \infty$ due to (19) and (20).

Let us associate with each pair of operators $b^\dagger_k, b_k$ the 'single-atom subsystems' \{s, k\} with the Hamiltonians $h^{(s)}_k = \epsilon_k b^\dagger_k b_k$. Suppose now, that each such atom is in the thermal equilibrium state characterized by the $k$-dependent inverse temperature

$$\beta_k = \epsilon_k^{-1} \log \frac{1 + \bar{n}(k)}{\bar{n}(k)}.$$  \hspace{1cm} (23)$$

This means, that the reduced density operator of the $k$-th atom has the Gibbs form,

$$\rho_G(k) = \frac{\exp[-\beta(k) h^{(s)}_k]}{Z^{(s)}_k} = \sum_{J=0}^{\infty} \frac{[\bar{n}(k)]^J}{[1 + \bar{n}(k)]^{J+1}} \frac{1}{J!} b^J_k |0\rangle \langle 0| b^J_k.$$  \hspace{1cm} (24)$$

Then, for arbitrary natural $M_1, M_2$, one can easily obtain the expectation value of the product $b_k^{M_1} b_k^{M_2}$ in this state

$$\text{Tr}^{(s, k)} \left[ b_k^{M_1} b_k^{M_2} \rho_G(k) \right] = M_1! \langle \bar{n}(k) \rangle^{M_1} \delta_{M_1, M_2},$$  \hspace{1cm} (25)$$

which coincides with the right-hand side of (21).

Thus, at large $N$, the huge majority of basis states (18) correspond to the partial equilibrium states with respect to the single-atom subsystems \{s, k\} in the sense of definition (1.3). The inverse
temperature $\beta_k$ of the $k$-th atom, generally speaking, depends on $k$, and is given by equations (23), (20).

Let us return to the chain of harmonic oscillator (1). For the bosonic annihilation operators $b_k$ and $a_l$ determined according to (A.3), the matrix $A_{kl}(N)$ introduced in (17) reduces at $\Omega = 0$ to the simple form $A_{kl} = N^{-1/2} \exp(2\pi i l/N)$, and $\epsilon_k = \Omega_0$. Parameter $\bar{n}(k)$ defined by (20) reduces to the average number of phonons in the chain $\bar{n} = N^{-1} \sum_{l=1}^{N} n_l$ and becomes $k$-independent, together with the inverse temperature (23). This proves (A.8) for all $\bar{n} > 0$.

2.2 Time evolution of the single-atom density operators

Relaxation of the macroscopic chain of harmonic oscillators from a nonequilibrium nonuniform initial state $|\psi(0)\rangle = (\mathcal{H}_0)^{-1/2} b_k^\dagger b_k |0\rangle$ was studied in Section 2 of [1]. First, the time evolution of the chain quantum state $|\psi(t)\rangle$ was determined in the leading order in the interaction constant $\Omega \to 0$. Then, representation (A.12) was obtained for the density operators $\rho(k,t)$ of the $k$-th atom at time $t$, which is asymptotically exact at $\Omega \to 0$. The full form of this expression reads as

$$
\rho(k,t) = \frac{\Omega}{N} \frac{r(k,t)}{J(\Omega - J)!} \left\{ \int_0^{\Omega} \frac{d\tau}{\pi} e^{i(\tau k - \omega_c,t)} \right\}^2 \left\{ 1 - \frac{r(k,t)}{N} \right\}^{\Omega - J},
$$

with

$$
r(k,t) = \sum_{\tau=1}^{N} \exp[i(\tau k - \omega_c,t)].
$$

Remind, that $\tau$ = $2\pi l/N$ and $\omega_c$ are the phonon quasimomentum and the energy, respectively,

$$
\omega_c = [\Omega_0^2 + 4\Omega^2 \sin^2(\tau/2)]^{1/2} = \Omega_0 + \frac{\Omega^2}{\Omega_0} (1 - \cos \tau) + O(\Omega^4).
$$

Parameter $r^2(k,t)$ is proportional to the energy $E(k,t)$, which is located at the $k$-th atom at the time moment $t$:

$$
E(k,t) = \Omega_0 \langle \psi(t) | b_k^\dagger b_k | \psi(t) \rangle = \Omega_0 \text{Tr} e^{i(k,t)} [\rho(k,t) b_k^\dagger b_k] = \mathcal{H} \Omega_0 \frac{r^2(k,t)}{N^2}.
$$

At small enough $t$, the sum in (27) can be replaced by the integral. This allows one to express the energy $E(k,t)$ normalized to the total energy in the chain in terms of the cylindric Bessel function $J_k(z)$,

$$
\frac{E(k,t)}{N\Omega_0} = \frac{r^2(k,t)}{N^2} \approx \left[ \int_0^{2\pi} \frac{d\tau}{2\pi} e^{i(\tau k - \omega_c,t)} \right]^2 = \left[ J_k(t \Omega^2/\Omega_0) \right]^2.
$$

The plot of this normalized energy versus $k$ and $t$ is shown in Figure 1. It is clear from (A.14) and Figure 1 that the energy perturbation spreads along the chain with the velocity $v = \Omega^2/\Omega_0$, which is just the maximum group velocity of phonons

$$
v_{ph}(\tau) = \frac{d\omega_c}{d\tau} = (\Omega^2/\Omega_0) \sin \tau + O(\Omega^4),
$$

$$
v = \max_{\tau} v_{ph}(\tau) = v_{ph}(\pi/2).
$$
Figure 1: Space and time dependence of the energy localized on the $k$-th atom normalized to the total energy in the chain, $E(k,t)/(N\Omega_0) = [J_k(t\Omega^2/\Omega_0)]^2$.

This feature of the relaxation dynamics known as 'the horizon effect' is typical in the quantum quench phenomenon [7].

2.3 Dispersion of the density operators

Now let us turn to the dynamics on the long time scale. When time $t$ becomes larger then the relaxation time $t_r = N/v = N\Omega_0/\Omega^2$, the energy perturbation reaches all atoms in the chain, all exponential terms in the sum in right-hand side of (27) completely dephase from each other, and this sum cannot be approximated by the integral, as it was done in (30). This leads to the qualitative change of of the chain evolution character from regular at $t \lesssim t_r$, to the 'stochastic' regime at $t \gtrsim t_r$, which is illustrated in Figure 2.

For the atom reduced density operators averaged over the infinite time interval, the canonical Gibbs distribution (A.17) with the site-number independent temperature was obtained in [4]. However, derivation of this result was incorrect, since it was based there on the erroneous equation (A.14a) in Page 24 see the footnote in this page. The fallacy in this equation came from the implicit and mistaken assumption, that the energy levels $E_n$ of the whole system are non-degenerate,

$$E_n \neq E_{n'}, \quad \text{if } n \neq n'.$$

(31)
Figure 2: The red line shows the time dependence of the quantity $r^2(0, t)/N^2$ defined by (27), which is proportional to the energy $E(0, t)$ localized on the 0-th atom, $E(0, t)/(N \Omega_0) = r^2(0, t)/N^2$. The blue line plots $|J_0(t \Omega^2/\Omega_0)|^2$. The model parameter values are taken as $N = 30$, $\Omega^2/\Omega_0 = 0.01$. Change of the evolution regime takes place at $t \approx t_r$, $t_r \Omega^2/\Omega_0 = 30$.

Really, the energy levels (measured from the ground state energy) in model (1) are given by

$$E_n = (n\omega) \equiv \sum_{\tau \in B} n_\tau \omega_\tau,$$

where summation in the quasimomentum $\tau$ runs over the Brillouin zone, $B = 2\pi \cdot ([Z \mod N])$. Due to the the mirror symmetry $\omega_\tau = \omega_{-\tau}$, of the phonon dispersion law (28), this energy spectrum can be rewritten in the form

$$E_n = n_0 \omega_0 + \sum_{0 < \tau < \pi} \left[ 1 + (-1)^N \right] \delta_{n_\tau, n_{-\tau}} \omega_\tau,$$

(33)

which indicates the strong degeneracy of the energy levels $E_n$ in model (1), in contrast to (31). Accordingly, one gets for the time average $\exp[it(E_n' - E_n)]$:

$$\exp[it(\omega(n' - n))] = \begin{cases} 
\delta_{n_0, n_0} \delta_{n_{-\tau}, n_{-\tau}} \prod_{0 < \tau < \pi} \delta_{n_\tau + n_{-\tau}, n'_{-\tau} + n'_{-\tau}}, & \text{for even } N, \\
\delta_{n_0, n_0} \prod_{0 < \tau < \pi} \delta_{n_\tau + n_{-\tau}, n'_{-\tau} + n'_{-\tau}}, & \text{for odd } N,
\end{cases}$$

(34)

instead of equation (A.14a). It turns out, however, that this correction does not change the final result (A.17) for the time averages of the reduced density operators almost for all atoms in the chain.
Proposition 2.2 In the thermodynamic limit, the time averages of the atom reduced density operators \( \rho(k, t) \) determined by equation (A.12) [or, equivalently, by equations (26), (27)] are given by the canonical Gibbs distributions with two different temperatures,

\[
\lim_{N \to \infty} \frac{\rho(k, t)}{N/N} = \begin{cases} 
\sum_{J=0}^{\infty} \left( \frac{2\bar{n}}{1+2\bar{n}} \right)^J |J\rangle\langle J|, & \text{for } k = 0, \\
\sum_{J=0}^{\infty} \left( \frac{\bar{n}^J}{1+n} \right)^J |J\rangle\langle J|, & \text{for } k = N/2 \text{ and even } \bar{n}, \\
\sum_{J=0}^{\infty} \frac{\bar{n}^J}{1+\bar{n}} |J\rangle\langle J|, & \text{otherwise},
\end{cases}
\]

(35)

where the time average is defined as

\[
\rho(k, t) \equiv \lim_{T \to \infty} \frac{1}{T} \int_0^T \rho(k, t) dt.
\]

(36)

Equation (35) corrects equation (A.17) for \( k = 0, \) and \( k = N/2. \)

Proof will be given only for the case of even \( N, \) since extension to the case of odd \( N \) is straightforward.

Let us introduce the \((N/2 + 1)\)-dimensional phase space with the points \( \phi = \{ \phi_\tau \}, \) where \( 0 \leq \phi_\tau < 2\pi, \) and \( \tau = \tau(l) = 2\pi l/N, \) with \( l = 0, 1, \ldots, N/2. \) Let us define the operator-valued function \( \rho(k, \phi) \) on this space which is obtained from (A.11) by the replacement

\[
t(n\omega) \to (n\phi) = n_0 \phi_0 + n_\pi \phi_\pi + \sum_{0<\tau<\pi} (n_\tau + n_{-\tau}) \phi_\tau,
\]

\[
t(n'\omega) \to (n'\phi) = n'_0 \phi_0 + n'_\pi \phi_\pi + \sum_{0<\tau<\pi} (n'_\tau + n'_{-\tau}) \phi_\tau,
\]

and averaging over the phases \( \{ \phi_\tau \} \) of the \( 2\pi \)-periodical functions \( f(\phi), \)

\[
\langle f(\phi) \rangle_\phi = \int_0^{2\pi} f(\phi) \prod_{l=0}^{N/2} \frac{\phi_\tau(l)}{2\pi} d\phi.
\]

Then, it follows from (34), that

\[
\exp[i t(\omega(n'-n))] = \langle \exp[i(\phi(n'-n))] \rangle_\phi.
\]

(37)

Applying this equality to (A.11), one can conclude, that the time average of the operator \( \rho(k, t) \) is equal to the phase average of the operator \( \rho(k, \phi) \). Therefore, the time average of the operator (26) can be written as

\[
\rho(k, t) = \sum_{J=0}^{\infty} |J\rangle\langle J| \rho(k, \phi) = C_{N/2}^J \left[ r(k, \phi)(N/2)^J \left[ 1 - r(k, \phi)(N/2)^J \right]\right]^{N-J} \langle \phi |,
\]

where

\[
r(k, \phi) = \sum_{l=0}^{N/2} w_{l}(k) \exp[i\phi_{\tau(l)}],
\]

\[
w_{l}(k) = \begin{cases} 
1, & \text{for } l = 0, \\
2 \cos[k \tau(l)], & \text{for } l = 1, \ldots, \frac{N}{2} - 1, \\
(-1)^k, & \text{for } l = \frac{N}{2}.
\end{cases}
\]
Accordingly, the matrix elements of the operator in the basis $|J\rangle = (J!)^{-1/2} b_k^{|J\rangle} |0\rangle$ take the form

$$\langle J'|\rho(k,t)|J\rangle = \delta_{J',J} \rho_J(k,t),$$

(39)

$$\rho_J(k,t) = \frac{2^J}{J!(2J)!} \int_0^\infty dr \frac{(r/N)^{2J}}{(1 - (r/N)^2)^J} p_N(k,r),$$

(40)

$$p_N(k,r) = \langle \delta[r - r(k,\phi)] \rangle.$$ (41)

After rescaling of the integration variable $r = \sqrt{N} x$ in the right-hand side of (40), the large-$N$ asymptotics of this equation can be written as

$$\rho_J(k,t) = \int_0^\infty dx \frac{n^J}{J!} \exp(-n x^2) \sqrt{N} p_N(k,r)|_{r=xN} + O(N^{-1}).$$

(42)

Function $p_N(k,r)$ defined by (41) is the probability density to find the total length $r$ of the sum of $N/2 + 1$ vectors in the plane which have arbitrary directions and different lengths $|w_l(k)|$, $l = 0, \ldots, N/2$. Straightforward calculations lead to the exact representation of this probability density in terms of the cylindrical Bessel function $J_0(z)$ [cf. equation (A.16) in Appendix],

$$p_N(k,r) = r \int_0^\infty dv v J_0(vr) \prod_{l=0}^{N/2} J_0[|w_l(k)|^2 v].$$

(43)

At large $N$, the main contribution to the integral in the right-hand side of (43) comes from small $v$, since the integrand vanishes at $v \gg N^{-1/2}$. So, in the thermodynamic limit we get from (43):

$$\sqrt{N} p_N(k,r)|_{r=xN} = N x \int_0^\infty dv v J_0(vx\sqrt{N}) \exp\left[-\frac{N v^2}{4} Y(k,N)\right] [1 + O(N^{-1})] = \frac{2x}{Y(k,N)} \exp[-x^2/Y(k,N)] + O(N^{-1}),$$

(44)

where

$$Y(k,N) = \frac{1}{N} \sum_{l=0}^{N/2} w_l(k)^2 = \begin{cases} 2 - \frac{2}{N}, & \text{if } k = 0, N/2, \\ 1 - \frac{2}{N}, & \text{if } k = 1, \ldots, \frac{N}{2} - 1. \end{cases}$$

(45)

Substitution of (44) and (45) into (42) yields finally to the result

$$\rho_J(k,t) = \left[\frac{n Y(k,N)}{1 + n Y(k,N)}\right]^J + O(N^{-1}) = \left[\frac{[\bar{n} Y(k,N)]^J}{(1 + 2\bar{n} Y(k,N))^{J+1}} + O(N^{-1})\right], \quad \text{if } k = 0, N/2,$$

(46)

$$\left[\frac{[\bar{n} Y(k,N)]^J}{(1 + n Y(k,N))^{J+1}} + O(N^{-1})\right], \quad \text{if } k = 1, \ldots, \frac{N}{2} - 1.$$}

Let us return now to the time evolution of the atom reduced density operators at large $t \gtrsim \tau$. At a fixed time moment $t \gtrsim \tau$, one can treat $r(k,t)$ as the absolute value of the sum of $N$ unit vectors on the plane which have 'stochastic' phases. Accordingly, it is again natural to rescale the 'length of the random walk path'

$$r(k,t) = \sqrt{N} x(k,t),$$

(47)
with \( x(k, t) \sim 1 \) for almost any \( t \geq t_r \). Substitution of (17) into (A.12) leads in the thermodynamic limit \( N \to \infty, \Omega \to \infty, \Omega/N = \bar{n} \) to the Poisson distribution

\[
\rho(k, t) = \sum_{j=0}^{\infty} |J\rangle \langle J| \frac{[\bar{n} x^2(k, t)]^j}{j!} \exp \left[-\bar{n} x^2(k, t)\right]
\]

(48)

for the atom density operators at almost any time moments \( t \gg t_r \). On the other hand, the time average of the density operator \( \rho(k, t) \) over the infinite time interval was proved to approach to the canonical Gibbs distributions in the thermodynamic limit, see (35). It follows from (35) and (48), that the reduced density operator \( \rho(k, t) \) of the \( k \)-th atom never approach to its time average (35) at any time moment. Similarly, the quantum averages \( \langle A_k(t) \rangle = \text{Tr}^{(s,k)}[A_k \rho(k, t)] \) of the local observables \( A_k \) relating to the \( k \)-th atom should also strongly fluctuate in time. This means, in turn, that the time dispersion

\[
D_{J,J'}(\rho) = \rho_{J,J'}(k, t) - \rho_{J,J'}(k, t)
\]

(49)

of the density operator matrix elements \( \rho_{J,J'}(k, t) = \langle J|\rho(k, t)|J\rangle \) remains considerable and does not vanish in the thermodynamic limit. Such type of evolution indicating lack of partial thermalization in model (1) was associated in [1] with the strong degeneracy of the energy level differences, see equation (A.18). Really, the dispersion (49) can be written as

\[
D_{J,J'}(\rho) = \sum_{n_1,n'_1,n_2,n'_2} \langle J|\text{Tr}^{(r,k)}[n_1]\rangle \langle n_1'|n_1\rangle |J\rangle \langle J'|\text{Tr}^{(r,k)}[n_2]\rangle \langle n_2'|n_2\rangle |J'| \cdot \langle n_1|\psi(0)\rangle \langle \psi(0)|n_1'\rangle \langle n_2|\psi(0)\rangle \langle \psi(0)|n_2'\rangle .
\]

\[
\left\{ \frac{\exp[it(E_{n_2} - E_{n_2'}) - E_{n_1} + E_{n_1'}]}{\exp[it(E_{n_2} - E_{n_2'})]} - \frac{\exp[it(E_{n_2} - E_{n_2'})]}{\exp[it(E_{n_1} - E_{n_1}')]} \right\},
\]

(50)

where \( E_n \) are the energy levels (32) in model (1). The last line in (50) has the structure

\[
\left\{ \frac{\exp[it(E_{n_2} - E_{n_2'} - E_{n_1} + E_{n_1'})]}{\exp[it(E_{n_2} - E_{n_2'})]} - \frac{\exp[it(E_{n_2} - E_{n_2'})]}{\exp[it(E_{n_1} - E_{n_1}')]} \right\} = \delta_{n_1,n_2} \delta_{n_1',n_2'} - \delta_{n_1,n_2} \delta_{n_2,n_1'} + C_{n_1,n_2,n_1',n_2'},
\]

(51)

where \( \delta_{n_1,n_2} \) is the Kronecker delta, and

\[
\delta_{n_1,n_2} = \begin{cases} 1, & \text{if } n_1 = n_2 = n_1' = n_2', \\ 0, & \text{otherwise}. \end{cases}
\]

The resonance term \( C_{n_1,n_2,n_1',n_2'} \) in the right-hand side of (51) is nonzero, in particular, at \( n_1' - n_1 = n_2' - n_2 = m \), and as well at \( n_2 - n_1 = n_2' - n_1' = m \) due to (A.18). It is precisely this term which is responsible for the strong time fluctuations of the density operator \( \rho(k, t) \) in model (1).

On the other hand, the resonance term \( C_{n_1,n_2,n_1',n_2'} \) vanishes in (51), if a weak anharmonic interaction is applied providing for the shifted energy levels that

\[
E_{n_1} - E_{n_1'} \neq E_{n_2} - E_{n_2'} \quad \text{unless} \quad \left\{ \begin{array}{ll} \text{either} & n_1 = n_1' \quad \text{and} \quad n_2 = n_2', \\
& \text{or} \quad n_1 = n_2 \quad \text{and} \quad n_1' = n_2'. \end{array} \right.
\]

(52)

\footnote{For the 0-th atom energy operator \( h^{(s)}_k \), the time fluctuations of its quantum expectation values \( E(0, t) \) are clearly seen in Figure 2 at \( \Omega^2 / \Omega_0 \gtrsim 30 \).}
In this case, one should expect, that the time dispersion \( D_{J',J}(\rho) \) would also vanish in the thermodynamic limit \( N \to \infty, \mathfrak{R}/N = \bar{n} \). For \( \bar{n} < 1 \), this was indeed proved in [1]. The crucial role of the 'non-resonance condition' (52) for ability of an isolated quantum system to thermalize was first established by von Neumann [22, 23], and confirmed later by many authors [20, 16, 18].

3 Time dispersion of the quantum expectation value of the atom energy

It is interesting to illustrate the dramatic effect of the nonlinear interaction on the time evolution of the quantum expectation value of the energy \( E(k,t) \) of a particular atom,

\[
E(k,t) = \langle \psi(t)| h^{(s)}_k |\psi(t)\rangle, \tag{53}
\]

where

\[
h^{(s)}_k = \Omega_0 b_k^\dagger b_k,
\]

is the Hamiltonian of the \( k \)-th atom, and \( |\psi(t)\rangle \) is the quantum state of the chain at time \( t \) which evolves from the initial state (A.10).

In the purely harmonic chain (1), the energy \( E(k,t) \) is determined by (29):

\[
E(k,t) = \mathfrak{R} \Omega_0 \frac{r^2(k,t)}{N^2}. \tag{54}
\]

Taking into account (27), one obtains from (54) for the time averages:

\[
\lim_{N \to \infty} E(k,t) = \begin{cases} 2\Omega_0 \bar{n}, & \text{if } k = 0, \\ 2\Omega_0 \bar{n}, & \text{if } k = N/2, \text{ and } N \text{ is even,} \\ \Omega_0 \bar{n}, & \text{otherwise,} \end{cases} \tag{55}
\]

\[
\lim_{N \to \infty} D(h^{(s)}_k) = \begin{cases} 4\Omega_0^2 \bar{n}^2, & \text{if } k = 0, \\ 4\Omega_0^2 \bar{n}^2, & \text{if } k = N/2, \text{ and } N \text{ is even,} \\ \Omega_0^2 \bar{n}^2, & \text{otherwise,} \end{cases} \tag{56}
\]

where

\[
D(h^{(s)}_k) \equiv \overline{E(k,t)^2} - \left[\overline{E(k,t)}\right]^2. \tag{57}
\]

Thus, the time dispersion \( D(h^{(s)}_k) \) of the quantum expectation value of the atom Hamiltonian remains finite in the thermodynamic limit in the purely harmonic chain.

On the other hand, in the chain perturbed by the extremely weak anharmonic interaction, the \( k \)-th atom energy (53) can be determined as

\[
E(k,t) = \text{Tr}^{(s,k)}[h^{(s)}_k \rho(k,t)], \tag{58}
\]
and the atom reduced density operator
\[
\rho(k,t) = \frac{\mathcal{N}!}{\mathcal{N}^N} \sum_{J=0}^{\mathcal{N}} \sum_{P=J}^{\mathcal{N}} P!(-1)^{P-J} \frac{1}{P!(P-J)!} \sum_{\tau, J_{\tau}=\mathcal{N}-P} \exp\{i[k(n\tau) - tE_n]\} \frac{N^P J!(P-J)!}{(n - l)!} \times \sum_{\tau, n_{\tau}=\mathcal{N}} \exp\{i[-k(n'\tau) + tE_{n'}]\} \frac{N^P J!(P-J)!}{(n' - l)!},
\]
(59)
can be obtained from (A.11) by replacement
\[
(\omega n) \rightarrow E_n = (\omega n) + \delta E_n,
\]
\[
(\omega n') \rightarrow E_{n'} = (\omega n') + \delta E_{n'},
\]
corresponding to the small shift of the energy levels.

If the perturbed energy levels \(E_n\) are not degenerate, averaging in time of (58) with the atom density operator \(\rho(k,t)\) given by (59) provides
\[
E(k,t) = \Omega_0 \bar{n},
\]
instead of (55). In turn, if the energy levels \(E_n\) satisfy the non-resonance condition (52), the time dispersion (57) can be written as
\[
D(h_k^{(s)}) = \Omega_0^2 \frac{\mathcal{N}!^2}{\mathcal{N}^{2\mathcal{N}+2}} \sum_{\tau, n_{\tau}=\mathcal{N}} \sum_{n_{\tau}', k_{\tau}=\mathcal{N}-1} \frac{1}{l!(n-l)!(n'-l)!} \frac{1}{k!(n-k)!(n'-k)!} = \Omega_0^2 \frac{\mathcal{N}!^2}{\mathcal{N}^{2\mathcal{N}+2}} \frac{N(N-1)}{N^2} \sum_{\tau, l_{\tau}=\mathcal{N}-1} \prod_{\tau} \frac{1}{l_{\tau}!} = \Omega_0^2 \frac{\mathcal{N}!^2}{\mathcal{N}^{2\mathcal{N}+2}} \frac{N(N-1)}{N^2} \int \frac{dx}{2\pi i x^{2\mathcal{N}-1}} [I_0(2x)]^N,
\]
(60)
where integration is performed in the complex \(x\)-plane along the circle centered at origin and going in the positive direction, and \(I_0(t)\) is the modified Bessel function of the first kind,
\[
I_0(t) = \sum_{j=0}^{\infty} \frac{(t/2)^{2j}}{j!^2}.
\]
(62)
In the thermodynamic limit \(N \to \infty, \bar{n} = \mathcal{N}/N = \text{Const}\), the integral in the right-hand side of
Figure 3: Function $W(\bar{n})$ determined by (66).

(62) is determined by contributions of two saddle points at $x = \pm x_0(\bar{n})$, where $x_0(\bar{n})$ is the positive solution of the equation

$$\left[ \frac{I_1(2x)}{I_0(2x)} - \frac{\bar{n}}{x} \right]_{x=x_0(\bar{n})} = 0.$$  \hspace{1cm} (63)

The saddle-point asymptotics of (62) in the thermodynamic limit reads as

$$D(h_k^{(s)}) = 2 \Omega_0^2 \bar{n} x_0(\bar{n}) \left[ \frac{2\pi N}{f''(x_0)} \right]^{1/2} [W(\bar{n})]^N \left[ 1 + O(N^{-1}) \right],$$  \hspace{1cm} (64)

where

$$f(x) = \log[I_0(2x)] - 2\bar{n} \log x,$$  \hspace{1cm} (65)

and

$$W(\bar{n}) = \left( \frac{\bar{n}}{e} \right)^{2\bar{n}} \frac{I_0[2 x_0(\bar{n})]}{[x_0(\bar{n})]^{2\bar{n}}}.$$  \hspace{1cm} (66)

The plot of function $W(\bar{n})$ is shown in Figure 3. This function has the following asymptotic behavior

$$W(\bar{n}) = \begin{cases} (\bar{n}/e^2)^{\bar{n}} \left[ 1 + \bar{n} + O(\bar{n}^2) \right], & \bar{n} \to +0, \\ (4\pi \bar{n})^{-1/2} \left[ 1 + O(\bar{n}^{-1}) \right], & \bar{n} \to +\infty, \end{cases}$$  \hspace{1cm} (67)
and monotonically decreases between values $W(0) = 1$ and \( \lim_{\bar{n} \to \infty} W(\bar{n}) = 0 \) in the half-axis \( 0 \leq \bar{n} < \infty \). Therefore, it follows from (54), that the time dispersion (57) of the quantum expectation value of the atom energy vanishes in the thermodynamic limit \( N \to \infty \) for all fixed \( \bar{n} > 0 \).

Acknowledgements

I am thankful to P. Calabrese, J. Cardy, H. W. Diehl, D. Huse, M. Olshanii and A. Silva for interesting discussions in the recent years. I am also grateful to M. Olshanii and A. Silva for their advise to publish the English translation of [1].

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Appendix

Relaxation Dynamics of a Quantum Chain of Harmonic Oscillators

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Abstract

The aim of the present paper is to trace the appearance of some statistical properties in an exactly solvable dynamic system - a quantum chain with weak harmonic interaction. The time dependence of the statistical single particle matrices is derived when the system relaxes from the non-equilibrium pure state. It is shown that the thermodynamic limit of the matrices in question is the Gibbs distribution. Moreover, the presence of any weak anharmonic interaction in the system causes each oscillator to have a canonical distribution almost at any moment.

Introduction

The statistical mechanics, besides the dynamical laws, is based on certain additional probability hypothesis (the micro-canonical distribution postulate, the correlation weakness principle, etc.) which are justified finally by the good agreement of the theory with experiment. One can guess, that such additional hypothesis are in fact the consequences of the dynamical laws. This idea was realized in the Boltzmann's approach, for which ergodicity of the Hamiltonian flows plays an important role. Verification of the latter for real systems is a difficult problem. In [1] ergodicity of a system of $N$ hard spheres was proved. However, this proof can not be extended to oscillatory systems. In many papers [2, 3, 4] the ergodicity problem is analyzed analytically and numerically.

For quantum systems, justification of the micro-canonical distribution is even more problematic, since the matrix elements of the density operator calculated in the basis of the stationary states only change their phases and do not approach to the equilibrium distribution. Nevertheless, von Neumann [5] managed to prove some important statements, which could be treated as quantum basis of the classical statistical mechanics. In the von Neumann's approach, it is allowed to measure not all dynamical quantities, but only classical (macroscopic) variables which quantum operators mutually commute.

One can guess, that in a non-isolated system being in contact with the thermal bath, all dynamical variables are characterized by statistical properties. In other words, the density operator of such a system at almost all time moments is the Gibbs distribution. In the present paper this assumption is verified for the linear chain of harmonic oscillators - the system of interacting particles, which allows exact solution of the Schrödinger equation. The dynamics of relaxation in this system is studied as well.

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1 Model

We consider the periodical chain of harmonic oscillators. Each of them is coupled with two neighbours and with its equilibrium point \([6]\). The Hamiltonian has the form

\[
H = \sum_{k=0}^{N-1} \frac{1}{2} \left[ p_k^2 + U(|q_k - q_{k+1}|) + \Omega_0^2 q_k^2 \right], \quad q_N \equiv q_0. \tag{A.1}
\]

Here \(q_k, p_k\) are the coordinate and momentum of the \(k\)-th oscillator, \(k = 0, \ldots, N - 1\); \(N\) is the numbers of oscillators, \(U(|q_k - q_{k+1}|)/2\) is the interaction potential of the neighbouring oscillators, \(\Omega_0\) is their own frequency, the Plank constant and the oscillator mass are put to the unit value, periodical boundary conditions are chosen. The \(k\)-th oscillator will be called ‘the \(k\)-th atom’.

Model (A.1) has been studied in \([7]\) in order to calculate correlation functions and to estimate the Poincare periods in the thermodynamics limit.

The dynamical problem can be solved exactly if \(U(|q_k - q_{k+1}|) = \Omega_0^2 (q_k - q_{k+1})^2\). In this case the normal coordinate \(Q_\tau, P_\tau\) are introduced as

\[
q_k = \sum_{\tau} e^{ik\tau} Q_\tau / \sqrt{N}, \quad p_k = \sum_{\tau} e^{-ik\tau} P_\tau / \sqrt{N}, \tag{A.2}
\]

with integer \(l\). Two sets of secondary quantization operators are related with \(q, p, Q, P\):

\[
b_k = \frac{\Omega_0 q_k + ip_k}{\sqrt{2\Omega_0}}, \quad b_k^\dagger = \frac{\Omega_0 q_k - ip_k}{\sqrt{2\Omega_0}},
\]

\[
a_\tau = \frac{\omega_\tau Q_\tau + iP_\tau}{\sqrt{2\omega_\tau}}, \quad a_\tau^\dagger = \frac{\omega_\tau Q_\tau^\dagger - iP_\tau}{\sqrt{2\omega_\tau}}, \tag{A.3}
\]

where \(\omega_\tau^2 = \Omega_0^2 + \Omega^2 (2\sin \frac{\tau}{2})^2\).

The Hamiltonian can be rewritten in the form

\[
H = \sum_{\tau} (a_\tau^\dagger a_\tau + 1/2) \omega_\tau, \tag{A.4}
\]

which shows that the normal modes (phonons) do not interact. The eigenstate of the Hamiltonian reads as

\[
|n_1, \ldots, n_N\rangle = (n_1! \ldots n_N!)^{-1/2} (a_1^\dagger)^{n_1} \ldots (a_N^\dagger)^{n_N} |0\rangle, \tag{A.5}
\]

where \(|0\rangle\) is the ground state, \(n_i\) is the number of phonons with the quasi-momentum \(\tau_i, \tau_i < \tau_{i+1}\). If \(\Omega \ll \Omega_0\), each atom can be considered as a subsystem which interacts weakly with surrounding (the thermal bath).

2 Relaxation of the one-particle density operator

If \(\Omega\) is small, one can follow the relaxation dynamics of the single-atom density operator for the system prepared in some realistic non-equilibrium initial state.
Let us introduce the following notations:

\[ a^n = \prod_{\tau} a^n_{\tau}, \quad n = \{n_{\tau}\}, \quad |n\rangle = \{|n_1, \ldots, n_N\rangle\}, \quad n! = \prod_{\tau} n_{\tau}!, \]

\[ C_n = \frac{n!}{l!(n-l)!}, \quad \text{etc.} \quad (A.6) \]

If the whole system is described by the density operator \( \rho = \rho_{nn'}|n\rangle\langle n'| \), then the atom with the number \( k = 0 \) in the chain has the density operator \( \text{Tr}^{(r)} \rho = \text{Tr}^{(r)} |n\rangle\langle n'| \), where

\[
\text{Tr}^{(r)} A = \sum_{m=0}^{\infty} \sum_{m'=0}^{\infty} \sum_{m_{N-1}=0}^{\infty} \frac{1}{\sqrt{m_0!m_1!\cdots m_{N-1}!}} (b_0^\dagger)^m_0 |0\rangle \times \langle 0|b_0^{m'_0}b_1^{m_1} \cdots A \ldots (b_1^\dagger)^m_1 (b_0^\dagger)^{m'_0}|0\rangle \langle 0|^0_{m'_0}.
\]

We have calculated the quantities \( \text{Tr}^{(r)} |n\rangle\langle n'| \) only at \( \Omega = 0 \):

\[
\text{Tr}^{(r)} |n\rangle\langle n'| = \sum_{J} |J\rangle \langle J| \sum_{P} \frac{P!^2(-1)^{P-J}}{N^P J!(P-J)!} \sum_{l,l'=-P}^{l} \sqrt{\alpha^n n^n \tau} \frac{\sqrt{\alpha^n n^n \tau}}{l!(n-l)!(n'-l)!}.
\]

where \( |J\rangle = (b_0^\dagger)^{J}|0\rangle \), \( N = \sum_{\tau} n_{\tau} = \sum_{\tau} n_{\tau}' \). The state \( |n\rangle \) has the energy \( E_n = E_0 + \Omega_0 \mathcal{R} \), where \( E_0 \) is the ground state energy.

Using (A.7) it is possible to show that the atom’s density operator which corresponds to the stationary state \( |n\rangle \) of the system, has the form of the Gibbs distribution in the thermodynamic limit \( (N \to \infty, \mathcal{R}/N = \bar{n} = \text{const}) \) at least for \( \bar{n} < 1 \), if the number \( \alpha N \) of nonzero integers in the set \( n = \{n_{\tau}\} \) is macroscopic (i.e. \( \alpha \sim 1 \)):

\[
\text{Tr}^{(r)} |n\rangle\langle n| = \frac{1}{1 + \bar{n}} \sum_{J} \left( \frac{\bar{n}}{1 + \bar{n}} \right)^J |J\rangle \langle J| \left[ 1 + O(N^{-1}) \right]. \quad (A.8)
\]

Perhaps, this result holds to some extent in other dynamical systems.

Let us show, how the evolution of the system from some non-equilibrium initial state can be described. Let

\[
\Omega(t) = \begin{cases} 0, & t \leq 0, \\ \Omega, & 0 < t < T, \\ 0, & t \geq T, \end{cases} \quad (A.9)
\]

and \( \Omega \) is so small, that one can neglect the terms of order \( \epsilon \) in

\[
\langle n'|\Omega(t') = \Omega|n\rangle \Omega(t) = 0 \rangle = \delta_{nn'} + \epsilon_{nn'},
\]

i.e. interaction almost does not change the stationary states \( |n\rangle \). At \( t \leq 0, t \geq T \) one can use expression (A.7), and at \( 0 < t < T \) the system relaxes due to the weak interaction.

If at \( t = 0 \) the system is in the stationary state \( |n\rangle \), then at time \( T \) its state vector is given by \( |n\rangle \exp[-i(n\omega)T] \) (the terms of order \( \epsilon \) are omitted), where \( (\omega n) = \sum_{\tau} \omega_{\tau} n_{\tau} \).
Let us choose the non-equilibrium initial state as

$$|\psi(t)|_{t=0} = \frac{(b_0^\dagger)^n}{\sqrt{\mathcal{N}!}} |0\rangle = \frac{1}{\sqrt{\mathcal{N}!}} \sum_{n=\mathcal{N}} \frac{\mathcal{N}!}{n!} (a_0^\dagger)^n |0\rangle,$$

(A.10)

the 0-th atom is exited to the energy \(\mathcal{N}\Omega_0\), while all the rest atoms remain unexcited. Then one gets from (A.7), (A.10)

$$\rho(k,t)|_{t=T} = \frac{\mathcal{N}!}{\mathcal{N}^k} \sum_J |J\rangle \langle J| \sum_P \frac{P!^2(-1)^J}{N^P!J!(P-J)!} \sum_{l_\tau=\mathcal{N}-P} \frac{1}{l_\tau!} \times \sum_{n_\tau=\mathcal{N}} \frac{\exp\{ik(n\tau) - t(n\Omega)\}}{(n-l)!} \sum_{n_\tau'=\mathcal{N}} \frac{\exp\{-k(n'\tau) + t(n'\Omega)\}}{(n'-l)!},$$

(A.11)

where \(\rho(k,t)\) is the density operator of the \(k\)-th atom \((k = 0, 1, \ldots, N-1)\) at the time \(t\), and \((n\tau) = \sum \tau n_\tau\). Straightforward calculations yield

$$\rho(k,t) = \sum_J |J\rangle \langle J| \frac{\mathcal{N}!}{J!(\mathcal{N} - J)!} \left( \frac{r}{N} \right)^{2J} \left[ 1 - \left( \frac{r}{N} \right)^2 \right]^{\mathcal{N}-J},$$

(A.12)

where

$$r(k,t) = \left| \sum_\tau \exp(i(k\tau - \omega_\tau t)) \right|. \quad \text{(A.13)}$$

Keeping the linear terms in \((\Omega/\Omega_0)^2\) in the expansion of \(\omega_\tau\), and replacing the sum in \(\tau\) in \(r(q,t)\) by the integral, we come to the integral representation of the Bessel function of the \(q\)-th order:

$$r(k,t) = \left| N_J^k |\Omega_0(\Omega/\Omega_0)^2 t| \right|. \quad \text{(A.13)}$$

One can safely replace the sum by the integral at large \(N\) and if \(t \ll N/[\Omega_0(\Omega/\Omega_0)^2]\) (the period of the integrand is much large than \(\Delta \tau = 2\pi/N\)).

One can easily see, that the energy of the \(k\)-th atom at the time \(t\) exceeds the ground state energy by the quantity

$$\Omega_0(J)_{\rho(k,t)} = \Omega_0 \mathcal{N} J_k^2 [\Omega_0(\Omega/\Omega_0)^2 t]. \quad \text{(A.14)}$$

Perturbation reaches the \(k\)-th atom after the time of order \(k/[\Omega_0(\Omega/\Omega_0)^2]\), and after that the energy of this atom oscillates slowly with decreasing amplitude. When the excitation energy distributes throughout the whole chain, one can not any more replace the sum (A.12) by the integral. For the classical harmonic chain, formula (A.14) was obtained in [7].

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3 Time average and dispersion of one-particle density operator

Let us introduce the following notations for the average quantities:

\[ \langle A \rangle_{\rho}(t) = \text{Tr} A \rho(t), \]

\[ \bar{f} = \lim_{T \to \infty} \frac{1}{T} \int_0^T f(t) dt, \]

where \( A, f \) are an operator a function of time, respectively.

In order to calculate \( \langle \bar{A} \rangle_{\rho} \), it is sufficient to know \( \bar{\rho} \). Consider the space of phases with points \( \phi = (\phi_1, \ldots, \phi_N) \), \( 0 \leq \phi_i < 2\pi \) (we use the same notations for indexes as in formula (A.5), and the measure \( d\phi = \prod_\tau d\phi_\tau/(2\pi) \)). Let us define the operator-valued function \( \rho(k, \phi) \) on this space which is obtained from (A.11) by the replacement

\[ t(n\omega) \to (n\phi), \quad t(n'\omega) \to (n'\phi) = \sum_\tau n_\tau \phi_\tau. \]

Due to the equality

\[ \exp[it(\phi(n' - n))] = \langle \exp[i(\phi(n' - n))] \rangle_\phi = \delta_{nn'}, \quad (A.14a) \]

one can conclude from (A.11), that the time average of the operator \( \rho(k, t) \) equals to the phase average of the operator \( \rho(k, \phi) \). This allows us to write the time average of the operator (A.12) in the form

\[ \bar{\rho} = \sum_J |J \rangle \langle J | C^J_0 \left[ r(\phi)/N \right]^{2J} \left[ 1 - [r(\phi)/N]^2 \right]^{N - J} \right]_\phi, \quad (A.15) \]

where

\[ r(\phi) = \left| \sum_\tau \exp(i\phi_\tau) \right|. \]

The problem is reduced to the random walk problem, which was studied in [8]. Using formulas (51)-(53), (103), (104) of reference [8] we find

\[ p_N(r) \equiv \langle \delta(r - r(\phi)) \rangle_\phi = r \int_0^\infty d\rho \rho J^N_0(\rho) J_0(r \rho), \]

\[ p_N(r) \to \frac{2r}{N} e^{-r^2/N}, \quad \text{at} \quad N \to \infty. \quad (A.16) \]

\[ \text{[S.R. 2012]} \] The first equality in equation (A.14a) is wrong, since it does not take into account that the energy spectrum \( E_n = (\omega n) \) of model (A.1) is strongly degenerate. The corrected form of this equation is given by formula (34) in Subsection 2.3. This correction induces also certain modifications into the calculation of \( \bar{\rho} \) in this page and into the final result (A.17). These modifications are described in Proposition 2.2 and equation (45) in Subsection 2.3. Fortunately, the above mentioned modifications are minimal, and equation (A.17) holds for all but one or two atoms in the chain, depending on the parity of \( N \). On the other hand, application of a weak anharmonic interaction breaking the energy spectrum degeneracy restores the result (A.17): the time average of the reduced density operators of all atoms in the chain is given by the Gibbs distribution with the same temperature.
Using the above large-\(N\) asymptotics for \(p_N(r)\) and for the asymptotic formula 
\[
[1 - (r/N)^2]^{\frac{r}{N} - J} \to \exp[-r^2\theta/N^2], \quad \text{at} \quad N \to \infty,
\]
we get
\[
\lim_{N \to \infty} \bar{\rho}_N = \sum_J \frac{1}{1 + \bar{n}} \left( \frac{\bar{n}}{1 + \bar{n}} \right)^J |J\rangle\langle J|.
\] (A.17)
The canonical distribution is obtained for all values of \(\bar{n}\).

It is clear from (A.12) that the time fluctuations of the density operator do not vanish in the thermodynamic limit. This behavior is caused by the degeneracy of the system in the differences of the energy levels of the stationary states:
\[
(\omega n) - (\omega n') = (\omega(n + m)) - (\omega(n' + m)).
\] (A.18)

If a weak enough anharmonic interaction is applied
(a) this will not change substantially \(\bar{\rho}\),
(b) at least at \(\bar{n} < 1\), the dispersion
\[
D_{JJ'}(\rho) = (\rho_J - \bar{\rho}_J)^* (\rho_{J'} - \bar{\rho}_{J'})
\]
vanishes in the thermodynamic limit.

A weak anharmonic interaction can be described as a perturbation leading to a small shift of each energy level
\[
E_n = (\omega n) + \delta E_n.
\]

Therefore, in equation (A.11), we should replace now \((n\omega)\) by \(E_n\), and \((n'\omega)\) by \(E_{n'}\), and the statement (a) becomes evident.

Let us prove (b). One obtains from (A.12)
\[
D_{JJ'}(\rho) = \frac{\mathcal{N}^2}{N^{2\mathcal{N}}} \sum_{PQ} \frac{P^l(-1)^{P-J}Q^q(-1)^{Q-J'}}{N^P P! (P-J)! N^Q Q! (Q-J')!} \times
\]
\[
\sum_{\tau \neq \tau'} \frac{1}{l!(n-l)!(n'-l)!} \frac{1}{k!(n-k)!(n'-k)!}.
\] (A.19)

In the sum (A.19), the following inequality holds \(\|n - n'\| \leq 2 \min(P, Q)\), where \(\|n\| = \sum_{\tau} |n_{\tau}|\).

Since
\[
\frac{\mathcal{N}^2}{N^{2\mathcal{N}}} \sum_{\tau \neq \tau'} \frac{1}{l!(n-l)!(n'-l)!} \frac{1}{k!(n-k)!(n'-k)!} \leq \frac{\mathcal{N}^2}{N^{2\mathcal{N}}} \sum_{\tau \neq \tau'} \frac{1}{n! n'!} \leq \frac{\mathcal{N}^2}{P! Q!} \frac{\mathcal{N}^2}{N^{2\mathcal{N}}} \sum_{\tau \neq \tau'} \frac{1}{n! n'!} \leq \frac{\mathcal{N}^2}{P! Q!},
\] (A.20)
the series in \( (A.19) \) uniformly converges at \( \bar{n} < 1 \). Therefore, one can treat \( P \) and \( Q \) as finite numbers. Let \( P < Q \). The number of terms in the sum

\[
\sum_{n' = 0}^{\bar{n}} \frac{1}{n!}
\]

is smaller than

\[
\frac{\sqrt{P!(N-1)!}}{N^{2N}} \leq \frac{\bar{n}!N^{2P}}{P!(N-1)!} \leq \frac{\bar{n}!N^{2P}}{P!(N-1)!}, \quad (A.21)
\]

which proves statement (b). It is quite possible that \( (A.8) \) and (b) hold also for \( \bar{n} \geq 1 \).

In conclusion let us note that the considered model can be useful for many other applications. Since in the case of the harmonic interaction, its dynamics is integrable, the model can be used to verify different approximate methods of studying relaxation processes. In the case of the anharmonic interaction, one can study analytically or numerically the relaxation dynamics in a nonlinear system. The model could be useful also for analyzing the arising statistical properties in a non-macroscopic systems, like three-atom molecules.

The author is grateful to S. V. Peletminski for the discussion of the results of this work.

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