Quantum kinetic equation before and after Big Bang

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Abstract

The energy dissipation in a gas of structured objects, e.g. molecules, is considered in density matrix formalism. It is shown that the macroscopic irreversibility of the kinetic processes can be considered as a consequence of the microscopic operator ordering. Our approach is free of any special assumptions on the space-time geometry, except for the general causality assumptions, so it can be applied to a wide variety of processes, from the cosmological processes at Big Bang stage till the energy dissipation in molecular gases.

1 Introduction

Kinetic equations describe the evolution of the distribution function of matter in phase space at the presence of particle collisions. They lay the foundation of many cosmological models, describing the formation of present barionic matter from initial plasma. The problem with kinetic approach is that at the Plank times, \( \tau \sim 10^{-44} \text{sec} \), the era of quantum gravity, the Riemann space-time itself did not exist, so neither the Boltzmann kinetic equation of the form

\[
\frac{\partial f(X, P, t)}{\partial t} + F \frac{\partial f(X, P, t)}{\partial P} + \frac{P}{m} \frac{\partial f(X, P, t)}{\partial X} = I_{\text{col}}[f],
\]

nor its relativistic generalisation is valid for that stage.

The situation with the quantum mechanical description of the Early Universe is a little better. In quantum mechanics the evolution of quantum system is described as the evolution of the density operator \( \hat{\rho} \) obeying the von Neumann equation

\[
\hat{H} \frac{\partial}{\partial t} \hat{\rho} = \{ \hat{H}, \hat{\rho} \},
\]
where $\hat{H}$ is the Hamiltonian of the system. For the evolution equation (2) it does not mean whether the spacetime is continuous, differentiable, Archimedian. What is significant is the evolution: the existence of time $t$ and the dependence of the state on $t$ just means the evolution; if there is no evolution there is no change in quantum state.

It is important for the kinetic approach that the evolution equation for the classical distribution function in phase space $f(X, P, t)$ should be obtained as the classical limit $\hbar \to 0$ of a more fundamental quantum equation (2) at the assumption of the existence of classical trajectory $X = X(t)$ for each particle. This is called the macroscopic limit.

In a purely quantum case, i.e. when $\hbar$ cannot be treated as a small parameter, it is impossible to assign any trajectory $X(t)$ to a given particle. This is the case for dense plasma, lasers, microelectronics etc. This is also the case for quantum gravity.

The present paper considers the effect of general causality assumptions on the evolution of the density operator and the kinetic equation, resulting from this evolution in macroscopic limit. The general causality assumptions, discussed in [1,2], are required for the construction of quantum field theory on a category space, which is not a manifold, i.e. when continuity and differentiability are not provided. This is the case for the quantum gravity era of the Early Universe, and hence before the light-cone causality of Minkovskian space have been set by Big Bang a more general causality assumptions should hold. In the limit of classical non relativistic gas the general theory drives us back to known results for the Boltzmann equation and the Klimontovich method for molecular gases, but ultimately leads to irreversibility if the internal degrees of freedom are involved.

The remainder of this paper is organized as follows. In Section 2 we remind the links between quantum description of hierarchic systems and causality. In Section 3 a semi-quantum kinetic equation for a gas of structured particles is constructed. Section 4 presents a toy model of a system of hierarchic quantum oscillators and imposes the operator ordering on this system. In Conclusion we summarize the basic ideas of our approach.

## 2 Density operator for hierarchic structures

Strictly speaking the von Neumann equation (2) holds only for closed systems – but the only system which is absolutely closed is the Universe as a whole. Therefore there should be some methods to treat the system of our interest as approximately closed, when its interaction with the rest of the Universe can be neglected, or treated perturbatively. In this case the state vector of the whole Universe can be casted in a form

$$|\psi\rangle = \sum_{i\alpha} c_{i\alpha} |\phi_i\rangle |\theta_{\alpha}\rangle,$$

where $|\phi_i\rangle$ are the states of the system, $|\theta_{\alpha}\rangle$ are the states of its environment, i.e. the rest part of the Universe. To get a tractable model the states of the environment are assumed to be mutually orthogonal

$$\langle \theta_\alpha | \theta_\beta \rangle = \delta_{\alpha\beta}.$$


In view of this assumption the matrix elements of the density operator of the whole Universe

\[ \hat{\rho} = |\psi\rangle\langle\psi| \]

in the basis of the states of system \( \phi \)

\[ \rho_{ij}^{\phi} = \sum_{\alpha} \bar{c}_{i\alpha} c_{i'\alpha} = \text{Tr}_{i'} \langle i'|\hat{\rho}|i \rangle. \]  

(5)

This means the probabilities of different states of a quantum system \( i \) are obtained by averaging over all states of its environment.

The mean value of arbitrary physical observable \( A \) for such system is equal to the trace of the product \( \hat{A}\hat{\rho} \) with respect to the states of the system \( \phi \):

\[ \langle A \rangle = \text{Tr} \hat{A}\hat{\rho} = \sum_{ji} A_{ij} \rho_{ji}^{\phi}. \]  

(6)

Since it is impossible to account for all degrees of freedom of the environment, what is done in practice is different from the summation (5) with orthonormality condition (4). Namely, considering a diluted gas of diatomic molecules in coordinate representation [3, 4], one uses the Wigner function

\[ \rho(R, P, r, r', t) = \frac{1}{(2\pi)^3} \int \rho_1(R - \frac{\hbar}{2}\gamma, R + \frac{\hbar}{2}\gamma, r_1', r_2', t) e^{-i\gamma P} d\gamma, \]  

(7)

where \( R \) is the center of mass coordinate of the molecule, \( P \) is its total momentum; \( r = r_1 - r_2 \) is the internal degree of freedom – the relative displacement of atoms in the molecule; \( \rho_1(r_1, r_2, r_1', r_2', t) \) is the density matrix of diatomic molecule in coordinate representation.

In the language of state vectors the Wigner function formalism corresponds to the change of basis (3) for the density operator (5) to a hierarchic one

\[ \hat{\rho} = |\psi\rangle\langle\psi|, \quad |\psi\rangle = \sum_{i_{\alpha}i_{\alpha-1}} c_{i_{\alpha}i_{\alpha-1}} |\phi_{i_{\alpha}}\rangle |\phi_{i_{\alpha}-1}\rangle, \]  

(8)

where \( (\alpha - 1) \) denotes the next to the studied system \( (\phi^{\alpha}) \) hierarchy level. (Say, in the case of diatomic gas \( |\phi^{\alpha-1}\rangle \) denotes the state vector of molecule, with \( |\phi^{\alpha}\rangle \) being the state of atom in this molecule.) The density matrix for the system \( (\phi^{\alpha}) \) can be casted in the form [5]:

\[ \hat{\rho}^{\alpha} = \text{Tr}_{\alpha-1} |\psi\rangle\langle\psi|, \]  

(9)

where \( |\psi\rangle \) is given by (3).

The hierarchic representation [5] poses the problem of ordering the operators acting at different hierarchy levels. The operator ordering rule “the coarse acts the first” was suggested.
by the author [2]. This corresponds to general cosmological idea of cascade process of the Universe origin from vacuum:

\[ |U_0⟩ = a_0^† |0⟩, |U_0U_0⟩ = a_i^† a_0^† |0⟩ = \{ |U_0⟩, |U_0i⟩ \}, \ldots. \quad (10) \]

At present stage of the Universe evolution the hierarchy level and the number of constituents are very large \( N \sim 2^n \) is expected to be of order of the Dirac-Eddington number \( N \sim 10^{80} \), or so, and we observe continuous Universe [6, 7].

This implies two types of causality: (i) the vertical causality \( a \subseteq b \) (\( a \) is a part of \( b \)); (ii) the horizontal causality \( a \prec b \) (\( a \) precedes \( b \)); in Fig. 1 \( U_{0i} \subseteq U_0, \quad U_{0i} \prec U_{0j} \). Consequently, two types of operator ordering are required to meet two types of partial order. The approach with two types of causality relations is a generalization of common light-cone causality of the Minkovsky space with \( T \)-ordering relation for the operators on more general spaces. It perfectly meets the needs of quantum gravity level cosmological models, when the the manifold structure is not provided [8, 9]. The details of this topological approach, known as region causality, can be found in [1].

What region causality says is quite natural not only for quantum gravity, but also for molecular physics: no experiment can detect a causal effect in a point – what is really observed is an effect in a region, the size of which is restricted, at best, by the Heisenberg uncertainty relation \( \Delta p \Delta x \geq \frac{\hbar}{2} \). So, in accordance to [1] we adopt two types of causality:

\[
\begin{align*}
    a & \subseteq b & a \text{ is a part of } b \\
    a & \prec b & b \text{ can see } a.
\end{align*}
\]

The latter corresponds to the light-cone causality; the former, supplied with the operator ordering “the coarse acts first”, just stands for the fact that it is impossible to change the state of the part without changing the state of the whole.
It is important for kinetic theory that the Bogolubov causality relations for the scattering matrix \[9\]
\[
\frac{\delta}{\delta g(x)} \left[ \frac{\delta S[g]}{\delta g(y)} S^\dagger[g] \right] = 0, \quad x \lessgtr y,
\]
originally formulated for the light-cone causality – \(x < y\) means \(x_0 < y_0\) and \(x \sim y\) means the interval between the events \(x\) and \(y\) is space-like interval – without significant changes are generalized to the vertical causality as well. This can be easily seen by introducing \(p\)-adic coordinate \(x \in \mathbb{Z}_p\) on the branching tree. The research in quantum gravity have stimulated the extension of the \(S\)-matrix formalism to non-Archimedean numeric fields, namely to the field of \(p\)-adic numbers \([10]\). Hence the Bogolubov causality relation \((11)\) can be given for the quantum fields depending on \(p\)-adic arguments, and therefore the fields defined on the vertexes of \(p\)-adic tree can be ordered in analogy to the \(T\)-ordering causality.

In \(p\)-adic metric the partial order is given by \(p\)-adic metric \(| \cdot |_p\):
\[
x < y \text{ if } |x|_p < |y|_p - \text{ vertical ordering;}
\]
\[
\text{if } |x|_p = |y|_p \text{ then } x \text{ and } y \text{ are ordered by the first nonzero coefficients} - \text{ this is horizontal ordering in the ring of natural numbers} \([10][11]\). \text{ So, if } x, y \in \mathbb{Z}_p \text{ in } (11) \text{ the Bogolubov causality relation is defined on the branching tree. A toy-model of such field theory is presented in} [12].
\]

In topology the causality of regions is axiomatising by means of partial order relations in a form of causal sets \([8][13]\). The causality at quantum gravity level – we would say before the Big Bang – will be the \textit{region causality} with two causality relations \(A \subset B\) and \(A \propto B\), that is called a causal site. The axiomatics of causal site given in \([1]\) is presented in Appendix.

In a (pseudo-) Euclidean space the structure of the causal sites implies causal paths and the geodesic coinciding with light-cone causality. However at quantum gravity level, when the Archimedean axiom does not hold, the vertical causality relation \(\subseteq\) is expected to play the important role. We do not know the concrete scheme of the present Universe formation from initial object, but without loss of generality we can assume that at initial time \(t = 0\) there was only one initial object \(U_0\). At the next instant of time \(t\) it branched into \(p \geq 2\) parts, each of those continued further branching in a tree-like matter – therefore a hierarchic structure have been formed \([14]\). This hierarchic structure endowed with certain system of relations between its elements has formed our space-time.

The axiomatics of causal site is rather general and should be applied not only at quantum gravity level, but also for quantum systems of present life, such as molecular gases. To see this, we have to cast the density operator in a hierarchic basis \([8]\). Let us consider a hierarchic system \(O\) consisting of two parts \(I\) and \(J\), each of those consists of its own two parts, \((i, i')\) and \((j, j')\), respectively, see Fig. \([2]\). For definiteness, let us consider the particle “\(i\)” of the finest hierarchy level of the system above. The mean value of an observable \(A\) related to \(i\) can be evaluated in two different ways:
Figure 2: Hierarchic binary system. Two means of calculating partial density matrices of the sub-parts can be applied

1. with the density matrix averaged over all states of \( i' \):
   \[
   \hat{\rho}_i = \sum_{i'} \langle i' | \hat{\rho} | i' \rangle;
   \]

2. with the density matrix averaged over the states of \( I \) – the “parent” of \( i \):
   \[
   \hat{\rho}_i = \sum_I \langle I | \hat{\rho} | I \rangle.
   \]

The former case is a standard way of the partial density matrix for a multi-particle system \[3\], the latter is presented in \[5\]. In the latter case the state vectors are represented in a tree-like form

\[
| \Phi_I \rangle = \{ | I \rangle, | II \rangle, \ldots \}, \quad \hat{\rho} = | \Phi_I \rangle \langle \Phi_I |,
\]

with index \( O \) being dropped as omnipresent.

To provide the equivalence of these two approaches the effect of the other particles \( J \neq I \) on the parts of \( I \), \( i.e. \) on \( i, i' \), should exist only via change the state of \( I \). This the effect of the whole to its parts. In thermodynamics it corresponds to adiabatic insulation of the system \( I \), when the energy can be transferred to the system as a whole, but not to its internal degrees of freedom.

### 3 Quantum kinetic equation for the gas of oscillators

Let us consider a simple example. A homogeneous gas of molecules with the distribution function \( f(P) \). The molecules can transfer part of their kinetic energy to their internal degrees of freedom, represented by quantum harmonic oscillators. The molecules do not interact beyond the interaction zone \( |x_1 - x_2| > 2r_0 \), with \( r_0 \) being the typical radius of the molecule. This approximation is valid since the energy of oscillatory degrees of freedom is much bigger than that of rotational degrees of freedom, but much less than the energy of electron transitions:

\[
E_{el} \gg E_{osc} \gg E_{rot}.
\]
So, in a certain range of energies, corresponding to infrared radiation energy, the kinetic energy of molecules is transferred into oscillatory degrees of freedom by means of binary collisions between molecules.

The energy levels of quantum harmonic oscillator, representing the oscillatory degrees of freedom of the molecules, are

\[ E_n = \hbar \omega \left( n + \frac{1}{2} \right), \quad n = 0, 1, \ldots \]  

\[ (14) \]

The state of each molecule in this semi-quantum approximation is given by three variables \((X, P, n)\) – position, momentum and excitation number. The rotations are ignored in this approximation \[(13)\]. The gas is assumed to be homogeneous (to be in a constant force field), therefore the total momentum is conserved in each binary collision, the energy can be transferred to the internal degrees of freedom only by quanta \(\Delta E = \hbar \omega\), but not in a continuous manner. To make the model consistent we assume the oscillator degrees of freedom to be in thermodynamic equilibrium with radiation at temperature \(T\).

Taking into account that in quantum description \((2)\) the density matrix can be cast in terms of the Wigner functions, we can derive the kinetic equation for the probability density functions \(f_n(X, P, t)\) with the initial condition \(f_{n>0}(X, P, 0) = 0\). The causality condition “the coarse acts first” will manifest itself in the restriction that the energy transfer from the macroscopic \((X, P)\) degrees of freedom to the microscopic \(n\) is allowed, while inverse is not: the excess of energy is relaxed into radiation only.

Let us denote the momenta of two colliding molecules (in centre mass system) before the collision as \(P\) and \(P_1\), and \(P'\) and \(P_1'\) after collision, respectively. The momentum and energy conservation laws for binary collision imply

\[ P + P_1 = P' + P_1' \]

\[ \frac{P^2}{2m} + \frac{P_1^2}{2m} + \hbar \omega (n + n_1) = \frac{P'^2}{2m} + \frac{P_1'^2}{2m} + \hbar \omega (n' + n_1'). \]  

\[ (15) \]

As a simplest model the assume the probability of transfer of \(N\) quanta of energy into internal degrees of freedom is proportional to the number of means \(g(N)\) this energy can be distributed between two oscillators:

\[ P(\Delta Q) = \frac{\sum_{N=0}^{N_{\max}} g(N)\delta(\Delta Q - \Delta E_N)}{\sum_{N=0}^{N_{\max}} g(N)}, \quad g(N) = N + 1, \quad \Delta E_N = \hbar \omega N. \]  

\[ (16) \]

The sums in \((16)\) should be bounded by some reasonable integer \(N_{\max} > 0\), which guaranties the condition \((13)\) holds.

The collision integral for our model, \(i.e.\) the change of particle density per unit of phase
space volume, is given by

\[ I_{\text{col}} = \int d\Gamma_1 d\Gamma' d\Gamma'_1 w'(f' f'_1 P(-\Delta Q) - f f_1 P(\Delta Q)), \]

\[ d\Gamma = \frac{dX dP}{(2\pi \hbar)^3}, \]

\[ w' \equiv w'(P', P'_1 \rightarrow P, P_1) \sim \delta(P' + P'_1 - P - P_1), \]

\[ f' \equiv f_n'(X', P', t), \]

\[ \Delta Q = \frac{P^2}{2m} + \frac{P_1^2}{2m} - \frac{P'^2}{2m} - \frac{P'_1^2}{2m}. \]  

(17)

The detailed balance principle does not hold for the kinetic equation

\[ \frac{\partial f_n(X, P, t)}{\partial t} + F \cdot \frac{\partial f_n(X, P, t)}{\partial P} + \frac{P}{m} \cdot \frac{\partial f_n(X, P, t)}{\partial X} + \sum_l \kappa_{nl} f_l(X, P, t) = I_{\text{col}}[f] \]  

(18)

for \( P(\Delta Q) \neq P(-\Delta Q) \). The coefficients \( \kappa_{nl} \) account for the interaction of the internal degrees of freedom with radiation.

If the internal degrees of freedom, i.e. the oscillators \((14)\), are in thermodynamic equilibrium with radiation at temperature \( T \), the ratios of the energy level populations are given by

\[ \frac{n_j}{n_k} = \exp\left(-\frac{E_j - E_k}{k_B T}\right), \]

(19)

where \( n_j = \int f_j(X, P, t) d\Gamma \), \( k_B \) – is the Boltzmann constant; for definiteness we assume \( E_j > E_k \). In thermodynamic equilibrium the transition rate from \( j \) to \( k \) is equal to that from \( k \) to \( j \). Since the population of each energy level is kept stationary

\[ \frac{dn_j}{dt} = k_{jk} n_k - k_{kj} n_j = 0, \quad k_{kj} = k_{jk}, \]

(20)

where the first term stands for the excitations \( k \rightarrow j \) and the second – for relaxations \( j \rightarrow k \).

For molecular oscillators the typical frequencies are infrared \( \omega_{jk} \sim 10^{14} \text{sec}^{-1} \). In dipole approximation (see e.g. \([15]\))

\[ k_{jk} = \frac{4\omega_{jk}^3 d_{jk}^2}{3\hbar c^3} \cdot \frac{1}{\exp\left(\frac{\hbar \omega_{jk}}{k_B T}\right) - 1}, \]

(21)

where \( d_{jk} \) is the matrix element of dipole moment operator for the \( j \rightarrow k \) transition. For molecular oscillators the equilibrium transition rate \((21)\) has the order of magnitude \( 10^2 \text{sec}^{-1} \).

For our case of the relaxation of the kinetic energy of macroscopic degrees of freedom into the microscopic oscillators the spontaneous and stimulated emission is of paramount importance. Spontaneous emission rate \( A_{kj} \) is the probability of downward transition \( j \rightarrow k \),
extra to the equilibrium one $k_{kj}$ \(^{(20)}\). In thermodynamic equilibrium the total numbers of upward and downward transitions are equal

\[ k_{jk} n_k = (k_{kj} + A_{kj}) n_j \]  \(^{(22)}\)

from where, with the symmetry relation $k_{kj} = k_{kj}$ and the equilibrium populations \(^{(19)}\), the spontaneous emission rate is found to be

\[ A_{jk} = \frac{4 \omega_{jk}^3 q_{jk}^2}{3 \hbar c^3}. \]  \(^{(23)}\)

For the low temperatures, $\hbar \omega_{jk} \gg k_B T$, the spontaneous emission dominates over the equilibrium transitions

\[ A_{jk} \gg k_{jk}. \]

For typical molecular frequencies the order of magnitude of the spontaneous emission rate is as high as $A_{jk} \sim 40 \text{sec}^{-1}$ \cite{15}.

If the time before collisions is much less than spontaneous emission time

\[ \tau_{col} \ll \frac{1}{A_{kj}}, \]

which is often so in molecular collisions, than the macroscopic collision plays the role of the measuring device with respect to quantum oscillator degrees of freedom, i.e. collisions force the spontaneous emission – that is they result in stimulated emission.

The direct, i.e. the photon-less, energy transfer of the excitation energies of colliding molecules into their kinetic energy seems to be impossible. If the molecules are in excited state $j$ and during the collision they relax to the lower energy states $k$ the energy $E_j - E_k$ of the molecules is released in the form of photons with frequencies

\[ \omega_{jk} = \frac{E_j - E_k}{\hbar} \]

and the momentum

\[ p_{jk} = \frac{\omega_{jk}}{c} = \frac{E_j - E_k}{c}, \]

see Fig. 3. Due to the conservation of total momentum, the momentum of each molecule is changed by $-p_{jk}$, and its energy is increased by

\[ \Delta E \approx \frac{p_{jk}^2}{2m} \]

(in non-relativistic approximation, since momentum transfer is small).

Suppose now, the photons are virtual, rather than real. If so, the photon emitted by molecule 1 is absorbed by the molecule 2, and drives it back to the excited state $j$; the
photon emitted by the molecule 2 is absorbed by the molecule 1 and drives it back to the excited state \( j \). In such a way we have increased the kinetic energy of colliding molecules without changing their internal states. This is a kind of *perpetum mobile* and is therefore forbidden. In the language of hierarchic state vectors (8) such process of energy transfer from \( |\phi^{\alpha}\rangle \) to \( |\phi^{\alpha-1}\rangle \) is prohibited by the operator ordering rule “the coarse (\( \alpha - 1 \)) acts first”.

Similarly, the molecules in Fig. 3 may be two mesons in excited states. In that case the quark confinement prohibits the transfer of internal excitation energy into the meson kinetic energy.

## 4 Oscillator toy model

In previous section we considered a gas of molecules where the kinetic energy of colliding particles is redistributed into internal excitation energy of particles by means of inelastic collisions. The particle motion in phase space was described classically, but the internal degrees of freedom were treated as quantum oscillators. It is possible to construct a toy hierarchic model treating where all degrees of freedom are quantized.

Let us consider a system of equally spaced particles of mass \( m_0 \) located at \( x = s_0^0, s_1^0, s_2, \ldots \), such that each \( (2i) \)-th particle is connected to its neighbour \( (2i + 1) \)-particle by a harmonic potential of rigidity \( k_0 \). The hierarchic structure is constructed in a way that two “atomic” particles. \( (2i, 2i + 1) \), form the \( i \)-th molecule of mass \( m_1 = 2m_0 \); the molecules, in their turn interact to each other in the same hierarchic way as atoms, but with different rigidity constant \( k_1 \), see Fig. 4. The Hamiltonian of the hierarchic two-level system shown in Fig. 4 has the form

\[
H = \frac{m_0}{2} \sum_{i=0}^{3} \left( \dot{s}_i^0 \right)^2 + \frac{k_0}{2} \sum_{i=0}^{1} \left( \dot{d}_i^1 \right)^2 + \frac{k_1}{2} \sum_{i=0}^{0} \left( \dot{d}_i^2 \right)^2 ,
\]

where we have introduced the hierarchic centre mass coordinates

\[
s_{i+1}^j = \frac{s_{2i}^j + s_{2i+1}^j}{2}
\]

and the displacements

\[
d_{i+1}^j = s_{2i}^j - s_{2i+1}^j;
\]

Figure 3: Simultaneous energy relaxation by two molecules in a binary collision
so that the inverse transform is

\[ s^j_{2i} = s^{j+1}_i + \frac{d^{j+1}_i}{2}, \quad s^j_{2i+1} = s^{j+1}_i - \frac{d^{j+1}_i}{2}. \]  

(27)

The straightforward algebra gives

\[
H = m_0 \sum_{i=0}^1 \left( \dot{s}^1_i \right)^2 + m_0 \sum_{i=0}^1 \left( \dot{d}^1_i \right)^2 + k_0 \sum_{i=0}^1 \left( d^1_i \right)^2 + k_1 \sum_{i=0}^0 \left( d^2_i \right)^2,
\]

or, after simplification,

\[
H = m_0 \left[ \left( \dot{s}_0^2 + \frac{\dot{d}_0^2}{2} \right)^2 + \left( \dot{s}_0^1 + \frac{\dot{d}_0^1}{2} \right)^2 \right] + k_1 \left( d_0^2 \right)^2 + m_0 \sum_{i=0}^1 \left( \dot{d}^1_i \right)^2 + k_0 \sum_{i=0}^1 \left( d^1_i \right)^2.
\]

Since \( \dot{s}_0^2 = 0 \) because of the zero total momentum, the final equation for the Hamiltonian is a sum of two independent oscillators, belonging to “0” and “1” scales, respectively

\[
H = m_0 \left[ \left( \dot{s}_0^2 + \frac{\dot{d}_0^2}{2} \right)^2 + \left( \dot{s}_0^1 + \frac{\dot{d}_0^1}{2} \right)^2 \right] + \frac{k_1}{2} \left( d_0^2 \right)^2 + \frac{m_0}{4} \sum_{i=0}^1 \left( \dot{d}^1_i \right)^2 + \frac{k_0}{2} \sum_{i=0}^1 \left( d^1_i \right)^2.
\]

(28)

For each level of the hierarchy it is possible to substitute creation and annihilation operators \( a^\dagger, a \) and the number of excitation. In this way the scattering of two molecules described by \( d_0^2 \) coordinate will result in relaxation of the excitation and redistribution of this energy into the modes \( d_0^1, d_1^1 \), so that

\[
\hbar \omega_2 \Delta n_0^2 = \hbar \omega_1 (\Delta n_0^1 + \Delta n_1^1).
\]

(29)

In classical toy models, like the Toda chains of oscillators there is no such independence of oscillations of different scales as in our model considered above. If the particles are
allowed to interact with all the neighbours, including that in the next block, the interaction Hamiltonian will have an extra term. Say, for the system shown in Fig. 4 this will be the term

\[ H_{ib} = \frac{\tilde{k}_0}{2} \sum_i (s_{2i+1}^0 - s_{2i+2}^0)^2. \]

For the first two blocks this gives the contribution

\[ \Delta H_{ib} = \frac{\tilde{k}_0}{2} (s_1^0 - s_2^0)^2 = \frac{\tilde{k}_0}{2} \left( d_0^2 - \frac{d_0^2 + d_1^2}{2} \right)^2, \]

which produces the inter-scale energy transfer.

The Hamiltonian (28) does not contain any cross-scale interaction terms. Therefore the equation (29) is just a formal equation for energy conservation without any specification of the processes of energy exchange. If the cross-scale interaction (30) is introduced, the free oscillators can be cast in terms of creation and annihilation operators \( a^\dagger, a \) and \( A^\dagger, A \)

\[ d_0^2 = \sqrt{\frac{\hbar}{\sqrt{m_0k_0}}} \frac{A + A^\dagger}{2}, \quad d_i^1 = \sqrt{\frac{\hbar}{\sqrt{\mu_0k_0}}} \frac{a_i + a_i^\dagger}{2}, \quad i = 0, 1, \]

where \( \mu_0 = m_0/2 \). The operators \( a \) and \( a^\dagger \) are related to the normal modes \( \Omega = \sqrt{k_1/m_0}, \omega = \sqrt{k_0/\mu_0} \) coordinate and momenta

\[ d_i^1 = \sqrt{\frac{\hbar}{\mu_0\omega}} \frac{a_i + a_i^\dagger}{2}, \quad p_i^1 = \sqrt{\hbar\mu_0\omega} \frac{a_i - a_i^\dagger}{2}. \]

The inter-scale interaction Hamiltonian (30) in second quantization formalism has the form

\[ H_{ib} = \frac{\tilde{k}_0\hbar}{2} \left[ \frac{1}{(k_1m_0)^{1/4}} \frac{A + A^\dagger}{2} - \frac{1}{2} \frac{1}{(k_0\mu_0)^{1/4}} \sum_{i=0}^1 \frac{a_i + a_i^\dagger}{2} \right]^2. \]

If we assume the scale ordering – an analog of \( T \)-ordering, – then only the terms of the form \( a_i^\dagger A \) will contribute to cross-scale interaction.

5 Conclusion

In classical theory of molecular gases the kinetic energy of molecules can be transformed into the heat energy of their internal degrees of freedom and vice versa: the energy accumulated in the internal degrees of freedom can be relaxed into kinetic energy of scattering particles, see Fig 5. In purely quantum case, when momentum and position become operators, the
Figure 5: Classical accumulation of mechanic energy: the potential energy of contracted springs of two oscillators can be relaxed in the form of kinetic energy of scattered oscillators.

Direct energy transfer from internal (microscopic) to macroscopic degrees of freedom seems to be impossible.

The mathematical reason for that is the need to order the operators related the part and the whole (the micro and the macro) degrees of freedom. Apart from the requirement of finiteness, which is not discussed in this paper, this need stems from the fact that the state of the part cannot be affected unless the state of the whole is affected (measured) first. This is axiomatized by the operator ordering rule “the coarse acts first” \[2\]. The set of axioms with two partial ordering operations \[1\], aimed for the development of quantum gravity theory, may or may not be self-evident at common scales \(l \gg l_{Pl}\). However, there exists a simple example illustrating the impossibility of the process, shown in Fig. 5 for a pair of quantum oscillators.

Indeed, in classical system the potential energy is accumulated into the springs by decreasing the size of oscillators, the relaxation of potential energy into kinetic energy of scattered particles goes through the expansion – the increase of oscillator sizes. For the quantum oscillator in the \(n\)-th excited state the mean squared size is

\[
\langle \xi^2 \rangle_n = n + \frac{1}{2}, \quad E_n = \hbar \omega \langle \xi^2 \rangle_n.
\]

Thus the relaxation from high to low energy level results in “contraction” of oscillator, rather than in expansion. So, no scattering takes place unless an extra momentum is injected.

In the final end the axiomatizing of operator ordering used above provides a reformulation of the second thermodynamics’s law on the microscopic level. For a microscopic system, described classically, the heating of internal degrees of freedom cannot result in macroscopic movement if it is accompanied by the decrease of entropy. In quantum case the decrease of entropy can be prevented by operator ordering.

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Axiomatic structure of causal sites

A causal site is a set of “regions” with two binary relations denoted $\subseteq$ and $\prec$ satisfying the axioms:

1. $\forall A, B, C$
   (a) $A \subseteq B \land B \subseteq C \Rightarrow A \subseteq C$,  
   (b) $A \subseteq A$,  
   (c) $A \subseteq B \land B \subseteq A \Rightarrow A = B$.
2. The partial order $\subseteq$ has a minimum element $\phi$, called an empty region.
3. The partial order $\subseteq$ has unions: $\forall A, B \exists A \cup B$, so that
   (a) $A \subseteq A \cup B \land B \subseteq A \cup B$,  
   (b) $A \subseteq C \land B \subseteq C \Rightarrow A \cup B \subseteq C$.
4. The partial order $\prec$ induces a strict partial order on the nonempty regions:
   (a) $A \prec B \land B \prec C \Rightarrow A \prec C$,  
   (b) $A \not\prec A$.
5. $\forall A, B, C$
   (a) $A \subseteq B \land B \prec C \Rightarrow A \prec C$,  
   (b) $A \subseteq B \land C \prec B \Rightarrow C \prec A$,  
   (c) $A \prec C \land B \prec C \Rightarrow A \cup B \prec C$.
6. $\forall A, B \exists B_A$, cutting of $A$ by $B$, so that
   (a) $B_A \prec A \land B_A \subseteq B$,  
   (b) $D \prec A \land D \subseteq B \Rightarrow D \subseteq B_A$.
7. If $A \prec C$ are nonempty regions, and $\exists D : A \prec D \prec C$, then $\exists B$ complete with respect to $A \prec C$
   
   Def.: If $A \prec B \prec C$, then $B$ is said to be complete with respect to a causal pair $A \prec C$, if any causal path from $A$ to $C$ can be refined to a causal path from $A$ to $C$, on of whose members is contained in $B$.

   Def.: A causal path $P$ is a sequence of nonempty regions $A_1 \prec A_2 \prec \ldots \prec A_n$.

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