Statistical mechanics of non-hamiltonian systems: Traffic flow

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Abstract: Statistical mechanics of a small system of cars on a single-lane road is developed. The system is not characterized by a Hamiltonian but by a conditional probability of a velocity of a car for the given velocity and distance of the car ahead. Distribution of car velocities for various densities of a group of cars are derived as well as probabilities of density fluctuations of the group for different velocities. For high braking abilities of cars free-flow and congested phases are found. Platoons of cars are formed for system of cars with inefficient brakes. A first order phase transition between free-flow and congested phase is suggested.

Keywords: non-Hamiltonian systems, microcanonical, canonical, traffic flow

PACS: 05.20.Gg, 05.50.+g, 05.60.Cd, 89.40.Bb

1 Introduction

In classical equilibrium statistical mechanics Hamiltonian plays a decisive role in determination of statistical properties of a system of interacting particles. In most cases it represents energy as a function of momenta and spatial coordinates of the particles. The system may be treated microcanonically or canonically. In a microcanonical ensemble all the states are equally probable and the number of states of a given energy determines the entropy of the system. In a canonical ensemble the probability of states of a subsystem are proportional to \( e^{-\beta E_s} \), where \( \beta \) is the inverse temperature and \( E_s \) is the energy of the subsystem. The sum of probabilities of all the states is called partition function and determines thermodynamic properties of the system. The subsystem may be taken as small as one particle, and the expression \( e^{-\beta (E_i(q_i,r_i)+E(C_{i,j}))} \) determines the conditional probability that a particle has momentum \( q_i \), coordinate \( r_i \) if its energy is \( E_i \) and interaction energy with neighbouring particles of generalized coordinates \( C_{i,j} \) is \( E_{i,j}(C_{i,j}) \).

In our approach, we do not start from the Hamiltonian of a system of particles, which we is not even introduced, but from the knowledge of conditional probabilities of generalized coordinates of each particle. It is assumed that the conditional probability depends only on the state of the neighbouring particles, and it can be determined from the behaviour of a small system experimentally.

This non-Hamiltonian approach is applied to a system of cars on a single-lane road while the behaviour of the cars is described by conditional probabilities of the velocity of each car depending on the distance and velocity of the car ahead.

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Traffic flow of a system of identical cars on a single-lane road has been intensively studied in the recent decade using dynamical or kinetic description of car behaviour [1,2]. The models used were continuous (fluid dynamical models), car-following models [3], or discrete particle hopping models related to cellular automaton models with stochastic behaviour [4].

In the approach of Mahnke et al. [5] the group of cars is represented by a grandcanonical ensemble, number of cars in which is not fixed, and its chemical potential is a function of parameters of a master equation.

In the last years we could observe a revival of the microcanonical approach to the problems of statistical mechanics [6–10]. One of the reasons for that was identification of the region where the entropy of a finite system is convex, instead of the standard concave shape of it, with a point or line in the phase space where the first-order phase transition in the corresponding infinite system takes place. As the number of observed cars in normal traffic is not too large, the techniques developed in statistical physics for small systems are convenient in this case. The term “phase transition” in this paper is used in the sense of the above-cited works.

Statistical mechanics of 1D non-Hamiltonian models is developed in Section 2. In Section 3 a traffic model inspired by the above-mentioned car following and discrete particle hopping models is introduced. In Sections 3 and 4 formulas for microcanonical and canonical treatment of our model are derived. The results for a subsystem of 5 cars are presented in Section 5.

2 Statistical mechanics of 1D non-Hamiltonian systems

A single-lane road represents a one-dimensional system so we shall further confine ourselves to 1D systems of particles with nearest neighbour interactions. The conditional probability that the particle has velocity \( v_i \) and coordinate \( r_i \) while the velocity and coordinate of its neighbouring particles are \( v_{i+1} \) and \( r_{i+1} \), respectively, will be denoted as

\[
p(v_i, r_i | v_{i+1}, r_{i+1}) \equiv p(v_i, r_i, v_{i+1}, r_{i+1})/p(v_{i-1}, r_{i-1}, v_i, r_i)
\]

and taken as an input to the theory. The probability of velocities and coordinates of all \( n \) particles of the system can be easily calculated from slightly different conditional probabilities

\[
p(v_1, r_1, \ldots, v_n, r_n) = p(v_1, r_1 | v_2, r_2)p(v_2, r_2 | v_3, r_3) \ldots p(v_{n-1}, r_{n-1} | v_n, r_n)p(v_n, r_n)
\]

where \( p(v_i, r_i | v_{i+1}, r_{i+1}) = p(v_i, r_i, v_{i+1}, r_{i+1})/p(v_{i+1}, r_{i+1}) \).

Probabilities \( p(v_i, r_i | v_{i+1}, r_{i+1}) \) are unknown, but they are closely related to the probabilities \( p(v_i, r_i | v_{i-1}, r_{i-1}, v_{i+1}, r_{i+1}) \) characterizing our system. They can be calculated from the following system of equations:

\[
p(v_i, r_i | v_{i+1}, r_{i+1}) = \sum_{v_{i-1}, r_{i-1}} p(v_{i-1}, r_{i-1} | v_{i+1}, r_{i+1})p(v_i, r_i | v_{i-1}, r_{i-1}, v_{i+1}, r_{i+1})
\]

\[
p(v_{i-1}, r_{i-1} | v_{i+1}, r_{i+1}) = \sum_{v_i, r_i} p(v_{i-1}, r_{i-1} | v_i, r_i)p(v_i, r_i | v_{i+1}, r_{i+1}).
\]

\( p(v, r) \) in a homogeneous system can be obtained by summation of \( p(v_1, r_1, \ldots, v_n, r_n) \) over all coordinates of the system but one. In a finite system \( p(v_n, r_n) \) represents a boundary
condition, which in our case is the probability of the velocity and coordinate of the first particle of a large reservoir. The spatial coordinates of the reservoir particles satisfy \( r_m > r_{n-1} \).

In the system of cars on a single-lane road the driver behaviour is assumed to depend only on the previous car. In such a system the conditional probability of velocity and coordinate of particle 1 depends only on the velocity and coordinate of particle 2 ahead of it: \( p \equiv p(v_1, r_1| v_2, r_2) \). Then the equations (3) are superfluous and the probabilities of the whole system are given directly by (2). These probabilities will be used for calculations of the sum of probabilities of the system as a function of length and total velocity (sum of velocities of all cars of the system).

The terms microcanonical and canonical will be used in the case of non-Hamiltonian systems as well, but they will be related rather to the \textit{length} of the system than to its \textit{energy}, which is not introduced.

In the canonical ensemble of a Hamiltonian system the usually calculated quantity is the partition function, which is sum of the probabilities of all possible states of the system. In the microcanonical ensemble, the probability to find the system in a state is same for all of them. Logarithm of their sum for some fixed quantities is called entropy. In our non-Hamiltonian approach, we calculate sum of the probabilities of states (SPS) as a function of length of the system and sum of velocities of the particles.

In the microcanonical approach the length of a group of cars is fixed, and it is influenced by the reservoir only through boundary conditions. The properties of the system are given by the sum of the probabilities of states with the same total velocity.

In the canonical approach the group of cars represents only a subsystem of a large system whose remaining part is a reservoir. The length of the whole system is constant, and the length of the subsystem is changed only at the expense of the length of the reservoir. The properties of the subsystem are given by sum of the probabilities of states of the \textit{whole system} having the same total velocity of the cars in the \textit{subsystem}. The canonical approach is able to describe fluctuations of the length of the subsystem around its mean value.

3 Model

The cars are further represented by dimensionless points moving on a discrete one-dimensional lattice and are characterized by 2 quantities: discrete velocity \( v_i \) in the interval \((0, v_{\text{max}})\) and a discrete coordinate (site number) \( x_i \in [1, X - 1] \). \( v_{\text{max}} \) is the maximum velocity given by the construction of the car, and \( X \) is the length of the observed group (subsystem) of cars. The coordinate of each car is measured with respect to the last car of the group. Its coordinate is always 0, i.e., the origin of the coordinate system is moving with it. As the length of the group is \( X \), the coordinate of the last car of the group ahead is also \( X \). Number of cars in the group is \( N \). (The lattice constant is related to the car length). Car velocities and coordinates acquire only integer values.

Kinetics of the system of cars is given by reaction of each driver on the car ahead moving with velocity \( v_{i+1} \) at the distance \( x_{i,i+1} \). As the driver directly influences only velocity of his car his reaction is characterized by a conditional probability of a car velocity \( v_i \) parametrized by velocity and distance of the car ahead: \( p \equiv p(v_i| x_{i,i+1}, v_{i+1}) \). The probability could be found experimentally by long observation of two cars at all possible
situations. Since such data are not available yet, the probability is calculated from a simple model behaviour of a driver.

The probability distribution is assumed to be peaked around an optimal velocity $v_{\text{opt}}$, which is further chosen as 90% of maximal safe velocity $v_m$. The maximal safe velocity is determined from the requirement that two neighbouring cars, which start to decelerate at the same time with the same deceleration rate $a$, would stop without crash. Moreover, $v_m$ must not be greater than the maximum possible velocity of the car $v_{\text{max}}$, i.e., for every car

$$v_{\text{opt}}(v_2, x_{1,2}) = 0.9 v_m(v_2, x_{1,2}),$$

$$v_m(v_2, x_{1,2}) = \begin{cases} -a\tau + \sqrt{(a\tau)^2 + 2ax_{1,2} + v_2^2} & \text{if } v_m \leq v_{\text{max}} \\ v_{\text{max}} & \text{if } v_m > v_{\text{max}} \end{cases}$$

where $x_{1,2}$ and $v_2$ are the distance (headway) and velocity of the car ahead, respectively, $\tau$ is the reaction time of the driver of the car 1. (Problem of non-zero reaction time is discussed in more detail in [11].) As we use only integer values of velocities, the nearest integer value to $v_{\text{opt}}$ from (1) is taken for the actual optimal velocity in our further calculations. For very high densities, when discreteness of the lattice is not negligible, another condition $v_1 < v_2 + x_{1,2}$ must be imposed.

The way of driving of the observed drivers is characterized by distribution of probabilities of car velocities around the optimal velocity. Here we use an extremely simple distribution, in which the probability of optimal velocity is $p_0$, the probabilities of the velocities $v_{\text{opt}} \pm 1$ are $p_1$, while the probability of the car to have any other permitted velocity is $p_2$. The values of the probabilities for velocities higher then the maximal safe velocity are equal to 0. The sum of all probabilities for each car is equal to 1. The parameters $p_0, p_1$ and $p_2$ are the same for every car, and the distribution depends on the headway only by means of the value of optimal velocity.

### 3 Microcanonical description

In the microcanonical approach only such groups of $N$ cars, which length is $X$ and sum of their velocities is $V$, are studied. These groups of cars are not totally isolated. They are influenced by the velocity distribution of the car ahead of them with spatial coordinate $X$. The probability distribution of each car is given by the rule above as a function of headway and the velocity of the car ahead, while the distances between them are arbitrary and limited only by the length of the group.

The sum of probabilities of states (SPS) with total velocity $V$ of a group of $N$ cars and length $X$ will be denoted as $W(V, X)$. It can be calculated, using (2), recurrently

$$W_1(V_1, X_1 v_2) = p(V_1 | X_1, v_2)$$

$$:$$

$$W_i(V_i, X_i; v_{i+1}) = \sum_{v_i, x_{i, i+1}} W_{i-1}(V_i - v_i, X_i - x_{i, i+1}; v_i)p(v_i | x_{i, i+1}, v_{i+1})$$

for $i = 2, N - 1$

$$:$$

(4)
\[
W_N(V, X; v_{N+1}) = \\
= \sum_{v_N, x_{N,N+1}} W_{N-1}(V - v_N, X - x_{N,N+1}; v_N)p(v_N|x_{N,N+1}, v_{N+1})
\]

\[
W(V, X) = \sum_{v_{N+1}} W_N(V, X; v_{N+1})p(v_{N+1})
\]

where \(0 \leq v_j \leq v_{\text{max}}, 0 \leq V_j \leq j v_{\text{max}}, j \leq x_{j,j+1}, X_j \leq X - j\). Probability \(p(v_{N+1})\) in the last line of (4) is the velocity probability of the last car of a large group ahead (reservoir) of the studied group with the same car density.

SPS in the reservoir of length \(L_r\), number of cars \(N_r\), with the density \(\frac{N_r}{L_r} = \frac{N}{X}\), and fixed velocity of the last car \(v_{N+1}\) is

\[
W_r(v_{N+1}, L_r) = \sum_{x_{N+2}, \ldots, x_{N+N_r}} \prod_{i=N+1}^{N+N_r} p_i(v_i|x_{i,i+1}, v_{i+1})\delta_{L_r}\sum x_{i,i+1} (5)
\]

It depends, in principle, on the velocity of the first car of the reservoir, but numerical calculations show that for large \(N_r\) this dependence is negligible. The probability \(p(v_{N+1})\) is the normalized SPS

\[
p(v_{N+1}) = W_r(v_{N+1}, L_r) / \sum_{v_{N+1}} W_r(v_{N+1}, L_r) (6)
\]

The quantity \(W(V, X)\) in (4) comprises the probability that the sum of velocities of the cars in the group is \(V\) and the number of possible configurations of occupation of \(X\) sites by \(N\) cars. It is, in fact, a product of the probability and number of configurations \(\Omega\)

\[
W(V, X) = \frac{W(V, X)}{\sum_{V} W(V, X)} \cdot \sum_{V} W(V, X) \equiv P(V, X) \cdot \Omega(X). (7)
\]

Since for the fixed length of the subsystem, \(\Omega(X)\) is constant, only the normalized probability \(P(V, X)\) is presented in Results.

In the microcanonical approach only subsystems of cars with the constant density, the same as is the mean density of the whole system, are studied. To take into account also the density fluctuations, it is more convenient to use the canonical description with variable density of the subsystem due to its variable length.

### 4 Canonical description

In canonical approach the length of the subsystem varies, only the length of the whole system, subsystem + reservoir is fixed. The number of cars in the subsystem and in the reservoir remains constant, so the density of cars varies with varying length of the groups. Our canonical description differs from the grandcanonical approach of Mahnke et al. [5] where the density of the subsystem changes due to exchange of cars between the subsystem and reservoir.
In statistical mechanics the properties of a reservoir are usually not calculated, only the values of derivatives of its entropy (logarithm of number of states) with respect to the quantities, which are fixed in the whole system, are assumed to be known. They are, e.g., temperature, chemical potential, etc. Similarly, in our canonical description of the system of cars, a pressure of reservoir exerted on the subsystem could be introduced. Nevertheless, this quantity cannot be directly measured, and it would depend on the velocity of the last car of the reservoir, so we prefer a direct calculation of number of states of a large enough reservoir for given velocity of the last car and length of the reservoir.

The length of the system $L_s$ is the sum of the length of the subsystem and reservoir $X + L_r$. The number of cars in the subsystem and reservoir are fixed and denoted as $N$ and $N_r$, respectively. If $X \ll L_r$ and $N \ll N_r$, the properties of the subsystem does not depend on velocity of the first car in the reservoir.

SPS of the reservoir at given velocity of the last car is calculated according to (5). SPS of the whole system at given total velocity of the subsystem $V$ and its length $X$ can be obtained by the same way as in the microcanonical case, only in the last term in (3) – the probability of the velocity of the last reservoir car $p(v_{n+1})$ – is replaced by SPS of the reservoir. Last line of (3) now reads

$$W(V, X) = \sum_{v_{n+1}} W_n(V, X; v_{n+1}) W_r(v_{n+1}, L_s - X).$$

The mean density of the subsystem $N/\langle X \rangle$ is equal to the density of the whole system $(N + N_r)/L_s$.

The main difference between the microcanonical and canonical treatment is that in the first case only number of states of the subsystem is calculated while in the latter case the properties of the subsystem are given by the number of states of the whole system. In the microcanonical approach the reservoir is used only for calculation of boundary condition – probability distribution of the last car of the subsystem.

5 Results and discussion

The velocities and positions of cars are described by discrete variables in our model. Changing the values of its parameters, we can observe two different types of behaviour. In the first one, for high deceleration rate $a$ and low densities, the system behaves like a continuous one; in the SPS and probability of total velocity the underlying discrete structure of velocities is not seen. At small $a$ and high densities, total velocities of the system, which are integer multiples of number of particles, are more probable then the others. Platoons of cars of the same velocities are formed. This regime reminds a ferromagnetic Potts model where the total magnetization of the system points in many different directions of the space.

In all our calculations, car velocity acquires 21 values $v_i = i, i = 0, 20$. The probability of a car to move with a velocity $v_i$ depends on the velocity and distance of the car ahead by means of optimal velocity $v_{opt}(v, x)$. As stated above it acquires 3 values $p_0, p_1$ and $p_2$.

In the present calculations $p_1/p_0$ is fixed to 0.3 and $p_2$ is chosen for the free parameter, and the normalization condition is used.
Fig. 1. Probability of the total velocity of a microcanonical ensemble of 5 cars as a function of its total velocity $V$ and length $X$ for $a = 4.0$, $p_2/p_0 = 0.025$, $\tau = 0$. The density of the system varies from 0.033 to 1.

The position of a car with respect to the first one may be an integer between 1, and $X - 1$ if the site is not occupied by another car. A subsystem of 5 cars as a part of a system of 50 cars is further studied.

The main result of our calculations is the probability of the total velocity $P(V, X)$ of the subsystem as a function of the subsystem length $X$ for fixed number of cars in the microcanonical ensemble and SPS $W(V, X)$ in the canonical case. They are plotted in 3D graphs.

In the microcanonical case the density of the subsystem is the same as the density of the reservoir. The probabilities of the sum of the velocities of 5 cars for lengths of the group from 5 to 150, i.e. for car densities from 1 to 0.033, $a = 4$, $p_2/p_0 = 0.025$, $\tau = 0$ are shown in Fig. 1. This case represents a group of cars with good brakes (large deceleration rate $a$), medium spread of velocities of each car, and zero reaction time of the drivers. For high group length (low density) the cars mostly move freely with optimal velocity, nevertheless due to the car velocity spread, there is a nonzero probability of smaller velocities. With increasing density, number of cars with small velocity increases, and at $X = 52$ the most probable velocity discontinuously drops to a value smaller by 20 units. In analogy with to microcanonical approach to finite systems of statistical mechanics where the entropy is not concave [6], we call this phenomenon first order phase transition. For length of the group $< 30$, the total velocity decreases fast to zero and a jammed traffic is observed. For high densities discontinuous nature of car velocities is manifested, when peaks at multiples of five appear in the diagram. For $X = 5$ ($\rho = 1$) practically all the cars have velocity equal...
Fig. 2. Probability of the total velocity of a microcanonical ensemble of 5 cars as a function of its total velocity $V$ and length $X$ for $a = 4.0$, $p_2/p_0 = 0.015$, $\tau = 0.5$. The density of the system varies from 0.033 to 1.

to zero.

The system of cars may exist in two phases: a fast, free-flow phase and slow, jammed phase. Nevertheless, contrary to the standard models of statistical mechanics, they cannot coexist as a collision between fast and slow group would take place. Thus, the transition from a local maximum to absolute maximum of probability is very improbable, and a strong hysteresis occurs in the system, observed also experimentally [12].

If the reaction time of the drivers is nonzero, the velocity of cars decreases with group length faster, the most probable velocity decreases continuously, and no first order phase transition takes place. The transition between free-flow and jammed phase is continuous and probability of velocities, i.e., entropy as a function of velocities is concave. This case for reaction time $\tau = 0.5$ is shown in Fig. 2.

When the car velocity spread is large, $p_2/p_0 = 0.045$, most of the cars are in the jammed phase, as depicted in Fig. 3. Only a small peak of a free-flow traffic can be seen in the Figure.

For low braking abilities of cars, $a = 0.5$, no free flow, even for density $\rho = 0.033$, low velocity spread $p_2/p_0 = 0.005$, and zero reaction time, exists, as shown in Fig. 4. At high density, there is convenient for them not to brake at all, so that they form platoons in which all the cars have the same velocity – in our case an integer one. This is the reason why in Fig. 4 the most probable total velocities up to $V = 40$ are multiples of five.

In the microcanonical approach the subsystem and the reservoir have the same density. Density fluctuations are described in the canonical approach where the length of the
Fig. 3. Probability of the total velocity of a microcanonical ensemble of 5 cars as a function of its total velocity $V$ and length $X$ for $\alpha = 4.0$, $p_2/p_0 = 0.06$, $\tau = 0$. The density of the system varies from 0.033 to 1.

Fig. 4. Probability of the total velocity of a microcanonical ensemble of 5 cars as a function of its total velocity $V$ and length $X$ for $\alpha = 0.5$, $p_2/p_0 = 0.005$, $\tau = 0$. The density of the system varies from 0.033 to 1.
Fig. 5. SPS of a canonical ensemble of 5 cars as a function of its total velocity $V$ and length $X$ for $a = 4.0, p_2/p_0 = 0.025, \tau = 0$, and mean length $\langle X \rangle = 50$, i.e., mean density $\rho = 0.1$. subsystem changes while the total length of the system remains constant. The probability that the total velocity of the subsystem is $V$ and its length is $X$ in the system with mean density is $(N + N_r)/L_s$ is proportional to $W(V, X)$. It is depicted in Fig. 5 for $a = 4, p_2/p_0 = 0.025, \tau = 0$ and mean length $\langle X \rangle = 50$. Low and high density fluctuation are suppressed due to small number of states of the reservoir and subsystem, respectively.

For inefficient car brakes the platoon structure of is seen also in SPS of a canonical ensemble, but only for high density fluctuations. At low density the probability maxima disappear and the cars may easily change the velocity of the platoon. It is shown in Fig. 6 for $a = 0.5$.

Our results are in qualitative agreement with those obtained from the approach of Nagel and Schreckenberg [4]. As it may be seen from Fig. 1, for low densities the velocity of the cars with increasing density remains constant, i.e., the flow linearly increases. At the density where the confined regime starts, the velocity and flow sharply decreases, and at $\rho = 1$ the flow is practically equal to zero. We have got not only the mean velocity in the system but also distributions of velocities of small groups of cars for each density and probabilities of density fluctuations for various velocities. The distribution is widest near the phase transition point, where very high and very low velocities are equally probable.

A statistical approach to traffic flow was also chosen by Mahnke et al. [5] who, starting from grandcanonical ensemble, introduced thermodynamical potential of standard Hamiltonian statistical mechanics, potential energy of interactions between vehicles, etc. We have developed the statistics of the system in analogy with developing statistical mechanics, starting from a microcanonical ensemble, but now not fixing the energy but other
quantities characterizing the system. The conditional probabilities of car velocities for given headway and velocity of the car ahead were assumed to be known, and probabilities of states differing in other quantities were taken equally probable, satisfying the principle of maximum entropy.

Number of cars on the road is small, much smaller than number of particles in most physical systems studied in statistical mechanics. Therefore it represent a suitable area for application of ideas recently developed for very small physical systems [6-10].

Acknowledgement

We acknowledge support from VEGA grant No. 2/6071/2006.

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