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Application of thermodynamics to driven systems

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Abstract. Application of thermodynamics to driven systems is discussed. As particular examples, simple traffic flow models are considered. On a microscopic level, traffic flow is described by Bando's optimal velocity model in terms of accelerating and decelerating forces. It allows to introduce kinetic, potential, as well as total energy, which is the internal energy of the car system in view of thermodynamics. The latter is not conserved, although it has certain value in any of two possible stationary states corresponding either to fixed point or to limit cycle in the space of headways and velocities. On a mesoscopic level of description, the size n of car cluster is considered as a stochastic variable in master equation. Here $n = 0$ corresponds to the fixed-point solution of the microscopic model, whereas the limit cycle is represented by coexistence of a car cluster with $n > 0$ and free flow phase. The detailed balance holds in a stationary state just like in equilibrium liquid-gas system. It allows to define free energy of the car system and chemical potentials of the coexisting phases, as well as a relaxation to a local or global free energy minimum. In this sense the behaviour of traffic flow can be described by equilibrium thermodynamics. We find, however, that the chemical potential of the cluster phase of traffic flow depends on an outer parameter — the density of cars in the free-flow phase. It allows to distinguish between the traffic flow as a driven system and purely equilibrium systems.

PACS. 05.70.-a Thermodynamics – 05.10.Gg Stochastic analysis methods – 89.40.-a Transportation

1 Introduction

An extension of thermodynamic concepts from equilibrium to nonequilibrium or driven systems is one of the fundamental problems in physics. It refers also to so-called nonphysical systems, like traffic or granular flow, economics, biological systems, etc., where the laws of microscopic interaction and motion differ from those known in physics. Different approaches have been developed till now. In the geometrical formulation of thermodynamics [1], the latter is regarded as a theory arising in the analysis of dynamics. In this concept the equilibrium thermodynamics is represented by a manifold of time-independent equilibrium states, whereas the thermodynamics of driven system is represented by a manifold of slowly evolving states. A k-component system undergoing chemical reaction is considered as an example in [1]. A more widely discussed approach is based on the introduction of entropy [2,3] and usage of the entropy maximization principle in various applications, e.g., linear dissipative driven systems [3] and single-lane traffic [2]. An appropriate definition of temperature is a relevant question when we speak about a nonphysical system. In [2] the temperature T and pressure p of traffic flow have been introduced via derivatives of certain thermodynamic functions, and it has been found that T is negative at typical velocities. In another approach [4] similarities between traffic and granular flow have been discussed proposing two effective temperatures: one characterising fast or single-car dynamics, and another — slow or collective dynamics of traffic flow.

As mentioned in [2], entropy need not occupy a position of primacy in a general theory beyond the classical equilibrium thermodynamics. We have found that in cases where the stationary state of a driven system has the property of detailed balance in a space of suitable stochastic variable, the thermodynamic potential can be easily introduced based on this property in a complete analogy with equilibrium systems. This approach can prove to be useful in many applications due to its relative simplicity. As an example we consider formation of a car cluster in one-lane traffic and show its analogy with the phase separation in supersaturated vapour-liquid system.

The aggregation of particles out of an initially homogeneous situation is well known in physics, as well as in other branches of natural sciences and engineering. The formation of bound states as an aggregation process is related to self-organization phenomena [5–7]. The formation of car clusters (jams) at overcritical densities in traffic flow is an analogous phenomenon in the sense that cars can be

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considered as interacting particles [8–10]. The development of traffic jams in vehicular flow is an everyday example of the occurrence of nucleation and aggregation in a system of many point-like cars. For previous work focusing on the description of jam formation as a nucleation process, see [11–14]. It is related to phase separation and metastability in low-dimensional driven systems, a topic which has attracted much recent interest [15–19]. Metastability and hysteresis effects have been observed in real traffic, see, e.g., [20–26] for discussion of empirical data and the various different modelling approaches.

Here we focus on the application of thermodynamics to such a many-particle system as traffic flow. In a first step we do not consider real traffic with its very complicated behaviour but limit our investigations to simple models of a directional one-lane vehicular flow. We hope this will trigger further development to describe more realistic situations of multi-lane traffic as well as of synchronized flow [24]. We have found certain analogy with physical systems like supersaturated vapour-liquid, although there are also essential differences, since the traffic flow is a driven system. We would like to outline some basic ideas and concepts developed throughout the paper.

1. On a microscopic level traffic flow can be described by Bando's optimal velocity model. In this case the equations of motion can be written as Newton's law with accelerating and decelerating forces and one can define the potential V and the kinetic T energy of the car system, as well as the total energy $E = T + V$. The latter one has a thermodynamic interpretation as $\langle E \rangle = U$, where U is the internal energy of the system.
2. Traffic flow is a dissipative system of driven or active particles. It means that the total energy is not conserved, but we have an energy balance equation
$$\frac{dE}{dt} + \Phi = 0$$
with the energy flux Φ following from the equations of motion and consisting of dissipation (due to friction) and energy input (due to burning of petrol).
3. In the long-time limit the many-car system tends to certain stationary state. In the microscopic description it is either the fixed-point or the limit cycle in the phase space of velocities and headways depending on the overall car density and control parameters. The stationary state is characterised by certain internal energy.
4. On a mesoscopic level traffic flow can be described by stochastic master equation, where stochastic variable is the number of congested cars n, i.e., the size of car cluster. In this case the fixed-point solution corresponds to $n = 0$, and the limit cycle — to coexistence of a car cluster with $n > 0$ and free flow phase.
5. In the space of cluster size, the detailed balance holds for the stationary solution just like in equilibrium physical systems. It allows to describe various properties of the stationary state by equilibrium thermodynamics. In particular, we calculate free energy of the system and chemical potentials of coexisting phases in a complete analogy with the known treatment for a supersaturated liquid-gas system.
6. In distinction to equilibrium systems, the chemical potential of the cluster phase of traffic flow is not an internal property of this phase, since it depends on an outer parameter — the density of cars in the free-flow phase. It allows to distinguish between the traffic flow as a driven system and purely equilibrium systems.

2 Microscopic optimal velocity model of traffic flow

Traffic flow can be viewed as a random dynamical system [27,28] of active or intelligent particles [29–31]. To describe it on a microscopic level, here we use a simple version of Bando's optimal velocity (OV) model for point-like cars moving on a one-lane road with periodic boundary conditions. The model is defined by the following set of equations [32–34]

$$\frac{dv_i}{dt} = \frac{1}{\tau}\left(v_{opt}(\Delta x_i) - v_i\right), \tag{1}$$

$$\frac{dx_i}{dt} = v_i, \tag{2}$$

where the coordinate $x_i(t)$ as well as the velocity $v_i(t)$ of each car $i = 1, \ldots, N$ at every time moment t can be calculated out of the initial values by integrating the coupled equations of motion. Here

$$v_{opt}(\Delta x) = v_{max}\frac{(\Delta x)^2}{D^2 + (\Delta x)^2} \tag{3}$$

is the optimal velocity function depending on the headway distance $\Delta x_i = x_{i+1} - x_i$ proposed in [11–13,35,36]. It includes the maximal velocity v_{max} and the interaction distance D as parameters. Equation (1) can be written as

$$m\,\frac{dv_i}{dt} = F_{acc}(v_i) + F_{dec}(\Delta x_i), \tag{4}$$

where

$$F_{acc}(v_i) = \frac{m}{\tau}\left(v_{max} - v_i\right) \geq 0 \tag{5}$$

$$F_{dec}(\Delta x_i) = \frac{m}{\tau}\left(v_{opt}(\Delta x_i) - v_{max}\right) \leq 0 \tag{6}$$

are the accelerating and decelerating forces, respectively. Similar representation has been introduced already in [9,10]. The only distinguishing feature is that in our case the deceleration force is specified by (6), whereas in [9] it is related to a power-like interaction potential. The coordinate-dependent force term is due to interaction between cars

$$F_{dec}(\Delta x) = v_{max}\frac{m}{\tau}\left(\frac{(\Delta x)^2}{D^2 + (\Delta x)^2} - 1\right) \tag{7}$$

and is always negative, starting at $F_{dec}(\Delta x = 0) = -v_{max}m/\tau$, approaching zero at infinite distances. The

potential energy of car system can be defined as $V = \sum_{i=1}^{N} \phi(\Delta x_i)$, where $\phi(\Delta x_i)$ is the interaction potential of the ith car with the car ahead, which is given by

$$F_{dec}(\Delta x_i) = -\frac{\partial \phi(x_{i+1} - x_i)}{\partial x_i} = \frac{d\phi(\Delta x_i)}{d\Delta x_i}. \qquad (8)$$

By integrating this equation we get

$$\phi(\Delta x) = v_{max} \frac{D\,m}{\tau} \left[\frac{\pi}{2} - \arctan\left(\frac{\Delta x}{D} \right) \right], \qquad (9)$$

where the integration constant is chosen such that $\phi(\infty) = 0$. For comparison, the interaction potential of the form $\phi(\Delta x) \propto (\Delta x)^{-\alpha}$ has been considered in [9]. Note that $F_{dec}(\Delta x_i)$ is not given by $-\partial V/\partial x_i$, since the latter quantity includes an additional term $-\partial \phi(x_i - x_{i-1})/\partial x_i$. This term is absent in our definition of the force because the car behind does not influence the motion of the actual ith vehicle. It reflects the fact that, unlike in physical systems, the third Newton's law does not hold here.

The total time derivative of the potential energy is

$$\frac{dV}{dt} = \sum_{i=1}^{N} \left[\frac{\partial \phi(\Delta x_i)}{\partial x_i} \frac{dx_i}{dt} + \frac{\partial \phi(\Delta x_i)}{\partial x_{i+1}} \frac{dx_{i+1}}{dt} \right]$$
$$= \sum_{i=1}^{N} (v_{i+1} - v_i) F_{dec}(\Delta x_i). \qquad (10)$$

The total time derivative of the kinetic energy $T = \sum_{i=1}^{N} m v_i^2/2$ is obtained by multiplying both sides of (4) by v_i and summing over i. It leads to the following energy balance equation

$$\frac{dE}{dt} + \Phi = 0 \qquad (11)$$

for the total energy $E = T + V$ of the car system, where

$$\Phi = -\sum_{i=1}^{N} [v_i F_{acc}(v_i) + v_{i+1} F_{dec}(\Delta x_i)] \qquad (12)$$

is the energy flux. It includes both energy dissipation due to friction and energy input from the engine. Equation (11) shows that, in distinction to closed mechanical systems, the total energy is not conserved in traffic flow. Nevertheless, it approaches a constant value in the long-time limit, where the system converges to one of two possible stationary states: either to the fixed point $\Delta x_i = \Delta x_{hom}$, $v_i = v_{opt}\,(\Delta x_{hom})$ (where $\Delta x_{hom} = L/N$ is the distance between homogeneously distributed N cars over the road of length L), or to the limit cycle in the phase space of headways and velocities. Both situations are illustrated in Figure 1. At small enough density of cars there is a stable fixed point (solid circle), which lies on the optimal velocity curve (dotted line). An unstable fixed point (empty circle) exists at larger densities. In the latter case any small perturbation of the initially homogeneous fixed point situation leads to the limit cycle (solid line) in the long-time limit.

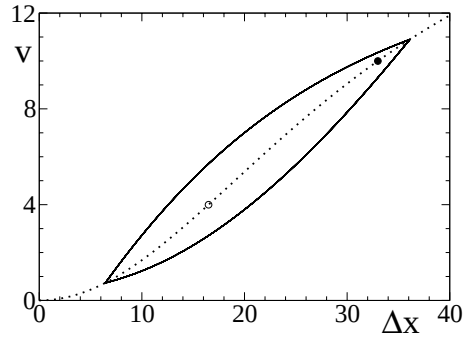

Fig. 1. Fixed points (circles) and limit cycle (solid line) in the space of headways Δx and velocities v of cars. The solid circle represents the stable fixed point at the car density $\rho = N/L = 0.0303$ m^{-1}. The empty circle is the unstable fixed point at a larger density $\rho = 0.0606$ m^{-1}, where the long-time trajectory for any car is the limit cycle shown. The fixed points lie on the optimal velocity curve (dotted line) given by (3). The parameters are chosen as $N = 60$, $D = 33$ m, $v_{max} = 20$ m/s, $\tau = 1.5$ s, and $m = 1000$ kg.

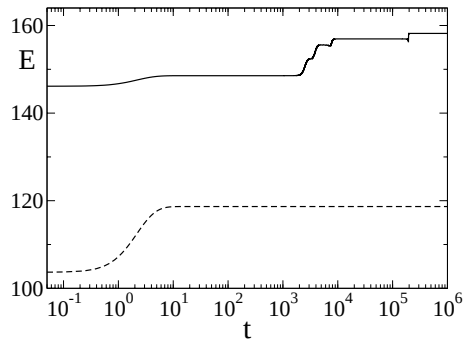

Fig. 2. The total energy E of the car system, measured in units of $mv_{max}^2/2$, depending on time t given in seconds. The same sets of parameters have been used as in Figure 1. The upper solid line corresponds to a larger density $\rho = 0.0606$ m^{-1} where the limit cycle forms, whereas the lower dashed line — to a smaller density $\rho = 0.0303$ m^{-1} where the convergence to stable fixed point is observed.

In the thermodynamic interpretation the mean energy $\langle E \rangle$ is the internal energy U of the system. The latter one thus has certain value in any one of the stationary states. The temporal behaviour of E for the same sets of parameters as in Figure 1 is shown in Figure 2. In the case of the convergence to the limit cycle (solid line) for $\rho = 0.0606$ m^{-1}, one can distinguish 6 plateau in the energy curve. The first one represents the short-time behaviour when starting from an almost homogeneous initial condition with zero velocities, and the second plateau is the unstable fixed point situation. Further on, 4 car clusters have been formed in the actual simulation, and this temporal situation is represented by the third relatively small plateau. The next three plateau with 3, 2, and finally 1 car clusters reflect the coarse graining or Ostwald ripening process. The dashed line shows the convergence to the stable fixed point value at $\rho = 0.0303$ m^{-1}.

Apart from the internal energy, other thermodynamic functions can be introduced as well. In the following

sections we will calculate the free energy F of the traffic flow. By using the known relation $F = U - T^* S$ we can calculate also the entropy S of traffic flow for a properly defined 'temperature' T^*.

Up to now we have considered purely deterministic equations of motion. Randomness can be included, e.g., by adding a multiplicative noise term to (4). It leads to stochastic differential equations

$$m\, dv_i(t) = (F_{acc}(v_i) + F_{dec}(\Delta x_i))dt + \sigma\, v_i dW_i(t), \quad (13)$$

$$dx_i(t) = v_i dt \quad (14)$$

considered and solved numerically in [13]. Here σ is the noise amplitude, and $dW_i(t)$ is the increment of Wiener process. Similar equation with additive noise term has been studied in [9,10]. An advantage of the version with multiplicative noise is that it guarantees the positiveness of velocities v_i. In the deterministic model the departure (leaving a cluster) times are strongly correlated in such a way that, in the stationary regime, one car leaves the cluster after each time interval of a given length τ_1. The arrival (adding to a cluster) times also are strongly correlated due to the repulsive forces. The noise makes these correlations weaker. It allows to apply the formalism of stochastic Markov processes to describe approximately the fluctuations of the cluster size, as discussed in the following section.

3 Mesoscopic stochastic model of traffic flow

It is easier to study the formation of a car congestion on a mesoscopic level, as it has been done in [11–13,35,36], where we do not follow each individual car, but only look for the number of congested cars n, i.e., the size of car cluster. In this description it is also very easy to introduce the randomness, by considering n as a stochastic variable. Following [11–13,35,36], in the simplest model only one cluster on a circular road is considered, and the probability $p(n,t)$ that it contains n cars at time t is given by one-step master equation

$$\begin{aligned}\frac{dp(n,t)}{dt} = {} & w_+(n-1)\, p(n-1,t) \\ & + w_-(n+1)\, p(n+1,t) \\ & - [w_+(n) + w_-(n)]\, p(n,t) \quad : \quad 0 < n < N.\end{aligned} \quad (15)$$

For $n = 0$ and $n = N$ the equations look different, i.e., terms with $p(-1,t)$ and $p(N+1,t)$ are absent. In the simplest version of the model of point-like cars the transition rates are $w_-(n) = 1/\tau$ and $w_+(n) = v_{opt}\left(\Delta x_{free}\right)/\Delta x_{free}$, where τ is a reaction time constant and $\Delta x_{free}(n) = L/(N-n)$ is the mean headway distance in the free flow phase. In this model no large stable cluster forms at low densities of cars, whereas a macroscopic fraction of them are condensed (jammed) into the cluster above certain critical density. The first situation corresponds to the fixed-point solution of the Bando model, whereas the second one — to the limit cycle. It is a remarkable fact that the stationary solution $p^{st}(n) = \lim_{t\to\infty} p(n,t)$ obeys the detailed balance condition $p^{st}(n)\, w_+(n) = p^{st}(n+1)\, w_-(n+1)$. It allows to describe some properties of the model by equilibrium thermodynamics in analogy to the liquid-vapour system, as discussed in the following sections, in spite of the fact that the traffic flow is a driven, i.e., nonequilibrium system.

4 Free energy of the liquid-gas system

The principle of detailed balance is useful to describe the equilibrium in a physical system. In particular, we analyse the condensation of supersaturated vapour to show how the free energy and chemical potentials can be derived based on this principle with the following idea to apply the same scheme for traffic flow.

For simplicity, we consider a situation where only one cluster of molecules coexists with the vapour phase. The number n of molecules called monomers binded in the cluster is a stochastic variable, whereas their total number N in a given volume V is fixed. The stochastic events of adding or removing one monomer are characterised by transition rates $w_+(n)$ and $w_-(n)$ depending on the actual cluster size n. Following [7,13], the detailed balance reads

$$\frac{w_+(n-1)}{w_-(n)} = \exp\left(-\frac{F(n) - F(n-1)}{k_B T}\right), \quad (16)$$

where T is temperature, k_B the Boltzmann constant, and $F(n)$ is the free energy of state (including all possible microscopic distributions of coordinates and momenta of free monomers) with cluster size n. For large enough n (16) can be approximated as

$$\frac{w_+(n)}{w_-(n)} \simeq \exp\left(-\frac{\partial F/\partial n}{k_B T}\right), \quad (17)$$

which leads to the equation

$$\ln\left[\frac{w_+(n)}{w_-(n)}\right] = -\frac{1}{k_B T}\frac{\partial F}{\partial n}. \quad (18)$$

From this we get

$$F = F_0 - k_B T \int_0^n \ln\left[\frac{w_+(n')}{w_-(n')}\right] dn', \quad (19)$$

where $F_0 = F(n=0)$ does not depend on the cluster size n. It is the free energy of the system without cluster, in this case the free energy of an ideal gas. We insert here the physical ansatz for the transition rates (see [13])

$$\frac{w_+(n)}{w_-(n)} = \frac{\lambda_0^3(T)(N-n)}{V} \exp\left(\frac{f_{n-1}(T) - f_n(T)}{k_B T}\right), \quad (20)$$

where V is the fixed volume of the system, $f_n(T)$ is the binding energy of a cluster of size n,

$\lambda_0(T) = h/(2\pi m k_B T)^{1/2}$ is the de Broglie wave length of a monomer, and h is the Planck's constant. By using the approximation $f_{n-1}(T) - f_n(T) \simeq -\partial f_n(T)/\partial n$, we obtain

$$F = F_0 - k_B T \int_0^n \ln\left[\frac{\lambda_0^3(T)(N-n')}{V}\right] dn' + f_n(T). \quad (21)$$

The integration, using $\int \ln x\, dx = x \ln x - x$, yields

$$F = F_0 - k_B T N \left[\ln\left(\lambda_0^3(T)\frac{N}{V}\right) - 1\right] + k_B T (N-n)\left[\ln\left(\lambda_0^3(T)\frac{N-n}{V}\right) - 1\right] + f_n(T). \quad (22)$$

The free energy of ideal system (gas) F_0 cannot be obtained from the detailed balance relation. It is given by $F_0 = -k_B T \ln Z_{id}$, where Z_{id} is the partition function of the ideal gas

$$Z_{id} = \frac{1}{N!}\prod_{\alpha=1}^{3N}\frac{1}{h}\int_0^L dx_\alpha \int_{-\infty}^{\infty} dp_\alpha \exp\left(-\frac{p_\alpha^2}{2mk_BT}\right) \quad (23)$$
$$= \frac{1}{N!}\left(\frac{L}{\lambda_0(T)}\right)^{3N}.$$

Hence, applying the Stirling formula $\ln N! \simeq N \ln N - N$, we obtain

$$F_0 = k_B T N \left[\ln\left(\lambda_0^3(T)\frac{N}{V}\right) - 1\right]. \quad (24)$$

By inserting (24) into (22) we recover the known expression

$$F = k_B T (N-n)\left[\ln\left(\lambda_0^3(T)\frac{N-n}{V}\right) - 1\right] + f_n(T) \quad (25)$$

for the free energy of liquid-gas system under isothermal and isochoric conditions. The binding energy $f_n(T)$ can be written as

$$f_n(T) = \mu_\infty(T) n + \sigma A(n), \quad (26)$$

where $\mu_\infty(T)n$ represents the volume contribution, $\mu_\infty(T) < 0$ being the chemical potential for a flat droplet interface (with infinite radius r), and $\sigma A(n)$ is the surface contribution. Here $\sigma > 0$ is the surface tension, whereas $A(n) = 4\pi r^2$ is the surface area of a droplet with radius r. Taking into account that the number of particles (molecules) in the cluster is $n = (c_{clust}\, 4\pi/3)\, r^3$, where c_{clust} is the particle density inside the cluster, equation (22) can be written as

$$\frac{F-F_0}{V k_B T} = \rho\Bigg\{\left(1-\frac{n}{N}\right)\left[\ln\left(1-\frac{n}{N}\right) - 1\right] + 1 - \frac{n}{N}\ln\left(\lambda_0^3(T)\rho\right) + \frac{\mu_\infty(T)}{k_B T}\frac{n}{N} + \frac{3}{2}\ell(T)\,(c_{clust}\,4\pi/3)^{1/3}\, N^{-1/3}\left(\frac{n}{N}\right)^{2/3}\Bigg\}, \quad (27)$$

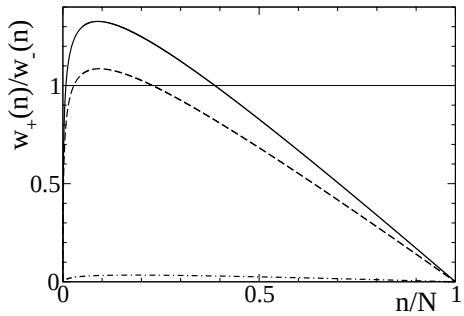

Fig. 3. The ratio of transition rates $w_+(n)/w_-(n)$ depending on the fraction of condensed particles n/N for three dimensionless densities $\tilde{\rho} = 5 \times 10^{-7}$ (dot-dashed line), $\tilde{\rho} = 10^{-5}$ (dashed line), and $\tilde{\rho} = 1.2 \times 10^{-5}$ (solid line).

where $\rho = N/V$ is the overall density and

$$\ell(T) = \frac{2\sigma}{c_{clust} k_B T} \quad (28)$$

is the diffusion length (width) of the liquid-gas interface.

Further on we introduce dimensionless density $\tilde{\rho} = \lambda_0^3(T)\rho$ and dimensionless volume $\widetilde{V} = V/\lambda_0^3(T)$. In this notation the equation (20) transforms to

$$\frac{w_+(n)}{w_-(n)} = \tilde{\rho}\left(1-\frac{n}{N}\right)\exp\left(-\frac{\mu_\infty(T)}{k_B T}\right) \times \exp\left(-\ell(T)\,(c_{clust}\,4\pi/3)^{1/3}\,\widetilde{V}^{-1/3}\tilde{\rho}^{-1/3}\left(\frac{n}{N}\right)^{-1/3}\right), \quad (29)$$

whereas (27) becomes

$$\frac{F-F_0}{\widetilde{V} k_B T} = \tilde{\rho}\Big\{\left(1-\frac{n}{N}\right)\left[\ln\left(1-\frac{n}{N}\right) - 1\right] + 1 - \frac{n}{N}\ln(\tilde{\rho}) + \frac{\mu_\infty(T)}{k_B T}\frac{n}{N} + \frac{3}{2}\ell(T)\,(c_{clust}\,4\pi/3)^{1/3}\,\widetilde{V}^{-1/3}\tilde{\rho}^{-1/3}\left(\frac{n}{N}\right)^{2/3}\Big\}. \quad (30)$$

These equations allow us to calculate the ratio $w_+(n)/w_-(n)$, as well as the normalised (dimensionless) free energy difference $(F-F_0)/(\widetilde{V} k_B T)$ depending on the fraction of condensed molecules n/N at a given overall density for fixed volume and temperature. The results of calculation for three different dimensionless densities $\tilde{\rho} = 5 \times 10^{-7}, 10^{-5}, 1.2 \times 10^{-5}$ at the values of dimensionless control parameters $\mu_\infty/(k_B T) = -12$ and $\ell(T)\,(c_{clust}\,4\pi/3)^{1/3}\,\widetilde{V}^{-1/3} = 0.003$ are shown in Figures 3 and 4. Note that the extrema of $F - F_0$ in Figure 4 correspond to the crossing points with the horizontal line $w_+(n)/w_-(n) = 1$ in Figure 3. At the smallest density (dot-dashed line) there are no crossing points and the free energy is a monotonously increasing function of n/N, showing that the stable state of the liquid-gas system contains no liquid droplet. Stable droplet appears at larger densities (dashed and solid lines) by overcoming a nucleation barrier (local free energy maximum in Fig. 4).

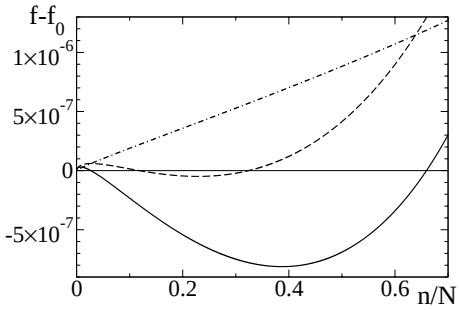

Fig. 4. Normalised free energy difference $(F-F_0)/(\widetilde{V}k_BT) = f-f_0$ depending on the fraction of condensed particles n/N for three dimensionless densities $\tilde{\rho} = 5\times10^{-7}$ (dot-dashed line), $\tilde{\rho} = 10^{-5}$ (dashed line), and $\tilde{\rho} = 1.2\times10^{-5}$ (solid line).

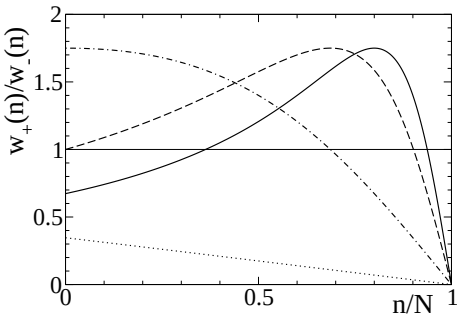

Fig. 5. The ratio of transition rates $w_+(n)/w_-(n)$ depending on the fraction of congested cars n/N for four dimensionless densities $\tilde{\rho} = 0.1$ (dotted line), $\tilde{\rho} = 1$ (dot-dashed line), $\tilde{\rho} = 3.186$ (dashed line), and $\tilde{\rho} = 5$ (solid line).

The parameters we have chosen are quite realistic, i.e., comparable with those of water at $T = 300$ K and $V = 5\times10^{-23}$ m^3 with about 37 250 molecules (mass $m = 2.99\times10^{-23}$ kg) at $\tilde{\rho} = 10^{-5}$. For water at $T = 300$ K we have $\lambda_0(T) = 2.377\times10^{-11}$ m and $c_{clust} = 3.346\times10^{28}$ m^{-3}. Hence, the dimensionless density in the cluster $\tilde{\rho}_{clust} = c_{clust}\lambda_0^3 = 4.491\times10^{-4}$ exceeds about 50 times the critical mean density $\tilde{\rho} = \tilde{\rho}_c \simeq 9.2\times10^{-6}$ at which the condensation (i.e., a minimum of free energy at $n/N > 0$) appears in our calculation. Assuming the above parameters of water, we obtain $\ell(T) = 8.953\times10^{-10}$ m for the width of the liquid-gas interface and surface tension $\sigma = 6.20\times10^8$ Nm/m^2. It is about 3 times the characteristic intermolecular distance in the cluster, which is roughly $c_{clust}^{-1/3} \simeq 3.1\times10^{-10}$ m. The critical density $\tilde{\rho}_c$ increases with temperature and becomes equal to the cluster density $\tilde{\rho}_{clust}$ at the critical temperature $T = T_c$. In our description the physically meaningful densities are restricted by $\tilde{\rho} \le \tilde{\rho}_{clust}$. It means that no condensation phase transition takes place for these physical densities at $T > T_c$. Assuming that μ_∞ and σ do not change with temperature and that the above given values of dimensionless control parameters correspond to $T = 300$ K, we find $T_c \simeq 430$ K in our example.

5 Free energy of traffic flow

Now we make similar calculation of free energy for the traffic flow model introduced in Section 3. Similar general relations (16) to (19) are valid to describe the stationary (quasi-equilibrium) properties in the space of car cluster size n, since the detailed balance is the property of the stationary solution of the one-dimensional one-step master equation for the probability distribution over n. Here we only replace k_BT with T^* which is the 'temperature' of traffic flow having energy dimension.

The ratio of transition rates in this case reads

$$\frac{w_+(n)}{w_-(n)} = \tau\frac{v_{opt}(\Delta x_{free})}{\Delta x_{free}}, \tag{31}$$

where $v_{opt}(\Delta x)$ is the optimal velocity function given by (3) and Δx_{free} is the headway distance in free flow phase. Assuming the model of point-like cars we have $\Delta x_{free}(n) = L/(N-n)$, where L is the length of the road and N is the total number of cars. It yields

$$\frac{w_+(n)}{w_-(n)} = v_{max}\tau\rho\frac{1-n/N}{1+\rho^2D^2(1-n/N)^2}, \tag{32}$$

where $\rho = N/L$ is the car density. Introducing the dimensionless density $\tilde{\rho} = \rho D$ and a dimensionless control parameter $\tilde{b} = D/(v_{max}\tau)$, it becomes

$$\frac{w_+(n)}{w_-(n)} = \frac{1}{\tilde{b}}\,\frac{\tilde{\rho}(1-n/N)}{1+\tilde{\rho}^2(1-n/N)^2}, \tag{33}$$

or

$$\ln\left[\frac{w_+(n)}{w_-(n)}\right] = \ln\left(\frac{\tilde{\rho}}{\tilde{b}}\right) + \ln\left[1-\frac{n}{N}\right] - \ln\left[1+\tilde{\rho}^2\left(1-\frac{n}{N}\right)^2\right]. \tag{34}$$

By inserting the latter relation into (19) (where $k_BT \to T^*$), the integration using $\int \ln\left(1+x^2\right)dx = 2\arctan x + x\ln\left(1+x^2\right) - 2x$ yields

$$\frac{F-F_0}{\widetilde{L}\,T^*} = \tilde{\rho}\left\{\left(1-\frac{n}{N}\right)\ln\left(1-\frac{n}{N}\right) - \frac{n}{N} - \frac{n}{N}\ln\left(\frac{\tilde{\rho}}{\tilde{b}}\right) - \left(1-\frac{n}{N}\right)\ln\left(1+\tilde{\rho}^2\left[1-\frac{n}{N}\right]^2\right) + \ln\left(1+\tilde{\rho}^2\right)\right\} + 2\arctan\tilde{\rho} - 2\arctan\left(\tilde{\rho}\left[1-\frac{n}{N}\right]\right), \tag{35}$$

where $\widetilde{L} = L/D$ is the dimensionless length of the road.

The results for $w_+(n)/w_-(n)$ and $(F-F_0)/(\widetilde{L}T^*)$ depending on the fraction of congested cars n/N at four different densities are shown in Figures 5 and 6. The value of the dimensionless control parameter has been chosen $\tilde{b} = 2/7 \approx 0.2857$. It corresponds, e.g., to $D = 24$ m, $v_{max} = 42$ m/s, and $\tau = 2$ s. Like in the case of the liquid-supersaturated vapour system, $w_+(n)/w_-(n)$ is never 1 and no stable car cluster forms at small densities (dotted line). In distinction to the liquid-vapour case, the cluster appears without a nucleation barrier in the actual traffic flow model at somewhat larger densities $\tilde{\rho}$ (dot-dashed

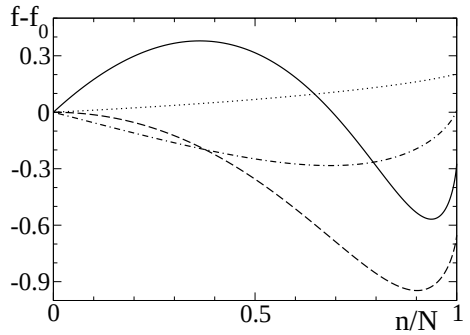

Fig. 6. Normalised free energy difference $(F - F_0)/(\widetilde{L}T^*) = f - f_0$ depending on the fraction of congested cars n/N for four dimensionless densities $\tilde{\rho} = 0.1$ (dotted line), $\tilde{\rho} = 1$ (dot–dashed line), $\tilde{\rho} = 3.186$ (dashed line), and $\tilde{\rho} = 5$ (solid line).

line), whereas the nucleation barrier (free energy maximum) shows up only at even larger $\tilde{\rho}$ values (solid line).

In the above calculation we have determined only the difference $F - F_0$, but not the free energy F_0 of the ideal system without car cluster. Like in the case of supersaturated vapour, the latter cannot be derived from the detailed balance. It should be calculated from a microscopic model. Now, however, we should take into account that the distribution over momenta for cars is not the same as that for molecules in an ideal gas. As a first approximation we may assume similar Gaussian distribution with only shifted mean value $\langle p \rangle = m\langle v \rangle = m v_{opt}\,(\Delta x_{hom})$ in accordance with the optimal velocity $v_{opt}\,(\Delta x_{hom})$ in the homogeneous flow of cars with the mean headway distance $\Delta x_{hom} = L/N = 1/\rho$. The Gaussian form of the distribution is well consistent with the simulation results for the stochastic car-following models [9,10,13]. We should take into account also that cars are moving always in one direction, i.e., momentum $p > 0$ always holds. Finally, in distinction to the ideal gas of molecules, the coordinates and momenta of cars are one-dimensional. Hence, by analogy to (36) we can write

$$Z_{id} = \frac{1}{N!}\prod_{\alpha=1}^{N}\frac{1}{h}\int_0^L dx_\alpha \int_0^\infty dp_\alpha \, \exp\left(-\frac{(p_\alpha - \langle p \rangle)^2}{2mT^*}\right) \approx \frac{1}{N!}\left(\frac{L}{\lambda_0(T^*)}\right)^N, \tag{36}$$

where $\lambda_0(T^*) = h/(2\pi m T^*)^{1/2}$. The latter approximate equality in (36) holds when $\langle p \rangle^2/(2mT^*) \gg 1$ or, in other words, when the width of the velocity distribution is narrow as compared to the mean velocity. The latter condition is well satisfied for the model (13)–(14) with certain set of control parameters used in the simulations of [13] (see Fig. 40 there). The distribution width, however, increases with the noise amplitude. In fact, the approximation (36) is good enough when the distribution function has small value at zero momentum $p = 0$, as in the simulation results of [9,10]. According to the above consideration, temperature in traffic flow is a parameter which controls this distribution width or the amplitude of velocity and momentum fluctuations, like in the ideal gas of molecules. According to (36), the ideal part of free energy reads

$$F_0 = -T^*\left[N \ln\left(L/\lambda_0(T^*)\right) - \ln N!\right] \simeq T^* N\left[\ln\left(\rho\lambda_0(T^*)\right) - 1\right]. \tag{37}$$

This expression is analogous to (24).

6 Relaxation to a free energy minimum

Now we consider the general behaviour of a system (equally valid for liquid-gas system with $T^* = k_B T$ and traffic flow) in vicinity of a local or global minimum of $F(n)$. In this case the argument of exponent in (17) is small and we can make a Taylor expansion

$$\frac{w_+(n)}{w_-(n)} \simeq \exp\left(-\frac{\partial F/\partial n}{T^*}\right) \simeq 1 - \frac{1}{T^*}\frac{\partial F}{\partial n}. \tag{38}$$

It can be rewritten as

$$w_+(n) - w_-(n) \simeq -\frac{w_-(n)}{T^*}\frac{\partial F}{\partial n}. \tag{39}$$

On the other hand, we can write in a deterministic approximation

$$\frac{dn}{dt} = w_+(n) - w_-(n). \tag{40}$$

Comparing (39) and (40), we obtain

$$\frac{dn}{dt} \simeq -\frac{w_-(n)}{T^*}\frac{\partial F}{\partial n}. \tag{41}$$

Like in the Landau theory of phase transitions, we can expand the free energy around the minimum point $n = n_0$ defined by

$$\left.\frac{\partial F}{\partial n}\right|_{n=n_0} = 0. \tag{42}$$

In the first approximation, where we retain only the leading term, we have also $w_+(n) = w_-(n) = w_\pm\,(n_0)$. It leads to the kinetic equation

$$\frac{dn}{dt} \simeq -\Gamma_0\,(n - n_0)\,, \tag{43}$$

where

$$\Gamma_0 = \frac{w_\pm\,(n_0)}{T^*}\left.\frac{\partial^2 F}{\partial n^2}\right|_{n=n_0} \tag{44}$$

is the relaxation rate. For $\Gamma_0 > 0$, what corresponds to minimum of F, the solution is the exponential relaxation to $n = n_0$, i.e.,

$$n(t) = n_0 + (n(0) - n_0)\, e^{-\Gamma_0 t}. \tag{45}$$

This solution is valid also for $\Gamma_0 < 0$, in which case n_0 corresponds to a free energy maximum. In this case it describes the deviation from this maximum point.

7 Chemical potentials

Our system can be considered as consisting of two phases: the cluster phase with n particles and free energy $F_{cl}(n)$, and the ideal gas phase with $N_{id} = N - n$ particles and free energy $F_{id}(N_{id})$. The total free energy then is $F = F_{cl} + F_{id}$. While the total number of particles N is fixed, the number of particles in any of the phases fluctuates. According to the definition, we can write $\mu_{cl} = \partial F_{cl}/\partial n$ and $\mu_{id} = \partial F_{id}/\partial N_{id} = -\partial F_{id}/\partial n$ for the chemical potentials of these phases. Hence

$$\frac{\partial F}{\partial n} = \frac{\partial F_{cl}}{\partial n} + \frac{\partial F_{id}}{\partial n} = \mu_{cl} - \mu_{id} \tag{46}$$

and the kinetic equation (41) can be written as

$$\frac{dn}{dt} \simeq -\frac{w_{\pm}(n_0)}{T^*}\,(\mu_{cl} - \mu_{id})\,. \tag{47}$$

The latter equation has certain physical interpretation: the driving force pushing the system to the phase equilibrium is the difference of chemical potentials in both phases. The equilibrium is reached when the chemical potentials of the coexisting phases are equal, i.e., $\mu_{cl} = \mu_{id}$.

For the liquid-gas system $F_{id}(T, V, N, n)$ is given by (24), where N is replaced with $N_{id} = N - n$, i.e.,

$$F_{id}(T, V, N, n) = k_B T(N - n)\left[\ln\left(\lambda_0^3(T)\frac{N-n}{V}\right) - 1\right]. \tag{48}$$

Hence the total free energy (25) can be written as

$$F = F_{id}(T, V, N, n) + f_n(T). \tag{49}$$

The chemical potential of the liquid phase is thus given by the derivative of the binding energy $f_n(T) \equiv F_{cl}(T, V, N, n)$, i.e.,

$$\mu_{cl} = \mu_\infty(T) + \sigma\,\frac{\partial A(n)}{\partial n} = \mu_\infty(T) + k_B T\,\ell(T) k(n), \tag{50}$$

where

$$k(n) = \frac{1}{r} = (c_{clust}\,4\pi/3)^{1/3}\,n^{-1/3} \tag{51}$$

is the curvature of the liquid surface for a droplet with radius r and surface area $A(n) = 4\pi r^2$. The chemical potential of the gaseous phase calculated from (48) is

$$\begin{aligned}\mu_{id} &= -\frac{\partial F_{id}}{\partial n} = k_B T\,\ln\left(\lambda_0^3(T)\frac{N-n}{V}\right)\\ &= k_B\,T \ln\left(\tilde\rho_{gas}\right),\end{aligned} \tag{52}$$

where $\tilde\rho_{gas} = \lambda_0^3(T)(N-n)/V$ is the dimensionless density of molecules in the gaseous phase. According to these expressions for the chemical potentials, the ansatz (20) can be written as

$$\begin{aligned}\frac{w_+(n)}{w_-(n)} &= \exp\left(\frac{\mu_{id}}{k_B T}\right)\,\exp\left(\frac{f_{n-1}(T) - f_n(T)}{k_B T}\right)\\ &\simeq \exp\left(-\frac{\mu_{cl} - \mu_{id}}{k_B T}\right).\end{aligned} \tag{53}$$

The latter relation is consistent with (17) and (46).

By analogy, the free energy of the free flow phase in traffic is

$$F_{id}(T^*, L, N, n) = T^*(N - n)\left[\ln\left(\lambda_0(T^*)\frac{N-n}{L}\right) - 1\right], \tag{54}$$

as consistent with (37) where we put $N \to N_{id} = N - n$ and $\rho \to N_{id}/L$. From (54) we get

$$\begin{aligned}\mu_{id} &= -\frac{\partial F_{id}}{\partial n} = T^*\,\ln\left(\lambda_0(T^*)\frac{N-n}{L}\right)\\ &= T^* \ln\left(\frac{\lambda_0(T^*)}{D}\,\tilde\rho_{free}\right),\end{aligned} \tag{55}$$

where $\tilde\rho_{free} = D(N-n)/L$ is the dimensionless density of cars in the free flow phase. The chemical potential of the cluster phase can be easily calculated from equations (18), (34), and (46). It yields

$$\begin{aligned}\mu_{cl} &= -T^*\left\{\ln\left(\frac{D}{\lambda_0\tilde b}\right) - \ln\left[1 + \tilde\rho^2\left(1 - \frac{n}{N}\right)^2\right]\right\}\\ &= -T^*\left\{\ln\left(\frac{D}{\lambda_0\tilde b}\right) - \ln\left[1 + \tilde\rho_{free}^2\right]\right\}.\end{aligned} \tag{56}$$

It is remarkable that, in distinction to the liquid-gas system, the chemical potential of the cluster phase is not an internal property of this phase, since it depends on the outer parameter — the density of the surrounding free-flow phase $\tilde\rho_{free}$. The physical interpretation of this fact is that the traffic flow is a driven system, which approaches a stationary rather than equilibrium state in the usual sense. However. as we have shown here, various properties of this stationary state can be described by equilibrium thermodynamics.

Free energy of the cluster phase can be calculated consistently from (35), (37), and (54) according to $F = F_{cl} + F_{id}$. The result is

$$F_{cl}(T^*, L, N, n) = T^* N\left\{-\frac{n}{N}\left(2 + \ln\left(\frac{D}{\lambda_0\tilde b}\right)\right)\right. \tag{57}$$

$$+\,\frac{2}{\tilde\rho}\left[\arctan\tilde\rho - \arctan\left(\tilde\rho\left[1 - \frac{n}{N}\right]\right)\right] \tag{58}$$

$$\left. -\left(1 - \frac{n}{N}\right)\ln\left(1 + \tilde\rho^2\left[1 - \frac{n}{N}\right]^2\right) + \ln\left(1 + \tilde\rho^2\right)\right\}. \tag{59}$$

It is consistent with $\mu_{cl} = \partial F_{cl}/\partial n$.

8 Conclusions

1. In the current paper we have shown how thermodynamics can be applied to such a many-particle system as traffic flow, based on a microscopic (car-following) as well as a mesoscopic (stochastic cluster) description, in analogy to equilibrium physical systems like supersaturated vapour forming liquid droplets. The basic idea here is to derive the free energy function and chemical potentials by using the detailed balance, which holds in the stationary state of traffic flow in the space of car cluster sizes.

2. Distinguishing features between the traffic flow and equilibrium physical systems have been outlined. In particular, we have found that the third Newton's law does not hold on the level of "microscopic" equations of motion for individual cars. Besides, the traffic flow is a dissipative system with inflow and outflow of total energy. Unlike in equilibrium systems, the chemical potential of the phase of congested cars is not an internal property of this phase, since the traffic flow is a driven system.

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