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Latent heat and the Fourier law

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ABSTRACT

We present computer simulations run with a stochastic cellular automaton which describes $d = 1$ particle systems connected to reservoirs which keep two different densities at the endpoints. We fix the parameters so that there is a phase transition (of the van der Waals type) and observe that if the densities at the boundaries are metastable then, after a transient, the system reaches an apparently stationary regime where the current flows from the reservoir with smaller density to the one with larger density.

1. Introduction

The Fourier law states that the heat flux is proportional to minus the gradient of the temperature, analogously the Fick law says that the mass flux is proportional to minus the gradient of the mass density. Both laws state that a gradient gives rise to a current. On the other hand in the presence of a first order phase transition there is a spontaneous separation of phases giving rise to a gradient (of the corresponding order parameter) without a current. Purpose of this article is to investigate how this fits with the Fourier or the Fick law, in particular to understand the role of the latent heat in heat conduction. In the sequel we will however refer to mass transport (hence to the Fick law), as we will study particles models.

The physical system we have in mind is made by a channel containing a gas of particles and by two density reservoirs which are respectively connected to the right and to the left of the channel and which fix the density of the gas at the endpoints of the channel at values ρ_+ and, respectively, ρ_-. We further suppose that the temperature is fixed throughout the channel at a value for which there is a phase transition.

We model the channel as one-dimensional and the gas as a system of particles which interact via a two-body attractive Kac potential, which in the Kac scaling limit gives rise to a van der Waals phase transition. We actually consider two models, the first one (described in Section 3) is a lattice gas with Kawasaki dynamics and Kac potential, the second one (described in Section 2) is a stochastic cellular automaton (CA) whose updating rules mimic the Kawasaki dynamics of the first one. While the first model is convenient for a theoretical analysis, the second one is amenable to computer simulations. Unfortunately, we cannot go very far theoretically and our results rely essentially on the simulations.

The simulations exhibit two totally unexpected phenomena when the reservoirs densities ρ_- and ρ_+ are such that $\rho_- < \rho_+$, and for the gas in the channel these values are minus/plus metastable (i.e. metastable and in the two different phases). In such a case the system seems to reach a stationary state such that (1) the current in the channel becomes positive so that mass goes from the reservoir at lower density to the one with larger density; (2) in a large fraction of the volume the density is metastable. We will argue in Section 3 that this does not contradict the Fick law, but our arguments are not mathematically complete. A consequence of (1) is the theoretical possibility of constructing circuits made of the above channel connected to two large but finite reservoirs which also exchange mass with each other (either directly or via a second channel where the gas has no phase transitions). Preliminary simulations seem to indicate that, in the circuit, after a transient, there is a stationary current which runs in the absence of an external bias. We believe that such a state is metastable with a very long life, but that in the long run the system will eventually decay to a state with no current.

2. The simulations

Our simulations use a CA introduced in [1] to simulate the time evolution of a system of particles which undergoes a phase transition of van der Waals type. The CA describes a system of particles

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in the interval $[1, L]$ of $\mathbb{Z}$, hereafter called "channel". The particles have only velocities $v \in \{-1, 1\}$ and we impose single occupancy, namely there cannot be two particles at same site with same velocity, $\eta(x, v) \in \{0, 1\}$ being the occupation variable at (x, v).

The definition of the CA involves five parameters, L, $\gamma : \gamma^{-1} \in \mathbb{N}$, $C > 0$ and $0 \le \rho_- < \rho_+ \le 1$. We use the following notation: for $x \in [1, L]$, $\eta(x) := \eta(x, -1) + \eta(x, 1)$; for $x \ge 1$, $\eta^{(+)}(x) = \eta(x)$ if $x \in [1, L]$ and $\eta^{(+)}(x) = 2\rho_+$ if $x > L$; for $x \le L$, $\eta^{(-)}(x) = \eta(x)$ if $x \in [1, L]$ and $\eta^{(-)}(x) = 2\rho_-$ if $x < 1$; finally for $x \in [1, L]$ we call

$$N_{+,x,\gamma} = \sum_{y=x+1}^{x+\gamma^{-1}} \eta^{(+)}(y),\ N_{-,x,\gamma} = \sum_{y=x-\gamma^{-1}}^{x-1} \eta^{(-)}(y)$$

We are now ready to define how the CA operates. The unit time step updating is obtained as the result of two successive operations: (1) *velocity flip*. At all sites $x \in [1, L]$ where there is only one particle we update the velocity of the particle to become $+1$ with probability $\frac{1}{2} + \epsilon_{x,\gamma}$ and -1 with probability $\frac{1}{2} - \epsilon_{x,\gamma}$, $\epsilon_{x,\gamma} = C\gamma^2[N_{+,x,\gamma} - N_{-,x,\gamma}]$. At all other sites the occupation numbers are left unchanged. Moreover, after adding two auxiliary sites 0 and $L+1$, we put a particle in 0 with velocity $+1$ with probability ρ_-, while we leave it empty with complementary probability; analogously we put a particle in $L+1$ with velocity -1 with probability ρ_+ while we leave it empty with complementary probability. (2) *advection*. Each particle moves by one lattice step in the direction of its velocity, if it goes to $L+1$ or to 0 it is deleted.

Remarks. $\epsilon_{x,\gamma}$ is a "small bias" (for γ small) which directs the velocity towards regions with higher density. As discussed in the next section, this can be interpreted as the action of two-body "long range" attractive forces; in such a context the constant C is proportional to the inverse temperature β, $2C = \beta$, and in the limit as $\gamma \to 0$ the equilibrium phase diagram exhibits a van der Waals phase transition for all $C > 0.5$. The addition of the extra sites 0 and $L+1$ in the definition of the CA simulates the action of the two reservoirs which after each time step put a new particle at 0 and at L with probability ρ_- and respectively ρ_+. The action of the reservoirs is however twofold: in fact, besides the aforementioned insertion of particles in the channel with probabilities ρ_+ and ρ_-, it also enters in the definition of $\epsilon_{x,\gamma}$, where the occupation numbers at $y > L$ and $y < 1$ are replaced by the average reservoir densities ρ_+ and, respectively, ρ_-.

We have run several Monte Carlo simulations for different values of the parameters defining the CA, we report here results in the case $C = 1.25$, $\gamma^{-1} = 30$, $L = 600$ and $\rho_- < \rho_+ = 1 - \rho_-$. We have computed the local particles density $\rho(x, t)$ by taking the time average $\frac{1}{2T}\sum_{s=t}^{t+T-1} \eta_s(x)$, $\eta_s(x)$ the number of particles at x at time s, $T = L^2$; however, instead of $\rho(x, t)$ we have plotted $m(r, t) = 2\rho(\gamma^{-1}r, t) - 1$, thus the unit space length becomes γ^{-1} (the interaction range) and the density is written in "magnetization variables" so that the magnetization at the endpoints is $m_+ = -m_-$.

In Fig. 1 we report what observed when $m_\pm = \pm 1$ while the initial configuration has $m_{0,x} = -1$ for $x \le 3L/4$ and $m_{0,x} = +1$ elsewhere. On the time scale L^2 we see the initial step to smoothen out: the profile becomes a curve starting on the left at $m_- = 1$ and increasing slowly, almost linearly, till $3L/4$ where it has a value $\approx -m_\beta$, $m_\beta = 0.985$, then there is a transition region where the magnetization increases quite abruptly from $-m_\beta$ to m_β; afterwards the profile goes again slowly, almost linearly, up to $m_+ = 1$ which is reached at the right endpoint. As time increases the profile moves rigidly towards the middle of the channel which is reached on times $\le L^3$ and in the time of our simulations it remains unchanged except for small fluctuations. In the next section we will interpret the values $\pm m_\beta$ as the equilibrium magnetization densities when the inverse temperature is $\beta = 2C$.

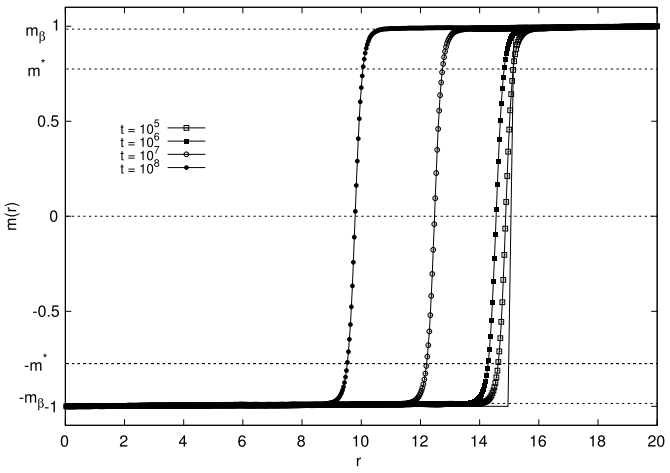

Fig. 1. Magnetization profiles for $C = 1.25$ and $m_+ = 1$ with space in γ^{-1} $(= 30)$ units. The parameters m_β and m^* have values $m_\beta = 0.985$ and $m^* = 0.775$. The different curves in the plot correspond to the averaged magnetization computed at different times: $t = 10^5$ (empty squares), $t = 10^6$ (filled squares), $t = 10^7$ (empty circles) and $t = 10^8$ (filled circles). The black thin line denotes the initial configuration, corresponding to a step function centered at $r = 15$.

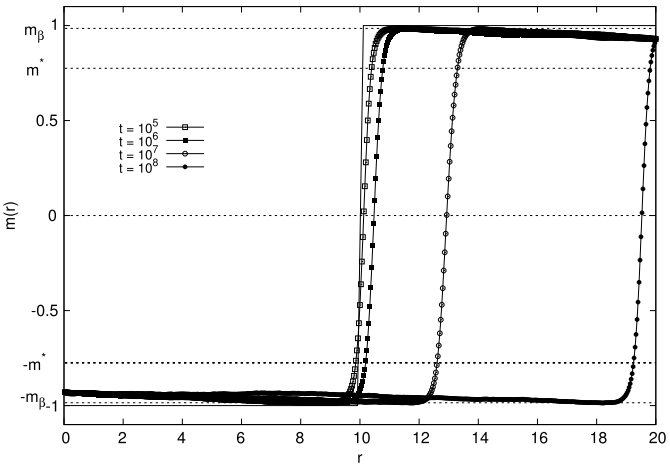

Fig. 2. Magnetization profiles for $C = 1.25$, $m_\beta = 0.985$ and $m^* = 0.775$, and with $m_+ = 0.93$. The curves in the plot have the same meaning of those illustrated in Fig. 1. The initial datum is a step function centered at $r = 10$.

If we decrease m_+ till m_β we see the same pattern with a transition region which is essentially unchanged and the quasi-linear parts with a smaller slope. However if m_+ decreases past m_β keeping $m_+ > m^* = 0.775$ we see a completely different picture (as argued in the next section, the values $|m| \le m^*$ are to be regarded as unstable, $m^* < |m| < m_\beta$ as metastable, and $|m| \ge m^*$ as stable). In Fig. 2 we report simulations with $m_+ = 0.93$. We start now from an initial configuration which has $m_{0,x} = -1$ for $x \le L/2$ and $m_{0,x} = +1$ elsewhere. We observe, after a short transient, a pattern similar to the one in Fig. 1, i.e. with a transition region around the middle which is very similar to the previous one. To its right and left there are again approximately linear profiles but now they are decreasing (because $m_+ < m_\beta$). In contrast to the previous case as time increases on the scale L^2 the transition region moves away from the middle and on times L^3 it "collides" with an endpoint of the channel: in Fig. 2 it is represented by a bump on the right of the channel where the magnetization rapidly increases from $-m_\beta$ to m_+, m_+ the magnetization forced by the right reservoir. If we change the seed of the random generator we may as well see the bump on the left. Such a profile seems stationary as it stays unchanged (modulo small fluctuations) for very long times, our longest simulation has $t = 10^{11}$.