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The Nearest Neighbor Gradient System. A Rigorous Model for a Version of the Minimal Entropy Production Principle

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We prove that a version of the minimal entropy production principle holds rigorously for the nearest neighbor gradient system, whose hydrodynamic behavior we treated in an earlier paper, and study its relation to the macroscopic mass current and local equilibrium of higher order.

KEY WORDS: Minimal entropy production; nearest neighbor gradient system; macroscopic mass current; nonlinear diffusion.

1. INTRODUCTION

The principle of minimal entropy production was noticed already by Kirchhoff in 1848 in his generalization of Ohm's law and thus is even older than Gibbs' variational principle. In the middle of the present century Prigogine and co-workers used it in nonequilibrium thermodynamics to characterize steady states with constraints. For a historical review see Jaynes.[(1)]

An important new application of the minimal entropy production principle seems to be the possibility to derive from it the macroscopic flux via first-order correction of local equilibrium in the transition from microscopic dynamics to macroscopic dynamics in the hydrodynamic limit (see Spohn[(2)] for a detailed heuristic discussion). Nevertheless, its precise meaning, including the assumptions under which it holds, and its significance for the derivation of hydrodynamic equations remain unclear.

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In this situation the rigorous study of simplified molecular models and their macroscopic behavior may help to understand these problems.

One step in this direction is the use of Lyapunov functionals with bounded decay rates as a basic tool in the derivation of the hydrodynamic limit of a deterministic gradient system with nearest neighbor interaction in our paper[3] and of a system of diffusions with nearest neighbor interaction by Guo *et al.*[4] This functional is the negative entropy in the latter model and the energy in ours. Lang[5] characterized the equilibrium states of the same system without the nearest neighbor restriction by the minimality of the energy, whose proof directly can be transferred to our model. Furthermore, the energy strictly decreases otherwise. Thus, it satisfies the characteristic properties of a Lyapunov functional. Already Kirchhoff's case was that of minimal energy dissipation. For our model we shall prefer the notion energy decay, since the energy decreases and does not dissipate into form of energy.

It is the purpose of this paper to study the model of ref. 3 in more detail, with special attention to the minimal entropy production in its present version of the energy decay principle. The main result is its verification for strictly positive macroscopic times in the hydrodynamic limit (Theorem 3.3). We also study the relation between the minimal energy decay, the macroscopic mass current, and local equilibrium of higher order. On a heuristic level we trace the minimal energy decay and the macroscopic mass current back to the validity of local equilibrium of higher order. Rigorously, we derive the macroscopic mass current from the boundedness of the energy decay (Proposition 2.5) and characterize minimal energy decay by a weak from of local equilibrium of higher order (Corollary 2.6). In contrast to Spohn's procedure,[2] who heuristically derived the mass current from a similar characterization, we use in the proof of this characterization the already established mass current.

We often rely on the results of ref. 3, but in order to make the paper self-contained, we first briefly describe the model with the basic results of ref. 3.

The gradient system itself is the time evolution of particles in the Euclidean space $\mathbf{R}^d$, given by the system of equations

$$\frac{dx_i}{dt} = \sum_{j \neq i} \mathbf{F}(x_i - x_j) \qquad (i \in I \subset Z)$$

The force $\mathbf{F}$ is the negative gradient of a symmetric potential Φ. For $d = 1$, e.g. the index set I is either $\mathbf{Z}$ (the infinite case) or $\{1,..., N\}$ (the finite case).

Our model, the finite one-dimensional gradient system with interaction only between neighbor particles, is given by the system of equations

$$\frac{dx_i}{dt} = \sum_{j:\,|j-i|=1} \mathbf{F}(x_i - x_j) = -\mathbf{F}(x_{i+1} - x_i) + \mathbf{F}(x_i - x_{i-1}) \qquad (1 \leqslant i \leqslant N)$$

with $x_i < x_{i+1}$ for $1 \leqslant i \leqslant N-1$.

We consider for $0 < \varepsilon \leqslant \varepsilon_0$ the rescaled system:

$$q_i^\varepsilon(t) := \varepsilon x_i(\varepsilon^{-2} t) \qquad (1 \leqslant i \leqslant N^\varepsilon)$$

which evolves according to the system of equations

$$\frac{dq_i}{dt} = \varepsilon^{-1} \left\{ -\mathbf{F}\left(\frac{q_{i+1} - q_i}{\varepsilon}\right) + \mathbf{F}\left(\frac{q_i - q_{i-1}}{\varepsilon}\right) \right\} \qquad (1 \leqslant i \leqslant N) \quad (1.1)$$

and study its behavior in the hydrodynamic limit, as ε tends to 0. For the sake of transparency we omit the explicit quotation of ε in the notation of the configuration and derived quantities, if this causes no confusion.

There is only one conserved quantity, the particle number, resp. mass, whose local distribution is represented by its empricial measure:

$$\rho_t^\varepsilon := \varepsilon \sum_i \delta_{q_i(t)} \qquad (1.2)$$

The equilibrium states corresponding to a given constant density ρ are characterized by equidistance equal to ρ^{-1} of the particles, except for the case of finite radius R of the range of the potential and density $\rho > R^{-1}$, where the particles only have to have a distance $\geqslant R^{-1}$. One can summarize both cases by claiming equality of the force $\mathbf{F}$ applied to the distance. This conception will turn out to be more natural, as we shall see later.

The main result of ref. 3 is the weak convergence of the measures (1.2) to measures with smooth density ρ_t satisfying the nonlinear diffusion equation

$$\frac{\partial}{\partial t} \rho_t(q) = \frac{\partial^2}{\partial q^2} \left(\mathbf{F}\left(\frac{1}{\rho_t(q)} \right) \right) \qquad (1.3)$$

in a weak sense (see also Theorem 3.1 below).

The proof consists of three steps[3]: compactness of the empirical distributions (1.2), the properties of limit measures with the derivation of Eq. (1.3), and the uniqueness of its solution with prescribed initial distribution. The most difficult part is the second step and it is just there where bounded energy decay is important. The results of the present paper, mainly Theorem 3.1, improve the procedure of this step.

2. VARIATIONAL INEQUALITIES

First we state the assumptions on the potential Φ.

Let Φ: $\mathbf{R}\backslash\{0\} \to \mathbf{R}^+$ be a twice continuously differentiable function with the following properties:

1. Symmetry: $\Phi(q) = \Phi(-q)$ for $q \neq 0$.
2. Convexity: there exists $0 < R \leqslant \infty$ such that Φ is strictly convex on $(0, R]$ and identically 0 on $[R, \infty)$, if $R < \infty$, resp. decreases to 0, as $q \to \infty$, if $R = \infty$.
3. Singularity at 0: (a) $\Phi(q) \to \infty$ as $|q| \to 0$; (b) there exists $\alpha > 0$ such that $|q \cdot \Phi'(q)| \leqslant \alpha\Phi(q)$ for $|q|$ sufficiently small. This condition prevents singularities of infinite order at 0. Remark that we do not need it in the stronger version of ref. 3.

In this section we shall prove asymptotic variational inequalities for the energy and its decay rate as the particle configuration given by (1.2) weakly converges to a given limit measure.

The energy of the configuration $\rho_t^\varepsilon = \varepsilon \sum_i \delta_{q_i(t)}$ is given by

$$H(\rho_t^\varepsilon) := \frac{\varepsilon}{2} \sum_{i,j:\,|i-j|=1} \Phi\left(\frac{q_i - q_j}{\varepsilon}\right) = \varepsilon \sum_i \Phi(d_i) \tag{2.1}$$

with $d_i := (q_{i+1} - q_i)/\varepsilon$ denoting the distances of the particles on the microscopic scale.

The decay rate of the energy

$$\frac{d}{dt} H(\rho_t^\varepsilon) = -D(\rho_t^\varepsilon) \tag{2.2}$$

is easily calculated (see ref. 3):

$$D(\rho_t^\varepsilon) = \varepsilon \sum_i v_i(t)^2 \qquad \text{with} \quad v_i = \varepsilon^{-1}\{-\mathbf{F}(d_i) + \mathbf{F}(d_{i-1})\}$$

[see (1.1)]. Remark that the velocities v_i are functions of the configuration and not independent variables as in the classical dynamics.

The inequalities which we are going to prove are valid for fixed times and do not depend on the dynamics except for the dynamical meaning of the estimated quantities. So we assume that for $0 < \varepsilon \leqslant \varepsilon_0$ we are given configurations $\rho^\varepsilon = \varepsilon \sum_i \delta_q \delta_{q_i}$, which weakly converge to a measure ρ as $\varepsilon \to 0$.

For a heuristic derivation of an asymptotic lower bound of the energy we assume that local equilibrium holds, i.e., d_i is asymptotically locally constant. Then it is easy to see that the limit measure ρ has a density, which we again denote by ρ, and that at least formally $H(\rho^\varepsilon)$ tends to $\int \Phi(1/\rho(q))\,\rho(q)\,dq$. The integrand is taken to be 0 for $\rho(q)=0$, as will be done with similar functions in the sequel without further mentioning. We shall show now that this is indeed an asymptotic lower bound of the energy.

Theorem 2.1. Let $\rho^\varepsilon = \varepsilon \sum_i \delta_{q_i} \to \rho$ weakly as $\varepsilon \to 0$ with $\underline{\lim}_{\varepsilon \to 0} H(\rho^\varepsilon) < \infty$. Then ρ has a density and

$$\underline{\lim}_{\varepsilon \to 0} H(\rho^\varepsilon) \geqslant \int \Phi\left(\frac{1}{\rho(q)}\right) \rho(q)\, dq$$

holds. If $\{D(\rho^\varepsilon),\ 0 < \varepsilon \leqslant \varepsilon_0\}$ is bounded, then

$$H(\rho^\varepsilon) \to \int \Phi\left(\frac{1}{\rho(q)}\right) \rho(q)\, dq \qquad \text{as} \quad \varepsilon \to 0$$

Proof. Let I be a bounded interval with $\rho(\partial I)=0$ and length $|I|$. For i with $q_i,\ q_{i+1} \in I$ there holds by the convexity of Φ

$$\Phi(d_i) \geqslant \Phi(\underline{d}) + \Phi'(\underline{d})(d_i - \underline{d})$$

with the mean value of the inner distances

$$\underline{d} := \frac{\sum_{i:[q_i,q_{i+1}] \subset I} d_i}{\varepsilon^{-1}\rho^\varepsilon(I) - 1} = \frac{\sum_{i:[q_i,q_{i+1}] \subset I} (q_{i+1} - q_i)}{\rho^\varepsilon(I) - \varepsilon} \leqslant \frac{|I|}{\rho^\varepsilon(I) - \varepsilon}$$

By summation over i we get

$$\varepsilon \sum_{i:[q_i,q_{i+1}] \subset I} \Phi(d_i) \geqslant [\rho^\varepsilon(I) - \varepsilon]\, \Phi(\underline{d})$$

since

$$\sum_{i:[q_i,q_{i+1}] \subset I} (d_i - \underline{d}) = 0$$

With $\varepsilon \to 0$ there follows

$$\underline{\lim}_{\varepsilon \to 0}\ \varepsilon \sum_{i:\,[q_i,q_{i+1}] \subset I} \Phi(d_i) \geqslant \rho(I)\, \Phi\left(\frac{|I|}{\rho(I)}\right) \tag{2.3}$$

By approximation this holds for every interval I, and, as in the proof of Theorem 3.1 of ref. 3, it follows that ρ is absolutely continuous with respect to the Lebesgue measure.

We fix again a bounded interval I and denote by $\Pi(I)$ the set of all partitions $\pi = \{I_1,..., I_m\}$ of I into subintervals equipped with the partial order induced by refinement. From (2.3) applied to the subintervals we get

$$\underline{\lim}_{\varepsilon \to 0} \varepsilon \sum_{i:[q_i, q_{i+1}] \subset I} \Phi(d_i) \geqslant \sum_{k=1}^{m} \rho(I_k) \, \Phi\left(\frac{|I_k|}{\rho(I_k)}\right) \tag{2.4}$$

If we attach to each partition $\pi = \{I_1,..., I_m\}$ the function J_π on I with constant value equal to $|I_k|/\rho(I_k)$ on each I_k, then $\{J_\pi;\ \pi \in \Pi\}$ is a martingale on I with respect to the normalized restriction of ρ to I. Furthermore, since Φ is convex, $\{\Phi(J_\pi);\ \pi \in \Pi(I)\}$ is a submartingale with

$$\int_I \Phi(J_\pi)\, d\rho = \sum_{k=1}^{m} \rho(I_k) \Phi\left(\frac{|I_k|}{\rho(I_k)}\right) \qquad \text{with} \quad \pi = \{I_1,..., I_m\}$$

By martingale convergence it follows that in the limit as π becomes arbitrarily fine, $J_\pi(q)$ converges to $\rho(q)^{-1}$, hence $\Phi(J_\pi(q))$ to $\Phi(\rho(q)^{-1})$ a.s. with respect to ρ and

$$\lim_{\pi} \int_I \Phi(J_\pi)\, d\rho = \sup_{\pi} \int_I \Phi(J_\pi)\, d\rho = \int_I \Phi\left(\frac{1}{\rho(q)}\right) \rho(q)\, dq$$

The last statement holds, since $\int_I \Phi(J_\pi)\, d\rho$ is increasing in π with

$$\int_I \Phi(J_\pi)\, d\rho \leqslant \int_I \Phi\left(\frac{1}{\rho(q)}\right) \rho(q)\, dq \qquad \text{for all} \quad \pi \in \Pi(I) \tag{2.5}$$

by Jensen's inequality and

$$\sup_{\pi} \int_I \Phi(J_\pi)\, d\rho \geqslant \int_I \Phi\left(\frac{1}{\rho(q)}\right) \rho(q)\, dq$$

(see, e.g., Billingsley,[6] Theorem 35.4). Since (2.4) is valid for all π, we finally get

$$\underline{\lim}_{\varepsilon \to 0} \varepsilon \sum_{i:q_i \in I} \Phi(d_i) \geqslant \underline{\lim}_{\varepsilon \to 0} \varepsilon \sum_{i:[q_i, q_{i+1}] \subset I} \Phi(d_i) \geqslant \int_I \Phi\left(\frac{1}{\rho(q)}\right) \rho(q)\, dq \tag{2.6}$$

which by approximation also holds for unbounded intervals. For $I = \mathbf{R}$ we get the estimate of Theorem 2.1. But remark that we derived it also locally.

For the derivation of conditions under which the energy becomes asymptotically minimal, we proceed as above with similar, reversed inequalities.

First we notice that accordingly it is sufficient to prove

$$\overline{\lim_{\varepsilon \to 0}}\, \varepsilon \sum_{i:q_i \in I} \Phi(d_i) \leqslant \int_I \Phi\left(\frac{1}{\rho(q)}\right) \rho(q)\, dq$$

for bounded intervals I.

So let I be a bounded interval. For i with q_{i-1} or $q_i \in I$ there holds

$$\Phi(\bar{d}) \geqslant \Phi(d_i) + \Phi'(d_i)(\bar{d} - d_i)$$

with the mean value of the enclosing particle distances

$$\bar{d} := \frac{\sum_{i:[q_{i-1}, q_i] \cap I \neq \varnothing} d_i}{\varepsilon^{-1} \rho^\varepsilon(I) + 1} = \frac{\sum_{i:[q_{i-1}, q_i] \cap I \neq \varnothing} (q_{i+1} - q_i)}{\rho^\varepsilon(I) + \varepsilon} \geqslant \frac{|I|}{\rho^\varepsilon(I) + \varepsilon} \tag{2.7}$$

By summation we get

$$\begin{aligned} &\varepsilon \sum_{i:[q_{i-1}, q_i] \cap I \neq \varnothing} \Phi(d_i) \\ &\quad \leqslant [\rho^\varepsilon(I) + \varepsilon]\, \Phi(\bar{d}) + \varepsilon \sum_{i:[q_{i-1}, q_i] \cap I \neq \varnothing} \mathbf{F}(d_i)(\bar{d} - d_i) \\ &\quad \leqslant [\rho^\varepsilon(I) + \varepsilon]\, \Phi\left(\frac{|I|}{\rho^\varepsilon(I) + \varepsilon}\right) + \varepsilon \sum_{i:[q_{i-1}, q_i] \cap I \neq \varnothing} [\mathbf{F}(d_i) - \mathbf{F}(\bar{d})] \cdot (\bar{d} - d_i) \end{aligned}$$

The added term vanishes, but makes the significance of the sum more transparent, since all its terms become positive by the monotonicity of **F**.

We now take the upper limit as $\varepsilon \to 0$ and apply as above the corresponding inequality to a partition $\pi \in \Pi(I)$. Because of (2.5) the first term of the obtained upper bound can be estimated by the required integral and we finally arrive at the following sufficient condition for asymptotic minimality of the energy.

Lemma 2.2. In addition to the the general assumption of Theorem 2.1, suppose that for every bounded interval I

$$\inf_{\pi \in \Pi(I)} \overline{\lim_{\varepsilon \to 0}} \sum_{k=1}^{m} \varepsilon \sum_{i:[q_{i-1}, q_i] \cap I \neq \varnothing} [\mathbf{F}(d_i) - \mathbf{F}(\bar{d}_k)] \cdot (\bar{d}_k - d_i) = 0$$

with $\pi = \{I_1, \ldots, I_m\}$ and $\bar{d}_k$ defined by (2.7) according to I_k. Then

$$H(\rho^\varepsilon) \to \int \Phi\left(\frac{1}{\rho(q)}\right) \rho(q)\, dq \qquad \text{as} \quad \varepsilon \to 0$$

The condition assumed in this lemma requires that the force applied to the distances of the particles are in the mean asymptotically locally constant, and thus is a weak form of local equilibrium.

To finish the proof of Theorem 2.1, it remains to show that this condition is satisfied in the case of bounded energy decay.

We need the following estimate, which we shall also frequently use later.

Lemma 2.3. For every interval I and $i<j$ with $q_{i+1},\ q_j \in I$ there holds

$$|\mathbf{F}(d_i) - \mathbf{F}(d_j)|^2 \leqslant \rho^\varepsilon(I) \cdot \left(\varepsilon \sum_{k:q_k \in I} v_k^2\right)$$

Proof. By (1.1) there follows

$$|\mathbf{F}(d_j) - \mathbf{F}(d_i)|^2 = \left|\varepsilon \sum_{k=i+1}^{j} v_k\right|^2 \leqslant \varepsilon(j-i)\left(\sum_{k=i+1}^{j} v_k^2\right) \leqslant \rho^\varepsilon(I) \cdot \left(\sum_{k:\, q_k \in I} v_k^2\right)$$

Now let I be a bounded interval and $C>0$ with $D(\rho^\varepsilon) \leqslant C$ for $0<\varepsilon\leqslant\varepsilon_0$. To a given $\eta>0$ there exists $\pi=\{I_1,..., I_m\} \in \Pi(I)$ with $\rho(I_k)\leqslant\eta$ for $1\leqslant k\leqslant m$ and $0<\varepsilon_1\leqslant\varepsilon_0$ such that $\rho^\varepsilon(I_k)\leqslant 2\eta$ for $0<\varepsilon\leqslant\varepsilon_1$ and $1\leqslant k\leqslant m$.

For $1\leqslant k\leqslant m$ we apply Lemma 2.3 to the interval I_k^ε, which slightly enlarges I_k to include the nearest particle to the left and right of I_k. By taking a smaller value of ε_1, if necessary, we may assume that I_k^ε satisfies the same estimate as I_k and that additionally $|I_k^\varepsilon| \leqslant (1+\eta)\,|I_k|$ holds for $0<\varepsilon\leqslant\varepsilon_1$. In the exceptional case that the distance of I_k to the nearest particle to the left, resp. right, does not converge to 0—which can only happen if the density ρ is essentially 0 at the boundary points—we can add, resp., a particle whose distance to I_k tends to 0 macroscopically, but to ∞ on the microscopic scale as $\varepsilon\to 0$, without changing the limit behavior.

We thus get for i, j with $[q_{i-1}, q_i]\cap I_k \neq \varnothing$ and $[q_{j-1}, q_j]\cap I_k \neq \varnothing$,

$$|\mathbf{F}(d_i) - \mathbf{F}(d_j)|^2 \leqslant 2\eta C$$

If we fix i, we may replace d_j by their mean value $\bar{d}_k$:

$$|\mathbf{F}(d_i) - \mathbf{F}(\bar{d}_k)|^2 \leqslant 2\eta C \qquad \text{for } i \text{ with } [q_{i-1}, q_i]\cap I_k \neq \varnothing$$

and thus

$$\begin{aligned} &\sum_{k=1}^{m} \varepsilon \sum_{i:[q_{i-1},q_i]\cap I_k\neq\varnothing} [\mathbf{F}(d_i) - \mathbf{F}(\bar{d}_k)] \cdot (\bar{d}_k - d_i) \\ &\leqslant \sum_{k=1}^{m} \varepsilon \sum_{i:[q_{i-1},q_i]\cap I_k\neq\varnothing} (2\eta C)^{1/2}\, |\bar{d}_k - d_i| \\ &\leqslant \sum_{k=1}^{m} (2\eta C)^{1/2} 2(1+\eta)\,|I_k| = 2(2\eta C)^{1/2}(1+\eta)\,|I| \end{aligned}$$

Since $\eta > 0$ was arbitrary, the condition of Lemma 2.2 is satisfied, as required.

For a heuristic derivation of an asymptotic lower bound of the energy decay, the assumption of local equilibrium is too weak, since it does not determine its value uniquely. We have to claim an even smoother behavior and assume that the rescaled differences $(d_{i+1} - d_i)/\varepsilon$ of the microscopic distances d_i of the particles are asymptotically locally constant. This implies, formally, that the limit density is sufficiently smooth and that $(d_{i+1} - d_i)/\varepsilon$ is approximately equal to $\{(\partial/\partial q)[1/\rho(q)]\} \cdot [1/\rho(q)]$ for q_i near q.

From this we conclude

$$v_i \approx -\left\{\frac{\partial}{\partial q}\mathbf{F}\left(\frac{1}{\rho(q)}\right)\right\}\cdot\frac{1}{\rho(q)} \quad \text{for} \quad q_i \approx q \tag{2.8}$$

$$D(\rho^\varepsilon) \approx \int \left[\left\{\frac{\partial}{\partial q}\mathbf{F}\left(\frac{1}{\rho(q)}\right)\right\}\cdot\frac{1}{\rho(q)}\right]^2 \rho(q)\,dq$$

$$= \int \left\{\frac{\partial}{\partial q}\mathbf{F}\left(\frac{1}{\rho(q)}\right)\right\}^2 \cdot\frac{1}{\rho(q)}\,dq$$

It seems likely that the energy decay corresponding to these states is minimal, which is established in the following theorem. Later we shall characterize minimal energy decay by a rigorous version of local equilibrium of higher order.

Theorem 2.4. Let $\rho^\varepsilon \to \rho$ as $\varepsilon \to 0$ with $\underline{\lim}_{\varepsilon \to 0} D(\rho^\varepsilon) < \infty$. Then ρ has a bounded density, which can be chosen such that $\mathbf{F}(1/\rho)$ is an absolutely continuous function with

$$\underline{\lim}_{\varepsilon \to 0}\, D(\rho^\varepsilon) \geq \int \left\{\frac{\partial}{\partial q}\mathbf{F}\left(\frac{1}{\rho(q)}\right)\right\}^2 \cdot\frac{1}{\rho(q)}\,dq$$

Proof. In order to show that ρ has a bounded density, we may assume without restriction that $\{D(\rho^\varepsilon),\ 0 < \varepsilon \leq \varepsilon_0\}$ is bounded by using only a suitable subsequence. Then by Lemma 2.3 applied to $I = \mathbf{R}$ it follows that $|\mathbf{F}(d_i) - \mathbf{F}(d_j)|$ is bounded independently of $0 < \varepsilon \leq \varepsilon_0$ and i, j. Since there is evidently one i for each ε such that $|\mathbf{F}(d_i)|$ is bounded, $|\mathbf{F}(d_j)|$ is bounded independently of ε and j. By the singularity of $\mathbf{F}$ the rescaled distances d_j are bounded away from 0 and thus ρ has a bounded density.

We fix a bounded interval of the form $I = [a, b)$ $(a < b)$ and take $0 < \delta < (b-a)/2$. First we assume $\rho([a, a+\delta)) \leq \rho([b-\delta, b))$. There exists $q_i \in [a, a+\delta)$ with

$$\varepsilon d_i = q_{i+1} - q_i \geq \frac{\delta}{\varepsilon^{-1}\rho^\varepsilon([a, a+\delta))}$$

and $q_j \in [b-\delta, b)$ with

$$\varepsilon d_j = q_{j+1} - q_j \leqslant \frac{\delta}{\varepsilon^{-1}\rho^{\varepsilon}([b-\delta, b))}$$

such that

$$\mathbf{F}(d_j) - \mathbf{F}(d_i) \geqslant \mathbf{F}\left(\frac{\delta}{\rho^{\varepsilon}([a, a+\delta))}\right) - \mathbf{F}\left(\frac{\delta}{\rho^{\varepsilon}([b-\delta, b))}\right)$$

As $\varepsilon \to 0$ the right-hand side becomes positive, and it follows from Lemma 2.3 that

$$\left|\mathbf{F}\left(\frac{\delta}{\rho([a, a+\delta))}\right) - \mathbf{F}\left(\frac{\delta}{\rho([b-\delta, b))}\right)\right|^2 \leqslant \rho(I) \cdot \varliminf_{\varepsilon \to 0}\left(\varepsilon \sum_{k: q_k \in I} v_k^2\right)$$

One derives the same estimate analogously in the case $\rho([a, a+\delta)) \geqslant \rho([b-\delta, b))$. As in the proof of Theorem 2.1 it follows that $\rho(I_\delta)/|I_\delta| \to \rho(q)$ as $|I_\delta| \to 0$ with $q \in I_\delta$ for all q outside a set of Lebesgue measure 0.

For a, b outside this set we get, as $\delta \to 0$,

$$\varliminf_{\varepsilon \to 0}\left(\varepsilon \sum_{k: q_k \in I} v_k^2\right) \geqslant \frac{1}{\rho([a, b))}\left|\mathbf{F}\left(\frac{1}{\rho(b)}\right) - \mathbf{F}\left(\frac{1}{\rho(a)}\right)\right|^2 \tag{2.9}$$

We understand the right-hand side as 0 if $\rho([a, b)) = 0$.

In the following we set $C = \varliminf_{\varepsilon \to 0}(\varepsilon \sum_k v_k^2)$.

For disjoint intervals $I_k = [a_k, b_k)$ $\{1 \leqslant k \leqslant m\}$ with a_k, b_k outside the set of measure 0 there follows from (2.9)

$$\sum_{k=1}^{m} \frac{1}{\rho([a_k, b_k))}\left|\mathbf{F}\left(\frac{1}{\rho(b_k)}\right) - \mathbf{F}\left(\frac{1}{\rho(a_k)}\right)\right|^2 \leqslant C \tag{2.10}$$

and

$$\begin{aligned}
&\sum_{k=1}^{m}\left|\mathbf{F}\left(\frac{1}{\rho(b_k)}\right) - \mathbf{F}\left(\frac{1}{\rho(a_k)}\right)\right| \\
&\quad \leqslant \left\{\sum_{k=1}^{m} \frac{1}{\rho([a_k, b_k))}\left|\mathbf{F}\left(\frac{1}{\rho(b_k)}\right) - \mathbf{F}\left(\frac{1}{\rho(a_k)}\right)\right|^2\right\}^{1/2}\left\{\sum_{k=1}^{m} \rho([a_k, b_k))\right\}^{1/2} \\
&\quad \leqslant \sqrt{C}\left\{\sum_{k=1}^{m} \rho([a_k, b_k))\right\}^{1/2}
\end{aligned}$$

Thus, we can choose the value of ρ on the set of measure 0 such that $\mathbf{F}(1/\rho)$ is an absolutely continuous function with respect to ρ and consequently with respect to the Lebesgue measure, too.

Now we fix $I = [a, b)$ and apply the estimates above to the case that $I_k = [a_k, a_{k+1})$ $\{1 \leqslant k \leqslant m\}$ is a partition of I into subintervals. If we attach to this partition the function with constant value equal to

$$\frac{1}{\rho([a_k, a_{k+1}))}\left[\mathbf{F}\left(\frac{1}{\rho(a_{k+1})}\right) - \mathbf{F}\left(\frac{1}{\rho(a_k)}\right)\right]$$

on each I_k, this is again a martingale with respect to the same partial order and measure as in the proof of Theorem 2.1. By (2.10) its $L^2(\rho|_I)$-norms are bounded independently of the partition. Hence, in the limit as the partition becomes arbitrarily fine, the martingale converges a.s. with respect to ρ and in $L^2(\rho|_I)$ to the function

$$\left\{\frac{1}{\rho(q)} \cdot \frac{\partial}{\partial q} \mathbf{F}\left(\frac{1}{\rho(q)}\right)\right\}$$

Thus, (2.10) becomes in the limit

$$\int_I \left\{\frac{\partial}{\partial q} \mathbf{F}\left(\frac{1}{\rho(q)}\right)\right\}^2 \cdot \frac{1}{\rho(q)}\, dq \leqslant C = \varliminf_{\varepsilon \to \infty} \left(\varepsilon \sum_k v_k^2\right)$$

and with $I \uparrow \mathbf{R}$ the desired estimate follows.

We now determine the macroscopic flux, in our case the mass current, under the assumption of the boundedness of the energy decay. The mass current turns out to be the same as one formally gets by the approximation (2.8).

Proposition 2.5. Let $\rho^\varepsilon \to \rho$ as $\varepsilon \to 0$ with bounded $\{D(\rho^\varepsilon), 0 < \varepsilon \leqslant \varepsilon_0\}$. Then the empirical velocity distribution $v^\varepsilon := \varepsilon \sum_i v_i \delta_{q_i}$ converges weakly to the signed measure with the density $-(\partial/\partial q)\, \mathbf{F}(1/\rho(q))$.

Proof. Let $q \in \mathbf{R}$ be such that $\rho(I_\delta)/|I_\delta| \to \rho(q)$ as $\delta \to 0$ with $I_\delta = [q - \delta, q + \delta]$. We can assume without restriction

$$d_{\min}(I_\delta) \cdot \rho^\varepsilon(I_\delta) \leqslant |I_\delta| \leqslant d_{\max}(I_\delta) \cdot \rho^\varepsilon(I_\delta) \tag{2.11}$$

with

$$d_{\min}(I_\delta) = \min\{d_i\colon [q_i, q_{i+1}] \subset I_\delta\}$$

and corresponding $d_{\max}(I_\delta)$. This relation might fail for finite ε because of particle distances at the boundary, but, as in the proof of Theorem 2.1, we can add a resp. particle near the boundary, if necessary, such that (2.11) strictly holds, without changing the limit behavior.

We apply Lemma 2.3 to $d_j = d_{\min}(I_\delta)$ and $d_{\max}(I_\delta)$ and get by (2.11) and the monotonocity of $\mathbf{F}$

$$\left|\mathbf{F}(d_i) - \mathbf{F}\left(\frac{|I_\delta|}{\rho^\varepsilon(I_\delta)}\right)\right|^2 \leqslant \rho^\varepsilon(I_\delta) \cdot \left(\varepsilon \sum_{k:q_k \in I_\delta} v_k^2\right) \tag{2.12}$$

for i with $[q_i, q_{i+1}] \subset I_\delta$.

We set $d^\varepsilon(q) = d_i$ with i such that $q_i < q \leqslant q_{i+1}$ holds, and hence

$$v^\varepsilon((-\infty, q)) = \varepsilon \sum_{k:q_k < q} v_k = -\mathbf{F}(d^\varepsilon(q))$$

Taking this i in (2.12), we get

$$\left|v^\varepsilon((-\infty, q)) + \mathbf{F}\left(\frac{|I_\delta|}{\rho^\varepsilon(I_\delta)}\right)\right|^2 \leqslant \rho^\varepsilon(I_\delta) \cdot \left(\varepsilon \sum_{k:q_k \in I_\delta} v_k^2\right)$$

By letting first ε and then δ tend to 0, there follows

$$v^\varepsilon((-\infty, q)) \to -\mathbf{F}\left(\frac{1}{\rho(q)}\right) \qquad \text{as} \quad \varepsilon \to 0$$

Since, by Theorem 2.4, the limit is an absolutely continuous function and we proved the convergence for q outside a set of Lebesgue measure 0, the result follows.

From (2.12) one can easily deduce the validity of local equilibrium in the following form:

To $\eta > 0$ and q there exist $\varepsilon_1 > 0$ and $\delta > 0$ with $|\mathbf{F}(d_i^\varepsilon) - \mathbf{F}(1/\rho(q))| \leqslant \eta$ for $0 < \varepsilon \leqslant \varepsilon_1$ and $0 \leqslant |q_i - q| \leqslant \delta$.

Here we marked the ε dependence of d_i for clearness.

Proposition 2.5 and its proof are improvements of Theorem 3.3 of ref. 3. The main difference consists in the fact that in ref. 3 we derived the limit of the empirical velocity distribution under the assumption that the limit exists. For the additional existence proof we needed the stronger assumption on the potential.

With Proposition 2.5 we are able to give the promised characterization of minimal energy decay. For that purpose let I be again a fixed, bounded interval and $\pi = \{I_1, ..., I_m\} \in \Pi(I)$. We approximate the velocities of the particles in each subinterval by their mean:

$$\langle v_k \rangle = \frac{\sum_{i:q_i \in I_k} v_i}{\varepsilon^{-1}\rho^\varepsilon(I_k)} = \frac{\varepsilon \sum_{i:q_i \in I_k} v_i}{\rho^\varepsilon(I_k)} \qquad (1 \leqslant k \leqslant m) \tag{2.13}$$

Then

$$\frac{\varepsilon \sum_{i:q_i \in I_k} (v_i - \langle v_k \rangle)^2}{\rho^\varepsilon(I_k)} = \frac{\varepsilon \sum_{i:q_i \in I_k} v_i^2}{\rho^\varepsilon(I_k)} - \langle v_k \rangle^2$$

$$\varepsilon \sum_{i:q_i \in I} v_i^2 = \sum_{k=1}^{m} \rho^\varepsilon(I_k) \langle v_k \rangle^2 + \varepsilon \sum_{k=1}^{m} \sum_{i:q_i \in I_k} (v_i - \langle v_k \rangle)^2$$

Since by Proposition 2.5

$$\sum_{k=1}^{m} \rho^\varepsilon(I_k) \langle v_k \rangle^2 \to \sum_{k=1}^{m} \rho^\varepsilon(I_k)^{-1} \left[\int_{I_k} -\frac{\partial}{\partial q} \mathbf{F}\left(\frac{1}{\rho(q)}\right) dq \right]^2 \qquad \text{as} \quad \varepsilon \to 0$$

and by the martingale convergence of Theorem 2.4

$$\lim_{\pi} \sum_{k=1}^{m} \rho^\varepsilon(I_k)^{-1} \left[\int_{I_k} -\frac{\partial}{\partial q} \mathbf{F}\left(\frac{1}{\rho(q)}\right) dq \right]^2 = \int_I \left\{ \frac{\partial}{\partial q} \mathbf{F}\left(\frac{1}{\rho(q)}\right) \right\}^2 \cdot \frac{1}{\rho(q)} dq$$

we get the following characterization.

Corollary 2.6. Under the assumptions of Theorem 2.4

$$D(\rho^\varepsilon) \to \int \left\{ \frac{\partial}{\partial q} \mathbf{F}\left(\frac{1}{\rho(q)}\right) \right\}^2 \cdot \frac{1}{\rho(q)} dq \qquad \text{as} \quad \varepsilon \to 0$$

if and only if

$$\lim_{\pi} \overline{\lim_{\varepsilon \to 0}} \, \varepsilon \sum_{k=1}^{m} \sum_{i:q_i \in I_k} (v_i - \langle v_k \rangle)^2 = 0$$

with $\langle v_k \rangle$ given by (2.3).

This condition says that the velocities are in the mean asymptotically locally constant. It requires not only that the force applied to the distances of the particles be asymptotically locally constant as in the condition of Lemma 2.2, but also their rescaled differences, and thus is a weak form of local equilibrium of a higher order.

Using states with this property, we see that Theorem 2.4 can be strengthened to a variational principle:

$$\inf_{\rho^\varepsilon \to \rho} D(\rho^\varepsilon) = \int \left\{ \frac{\partial}{\partial q} \mathbf{F}\left(\frac{1}{\rho(q)}\right) \right\}^2 \cdot \frac{1}{\rho(q)} dq$$

with a given density ρ.

3. VARIATIONAL PRINCIPLES

We return to the dynamics (1.1) and apply the results of the previous section to its empirical mass distribution ρ_t^ε. As mentioned in the introduction, we are not concerned with the derivation of the existence of limit distributions. So we assume that $\rho_t^\varepsilon \to \rho_t$ weakly as $\varepsilon \to 0$ for $0 \leqslant t \leqslant T$ for some $T > 0$, with bounded energy at time $t = 0$:

$$H(\rho_0^\varepsilon) \leqslant E \qquad \text{for} \quad 0 < \varepsilon \leqslant \varepsilon_0 \tag{3.1}$$

There follows for $0 < t \leqslant T$ and $0 < \varepsilon \leqslant \varepsilon_0$ (see Lemma 2.1 of ref. 3)

$$H(\rho_t^\varepsilon) \leqslant E \qquad \text{and} \qquad D(\rho_t^\varepsilon) \leqslant E/t$$

By the boundedness of the energy decay for $t > 0$, there follows from Theorem 2.1 the convergence of the energy to its minimal value. Before we derive the more difficult minimality of the energy decay, we deduce from Proposition 2.5 that the derived mass current really determines the macroscopic dynamics.

Theorem 3.1. Let $\rho_t^\varepsilon \to \rho_t$ weakly as $\varepsilon \to 0$ for $0 \leqslant t \leqslant T$ with (3.1). Then the limit distributions $\{\rho_t, 0 \leqslant t \leqslant T\}$ are weakly continuous in t and satisfy the nonlinear diffusion equation

$$\frac{\partial}{\partial t} \rho_t(q) = \frac{\partial^2}{\partial q^2} \left(\mathbf{F} \left(\frac{1}{\rho_t(q)} \right) \right)$$

in the weak sense:

$$\frac{d}{dt} \int \varphi(q)\, \rho_t(q)\, dq = -\int \varphi'(q) \frac{\partial}{\partial q} \left(\mathbf{F} \left(\frac{1}{\rho_t(q)} \right) \right) dq$$

for $0 < t < T$ and sufficiently smooth test functions φ.

The proof is an easy consequence of Proposition 2.5 (see proof of Corollary 3.4 of ref. 3).

For the proof of the minimality of the energy decay, we have to study the limit behavior of the energy and its decay rate in more detail. We denote their minimal values as functionals of the limit density:

$$\underline{H}(\rho) = \int \Phi \left(\frac{1}{\rho(q)} \right) \rho(q)\, dq$$

$$\underline{D}(\rho) = \int \left\{ \frac{\partial}{\partial q} \mathbf{F} \left(\frac{1}{\rho(q)} \right) \right\}^2 \cdot \frac{1}{\rho(q)}\, dq$$

Since $H(\rho_t^\varepsilon) \to \underline{H}(\rho_t)$ as $\varepsilon \to 0$ for $t>0$, $\underline{H}(\rho_t)$ is convex and decreasing in $t>0$. We shall show now that (2.2) holds for the minimal values, too, i.e., $\underline{D}(\rho_t)$ is the decay rate of $\underline{H}(\rho_t)$.

Lemma 3.2. For $0<s<t\leqslant T$ there holds

$$\underline{H}(\rho_t)-\underline{H}(\rho_s)=-\int_s^t \underline{D}(\rho_r)\,dr$$

As a consequence, $\underline{D}(\rho_t)$ is decreasing in $t>0$.

Proof. The proof uses methods of Alt and Luckhaus.[7] We consider the function

$$g(x)=x\Phi\left(\frac{1}{x}\right) \quad \text{for } x>0 \qquad \text{and} \qquad g(0)=0$$

such that $\underline{H}(\rho)=\int g(\rho(q))\,dq$ holds. Simple calculations show that g is increasing and convex and satisfies the relation

$$xg''(x)=\frac{d}{dx}\mathbf{F}\left(\frac{1}{x}\right)$$

By the convexity it follows for $r>0$, $h>0$ that

$$g(\rho_{r+h}(q))-g(\rho_r(q))\geqslant g'(\rho_r(q))\cdot[\rho_{r+h}(q)-\rho_r(q)]$$
$$g(\rho_r(q))-g(\rho_{r+h}(q))\geqslant g'(\rho_{r+h}(q))\cdot[\rho_r(q)-\rho_{r+h}(q)]$$

and by integration

$$\frac{\underline{H}(\rho_{r+h})-\underline{H}(\rho_r)}{h}\geqslant\int g'(\rho_r(q))\cdot\frac{\rho_{r+h}(q)-\rho_r(q)}{h}\,dq$$

$$\frac{\underline{H}(\rho_{r+h})-\underline{H}(\rho_r)}{h}\leqslant\int g'(\rho_{r+h}(q))\cdot\frac{\rho_{r+h}(q)-\rho_r(q)}{h}\,dq$$

Theorem 2.4 and the boundedness of the derivative[8,9] for strictly positive times [condition (4.4) of ref. 9 is easily verified in our case] allow the function $g'(\rho_r)$ to be chosen as a test function in Theorem 3.1. We integrate these inequalities with respect to time between s and t and take the limit $h\to 0$. By Theorem 3.1 one easily sees that both right-hand sides converge to

$$\int_s^t\left[\int\frac{\partial}{\partial q}g'(\rho_r(q))\cdot\frac{\partial}{\partial q}\mathbf{F}\left(\frac{1}{\rho_r(q)}\right)dq\right]dr$$
$$=-\int_s^t\left\{\int\frac{1}{\rho_r(q)}\cdot\left[\frac{\partial}{\partial q}\mathbf{F}\left(\frac{1}{\rho_r(q)}\right)\right]^2dq\right\}dr=-\int_s^t\underline{D}(\rho_r)\,dr$$

and the left-hand side by continuity

$$\int_s^t \frac{\underline{H}(\rho_{r+h})-\underline{H}(\rho_r)}{h}\,dr=\frac{1}{h}\int_t^{t+h}\underline{H}(\rho_r)\,dr-\frac{1}{h}\int_s^{s+h}\underline{H}(\rho_r)\,dr\to\underline{H}(\rho_t)-\underline{H}(\rho_s)$$

Finally we prove the minimality of the energy decay. With the already established minimality of the energy we have the following result.

Theorem 3.3. Let $\rho_t^\varepsilon\to\rho_t$ weakly as $\varepsilon\to 0$ for $0\leqslant t\leqslant T$ with (3.1). Then, as $\varepsilon\to 0$,

$\underline{H}(\rho_t^\varepsilon)\to\underline{H}(\rho_t)$ for $0<t\leqslant T$

$\underline{D}(\rho_t^\varepsilon)\to\underline{D}(\rho_t)$ for those $0<t\leqslant T$ at which $\underline{D}(\rho_t)$ is left-continuous, which holds except for at most countably many t

Proof. Let $\underline{D}(\rho_t)$ be left-continuous at a fixed $t>0$ and assume that the energy decay does not converge to its minimal value at t. Then there exists $\eta>0$ and a sequence $\varepsilon_n\to 0$ with

$$D(\rho_t^{\varepsilon_n})\geqslant\underline{D}(\rho_t)+\eta\qquad\text{for}\quad n\geqslant 1$$

Because of the left-continuity there exists $\delta>0$ with

$$\underline{D}(\rho_t)\leqslant\underline{D}(\rho_s)\leqslant\underline{D}(\rho_t)+\eta/2\qquad\text{for}\quad t-\delta\leqslant s\leqslant t$$

There follows

$$H(\rho_t^{\varepsilon_n})-H(\rho_{t-\delta}^{\varepsilon_n})=-\int_{t-\delta}^t D(\rho_s^{\varepsilon_n})\,ds\leqslant-\delta D(\rho_t^{\varepsilon_n})\leqslant-\delta(\underline{D}(\rho_t)+\eta)$$

$$\underline{H}(\rho_t)-\underline{H}(\rho_{t-\delta})=-\int_{t-\delta}^t\underline{D}(\rho_s)\,ds\geqslant-\delta(\underline{D}(\rho_t)+\eta/2)$$

which leads with $\varepsilon_n\to 0$ to a contradiction.

The fact that a monotone function has at most countably many discontinuities is well known.

NOTE ADDED IN PROOF

For a more detailed summary of ref. 3 and the present paper with additional results as e.g. the local behavior of the energy and the motion of a tagged particle see M. G. Mürmann. The hydrodynamic behavior of a one-dimensional nearest neighbor gradient system. (Unpublished manuscript, Universität Heidelberg, 1990.)

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REFERENCES

1. E. T. Jaynes, The minimum entropy production principle, in *Annual Review of Physical Chemistry*, S. Rabinovitch, ed. (Annual Reviews, Palo Alto, California, 1980).
2. H. Spohn, Large scale dynamics of interacting particles, Preprint (1989).
3. M. G. Mürmann, The hydrodynamic limit of a one-dimensional nearest neighbor gradient system, *J. Stat. Phys.* **48**:769–788 (1987).
4. M. Z. Guo, G. C. Papanicolaou, and S. R. S. Varadhan, Nonlinear diffusion limit for a system with nearest interactions, *Commun. Math. Phys.* **118**:31–59 (1988).
5. R. Lang, On the asymptotic behaviour of infinite gradient systems, *Commun. Math. Phys.* **65**:129–149 (1979).
6. P. Billingsley, *Probability and Measure*, 2nd ed. (Wiley, New York, 1986).
7. H. W. Alt and S. Luckhaus, Quasilinear elliptic-parabolic differential equations, *Math. Z.* **183**:311–341 (1983).
8. A. S. Kalashnikov, On the differential properties of generalized solutions of equations of the nonsteady-state filtration type, *Vestnik Moskov Univ. Ser. I Math. Mekh.* **29**:62–68 (transl. 48–53) (1974).
9. J. L. Vazquez, Behaviour of the velocity of one-dimensional flows in porous media, *Trans. Am. Math. Soc.* **286**:787–802 (1984).