Journal of Statistical Physics, Vol. 125, No. 3, November 2006 (© 2006)
DOI: 10.1007/s10955-006-9201-0

Lattice Gas with Finite-Range Interaction Under Gravity[1,2]

Karl Grill[3] and Christian Tutschka[4]

Received January 17, 2006; accepted August 28, 2006
Published Online: October 6, 2006

Existence of a phase separation is proved for a classical lattice gas with finite-range pair potential under the action of a weak gravitational field.

KEY WORDS: phase separation, lattice gas, finite-range, gravitational field, weak limits

1. INTRODUCTION

Recently, we uncovered a well-delineated phase separation for a one-dimensional classical fluid with next neighbor interactions in a weak gravitational field.[(2)] We showed that one can identify, with probability tending to one as the size of the system approaches infinity, three regions: a dense part at the bottom, which we called the condensate, a dilute part at the top, called the gas, and in between these two phases an interface whose relative width goes to zero as the number of particles goes to infinity.

The next step was clearly to drop the next neighbor assumption. The global effect of weak gravitational forces on the equilibrium structure of hard rods with finite-range interactions has been studied in Ref. 1. It turned out that the overall

[1] One of the authors (C.T.) is greatly indebted to the Schrödinger Institute for a Junior Research Fellowship in Mathematics and Mathematical Physics during the 2004/05 winter semester at which time this work was begun.

[2] We would like to dedicate this paper to Jerry Percus on the happy occasion of his 80th birthday.

[3] Institut für Statistik und Wahrscheinlichkeitstheorie, TU Wien, 1040 Wien, Austria; e-mail: grill@ci.tuwien.ac.at

[4] Institut für Theoretische Physik, TU Wien, 1040 Wien, Austria; e-mail: christian.tutschka@tuwien.ac.at

qualitative behavior we found for the special class of next neighbor interactions prevails in this more general situation. That is, the phenomenon appears to be robust with respect to changes in the interactions.

The purpose of the present paper is to extend this work to D-dimensional space. To allow for the phenomenology without unnecessary structural details, we consider a particle system in a subset Λ of the D-dimensional integer lattice $\mathbb{Z}^D$, with finite-range forces, and in a weak external (gravitational) field.

More specifically, pick $\Lambda = ([0, N] \cap \mathbb{Z})^D$, and for a configuration $x \in \{0, 1\}^\Lambda$ let the potential energy of the system be given by (see, e.g., Ruelle [8])

$$U_\Lambda(x) = \sum_{i,j\in\Lambda, i\neq j} V(i-j)x_i x_j + g\sum_{i\in\Lambda} i_1 x_i.$$

The pairwise interaction V is assumed to be finite, attractive, and of finite range r, so $-\infty < V \leq 0$ and $V(i) = 0$ if $\|i\| > r$ ($\|\ \|$ is the usual Euclidean norm). Furthermore, we suppose that V is symmetric

$$V(-i) = V(i), \tag{1.1}$$

translation invariant, and not identically zero. The second term of the formula for U_Λ represents the effect of a homogeneous gravitational field of strength g that exerts its force along the first coordinate. Here we selected units such that the mass of the particles equals one.

Classical equilibrium statistical mechanics is defined by the finite-volume Gibbs probability measure $\mathbb{P}_\Lambda$ which assigns to each configuration $x \in \{0, 1\}^\Lambda$ the probability (see, e.g., Ruelle [8])

$$\mathbb{P}_\Lambda(x) = \frac{1}{Z_\Lambda}\exp[-\beta H_\Lambda(x)]$$

with

$$H_\Lambda(x) = U_\Lambda(x) - \mu\sum_{i\in\Lambda} x_i$$

and the normalization

$$Z_\Lambda = \sum_{x\in\{0,1\}^\Lambda} \exp[-\beta H_\Lambda(x)].$$

The parameter β represents the reciprocal temperature, and μ is to be interpreted as chemical potential. The chemical potential is used to control the number of particles. Within the framework of the present article, the number of particles is close to its expectation with probability approaching one as N tends to infinity. So, for sufficiently large N, the isothermal measure (see, e.g., Ruelle [8]), which is obtained by conditioning on the total number of particles, is, essentially, equivalent to the Gibbs measure with appropriately chosen parameters.

2. THEOREM

The formulation of our theorem has been inspired by some experimental evidence due to Pierański.(7) He observed a separation of phases for a classical system of hard disks under gravity. This says that the general case might not differ too much from the case without attractive interactions and motivates the following definition.

For a subset I of Λ and a given configuration $x \in \{0, 1\}^I$, let

$$\mathbb{P}_I^0(x) = \frac{1}{Z_I^0} \exp\left[-\beta H_I^0(x)\right]$$

with

$$H_I^0(x) = g \sum_{i \in I} i_1 x_i - \mu \sum_{i \in I} x_i$$

and again the partition function

$$Z_I^0 = \sum_{x \in \{0,1\}^I} \exp\left[-\beta H_I^0(x)\right].$$

This distribution is very handy, because under this distribution the values x_i are independent with

$$\mathbb{P}_I^0(x_i = 1) = p_i = \frac{1}{1 + \exp[\beta(g i_1 - \mu)]}.$$

The two subsystems condensate and gas are defined next. Let us say that a particle is part of the condensate if it is connected to some other particle and call an assembly of unconnected particles gas. Here there are at least two reasonable definitions of what connected should mean. Namely that we can call two particles connected if they are next neighbors; i.e., their coordinates i and j satisfy $\|i - j\| = 1$, or we can call them connected if they interact via the attractive tail of the pair potential; i.e., $V(i - j) \neq 0$.(3) In this fashion we call two particles connected if $\|i - j\| \leq r$.

Moreover, consider the boundary of a set $I \subset \Lambda$ as the set of members of I that are connected to the outside,

$$\partial I = \{i \in I : \exists j \in \Lambda \setminus I : \|i - j\| \leq r\},$$

and introduce a few microscopic sums:

$$S_I(x) = \sum_{i \in I} x_i,$$

$$T_I(x) = \sum_{i \in I, \sum_{j \in I, i \neq j} V(i-j) x_j \neq 0} x_i,$$

$$V_I(x) = \sum_{i,j \in I, i \neq j} V(i-j) x_i x_j,$$

and

$$V_{I,J}(x) = \sum_{i \in I, j \in J} V(i-j) x_i x_j.$$

Now, we can formulate the following

Theorem. *Let $\beta \in (0, \infty)$ and $\rho \in (0, 1)$ be given and let $\mu = \mu_N$ and $g = g_N$ vary with N in such a way that*

$$\mu_N \to \infty \quad \textit{and} \quad \frac{\mu_N}{\log N} \to 0,$$

as well as

$$\frac{\mu_N}{g_N N} \to \rho.$$

Then, for any $\epsilon > 0$ there is a constant $M(\epsilon) \in (0, \infty)$ such that, for

$$N_1 = \frac{\beta \mu_N - M(\epsilon)}{\beta g_N}$$

and

$$N_2 = \frac{\beta \mu_N + M(\epsilon)}{\beta g_N},$$

with probability tending to one as N tends to infinity, the following conclusions hold.

(1) All connected subsets I of $[0, N_1] \times [0, N]^{D-1}$ with $x_i = 0$ for all $i \in I$ satisfy $|I| < \epsilon \log N$.
(2) All connected subsets I of $[N_2, N] \times [0, N]^{D-1}$ with $x_i = 1$ for all $i \in I$ satisfy $|I| < \epsilon \log N$.
(3) For all hypercubes $C = \prod_{i=1}^{D} [a_i, a_i + l]$ with $a_i \in [0, N - l]$, $l > N^\alpha$, $\alpha \in (0, 1)$, and $C \subset [0, N_1] \times [0, N]^{D-1}$,

$$S_C \geq (1 - \epsilon)|C|.$$

(4) For all hypercubes $C = \prod_{i=1}^{D} [a_i, a_i + l]$ with $a_i \in [0, N - l]$, $l > N^\alpha$, $\alpha \in (0, 1)$, and $C \subset [N_2, N] \times [0, N]^{D-1}$,

$$(1 - \epsilon)\mathbb{E}_C^0(S_C) \leq S_C \leq (1 + \epsilon)\mathbb{E}_C^0(S_C) \tag{2.1}$$

as well as

$$T_C \leq \epsilon \mathbb{E}_C^0(S_C). \tag{2.2}$$

3. REMARKS

(1) For a system of macroscopic size, we see, with high probability, a condensed phase at heights below N_1 which contains only small bubbles of a gaseous phase.

(2) At heights above N_2, we find a gaseous phase with only small drops of condensate, and, in addition, we have an approximate barometric equation (see, e.g., Kittel [5]), because the local density at height i_1 is close to p_i which in turn is about $\exp[-\beta(gi_1 - \mu)]$.

(3) We also see that the density $S_\Lambda/|\Lambda|$ tends to ρ in probability as $N \to \infty$.

(4) The relative width of the interface, i.e., $(N_2 - N_1)/N$, goes to zero slower than $1/\log N$ as $N \to \infty$. One could achieve a rate $O(1/\log N)$ just by letting $\beta\mu_N = c \log N$, but then one has to bound the exponent α away from zero, and if $\beta\mu_N$ is growing even faster, the probability that there is a particle above $N_1 + \epsilon N$ tends to zero, so the gas phase disappears completely. Hence, if we want a gaseous phase, the smallest order that can be achieved for the relative width of the interface is $1/\log N$.

(5) Let us point out that many-particle systems with a density profile going from minimum to maximum density over a relatively small interval arise in gravitational astrophysics and space science, as well (see, e.g., Stahl *et al.* [9]). There, local particle densities of core-atmosphere type signify the low temperature phase of a gravitational phase transition. The existence of a gravitational phase transition has been proved by Kiessling in 1989.[4]

(6) It may also be noted that local thermodynamics is adequate in the presence of a very slowly varying external field (cf. Percus [6]).

(7) We further observe that our approach to the one-dimensional case uses the one-sided Boltzmann factor and the fact that the relative distances of the particles have pleasant stochastic properties.[1,2] These features are not available in higher dimensions, and consequently a new method of proof is developed in Sec. 4.

(8) Finally, let us see if our theory can be put into weak quantitative agreement with Pierański's results. To present this comparison most effectively, it will be convenient to consider Fig. 4 from Ref. 7: We notice, first, that the relative volume has been 1.3 and that 7500 particles have been used, which translates at once to: $\rho = 0.769$ and $\Lambda = [0, 113] \times [0, 85]$ by means of Pierański's geometrical setup; second, that the values of the parameters β and g have not been specified. So let us complete our idealization of his system by adopting the simplest possible scaling, i.e., let us pick $\beta\mu = \log 113$ (cf. Remark 4). This gives $\beta g = 0.054$. Then we have from our results that the interface extends over one fifth of the height of the assembly ($1/\log 113 = 0.212$)

Fig. 1. Typical isothermal configuration for $D = 2$, $\Lambda = [0, 113] \times [0, 85]$, $V \equiv 0$, $\rho = 0.769$, and $\beta g = 0.054$.

and is centered at a relative height equal to 0.769. The former expectation agrees quite well with the configuration depicted in Fig. 4 of Ref. 7, while the latter expectation overestimates moderately the volume of the dense phase thereof. It is of course tempting to complement these findings with corresponding simulation results. Figure 1 shows a typical isothermal equilibrium state of our system on a 86×114 rectangle, at $\rho = 0.769$, $\beta g = 0.054$, and with V taken to be identically zero. One immediately sees that the condensed phase contains bubbles of gas (cf. part (1) of the theorem) in contrast to the dense phase of the state represented in Fig. 4 of Ref. 7 where none are visible. This may be interpreted as a lack of ergodicity of Pierański's experimental setting.

4. PROOF

Throughout this section, we fix a density and a temperature. The proof of our theorem works by showing that the general case does not differ too much from the case without attractive tail. This is the essence of the following

Lemma 1. *For any $I \subseteq \Lambda$, $A \subseteq \{0, 1\}^I$, $B \subseteq \{0, 1\}^{\Lambda \setminus I}$, and $t > 0$, we have*

$$\mathbb{P}_\Lambda(AB) \leq \mathbb{P}_I(A)\mathbb{P}_{\Lambda\setminus I}(B)\exp(2K|\partial I|),$$

$$\mathbb{P}_I(A) \leq \exp(Kt)\mathbb{P}_I^0(A) + \mathbb{P}_I(T_I > t),$$

as well as

$$\mathbb{P}_I(T_I = t) \leq \exp(Kt)\mathbb{P}_I^0(T_I = t)$$

with $K = -\beta \inf_i V(i)(2r + 1)^D$.

Proof: By definition, for each $x \in \{0, 1\}^\Lambda$,

$$H_\Lambda(x) = H_I(x) + H_{\Lambda\setminus I}(x) + V_{I,\Lambda\setminus I}(x) + V_{\Lambda\setminus I,I}(x).$$

This implies by (1.1)

$$\exp[-\beta H_\Lambda(x)] = \exp[-\beta H_I(x)]\exp[-\beta H_{\Lambda\setminus I}(x)]\exp[-2\beta V_{I,\Lambda\setminus I}(x)],$$

and, using $-K|\partial I| \leq \beta V_{I,\Lambda\setminus I}(x) \leq 0$, we get

$$Z_\Lambda \geq Z_I Z_{\Lambda\setminus I}$$

as well as

$$\sum_{x\in A\times B} \exp[-\beta H_\Lambda(x)] \leq \left(\sum_{x\in A} \exp[-\beta H_I(x)]\right)$$
$$\times \left(\sum_{x\in B} \exp[-\beta H_{\Lambda\setminus I}(x)]\right) \exp(2K|\partial I|),$$

and these two inequalities together yield the first assertion of the lemma.

The second assertion is proved the same way, taking advantage of the fact that

$$\mathbb{P}_I(A) = \mathbb{P}_I(A \cap \{T_I \leq t\}) + \mathbb{P}_I(A \cap \{T_I > t\}) \tag{*}$$

and

$$-\beta H_I^0(x) \leq -\beta H_I(x) = -\beta[H_I^0(x) + V_I(x)] \leq -\beta H_I^0(x) + K T_I(x).$$

The third assertion is obtained by letting $A = \{T_I = t\}$ in (*). □

An estimate for the distributions without attractive component is stated next.

Lemma 2. *Let $X_1, \ldots, X_n$ be independent random variables with $X_i \in \{0, 1\}$ and $\mathbb{P}(X_i = 1) = p_i$. Furthermore, let $Y = \sum_i^n X_i$ and $m = \mathbb{E}(Y) = \sum_{i=1}^n p_i$. Then there is for any $\epsilon > 0$ a constant $c(\epsilon) > 0$ such that*

$$\mathbb{P}(|Y - m| \geq \epsilon m) \leq 2\exp(-mc(\epsilon)).$$

Proof: For any $t > 0$, we have by Markov's inequality

$$\mathbb{P}(Y \geq (1+\epsilon)m) \leq \exp(-(1+\epsilon)mt)\mathbb{E}(\exp(Yt)) =$$

$$\exp(-(1+\epsilon)mt)\prod_{i=1}^n(1 + p_i(\exp(t) - 1)) \leq \exp(-(1+\epsilon)mt + m(\exp(t) - 1)).$$

Minimizing over t yields

$$\mathbb{P}(Y \geq (1+\epsilon)m) \leq \exp[m(\epsilon - (1+\epsilon)\log(1+\epsilon))].$$

Alike, we infer

$$\mathbb{P}(Y \geq (1-\epsilon)m) \leq \exp[m(-\epsilon - (1-\epsilon)\log(1-\epsilon))].$$

The first expression is the larger one, so we get the assertion of the lemma with $c(\epsilon) = (1+\epsilon)\log(1+\epsilon) - \epsilon$. □

Note also that for any given $\delta > 0$, we can choose $M(\epsilon)$ in such a way that p_i is greater than $1-\delta$ for $i_1 < N_1$ and less than δ for $i_1 > N_2$.

We are now ready to prove the theorem.

As for part (1) of the theorem, recognize that we can enumerate the connected subsets I of Λ of size n by starting from one of its members, listing in lexicographical order all points that are at a distance at most r from it and belong to I, and proceed by doing the same for all points in the list until we have enumerated all the points of I. Thus, the number of connected subsets is the number of choices that we have to give the intersection of each point's neighborhood with I. For a given point, this number of choices is at most the number of all subsets of the neighborhood, so we find that there are at most $2^{n(2r+1)^D}$ connected subsets of Λ that have size n and contain a given point, and as we have $(N+1)^D$ choices for the starting point, the number of connected subsets of Λ of size n is at most $(N+1)^D 2^{n(2r+1)^D}$. Now, for a given connected subset I of $[0, N_1] \times [0, N]^{D-1}$ with $|I| = n$, the probability that $x_i = 0$ for all $i \in I$ is via Lemma 1

$$\mathbb{P}_\Lambda(S_I = 0) \leq \mathbb{P}_I(S_I = 0)\exp(2Kn) \leq \mathbb{P}_I^0(S_I = 0)\exp(2Kn) \leq (\delta\exp(2K))^n,$$

and the probability that $S_I = 0$ for all such I is therefore not greater than

$$(N+1)^D (2^{(2r+1)^D}\delta\exp(2K))^n.$$

If we choose $n = \epsilon\log N$ and $\delta < \exp(-2K - \epsilon^{-1}D)2^{-(2r+1)^D}$, then this probability tends to zero as N tends to infinity, and so the first assertion of the theorem is proved.

Part (2) of the theorem is proved the same way.

For the proof of part (3), observe that for a given $C \subset [0, N_1] \times [0, N]^{D-1}$, we have through Lemma 1

$$\begin{aligned}\mathbb{P}_\Lambda(S_C < (1-\epsilon)|C|) &\leq \mathbb{P}_C(S_C < (1-\epsilon)|C|)\exp(2K|C|)\\ &\leq \mathbb{P}_C^0(S_C < (1-\epsilon)|C|)\exp(3K|C|).\end{aligned}$$

Applying Lemma 2 to the number of zeros among the x_i with $i \in C$, we infer

$$\mathbb{P}_C^0(S_C < (1-\epsilon)|C|) \leq 2\exp(-\epsilon|C|(\log(\epsilon/\delta) - 1)).$$

If we choose $\delta < \epsilon \exp(-(3K+2)\epsilon^{-1})$, then

$$\mathbb{P}_\Lambda(S_C < (1-\epsilon)|C|) \leq 2\exp(-|C|) \leq 2\exp(-N^{\alpha D}),$$

and since the number of hypercubes $C \subset [0, N_1] \times [0, N]^{D-1}$ is not greater than $(N+1)^{D+1}$, we conclude that $\mathbb{P}_\Lambda(\bigcup_C \{S_C < (1-\epsilon)|C|\})$ tends to zero as $N \to \infty$. So, part (3) of the theorem is proved.

We finally prove part (4) of the theorem. Define, for every $C \subset [N_2, N] \times [0, N]^{D-1}$, $i \in \{0, \ldots, r\}^D$, and $j \in [-N, N]^D$,

$$R_C(i, j) = \{(k, l) \in C \times C : k - l = j, l = i \bmod (r+1), V(j) \neq 0\}$$

as well as

$$W_C(i, j) = \sum_{(k,l) \in R_C(i,j)} x_k x_l.$$

Therefore

$$T_C = \sum_{i \in \{0,\ldots,r\}^D, j \in [-N,N]^D} W_C(i, j),$$

so, if $T_C = n$, then there exist i and j such that $W_C(i, j) \geq n((r+1)(2r+1))^{-D}$. The summands in the definition of $W_C(i, j)$ are independent under $\mathbb{P}^0_C$. This implies that $\mathbb{E}^0_C(W_C(i, j))$ is not greater than δ times $\mathbb{E}^0_C(S_C)$. Furthermore, for any $\alpha' < \alpha$ and N large enough, the latter expectations are all greater than $N^{\alpha' D}$. In particular, we can choose α' such that

$$|\partial C| \leq \epsilon \mathbb{E}^0_C(S_C).$$

Assume that $n > \epsilon \mathbb{E}^0_C(S_C)$. Then Lemma 1 shows

$$\begin{aligned}\mathbb{P}_\Lambda(T_C = n) &\leq \exp(2K|\partial C|)\mathbb{P}_C(T_C = n) \leq \exp(K(2|\partial C| + n))\mathbb{P}^0_C(T_C = n)\\ &\leq \exp(3Kn) \sum_{i \in \{0,\ldots,r\}^D, j \in [-N,N]^D} \mathbb{P}^0_C(W_C(i, j) \geq n((r+1)(2r+1))^{-D}).\end{aligned}$$

Moreover, pick $\delta < ((r+1)(2r+1))^{-D} \epsilon \exp[-(3K+2)((r+1)(2r+1))^D]$. So, using Lemma 2, we have that $\mathbb{P}_\Lambda(T_C = n)$ is not greater than a constant times $\exp(-n)$. And since there are no more than $(N+1)^{D+1}$ hypercubes, we conclude that the probability that $T_C > \epsilon \mathbb{E}^0_C(S_C)$ for all hypercubes $C \subset [N_2, N] \times [0, N]^{D-1}$ tends to zero as $N \to \infty$. This yields (2.2).

In order to prove (2.1), we choose $\epsilon' < (9K)^{-1}\epsilon^2$ and define events

$$A = \{T_C \leq \epsilon' \mathbb{E}^0_C(S_C) \text{ for all } C \subset [N_2, N] \times [0, N]^{D-1}\}$$

as well as for every $C \subset [N_2, N] \times [0, N]^{D-1}$

$$B_C = \{|S_C - \mathbb{E}^0_C(S_C)| > \epsilon \mathbb{E}^0_C(S_C)\}.$$

What then remains to show is $\mathbb{P}_\Lambda(\bigcup_C B_C) \to 0$ as N tends to infinity. But since we already know that $\mathbb{P}_\Lambda(A^C)$ goes to zero as N goes to infinity, it is enough to establish $\mathbb{P}_\Lambda(\bigcup_C A \cap B_C) \to 0$ as $N \to \infty$. Now, for a given C,

$$\mathbb{P}_\Lambda(A \cap B_C) \leq \exp[K(2|\partial C| + \epsilon' \mathbb{E}_C^0(S_C))]\mathbb{P}_C^0(|S_C - \mathbb{E}_C^0(S_C)| > \epsilon \mathbb{E}_C^0(S_C)),$$

and via Lemma 2, we can estimate this from above by $2\exp(-\eta(\epsilon)\mathbb{E}_C^0(S_C))$ with some $\eta(\epsilon) > 0$. Thus

$$\mathbb{P}_\Lambda\Big(\bigcup_C A \cap B_C\Big) \leq 2(N+1)^{D+1} \exp(-\eta(\epsilon) N^{\alpha' D}),$$

and the last estimate tends to zero as $N \to \infty$. This completes the proof of the theorem.

REFERENCES

1. K. Grill, Finite-range interactions and phases. *Periodica Mathematica Hungarica* **50**:155 (2005).
2. K. Grill and C. Tutschka, One-dimensional falling bodies. *J. Stat. Phys.* **117**:1015 (2004).
3. P. Kasperkovitz and C. Tutschka, Cluster analysis of a one-dimensional continuous system with nearest-neighbor interaction. *Ukrainian J. Phys.* **45**:488 (2000).
4. M. K.-H. Kiessling, On the equilibrium statistical mechanics of isothermal classical self-gravitating matter. *J. Stat. Phys.* **55**:203 (1989).
5. C. Kittel, *Thermal Physics*. Wiley (1969).
6. J. K. Percus, Density functional theory in the classical domain. In J. M. Seminario, editor, *Recent Developments and Applications of Modern Density Functional Theory*, p. 151. Elsevier (1996).
7. P. Pierański, An experimental model of a classical many-body system. *Am. J. Phys.* **52**:68 (1984).
8. D. Ruelle, *Statistical Mechanics: Rigorous Results*. Benjamin (1969).
9. B. Stahl, M. K.-H. Kiessling, and K. Schindler, Phase transitions in gravitating systems and the formation of condensed objects. *Planetary and Space Sci.* **43**:271 (1995).