Journal of Statistical Physics, Vol. 117, Nos. 5/6, December 2004 (© 2004)

One-Dimensional Falling Bodies

Karl Grill[1] **and Christian Tutschka**[2]

Received May 24 2004; accepted July 26 2004

It is shown that a macroscopic system of classical hard rods with next neighbor interactions attains a phase separation under a weak gravitational field.

KEY WORDS: One-dimensional; classical fluid; next neighbor; gravitational field; phase separation

1. INTRODUCTION

We start out from a system of n (identical) hard rods with next neighbor pair interactions V. In this case, we can number the particles sequentially: $q_1 \leqslant \cdots \leqslant q_n$, where q_i denotes the position of particle i. We assume that the interaction between two particles at distance x has the form

$$V(x) = \mathcal{E}\, j(x) \tag{1a}$$

with $\mathcal{E} > 0$ and

$$j(x) = \begin{cases} \infty & \text{if } 0 \leqslant x < a, \\ h(x) \in [-1, 0] & \text{if } a \leqslant x \leqslant b, \\ 0 & \text{if } x > b. \end{cases} \tag{1b}$$

As a normalization, we suppose that h actually attains the value -1 in the interval $[a, b]$. Furthermore, we take h to be continuous. This form of

[1]Institut für Statistik und Wahrscheinlichkeitstheorie, TU Wien, Wiedner Hauptstraße 7, 1040 Wien, Austria; e-mail: grill@ci.tuwien.ac.at
[2]Erwin Schrödinger Institute for Mathematical Physics, Boltzmanngasse 9, 1090 Wien, Austria; e-mail: christian.tutschka@esi.ac.at

0022-4715/04/1200-1015/0

the pairwise potential means that we deal with one-dimensional hard cores of diameter a and that there is an attractive interaction of finite-range b which is bounded below by $-\mathcal{E}$, as well.

The aim of this article is to show that this simple one-dimensional fluid, which thermodynamically would have no phase transition at all (see, e.g., ref. 1, 5.6.7 Theorem (Van Hove)), attains one macroscopically under the action of a weak gravitational field.

So, let us add a homogeneous gravitational field to our model. Upon selecting units such that the mass of the particles equals 1, the external potential thus is

$$U(x) = gx, \tag{2}$$

where g is the acceleration due to gravity and x the coordinate parallel to the field. This completes the characterization of the Hamiltonian.

Classical equilibrium statistical mechanics is then determined by the (configurational) isothermal–isobaric (probability) measure thereof (see, e.g., ref. 1). If the first particle is fixed at the origin, i.e., $q_1 = 0$, and we let

$$x_i = q_{i+1} - q_i \quad \text{for} \quad 1 \leqslant i < n,$$

then the relative positions $x_1, \ldots, x_{n-1}$ turn into independent random variables, and their marginal densities are easily written down: The density of x_i is given by

$$f_i(x) = \Phi(\beta((n-i)g + p))^{-1} \exp(-\beta(V(x) + ((n-i)g + p)x)), \tag{3a}$$

where

$$\Phi(t) = \int_0^\infty \exp(-\beta V(x) - tx)\, dx. \tag{3b}$$

In this density, β represents the inverse (absolute) temperature, and the pressure p is to be identified with the additional external force exerted on particle n.

2. MAIN THEOREM

The rough idea is that our model system (as characterized by (1) and (2)) exhibits a non-uniform profile with a proper interface between a dense "condensate" and a dilute "gas". Here the key is the concept of clustered (connected or condensed) particles. We say that two particles are condensed if they interact through the attractive part of the pair potential (i.e., the distance between them is less than b). Then the "condensate" is to be interpreted as meaning a particle system wherein all pairs are condensed, and the "gas" is defined (complementary) as system composed of non-condensed particles (cf. ref. 2).

A direct application of this idea fails, however; namely, with a fixed external (gravitational) field (2), and in the (infinite-particle or thermodynamic) limit $n \to \infty$, there is no gas at all. Rather, almost all the particles end up stacked on top of each other (cf. ref. 3). We will resolve this problem by letting the strength of the field diminish gradually as n increases. Intuitively, this is in tune with our understanding of physics, as gravity is known to be the weakest among the fundamental forces.

We are now going to formulate our main theorem. To do so, fix $\epsilon > 0$ and let n_1 and n_2 be chosen as the largest numbers such that

$$\mathbb{P}(x_{n_1} > b) < \epsilon,$$

and

$$\mathbb{P}(x_{n_2} > b) < 1 - \epsilon.$$

By our assumptions, it is readily seen that the probability $\mathbb{P}(x_i > b)$ is increasing as i increases, so $n_1 < n_2$, and that this probability is $< \epsilon$ for all $i < n_1$, and $\geqslant 1 - \epsilon$ for $i > n_2$. Our theorem then states as follows.

Theorem 1. Let $\beta > 0$ and $p = 0$ be given and let $\mathcal{E}$ and g be chosen so that

$$\beta \mathcal{E} = c_1 \log n,$$

and

$$\beta g = c_2 \frac{\log n}{n}$$

with $0 < c_1 < 1$ and $c_2 > 0$. Then, as $n \to \infty$, the following limits hold in probability.

$$\frac{q_{n_1}}{q_n} \to \theta \in (0, 1)$$

as well as

$$\frac{q_{n_2} - q_{n_1}}{q_n} \to 0.$$

More precisely, it holds that

$$\frac{q_{n_2} - q_{n_1}}{n(\log n)^{-1}} \to \frac{1}{c_2} \log\left(\frac{1-\epsilon}{\epsilon}\right).$$

Proof. This theorem is proved by showing that q_{n_1}, q_{n_2}, and q_n obey the law of large numbers (see, e.g., ref. 4).

First, we look at q_n. Let

$$\Psi(t) = \log \Phi(t).$$

Then

$$\mathbb{E}(x_i) = -\Psi'(\beta(n-i)g),$$

and thus

$$\mathbb{E}(q_n) = -\sum_{i=1}^{n-1} \Psi'(\beta(n-i)g).$$

For all sufficiently large n, the sum can be approximated by an integral, so that

$$\mathbb{E}(q_n) = \frac{1}{\beta g}(\Psi(\beta g) - \Psi(\beta(n-1)g))(1 + o(1)).$$

Moreover, since h is a bounded continuous function on $[a, b]$, we have

$$\Psi(\beta g) = \log n(1 + o(1))$$

as well as

$$\Psi(\beta(n-1)g) = d \log n(1+o(1)),$$

where $d = \sup_{a \leqslant x \leqslant b}(-c_1 h(x) - c_2 x)$. Hence

$$\lim_{n\to\infty} \frac{\mathbb{E}(q_n)}{n} = \frac{1-d}{c_2} > a$$

as desired.

Next, let us consider

$$\mathbb{P}(x_i > b) = \frac{1}{1+\beta(n-i)g\exp(\beta(n-i)gb)\int_a^b \exp(-\beta(\mathcal{E}h(x)+(n-i)gx))dx}.$$

This probability tends to zero if

$$n - i = n^{1-c_1},$$

whereas it tends to one as n tends to infinity if

$$n - i = n^{1-c_1-\delta}$$

for any $\delta > 0$, and therefore

$$\lim_{n\to\infty} \frac{\log(n-n_1)}{\log n} = \lim_{n\to\infty} \frac{\log(n-n_2)}{\log n} = 1 - c_1.$$

Consequently, upon determining the leading order asymptotic behavior of the expectations as above, we find that

$$\lim_{n\to\infty} \frac{\mathbb{E}(q_n - q_{n_1})}{n} = \lim_{n\to\infty} \frac{\mathbb{E}(q_n - q_{n_2})}{n} = \frac{1-c_1}{c_2}.$$

In order to establish the convergence in probability that is claimed in the theorem, we take a look at the variances. To this end, we can regard the distribution of x_i as a mixture of a distribution concentrated on $[a,b]$ and an exponential distribution shifted to the right by b. Remembering that the variance of a random variable X that is the mixture of X_1 and X_2 with weights r and $s = 1-r$ is given by

$$\mathbb{V}(X) = r\mathbb{V}(X_1) + s\mathbb{V}(X_2) + rs(\mathbb{E}(X_1) - \mathbb{E}(X_2))^2,$$

we get the estimate

$$\mathbb{V}(x_i) \leqslant 2\Big(b^2 + \frac{1}{(\beta(n-i)g)^2}\Big)$$

and so

$$\mathbb{V}(q_n) = O\Big(\frac{n^2}{(\log n)^2}\Big).$$

The same inequality holds for the variances of q_{n_1} and q_{n_2}, of course, and as these are of smaller order than n^2, we obtain via the Chebyshev inequality (see, e.g., ref. 4), that in probability as n tends to infinity,

$$\lim_{n\to\infty} \frac{q_n}{n} = \frac{1-d}{c_2}$$

as well as

$$\lim_{n\to\infty} \frac{q_{n_1}}{n} = \lim_{n\to\infty} \frac{q_{n_2}}{n} = \frac{c_1-d}{c_2}.$$

Finally, let us derive the more precise law for the width of the interface. To do so, it is convenient to return to $\mathbb{P}(x_i > b)$. Taking advantage of the fact that $\beta(n-i)g$ tends to zero as n tends to infinity for $n_1 \leqslant i \leqslant n_2$, we can simplify this probability to

$$P(i) = \mathbb{P}(x_i > b) = \frac{1}{1+(n-i)/C}(1+o(1)) \quad \text{for} \quad n_1 \leqslant i \leqslant n_2,$$

where

$$C = \frac{1}{\beta g \int_a^b \exp(-\beta \mathcal{E} h(x))dx}.$$

From this, it readily follows that

$$i_1 = n - n_1 = \frac{1-\epsilon}{\epsilon} C(1+o(1)),$$

and

$$i_2 = n - n_2 = \frac{\epsilon}{1-\epsilon} C(1+o(1)).$$

Using again the mixture argument, the expectation of x_i is obtained as

$$\mathbb{E}(x_i) = y_i + P(i)\frac{1}{\beta(n-i)g} \quad \text{for} \quad n_1 \leqslant i \leqslant n_2$$

with $y_i \leqslant 2b$. So,

$$\begin{aligned}\lim_{n\to\infty} \frac{\mathbb{E}(q_{n_2} - q_{n_1})}{n(\log n)^{-1}} &= \lim_{n\to\infty} \frac{\mathbb{E}(\sum_{i=n_1}^{n_2-1} x_i)}{n(\log n)^{-1}} \\ &= \frac{1}{c_2} \lim_{n\to\infty} \sum_{k=i_2+1}^{i_1} \frac{1}{1+k/C}\frac{1}{k}(1+o(1)) \\ &= \frac{1}{c_2} \log\left(\frac{1-\epsilon}{\epsilon}\right).\end{aligned}$$

With the same method that we applied to the variance of q_n, we can show that the variance of $q_{n_2} - q_{n_1}$ satisfies

$$\mathbb{V}(q_{n_2} - q_{n_1}) = O\left(\frac{n^2}{n_1(\log n)^2}\right).$$

This establishes the convergence in probability and completes the proof of our theorem. ∎

3. DISCUSSION

We now interprete Theorem 1 physically. For large n, with high probability, the total volume q_n of our system consists of three regions. First, there is a (dense) part of size q_{n_1} which contains mostly condensate with a few "bubbles" of gas, then there is an interface where the two phases mix, and the remaining space is occupied by gas with only a few occasional "droplets" of condensate. Both the condensate and the gas use up an almost fixed fraction of the available space, whereas the width of the interface is small (i.e., of order $1/\log n$) in comparison to the total length of the system. Thus, with high probability, a separation of phases occurs.

We also observe that the condition $p = 0$ is handy for the calculations, but for the qualitative result it is only necessary that p is not too large. The case of non-zero p can be reduced to this special case by adding p/g particles at the top and considering only the first n particles of this enlarged system—see (3).

Finally, it is interesting to ask what the effect becomes in, say, the grand isothermal–isobaric format wherein the fixed number of particles n is replaced by a random number N (see, e.g., ref. 5). Let us choose the associated activity parameter in such a way that the probability for $N = k$ attains its maximum at $k = n$ (and the other parameters as before). Then one can show that the distribution of N is approximately normal with mean n and a variance of order $n/\log n$, so that, in a typical configuration, the number of particles is close to n. This means that for the purpose of deducing the behavior of our macroscopic system, the isothermal–isobaric measure and the grand isothermal–isobaric measure give essentially the same answers. In particular, the interface structure will not be averaged out in the grand isothermal–isobaric version.

ACKNOWLEDGMENTS

We thank the referee for his clarifying remarks. C.T. acknowledges the support by an Erwin Scrödinger Institute Junior Research Fellowship in Mathematics and Mathematical Physics.

REFERENCES

1. D. Ruelle, *Statistical Mechanics: Rigorous Results* (Benjamin, New York, 1969).
2. P. Kasperkovitz and C. Tutschka, Cluster analysis of a one-dimensional continuous system with nearest-neighbor interaction, *Ukr. J. Phys.* **45**:488 (2000).
3. C. Tutschka, Condensation in stable systems, PhD thesis (TU Wien, 1999).
4. W. Feller, *An Introduction to Probability Theory and Its Applications* (Wiley, New York, 1968).
5. J. K. Percus, Nonuniform classical fluid mixture in one-dimensional space with next neighbor interactions, *J. Stat. Phys.* **89**:249 (1997).