Physica 98A (1979) 274–288 © *North-Holland Publishing Co.*

ON THE CONFIGURATION OF SYSTEMS OF INTERACTING PARTICLE WITH MINIMUM POTENTIAL ENERGY PER PARTICLE

W.J. VENTEVOGEL and B.R.A. NIJBOER

Instituut voor Theoretische Fysica, Rijksuniversiteit Utrecht, Utrecht, The Netherlands

Received 15 May 1979

In continuation of previous work we extend the class of two-body potentials, either repulsive or of generalized Lennard–Jones type, for which it can be proved that among all configurations of an infinite one-dimensional system of interacting particles (with fixed density in the case of repulsive interaction) the configuration where all particles are equidistant has the minimum potential energy per particle. It is shown that this property does not hold for the repulsive potential $\phi(x) = (1+x^4)^{-1}$.

For infinite systems in n-dimensions it is stated that a necessary condition for an analogous property is that the Fourier transform $\hat{\phi}(k)$ of the potential be non-negative for all k. The proof of this statement will be given in a subsequent publication.

1. Introduction

In a previous paper[1]), to be referred to as I, we studied configurations of one-dimensional systems consisting of a finite or infinite number of equal particles interacting with two-body potentials $\phi(x)$. We assumed throughout $\phi(x) = \phi(-x)$ and $\phi(x)$ to be integrable at infinity.

With respect to these systems we proved a number of theorems among which were the following:

1) If $\phi''(x) > 0$ for $x \neq 0$, i.e. if the two-body interaction is given by a convex repulsive potential, then for an infinite system of arbitrary but fixed number density the configuration where all particles are equidistant has the minimum potential energy per particle.

2) If $\phi(x)$ is a Lennard–Jones potential (L.J. potential) defined by

$$\phi(x) = \epsilon \left\{ \left(\frac{\sigma}{|x|}\right)^l - \left(\frac{\sigma}{|x|}\right)^m \right\}, \quad l > m > 1, \epsilon > 0, \sigma > 0, \tag{1}$$

then, if

$$l - m \geqslant (m+1)(\zeta(m) - 1), \quad \text{with } \zeta(m) \equiv \sum_{n=1}^{\infty} n^{-m}, \tag{2}$$

for an infinite system among all configurations the one, where all particles are equidistant with lattice constant a_0, has the minimum potential energy per particle. a_0 is uniquely determined by the condition $\Sigma_{k=1}^{\infty} \phi(kx)$ has a minimum for $x = a_0$.

Furthermore we considered in I a more general though rather similar type of potentials than the L.J. potential, which we called type-A potentials. A potential $\phi(x)$ was called a type A-potential if i) there exists a positive number r_0, such that $\phi(x)$ is strictly decreasing for $0 < x \leq r_0$ and strictly increasing for $x \geq r_0$ and ii) $\int_0^\infty \phi(x)\,dx > 0$ (or ∞). It will be evident that a L.J. potential is of type-A, but the latter are more general. Theorem 2) may be generalized for a wider class of type-A potentials than the L.J. potential satisfying condition (2), however it was shown in I by a counter-example that it does not hold for all type-A potentials.

In the present paper we will continue the work reported in I and we will prove a number of theorems which extend the class of potentials for which the equidistant configuration proves to be the one with minimum potential energy per particle. For instance we will show that for a class of repulsive potentials which are *not* convex (in distinction from 1)) and which includes potentials like

$$\phi(x) = e^{-\alpha x^2} \quad (\alpha > 0) \tag{3}$$

and

$$\phi(x) = \frac{1}{(b^2 + x^2)^\alpha} \quad (\alpha > \tfrac{1}{2}, b > 0), \tag{4}$$

for infinite systems with a given arbitrary density the equidistant configuration has minimum potential energy per particle. On the other hand we show that the latter property does not hold for a potential as

$$\phi(x) = (1 + x^4)^{-1}. \tag{5}$$

Furthermore we have generalized the theorem 2) mentioned above to a subclass of type-A potentials (which are repulsive at short distance and attractive at large distance), which includes all L.J. potentials (1) and which we call type-C potentials. (Type-B potentials defined in I will not be considered here, but it may be noticed that not all B-potentials are C-potentials and neither are all C-potentials B-potentials.)

A type-C potential in a type-A potential for which a fixed number $\alpha > 0$ exists such that

$$(\alpha + 1)\phi'(x) + x\phi''(x) > 0 \quad \text{for all } x > 0. \tag{6}$$

All L.J. potentials (1) with $l > m > 1$ are of type-C, since $\phi(x)$ given by (1) will satisfy (6) for $l \geq \alpha \geq m$. However, type-C potentials are more general because any A-potential is of type-C as soon as its derivative can for $x > 0$ be written in the form:

$$\phi'(x) = x^{-\alpha-1}\theta(x),$$

where $\alpha > 0$ and $\theta(x)$ may be any differentiable strictly increasing function. On the other hand there are many A-potentials which are not of type-C, e.g.

$$\phi(x) = A\,\mathrm{e}^{-\lambda x} - B\,\mathrm{e}^{-\mu x} \quad (x, B, \mu > 0; \lambda > \mu; A\mu > B\lambda). \tag{7}$$

It seems plausible that theorem 2) also holds for the potential (7), but we have not yet been able to prove this. We have shown, however, that for potential (7) among all periodic configurations with 2 and 3 particles per unit cell and with a volume per particle $a \leq a_0$ the equidistant configuration with the same volume a per particle has the minimum potential energy per particle. Here a_0 is uniquely determined by the condition that $\Sigma_{k=1}^{\infty} \phi(kx)$ has a minimum for $x = a_0$. The proof of this statement will not be reproduced here.

While the present paper was being written we received a preprint by Gardner and Radin[2]) in which a one-dimensional system of particles interacting with a L.J. potential is considered. The authors show that for a finite system the configuration with minimum potential energy is unique and that it approaches uniform spacing in the limit of an infinite number of particles.

It has been mentioned in I already that unfortunately the proofs of the theorems mentioned above cannot be readily generalized for systems in two and three dimensions. In a subsequent publication, however, we will prove the following theorem valid for an infinite n-dimensional system:

Let $\phi(\boldsymbol{r})$ be a potential in n-dimensions with the following properties:

i) $\phi(\boldsymbol{r}) = \phi(-\boldsymbol{r})$.

ii) $\phi(\boldsymbol{r})$ is sufficiently well-behaved at $|\boldsymbol{r}| = 0$ and at $|\boldsymbol{r}| = \infty$.

iii) The Fourier transform $\hat{\phi}(\boldsymbol{k}) \equiv \int \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}}\phi(\boldsymbol{r})\,\mathrm{d}\boldsymbol{r}$ exists.

If a density ρ_0 exists such that for all given densities $\rho > \rho_0$ the potential energy per particle in an infinite periodic system of particles has a minimum for a Bravais-lattice (the unit-cell of which may be chosen in such a way that its linear dimensions approach 0 as $\rho \to \infty$) then $\hat{\phi}(\boldsymbol{k}) \geq 0$ for all $\boldsymbol{k}$.

2. Type-C potentials

It may be recalled (cf. I) that in the case of an infinite number of particles we have introduced a large but finite periodicity number N, such that $x_{N+n+1} - x_{N+n} = x_{n+1} - x_n$ for all n and the x_n are chosen so that $x_{n+1} - x_n > 0$.

Furthermore in this case the mean potential energy per particle is defined by

$$u(\{x_n\}) = N^{-1} \sum_{i=1}^{N} \sum_{l=1}^{\infty} \phi(x_{i+l} - x_i). \tag{8}$$

On the other hand for a finite system with N particles $u(\{x_n\})$ is defined by

$$u(\{x_n\}) = N^{-1} \sum_{i=1}^{N-1} \sum_{l=1}^{N-i} \phi(x_{i+l} - x_i). \tag{9}$$

In this section we will prove two theorems:

i) If $\phi(x)$ is a type-C potential (cf. (6)), the equation

$$\sum_{l=1}^{\infty} l\phi'(la) = 0 \quad \text{has a unique solution } a = a_0 > 0, \tag{10}$$

and for all finite or infinite configurations

$$u(\{x_n\}) \geq \sum_{l=1}^{\infty} \phi(la_0). \tag{11}$$

The equal sign holds iff $x_{n+1} - x_n = a_0$ for all n.

ii) If $\phi(x)$ is a type-C potential, for an infinite system with a given volume per particle $N^{-1}(x_N - x_0) \equiv a \leq a_0$ (i.e. the fixed density is larger than or equal to a_0^{-1} given by (10))

$$u(\{x_n\}) \geq \sum_{l=1}^{\infty} \phi(la). \tag{12}$$

Again the equal sign holds iff $x_{n+1} - x_n = a$ for all n.

The proof of these two theorems will be arranged in a few steps:

a) In I, appendix A it has been shown that for all type-A potentials and therefore in particular for all C-potentials the equation

$$\sum_{l=1}^{\infty} l\phi'(la) = 0$$

has at least one solution $a_0 > 0$.

From (6) we infer that the equation $\Sigma_{l=1}^{\infty} l\phi'(la_0) = 0$ implies

$$\sum_{l=1}^{\infty} l^2\phi''(la_0) = \frac{\mathrm{d}}{\mathrm{d}a}\left(\sum_{l=1}^{\infty} l\phi'(la)\right)_{a=a_0} > 0,$$

and therefore that the function $\Sigma_{l=1}^{\infty} l\phi'(la)$ is increasing in the neighbourhood of its zeroes. Hence $\Sigma_{l=1}^{\infty} l\phi'(la)$ has at most one zero for $a > 0$. From these observations we may conclude that a_0 is unique.

b) From (6) it follows that for $x > 0$ and $z > 0$

$$\int_x^z \left(1 - \left(\frac{y}{z}\right)^\alpha\right) \{y\phi''(y) + (\alpha+1)\phi'(y)\}\,dy \geq 0, \tag{13}$$

where the equal sign holds iff $x = z$. Integrating by parts we find

$$\int_x^z \left(1 - \left(\frac{y}{z}\right)^\alpha\right) y\phi''(y)\,dy = \left\{\left(\frac{x}{z}\right)^\alpha - 1\right\} x\phi'(x) + \int_x^z \left\{(\alpha+1)\left(\frac{y}{z}\right)^\alpha - 1\right\} \phi'(y)\,dy. \tag{14}$$

We now combine (13) and (14) and we find

$$\phi(z) - \phi(x) = \int_x^z \phi'(y)\,dy \geq -\alpha^{-1}\left\{\left(\frac{x}{z}\right)^\alpha - 1\right\} x\phi'(x), \tag{15}$$

where the equal sign holds iff $x = z$.

c) Applying (15) to (8) we find

$$u(\{x_n\}) - \sum_{l=1}^{\infty} \phi(la) \geq -\alpha^{-1} \sum_{l=1}^{\infty} \left[N^{-1} \sum_{i=1}^{N} \left\{\left(\frac{la}{x_{i+l} - x_i}\right)^\alpha - 1\right\}\right] la\phi'(la), \tag{16}$$

where for the moment a is an arbitrary positive number. The equal sign in (16) holds iff $x_{n+1} - x_n = a$ for all n. Now $\phi(x)$ is a type-A potential, hence there is a positive number r_0 such that $\phi'(x) < 0$ for $0 < x < r_0$ and $\phi'(x) > 0$ for $x > r_0$. Therefore if $a \geq r_0, \Sigma_{l=1}^{\infty} l\phi'(la) > 0$ and from this we infer that $a_0 < r_0$.

Let us choose the number a in (16) in such a way that

$$0 < a < r_0. \tag{17}$$

From (6) it follows that the condition $\phi'(x) \leq 0$ implies $\phi''(x) > 0$. Hence $\phi'(x)$ is a strictly increasing function of x in the interval $0 < x \leq r_0$.

Let l_0 be the largest integer for which $l_0 a \leq r_0$. It then follows that

$$\phi'(la) < \phi'((l+1)a) \leq 0 \quad \text{for } l+1 \leq l_0 \tag{18a}$$

and

$$\phi'(la) > 0 \quad \text{for } l > l_0. \tag{18b}$$

Now let t_m $(m = 1, 2, \ldots, j)$ be a set of numbers obeying $t_1 \geq t_2 \cdots \geq t_j \geq 0$. In appendix A we will prove that for any convex function $g(x)$ and if $l \geq j$:

$$\left\{\sum_{i=1}^{N} g\left(\frac{x_{i+l}-x_i}{l}\right)\right\}\left\{\sum_{m=1}^{j} mt_m\right\} \leq \sum_{i=1}^{N}\sum_{m=1}^{j} mt_m g\left(\frac{x_{i+m}-x_i}{m}\right). \tag{19}$$

where the equal sign holds iff $x_{n+l}-x_n$ is independent of n. We use the inequality (19) taking $j = l_0$, $t_m = -\phi'(ma)$ and we find for $l > l_0$

$$\phi'(la)\left\{\sum_{i=1}^{N} g\left(\frac{x_{i+l}-x_i}{l}\right)\right\}\left\{\sum_{m=1}^{l_0} m\phi'(ma)\right\}$$
$$\geq \phi'(la)\sum_{i=1}^{N}\sum_{m=1}^{l_0} m\phi'(ma) g\left(\frac{x_{i+m}-x_i}{m}\right). \tag{20}$$

We now make the choice $g(x) = (a/x)^\alpha - 1$ and we apply (20) to the summation $\Sigma_{l_0+1}^{\infty}$ which is part of the right-hand side of (16). As a result we find:

$$u(\{x_n\}) - \sum_{l=1}^{\infty}\phi(la) \geq -\frac{a}{N\alpha}\left\{\sum_{m=1}^{l_0} m\phi'(ma)\right\}^{-1}$$
$$\times\left\{\sum_{m=1}^{l_0}\sum_{i=1}^{N}\left(\left(\frac{ma}{x_{i+m}-x_i}\right)^{\alpha}-1\right) m\phi'(ma)\right\}\cdot\sum_{l=1}^{\infty} l\phi'(la). \tag{21}$$

If in particular we take for a the value a_0 as defined by (10), we conclude from (21) that

$$u(\{x_n\}) \geq \sum_{l=1}^{\infty}\phi(la_0), \tag{22}$$

where the equal sign holds iff $x_{n+1} - x_n = a_0$ for all n.
This proves, for infinite systems, the first theorem.

By the same arguments as given in I it may be shown that $\Sigma_{l=1}^{\infty}\phi(la_0)$ is also a lower bound on the energy per particle of a finite system and further that this lower bound can be approximated to any degree of accuracy by increasing the number of particles of the system.

d) In order to prove theorem ii) we now suppose that $N^{-1}(x_N - x_0) < a_0$ and in (21) we choose $a = N^{-1}(x_N - x_0)$, i.e. a is the fixed average volume per particle. We then have

$$\sum_{l=1}^{\infty} l\phi'(la) < 0; \tag{23}$$

because we know that $\Sigma_{l=1}^{\infty} l\phi'(la)$ has only one zero a_0, where the derivative of this function is positive.

From the fact that $(a/x)^\alpha - 1$ is a convex function of x and that $\phi'(ma) \leq 0$ for $m \leq l_0$ we conclude that

$$N^{-1}\sum_{i=1}^{N}\left\{\left(\frac{ma}{x_{i+m}-x_i}\right)^{\alpha}-1\right\} m\phi'(ma)$$
$$\leq\left\{\left((Nma)^{-1}\sum_{i=1}^{N}(x_{i+m}-x_i)\right)^{-\alpha}-1\right\} m\phi'(ma) = 0. \tag{24}$$

Combination of (21), (23) and (24) then leads to

$$u(\{x_n\}) \geq \sum_{l=1}^{\infty} \phi(la), \tag{25}$$

for $a = N^{-1}(x_N - x_0) < a_0$. The equal sign holds iff $x_{n+1} - x_n = a$ for all n. Q.E.D.

3. Repulsive potentials

In this section we consider again infinite one-dimensional systems of particles, but the two-body potential $\phi(x)$ will now belong to a class of repulsive potentials, which, however, will not be convex in distinction from those treated in I. We will prove that for the potential

$$\phi(x) = e^{-\alpha x^2} \quad (\alpha > 0) \tag{26}$$

the minimum potential energy per particle for all systems with a given, but arbitrary, density is assumed (and assumed only) for the configuration where all particles are equidistant.

It then follows immediately that potentials of the form

$$\phi(x) = \int_0^\infty W(\alpha)\, e^{-\alpha x^2}\, d\alpha, \quad \text{with } W(\alpha) \geq 0, \tag{27}$$

have the same property. For instance, choosing

$$W(\alpha) = \frac{\alpha^{n-1}}{\Gamma(n)} e^{-\alpha b^2}, \quad \text{with } n > \tfrac{1}{2}, \tag{28}$$

we see that the property mentioned also holds for the potential

$$\phi(x) = \frac{1}{(b^2 + x^2)^n}, \quad \text{with } n > \tfrac{1}{2}. \tag{29}$$

Here b is an arbitrary constant.

On the other hand we will show by a counter-example that the property does not hold for the potential

$$\phi(x) = \frac{1}{1 + x^4}. \tag{30}$$

In fact this might be inferred already from the necessary condition for the

Fourier transform of the potential, mentioned at the end of the introduction. The Fourier transform of (30) is given by[3])

$$\hat{\phi}(k) = \pi\, e^{-1/2\sqrt{2}|k|} \cos(\tfrac{1}{2}\sqrt{2}|k| - \tfrac{1}{4}\pi), \tag{31}$$

which is not positive definite.

Let us now proceed to the proof of our theorem for the potential $\phi(x) = e^{-x^2}$ (without loss of generality we take $\alpha = 1$ for simplicity). Let p be the positive root of the equation

$$e^{x^2} = 1 + 2x^2.$$

Numerical calculation gives $p \simeq 1.1209$.

We distinguish two cases: 1) $a \geqslant p$ and 2) $0 < a \leqslant p$, where $a = N^{-1}(x_N - x_0)$, i.e. the mean volume per particle.

1) We define a function $\phi_1(x)$ by

$$\begin{aligned} &\phi_1(x) = \phi(x) \quad \text{for } |x| \geqslant p, \\ &\phi_1(x) = 1 - 2|x|p\, e^{-p^2} \quad \text{for } |x| \leqslant p. \end{aligned} \tag{32}$$

Notice that $\phi_1(x)$ and its derivative are continuous in $x = p$. It is easily verified that $\phi_1(x)$ has the properties:

$$\begin{aligned} &\text{a) } \phi_1(x) < \phi(x) \quad \text{for } 0 < x < p, \\ &\text{b) } \phi_1''(x) \geqslant 0, \quad \textit{i.e. } \phi_1(x) \text{ is (not strictly) convex.} \end{aligned} \tag{33}$$

We can now conclude that

$$\begin{aligned} u(\{x_n\}) &\equiv N^{-1} \sum_{i=1}^{N} \sum_{l=1}^{\infty} \phi(x_{i+l} - x_i) \geqslant N^{-1} \sum_{i=1}^{N} \sum_{l=1}^{\infty} \phi_1(x_{i+l} - x_i) \\ &\geqslant \sum_{l=1}^{\infty} \phi_1 \left\{ N^{-1} \sum_{i=1}^{N} (x_{i+l} - x_i) \right\} = \sum_{l=1}^{\infty} \phi_1(la) = \sum_{l=1}^{\infty} \phi(la). \end{aligned} \tag{34}$$

This completes the proof for case 1).

2) This case is rather more complicated. The Fourier transform of $\phi(x)$ is given by

$$\hat{\phi}(k) = 2 \int_0^\infty \phi(x) \cos kx\, dx = \sqrt{\pi}\, e^{-1/4k^2}. \tag{35}$$

It is not difficult to verify by means of partial integrations that

$$\begin{aligned} \phi(x) &= \frac{1}{\pi} \int_0^\infty \hat{\phi}(k) \cos kx\, dk \\ &= \frac{1}{\pi} \int_0^{2\pi/a} \cos kx \left\{ \hat{\phi}(k) - \sum_{l=0}^{3} \frac{(k - 2\pi/a)^l}{l!}\, \hat{\phi}^{(l)}\left(\frac{2\pi}{a}\right) \right\} dk + \end{aligned}$$

$$+\frac{1}{\pi}\int_{2\pi/a}^{\infty} g(kx)k^4\hat{\phi}^{(4)}(k)\,\mathrm{d}k \equiv \phi_1(x)+\phi_2(x). \tag{36}$$

$\phi_1(x)$ and $\phi_2(x)$ are defined by the first and second integral respectively. $\hat{\phi}^{(n)}(x)$ denotes the nth derivative of $\hat{\phi}(k)$ and the function $g(y)$ is given by

$$g(y) = y^{-4}(\tfrac{1}{2}y^2+\cos y-1). \tag{37}$$

We note that $\hat{\phi}^{(4)}(k) = (1/16)\sqrt{\pi}(k^4-12k^2+12)\,\mathrm{e}^{-1/4k^2} > 0$ for $k > (6+2\sqrt{6})^{1/2} \simeq 3.3014$.

In the present case we have

$$\frac{2\pi}{a} \geqslant \frac{2\pi}{p} \simeq 5.6054 > (6+2\sqrt{6})^{1/2},$$

and therefore

$$\hat{\phi}^{(4)}(k) > 0 \quad \text{for } k \geqslant \frac{2\pi}{a}. \tag{38}$$

From its definition (36) it is evident that the Fourier-transform of $\phi_1(x)$ is given by

$$\hat{\phi}_1(k) = \hat{\phi}(k) - \sum_{l=0}^{3}\frac{(|k|-2\pi/a)^l}{l!}\,\hat{\phi}^{(l)}\left(\frac{2\pi}{a}\right) \quad \text{for } |k| \leqslant \frac{2\pi}{a}$$

and

$$\hat{\phi}_1(k) = 0 \quad \text{for } |k| \geqslant \frac{2\pi}{a}. \tag{39}$$

Further we remark that from the explicit expression for $\hat{\phi}(k)$ it may be shown that

$$\hat{\phi}_1(k) > 0 \quad \text{for } |k| < \frac{2\pi}{a} \text{ (cf. Appendix B).} \tag{40}$$

From Poisson's summation theorem[4]) we can now conclude that

$$\begin{aligned} &N^{-1}\sum_{i=1}^{N}\sum_{l=1}^{\infty}\phi_1(x_{i+l}-x_i) \\ &= \frac{1}{2a}\sum_{m=-\infty}^{+\infty}\hat{\phi}_1\left(\frac{2\pi m}{Na}\right)\left|N^{-1}\sum_{i=1}^{N}\mathrm{e}^{-2\pi i m x_i/Na}\right|^2 - \tfrac{1}{2}\phi_1(0) \\ &\geqslant \frac{1}{2a}\hat{\phi}_1(0) - \tfrac{1}{2}\phi_1(0) = \frac{1}{2a}\sum_{m=-\infty}^{+\infty}\hat{\phi}_1\left(\frac{2\pi m}{a}\right) - \tfrac{1}{2}\phi_1(0) \\ &= \sum_{l=1}^{\infty}\phi_1(la). \end{aligned} \tag{41}$$

We now show that a similar inequality can be proved for

$$\phi_2(x) \equiv \frac{1}{\pi} \int_{2\pi/a}^{\infty} g(kx)k^4\hat{\phi}^{(4)}(k)\,\mathrm{d}k. \tag{42}$$

Let us introduce a function $g_1(y)$ defined by

$$\begin{aligned} g_1(y) &= g(y) && \text{for } y \geqslant 2\pi \\ &= g(2\pi) + (y - 2\pi)g'(2\pi) && \text{for } 0 \leqslant y \leqslant 2\pi. \end{aligned} \tag{43}$$

$g_1(y)$ can simply be shown to have the following properties:

$$\begin{aligned} &\text{a) } g_1(y) \text{ is convex} && \text{for } y > 0, \\ &\text{b) } g(y) - g_1(y) > 0 && \text{for } 0 < y < 2\pi. \end{aligned} \tag{44}$$

It then follows that (cf. (38), (42), (43) and (44)):

$$\begin{aligned} &N^{-1}\sum_{i=1}^{N}\sum_{l=1}^{\infty}\phi_2(x_{i+l}-x_i) \\ &= (\pi N)^{-1}\sum_{i=1}^{N}\sum_{l=1}^{\infty}\int_{2\pi/a}^{\infty} g\{k(x_{i+l}-x_i)\}k^4\hat{\phi}^{(4)}\,\mathrm{d}k \\ &\geqslant (\pi N)^{-1}\sum_{l=1}^{\infty}\int_{2\pi/a}^{\infty}\sum_{i=1}^{N} g_1\{k(x_{i+l}-x_i)\}k^4\hat{\phi}^{(4)}(k)\,\mathrm{d}k \\ &\geqslant \pi^{-1}\sum_{l=1}^{\infty}\int_{2\pi/a}^{\infty} g_1\left\{kN^{-1}\sum_{i=1}^{N}(x_{i+l}-x_i)\right\}k^4\hat{\phi}^{(4)}(k)\,\mathrm{d}k \\ &= \pi^{-1}\sum_{l=1}^{\infty}\int_{2\pi/a}^{\infty} g_1(kla)k^4\hat{\phi}^{(4)}(k)\,\mathrm{d}k \\ &= \pi^{-1}\sum_{l=1}^{\infty}\int_{2\pi/a}^{\infty} g(kla)k^4\hat{\phi}^{(4)}(k)\,\mathrm{d}k \\ &= \sum_{l=1}^{\infty}\phi_2(la). \end{aligned} \tag{45}$$

Combination of (41) and (45) leads to the result that also in case 2)

$$u(\{x_n\}) = N^{-1}\sum_{i=1}^{N}\sum_{l=1}^{\infty}\phi(x_{i+l}-x_i) \geqslant \sum_{l=1}^{\infty}\phi(la). \tag{46}$$

It is easily verified that the equal sign in (46) holds iff $x_{n+1} - x_n = a$ for all n.

We will now show by a counter-example that the theorem proved in this section for a class of repulsive potentials is by no means true for all repulsive potentials. Let us consider the potential

$$\phi(x) = (1 + x^4)^{-1}. \tag{47}$$

First we calculate the mean potential energy per particle for the equidistant configuration:

$$x_n = \tfrac{1}{2}n \quad (\text{all } n). \tag{48}$$

The result is:

$$u(\{x_n\}) = \sum_{l=1}^{\infty} \phi(\tfrac{1}{2}l) = 1.7212. \tag{49}$$

Next consider the configuration:

$$\begin{aligned} x_{2n} &= n \quad (\text{all } n), \\ x_{2n+1} &= n \quad (\text{all } n). \end{aligned} \tag{50}$$

This configuration, where at each lattice point n two particles coincide, has the same density 2 as the equidistant configuration (48), but here the mean potential energy per particle is:

$$u(\{x_n\}) = \tfrac{1}{2}\phi(0) + 2\sum_{l=1}^{\infty} \phi(l) = 1.6570, \tag{51}$$

i.e. it has a smaller energy per particle than the equally dense equidistant configuration. It is easily verified that the configuration with 3 coincident particles (and the same density) has an even lower energy per particle.

Appendix A

Proof of (19)*

Let us first take $t_m = 1$ ($m = 1, 2, \ldots, j$), i.e. we will prove that

$$\left\{\sum_{i=1}^{N} g\left(\frac{x_{i+l} - x_i}{l}\right)\right\}\left(\sum_{m=1}^{j} m\right) \leqslant \sum_{i=1}^{N} \sum_{m=1}^{j} mg\left(\frac{x_{i+m} - x_i}{m}\right), \tag{A.1}$$

for any convex function $g(x)$ and for $l \geqslant j$. The equal sign will hold iff $x_{n+1} - x_n$ is independent of n. Let us call

$$\sum_{i=1}^{N} g\left(\frac{x_{i+m} - x_i}{m}\right) = \sum_{i=1}^{N} g\left(\frac{a_i + a_{i+1} + \cdots + a_{i+m-1}}{m}\right) \equiv G_m. \tag{A.2}$$

* We wish to thank Dr. J. Groeneveld for showing us the proof of (A.1) reproduced here, which is more elegant than ours.

Here $a_i \equiv x_{i+1} - x_i$ is the distance between particles i and $i+1$. ($a_{i+N} = a_i$). Hence we must prove

$$A_{jl} \equiv \sum_{m=1}^{j} m(G_m - G_l) \geqslant 0 \quad \text{for } l \geqslant j. \tag{A.3}$$

From the convexity of $g(x)$ we know that

$$G_l \leqslant \frac{k}{l} G_k + \frac{l-k}{l} G_{l-k} \quad \text{for } 0 \leqslant k \leqslant l. \tag{A.4}$$

Hence

$$\begin{aligned} A_{jl} &\geqslant \frac{k}{l} \sum_{m=1}^{j} m(G_m - G_k) + \frac{l-k}{l} \sum_{m=1}^{j} m(G_m - G_{l-k}) \\ &= \frac{k}{l} A_{jk} + \frac{l-k}{l} A_{j(l-k)}, \quad \text{for } 0 \leqslant k \leqslant l. \end{aligned} \tag{A.5}$$

Noticing further that $A_{jj} = A_{(j-1)j}$ we conclude from (A.5) that we can restrict ourselves in our proof to:

$$1 \leqslant j < l \leqslant 2j - 1. \tag{A.6}$$

Let us define

$$C_{kl} \equiv kG_k + (l-k)G_{l-k} - lG_l \quad \text{for } 0 \leqslant k \leqslant l. \tag{A.7}$$

From (A.4) it follows that

$$C_{kl} \geqslant 0. \tag{A.8}$$

Consider now $(l - j < j)$:

$$\begin{aligned} A_{jl} - A_{(l-j-1)l} &= \sum_{m=l-j}^{j} m(G_m - G_l) \\ &= (l-j)G_{l-j} + jG_j - lG_l \\ &\quad + (l-j+1)G_{l-j+1} + (j-1)G_{j-1} - lG_l + \cdots \\ &= \sum_{\nu=0}^{j} \theta(2j - l - 2\nu) C_{l-j+\nu, j-\nu} \geqslant 0, \end{aligned} \tag{A.9}$$

where

$$\theta(x) = \begin{cases} 1 & \text{for } x > 0 \\ \frac{1}{2} & \text{for } x = 0 \\ 0 & \text{for } x < 0. \end{cases}$$

Now obviously $A_{1l} \geqslant 0$ and as $l - j - 1 < j - 1$ we may conclude from (A.9) that we can successively show that $A_{jl} \geqslant 0$ for all j and l satisfying (A.6) and hence also for all $l \geqslant j \geqslant 1$. The proof of (A.1) is now complete. In (19) we had introduced a set of numbers t_m ($m = 1, 2, \ldots, j$) with $t_1 \geqslant t_2 \geqslant \cdots \geqslant t_j \geqslant 0$. We now multiply (A.1) with t_j, (A.1) with j replaced by $j-1$ with $t_{j-1} - t_j$, (A.1) with j replaced by $j-2$ with $t_{j-2} - t_{j-1}$ and so on.

Adding the resulting inequalities we find (19).

Appendix B

Proof of (40)

We start from (39):

$$\hat{\phi}_1(k) \equiv \hat{\phi}(k) - \sum_{l=0}^{3} \frac{(k - 2\pi/a)^l}{l!} \hat{\phi}^{(l)}\left(\frac{2\pi}{a}\right) \quad \text{for } 0 \leqslant k \leqslant \frac{2\pi}{a},$$

$$\hat{\phi}_1(k) \equiv 0 \quad \text{for } k \geqslant \frac{2\pi}{a}.$$

We want to show that $\hat{\phi}_1(k) > 0$ for $0 \leqslant k < 2\pi/a$. Let us call $2\pi/a = k_0$.

$$\hat{\phi}_1(0) = \hat{\phi}(0) - \sum_{l=0}^{3} \frac{(-1)^l}{l!} \hat{\phi}^{(l)}(k_0) k_0^l.$$

Therefore

$$\begin{aligned}
\frac{\partial}{\partial k_0}\{\hat{\phi}_1(0)\} &= -\sum_{l=1}^{3} \frac{(-1)^l}{(l-1)!} k_0^{l-1} \hat{\phi}^{(l)}(k_0) - \sum_{l=0}^{3} \frac{(-1)^l}{l!} k_0^l \hat{\phi}^{(l+1)}(k_0) \\
&= -\sum_{l=0}^{2} \frac{(-1)^{l+1}}{l!} k_0^l \hat{\phi}^{(l+1)}(k_0) - \sum_{l=0}^{3} \frac{(-1)^l}{l!} k_0^l \hat{\phi}^{(l+1)}(k_0) \\
&= \frac{k_0^3}{3!} \hat{\phi}^{(4)}(k_0) > 0 \quad \text{(cf. (38))}.
\end{aligned}$$

Hence $\hat{\phi}_1(0)$ is an increasing function of k_0. For $k_0 = 2\pi/p$ calculation gives:

$$\hat{\phi}_1(0) = 0.7460\sqrt{\pi},$$

and for all $k_0 \geqslant 2\pi/p$ (i.e. $0 < a \leqslant p$): $\hat{\phi}_1(0) > 0$. One verifies from $\hat{\phi}(k) = \sqrt{\pi}\, e^{-1/4k^2}$ that

$$(-1)^j \hat{\phi}^{(j)}(k_0) > 0 \quad (j = 0, 1, 2, 3, 4).$$

Further from (39):

$$\hat{\phi}_1^{(j)}(k) = \hat{\phi}^{(j)}(k) - \sum_{l=0}^{3-j} \frac{(k - k_0)^l}{l!} \hat{\phi}^{(l+j)}(k_0)$$

for $j = 0, 1, 2, 3$ and $0 \leqslant k \leqslant k_0$.

One can now show easily that

$$\hat{\phi}_1(0) > 0, \hat{\phi}_1^{(1)}(0) > 0, \hat{\phi}_1^{(2)}(0) < 0 \text{ and } \hat{\phi}_1^{(3)}(0) > 0$$

and also: (B.1)

$$\hat{\phi}_1(k_0) = \hat{\phi}_1^{(1)}(k_0) = \hat{\phi}_1^{(2)}(k_0) = \hat{\phi}_1^{(3)}(k_0) = 0.$$

Furthermore we know from (39) and the explicit expression for $\hat{\phi}^{(4)}(k)$ (cf. the line below (37)):

$$\hat{\phi}_1^{(4)}(k) = \hat{\phi}^{(4)}(k) > 0 \quad \text{for } 0 < k < (6 - 2\sqrt{6})^{1/2}$$
$$\text{and for } k_0 > k > (6 + 2\sqrt{6})^{1/2},$$
$$\hat{\phi}_1^{(4)}(k) = \hat{\phi}^{(4)}(k) < 0 \quad \text{for } (6 - 2\sqrt{6})^{1/2} < k < (6 + 2\sqrt{6})^{1/2},$$

i.e. $\hat{\phi}_1^{(3)}(k)$ is strictly increasing for $0 \leq k \leq (6 - 2\sqrt{6})^{1/2}$ and $k_0 \geq k \geq (6 + 2\sqrt{6})^{1/2}$, and is strictly decreasing for $(6 - 2\sqrt{6})^{1/2} \leq k \leq (6 + 2\sqrt{6})^{1/2}$.

If we combine this result with (B.1) we may conclude that a number z_3 exists with $(6 - 2\sqrt{6})^{1/2} < z_3 < (6 + 2\sqrt{6})^{1/2}$, such that

$$\hat{\phi}_1^{(3)}(k) > 0 \quad \text{for } 0 \leq k < z_3,$$
$$\hat{\phi}_1^{(3)}(k) < 0 \quad \text{for } z_3 < k < k_0,$$
$$\hat{\phi}_1^{(3)}(z_3) = 0.$$

Hence $\hat{\phi}^{(2)}(k)$ is strictly increasing for $0 \leq k \leq z_3$ and strictly decreasing for $z_3 \leq k \leq k_0$. We can continue in a similar way and we find: There is a number z_2 with $0 < z_2 < z_3$, such that

$$\hat{\phi}_1^{(2)}(k) < 0 \quad \text{for } 0 \leq k < z_2,$$
$$\hat{\phi}_1^{(2)}(k) > 0 \quad \text{for } z_2 < k < k_0,$$
$$\hat{\phi}_1^{(2)}(z_2) = 0.$$

Furthermore there is a number z_1 with $0 < z_1 < z_2$, such that

$$\hat{\phi}_1^{(1)}(k) > 0 \quad \text{for } 0 \leq k < z_1,$$
$$\hat{\phi}_1^{(1)}(k) < 0 \quad \text{for } z_1 < k \leq k_0,$$
$$\hat{\phi}_1(z_1) = 0.$$

And finally (cf. (B.1)):

$$\hat{\phi}_1(k) > 0 \quad \text{for } 0 \leq k < k_0. \quad \text{Q.E.D.}$$

References

1) W.J. Ventevogel, Physica **92A** (1978) 343.

2) C.S. Gardner and C. Radin, J. Stat. Phys., to be published.
3) F. Oberhettinger, Tabellen zur Fourier Transformation (Springer, Berlin, 1957) S.4.
4) R. Courant and D. Hilbert, Methoden der Mathematischen Physik (Springer, Berlin, 1931) S.64.