

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

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Previous work on infinite one-dimensional systems of interacting particles is continued. In the case of two-body potentials $\phi(x) = \phi(-x)$, whose Fourier transform $\hat{\phi}(k)$ exists, it is shown that a necessary condition that the equidistant configuration has for a certain range of densities minimum potential energy per particle among all configurations of the same density, is that $\hat{\phi}(k) \geq 0$ for all k . An analogous theorem is proved for systems of particles in two and three dimensions.

Furthermore some properties are discussed of one-dimensional systems for which $\hat{\phi}(k) \geq 0$ for all k and moreover $\hat{\phi}(k) = 0$ for $|k| \geq k_0$.

1. Introduction

In previous publications^{1,2}, to be referred to as I and II, respectively, we studied finite and infinite one-dimensional systems of particles interacting with a two-body potential $\phi(x)$. $\phi(x)$ was assumed to satisfy $\phi(x) = \phi(-x)$ and to be integrable at infinity. We were mainly interested in identifying classes of potentials $\phi(x)$ (either repulsive or of generalized Lennard-Jones (L.J.) type) for which in an infinite system the equidistant configuration could be shown to have the minimum potential energy per particle to the exclusion of all other configurations.

To be more specific we showed in I that for a *convex repulsive* potential $\phi(x)$ (i.e. $\phi''(x) > 0$ for $x \neq 0$) among all configurations of an infinite one-dimensional system with arbitrary but fixed number density the equidistant configuration has the smallest potential energy per particle. For these potentials the potential energy per particle of a finite system could be shown to have a minimum smaller than the minimum of the potential energy per particle of an infinite system of the same number density, but converging to the latter if the number of particles tends to infinity.

In II the first property (for infinite systems) has been proved also for a class of *non-convex* repulsive potentials, which includes potentials as $\phi(x) = e^{-\alpha x^2}$ ($\alpha > 0$) and $\phi(x) = (b^2 + x^2)^{-n}$ ($b > 0, n > \frac{1}{2}$). However, it was shown that this property does *not* hold for $\phi(x) = (1 + x^4)^{-1}$ (at least not for certain densities).

With regard to generalized L.J. potentials, we introduced in I a class of potentials (*A-potentials*) for which (1) 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 (2) $\int_0^\infty \phi(x) dx > 0$ (or ∞). Furthermore we defined in II a subclass of A-potentials, which we called *C-potentials*, for which in addition a fixed number $\alpha > 0$ exists such that

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

Notice that all L.J. potentials with exponents $l > m > 1$ are C-potentials. In II we proved for C-potentials two theorems.

(1) The equation

$$\sum_{l=1}^{\infty} l\phi'(la) = 0 \quad (2)$$

has a unique solution $a = a_0 > 0$, and for all finite or infinite configurations the potential energy per particle $u(\{x_n\})$ satisfies

$$u(\{x_n\}) \geq \sum_{l=1}^{\infty} \phi(la_0). \quad (3)$$

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

(2) For an infinite system with a given volume per particle $a \leq a_0$

$$u(\{x_n\}) \geq \sum_{l=1}^{\infty} \phi(la). \quad (4)$$

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

It is easily verified that theorem (2) does not hold for $a > a_0$. On the other hand theorem (1) does not hold for all A-potentials as was shown in I by a counter-example.

In continuation of the previous work briefly summarized above we will prove in the present paper the following theorem (which has been stated without proof already in II):

Let $\phi(x) = \phi(-x)$ be a two-body potential (either repulsive or of generalized L.J. type) for which the Fourier transform $\hat{\phi}(k) = 2 \int_0^\infty \phi(x) \cos kx dx$ exists and for which $\phi''(x)$ is continuous and sufficiently well-behaved at infinity. We consider periodic configurations $\{x_n\}$, such that $x_{n+1} > x_n$ (all n) and $x_{n+N} - x_n = Na$ (all n). N is a large but arbitrary periodicity number and a is the average volume per particle. If a number a_1 exists, such that for all $a(0 < a \leq a_1)$ and independently of N

$$u(\{x_n\}) \equiv \frac{1}{N} \sum_{i=1}^N \sum_{j=1}^{\infty} \phi(x_{i+j} - x_i) \geq \sum_{j=1}^{\infty} \phi(ja), \quad (5)$$

then

$$\hat{\phi}(k) \geq 0 \quad \text{for all } k. \quad (6)$$

We have here a necessary condition pertaining to potentials which have a Fourier transform. Furthermore we will show that this theorem may be generalized to systems in more dimensions. Finally we will discuss (without giving here all the proofs) some results for potentials for which

$$\hat{\phi}(k) \geq 0 \quad \text{and} \quad \hat{\phi}(k) = 0 \quad \text{for } |k| \geq k_0. \quad (7)$$

We would like to mention that related work by C. Radin et al.³⁾ is in course of publication in J. Stat. Phys.

2. Proof of necessary condition for one-dimensional systems

Suppose that for all a (a is volume per particle) smaller (or equal) than a given value a_1 and independently of the periodicity number N , the potential energy per particle

$$u(\{x_n\}) \geq \sum_{j=1}^{\infty} \phi(ja). \quad (5)$$

The right-hand side represents the potential energy per particle of the equidistant configuration. We define $y_n = x_n - na$. We then have

$$y_{i+N} = y_i \quad \text{for all } i \quad \text{and} \quad \sum_{i=1}^N (y_{i+j} - y_i) = 0, \quad (8)$$

because $\sum_{i=1}^N (x_{i+j} - x_i) = jNa$.

For small values of y_n

$$u(\{x_n\}) \approx \sum_{j=1}^{\infty} \phi(ja) + \frac{1}{2} \sum_{j=1}^{\infty} \left\{ N^{-1} \sum_{i=1}^N (y_{i+j} - y_i)^2 \right\} \phi''(ja). \quad (9)$$

Hence for each set $\{y_i\}$ satisfying (8) we have for $0 < a \leq a_1$:

$$\sum_{j=1}^{\infty} \left\{ N^{-1} \sum_{i=1}^N (y_{i+j} - y_i)^2 \right\} \phi''(ja) \geq 0. \quad (10)$$

For complex values of $\{y_i\}$ we conclude by considering the real and imaginary part separately that also

$$\sum_{j=1}^{\infty} \left\{ N^{-1} \sum_{i=1}^N |y_{i+j} - y_i|^2 \right\} \phi''(ja) \geq 0 \quad \text{for } 0 < a \leq a_1. \quad (10a)$$

We now make the special choice

$$y_n = \epsilon e^{2\pi i n m / N}, \quad (m \text{ integer, } \epsilon \text{ is a small number}) \quad (11)$$

which satisfies (8). It then follows from (10a) that

$$\sum_{j=1}^{\infty} \left(1 - \cos \frac{2\pi j m}{N}\right) \phi''(ja) \geq 0 \quad \text{for } 0 < a \leq a_1, \quad (12)$$

for all integer m . As (12) was supposed to hold independently of N we may conclude that for all real x

$$\sum_{j=1}^{\infty} (1 - \cos jx) \phi''(ja) \geq 0 \quad \text{for } 0 < a \leq a_1. \quad (13)$$

Hence

$$\lim_{a \downarrow 0} a \sum_{j=1}^{\infty} \frac{1 - \cos jka}{k^2} \phi''(ja) = \int_0^{\infty} \frac{1 - \cos ky}{k^2} \phi''(y) dy \geq 0. \quad (14)$$

But

$$\int_0^{\infty} \frac{1 - \cos ky}{k^2} \phi''(y) dy = \frac{1}{2} \hat{\phi}(k) \quad (\text{by partial integration}).$$

We therefore find:

$$\hat{\phi}(k) \geq 0 \quad \text{for all } k. \quad \text{Q.E.D.} \quad (15)$$

For convex repulsive potentials we proved in I and for the class of repulsive potentials $\phi(x) = \int_0^{\infty} W(\alpha) e^{-\alpha x^2} d\alpha$ (with $W(\alpha) \geq 0$ but further arbitrary) we proved in II, that for arbitrary values of the volume a per particle the equidistant configuration has the smallest potential energy per particle. One can easily verify that for these potentials (if their Fourier transform exists) indeed $\hat{\phi}(k) \geq 0$ for all k . On the other hand it was shown in II that for $\phi(x) = (1 + x^4)^{-1}$ for certain densities the equidistant configuration is not the one with minimum potential energy per particle. It was pointed out in II that $\phi(k) = \pi \exp(-\frac{1}{2}\sqrt{2}|k|) \cos(\frac{1}{2}\sqrt{2}|k| - \frac{1}{4}\pi)$ is not positive definite. We may even conclude from the theorem proved above that for any value of a_1 there must be values of a with $0 < a \leq a_1$ for which there are configurations with smaller potential energy per particle than that of the equidistant configuration.

Let us consider for a moment also potentials of type-A. For a subclass of A-potentials, introduced in I and called B-potentials, it has been proved there that $\hat{\phi}(k) \geq 0$, if it does exist. In Appendix A we will show that for A-potentials a sufficient condition that $\hat{\phi}(k) \geq 0$ if it exists, is that a positive

number γ can be found such that

$$\gamma\phi'(x) + \phi''(x) > 0 \quad \text{for all } x > 0. \quad (15a)$$

This condition is satisfied e.g. for the potential

$$\phi(x) = Ae^{-\lambda x} - Be^{-\mu x}, \quad (\lambda > \mu > 0; A\mu > B\lambda > 0)$$

considered in II, because

$$\mu\phi'(x) + \phi''(x) = A\lambda(\lambda - \mu)e^{-\lambda x}.$$

By the way the criterion (15a) is also satisfied by all C-potentials. However, the Fourier transform of C-potentials does not exist in general.

Though we have found that the criterium $\hat{\phi}(k) \geq 0$ (for all k) is a *necessary* condition for the theorems mentioned in the Introduction to hold (i.e. for potentials for which $\hat{\phi}(k)$ exists), it cannot be a sufficient condition on the two-body potential. In Appendix B we will prove that for any function $\phi(x) = \phi(-x)$, for which $|\phi(x)|$ is integrable at infinity and for which $\int_b^\infty |\phi''(x)|dx < \infty$ for all $b > 0$, we can find for every $a > 0$ a function $\psi_a(x)$, such that

$$\psi_a(x) = \phi(x) \quad \text{for } x \geq a$$

and

$$\psi_a(k) \geq 0. \quad (16)$$

Hence we may modify e.g. the function $\phi(x) = (1 + x^4)^{-1}$ in an arbitrary small interval around $x = 0$ in such a way that the modified function has a non-negative Fourier transform. And it will be evident that for this modified potential the equidistant configuration cannot have the minimum potential energy per particle for all densities. Indeed, from the discussion in II it follows that one can find a value of ϵ small enough in order that the configuration $x_{2n} = n$, $x_{2n+1} = n + \epsilon$ has smaller potential energy per particle than the equidistant configuration of the same density. One can then modify $\phi(x)$ in an interval smaller than ϵ around $x = 0$ in such a way that the Fourier transform of the modified function becomes non-negative.

3. Proof of necessary condition for three-dimensional systems

The proof given in section 2 for one-dimensional systems may be generalized to systems in more dimensions. However, we prefer to give an alternative proof, in which for definiteness we assume the system to be three-dimensional.

Suppose that the three-dimensional two-body potential has the following properties:

- (1) $\phi(\mathbf{r}) = \phi(-\mathbf{r})$ and is sufficiently well-behaved at 0 and ∞ ;
- (2) The Fourier transform $\hat{\phi}(\mathbf{k}) \equiv \int \phi(\mathbf{r}) e^{i\mathbf{k} \cdot \mathbf{r}} d\mathbf{r}$ exists;
- (3) $\lim_{k \rightarrow \infty} \hat{\phi}(\mathbf{k}) = 0$.

If now 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 (with arbitrarily large periodicity number N) 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 $\rho \rightarrow \infty$, then $\hat{\phi}(\mathbf{k}) \geq 0$ for all \mathbf{k} .

Notice that we need not assume here (and this applies equally to the one-dimensional case treated in section 2) that the Bravais-lattice is the only configuration for which the potential energy takes the minimum value for given density. And furthermore for another density $\rho > \rho_0$ this Bravais-lattice may be of different type.

Let for given density $\rho > \rho_0$ the basic vectors of the Bravais-lattice having minimum potential energy be denoted by \mathbf{e}_j ($j = 1, 2, 3$).

Consider also a large parallelepiped as periodicity volume with basic vectors $L_j \mathbf{e}_j$ (L_j integer), in which there are $N = L_1 L_2 L_3$ particles. In an infinite periodic system the positions of the particles are given by:

$$\mathbf{r}_n + \mathbf{K}_m \quad \text{with} \quad \mathbf{K}_m = \sum_{j=1}^3 m_j L_j \mathbf{e}_j \quad (m_j \text{ integers, } n = 1, 2, \dots, N).$$

From Poisson's summation theorem⁽⁴⁾ it follows that the potential energy per particle $u(\{\mathbf{r}_n\})$ in this infinite periodic system is given by

$$\begin{aligned} u(\{\mathbf{r}_n\}) &= (2N)^{-1} \sum_{n=1}^N \sum_{l \neq n} \phi(\mathbf{r}_l - \mathbf{r}_n) \\ &= -\frac{1}{2} \phi(0) + \frac{N}{2V} \sum_{\mathbf{m}} \hat{\phi}(\mathbf{P}_m) \left| N^{-1} \sum_{j=1}^N e^{-i\mathbf{P}_m \cdot \mathbf{r}_j} \right|^2, \end{aligned} \quad (17)$$

where V is the volume of the large parallelepiped and $\mathbf{P}_m = 2\pi \sum_{j=1}^3 m_j L_j^{-1} \mathbf{f}_j$ with $\mathbf{f}_j \cdot \mathbf{e}_k = \delta_{jk}$. The summation over l is over all particles except the one in \mathbf{r}_n and including all particles outside the volume V . For the particular configuration of the Bravais-lattice we have

$$u(\{\mathbf{r}_n\}) = -\frac{1}{2} \phi(0) + \frac{1}{2v} \sum_{\mathbf{n}} \hat{\phi}(\mathbf{p}_n), \quad (18)$$

where $v = V/N$ is the volume of the unit cell and $\mathbf{p}_n = 2\pi \sum_{j=1}^3 n_j \mathbf{f}_j$. Because we have supposed that the linear dimensions of the unit cell of the Bravais-lattice approach 0 as $\rho \rightarrow \infty$, it follows that $\lim_{\rho \rightarrow \infty} |\mathbf{p}_n| = \infty$ for all \mathbf{n} unequal to the nullvector. And as $\hat{\phi}(\mathbf{k}) \rightarrow 0$ as $k \rightarrow \infty$ we may conclude that $(\rho = 1/v)$:

$$\lim_{\rho \rightarrow \infty} \rho^{-1} \min u(\{r_n\}) = \frac{1}{2} \hat{\phi}(0). \quad (19)$$

Now suppose for a moment that there is a vector k_0 for which $\hat{\phi}(k_0) < 0$. Without loss of generality we take $k_0 = (k_0, 0, 0)$. Now consider a configuration with particles in positions $r = (x, y, z)$ such that

$$\rho^{1/3} \frac{(k_0 x + \sin k_0 x)}{k_0}, \rho^{1/3} y, \rho^{1/3} z \text{ are integers.}$$

These particles are *not* on a Bravais-lattice. Let us assume that $2\pi k_0^{-1} \rho^{1/3}$ is an integer number. As we are interested in very large densities this is not a serious restriction. We now have a periodicity volume which is a rectangular parallelepiped with edges $L_1 = 2\pi k_0^{-1}$, $L_2 = L_3 = \rho^{-1/3}$. Inside this volume there are $2\pi k_0^{-1} \rho^{1/3}$ particles and the density is ρ .

The vectors P_m in (17) are now: $P_m = (m_1 k_0, 2\pi \rho^{1/3} m_2, 2\pi \rho^{1/3} m_3)$ with m_j integer, and

$$N^{-1} \sum_{j=1}^N e^{-iP_m \cdot r_j} = N^{-1} \sum_{j=1}^N e^{-im_1 x_j k_0} \quad \text{with } N = 2\pi k_0^{-1} \rho^{1/3}.$$

As ρ increases indefinitely, the number of integer values of $\rho^{1/3} k_0^{-1} (k_0 x + \sin k_0 x)$ between x and $x + dx$ will be approximated to any degree of accuracy by $\rho^{1/3} (1 + \cos k_0 x) dx$ and hence

$$\begin{aligned} \lim_{\rho \rightarrow \infty} N^{-1} \sum_{j=1}^N e^{-im_1 x_j k_0} &= \lim_{\rho \rightarrow \infty} \frac{k_0}{2\pi \rho^{1/3}} \int_0^{2\pi/k_0} e^{-im_1 x k_0} \rho^{1/3} (1 + \cos k_0 x) dx \\ &= (2\pi)^{-1} \int_0^{2\pi} (1 + \cos u) e^{-im_1 u} du \\ &= \begin{cases} 1 & \text{for } m_1 = 0 \\ \frac{1}{2} & \text{for } m_1 = \pm 1 \\ 0 & \text{for all other values of } m_1. \end{cases} \end{aligned} \quad (20)$$

For this particular configuration we therefore find from (17)

$$\lim_{\rho \rightarrow \infty} \rho^{-1} u(\{r_n\}) = \frac{1}{2} \hat{\phi}(0) + (1/8) \hat{\phi}(k_0) + (1/8) \hat{\phi}(-k_0) < \frac{1}{2} \hat{\phi}(0). \quad (21)$$

This is in contradiction to (19) and we come to the conclusion that $\hat{\phi}(k) \geq 0$ for all k .

Similarly as for one-dimensional systems, $\phi(r) = 1/(1+r^4)$ is an example of a potential for which in three dimensions the necessary condition $\hat{\phi}(k) \geq 0$ is not satisfied ($\hat{\phi}(k) = \pi^2 \sqrt{2} k^{-1} \exp(-\frac{1}{2} \sqrt{2} k) \sin \frac{1}{2} \sqrt{2} k$). However, again as in section 2 we can show that under mild conditions any function $\phi(r)$ may be

modified in an arbitrarily small region around the origin in such a way that the Fourier transform of the modified function is everywhere non-negative.

4. Potentials with $\hat{\phi}(k) \geq 0$ (all k) and $\hat{\phi}(k) = 0$ for $|k| \geq k_0$

In this section we return to one-dimensional systems. Suppose that the Fourier transform of the two-body potential $\phi(x) = \phi(-x)$ has the following properties:

- (1) $\hat{\phi}(k) \geq 0$ for all k ;
- (2) $\hat{\phi}(k) = 0$ for $|k| \geq k_0 > 0$. (22)

Let us consider infinite periodic systems with arbitrarily large periodicity number N and let the volume per particle be $a = 1/\rho$ (ρ is the number density). We will now prove that for $\rho \geq k_0/2\pi$ ($a \leq 2\pi/k_0$) the potential energy per particle $u(\{x_n\})$ takes its minimum value for the equidistant configuration.

From Poisson's summation theorem (cf. section 3) it follows that

$$\begin{aligned} u(\{x_n\}) &\equiv N^{-1} \sum_{i=1}^N \sum_{l=1}^{\infty} \phi(x_{i+l} - x_i) \\ &= \frac{1}{2a} \sum_{m=-\infty}^{+\infty} \hat{\phi}\left(\frac{2\pi m}{Na}\right) \left| N^{-1} \sum_{j=1}^N \exp(-2\pi i m x_j / Na) \right|^2 - \frac{1}{2} \phi(0). \end{aligned} \quad (23)$$

If $\hat{\phi}(k) \geq 0$ we see, by keeping only the term $m = 0$ in the above sum, that

$$u(\{x_n\}) \geq \frac{1}{2a} \hat{\phi}(0) - \frac{1}{2} \phi(0). \quad (24)$$

For the equidistant configuration $x_j = ja$ (23) reduces to

$$u(\{na\}) = \frac{1}{2a} \sum_{m=-\infty}^{+\infty} \hat{\phi}\left(\frac{2\pi m}{a}\right) - \frac{1}{2} \phi(0). \quad (25)$$

Now if $\hat{\phi}(k) = 0$ for $|k| \geq k_0$, we conclude that for $a \leq 2\pi/k_0$

$$u(\{na\}) = \frac{1}{2a} \hat{\phi}(0) - \frac{1}{2} \phi(0), \quad (26)$$

and this according to (24) is indeed the minimum of the potential energy per particle for all configurations with volume a per particle. However, it will be evident from (22) that this minimum value will be reached by every periodic structure with period $\leq 2\pi/k_0$.

Let us finally consider a configuration consisting of two equidistant

configurations superposed, in which particles occupy the positions ("composite crystal"):

$$\begin{aligned}x_n^{(1)} &= na, \quad a > 0, \\x_n^{(2)} &= nb + c, \quad b > 0, \quad 0 \leq c \leq b.\end{aligned}\tag{27}$$

The mean volume per particle is given by

$$\frac{1}{v} = \frac{1}{a} + \frac{1}{b}.$$

If a/b is rational, the configuration considered is strictly periodic, if a/b is irrational it is not.

We can show that for potentials satisfying (22), at given density $\rho > k_0/\pi$ the minimum potential energy per particle $(1/2v)\hat{\phi}(0) - \frac{1}{2}\phi(0)$ is assumed for all configurations (27) as long as $a \leq 2\pi/k_0$ and $b \leq 2\pi/k_0$. Among these configurations are periodic as well as non-periodic ones.

And furthermore that for $\rho = k_0/2\pi$ the equidistant configuration is the *only* configuration for which $u(\{x_n\})$ takes its minimum value. The proofs of these last two statements, which are somewhat more complicated, will not be reproduced here.

Appendix A

Proof that $\hat{\phi}(k) \geq 0$ (all k) for all A-potentials for which $\hat{\phi}(k)$ exists and which satisfy the relation

$$\gamma\phi'(x) + \phi''(x) > 0 \quad \text{for all } x > 0 \quad \text{and for fixed } \gamma > 0.\tag{A.1}$$

It is obvious that all C-potentials obey (A.1). For if x_0 is the unique solution of $\phi'(x_0) = 0$, we have

$$(x - x_0)\phi'(x) \geq 0 \quad (x > 0).\tag{A.2}$$

From the definition of C-potentials (cf. the Introduction)

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

Hence

$$x\{(\alpha + 1)\phi'(x) + x_0\phi''(x)\} \geq x_0\{(\alpha + 1)\phi'(x) + x\phi''(x)\} > 0,\tag{A.3}$$

and (A.1) is satisfied with $\gamma = (\alpha + 1)/x_0$. From (A.1) follows by integration for $x > 0$

$$\gamma\phi(x) + \phi'(x) < 0,$$

and therefore

$$\phi''(x) - \gamma^2 \phi(x) = \phi''(x) + \gamma \phi'(x) - \gamma(\phi'(x) + \gamma \phi(x)) > 0, \quad \text{for } x > 0. \quad (\text{A.4})$$

As $\phi(-x) = \phi(x)$ we see from (A.4) that

$$\phi''(x) - \gamma^2 \phi(x) > 0 \quad \text{for all } x. \quad (\text{A.5})$$

Now

$$k^2 \hat{\phi}(k) = 2 \int_0^\infty (1 - \cos kx) \phi''(x) dx,$$

$$\gamma^2 \hat{\phi}(k) = 2 \int_0^\infty \gamma^2 \cos kx \phi(x) dx,$$

$$\gamma^2 \hat{\phi}(0) = 2 \int_0^\infty \gamma^2 \phi(x) dx$$

and hence from (A.5):

$$(k^2 + \gamma^2) \hat{\phi}(k) - \gamma^2 \hat{\phi}(0) = 2 \int_0^\infty (1 - \cos kx)(\phi'' - \gamma^2 \phi(x)) dx \geq 0,$$

$$\hat{\phi}(k) \geq \frac{\gamma^2}{k^2 + \gamma^2} \hat{\phi}(0) > 0. \quad \text{Q.E.D.}$$

Appendix B

Proof of equation (16)

We suppose that $\phi(x) = \phi(-x)$, $|\phi(x)|$ is integrable at infinity and $\int_b^\infty |\phi''(x)| dx < \infty$ for all $b > 0$. We will prove that for all $a > 0$ a function $\psi_a(x)$ can be found such that

$$\psi_a(x) = \phi(x) \quad \text{for } x \geq a,$$

$$\hat{\psi}_a(k) \geq 0 \quad \text{for all } k.$$

We define the function $\bar{\psi}_a(x)$ by

$$\bar{\psi}_a(x) = \phi(x) \quad \text{for } x \geq a,$$

$$\bar{\psi}_a(x) = \phi(a) + (x - a)\phi'(a) \quad \text{for } 0 \leq x \leq a, \quad (\text{B.1})$$

$$\bar{\psi}_a(-x) = \bar{\psi}_a(x).$$

Then

$$\begin{aligned}\hat{\psi}_a(k) &= 2 \int_0^\infty \bar{\psi}_a(x) \cos kx \, dx = \frac{2}{k^2} \int_0^\infty (1 - \cos kx) \bar{\psi}_a''(x) \, dx \\ &= \frac{2}{k^2} \int_0^\infty (1 - \cos kx) \phi''(x) \, dx.\end{aligned}$$

Hence

$$|\hat{\psi}_a(k)| \leq 2 \int_0^\infty |\bar{\psi}_a(x)| \, dx$$

and

$$|\hat{\psi}_a(k)| \leq \frac{4}{k^2} \int_0^\infty |\phi''(x)| \, dx. \quad (\text{B.2})$$

We conclude that there are positive numbers A and B , such that

$$\hat{\psi}_a(k) \geq -\min(A, Bk^{-2}). \quad (\text{B.3})$$

We now define the function $g(x)$ by

$$\begin{aligned}g(x) &= (a - x)^2 \quad \text{for } 0 \leq x \leq a, \\ g(x) &= 0 \quad \text{for } x \geq a, \\ g(-x) &= g(x).\end{aligned} \quad (\text{B.4})$$

Then

$$\begin{aligned}\hat{g}(k) &= 2 \int_0^a (a - x)^2 \cos kx \, dx = 4k^{-2} \int_0^a (1 - \cos kx) \, dx \\ &= 4k^{-3}(ka - \sin ka) > 0.\end{aligned} \quad (\text{B.5})$$

We choose the number h so large that $h\hat{g}(k) \geq \min(A, Bk^{-2})$. That this is possible may be seen as follows:

$$\lim_{k \rightarrow \infty} \hat{g}(k) \{\min(A, Bk^{-2})\}^{-1} = \frac{4a}{B} > 0.$$

Moreover the function $\hat{g}(k) \{\min(A, Bk^{-2})\}^{-1}$ is a continuous positive function of k . Therefore this function has either a positive minimum or it is $> 4a/B$ for all k . We call this minimum (or $4a/B$ in the alternative case) h^{-1} . Then

$$h\hat{g}(k) \geq \min(A, Bk^{-2}). \quad (\text{B.6})$$

We finally define $\psi_a(x) = \bar{\psi}_a(x) + \hbar g(x)$. (B.7)

It then follows from (B.3) and (B.6) that

$$\hat{\psi}_a(k) \geq 0 \quad \text{for all } k.$$

References

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