Dynamical phase transition in the simplest molecular chain model

V. A. Malyshev, S. A. Muzychka

Abstract

We consider the dynamics of the simplest chain of large number $N$ of particles. We find, in the double scaling limit, the partition of the parameter space onto two domains, where for one domain the supremum (over all time interval $(0, \infty)$ of relative extension tends to 1 as $N \to \infty$, and for the other this supremum tends to infinity as $N \to \infty$.

1 Introduction

For mathematical models of equilibrium statistical physics one needs stability, that is finiteness of the partition function in the finite volume. This stability condition provides good approximation for many phenomena in gases, liquids and even condensed matter. However, for example, any analysis of the models for expansion or destruction of condensed matter rests on the problem that the volume is not fixed and it is necessary to consider finite number of particles in the infinite volume. For realistic interactions (when the potential disappears at infinity) such system is not stable that is Gibbs distribution does not exist. It is common to say that the system is metastable, see for example \cite{1}.

For finite number of particles, it is necessary then to prove that the system does not quit some bounded region of the phase space (does not dissociate into pieces). As this region depends on all parameters of the model, for large number of particles it is convenient to use the method, the so called double (sometimes it is better to say multiple) scaling limit in physics. In our case all parameters are scaled with respect to large number $N$ of particles. Then one can get asymptotic estimates in the large $N$ limit, exhibiting the phase transition domain of parameters.

We consider one-dimensional system of $N$ classical point particles (molecules) of the same mass $m$ and initial configuration at time $t = 0$

$$0 = z_0(0) < z_1(0) = a < z_2(0) = 2a < \ldots < z_{N-1}(0) = (N-1)a$$

for some $a > 0$. The dynamics of such system is defined by the following Hamiltonian

$$H = \sum_{k=1}^{N-1} \frac{p_k^2}{2m} + \sum_{k=1}^{N-1} V(z_k - z_{k-1}) - f z_{N-1}$$

It is assumed that one of the particles $z_0$ stays permanently at zero, and $z_{N-1}$ is subjected to the constant external force $f > 0$. Concerning the function $V(z)$ it is assumed that $V(z) \to \infty$ as $z \to 0$, $V(z) \to 0$ as $z \to \infty$, $V(z)$ is convex on the interval $(0, b)$, concave on $(b, \infty)$ and has the unique minimum $V(a) < 0$ at some $a > 0$, where $a < b < \infty$. Of course, Gibbs distribution with such Hamiltonian does not exist, and two approaches are possible:

1. to change $V(z)$ for large $z$ so that $V(z) \to \infty$ as $x \to \infty$, then one can use Gibbs ideology to study thermal and elastic extension in equilibrium. See the book \cite{12} where there are many related applied problems, and, in particular, by simple calculation for harmonic chain, the growth of variance of extension, linear in temperature, had been demonstrated. However, as it was shown earlier in \cite{2}, the mean extension can be linear in $T$ only for non-harmonic case.

2. to find a neighborhood $O(a)$ of the minimum such that, for initial data \cite{11} the trajectory stays in $O(a)$ forever.
Here we follow the second approach, assuming additionally that in the vicinity of point \( a \) the potential has the quadratic form
\[
V(z) = \frac{\kappa}{2}(z - a)^2
\]
Now we formulate this more exactly. It is not difficult to calculate the extension of such chain in the static situation (at zero temperature), that is to find the unique fixed point (minimum of \( H \)), see below. However it is logical to study the dynamics of this particle system and get good estimates for the functional
\[
A = A(N, l, f, \kappa, m) = \max_{1 \leq k, k+l \leq N-1} \sup_{t \in (0, \infty)} |z_{k+l}(t) - z_k(t)|
\]
for large \( N \) and various \( l > 0 \). In despite of evident simplicity of the model, the main result of the paper - estimates for the maximal (over all time interval) deviations from the initial crystal structure is nontrivial and uses some facts from number theory. The question is that, although the model has a simple fixed point, but the following inequalities hold
\[
\text{for large } N \text{ and various } l > 0.
\]

We want to note that there are many papers concerning other problems for one-dimensionnal models. Most popular are the Fermi-Pasta-Ulam models \( [5] \) and the Frenkel-Kontorova model \( [6] \). One should also mention the papers \( [10, 6, 9, 7, 8] \), erasing from the book \( [11] \), where multi-dimensional static models were considered with the goal to derive equations of linear elasticity from micromodels.

### 2 Main result

Defining the deviations \( x_k(t) = z_k(t) - ka, k = 0, \ldots, N - 1 \), we have the following hamiltonian system of linear equations
\[
\begin{aligned}
\ddot{x}_0(t) &= 0, \\
\ddot{x}_k(t) &= \omega_0^2(x_{k-1} - 2x_k + x_{k+1}), \quad k = 1, \ldots, N - 2 \\
\ddot{x}_{N-1}(t) &= \omega_0^2(-x_{N-2} + x_{N-1}) + f_0,
\end{aligned}
\]
with initial data \( (1) \) and \( v_k(0) = \dot{x}_k(0) = 0, k = 1, \ldots, N - 1 \). Here we denoted the proper frequency \( \omega_0^2 = \kappa/m \), and \( f_0 = f/m \).

Introduce the following auxiliary function
\[
F_N(x) = x \ln \frac{N}{x}, \quad x > 0,
\]
and our main parameter \( \sigma = \frac{\kappa}{\omega_0^2} = f_0/\omega_0^2 \). Let is agree that the constants denoted further by \( c, c_i, \text{const} \), do not depend on \( N, l, f_0, \omega_0 \) and \( a \). The main estimate is as follows.

**Theorem 1** Fix some \( \varepsilon \in (0, 1) \), then for any \( k, l \in \mathbb{N} \), such that
\[
0 \leq k < l \leq (1 - \varepsilon)N,
\]
the following inequalities hold
\[
\begin{aligned}
\sigma(l + c_1F_N(l)) &\leq \sup_{t \geq 0} (x_{k+l}(t) - x_k(t)) \leq \sigma(l + c_2F_N(l)) \quad (8) \\
\sigma(l - c_3F_N(l)) &\leq \inf_{t \geq 0} (x_{k+l}(t) - x_k(t)) \leq \sigma(l - c_4F_N(l)) \quad (9)
\end{aligned}
\]
for some \( c_1, c_2, c_3, c_4 > 0 \), where \( c_1, c_2 \) may depend on \( \varepsilon \).

Further on we use the procedure, called in physics «double scaling limit». Namely, we put \( a = \frac{1}{N} \) and will consider various scalings of \( \sigma = \sigma(N) \).

We use the following notation: for positive functions \( f(x) \simeq g(x), x \in \Lambda \), for some domain \( \Lambda \), if there exist such \( c_1, c_2 > 0 \), that on all domain of definition \( c_1g(x) \leq f(x) \leq c_2g(x) \).
Corollary 1 Under the conditions of theorem 1

\[ |x_{k+l}(t) - x_k(t)| \approx \sigma(N)l \ln \frac{N}{l} \]

As the characteristics of this phase transition we use the maximal relative extension (for \( l = 1 \))

\[ \frac{A}{a} = NA \]

under the strength \( f \). We have \( a^{-1}A \to 1 \), if \( \sigma(N)N \ln N \to 0 \) as \( N \to \infty \), and \( a^{-1}A \to \infty \), if \( \sigma(N)N \ln N \to \infty \).

More exactly, if \( \sigma < \frac{c}{N \ln N} \) for sufficiently small \( c > 0 \), then the distances will never leave some neighborhood \((1 - \epsilon N, 1 + \epsilon N)\) of \( \frac{1}{N} \).

Comparison with equilibrium phase transition For quadratic hamiltonian (3) a fixed point always exists and is unique, and moreover for any \( k \) the distances \( z_k - z_{k-1} = h = a + \sigma \). That is why the static phase transition is as follows:

\[ h \to \infty \], if \( \sigma N \to \infty \) and \( h \to 1 \), if \( \sigma N \to 0 \). Thus static and dynamic phase transition differ only by logarithmic factor.

The similar fact takes place for more general interactions. Namely, usually the interaction is assumed to be

\[ V(r) = -\frac{c_n}{r^n} + \frac{c_m}{r^m} \quad \text{(10)} \]

Note that for arbitrary \( 0 < n < m, c_n > 0, c_m > 0 \) the function \( V(r) \) satisfies all properties, formulated above, and moreover the following holds. If \( \max_{a < h \leq b} \frac{dV(h)}{dh} \geq f \) then the hamiltonian (2) has the unique minimum, for which all \( b \geq z_k - z_{k-1} = h > a > 0 \), and the value \( h \) is defined from the equation

\[ \frac{dV(h)}{dh} = f \quad \text{(11)} \]

But if \( \max_{a < h \leq b} \frac{dV(h)}{dh} < f \), then fixed points do not exist and, under the action of the force \( f \) the chain falls apart. The following statement concerns the static phase transition for the interaction (10).

Lemma 1 If \( a = \frac{1}{N} \), then a fixed point exists iff

\[ \sigma = \frac{f}{\kappa} \leq \frac{1}{N} C \]

where

\[ \kappa = V''(a), \quad C = C(n, m) = \frac{1}{m-n} \left( \frac{m+1}{n+1} - \frac{n+1}{m-n} \right) - \left( \frac{m+1}{n+1} \right)^{-\frac{n+1}{m-n}} - \left( \frac{m+1}{n+1} \right)^{-\frac{n+1}{m-n}} \]

Remark 1 For the existence of the Gibbs distribution it is necessary that \( V(x) \to \infty \) as \( x \to \infty \). Then one can say that for non-zero temperature the existence of the thermal expansion depends on the third term of the expansion of \( V \) at the point \( a \), see[2].

3 Proofs

3.1 Auxiliary results

In this section we prove some auxiliary results necessary for the proof of the main theorem.

Lemma 2 The system (5) has the solution

\[ x_n(t) = \sigma \left[ n - \frac{1}{2N-1} \sum_{m=1}^{2N-2} \gamma_{m,n} \cos \omega_m t \right], \quad \text{(12)} \]

where

\[ \gamma_{m,n} = \frac{1}{\sin^2 \frac{\pi m}{8N-4} \sin \frac{\pi m}{4N-2} \sin \frac{\pi mn}{2N-1}}, \quad \omega_m = 2\omega_0 \sin \frac{\pi m}{8N-4}. \quad \text{(13)} \]
Proof. Consider the following auxiliary system of $4N - 2$ equations on the circle (all indices are modulo $4N - 2$):

$$
\ddot{y}_n = \omega_0^2(y_{n-1} - 2y_n + y_{n+1}) + f_0(\delta_{n,N-1} + \delta_{n,N} - \delta_{n,3N-2} - \delta_{n,3N-1}), \quad n = 0, \ldots, 4N - 3
$$

(14)

with zero initial conditions. Then we claim that for any $t$

$$
\ddot{x}_n(t) \equiv y_n(t), \quad n = 0, \ldots, N - 1.
$$

In fact firstly, from symmetry of the equations it follows that

$$
y_n = y_{2N-1-n} = -y_n = -y_{2N-1+n}, \quad n = 0, \ldots, N - 1.
$$

Thus, $\ddot{y}_0 = \omega_0^2(y_0 - 2y_0 + y_1) = -2\omega_0^2y_0$, and, taking the initial conditions into account, it follows that $y_0(t) = x_0(t) \equiv 0$. Then for $n = 1, \ldots, N - 2$

$$
\ddot{y}_n = \omega_0^2(y_{n-1} - 2y_n + y_{n+1}).
$$

And finally for $n = N - 1$

$$
\ddot{y}_{N-1} = \omega_0^2(y_{N-2} - 2y_{N-1} + y_N) + f_0 = \omega_0^2(y_{N-2} - y_{N-1}) + f_0.
$$

Thus, the solutions of equations for $x_n$ and $y_n$ completely coincide, and we have the result.

Then the system of equations (14) is easily solved using Fourier transform

$$
x_n = y_n = \frac{1}{4N-2} \sum_{m=0}^{4N-3} \alpha_m e^{-2\pi im/(4N-2)},
$$

(15)

where

$$
\alpha_m = \sum_{n=0}^{4N-3} y_n e^{2\pi im/(4N-2)}
$$

is the solution of the following system of ODE with zero initial conditions

$$
\ddot{\alpha}_m + \omega_m^2\alpha_m = f_0 \left( e^{\frac{2\pi im(N-1)}{4N-2}} + e^{\frac{2\pi im}{4N-2}} - e^{\frac{2\pi im(N+1)}{4N-2}} - e^{-\frac{2\pi im}{4N-2}} \right) = f_0 \left( e^{\frac{\pi im}{2N-2}} - e^{-\frac{\pi im}{2N-2}} \right) \left( e^{\frac{\pi im}{2N-2}} + e^{-\frac{\pi im}{2N-2}} \right) = 4if_0 \cos \frac{\pi m}{4N-2} \sin \frac{\pi m}{2}.
$$

(16)

It follows

$$
\alpha_m(t) = \frac{4if_0}{\omega_m^2} \cos \frac{\pi m}{4N-2} \sin \frac{\pi m}{2} \left( 1 - \cos \omega_m t \right) = \frac{if_0}{\omega_0^2} \frac{1}{\sin^2 \frac{\pi m}{8N-4}} \cos \frac{\pi m}{4N-2} \sin \frac{\pi m}{2} \left( 1 - \cos \omega_m t \right).
$$

As $y_n = -y_n$, then $\alpha_m = -\alpha_{-m}$, and thus

$$
x_n = y_n = \frac{1}{4N-2} \sum_{m=0}^{2N-2} \alpha_m \left( e^{-2\pi im/(4N-2)} - e^{2\pi im/(4N-2)} \right) = -\frac{2i}{4N-2} \sum_{m=1}^{2N-2} \alpha_m \sin \frac{\pi m}{2N-1}.
$$

(17)

Finally we have the following formula

$$
y_n = \sigma \frac{1}{2N-1} \sum_{m=1}^{2N-2} \gamma_{m,N,n} \left( 1 - \cos \omega_m t \right).
$$

To finish the proof we have to verify that

$$
\frac{1}{2N-1} \sum_{m=1}^{2N-2} \gamma_{m,N,n} = n.
$$
Lemma 3

The following assertions hold:

1. and then, from (17), where

2. and assertion 5 follows. Finally we have for any

3. is not zero for all

4. Consider the same system (14), but with initial conditions

5. It is easy to check that then the system is in the equilibrium \( y_n(t) \equiv y_n(0) \). As a corollary, \( \alpha_m(t) \) also does not change with time. From (16) it follows that the latter is possible only if

6. and get the desired statement.

7. Direct substitution of (12) shows that we have the following identity

8. where

9. We will need also the following facts concerning \( a_m \) and \( b_m \).

**Lemma 3** The following assertions hold:

1. \(|b_m| \leq 1 \) for any \( m \in \mathbb{Z} \);
2. \( a_m = 0 \) for any even \( m \);
3. \(|a_m| \leq \text{const} \frac{N^2}{m^2} \) for all \( 1 \leq m \leq 2N \);
4. \(|a_m| \approx \frac{Nl}{m} \) for any odd \( 1 \leq m \leq N/l \);
5. \( \frac{|b_m|}{m} + \frac{|b_{m+2}|}{m+2} \geq \text{const} \frac{m}{m} \) for all \( m > 0 \).

Proof. The first and second assertions are evident. The third follows from

\[
|a_m| \leq \sin^{-2} \frac{\pi m}{8N - 4} \leq \text{const} \cdot \frac{N^2}{m^2},
\]

and the fourth follows from the fact that for \( 1 \leq m \leq N/l \)

\[
\sin \frac{\pi m}{8N - 4} \approx \frac{m}{N}, \quad \cos \frac{\pi m}{4N - 2} \approx 1, \quad \sin \frac{\pi ml}{4N - 2} \approx \frac{ml}{N}.
\]

To prove the assertion 5 we should check that there exists such \( c > 0 \), that for any \( m \in \mathbb{Z} \) at least one of the numbers \(|b_m|, |b_{m+2}|\) is not less than \( c \). But from condition (7) it follows that

\[
2k + l \leq 2(k + l) \leq 2(1 - \varepsilon)N \Rightarrow 0 \leq \frac{\pi(2k + l)}{2N - 1} \leq \pi(1 - \varepsilon),
\]

and hence, the function

\[
g(x) = \min \left( |\cos x|, |\cos \left( x + \frac{\pi(2k + l)}{2N - 1} \right) | \right)
\]

is not zero for all \( x \in \mathbb{R} \), then from periodicity of \( g(x) \) it follows that \( \inf_x g(x) > 0 \). But

\[
\min(|b_m|, |b_{m+2}|) = g(\pi m(k + l/2)/(2N - 1)) \geq \inf_x g(x),
\]

and assertion 5 follows. Finally we have for any \( m > 0 \)

\[
\frac{|b_m|}{m} + \frac{|b_{m+2}|}{m+2} \geq \frac{\inf_x g(x)}{m} \geq \text{const} \frac{m}{m}. \]
Lemma 4 There exists such $c > 0$, that for any $N \in \mathbb{N}$ and

$$M = M(N, c) = \lfloor cN/ \ln \ln N \rfloor$$

the numbers

$$\omega_1/2\omega_0, \omega_2/2\omega_0, \ldots, \omega_M/2\omega_0$$

are rationally independent (that is there are integers $a_0, a_1, \ldots, a_M \in \mathbb{Z}$, that $\sum_{m=1}^M a_m (\omega_m/2\omega_0) = a_0$).

Proof. In this proof we need some facts from the number theory.

1. ([3], chapter 3) The algebraic degree of the number $e^{2\pi i/n}, n \in \mathbb{N}$, equals $\varphi(n)$, where $\varphi(\cdot)$ is the Euler function.

2. ([H], theorem 328) The following asymptotics holds

$$\lim_{n \to \infty} \frac{\varphi(n) \ln \ln n}{n} = e^{-\gamma},$$

where $\gamma$ is the Euler-Mascheroni constant.

For the proof assume the contrary. Putting $z = e^{2\pi i/n}$, the rational independence condition can be rewritten as follows

$$\frac{1}{2i} \sum_{m=1}^M a_m (z^m - z^{-m}) = a_0 \Rightarrow \left( \sum_{m=1}^M a_m (z^m - z^{-m}) \right)^2 + 4a_0^2 = 0 \Rightarrow \left( \sum_{m=1}^M a_m (z^{M+m} - z^{M-m}) \right)^2 + 4a_0^2 2^{2M} = 0.$$

As in the left-hand side of this equality we have the polynomial of degree not greater than $4M$, then the algebraic degree of the number $z$ does not exceed $4cN/ \ln \ln N$. At the same time from these two number theoretical facts it follows that there exists $c' > 0$, such that the algebraic degree of $z$ is not less than $c'/N/ \ln \ln N$. Then, as $c$ is arbitrary, we get the contradiction.

Corollary 2 Under the conditions of lemma 4 for any $a_1, \ldots, a_M \in \mathbb{R}$

$$\sup_{t \geq 0} \sum_{m=1}^M a_m \cos \omega_m t = - \inf_{t \geq 0} \sum_{m=1}^M a_m \cos \omega_m t = \sum_{m=1}^M |a_m|.$$

Proof. From lemma 4 it follows that the trajectory $(\omega_1 t, \omega_2 t, \ldots, \omega_M t)$ is everywhere dense on the corresponding $M$-dimensional torus $T$. From this we have the desired assertion.

3.2 Proof of the theorem

We will check only ([3]). The formula (9) can be checked similarly.

Lower bound We subdivide the sum in (18) into two parts

$$I_{N,k,l}(t) = I_{N,k,l}^1(t) + I_{N,k,l}^2(t) := \sum_{m \leq M(N)} + \sum_{m > M(N)}$$

and estimate them separately.

1) From the corollary 2 it follows that

$$\sup_{t \geq 0} I_{N,k,l}^1(t) = \frac{2}{2N} \sum_{m=1, m \neq \text{even}}^{M(N)} |a_m b_m| \geq \frac{2}{(2N-1)} \sum_{m=1, m \neq \text{even}}^{M(N) \wedge \lfloor N/2 \rfloor} |a_m b_m| \geq \text{const} \cdot l \cdot \sum_{m=1, m \neq \text{even}}^{M(N) \wedge \lfloor N/2 \rfloor} \frac{|b_m|}{m} = \text{const} \cdot l \cdot \sum_{m=1, m \neq \text{even}}^{[\lfloor M(N) \wedge \lfloor N/2 \rfloor \rfloor]/4} \left( \frac{|b_{4m+1}|}{4m+1} + \frac{|b_{4m+3}|}{4m+3} \right) \geq \text{const} \cdot l \cdot \sum_{m=1}^{[\lfloor M(N) \wedge \lfloor N/2 \rfloor \rfloor]/4} \frac{1}{m} \geq \text{const} \cdot l \cdot \sum_{m=1}^{[\lfloor M(N) \wedge \lfloor N/2 \rfloor \rfloor]/4} \frac{1}{m} \geq $
\[
\geq \text{const} \cdot \ln \left( \frac{1}{4} (M(N) \land \lfloor N/l \rfloor) \right) \geq \text{const} \cdot \ln \left( \text{const} \cdot \frac{N}{l \land \ln \ln N} \right) \geq \text{const} \cdot F_N(l)
\]

where \( \lfloor . \rfloor \) is the integer part and \( \land \) is the minimum). Here in the first inequality, we discarded some terms in the sum. In the second one we used assertion 4. In the third one we used assertion 5 of the lemma. In the fourth we used the fact that
\[
\sum_{m=1}^{n} \frac{1}{m} \simeq \ln n, n \in \mathbb{Z}
\]

The inequality 5 follows from the definition of \( M(N) \). The sixth one can be obtained by separation of two cases: for \( l \geq \ln \ln N \) the left-hand part exactly equals the right-hand part, and for \( l < \ln \ln N \) we have
\[
\ln \left( \text{const} \cdot \frac{N}{\ln \ln N} \right) = \text{const} \cdot \ln \text{ln} \ln N
\]

2) We have
\[
\sup_{t \geq 0} |J_{N,k,l}^2(t)| \leq \text{const} \cdot N \cdot \sum_{m=M(N)+1}^{2N-1} \frac{1}{m^2} \leq \text{const} \cdot N \int_{M(N)}^{\infty} \frac{dx}{x^2} = \text{const} \cdot \frac{N}{M(N)} \leq \text{const} \cdot \ln \ln N
\]

Here in the first inequality we used the statement 3 of lemma 3, and in the second we used (21).

In the last inequality we substituted the definition of the function \( M(N) \).

Joining two cases together we have
\[
\sup_{t \geq 0} I_{N,k,l}(t) \geq \sup_{t \geq 0} I_{N,k,l}^1(t) - \sup_{t \geq 0} |J_{N,k,l}^2(t)| \geq \text{const} \cdot F_N(l) - \text{const} \cdot \ln \ln N \geq \text{const} \cdot F_N(l).
\]

**Upper bound**

Now we subdivide the sum (18) differently
\[
I_{N,k,l}(t) = J_{N,k,l}^1(t) + J_{N,k,l}^2(t) := \sum_{m \leq N/l} + \sum_{m > N/l}
\]

and again estimate them separately.

1) We have
\[
\sup_{t \geq 0} |J_{N,k,l}^1(t)| \leq \text{const} \cdot \frac{N}{l} \sum_{m \leq N/l} \frac{N}{m} = \text{const} \cdot \ln \frac{N}{l} \sum_{m \leq N/l} \frac{1}{m} \leq \text{const} \cdot \ln \frac{N}{l} = \text{const} \cdot F_N(l)
\]

Here in the first inequality we used assertions 2 and 4 of lemma 3, and in the third we used (21).

2) We have
\[
\sup_{t \geq 0} |J_{N,k,l}^2(t)| \leq \text{const} \cdot N \cdot \sum_{m=\lfloor N/l \rfloor}^{2N-1} \frac{1}{m^2} \leq \text{const} \cdot N \int_{N/l}^{\infty} \frac{dx}{x^2} = \text{const} \cdot l \leq \text{const} \cdot F_N(l)
\]

In the first inequality we used the assertion 3 of lemma 3, in the second we used (22), and in the last one we used the definition (6). Joining the results together we have the desired bound from above
\[
\sup_{t \geq 0} |I_{N,k,l}(t)| \leq \sup_{t \geq 0} |J_{N,k,l}^1(t)| + \sup_{t \geq 0} |J_{N,k,l}^2(t)| \leq \text{const} \cdot F_N(l).
\]
3.3 Proof of lemma 1

We have three equations for the potential at the point \( a = \frac{1}{N} \)

\[
V(a) = -c_n N^n + c_m N^m \tag{23}
\]

\[
V'(a) = 0 = nc_n N^{n+1} - mc_m N^{m+1} \tag{24}
\]

\[
V''(a) = \kappa = -n(n+1)c_n N^{n+2} + m(m+1)c_m N^{m+2} \tag{25}
\]

However, in the first equation we do not know the value \( V(a) \). From (23) and (24) we have

\[
c_m = \frac{n}{m-n} N^{-m} V(a), \quad c_n = \frac{1}{m-n} N^{-n} V(a) \tag{26}
\]

and from (24) and (25)

\[
c_m = \frac{\kappa}{m(m-n)} N^{-2-m}, \quad c_n = \frac{\kappa}{n(m-n)} N^{-2-n} \tag{27}
\]

From this we can find \( V(a) = -\frac{\kappa}{m,n} N^{-2} \). Also we need the inflection point \( b > a > 0 \), which can be found from the condition

\[
V''(b) = -n(n+1)c_n b^{-(n+2)} + m(m+1)c_m b^{-(m+2)} = 0, \tag{28}
\]

thus

\[
b = \frac{1}{N} \left( \frac{m+1}{n+1} \right)^{m-n}
\]

and

\[
V'(b) = nc_n b^{-n-1} - mc_m b^{-m-1}
\]

Using (24) together with the equation (11) for \( h = b \), we find \( \sigma(N) = \frac{f}{\kappa} \). From (28) we have

\[
\frac{f}{\kappa} = \frac{C}{N}, \quad C = C(n,m) = \frac{1}{m-n} \left( \frac{m+1}{n+1} \right)^{-\frac{n-1}{m-n}} - \left( \frac{m+1}{n+1} \right)^{-\frac{n-1}{m-n}}
\]

References

[1] O. Penrose. Statistical mechanics of nonlinear elasticity. Markov Processes and Related Fields, 2002, 8, no.2, 351-364.

[2] V.A. Malyshev. One-dimensional mechanical networks and crystals. Moscow Mathematical Journal, 2006, v, 6, No. 2, 353-358.

[3] I. Niven. Irrational numbers. 1956, Math. Ass. of America.

[4] G. H. Hardy, E. M. Wright An Introduction to the Theory of Numbers. 4th edition, Oxford, 1975.

[5] G. Gallavotti (ed.). The Fermi-Pasta-Ulam problem. Lecture Notes in Physics, 728. Springer, 2008.

[6] O. M. Braun, Y. S. Kivshar. The Frenkel-Kontorova model, 2004. Springer.

[7] Weinan E, Pingbing Ming.Cauchy-Born rule and the stability of crystalline solids: static problems. Arch. Rational Mech.Anal., 2006.

[8] Weinan E, Pingbing Ming.Cauchy-Born rule and the stability of crystalline solids: dynamic problems.

[9] J. Braun, B. Schmidt. On the passage from atomistic systems to nonlinear elasticity theory. 2012.

[10] A. Braides, M. Solci, E. Vitali. A derivation of linear elastic energies from pair-interaction atomistic systems.

[11] M. Born, K. Huang. Dynamical theory of crystal lattices. 1964. Oxford.

[12] M. Kardar. Problems and Solutions for Statistical Physics, MIT, 2008.