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Markov Processes and Related Fields

Introduction to Micro Life of Graphs. I.

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Abstract. Multiparticle systems on complicated metric graphs might have many applications in physics, biology and social life. But the corresponding science still does not exist. Here we start it with simplest examples where there is quadratic interaction between neighboring particles and deterministic external forces. In this introduction we consider stable configurations and stable flows on one and two edge graphs. Moreover, distribution of mean (as in virial theorem) kinetic and potential energies along the graph is considered.

KEYWORDS: metric graphs, multi particle systems, virial theorem, deterministic equilibrium, non-equilibrium

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Contents

1. Introduction

Mathematician, who besides pure mathematical problems, wants to do something else, might ask the question – could mathematics give some ideas why our life is so short.

More exact question could be like this: can mathematics provide some kind of broad view on bio organism using small number of axioms at the upper level but many examples on the lower.

Immediately mathematician sees that the amount of information concerning physics, chemistry and biology of bio organisms is already immense but is still growing faster and faster. Moreover, even the existence of long molecules and solids does not have rigorous proofs neither in classical (assuming only Newton equation with Coulomb force), nor in quantum mathematical physics. This suggests the answer to this question – obviously NOT.

However, some of us can remember that "toy models" were popular in mathematical statistical physics in second half of last century. So, we could try to find toy models of our own health, in particular due to harmful external influence.

The components of such toy models are the following:

1) we consider large systems of point particles such that their micro behavior gives rise to macro effects which everyone knows when feels his own body;

2) this system, as a whole, can be imagined as "body", and edges (or subsets of edges) are the parts of this body. For sufficiently large graphs one can imagine even more complicated hierarchy;

3) for such system there are different static and dynamical problems. For example, stable state (no dynamics) is the minimum of the potential energy. It is important to understand what (potential and kinetic) energy distribution can be over living "body". If the initial conditions are not stable, or if external forces are time-dependent, then potential and kinetic energy can be quite differently distributed over the "body". It is obvious that any part of the body should have sufficient energy to survive;

4) if our graph has cycles, then stationary flows (like electric current for Coulomb forces) along some or all cycles are possible;

5) in the first model the particles move in their local potential wells which are formed by neighboring particles. Next development of the model is to introduce external media and flows in this media. Moreover, this interaction allows, for any edge, departure and arrival of particles. Departure can be in cases when dynamical situation leads to collisions or too close rapprochement of neighboring particles. On the contrary, arrival can occur if neighboring particles on the edge become too far apart from each other;

6) growth of graph becomes also possible if we consider the edge not as the segment of fixed length, but of the length which is defined as the sum of distances between neighboring edges. Then the breaks and growth of edges and even appearance of new edges is possible.

Now we start rigorous definitions.

Static metric graph In this case we consider many-particle systems on metric graphs, where (static) metric graph G is a graph with metrics, where each edge is metrically isomorphic to a segment of the real line, and the distance between two points is the minimal length of path between these points.

On each edge l there is large system of identical particles. Potential energy of such system is the sum

$$U = \sum_{(i,j)} u(\rho_{ij})$$

over pairs i, j of particles, for which there exists a path between i and j such that does not pass over any other particle. And ρ_{ij} is the minimal length of such path. In this paper we start with the case when the interaction is quadratic, that is

$$u(\rho_{ij}) = \frac{\omega_{ij}^2}{2} \rho_{ij}^2.$$

Moreover, external forces can act on some or all particles.

Dynamic graph Here abstract graph G is fixed. We assume it connected and not more than one edge between any two vertices. Vertices of graph may be called point particles and numerated as $i = 1, \dots, N$. Existence of edge $l = (i.j)$ between vertices means that these two "particles" interact. Each edge has variable length $q_l = q_{ij} > 0$. Dynamics of these lengths is defined by Newton equations

$$\frac{d^2 q_l}{dt^2} = F_l(q_l) + \sum_{m:m \neq l} F_{lm}(q_l, q_m),$$

where the summation is over all edges m such that have common vertex with edge l. And F_l, F_{lm} are forces – real functions of one and two variables correspondingly.

In this introduction we consider only static graphs and give an introduction to the statics of such systems for three simplest graphs – segment, circle and graph with 2 edges. The first interesting topics – ground states of such systems.

Ground states with different interactions, but without external force, for classical finite and infinite particle systems were intensively studied during last 30 years, see for example [1–6]. Main results in these papers concern periodicity of the ground states. In the papers [7–14] mostly Coulomb systems were considered.

Other question in our paper: 1) flow of particles along the cycle; 2) energy distribution on parts of the graph.

2. Stationary flow of point particles

Periodic equilibrium configurations Let $S = S_L$ be circle of length L, or segment $[0, L]$ with identified end points. Consider N point particles $0, 1, \ldots,$ $N-1$ with coordinates

$$0 = x_0 < x_1 < \ldots < x_{N-1} < L \tag{2.1}$$

or infinite periodic sequence (with period L) on the real axis R

$$\ldots < x_{-1} < 0 = x_0 < x_1 < \ldots < x_{N-1} < x_N = L < x_{N+1} < \ldots$$

where $x_{k+N} = x_k + L$ for any k. We assume formal potential energy

$$U = \frac{\omega^2}{2} \sum_{k \in Z} (x_k - x_{k-1} - a)^2$$

with $a = L/N$, and moreover there are the following external forces:

1. constant force $f > 0$ on the particle 0, or on any particle $iN, i \in Z,$;
2. constant forces $-\varphi < 0$ (that is $\varphi > 0$) on any particle.

Define ε_k as

$$\Delta_k = x_k - x_{k-1} = \frac{L}{N} + \frac{\varepsilon_k}{N^2}.$$

Then: the sequence ε_k is also periodic, $-LN < \varepsilon_k$ for any k, and

$$\sum_{k=1}^{N} \varepsilon_k = 0. \tag{2.2}$$

Configuration is called equilibrium, if the force, acting on any particle, is zero.

Theorem 2.1. *There exists fixed* (*equilibrium*) *configuration, satisfying condition* (2.1), *iff the following two conditions hold:*

1) $\varphi = f/N$,

2) $\dfrac{f}{2\omega^2 L} < \dfrac{1}{N(1 - 1/N)}$.

This configuration is unique and is defined by

$$\varepsilon_1 = -\frac{fN(N-1)}{2\omega^2}, \quad \varepsilon_N = \frac{fN(N-1)}{2\omega^2},$$

$$\varepsilon_k = \varepsilon_1 + (k-1)\frac{fN}{\omega^2}, \quad k = 1, \ldots, N-1.$$

If moreover

$$\frac{f}{2\omega^2 L} < \frac{C}{N^2}$$

for some fixed constant $C > 0$, then, in such scaling, $\varepsilon_k = O(1)$ uniformly in $k = 1, \ldots, N$.

Proof. The condition that the total force on particles $k = 1, \dots, N-1$ is zero can be written as follows

$$\omega^2\Big(\frac{\varepsilon_{k+1}}{N^2} - \frac{\varepsilon_k}{N^2}\Big) = \varphi \Longleftrightarrow \varepsilon_{k+1} - \varepsilon_k = \frac{\varphi N^2}{\omega^2} \tag{2.3}$$

and on the particle 0 (or N)

$$f + \omega^2\Big(\frac{\varepsilon_1}{N^2} - \frac{\varepsilon_N}{N^2}\Big) = \varphi \Longleftrightarrow \varepsilon_1 - \varepsilon_N = \frac{N^2}{\omega^2}(-f + \varphi). \tag{2.4}$$

Summation of (2.4) and all (2.3) gives

$$(N-1)\varphi - f + \varphi = 0 \Longleftrightarrow \varphi = \frac{f}{N}. \tag{2.5}$$

Thus, condition 1) of the Theorem is a necessary condition.

And we can rewrite conditions (2.3) and (2.4) as

$$\varepsilon_{k+1} - \varepsilon_k = \frac{fN}{\omega^2}, \quad \varepsilon_1 - \varepsilon_N = -\frac{fN(N-1)}{\omega^2}.$$

Then

$$\varepsilon_k = \varepsilon_1 + (k-1)\frac{fN}{\omega^2}, \quad k = 2, \dots, N-1, \quad \varepsilon_N = \varepsilon_1 + \frac{fN(N-1)}{\omega^2}.$$

Substituting to (2.2) we get

$$N\varepsilon_1 + \frac{fN}{\omega^2}\sum_{k=2}^{N-1}(k-1) + \frac{fN(N-1)}{\omega^2} = N\varepsilon_1 + \frac{fN}{\omega^2}\sum_{k=2}^{N}(k-1) =$$

$$= N(\varepsilon_1 + \frac{fN(N-1)}{2\omega^2}) = 0$$

or

$$\varepsilon_1 = -\frac{fN(N-1)}{2\omega^2}$$

and then

$$\varepsilon_N = \frac{fN(N-1)}{2\omega^2}.$$

Also for all $k = 1, \dots, N-1$

$$\varepsilon_k = \varepsilon_1 + (k-1)\frac{fN}{\omega^2}.$$

Note that

$$x_k > x_{k-1} \Longleftrightarrow \frac{\varepsilon_k}{N^2} > -\frac{L}{N} \Longleftrightarrow \frac{\varepsilon_1}{N^2} = -\frac{fN(N-1)}{2\omega^2 N^2} > -\frac{L}{N} \Longleftrightarrow$$

$$\Longleftrightarrow \frac{f}{2\omega^2} < \frac{L}{N(1-1/N)} \Longleftrightarrow \frac{f}{2\omega^2 L} < \frac{1}{N(1-1/N)}. \tag{2.6}$$

That is for fixed L, the parameters f, ω should be scaled (with respect to N) so that $f/(2\omega^2 L) < 1/N$ hold.

Stationary flow Now we want to prove that there exists stationary periodic flow of particles as

$$x_k(t) = x_k(0) + vt,$$

where $v > 0$ and $x_k(0) = x_k$, defined in the Theorem. That is the particles move with the same velocity $v > 0$. This flow is driven by the constant force $f > 0$ acting only on the particle 0 and by some dissipative force which acts on any particle and depends only on its velocity. Such dissipative forces $-g(v)$, where $g(v)$ is positive smooth increasing function) (often used is $g(v) = \alpha v$ with some $\alpha > 0$). Assume that we fixed this function g. Then there exists unique $v > 0$ such that $g(v) = \varphi = f/N$.

This construction is resembles the famous Drude's model of electric current (one can find it in any text book on electricity) where particles move without interaction under the influence of external constant force and dissipative force, acting on all particles. Here however the particles move due to the driven force acting on only one particles.

Even more realistic model with Coulomb interaction forces see in [12].

3. Static equilibrium

Here we give 5 examples of 1-dimensional stable equilibrium configurations.

External force on one particle Consider $N+1$ particles $i = 0, 1, \ldots, N$ on R with coordinates x_i. Potential energy is assumed to be

$$U = -fx_0 + \frac{\omega_0^2}{2} x_0^2 + \frac{\omega_1^2}{2} \sum_{i=1}^{N} (x_i - x_{i-1} - a)^2. \tag{3.1}$$

That is there is constant force f which acts only on particle 0. Moreover, particle N is assumed to be tightly fixed, that is $x_N \equiv L > 0$. We see from (3.1) that particle 0 is attached to $0 \in R$ by harmonic force.

Theorem 3.1. *For any parameters $f, L > 0, \omega_0, \omega_1 > 0$ equilibrium configuration exists and is unique. Two cases are possible:*

1) If $f < \omega_0^2 L + \omega_1^2 a$ then

$$x_0 = \frac{\omega_1^2 (L - Na) + Nf}{\omega_1^2 + \omega_0^2 N},$$

$$x_k = x_0 + \frac{\omega_0^2 L + \omega_1^2 a - f}{\omega_1^2 + \omega_0^2 N} k, \quad k = 1, \ldots, N-1.$$

It follows that $x_0 < x_1 < \cdots < x_N = L$.

2) If $f \geq \omega_0^2 L + \omega_1^2 a$ then $x_0 = x_1 = \cdots = x_N = L$.

In all cases this equilibrium is stable, that is the minimum of U.

Note that a "natural order" $0 \le x_0 < x_1 < \cdots < x_N = L$ holds iff

$$\omega_1^2\Big(a - \frac{L}{N}\Big) \le f < \omega_0^2 L + \omega_1^2 a.$$

Now consider the case when x_N is not fixed but the potential energy is

$$U = -fx_0 + \frac{\omega_0^2}{2}x_0^2 + \frac{\omega_0^2}{2}(x_N - L)^2 + \frac{\omega_1^2}{2}\sum_{i=1}^{N}(x_i - x_{i-1} - a)^2.$$

Theorem 3.2. *For any parameters equilibrium configuration exists and is unique. It is given by*

$$x_0 = \frac{\omega_1^2\big(L + N(f/\omega_1^2 - a)\big) + \omega_1^2\omega_0^{-2}f}{2\omega_1^2 + N\omega_0^2},$$

$$x_k = x_0 + \frac{\omega_0^2 L + 2\omega_1^2 a - f}{2\omega_1^2 + N\omega_0^2}k, \quad k = 1, \ldots, N.$$

There can be 3 types of equilibrium configurations:

$$x_0 < x_1 < \cdots < x_N \Longleftrightarrow f < \omega_0^2 L + 2\omega_1^2 a$$

$$x_0 = x_1 = \cdots = x_N = L + \frac{\omega_1^2 a(N + 2\omega_1^2\omega_0^{-2})}{2\omega_1^2 + N\omega_0^2} \Longleftrightarrow f = \omega_0^2 L + 2\omega_1^2 a$$

$$x_0 > x_1 > \cdots > x_N > L \Longleftrightarrow f > \omega_0^2 L + 2\omega_1^2 a$$

Note that $0 \le x_0 < x_1 < \cdots < x_N \le L$ iff $L \ge aN$ and

$$-\frac{\omega_1^2(L - aN)}{N + \omega_1^2\omega_0^{-2}} \le f \le \omega_0^2(L - aN).$$

Forces on both extreme points Here we assume that force f acts on particle 0, and the force $-f$ acts on the particle N. That is the potential energy is

$$U = \frac{\omega_0^2}{2}x_0^2 + \frac{\omega_0^2}{2}(x_N - L)^2 + \frac{\omega_1^2}{2}\sum_{i=1}^{N}(x_i - x_{i-1} - a)^2 - fx_0 + fx_N.$$

Theorem 3.3.

1) *For any parameters equilibrium configuration exists, is unique and the coordinates are given by*

$$x_0 = \frac{\omega_1^2\big(L + N(f/\omega_1^2 - a)\big)}{2\omega_1^2 + N\omega_0^2},$$

$$x_k - x_{k-1} = \frac{\omega_0^2 L + 2\omega_1^2 a - 2f}{2\omega_1^2 + N\omega_0^2}, \quad k = 1, \ldots, N-1.$$

2) *3 types of configuration are possible:*

$$x_0 < x_1 < \dots < x_N \Longleftrightarrow f < \frac{\omega_0^2 L + 2\omega_1^2 a}{2},$$

$$x_0 = x_1 = \dots = x_N \Longleftrightarrow f = \frac{\omega_0^2 L + 2\omega_1^2 a}{2},$$

$$x_0 > x_1 > \dots > x_N \Longleftrightarrow f > \frac{\omega_0^2 L + 2\omega_1^2 a}{2}.$$

Note that condition $0 \leq x_0 < x_1 < \dots < x_N \leq L$ holds iff

$$0 \leq x_0 < x_1 < \dots < x_N \leq L \Longleftrightarrow \omega_1^2 a - \frac{\omega_1^2 L}{N} \leq f < \frac{\omega_0^2 L + 2\omega_1^2 a}{2}.$$

Force on all particles Here we assume that constant force f acts on each particle.

Theorem 3.4. *Assume that $x_N \equiv L$ and the potential energy is*

$$U = \frac{\omega_0^2}{2} x_0^2 + \frac{\omega_1^2}{2} \sum_{i=1}^{N} (x_i - x_{i-1} - a)^2 - f(x_0 + x_1 + \ldots + x_{N-1})$$

where $f > 0$. Then:
1) for any given parameters stable equilibrium exists and is unique;
2) condition $0 \leq x_0 < x_1 < \dots < x_N = L$ holds iff

$$-\frac{2\omega_1^2(L - aN)}{N(N+1)} \leq f < \frac{2\omega_1^2 \left(\omega_0^2 L + a\omega_1^2\right)}{N(2\omega_1^2 + \omega_0^2(N-1))}$$

and the coordinates are given by

$$x_0 = \frac{\omega_1^2(L + N(N+1)f/(2\omega_1^2) - Na)}{\omega_1^2 + \omega_0^2 N}$$

$$x_k - x_{k-1} = -\frac{fk}{\omega_1^2} + \frac{\omega_0^2\big(L + N(N+1)f/(2\omega_1^2)\big) + a\omega_1^2}{\omega_1^2 + \omega_0^2 N}, \quad k = 1, \dots, N-1$$

Note that under scaling $a = a_0 N^{-1}$, $f = f_0 N^{-1}$, $\omega_1^2 = w_1^2 N$ we will have

$$0 \leq x_0 < x_1 < \dots < x_N = L \Longleftrightarrow -\frac{2w_1^2(L - a_0)}{1 + N^{-1}} \leq f_0 < \frac{2w_1^2 \left(\omega_0^2 L + a_0 w_1^2\right)}{2w_1^2 + \omega_0^2(1 - N^{-1})}.$$

Theorem 3.5. *Assume that the potential energy is*

$$U = \frac{\omega_0^2}{2} x_0^2 + \frac{\omega_0^2}{2}(x_N - L)^2 + \frac{\omega_1^2}{2}\sum_{i=1}^{N}(x_i - x_{i-1} - a)^2 - f(x_0 + x_1 + \ldots + x_N).$$

Then:

1) For any given parameters stable equilibrium exists and is unique. Coordinates are given by:

$$x_0 = \frac{\omega_1^2(L + N(N+1)f/(2\omega_1^2) - Na) + \omega_1^2\omega_0^{-2} f(N+1)}{2\omega_1^2 + N\omega_0^2},$$

$$x_k - x_{k-1} = -\frac{fk}{\omega_1^2} + \frac{\omega_0^2(L + N(N+1)f/(2\omega_1^2)) + f(N+1) + 2\omega_1^2 a}{2\omega_1^2 + N\omega_0^2}, \quad k = 1, \ldots, N.$$

2) Condition $x_0 < x_1 < \cdots < x_N$ holds iff

$$|f| < \frac{2\omega_1^2\left(\omega_0^2 L + 2\omega_1^2 a\right)}{(N-1)\left(2\omega_1^2 + N\omega_0^2\right)}.$$

3) Condition $0 \leq x_0 < x_1 < \cdots < x_N \leq L$ holds iff $L \geq Na$ and

$$\frac{-2\omega_1^2\omega_0^2(L - Na)}{(2\omega_1^2 + N\omega_0^2)(N+1)} \leq f \leq \frac{\omega_1^2\omega_0^2(L - Na)}{(2\omega_1^2 + N\omega_0^2)(N+1)}.$$

Under the scaling $a = a_0 N^{-1}$, $f = f_0 N^{-1}$, $\omega_1^2 = w_1^2 N$ we will have

$$0 \leq x_0 < x_1 < \cdots < x_N \leq L \Longleftrightarrow$$

$$-\frac{2w_1^2\omega_0^2(L - a_0)}{(2w_1^2 + \omega_0^2)(1 + N^{-1})} \leq f_0 \leq \frac{2w_1^2\omega_0^2(L - a_0)}{(2w_1^2 + \omega_0^2)(1 + N^{-1})}, \quad L > a_0.$$

Example of regular continuum system of particles Here we assume that the reader knows the main definitions in the paper [16]. Assume that we are in the situation of Theorem 3.4. We assume further on that $\omega_0 = 0, a = L/N$. The potential energy is the sum of two terms interaction energy and external field energy:

$$U = U_{int} + U_{ext} = \frac{\omega_1^2}{2}\sum_{i=1}^{N}(x_i - x_{i-1} - a)^2 - f(x_0 + x_1 + \ldots + x_{N-1}).$$

We want to show that the scaling limits of U for the configuration $x_k = ka, k = 1, \ldots, N-1$

$$\lim_{N\to\infty} U = \lim_{N\to\infty} U_{ext} = -\frac{f_1 L}{2},$$

and for the equilibrium configuration

$$\lim_{N\to\infty} U = \lim_{N\to\infty} U_{ext} + \lim_{N\to\infty} U_{int} = -\frac{f_1 L}{2}$$

are equal.

By Theorem 3.4 the condition $f < a\omega_1^2/N = L\omega_1^2/N^2$ should hold. Put

$$f = \frac{f_1}{N}, \quad \omega_1^2 = w_1 N,$$

where $f_1 < Lw_1$. And, by the same Theorem, as $N \to \infty$,

$$x_0 = \frac{N(N+1)f}{2\omega_1^2} \sim \frac{f_1}{2w_1},$$

$$x_k - x_{k-1} = -\frac{fk}{\omega_1^2} + a = -\frac{fk}{\omega_1^2} + \frac{L}{N} = \frac{L}{N} - \frac{f_1 k}{w_1 N^2} + o(N^{-2}),$$

$$x_k = -\frac{fk(k+1)}{\omega_1^2} + ka + x_0.$$

Potential energy of the configuration $x_k = ka,\ k = 1, \ldots, N-1$ is

$$U_0 = -fa\frac{N(N-1)}{2} \sim -\frac{f_1 L}{2}.$$

Potential energy of the equilibrium configuration is

$$U = \frac{\omega_1^2}{2}\sum_{k=1}^{N}\left(\frac{fk}{\omega_1^2}\right)^2 - f\sum_{k=1}^{N-1}\left(-\frac{fk(k+1)}{\omega_1^2} + ka + x_0\right) =$$

$$= \frac{3\omega_1^2}{2}\sum_{k=1}^{N}\left(\frac{fk}{\omega_1^2}\right)^2 + \sum_{k=1}^{N}\frac{f^2 k}{\omega_1^2} - fa\frac{N(N-1)}{2} - fNx_0.$$

Then, as $N \to \infty$,

$$\frac{3\omega_1^2}{2}\sum_{k=1}^{N}\left(\frac{fk}{\omega_1^2}\right)^2 = \frac{3f_1^2}{2w_1}\frac{1}{N}\sum_{k=1}^{N}\frac{k^2}{N^2} \to \frac{3f_1^2}{2w_1}\int_0^1 x^2 dx = \frac{f_1^2}{2w_1}.$$

It follows that

$$U \to -\frac{f_1 L}{2}.$$

Now for given N and given configuration X, denote by $U_N(a,b,X)$, where $0 \le a < b \le L$, the potential energy of all particles x_k such that $x_k \in (a,b)$. The potential energy of the particle k is defined as

$$U_k = \frac{\omega_1^2}{4}(x_k - x_{k-1} - a)^2 + \frac{\omega_1^2}{4}(x_{k+1} - x_k - a)^2 - fx_k =$$

$$= \frac{\omega_1^2}{4}\left(\frac{fk}{\omega_1^2}\right)^2 + \frac{\omega_1^2}{4}\left(\frac{f(k+1)}{\omega_1^2}\right)^2 - f\Big(-\frac{fk(k+1)}{\omega_1^2} + ka + x_0\Big) =$$

$$= -\frac{f_1^2}{2w_1 N} - \frac{f_1 Lk}{N^2} + \frac{3f_1^2}{2w_1}\frac{k^2}{N^3} + o(N^{-3}).$$

Then there exists

$$u(x) = \lim_{\Delta x\to 0}\frac{1}{\Delta x}\lim_{N\to\infty}(U_{int,N}(x, x+\Delta x, X) + U_{ext,N}(x, x+\Delta x, X))$$

correspondingly for the configuration $x_k = ka, k = 1, \dots, N-1$ and for the equilibrium configuration.

For the configuration $X = \{x_k = ka, k = 1, \dots, N-1\}$ we have

$$U_{int,N}(x, x+\Delta x, X) = 0$$

and

$$U_{ext,N}(x, x+\Delta x, X) = -\frac{f_1}{N}\sum\frac{kL}{N},$$

where the sum is over k such that $x \le \frac{kL}{N} \le x + \Delta x$. So

$$\lim_{N\to\infty} U_{ext,N}(x, x+\Delta x, X) = -\frac{f_1}{L}\int_x^{x+\Delta x} y dy$$

and

$$u(x) = -\frac{f_1}{L}x.$$

For the equilibrium configuration X we have

$$U_{int,N}(x, x+\Delta x, X) = \frac{f_1^2}{2w_1}\sum\frac{k^2}{N^3} = \frac{f_1^2}{2L^3 w_1}\frac{L}{N}\sum\frac{k^2L^2}{N^2}$$

where the sum is over k such that $x \le kL/N \le x + \Delta x$, because of $x_k - x_{k-1} \sim L/N$, as $N \to \infty$. So

$$\lim_{N\to\infty} U_{int,N}(x, x+\Delta x, X) = \frac{f_1^2}{2L^3 w_1}\int_x^{x+\Delta x} y^2 dy$$

and

$$\lim_{\Delta x\to 0}\frac{1}{\Delta x}\lim_{N\to\infty} U_{int,N}(x, x+\Delta x, X) = \frac{f_1^2 x^2}{2L^3 w_1}.$$

Similarly one can show

$$\lim_{\Delta x\to 0}\frac{1}{\Delta x}\lim_{N\to\infty} U_{ext,N}(x, x+\Delta x, X) = \frac{f_1^2 x^2}{L^3 w_1} - \frac{f_1}{L}x - \frac{f_1^2}{2w_1}.$$

Hence, for the equilibrium configuration X we have

$$u(x) = \frac{3f_1^2 x^2}{2L^3 w_1} - \frac{f_1}{L}x - \frac{f_1^2}{2w_1}.$$

Note that in both cases the integral $\int_0^L u(x)dx = -f_1 L/2$.

Two edges Here we consider graph with two edges and common vertex which we denote 0. On the first edge of length L_1 there are N_1 particles with coordinates

$$0 \leq x_1 < \ldots < x_{N_1 - 1} < x_{N_1} \equiv L_1, \tag{3.2}$$

and on the second edge of length L_2 there are N_2 particles with coordinates

$$0 \leq y_1 < \ldots < y_{N_2} \equiv L_2. \tag{3.3}$$

It is important that coordinates x_{N_1} and y_{N_2} are tightly fixed and cannot move. Potential energy is given by

$$U = \frac{\omega_2^2}{2} \sum_{i=1}^{N_2 - 1} \Big(y_{i+1} - y_i - \frac{a_2}{M} \Big)^2 + \frac{\omega_1^2}{2} \sum_{i=1}^{N_1 - 1} \Big(x_{i+1} - x_i - \frac{a_1}{M} \Big)^2 + \frac{\omega_0^2}{2} \Big(x_1 + y_1 - \frac{a_0}{M} \Big)^2$$

where all parameters $a_j, \omega_j > 0$ and $b = N/M$, $c = N_1/N < 1$ are of order 1, but $M, N_1, N_2, N = N_1 + N_2$ are sufficiently large but of the same order.

Put

$$r_0 = \frac{L_1 + L_2 - a_1 cb - a_2 (1 - c) b - a_0 M^{-1}}{M^{-1} + b\omega_0^2 \left(\omega_1^{-2} c + \omega_2^{-2} (1 - c) \right)}. \tag{3.4}$$

Theorem 3.6. *1) For fixed parameters a_j, ω_j, b, c there exists equilibrium state, satisfying conditions* (3.2) *and* (3.3), *iff the following two inequalities hold:*

$$\frac{\omega_0^2 r_0}{\omega_1^2} + a_1 > 0, \quad \frac{\omega_0^2 r_0}{\omega_2^2} + a_2 > 0.$$

In this case equilibrium state is unique and is defined by

$$x_{k+1} - x_k = \Big(\frac{\omega_0^2 r_0}{\omega_1^2} + a_1 \Big) \frac{1}{M},$$

$$y_{l+1} - y_l = \Big(\frac{\omega_0^2 r_0}{\omega_2^2} + a_2 \Big) \frac{1}{M},$$

for all $k = 1, \ldots, N_1 - 1$ and $l = 1, \ldots, N_2 - 1$.

2) This equilibrium state defines also the unique minimum of U, which is equal to

$$U(b, c, M) = \frac{\omega_0^2 (L_1 + L_2 - a_1 cb - a_2 (1 - c) b - a_0 M^{-1})^2}{2bM (\omega_0^2 \left(\omega_1^{-2} c + \omega_2^{-2} (1 - c) \right) + (bM)^{-1})}.$$

Remark 3.1. To get macroscopic (of the order 1) values for U one should scale also all frequencies as $\omega_i^2 \sim c_i M$. Then we will get finite "thermodynamic limit" of U as $M \to \infty$.

4. Proofs

Proof of Theorem 3.1 We get linear system of N equations for the forces F_k acting on the particles $k = 1, 2, \dots, N$, using the fact that the total force on each of the particles $k = 0, 1, \dots, N-1$ equals zero:

$$F_0 = -\omega_0^2 x_0 + \omega_1^2(x_1 - x_0 - a) + f = 0, \tag{4.1}$$

$$F_k = \omega_1^2(x_{k+1} - x_k - a) - \omega_1^2(x_k - x_{k-1} - a) = 0, \quad k = 1, \dots, N-1, \tag{4.2}$$

where the coordinates satisfy the conditions: $x_k \le L, k = 1, \dots, N-1$ and $x_N = L$.

From equation (4.2) it follows that the difference $x_k - x_{k-1}$ does not depend on $k = 1, \dots, N$. Put $r = x_k - x_{k-1} - a$. Then

$$x_k = x_0 + k(r + a), \quad k = 1, \dots, N.$$

Using the condition $x_N = L$ we get one more equation:

$$x_N = x_0 + N(r + a) = L \Longleftrightarrow r + a = \frac{L - x_0}{N}.$$

Finally we get system of two linear equations for two unknowns x_0, r:

$$-\omega_0^2 x_0 + \omega_1^2 r + f = 0 \tag{4.3}$$

$$x_0 + N(r + a) = L. \tag{4.4}$$

Multiplying second equation on ω_0^2 and adding both equations we can find r

$$(\omega_1^2 + \omega_0^2 N)r + \omega_0^2 N a + f = \omega_0^2 L \Longleftrightarrow r = \frac{\omega_0^2 L - f - \omega_0^2 N a}{\omega_1^2 + \omega_0^2 N}.$$

Then

$$x_k - x_{k-1} = r + a = \frac{\omega_0^2 L - f - \omega_0^2 N a}{\omega_1^2 + \omega_0^2 N} + a = \frac{\omega_0^2 L + a\omega_1^2 - f}{\omega_1^2 + \omega_0^2 N}.$$

From equation (4.3)

$$-\omega_0^2 x_0 + \omega_1^2\Big(\frac{L - x_0}{N} - a\Big) + f = 0 \Longleftrightarrow -\Big(\omega_0^2 + \frac{\omega_1^2}{N}\Big)x_0 + \omega_1^2\Big(\frac{L}{N} - a\Big) + f = 0$$

we get

$$x_0 = \frac{\omega_1^2(L - Na) + Nf}{\omega_1^2 + \omega_0^2 N}.$$

Thus, the solution of the system (4.1), (4.2) is

$$x_k = x_0 + k\frac{\omega_0^2 L + a\omega_1^2 - f}{\omega_1^2 + \omega_0^2 N} = \frac{(\omega_1^2 + \omega_0^2 k)L - \omega_1^2(N - k)a + (N - k)f}{\omega_1^2 + \omega_0^2 N} \tag{4.5}$$

where $k = 1, \dots, N-1$.

According to (4.5) the condition that $x_k \le L$ for $k = 1, \dots, N-1$ is equivalent to the condition $f \le \omega_0^2 L + \omega_1^2 a$. For $f < \omega_0^2 L + \omega_1^2 a$ we get the condition

$$x_0 < x_1 < \cdots < x_{N-1} < x_N = L.$$

For $f = \omega_0^2 L + \omega_1^2 a$ we get the solution $x_k \equiv L, k = 0, 1, \dots, N$. For $f > \omega_0^2 L + \omega_1^2 a$ the solution (4.5) does not have sense as by (4.5) we have

$$x_0 > x_1 > \cdots > x_{N-1} > x_N = L,$$

what is impossible if we assume that the particles cannot jump through fixed particle $x_N = L$. Thus, for $f > \omega_0^2 L + \omega_1^2 a$ we get the equilibrium as $x_k \equiv L, k = 0, 1, \dots, N$.

Note that the uniqueness of equilibrium configuration for $f \le \omega_0^2 L + \omega_1^2 a$ follows from uniqueness of solution of the linear system (4.3), (4.4).

As the equilibrium configuration is unique and the potential energy U is bounded from below (and unbounded from above) quadratic function, then this point is the unique minimum of U.

Proof of Theorem 3.2 We have the following system of equations for the forces F_k acting on the particles $k = 1, 2, \dots, N$:

$$F_0 = -\omega_0^2 x_0 + \omega_1^2 (x_1 - x_0 - a) + f = 0, \tag{4.6}$$

$$F_k = \omega_1^2 (x_{k+1} - x_k - a) - \omega_1^2 (x_k - x_{k-1} - a) = 0, \quad k = 1, \dots, N-1 \tag{4.7}$$

$$F_N = -\omega_0^2 (x_N - L) - \omega_1^2 (x_N - x_{N-1} - a) = 0. \tag{4.8}$$

From (4.7) it follows that the difference $x_k - x_{k-1}$ does not depend on k. Put $r = x_k - x_{k-1} - a$. Then

$$x_k = x_0 + k(r + a), \quad k = 1, \dots, N.$$

Substituting $x_N = x_0 + N(r + a)$ and $r = x_N - x_{N-1} - a$ to equation (4.8) we get system of two equations with respect to x_0, r:

$$-\omega_0^2 x_0 + \omega_1^2 r + f = 0, \tag{4.9}$$

$$-\omega_0^2 x_0 - (\omega_1^2 + N\omega_0^2) r - \omega_0^2 N a + \omega_0^2 L = 0. \tag{4.10}$$

Subtracting second equation from the first we get, we find r:

$$(2\omega_1^2 + N\omega_0^2) r + f + \omega_0^2 N a - \omega_0^2 L = 0 \Longleftrightarrow r = \frac{\omega_0^2 (L - Na) - f}{2\omega_1^2 + N\omega_0^2},$$

$$x_k - x_{k-1} = r + a = \frac{\omega_0^2 L + 2\omega_1^2 a - f}{2\omega_1^2 + N\omega_0^2}, \quad k = 1, \dots, N \tag{4.11}$$

and x_0 we find from equation (4.9)

$$x_0 = \frac{\omega_1^2 r + f}{\omega_0^2} = \frac{\omega_1^2 (L - Na) + Nf + \omega_1^2 \omega_0^{-2} f}{2\omega_1^2 + N\omega_0^2}.$$

Finally also for other coordinates in equilibrium

$$\begin{aligned} x_k &= x_0 + k\frac{\omega_0^2 L + 2\omega_1^2 a - f}{2\omega_1^2 + N\omega_0^2} \\ &= \frac{(\omega_1^2 + k\omega_0^2)L + (N-k)f + \omega_1^2\omega_0^{-2} f - \omega_1^2 (N-k)a + k\omega_1^2 a}{2\omega_1^2 + N\omega_0^2}, \\ x_N &= \frac{(\omega_1^2 + N\omega_0^2)L + \omega_1^2\omega_0^{-2} f + N\omega_1^2 a}{2\omega_1^2 + N\omega_0^2}. \end{aligned}$$

Accordingly to (4.11), we get the following equivalences

$$x_0 < x_1 < \ldots < x_N \iff f < \omega_0^2 L + 2\omega_1^2 a;$$

$$x_0 = x_1 = \ldots = x_N \iff f = \omega_0^2 L + 2\omega_1^2 a;$$

$$x_0 > x_1 > \ldots > x_N \iff f > \omega_0^2 L + 2\omega_1^2 a;$$

$$x_N \le L \iff \frac{(\omega_1^2 + N\omega_0^2)L + \omega_1^2\omega_0^{-2} f + N\omega_1^2 a}{2\omega_1^2 + N\omega_0^2} \le L \iff f \le \omega_0^2 (L - Na);$$

$$x_0 \ge 0 \iff \frac{\omega_1^2 (L - Na) + Nf + \omega_1^2\omega_0^{-2} f}{2\omega_1^2 + N\omega_0^2} \ge 0 \iff f \ge -\frac{\omega_1^2 (L - Na)}{N + \omega_1^2 \omega_0^{-2}}.$$

It follows that the condition, $0 \le x_0 < x_1 < \ldots < x_N \le L$ is equivalent to

$$-\frac{\omega_1^2 (L - Na)}{N + \omega_1^2 \omega_0^{-2}} \le f \le \omega_0^2 (L - Na)$$

as from $f \le \omega_0^2 (L - Na)$ it follows that $f < \omega_0^2 L + 2\omega_1^2 a$.

As in Theorem 3.1 this equilibrium configuration is unique and stable.

Proof of Theorem 3.3 The system of equations is

$$F_0 = -\omega_0^2 x_0 + \omega_1^2 (x_1 - x_0 - a) + f = 0,$$

$$F_k = \omega_1^2 (x_{k+1} - x_k - a) - \omega_1^2 (x_k - x_{k-1} - a) = 0, \quad k = 1, \ldots, N-1,$$

$$F_N = -\omega_0^2 (x_N - L) - \omega_1^2 (x_N - x_{N-1} - a) - f = 0.$$

Also $x_k - x_{k-1}$ does not depend on k, and we put

$$x_k = x_0 + k(r + a), \quad k = 1, \ldots, N$$

where $r = x_k - x_{k-1} - a$.

Substituting $x_N = x_0 + N(r+a), r = x_N - x_{N-1} - a$ to equation $F_N = 0$, we get the system of two equations w.r.t. x_0, r:

$$-\omega_0^2 x_0 + \omega_1^2 r + f = 0,$$

$$-\omega_0^2 x_0 - (\omega_1^2 + N\omega_0^2) r - \omega_0^2 N a + \omega_0^2 L - f = 0,$$

from where we get

$$r = \frac{\omega_0^2 (L - Na) - 2f}{2\omega_1^2 + N\omega_0^2}, \quad x_0 = \frac{\omega_1^2 (L - Na) + Nf}{2\omega_1^2 + N\omega_0^2}.$$

It follows $x_0 \geq 0 \Longleftrightarrow \omega_1^2 (L - Na) + Nf > 0 \Longleftrightarrow f \geq \omega_1^2 (a - L/N)$. And then

$$x_k - x_{k-1} = r + a = \frac{\omega_0^2 L + 2\omega_1^2 a - 2f}{2\omega_1^2 + N\omega_0^2}, \quad k = 1, \ldots, N,$$

and

$$\begin{aligned} x_k = x_0 + k \frac{\omega_0^2 L + 2\omega_1^2 a - 2f}{2\omega_1^2 + N\omega_0^2} = \\ = \frac{(\omega_1^2 + k\omega_0^2) L + (N - 2k) f - \omega_1^2 (N - k) a + k\omega_1^2 a}{2\omega_1^2 + N\omega_0^2}. \end{aligned}$$

Thus,

$$x_0 < x_1 < \ldots < x_N \Longleftrightarrow 2f < \omega_0^2 L + 2\omega_1^2 a.$$

In particular,

$$x_N = \frac{(\omega_1^2 + N\omega_0^2) L - Nf + N\omega_1^2 a}{2\omega_1^2 + N\omega_0^2},$$

$$x_N \leq L \Longleftrightarrow \frac{(\omega_1^2 + N\omega_0^2) L - Nf + N\omega_1^2 a}{2\omega_1^2 + N\omega_0^2} \leq L \Longleftrightarrow f \geq \omega_1^2 \Big(a - \frac{L}{N} \Big) a.$$

Finally

$$0 \leq x_0 < x_1 < \ldots < x_N \leq L \Longleftrightarrow \omega_1^2 \Big(a - \frac{L}{N} \Big) a \leq f < \frac{\omega_0^2 L + 2\omega_1^2 a}{2}.$$

Proof of Theorem 3.4 The system of equations is

$$F_0 = -\omega_0^2 x_0 + \omega_1^2 (x_1 - x_0 - a) + f = 0, \tag{4.12}$$

$$F_k = \omega_1^2 (x_{k+1} - x_k - a) - \omega_1^2 (x_k - x_{k-1} - a) + f = 0, \ k = 1, \ldots, N-1, \tag{4.13}$$

where the coordinates x_k should also satisfy the conditions: $x_k \leq L, k = 1, \ldots, N-1$ and $x_N = L$.

Put $r_k = x_k - x_{k-1} - a$. Then the system (4.12) and (4.13) can be rewritten as:

$$r_1 = -\frac{f}{\omega_1^2} + \frac{\omega_0^2 x_0}{\omega_1^2}, \quad r_k = -\frac{f}{\omega_1^2} + r_{k-1}, \quad k = 2, \dots, N.$$

Then

$$r_k = -\frac{f}{\omega_1^2} k + \frac{\omega_0^2 x_0}{\omega_1^2}, \quad k = 1, \dots, N.$$

Using the last formula we write $x_k, k = 1, \dots, N-1$ in terms of x_0 :

$$x_k = x_0 + \sum_{l=1}^{k} (x_k - x_{k-1} - a) + ka = x_0 + \sum_{l=1}^{k} r_l + ka =$$

$$= x_0 + \sum_{l=1}^{k} \left(-\frac{f}{\omega_1^2} l + \frac{\omega_0^2 x_0}{\omega_1^2} \right) + ka = x_0 + k\Big(\frac{\omega_0^2 x_0}{\omega_1^2} + a \Big) - \frac{f}{\omega_1^2} \frac{k(k+1)}{2}.$$

Then,

$$x_k = x_0 + k\Big(\frac{\omega_0^2 x_0}{\omega_1^2} + a \Big) - \frac{k(k+1)f}{2\omega_1^2},$$

$$x_k - x_{k-1} = r_k + a = -\frac{f}{\omega_1^2} k + \frac{\omega_0^2 x_0}{\omega_1^2} + a. \tag{4.14}$$

From the condition $x_N = L$ we get the equation for x_0

$$x_0 + N\Big(\frac{\omega_0^2 x_0}{\omega_1^2} + a \Big) - \frac{N(N+1)f}{2\omega_1^2} = L \Longleftrightarrow$$

$$x_0 = \frac{\omega_1^2 \big(L + N(N+1) f/(2\omega_1^2) - Na \big)}{\omega_1^2 + \omega_0^2 N}.$$

It is easy to see that

$$x_0 \geq 0 \Longleftrightarrow \omega_1^2 \Big(L + \frac{N(N+1)f}{2\omega_1^2} - Na \Big) > 0 \Longleftrightarrow f \geq -\frac{2\omega_1^2 (L - Na)}{N(N+1)}.$$

Then by (4.14) we have

$$x_k - x_{k-1} = -\frac{fk}{\omega_1^2} + \frac{\omega_0^2 \big(L + N(N+1) f/(2\omega_1^2) \big) + a\omega_1^2}{\omega_1^2 + \omega_0^2 N}, \ k = 1, \dots, N-1.$$

Assume that $f > 0$. Then the condition $x_0 < x_1 < \ldots < x_{N-1} < L$ is equivalent to

$$-\frac{fk}{\omega_1^2} + \frac{\omega_0^2 (L + N(N+1) f/(2\omega_1^2)) + a\omega_1^2}{\omega_1^2 + \omega_0^2 N} > 0, \ \forall k = 1, \dots, N \Longleftrightarrow$$

$$\frac{\omega_0^2(L+N(N+1)f/(2\omega_1^2))+a\omega_1^2}{\omega_1^2+\omega_0^2N} > \frac{fN}{\omega_1^2} \Longleftrightarrow f < \frac{2\omega_1^2\left(\omega_0^2L+a\omega_1^2\right)}{N(2\omega_1^2+\omega_0^2(N-1))}.$$

Thus for $f>0$ the condition $0 \le x_0 < x_1 < \ldots < x_{N-1} < x_N = L$ is equivalent to

$$-\frac{2\omega_1^2(L-Na)}{N(N+1)} \le f < \frac{2\omega_1^2\left(\omega_0^2L+a\omega_1^2\right)}{N(2\omega_1^2+\omega_0^2(N-1))}.$$

If $f<0$ the condition $x_k > x_{k-1}$ for any $k=1,\ldots,N$ is equivalent to

$$-\frac{fk}{\omega_1^2} + \frac{\omega_0^2(L+N(N+1)f/(2\omega_1^2))+a\omega_1^2}{\omega_1^2+\omega_0^2N} > 0\ \forall k=1,\ldots,N \Longleftrightarrow$$

$$-\frac{f}{\omega_1^2} + \frac{\omega_0^2(L+N(N+1)f/(2\omega_1^2))+a\omega_1^2}{\omega_1^2+\omega_0^2N} > 0 \Longleftrightarrow f < -\frac{2\omega_1^2(\omega_0^2L+a\omega_1^2)}{\omega_0^2N(N-1)-2\omega_1^2}.$$

And in general, for $f<0$ the condition $0 \le x_0 < x_1 < \ldots < x_{N-1} < x_N = L$ is equivalent to

$$-\frac{2\omega_1^2(L-Na)}{N(N+1)} \le f < -\frac{2\omega_1^2(\omega_0^2L+a\omega_1^2)}{\omega_0^2N(N-1)-2\omega_1^2}.$$

Proof of Theorem 3.5 The equations are

$$F_0 = -\omega_0^2x_0 + \omega_1^2(x_1-x_0-a)+f=0, \tag{4.15}$$

$$F_k = \omega_1^2(x_{k+1}-x_k-a) - \omega_1^2(x_k-x_{k-1}-a)+f=0,\ k=1,\ldots,N-1, \tag{4.16}$$

$$F_N = -\omega_0^2(x_N-L) - \omega_1^2r_N + f = 0. \tag{4.17}$$

Putting $r_k = x_k - x_{k-1} - a$ and as Theorem 3.4, from equations (4.15), (4.16) we find

$$r_k = -\frac{fk}{\omega_1^2} + \frac{\omega_0^2x_0}{\omega_1^2} \Longleftrightarrow x_k - x_{k-1} = -\frac{fk}{\omega_1^2} + \frac{\omega_0^2x_0}{\omega_1^2} + a, \tag{4.18}$$

$$x_k = x_0 + k\Big(\frac{\omega_0^2x_0}{\omega_1^2}+a\Big) - \frac{f}{\omega_1^2}\frac{k(k+1)}{2}$$

for $k=1,\ldots,N$. Substituting

$$x_N = x_0 + N\Big(\frac{\omega_0^2x_0}{\omega_1^2}+a\Big) - \frac{N(N+1)f}{2\omega_1^2}, \quad r_N = -\frac{f}{\omega_1^2}N + \frac{\omega_0^2x_0}{\omega_1^2}$$

to (4.17), we can get x_0 :

$$x_0 = \frac{\omega_1^2(L+N(N+1)f/(2\omega_1^2)-Na)+\omega_1^2\omega_0^{-2}f(N+1)}{2\omega_1^2+N\omega_0^2}. \tag{4.19}$$

According to (4.18) we have

$$x_k - x_{k-1} = -\frac{fk}{\omega_1^2} + \frac{\omega_0^2 x_0}{\omega_1^2} + a =$$

$$= -\frac{fk}{\omega_1^2} + \frac{\omega_0^2(L + N(N+1)f/(2\omega_1^2)) + f(N+1) + 2\omega_1^2 a}{2\omega_1^2 + N\omega_0^2}, \ k = 1, \dots, N. \quad (4.20)$$

For $f > 0$ the condition $x_k > x_{k-1}$ for any $k = 1, \dots, N$ is equivalent to

$$\frac{\omega_0^2(L + N(N+1)f/(2\omega_1^2)) + f(N+1) + 2\omega_1^2 a}{2\omega_1^2 + N\omega_0^2} > \frac{fk}{\omega_1^2} \ \forall k = 1, \dots, N \iff$$

$$\frac{\omega_0^2(L + N(N+1)f/(2\omega_1^2)) + f(N+1) + 2\omega_1^2 a}{2\omega_1^2 + N\omega_0^2} > \frac{fN}{\omega_1^2} \iff$$

$$f < \frac{2\omega_1^2\left(\omega_0^2 L + 2a\omega_1^2\right)}{(N-1)(2\omega_1^2 + \omega_0^2 N)}.$$

For $f < 0$ the condition $x_k > x_{k-1}$ for any $k = 1, \dots, N$ is equivalent to

$$\frac{-\omega_0^2(L + N(N+1)f/(2\omega_1^2)) - f(N+1) - 2\omega_1^2 a}{2\omega_1^2 + N\omega_0^2} < -\frac{fk}{\omega_1^2} \ \forall k = 1, \dots, N \iff$$

$$\frac{-\omega_0^2(L + N(N+1)f/(2\omega_1^2)) - f(N+1) - 2\omega_1^2 a}{2\omega_1^2 + N\omega_0^2} < -\frac{f}{\omega_1^2} \iff$$

$$-f < \frac{2\omega_1^2\left(\omega_0^2 L + 2a\omega_1^2\right)}{(N-1)(2\omega_1^2 + \omega_0^2 N)}.$$

And then

$$x_0 < x_1 < \ldots < x_N \iff |f| < \frac{2\omega_1^2\left(\omega_0^2 L + 2a\omega_1^2\right)}{(N-1)(2\omega_1^2 + \omega_0^2 N)}.$$

From (4.19), (4.20) we have

$$x_N = \frac{N(N+1)f/2 + \omega_1^2\omega_0^{-2} f(N+1) + \omega_1^2(L + Na) + N\omega_0^2 L}{2\omega_1^2 + N\omega_0^2}.$$

Then

$$x_N \le L \iff f \le \frac{\omega_1^2\omega_0^2(L - Na)}{(2\omega_1^2 + N\omega_0^2)\,(N+1)}.$$

By (4.19)

$$x_0 \ge 0 \iff f \ge \frac{-2\omega_1^2\omega_0^2(L - Na)}{(2\omega_1^2 + N\omega_0^2)\,(N+1)}.$$

Denote

$$A = \frac{2\omega_1^2\left(\omega_0^2 L + 2a\omega_1^2\right)}{(N-1)(2\omega_1^2+\omega_0^2 N)},$$

$$B = \frac{\omega_1^2\omega_0^2(L-Na)}{(2\omega_1^2+N\omega_0^2)\,(N+1)}.$$

Note that $0 < 2B < A$ is equivalent to

$$f \le \frac{\omega_1^2\omega_0^2(L-Na)}{(2\omega_1^2+N\omega_0^2)\,(N+1)} < \frac{2\omega_1^2\left(\omega_0^2 L + 2a\omega_1^2\right)}{(N-1)(2\omega_1^2+\omega_0^2 N)}.$$

As $2B < A$, the condition $0 \le x_0 < x_1 < \ldots < x_N \le L$ is equivalent to the condition that $-2B \le f \le B$ and $B > 0$.

Proof of Theorem 3.6 We get the following system of equations from the condition that forces on each particle equal zero:

$$\omega_1^2\Big(x_{k+1}-x_k-\frac{a_1}{M}\Big)-\omega_1^2\Big(x_k-x_{k-1}-\frac{a_1}{M}\Big)=0,\ k=2,\ldots,N_1-1,$$

$$\omega_1^2\Big(x_2-x_1-\frac{a_1}{M}\Big)-\omega_0^2\Big(x_1+y_1-\frac{a_0}{M}\Big)=0,$$

$$\omega_2^2\Big(y_2-y_1-\frac{a_2}{M}\Big)-\omega_0^2\Big(x_1+y_1-\frac{a_0}{M}\Big)=0,$$

$$\omega_2^2\Big(y_{i+1}-y_i-\frac{a_2}{M}\Big)-\omega_2^2\Big(y_i-y_{i-1}-\frac{a_2}{M}\Big)=0,\ i=2,\ldots,N_2-1.$$

Denote

$$R_k = x_{k+1}-x_k-\frac{a_1}{M},\ \ k=1,\ldots,N_1-1,$$

$$R_0 = x_1+y_1-\frac{a_0}{M},$$

$$Q_i = y_{i+1}-y_i-\frac{a_2}{M},\ \ i=1,\ldots,N_2-1.$$

Then

$$R_1=\ldots=R_{N_1-1}=\frac{\omega_0^2 R_0}{\omega_1^2},$$

$$Q_1=\ldots=Q_{N_2-1}=\frac{\omega_0^2 R_0}{\omega_2^2},$$

and it follows

$$x_{k+1}-x_k-\frac{a_1}{M}=\frac{\omega_0^2 R_0}{\omega_1^2}\Longleftrightarrow x_{k+1}=x_1+\left(\frac{\omega_0^2(x_1+y_1-a_0/M)}{\omega_1^2}+\frac{a_1}{M}\right)k,$$

$$y_{i+1} - y_i - \frac{a_2}{M} = \frac{\omega_0^2 R_0}{\omega_2^2} \iff y_{i+1} = y_1 + \left(\frac{\omega_0^2 (x_1 + y_1 - a_0/M)}{\omega_2^2} + \frac{a_2}{M} \right) i.$$

By conditions (3.2) and (3.3) it should be

$$x_{k+1} > x_k \iff \frac{\omega_0^2 R_0}{\omega_1^2} + \frac{a_1}{M} > 0 \iff R_0 > -\frac{\omega_1^2 a_1}{\omega_0^2 M},$$

$$y_{k+1} > y_k \iff \frac{\omega_0^2 R_0}{\omega_2^2} + \frac{a_2}{M} > 0 \iff R_0 > -\frac{\omega_2^2 a_2}{\omega_0^2 M}$$

and then

$$x_1 + y_1 - \frac{a_0}{M} > -\min\Big(\frac{\omega_1^2 a_1}{\omega_0^2 M}, \frac{\omega_2^2 a_2}{\omega_0^2 M} \Big).$$

The potential energy is then

$$\begin{aligned} U &= \frac{\omega_0^4 R_0^2 (N_2 - 1)}{2\omega_2^2} + \frac{\omega_0^2 R_0^2}{2} + \frac{\omega_0^4 R_0^2 (N_1 - 1)}{2\omega_1^2} = \\ &= \frac{\omega_0^2}{2} \left(\omega_0^2 \left(\frac{N_2 - 1}{\omega_2^2} + \frac{N_1 - 1}{\omega_1^2} \right) + 1 \right) \left(x_1 + y_1 - \frac{a_0}{M} \right)^2 \\ &= \frac{\omega_0^2 N}{2} \left(\omega_0^2 \left(\omega_1^{-2} c + \omega_2^{-2} (1 - c) \right) + N^{-1} \right) \\ &\quad \times \left(x_1 + y_1 - \frac{a_0}{M} \right)^2. \end{aligned}$$

Finally, from equations

$$x_{N_1} = x_1 + \left(\frac{\omega_0^2 (x_1 + y_1 - a_0/M)}{\omega_1^2} + \frac{a_1}{M} \right) cN = L_1,$$

$$y_{N_2} = y_1 + \left(\frac{\omega_0^2 (x_1 + y_1 - a_0/M)}{\omega_2^2} + \frac{a_2}{M} \right) (1 - c) N = L_2,$$

we have

$$x_1 + y_1 - \frac{a_0}{M} = \frac{L_1 + L_2 - a_1 cb - a_2 (1 - c) b - a_0 M^{-1}}{1 + bM\omega_0^2 \left(\omega_1^{-2} c + \omega_2^{-2} (1 - c) \right)}$$

and it should be

$$\frac{L_1 + L_2 - a_1 cb - a_2 (1 - c) b - a_0 M^{-1}}{1 + bM\omega_0^2 \left(\omega_1^{-2} c + \omega_2^{-2} (1 - c) \right)} > -\min\Big(\frac{\omega_1^2 a_1}{\omega_0^2 M}, \frac{\omega_2^2 a_2}{\omega_0^2 M} \Big),$$

and the potential energy is easily calculated.

5. Distribution of kinetic and potential energies

5.1. Necessary definitions

Here we give well-known definitions (more general than necessary) for better understanding the results below.

We consider systems with N_0 particles in R^d, denote $N = dN_0$ the number of coordinates $x_i = q_i \in R, i = 1, \ldots, N$, velocities v_i, masses $m_i > 0$ and momenta $p_i = m_i v_i, v_i = \dot{x}_i$, of these particles. The dynamics (trajectories) $x_i(t), 0 \leq t < \infty$, is defined by the Hamiltonian $H = T + U$, with kinetic T and potential U energies

$$T = \sum_{i=1}^{N} \frac{m_i v_i^2}{2}, \quad U = U_0(x_1, \ldots, x_N) + U_{ext},$$

where

$$U_{ext} = U_{ext}(t, x_1, \ldots, x_N) = -\sum_{i=1}^{N} f_i(t) x_i.$$

The equations are

$$m_i \frac{d^2 x_i}{dt^2} = -\frac{\partial U}{\partial x_i} = -\frac{\partial U_0}{\partial x_i} + f_i(t)$$

with initial conditions $x_i(0), v_i(0)$. Here U_0 corresponds to interaction between particles and $f_i(t)$ are external forces.

Time averages of the energies are defined as the limits (if they exist)

$$\langle T \rangle = \lim_{t \to \infty} \frac{1}{t} \int_0^t T(s) ds, \quad \langle U \rangle = \lim_{t \to \infty} \frac{1}{t} \int_0^t U(s) ds.$$

General virial theorem It is the following equality:

$$\langle T \rangle = -\sum_{i=1}^{N} \langle (f_i, r_i) \rangle \tag{5.1}$$

where f_i is the force on the i-th coordinate, r_i - its coordinate vector.

Proof. Let

$$G = \sum_{i=1}^{N} (p_i, r_i).$$

Then

$$\dot{G}_t = \sum_{i=1}^{N} (f_i, r_i) + 2T.$$

If all p_i and r_i stay uniformly bounded then virial theorem follows as

$$\frac{1}{t}\int_0^t \dot{G}dt = \frac{1}{t}(G(t) - G(0)) \to 0.$$

Virial theorem for quadratic potential For general quadratic potential energy

$$U(x) = \frac{1}{2}(x, Vx),$$

where $x \in R^N$, $V = (v_{ij})$ is positive definite symmetric $(N \times N)$-matrix. Then the force F_i on particle i

$$F_i = -\nabla_{x_i} U(x) = -\sum_{j=1}^{N} v_{ij} x_j.$$

Then

$$\sum_{i=1}^{N} F_i x_i = -\sum_{i=1}^{N}\sum_{j=1}^{N} v_{ij} x_i x_j = -(Vx, x) = -2U(x).$$

Put

$$G = \sum_{i=1}^{N} m_i v_i x_i.$$

Then

$$\dot{G}_t = \sum_{i=1}^{N} m_i v_i^2 + \sum_{i=1}^{N} m_i \dot{v}_i x_i = 2T + \sum_{i=1}^{N} F_i x_i = 2T - 2U \tag{5.2}$$

and for the averages

$$2\left(\langle T\rangle - \langle U\rangle\right) = \langle \dot{G}_t\rangle = \lim_{t\to\infty} \frac{G(t) - G(0)}{t} = 0$$

as $G(t)$ is uniformly bounded. To see this note first that the kinetic and potential energies are positive and due to energy conservation are uniformly bounded. Then the system stays in bounded volume.

It follows that kinetic and potential energies are equal

$$\langle T\rangle = \langle U\rangle. \tag{5.3}$$

Now assume also time-dependent external forces. For example, a harmonic force $f_i(t) = \sin \omega_i t$ on particle i. Then the potential energy is

$$U(x) = \frac{1}{2}(x, Vx) - \sum_{i=1}^{N} f_i x_i.$$

Similarly to (5.2) we get

$$\langle \dot{G}_t \rangle = 2\left(\langle T \rangle - \langle U \rangle\right).$$

Let $\nu_1, \ldots, \nu_N$ be eigenvalues of V. They are positive and assume that for all i, j

$$\omega_i \neq \sqrt{\nu_j}.$$

Then $\langle \dot{G}_t \rangle = 0$ due to boundedness of $G(t)$ and $\langle T \rangle = \langle U \rangle$.

More interesting is analogs of virial theorem for local parts of a large system of particles. For example, in biological organism (or even in social organism) one part of the system can move more intensively (large $< T >$, small $< U >$) and another part could be the contrary. We consider here simple system and try to understand when could this be. For calculations we will use explicit calculations – direct but cumbersome. Our example is the following.

5.2. Simplest system under periodic boundary force

Consider the chain of $N+1$ particles with coordinates $x_0 \equiv 0, x_1, \ldots, x_N$. We assume that particle 0 is fixed at 0 and on the particle N acts periodic force $f(t) = c \sin \omega t$. Potential energy of the system is

$$U(x) = \frac{\omega_1^2}{2} \sum_{i=1}^{N} (x_i - x_{i-1} - a)^2 - x_N c \sin \omega t$$

and the equations are

$$\begin{aligned} \ddot{x}_k &= -\omega_1^2 (x_k - x_{k-1} - a) + \omega_1^2 (x_{k+1} - x_k - a) \\ &= \omega_1^2 (x_{k+1} - 2x_k + x_{k-1}), \quad k = 1, \ldots, N-1, \\ \ddot{x}_N &= -\omega_1^2 (x_N - x_{N-1} - a) + c \sin \omega t \end{aligned}$$

with initial conditions $x_k(0) = ka, v_k(0) = 0$.

After change

$$q_k = x_k - ka, \;\; k = 0, 1, \ldots, N$$

the equations will be

$$\ddot{q}_k = \omega_1^2 (q_{k+1} - 2q_k + q_{k-1}), \;\; k = 1, \ldots, N-1,$$

$$\ddot{q}_N = -\omega_1^2 (q_N - q_{N-1}) + c \sin \omega t.$$

In the matrix form they can be rewritten as

$$\ddot{q} = -Vq + c \sin \omega t e_N, \quad e_N = (\delta_{1,N}, \ldots, \delta_{N,N}) = (0, \ldots, 0, 1),$$

where V is the following tridiagonal matrix $N \times N$

$$V = \begin{pmatrix} 2\omega_1^2 & -\omega_1^2 & & \\ -\omega_1^2 & 2\omega_1^2 & -\omega_1^2 & \\ \dots & \dots & \dots & \dots \\ & & -\omega_1^2 & \omega_1^2 \end{pmatrix}$$

In the last row there is ω_1^2, all the rest are $2\omega_1^2$.

Spectrum of matrix *V* Denote λ_k the eigenvalues of V and let $\{h_k, k = 1, \dots, N\}$ be the corresponding eigenvectors $Vh_k = \lambda_k h_k$ with coordinates $h_k = (h_k^{(j)}, j = 1, \dots, N)$.

Lemma 5.1. *The eigenvalues and eigenvectors of V are*

$$\lambda_k = 2\omega_1^2 \left(\cos\left(\frac{\pi k}{N + 1/2} \right) + 1 \right), \quad k = 1, \dots, N$$

$$h_k^{(j)} = \frac{\sin\left(\frac{j(N-k+1/2)\pi}{N+1/2}\right)}{\sin\left(\frac{(N-k+1/2)\pi}{N+1/2}\right)}, \quad j = 1, \dots, N.$$

As all eigenvalues are positive, we can denote them as $\lambda_k = \nu_k^2, \ k = 1, \dots, N$, where it will be convenient to assume all ν_k also positive. Denote by g_k the normalized eigenvectors

$$g_k = \frac{h_k}{\sqrt{(h_k, h_k)}}, \ \ k = 1, \dots, N,$$

which form an orthonormal basis.

The energy of the system then is

$$H(\psi(t)) = U(\psi(t)) + T(\psi(t)) - f(t)q_N.$$

where $\psi = (q_1, \dots, q_N, p_1, \dots, p_N)$ and

$$U(\psi(t)) = \frac{1}{2} \sum_{1 \le j,l \le N} V_{j,l} q_j q_l = \frac{1}{2}(q, Vq), \quad T(\psi(t)) = \sum_{j=1}^{N} \frac{p_j^2}{2} = \frac{1}{2}(p, p),$$

are internal potential and kinetic energy of the system. Then the dynamics satisfies the following system of equations:

$$\ddot{q}_j = -\sum_l V_{j,l} q_l + f(t)\delta_{j,N}, \ \ j = 1, \dots, N,$$

where $\delta_{j,N}$ is the Kronecker symbol. Let us rewrite this in Hamiltonian form:

$$\begin{cases} \dot{q}_j = p_j, \\ \dot{p}_j = -\sum_l V_{j,l} q_l + f(t)\delta_{j,N}, \end{cases}$$

and in vector notation:

$$\dot{\psi} = A_0 \psi + f(t) g_N, \tag{5.4}$$

where

$$A_0 = \begin{pmatrix} 0 & E \\ -V & 0 \end{pmatrix}$$

is $(2N \times 2N)$-matrix, E is the unit $(N \times N)$-matrix, and

$$r_N = (0, \dots, 0, e_N)^T \in \mathbb{R}^{2N}, \quad e_N = (\delta_{1,N}, \dots, \delta_{N,N}).$$

It is well-known that the solution of (5.4) is:

$$\psi(t) = e^{A_0 t}\psi(0) + \int_0^t e^{A_0(t-s)} f(s) r_N ds \tag{5.5}$$

with

$$e^{A_0 t} = \begin{pmatrix} \cos(\sqrt{V}t) & (\sqrt{V})^{-1}\sin(\sqrt{V}t) \\ -\sqrt{V}\sin(\sqrt{V}t) & \cos(\sqrt{V}t) \end{pmatrix},$$

where matrix sine and cosine are defined, similar to matrix exponent by corresponding series. Then we can write down the solution as:

$$\begin{aligned} q(t) &= \cos(\sqrt{V}t)q(0) + (\sqrt{V})^{-1}\sin(\sqrt{V}t)p(0) \\ &\quad + \int_0^t f(s)(\sqrt{V})^{-1}\sin(\sqrt{V}(t-s))e_N ds, \end{aligned} \tag{5.6}$$

$$p(t) = -\sqrt{V}\sin(\sqrt{V}t)q(0) + \cos(\sqrt{V}t)p(0) + \int_0^t f(s)\cos(\sqrt{V}(t-s))e_N ds. \tag{5.7}$$

Let us expand the vectors $e_N, q(0), p(0)$ in the basis of eigenvectors of V:

$$e_N = \sum_{k=1}^N (g_k, e_N) g_k, \quad q(0) = \sum_{k=1}^N (g_k, q(0)) g_k, \quad p(0) = \sum_{k=1}^N (g_k, p(0)) g_k.$$

Then, as

$$\begin{aligned} (\sqrt{V})^{-1} g_k &= \frac{1}{\nu_k} g_k, \\ \sin(\sqrt{V}t) g_k &= g_k \sin(\nu_k t), \\ \cos(\sqrt{V}t) g_k &= g_k \cos(\nu_k t), \end{aligned}$$

we have

$$q(t) = \sum_{k=1}^{N} \Bigg[(g_k, e_N) \int_0^t f(s) \frac{\sin(\nu_k(t-s))}{\nu_k} ds + (g_k, q(0)) \cos(\nu_k t) + (g_k, p(0)) \frac{\sin(\nu_k t)}{\nu_k} \Bigg] g_k, \tag{5.8}$$

$$p(t) = \sum_{k=1}^{N} \Bigg[(g_k, e_N) \int_0^t f(s) \cos(\nu_k(t-s)) ds - (g_k, q(0)) \nu_k \sin(\nu_k t) + (g_k, p(0)) \cos(\nu_k t) \Bigg] g_k. \tag{5.9}$$

We have to find functions

$$\hat{q}_k(t) = \nu_k^{-1} \int_0^t f(s) \sin(\nu_k(t-s)) ds,$$

$$\hat{p}_k(t) = \int_0^t f(s) \cos(\nu_k(t-s)) ds.$$

Since $f(t) = c \sin \omega t$, for $\omega \neq \nu_k$ we have

$$\hat{q}_k(t) = \frac{c\omega}{\nu_k^2 - \omega^2} \left(\frac{\sin(\omega t)}{\omega} - \frac{\sin(\nu_k t)}{\nu_k} \right), \tag{5.10}$$

$$\hat{p}_k(t) = \frac{c\omega}{\nu_k^2 - \omega^2} \left(\cos(\omega t) - \cos(\nu_k t) \right).$$

Further on we consider zero initial conditions, then coordinates and momenta of particle j are:

$$q_j(t) = \sum_{k=1}^{N} (g_k, e_N)(g_k, e_j) \hat{q}_k(t), \tag{5.11}$$

$$p_j(t) = \sum_{k=1}^{N} (g_k, e_N)(g_k, e_j) \hat{p}_k(t).$$

5.3. Kinetic energy

Now we can find kinetic energy of particle j:

$$T_j(t) = \frac{1}{2} \sum_{k=1}^{N} \sum_{l=1}^{N} (g_k, e_N)(g_k, e_j)(g_l, e_N)(g_l, e_j) \hat{p}_k(t) \hat{p}_l(t),$$

where

$$\hat{p}_k(t) = \frac{c\omega}{\nu_k^2 - \omega^2} \left(\cos(\omega t) - \cos(\nu_k t) \right), \quad k = 1, \ldots, N,$$

$$\nu_k^2 = 2\omega_1^2 \Big(\cos\Big(\frac{\pi k}{N + 1/2} \Big) + 1 \Big), \quad k = 1, \ldots, N,$$

$$(g_k, e_j) = \frac{h_k^{(j)}}{\sqrt{(h_k, h_k)}} = \frac{1}{\sqrt{(h_k, h_k)}} \frac{\sin\left(\frac{j(N-k+1/2)\pi}{N+1/2} \right)}{\sin\left(\frac{(N-k+1/2)\pi}{N+1/2} \right)}, \quad k, j = 1, \ldots, N.$$

Note also that

$$\sin\left(\frac{j(N-k+1/2)\pi}{N+1/2} \right) = \sin\left(j\pi - \frac{jk\pi}{N+1/2} \right) = (-1)^{j-1} \sin\left(\frac{jk\pi}{N+1/2} \right),$$

$$(g_k, e_j) = \frac{1}{\sqrt{(h_k, h_k)}} \frac{(-1)^{j-1} \sin\left(\frac{jk\pi}{N+1/2} \right)}{\sin\left(\frac{k\pi}{N+1/2} \right)}. \tag{5.12}$$

Then

$$(h_k, h_k) = \sin^{-2}\left(\frac{k\pi}{N+1/2} \right) \sum_{j=1}^{N} \sin^2\left(\frac{jk\pi}{N+1/2} \right).$$

Now we want to find the mean kinetic energy of the particle j

$$\langle T_j \rangle = \frac{\langle p_j^2(t) \rangle}{2}.$$

Theorem 5.1. *If $\omega \neq \nu_k$ for any k then (for zero initial conditions)*

$$\langle T_j \rangle = \frac{1}{4} \left(\sum_{k=1}^{N} (g_k, e_N)(g_k, e_j) \frac{\omega c}{\nu_k^2 - \omega^2} \right)^2 + \frac{1}{4} \sum_{k=1}^{N} (g_k, e_N)^2 (g_k, e_j)^2 \left(\frac{\omega c}{\nu_k^2 - \omega^2} \right)^2 \tag{5.13}$$

Proof. By (5.9),

$$p_j(t) = \sum_{k=1}^{N} (g_k, e_N)(g_k, e_j) \hat{p}_k(t),$$

where

$$\hat{p}_k(t) = A_k \left(\cos(\omega t) - \cos(\nu_k t) \right), A_k = \frac{\omega c}{\nu_k^2 - \omega^2},$$

then we can show that

$$\langle p_j^2(t) \rangle = \sum_{k=1}^{N} \sum_{l=1}^{N} (g_k, e_N)(g_k, e_j)(g_l, e_N)(g_l, e_j) \langle \hat{p}_k(t) \hat{p}_l(t) \rangle,$$

where

$$\langle \hat{p}_k(t)\hat{p}_l(t)\rangle = \begin{cases} A_k^2 & k=l, \\ \frac{1}{2}A_kA_l & k\neq l. \end{cases}$$

In fact, for $\omega \neq \nu_k$

$$\langle \hat{p}_k^2(t)\rangle = A_k^2\langle(\cos(\omega t)-\cos(\nu_k t))^2\rangle = A_k^2\left(\langle\cos^2(\omega t)\rangle + \langle\cos^2(\nu_k t)\rangle\right) = A_k^2$$

and for $k \neq l$

$$\begin{aligned}\langle \hat{p}_k(t)\hat{p}_l(t)\rangle &= A_kA_l\langle(\cos(\omega t)-\cos(\nu_k t))(\cos(\omega t)-\cos(\nu_l t))\rangle \\ &= A_kA_l\langle\cos^2(\omega t)\rangle = \frac{A_kA_l}{2}.\end{aligned}$$

Then

$$\frac{\langle p_j^2(t)\rangle}{2} = \frac{1}{2}\sum_{k=1}^{N}(g_k,e_N)^2(g_k,e_j)^2A_k^2 +$$

$$+\frac{1}{4}\sum_{k\neq l}^{N}(g_k,e_N)(g_l,e_N)(g_k,e_j)(g_l,e_j)A_kA_l =$$

$$= \frac{1}{4}\sum_{k=1}^{N}(g_k,e_N)^2(g_k,e_j)^2A_k^2 +$$

$$+\frac{1}{4}\sum_{k,l=1}^{N}(g_k,e_N)(g_l,e_N)(g_k,e_j)(g_l,e_j)A_kA_l =$$

$$= \frac{1}{4}\sum_{k=1}^{N}(g_k,e_N)^2(g_k,e_j)^2A_k^2 + \frac{1}{4}\left(\sum_{k=1}^{N}(g_k,e_N)(g_k,e_j)A_k\right)^2.$$

Theorem 5.2. *Assume that $\omega^2 > 4\omega_1^2$. Then there exist limits*

$$\lim_{N\to\infty}\langle T_1\rangle = 0, \qquad \lim_{N\to\infty}\langle T_N\rangle = K > 0.$$

Proof. By (5.13),

$$\langle T_1\rangle = \frac{1}{4}\left(\sum_{k=1}^{N}(g_k,e_N)(g_k,e_1)\frac{\omega c}{\nu_k^2-\omega^2}\right)^2 + \frac{1}{4}\sum_{k=1}^{N}(g_k,e_N)^2(g_k,e_1)^2\left(\frac{\omega c}{\nu_k^2-\omega^2}\right)^2,$$

$$\langle T_N\rangle = \frac{1}{4}\left(\sum_{k=1}^{N}(g_k,e_N)^2\frac{\omega c}{\nu_k^2-\omega^2}\right)^2 + \frac{1}{4}\sum_{k=1}^{N}(g_k,e_N)^4\left(\frac{\omega c}{\nu_k^2-\omega^2}\right)^2.$$

According to (5.12),

$$(g_k, e_1) = \frac{1}{\sqrt{(h_k, h_k)}},$$

$$(g_k, e_N) = \frac{(-1)^{N-1}}{\sqrt{(h_k, h_k)}} \frac{\sin\left(\frac{k\pi}{1+1/(2N)}\right)}{\sin\left(\frac{k\pi}{N+1/2}\right)}.$$

Then

$$\langle T_1 \rangle = \frac{1}{4} \left(\sum_{k=1}^{N} \frac{1}{(h_k, h_k)} \frac{\sin\left(\frac{k\pi}{1+1/(2N)}\right)}{\sin\left(\frac{k\pi}{N+1/2}\right)} \frac{\omega c}{\nu_k^2 - \omega^2} \right)^2 + \frac{1}{4} \sum_{k=1}^{N} \frac{1}{(h_k, h_k)^2} \frac{\sin^2\left(\frac{k\pi}{1+1/(2N)}\right)}{\sin^2\left(\frac{k\pi}{N+1/2}\right)} \left(\frac{\omega c}{\nu_k^2 - \omega^2} \right)^2, \tag{5.14}$$

$$\langle T_N \rangle = \frac{1}{4} \left(\sum_{k=1}^{N} \frac{1}{(h_k, h_k)} \frac{\sin^2\left(\frac{k\pi}{1+1/(2N)}\right)}{\sin^2\left(\frac{k\pi}{N+1/2}\right)} \frac{\omega c}{\nu_k^2 - \omega^2} \right)^2 + \frac{1}{4} \sum_{k=1}^{N} \frac{1}{(h_k, h_k)^2} \frac{\sin^4\left(\frac{k\pi}{1+1/(2N)}\right)}{\sin^4\left(\frac{k\pi}{N+1/2}\right)} \left(\frac{\omega c}{\nu_k^2 - \omega^2} \right)^2, \tag{5.15}$$

where

$$\nu_k^2 = 2\omega_1^2 \left(\cos\left(\frac{\pi k}{N+1/2} \right) + 1 \right), \quad k = 1, \dots, N,$$

$$(h_k, h_k) = \sin^{-2}\left(\frac{k\pi}{N+1/2} \right) \sum_{j=1}^{N} \sin^2\left(\frac{jk\pi}{N+1/2} \right), \quad k = 1, \dots, N.$$

Note that as $N \to \infty$

$$\frac{k\pi}{N} \sum_{j=1}^{N} \sin^2\left(\frac{jk\pi}{N+1/2} \right) \sim \frac{k\pi}{N} \sum_{j=1}^{N} \sin^2\left(\frac{jk\pi}{N} \right) \to \int_0^{k\pi} \sin^2 u du = k \int_0^{\pi} \sin^2 u du = \frac{k\pi}{2}.$$

It follows

$$\sum_{j=1}^{N} \sin^2\left(\frac{jk\pi}{N+1/2} \right) \sim \frac{N}{2}, \quad N \to \infty. \tag{5.16}$$

Consider the first term in (5.14)

$$I_1 = \sum_{k=1}^{N} \frac{1}{(h_k, h_k)} \frac{\sin\left(\frac{k\pi}{1+1/(2N)}\right)}{\sin\left(\frac{k\pi}{N+1/2}\right)} \frac{\omega c}{\nu_k^2 - \omega^2} =$$

$$= \sum_{k=1}^{N} \frac{\sin\left(\frac{k\pi}{N+1/2}\right)}{\sum_{j=1}^{N} \sin^2\left(\frac{jk\pi}{N+1/2}\right)} \sin\left(\frac{k\pi}{1+1/(2N)}\right) \frac{\omega c}{\nu_k^2 - \omega^2}.$$

Since

$$\sin\left(\frac{k\pi}{1+1/(2N)}\right) = (-1)^{k-1}\frac{k\pi}{2N} + O(N^{-3}) \tag{5.17}$$

we have

$$I_1 \sim S = -\frac{1}{\pi}\sum_{k=1}^{N} \frac{\pi}{N}(-1)^k \frac{k\pi}{N} \sin\left(\frac{k\pi}{N}\right) \frac{\omega c}{2\omega_1^2\left(\cos\left(\pi k/N\right)+1\right) - \omega^2}.$$

Firstly, we sum up separately in even and odd k. That is, we can write

$$S = S_1 + S_2,$$

where

$$S_1 = -\frac{1}{2\pi}\sum_{k=1}^{[N/2]} \frac{2\pi}{N}\frac{2k\pi}{N} \sin\left(\frac{2k\pi}{N}\right) \frac{\omega c}{2\omega_1^2\left(\cos\left(2\pi k/N\right)+1\right) - \omega^2},$$

$$S_2 = \frac{1}{2\pi}\sum_{k=1}^{[N/2]} \frac{2\pi}{N}\frac{(2k+1)\pi}{N} \sin\left(\frac{(2k+1)\pi}{N}\right) \frac{\omega c}{2\omega_1^2\left(\cos\left((2k+1)\pi/N\right)+1\right) - \omega^2}.$$

As $N \to \infty$

$$S_1 \to -\frac{1}{\pi}\int_0^{\pi} \frac{u \sin u \, du}{2\omega_1^2\left(\cos u + 1\right) - \omega^2},$$

$$S_2 \to \frac{1}{\pi}\int_0^{\pi} \frac{u \sin u \, du}{2\omega_1^2\left(\cos u + 1\right) - \omega^2}.$$

Then, $I_1 \to 0$. Thus the first term in (5.14) tends to 0.

Consider now the first term in (5.15)

$$I_2 = \sum_{k=1}^{N} \frac{1}{(h_k, h_k)} \frac{\sin^2\left(\frac{k\pi}{1+1/(2N)}\right)}{\sin^2\left(\frac{k\pi}{N+1/2}\right)} \frac{\omega c}{\nu_k^2 - \omega^2} =$$

$$= \sum_{k=1}^{N} \frac{\sin^2\left(\frac{k\pi}{1+1/(2N)}\right)}{\sum_{j=1}^{N}\sin^2\left(\frac{jk\pi}{N+1/2}\right)} \frac{\omega c}{\nu_k^2 - \omega^2}.$$

According to (5.16) and (5.17)

$$I_2 \sim \frac{1}{\pi}\sum_{k=1}^{N} \frac{\pi}{N}\left(\frac{k\pi}{N}\right)^2 \frac{\omega c}{2\omega_1^2\left(\cos\left(\pi k/N\right)+1\right)-\omega^2}$$

as $N \to \infty$. Thus

$$I_2 \to \frac{c}{\pi}\int_0^\pi \frac{u^2\,du}{2\omega_1^2\left(\cos u+1\right)-\omega^2}.$$

The integral is not 0, as the integrand has constant sign.

It is not difficult to show that the second terms in (5.14) and in (5.15) tend to 0. Finally, we get

$$\langle T_N\rangle \to \frac{c^2}{4\pi^2}\left(\int_0^\pi \frac{u^2\,du}{2\omega_1^2\left(\cos u+1\right)-\omega^2}\right)^2, \quad \langle T_1\rangle \to 0.$$

5.4. Potential energy

We define potential energy of the particle j

$$\langle U_j\rangle = \frac{\omega_1^2}{4}\left(\langle (q_j - q_{j-1})^2\rangle + \langle (q_{j+1}-q_j)^2\rangle\right)$$

for $j = 2, \ldots, N-1$. Here $1/4$ appears because we take only half of the interaction energy of the particle j with its neighbors.

For $j = 1, N$ we have:

$$\langle U_1\rangle = \frac{\omega_1^2}{2}\langle q_1^2\rangle + \frac{\omega_1^2}{4}\langle (q_2-q_1)^2\rangle,$$

$$\langle U_N\rangle = \frac{\omega_1^2}{4}\langle (q_N - q_{N-1})^2\rangle - c\langle q_N \sin\omega t\rangle.$$

Theorem 5.3. *Assume that* $\omega^2 > 4\omega_1^2$. *Then the following limits exist*

$$\lim_{N\to\infty}\langle U_1\rangle = 0,$$

$$\lim_{N\to\infty}\langle U_N\rangle = \frac{1}{2}\left(\frac{\omega_1}{\pi}\int_0^\pi \frac{cu^2\,du}{2\omega_1^2\left(\cos u+1\right)-\omega^2}\right)^2 - \frac{1}{4\pi}\int_0^\pi \frac{cu^2\,du}{2\omega_1^2\left(\cos u+1\right)-\omega^2} > 0.$$

Proof. Using

$$q_j(t) = \sum_{k=1}^{N} (g_k, e_N)(g_k, e_j)\hat{q}_k(t)$$

where

$$\hat{q}_k(t) = \frac{c\omega}{\nu_k^2 - \omega^2} \left(\frac{\sin(\omega t)}{\omega} - \frac{\sin(\nu_k t)}{\nu_k} \right)$$

we get

$$\langle U_1 \rangle = \frac{\omega_1^2}{2} \sum_{k,l=1}^{N} (g_k, e_N)(g_l, e_N)(g_k, e_1)(g_l, e_1)\langle \hat{q}_k(t)\hat{q}_l(t)\rangle +$$

$$+\frac{\omega_1^2}{4} \sum_{k,l=1}^{N} (g_k, e_N)(g_l, e_N)((g_k, e_2) - (g_k, e_1))((g_l, e_2) - (g_l, e_1))\langle \hat{q}_k(t)\hat{q}_l(t)\rangle,$$

where

$$\langle \hat{q}_k(t)\hat{q}_l(t)\rangle = \begin{cases} \frac{A_k^2}{2}\left(\omega^{-2} + \nu_k^{-2}\right) & k = l, \\ \frac{A_k A_l}{2\omega^2} & k \neq l. \end{cases}$$

In fact, in more details

$$\begin{aligned} \langle \hat{q}_k^2(t)\rangle &= A_k^2 \Big\langle \Big(\frac{\sin(\omega t)}{\omega} - \frac{\sin(\nu_k t)}{\nu_k} \Big)^2 \Big\rangle \\ &= A_k^2 \Big(\frac{1}{\omega^2} \langle \sin^2(\omega t)\rangle + \frac{1}{\nu_k^2} \langle \sin^2(\nu_k t)\rangle \Big) \\ &= \frac{A_k^2}{2}\left(\omega^{-2} + \nu_k^{-2}\right) \end{aligned}$$

and for $k \neq l$

$$\begin{aligned} \langle \hat{q}_k(t)\hat{q}_l(t)\rangle &= A_k A_l \Big\langle \Big(\frac{\sin(\omega t)}{\omega} - \frac{\sin(\nu_k t)}{\nu_k} \Big)\Big(\frac{\sin(\omega t)}{\omega} - \frac{\sin(\nu_l t)}{\nu_l} \Big) \Big\rangle \\ &= \frac{A_k A_l}{\omega^2} \langle \sin^2(\omega t)\rangle = \frac{A_k A_l}{2\omega^2}. \end{aligned}$$

Finally we get

$$\langle U_1 \rangle = \frac{\omega_1^2}{4\omega^2} \sum_{k,l=1}^{N} (g_k, e_N)(g_l, e_N)(g_k, e_1)(g_l, e_1)A_k A_l +$$

$$+\frac{\omega_1^2}{4} \sum_{k,l=1}^{N} (g_k, e_N)^2 (g_k, e_1)^2 \frac{A_k^2}{\nu_k^2} +$$

$$+\frac{\omega_1^2}{8\omega^2}\sum_{k,l=1}^{N}(g_k,e_N)(g_l,e_N)((g_k,e_2)-(g_k,e_1))((g_l,e_2)-(g_l,e_2))A_kA_l+$$

$$+\frac{\omega_1^2}{8}\sum_{k=1}^{N}(g_k,e_N)^2((g_k,e_2)-(g_k,e_1))^2\frac{A_k^2}{\nu_k^2}=$$

$$=\frac{\omega_1^2}{4\omega^2}\left(\sum_{k=1}^{N}(g_k,e_N)(g_k,e_1)A_k\right)^2+\frac{\omega_1^2}{4}\sum_{k,l=1}^{N}(g_k,e_N)^2(g_k,e_1)^2\frac{A_k^2}{\nu_k^2}+$$

$$+\frac{\omega_1^2}{8\omega^2}\left(\sum_{k=1}^{N}(g_k,e_N)((g_k,e_2)-(g_k,e_1))A_k\right)^2+$$

$$+\frac{\omega_1^2}{8}\sum_{k,l=1}^{N}(g_k,e_N)^2((g_k,e_2)-(g_k,e_1))^2\frac{A_k^2}{\nu_k^2}.$$

Using formula (5.12) for (g_k,e_j), we get

$$\langle U_1\rangle=\frac{\omega_1^2}{4\omega^2}\left(\sum_{k=1}^{N}\frac{1}{(h_k,h_k)}\frac{\sin\left(\frac{Nk\pi}{N+1/2}\right)}{\sin\left(\frac{k\pi}{N+1/2}\right)}\frac{c\omega}{\nu_k^2-\omega^2}\right)^2+$$

$$+\frac{\omega_1^2}{4}\sum_{k=1}^{N}\frac{1}{(h_k,h_k)^2}\frac{\sin^2\left(\frac{Nk\pi}{N+1/2}\right)}{\sin^2\left(\frac{k\pi}{N+1/2}\right)}\left(\frac{c\omega}{\nu_k\left(\nu_k^2-\omega^2\right)}\right)^2+$$

$$+\frac{\omega_1^2}{8\omega^2}\left(\sum_{k=1}^{N}\frac{1}{(h_k,h_k)}\frac{\sin\left(\frac{Nk\pi}{N+1/2}\right)\left(-\sin\left(\frac{2k\pi}{N+1/2}\right)-\sin\left(\frac{k\pi}{N+1/2}\right)\right)}{\sin^2\left(\frac{k\pi}{N+1/2}\right)}\frac{c\omega}{\nu_k^2-\omega^2}\right)^2+$$

$$+\frac{\omega_1^2}{8}\sum_{k=1}^{N}\frac{1}{(h_k,h_k)^2}\frac{\sin\left(\frac{Nk\pi}{N+1/2}\right)^2\left(\sin\left(\frac{2k\pi}{N+1/2}\right)+\sin\left(\frac{k\pi}{N+1/2}\right)\right)^2}{\sin^4\left(\frac{k\pi}{N+1/2}\right)}\times$$

$$\times\left(\frac{c\omega}{\nu_k\left(\nu_k^2-\omega^2\right)}\right)^2.$$

Now we can prove that $\langle U_1\rangle\to 0$ as $N\to\infty$, similarly to the proof of the fact that $\langle T_1\rangle\to 0$ in the Theorem 5.2.

Now we find

$$\langle(q_N(t)-q_{N-1}(t))^2\rangle=\left(\frac{1}{2\omega^2}\sum_{k=1}^{N}(g_k,e_N)((g_k,e_N)-(g_k,e_{N-1}))\frac{c\omega}{\nu_k^2-\omega^2}\right)^2+$$

$$+\frac{1}{2}\sum_{k=1}^{N}(g_k,e_N)^2((g_k,e_N)-(g_k,e_{N-1}))^2\left(\frac{c\omega}{\nu_k\,(\nu_k^2-\omega^2)}\right)^2,$$

and using (5.12), we find

$$\langle (q_N(t)-q_{N-1}(t))^2\rangle =$$

$$=\frac{1}{2\omega^2}\left(\sum_{k=1}^{N}\frac{1}{(h_k,h_k)}\frac{\sin\left(\frac{k\pi}{1+1/(2N)}\right)}{\sin^2\left(\frac{k\pi}{N+1/2}\right)}\times\right.$$

$$\left.\times\left(\sin\left(\frac{k\pi}{1+1/(2N)}\right)+\sin\left(\frac{k\pi}{1+3/(2(N-1))}\right)\right)\frac{c\omega}{\nu_k^2-\omega^2}\right)^2+$$

$$+\frac{1}{2}\sum_{k=1}^{N}\frac{1}{(h_k,h_k)^2}\frac{\sin^2\left(\frac{k\pi}{1+1/(2N)}\right)\left(\sin\left(\frac{k\pi}{1+1/(2N)}\right)+\sin\left(\frac{k\pi}{1+3/(2(N-1))}\right)\right)^2}{\sin^4\left(\frac{k\pi}{N+1/2}\right)}\times$$

$$\times\left(\frac{c\omega}{\nu_k\,(\nu_k^2-\omega^2)}\right)^2.$$

Denote by J_1 and J_2 correspondingly the first and second terms in the last expressions.

Using formulas (5.16), (5.17) we get that as $N\to\infty$,

$$J_1\sim\frac{2}{\omega^2\pi^2}\left(\sum_{k=1}^{N}\frac{\pi}{N}\,(k\pi/N)^2\,\frac{c\omega}{2\omega_1^2\,(\cos{(\pi k/N)}+1)-\omega^2}\right)^2\to$$

$$\to 2\left(\frac{1}{\pi}\int_0^{\pi}\frac{cu^2\,du}{2\omega_1^2\,(\cos u+1)-\omega^2}\right)^2.$$

Similarly to Theorem 5.2 one can show that $J_2\to 0$.

We should find also the mean value

$$\langle q_N\sin\omega t\rangle=\sum_{k=1}^{N}(g_k,e_N)^2\langle\hat{q}_k(t)\sin\omega t\rangle=\frac{1}{2}\sum_{k=1}^{N}(g_k,e_N)^2\frac{c}{\nu_k^2-\omega^2}=$$

$$=\frac{1}{2}\sum_{k=1}^{N}\frac{1}{(h_k,h_k)}\frac{\sin^2\left(\frac{k\pi}{1+1/(2N)}\right)}{\sin^2\left(\frac{k\pi}{N+1/2}\right)}\frac{c}{\nu_k^2-\omega^2}.$$

Then quite similarly as for J_1 we get that, as $N\to\infty$,

$$\langle q_N\sin\omega t\rangle\sim\frac{1}{2\pi}\sum_{k=1}^{N}\frac{2\pi}{N}\left(\frac{k\pi}{2N}\right)^2\frac{c}{2\omega_1^2\,(\cos{(\pi k/N)}+1)-\omega^2}$$

$$\to \frac{c}{4\pi}\int_0^\pi \frac{u^2\,du}{2\omega_1^2(\cos u+1)-\omega^2}$$

and finally

$$\langle U_N\rangle \to \frac{1}{2}\left(\frac{\omega_1}{\pi}\int_0^\pi \frac{cu^2\,du}{2\omega_1^2(\cos u+1)-\omega^2}\right)^2 - \frac{1}{4\pi}\int_0^\pi \frac{cu^2\,du}{2\omega_1^2(\cos u+1)-\omega^2}$$

as $N\to\infty$.

5.5. Conservation of initial order of particles (no collisions)

Assume that initial conditions are $q_j(0)=0 \Longleftrightarrow x_j(0)=ja, v_j(0)=0$.

If $\omega^2 > 4\omega_1^2$ (in particular, no resonance), then we will show that, if the constant c is sufficiently small with respect to a, for any t the initial order will not change, that is there will not be collisions of particles, that is

$$x_1(t) < x_2(t) < \ldots < x_N(t).$$

By (5.10)

$$|\hat{q}_k(t)| \le \frac{c\omega}{\omega^2-\nu_k^2}\left(\frac{1}{\omega}+\frac{1}{\nu_k}\right) = cb_k.$$

As $\omega^2 > 4\omega_1^2$ the constants $b_k>0$, as $\nu_k^2 < 4\omega_1^2$. Then using (5.11) we get

$$|q_j(t)| \le c\sum_{k=1}^N |(g_k,e_N)(g_k,e_j)|b_k.$$

By (5.12)

$$|(g_k,e_N)(g_k,e_j)| = \frac{1}{(h_k,h_k)}\frac{\left|\sin\left(\frac{Nk\pi}{N+1/2}\right)\sin\left(\frac{jk\pi}{N+1/2}\right)\right|}{\sin^2\left(\frac{k\pi}{N+1/2}\right)}$$
$$\le \frac{1}{(h_k,h_k)}\frac{\left|\sin\left(\frac{k\pi}{1+1/(2N)}\right)\right|}{\sin^2\left(\frac{k\pi}{N+1/2}\right)}.$$

Further, using (5.16), (5.17), we get

$$|q_j(t)| \le \frac{cB}{N^2}\sum_{k=1}^N b_k = \frac{cB}{N^2}\sum_{k=1}^N\left(\frac{1}{\omega^2-\nu_k^2}+\frac{1}{\nu_k}\right) \tag{5.18}$$

for some constant $B>0$. Since $\omega^2-\nu_k^2 > \omega^2-4\omega_1^2>0$, we have

$$\frac{1}{N^2}\sum_{k=1}^N\frac{1}{\omega^2-\nu_k^2} \le \frac{1}{N}\frac{1}{\omega^2-4\omega_1^2} \to 0, \quad N\to\infty.$$

Finally, from $\nu_1 > \nu_2 > \ldots > \nu_N$, where

$$\nu_k^2 = 2\omega_1^2 \left(\cos\left(\frac{\pi k}{N+1/2} \right) + 1 \right), \quad k = 1, \ldots, N,$$

it follows

$$\sum_{k=1}^{N} \frac{1}{\nu_k} \leq \frac{N}{\nu_N}.$$

Note that

$$\cos\left(\frac{\pi N}{N+1/2} \right) + 1 = O(N^{-2}).$$

Hence, $\nu_N^{-1} = O(N)$ and

$$\sum_{k=1}^{N} \frac{1}{\nu_k} = O(N^2).$$

So the right hand side of the inequality (5.18) is equal to $O(1)$ as $N \to \infty$.

It follows that one can choose parameters c and a so that for all N

$$|q_j(t)| < \frac{a}{2}, \quad j = 1, \ldots, N.$$

Another case was considered in [15], where frequencies and constant a are scaled so that this property (called regularity in [16]) holds for all N.

6. Conclusion

In all examples of ground states above, it can be easily proved that for the system of equations

$$\frac{d^2 x_k(t)}{dt^2} = F_k - \alpha_k v_k(t), \quad k = 0, 1, \ldots, N, \tag{6.1}$$

where $v_k = dx_k/dt$ and $\alpha_k \geq \alpha$ for some $\alpha > 0$, the following statement holds: for any initial conditions $x_k(0), v_k(0)$ the solution converges to the corresponding minimum of potential energy. The proof is exactly the same as in ([10]) for Coulomb systems. More difficult is the question whether it is true when some $\alpha_k = 0$.

One of the next problems is the following. Assume that we define the system to be "healthy" if the configuration is close to the ground state in l_1-metrics that is if for some $\varepsilon > 0$ and all k we have $|x_k(t) - a| < \varepsilon$. The question is the following: is this domain invariant w.r.t. dynamics (6.1), or some differences $|x_k(t) - x_{k-1}(t)|$ between nearest neighbors can become too small (or even collide) or can become "too big". Obviously, it is for the scaled parameters for which the ground state satisfies condition $x_0 < x_1 < \ldots < x_N$.

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