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Asymptotically Solid Systems of Point Particles

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Abstract. We define a solid N-particle system with the fixed distances $r(i,j) = c(i,j)$ between any two particles i and j. Its dynamics is defined as the limit of the dynamics for the system where the Hamiltonian is the sum of the terms $w^2(r(i,j) - c(i,j))^2$ as w^2 tends to infinity. Three concrete examples are considered.

Keywords: point particles, solid collection, hamiltonian systems, dynamical equations

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1. Introduction

We call a collection (system) of point particles $x_1(t), \ldots, x_N(t) \in R^d$ a *solid collection* if the distances $\rho(x_i(t), x_j(t)) = |x_i(t) - x_j(t)|$ between any two particles remain fixed forever. One can define dynamics for such collection similar to Euler equations for ideal solids. If the density of particles tends to infinity then it could be the natural model for real solid. Obviously, such systems cannot be Newtonian or Hamiltonian without introducing forces of infinite strength. Our goal is to deduce dynamical equations for solid particle collections from Newtonian point particle dynamics. For this we use a weaker notion – asymptotically (with respect to some parameter ω in the interaction potential) solid systems of point particles where $\rho(x_i(t), x_j(t))$ tend to some constants r_{ij} as $\omega \to \infty$.

2. 1-dim two-particle problem

Two point particles with masses m_1, m_2 and Hamiltonian

$$H = \frac{m_1 v_1^2}{2} + \frac{m_2 v_2^2}{2} + \frac{\omega^2}{2}(x_1 - x_2 - a)^2 + U(x_2)$$

where $a > 0$. We consider the simplest case when $U = -Fx_2$ with constant $F > 0$. The equations are

$$m_1 \frac{d^2 x_1}{dt^2} = -\omega^2(x_1 - x_2 - a),$$

$$m_2 \frac{d^2 x_2}{dt^2} = \omega^2(x_1 - x_2 - a) + F.$$

Introduce a new variable $y = m_1 x_1 + m_2 x_2$. The sum of two equations gives

$$\ddot{y} = F \implies y = y(0) + \dot{y}(0)t + F\frac{t^2}{2},$$

that is, y moves as particle of mass 1. And the mass center

$$X = \frac{y}{m_1 + m_2} = \frac{m_1 x_1 + m_2 x_2}{m_1 + m_2}$$

moves as the particle of mass $M = m_1 + m_2$. This is of course quite known even for more general particle systems.

Now we should understand the motion of $z = x_1 - x_2 - a$.

Proposition 1. *Let $z(\omega, t)$ be the trajectory of z with initial conditions $z(0) - 0, \dot{z}(0) = v_0$. Then for fixed v_0, F, m_1, m_2, a, as $\omega \to \infty$,*

$$|z(\omega, t)| \to 0$$

uniformly in t.

That is, in this limit the distance

$$\rho(x_1 - x_2) = |x_1 - x_2|$$

does not change at all, despite the constant force F, only the center of mass moves.

Proof. We have

$$\ddot{z} = -\omega^2\Big(\frac{1}{m_1} + \frac{1}{m_2}\Big)z - \frac{F}{m_2} = -k^2 z - \frac{F}{m_2}$$

where

$$k^2 = \omega^2\Big(\frac{1}{m_1} + \frac{1}{m_2}\Big).$$

The general solution is

$$z = -\frac{F}{m_2 k^2} + C_1 \cos kt + C_2 \sin kt$$

where

$$C_1 = \frac{F}{m_2 k^2}, \quad C_2 = \frac{v(0)}{k} \Longrightarrow z = \frac{F}{m_2 k^2}(\cos kt - 1) + \frac{v(0)}{k} \sin kt. \qquad (1)$$

The proposition follows as $k \to \infty$. □

Note that for large ω^2 the particles never collide. That is, if for example $x_1(0) > x_2(0)$, equation (1) gives conditions for no collision, i.e. $x_1(t) > x_2(t) \Longleftrightarrow z(t) > -a$ for all $t > 0$.

3. Restricted two particle problem in R^2

Here one particle is fixed at 0 and the second with coordinates $x = (x_1, x_2)$ moves in the shifted quadratic potential and constant force $F = (f_1, f_2)$

$$U(x) = \frac{\omega^2}{2}(r - a)^2 - (F, x), r = \sqrt{x_1^2 + x_2^2}.$$

Equations (nonlinear) are (we take $m = 1$)

$$\ddot{x}_1 = -\omega^2(x_1 - a\frac{x_1}{\sqrt{x_1^2 + x_2^2}}) + f_1,$$

$$\ddot{x}_2 = -\omega^2(x_2 - a\frac{x_2}{\sqrt{x_1^2 + x_2^2}}) + f_2.$$

Remak 1. One can easily check that for $F = 0$ one of the possible solutions is

$$x_1(t) = R\cos\omega_0 t, x_2 = R\sin\omega_0 t$$

for any fixed $R \geq a$ and

$$-\omega_0^2 = -\omega^2\Big(1 - \frac{a}{R}\Big) \Longrightarrow \omega_0 = \omega\sqrt{1 - \frac{a}{R}}.$$

Note that if we choose R close to a, then ω_0 will be much less than ω. For $R = a$ there will not be rotation, that is the particle will not move at all. Note that $R < a$ is impossible as there will not be balancing centrifugal force.

To get a wider class of solutions we will use conservation of energy H and of kinetic momentum $L = [x, p]$.

In polar coordinates

$$v = (\dot{r}\cos\phi - r\dot{\phi}\sin\phi, \dot{r}\sin\phi + r\dot{\phi}\cos\phi).$$

Then

$$\frac{m}{2}v^2 = \frac{m}{2}\Big(\Big(\frac{dr}{dt}\Big)^2 + r^2\Big(\frac{d\phi}{dt}\Big)^2\Big),$$

$$\begin{aligned}\frac{L}{m} &= [x, v] = x_1 v_2 - x_2 v_1 \\ &= r\cos\phi\dot{r}\sin\phi + r^2\dot{\phi}\cos^2\phi - \dot{r}\cos\phi r\sin\phi + r^2\dot{\phi}\sin^2\phi = r^2\dot{\phi},\end{aligned}$$

It follows that

$$\begin{aligned}H(t) &= \frac{m}{2}v^2 + U = \frac{m}{2}\Big(\frac{dr}{dt}\Big)^2 + \frac{m}{2}r^2\Big(\frac{d\phi}{dt}\Big)^2 + \frac{\omega^2}{2}(r-a)^2 - (F, x) \\ &= \frac{m}{2}\Big(\frac{dr}{dt}\Big)^2 + \frac{L^2(0)}{2mr^2} + \frac{\omega^2}{2}(r-a)^2 - (F, x).\end{aligned}$$

Then

$$H(0) = \frac{m}{2}\Big(\frac{dr}{dt}\Big)^2 + \frac{L^2(0)}{2mr^2} + \frac{\omega^2}{2}(r-a)^2 - (F, x).$$

It follows that for $R(t) = r(t) - a$ we have

$$H(0) + (F, x) - \frac{\omega^2}{2}(r(t) - a)^2 \geq 0 \Longrightarrow R^2(t) \leq \frac{2(H(0) + (F, x))}{\omega^2}.$$

Proposition 2. *For any initial conditions the particle, for sufficiently large ω stays always in a narrow ring, around the circle $r = a$. The width of this ring tends to 0 as $\omega \to \infty$.*

Proof. If $||x|| < 2a$ we use the last inequality. If $||x|| \geq 2a$ then $|R| \geq a$ and $R^{-1}||x|| < 2$ and we can use inequality

$$|R(t)| \leq \frac{2(H(0) + (F, x))}{\omega^2 |R|}.$$

If $F = 0$ then we get the following first order equation for $r(t)$, or for $R(t) = r(t) - a$,

$$\frac{dR}{dt} = \sqrt{\frac{2H(0)}{m} - \frac{\omega^2}{m}R^2 - \frac{L^2(0)}{2m(a+R)^2}}. \tag{1}$$

After solving this equation, we get the first order equation for $\phi(t)$

$$\dot{\phi} = \frac{L(0)}{m(a + R(t))^2} \Longrightarrow \phi(t) = \phi(0) + \frac{L(0)}{m}\int_0^t (a + R(t))^{-2} dt. \tag{2}$$

In particular, if $r(0) = a$, then $\phi(t) = \omega_0 t$, where $\omega_0 = L(0)r^{-2}$. □

From all this the following statement follows.

We would like to get limiting Euler equations for this model. To do this for the point $(x, y) = (r, \varphi)$ denote by $n_1(x, y) = n_1(r, \varphi)$ the unit vector parallel to vector r and $n_2(x, y) = n_2(r, \varphi)$ the unit tangent vector perpendicular to vector r at the point (r, φ). Then for any (r, φ) vector F will be the sum of two vectors: $P_{r,\varphi} = (F, n_1(r, \varphi))n_1(r, \varphi)$ and $T_{r,\varphi} = (F, n_2(r, \varphi))n_2(r, \varphi)$. Then the components $r(t)$ and $\varphi(t)$ satisfy the system of differential equations

$$\ddot{r}(t) = -\omega^2(r - a) + (F, n_1(r, \varphi)),$$
$$\ddot{\varphi}(t) = (F, n_2(r, \varphi)).$$

And the limiting equations will be

$$r(t) \equiv a,$$
$$\ddot{\varphi} = (F, n_2(r, \varphi)).$$

4. *N*-particles in dim 1

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

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

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

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

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, ∞) and has the unique minimum $V(a) < 0$ at some $a > 0$, where $a < b < \infty$.

4.1. Equilibrium stability

Fixed points For quadratic Hamiltonian

$$V(z) = \frac{\omega^2}{2}(z - a)^2$$

fixed point always exists and is unique, and moreover for any ω^2 the distances $z_k - z_{k-1} = h = a + \sigma$, where

$$\sigma = \frac{f}{\omega^2}.$$

That is why the static phase transition is as follows: $h/a \to \infty$ if $\sigma N \to \infty$, and $h/a \to 1$ if $\sigma N \to 0$. We will see that static and dynamic phase transition differ only by logarithmic factor.

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

$$V(r) = -\frac{c_n}{r^n} + \frac{c_m}{r^m}. \tag{3}$$

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 $\max_{a<h\leq b} dV(h)/dh \geq f$ then the Hamiltonian (2) has the unique minimum, for which all $z_k - z_{k-1} = h > a > 0$, and the value h is defined from the equation

$$\frac{dV(h)}{dh} = f. \tag{4}$$

But if $\max_{a<h\leq b} dV(h)/dh < f$, 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 (3).

Proposition 3. *If $a = 1/N$, then a fixed point exists iff*

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

where

$$\kappa = V''(a),$$
$$C = C(n,m) = \frac{1}{m-n}\left(\left(\frac{m+1}{n+1}\right)^{-(n-1)/(m-n)} - \left(\frac{m+1}{n+1}\right)^{-(m-1)/(m-)n}\right).$$

Non-zero temperature For non-zero temperature fixed point becomes Gibbs distribution. 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].

4.2. Dynamical stability

Now we will consider the dynamics of this particle system and get estimates for the functional

$$A = A(N, l, f, \omega^2, m) = \max_{1\leq k, k+l \leq N-1} \sup_{t\in(0,\infty)} |z_{k+l}(t) - z_k(t)| \tag{5}$$

for large N and various $l > 0$. In despite of apparent simplicity of the quadratic interaction, the main result of the paper – estimates for the maximal (over all time interval) deviations from the initial crystal structure are nontrivial and use some facts from number theory. The question is that, although the model has a simple fixed point, but as the model is Hamiltonian, then there is no any convergence to this fixed point.

We consider finite number N of particles and find the neighborhood which the trajectory never leaves. Then in the limit $N \to \infty$. we find the phase transition using scaling of the parameters, for which the crystal structure changes only slightly on all time interval, and the scaling for which this supremum grows with N.

We want to note that there are many papers concerning other problems for one-dimensional models. Most popular are the Fermi – Pasta – Ulam models [5] and the Frenkel – Kontorova model [6].

Defining the deviations $x_k(t) = z_k(t) - ka, k = 0, \ldots, N-1$, we have the following Hamiltonian system of linear equations (assuming $m = 1$)

$$\begin{cases} \ddot{x}_0(t) = 0, \\ \ddot{x}_k(t) = \omega^2(x_{k-1} - 2x_k + x_{k+1}), & k = 1, \ldots, N-2, \\ \ddot{x}_{N-1}(t) = \omega^2(-x_{N-2} + x_{N-1}) + f, \end{cases} \tag{6}$$

with initial data (1) and $v_k(0) = \dot{x}_k(0) = 0,\ k = 1, \ldots, N-1$.

Introduce the following auxiliary function

$$F_N(x) = x \ln \frac{N}{x},\ x > 0. \tag{7}$$

Let us agree that the constants denoted further by $c, c_i, const$, do not depend on N, l, f, ω 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*

$$0 \le k < k + l \le (1-\varepsilon)N, \tag{8}$$

the following inequalities hold

$$\sigma(l + c_1 F_N(l)) \le \sup_{t \ge 0} (x_{k+l}(t) - x_k(t)) \le \sigma(l + c_2 F_N(l)), \tag{9}$$

$$\sigma(l - c_3 F_N(l)) \le \inf_{t \ge 0} (x_{k+l}(t) - x_k(t)) \le \sigma(l - c_4 F_N(l)) \tag{10}$$

for some $c_1, c_2, c_3, c_4 > 0$, where c_1, c_3 may depend on ε.

See these results and proofs in [1].

Further on we use the procedure, called in physics “double scaling limit”. Namely, we put $a = 1/N$ 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 Λ, if there exist such $c_1, c_2 > 0$, that on all domain of definition $c_1 g(x) \leq f(x) \leq c_2 g(x)$.

Corollary 1. *Under the conditions of Theorem 1*

$$|x_{k+l}(t) - x_k(t)| \simeq \sigma(N) l \ln \frac{N}{l}.$$

As the indicator of the 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 $\sigma < c/(N \ln N)$ for sufficiently small $c > 0$, then the distances will never leave some neighborhood $\big((1-\varepsilon)/N, (1+\varepsilon)/N\big)$ of $1/N$.

Again we get that for $\omega^2 \to \infty$ we have a solid collection of particles.

5. Conclusion

So, we saw that asymptotically solid collection of point particles can be defined by various types of interaction Hamiltonian. Further plans in this direction could be to use this micro approach to such macro sciences as elasticity and plasticity of solid matter, or even to soft matter.

The simplest gas collection can be defined, for example, by repulsive potential with small finite support: $V(|x_i - x_j|) = \infty$ if $|x_i - x_j| < \varepsilon$. Or, by quite general potential where the particles cannot collide. For example, potential $V(|x_i - x_j|)$ with quadratic minimum at $|x_i - x_j| = a$, as it was done for derivation of Euler equations for Chaplygin gas, see [4].

What is necessary to do now: 1) find models of "asymptotically liquid" particle systems, 2) to have complete review of rigorous results and non-rigorous ideas concerning point particle models of continuum mechanics – possible starting papers for such report are [3,5–18].

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