Emergence of sub-micro-scales in many particle Hamiltonian systems

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Introduction Mathematical statistical physics of the last 50-60 years may be characterized by tight connection with physics itself and with many classical fields of mathematics. Its main goal was to study and develop various models, describing qualitatively what occurs in nature, although most of them cannot be readily applied in experimental physics. Even more ambitious goal could be to verify the logical structure of physics, that is to construct models based on basic physical laws.

Lattice models of statistical physics prevailed, both with fixed lattice spacing and/or various scaling limits (for example, euclidean field theory). As a result, many problems of lattice statistical mechanics are now well understood. Second direction of research was statistical physics of point particles in R^d. It described gaseous phases, based on the ideas of Boltzmann and Gibbs, in both equilibrium and non-equilibrium aspects (with classical Hamiltonian or quantum dynamics).

However, for other physical media, there are still many unsolved fundamental problems. First example are gases with chemical reactions. Here even the basic molecular dynamics is poorly understood. Normally it is taken to be a mixture of Hamiltonian dynamics and random reactions. This field has now very limited results (see [10, 9]), because random dynamics does not belong to the basic physical laws, rather it should be deduced from them (which had never been done). Also, condensed matter (without apriori fixed lattice spaceing), and even more liquids, are still lacking mathematically rigorous description based on the basic physical laws. However, crystalline classical ground states were intensively studied, see [1]-[7]). The problem however is that condensed matter should be considered as a metastable state at any nonzero temperature, and liquids possibly have metastable clusters on various space and time scales (that is even more difficult to describe than chemical reactions between stable particles).

There is however one more problem to which I refer in this note. In mathematical physics papers, two scales are normally present (explicitly or not) - macro scale and micro scale. Micro scales depend on the model, but normally they are characterized by $\frac{|\Lambda|}{N}$ where Λ is the volume and N is the number of particles. It is a folklore, or even some philosophical principle, that all macro phenomena can be deduced from the behaviour of micro-variables on the corresponding scale. I want to show here that it is not always the case.

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Already Wigner in 1934 suggested that the configuration of electron gas with minimal potential energy could be a body-centered cubic lattice. We consider one-dimensional classical point particle systems with the strong Coulomb repulsion and external field. We study ground and Gibbs states on the segment and on the circle, and also Hamiltonian dynamics on the circle. Physically, first problem is how the electrons are situated on the broken circuit undet nonzero voltage, the second is a model of direct electric current. It appeared that, for example in the second cases, the effective accelerating force cannot be seen on normal microscale $\frac{1}{N}$, but is formed only on much smaller scale, of order $\frac{1}{N^2}$.

The model Consider the system

$$0 \leq x_1(t) < ... < x_N(t) < L \tag{1}$$

of identical classical point particles on the interval $[0, L]$ with periodic boundary conditions (b.c.), that is on the circle S of length L, or with completely inelastic b.c. (here one allows $x_N(t) = L$). This means that if one of the extreme particles reaches the corresponding end point of the interval, it stops and can leave this point only if the resulting force becomes directed to inside the interval.

The dynamics of this system of points is defined by the system of N equations

$$m\frac{d^2x_i}{dt^2} = -\frac{\partial U}{\partial x_i} + F(x_i) \tag{2}$$

where $F(x)$ is the external force, and the interaction for periodic b.c. is given by

$$U(x_1, ..., x_N) = V(x_2 - x_1) + V(x_3 - x_2) + ... + V(x_N - x_{N-1}) + V(x_1 - x_N)$$

where $x_1 - x_N$ should be understood as $x_1 + (L - x_N)$, otherwise speaking, For completely inelastic b.c. the term $V(x_1 - x_N)$ is excluded. It is assumed that the potential V is symmetric and repulsive (we consider in this note only Coulomb case)

$$V(x) = V(-x) > 0, V(r) = r^{-1} > 0, r = |x|$$

The interaction force then is

$$f(r) = -\frac{dV(r)}{dr} = r^{-2} > 0 \tag{3}$$

Fixed points If $F \equiv 0$, then it is evident that the fixed configuration is unique (up to translation if on the circle), and for any i

$$|x_{i+1} - x_i| = \frac{L}{N}$$

If F is not identically zero, the situation is essentially more complicated. Consider first periodic b.c. Here we have the following general result.

Theorem 1 *Let the external force $F(x)$ be any bounded function. Assume that there exists a sequence $(x_1^{(p)}, ..., x_{N_p}^{(p)}), p = 1, 2, ...,$ of fixed configurations with $N_p \to \infty$. Then for $p \to \infty$ uniformly in $i = 1, ..., N_p$*

$$|x_{i+1}^{(p)} - x_i^{(p)}| \sim \frac{L}{N_p}$$

Thus it means that F can be seen only in the second term of the expansion. In the following result the second term is explicit, and is $O(N^{-2})$.

Theorem 2 *Consider completely inelastic b.c. and assume that the external force $F > 0$ is constant. Then for sufficiently large N the fixed point $(x_1, x_2, ..., x_N)$ exists and is unique. Moreover $x_1 = 0, x_N = L$ and for any $k = 1, ..., N-1$ we have as $N \to \infty$*

$$(x_{k+1} - x_k) - \frac{L}{N-1} \sim \frac{FL^2}{2} N^{-3} (\frac{N}{2} - k)$$

Electric current We remind Ohm's law for DC (direct current)

$$U = RI$$

Microscopic picture of this law is the following. The elcctrons (having uniform density ρ) move around the circuit, accelerated by some external constant force F and slowed down by some media. Most studies in microscopic picture of Ohm's law consider one-particle problem with constant external force and various types of random media (the model of free electrons, as in all text books on condensed matter physics). If the media is such that the velocity of the particle stabilizes as $t \to \infty$ to some CONSTANT velocity $v = AF$, linearly depending on F, then the connection between macro amd micro variables of the electric current is (we do not care about the signs)

$$U = FL, I = \rho v, R = \frac{L}{\rho A}$$

However in reality the external force acts on the electrons only on a small part (battery, generator) of the circuit and equals zero on the remaining many kilometers of electric aerial lines. It follows that there should be some constant EFFECTIVE force, acting in any part of the circuit. We show that this effective force can be produced by the strong interaction between electrons and due to a specific self-organized process. We explain this on one-dimensional models of direct current.

Now we show how this problem is related to fixed points. Assume the external force $F(x)$ to be continuous (but not at all constant) on the circle $S = [0, L)$. We want to find a configuration of electrons on the circle at a given time $t = 0$ such that the EFFECTIVE force on each electron is constant, that is we want to find initial configuration of particle

$$0 \leq x_1 = x_1^{(N)} = x_1^{(N)}(0) < ... < x_N^{(N)} = x_N^{(N)}(0) < L$$

so that for some fixed $w > 0$ and any $i = 1, ..., N$

$$f(x_i - x_{i-1}) - f(x_{i+1} - x_i) + F(x_i) = w \tag{4}$$

where $x_0 = x_N, x_{N+1} = x_1$. We call w the effective constant force acting on each particle.

For fixed w call $\psi(x) = F(x) - w$ the virtual force. Assume that the virtual force is potential that is

$$\int_S \psi(x)dx = \int_S F(x)dx - Lw = 0 \tag{5}$$

The potential is

$$W(x) = -\int_0^x \psi(x)dx$$

Lemma 1 *If the virtual force is potential then the configuration $x_1 < ... < x_N$, satisfying (4), exists.*

In fact, such configuration is the fixed configuration for some new external force, equal to the virtual force. Then such fixed configuration exists as the minimum of the potential

$$U(x_1, ..., x_N) + \sum W(x_i)$$

The effective force $w > 0$ then can be found from (5). At the same time for fixed N, summing up the equations (4) we get

$$\sum F(x_i) - Nw = 0 \tag{6}$$

Then the effective force is

$$w = \frac{1}{N} \sum_{i=1}^{N} F(x_i)$$

Quasi-homogeneous dynamics Constructing the initial configuration with such homogeneous effective force is only the first (easier) step. We should also find initial velocities $v_i(0)$ of particles so that the homogeneity property conserved over all the time. It is impossible to conserve homogeneity even for small times, but possible to construct dynamics, conserving the following quasi-homogeneous picture.

Let us call a point $(x_i = x_i^{(N)}, v_i = v_i^{(N)}), i = 1, ..., N$, in the phase space $S^N \times R^N$ locally quasi-homogeneous, if there exist continuous functions $w(x), v(x), \rho(x), x \in [0, L)$, such that uniformly in $i = 1, ..., N$ the following conditions hold in the limit $N \to \infty$

1. (asymptotic local homogeneity of effective force)

$$w_i^{(N)} = w_i^{(N)}(x_{i-1}, x_i, x_{i+1}) = f(x_i - x_{i-1}) - f(x_{i+1} - x_i) + F(x_i) \to w(x_i)$$

2. (asymptotic local homogeneity of velocities) $v_i^{(N)} \to v(x_i)$;

3. (asymptotic local homogeneity of the particle density) for any interval $I \subset [0, L]$

$$\frac{N(I)}{N} \to \int_I \rho(x)dx$$

   where $N(l)$ is the number of particles on this interval.

We call this family quasi-homogeneous, if the functions $w(x), v(x), \rho(x)$ are constant and equal $w, v, \rho = L^{-1}$.

To construct solutions of the system (2), quasi-homogeneous at any time moment, we should choose the slowing-down media. We choose it adding the terms

$$\Phi(t, v_i) = -\sum_{l=1}^{\infty} \delta(t - ls)\Theta(v_i(ls)), s = \frac{L}{vN}$$

for some specially chosen function $\Theta(v)$, to the left-hand side of the equations (2)

The result is that a periodic solution of (2) exists and has quasi-homogeneous character.

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