Simulating N particles in a box

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1 Introduction

The N-particle Hamiltonian in a box has the from [RKT03]:

$$H = \sum_{n=1,\ldots,N} \sum_{i=1}^{d} \left[\frac{(p_i^{(n)})^2}{2} + V_i(q_i^{(n)}) \right] + \sum_{\substack{n,m=1,\ldots,N \\ n \neq m}} W(q^{(n)} - q^{(m)}), \tag{1}$$

where W is a repelling potential, C^∞ for $\|q^{(n)} - q^{(m)}\| > \rho$. We consider the limit of large energy per particle, and look for motions which are fast only in the last coordinate: we study the motion at the energy level $H = Nh$ for a fixed N and large h, with most of the particles' energy is at the vertical motion. We scale the vertical momenta $p_d^{(n)}$ by $\sqrt{2h}$, and the Hamiltonian transforms to

$$H = \sum_{n=1,\ldots,N} \left[\frac{(p_d^{(n)})^2}{2} + \delta V_d(q_d^{(n)}) \right] + \delta \sum_{n=1,\ldots,N} \sum_{i=1}^{d-1} \left[\frac{(p_i^{(n)})^2}{2} + V_i(q_i^{(n)}) \right] + \delta \sum_{\substack{n,m=1,\ldots,N \\ n \neq m}} W(q^{(n)} - q^{(m)}), \tag{2}$$

where $\delta = \frac{1}{2h}$; we study the behavior on the fixed energy level $H = \frac{N}{2}$, with

$$V_i(q_i) = \frac{1}{Q_i(q_i)^\alpha}, \quad \alpha > 0 \tag{3}$$

where the C^∞ function Q_i measures the distance to the box boundary in the i-th coordinate direction, i.e., $Q_i(0) = 0$, $Q_i(l_i) = 0$, $Q_i'(0) > 0$, $Q_i'(l_i) < 0$, and $Q_i(q_i) > 0$ for $q_i \in (0, l_i)$.

2 Specific example to be studied

Take $d = 2$ (so q_2 is the fast motion and q_1 is fixed for the periodic solutions) and small N (e.g. start with $N = 2$, then 3, and then maybe more..), and

$$Q_i(q_i) = q_i(l_i - q_i)(1 + P(q_i)), \qquad P_i(0) = 0, P_i(q_i) \geq 0, q_i \in (0, l_i). \tag{4}$$

so

$$Q_i'(q_i) = (l_i - q_i)(1+P_i(q_i)) - q_i(1+P_i(q_i)) + P_i'(q_i)q_i(l_i - q_i) = \{ \begin{array}{cc} l_i & q_i = 0 \\ -l_i(1+P_i(l_i)) & q_i = l_i \end{array} \tag{5}$$

and

$$W(q^{(n)} - q^{(m)}) = \frac{a}{\left\| q^{(n)} - q^{(m)} \right\|^{\beta}}, \qquad a, \beta > 0. \tag{6}$$

3 Assignment

1. Find the fixed points of (2) for $N = 2, 3$ (start with $P_i(q_i) = 0$ and $a = 0$, but also check what can you do for $a > 0$, and see if by preparing $P_1(q_1)$ to get more fixed points in the q_1 direction helps.
2. Write a code to find numerically the solutions of (2).
3. Look for periodic solutions in the q_2 direction.
4. Write a code for calculating the averaged potential and find the "minimizing phases" for it. See if we can observe islands of stability.

4 Answers

4.1 Finding the Fixed Points

Since there are N particles each living in d-dimensions, the system is of Nd degrees of freedom (each particle is described by d scalars). The fixed points of Hamiltonian systems are the points where the gradient of H vanishes. We find the partial derivatives of H. For $j = 1, \ldots, d, \quad k = 1, \ldots, N$,

$$\frac{\partial H}{\partial p_j^{(k)}} = p_j^{(k)}$$

Recall that:

$$V_j(q_j^{(k)}) = \frac{1}{Q_j(q_j^{(k)})^{\alpha}}$$

so

$$V_j'(q_j^{(k)}) = \frac{-\alpha \cdot Q_j'(q_j^{(k)})}{Q_j(q_j^{(k)})^{\alpha+1}}$$

$$W(q^{(n)} - q^{(m)}) = \frac{a}{\left\| q^{(n)} - q^{(m)} \right\|^{\beta}} = a \left(\sum_{i=1}^{d} \left(q_i^{(n)} - q_i^{(m)} \right)^2 \right)^{-\beta/2}$$

$$\frac{\partial}{\partial q_j^{(k)}} \sum_{\substack{n,m=1,\ldots,N \\ n\neq m}} W(q^{(n)} - q^{(m)}) =$$

$$= 2\frac{\partial}{\partial q_j^{(k)}} \sum_{\substack{n=1 \\ n\neq k}}^{N} W(q^{(k)} - q^{(n)}) =$$

$$= 2\frac{\partial}{\partial q_j^{(k)}} \sum_{\substack{n=1 \\ n\neq k}}^{N} a \left(\sum_{i=1}^{d} \left(q_i^{(k)} - q_i^{(n)} \right)^2 \right)^{-\beta/2} =$$

$$= 2a \sum_{\substack{n=1 \\ n\neq k}}^{N} \left(\sum_{i=1}^{d} \left(q_i^{(k)} - q_i^{(n)} \right)^2 \right)^{-(\beta+2)/2} \cdot \frac{-\beta}{2} \cdot 2 \left(q_j^{(k)} - q_j^{(n)} \right)$$

$$= -2a\beta \sum_{\substack{n=1 \\ n\neq k}}^{N} \frac{q_j^{(k)} - q_j^{(n)}}{\left\| q^{(k)} - q^{(n)} \right\|^{\beta+2}}$$

(The factor of 2 comes here, because we sum up the potential inflicted on the k-th particle and inflicted by the k-th particle, which are equal).
To summarize, the fixed points are where the momenta vanish and the particles' positions $q_j^{(k)}$ satisfy:

$$\frac{\alpha \cdot Q_j'(q_j^{(k)})}{Q_j(q_j^{(k)})^{\alpha+1}} + 2a\beta \sum_{\substack{n=1 \\ n\neq k}}^{N} \frac{q_j^{(k)} - q_j^{(n)}}{\left\| q^{(k)} - q^{(n)} \right\|^{\beta+2}} = 0$$

where

$$Q_j(q) = q(l_j - q)(1 + P(q))$$

and

$$Q_j'(q) = (l_j - q)(1 + P_j(q)) - q(1 + P_j(q)) + q(l_j - q)P_j'(q)$$

This system of equations is generally hard to solve. However, when taking $a = 0$, (i.e no repelling potential), the system is just a set of Nd separate equations, and the solution boils down to finding where the derivatives of the polynomials Q_j vanish.

Example 1 *For* $a = 0,\ P_j(q) = 0,$

$$Q_j(q) = q(l_j - q) \Longrightarrow Q_j'(q) = l_j - 2q \Longrightarrow q = \frac{l_j}{2}$$

Example 2 *For* $a = 0,\ P_j(q) = q,$

$$Q_j(q) = q(l_j - q)(1 + q) \Longrightarrow Q_j'(q) = -3q^2 + 2(l_j - 1)q + l_j$$
$$\Longrightarrow q = -\frac{2(1 - l_j) \pm \sqrt{4(l_j - 1)^2 + 12l_j}}{6}$$

Example 3 *For $a = 0$, $P_j(q) = 24q^3 - 30q^2 + 10, l_j = 1$, $Q_j(q)$ has 3 critical points as shown in the Figure 1:*

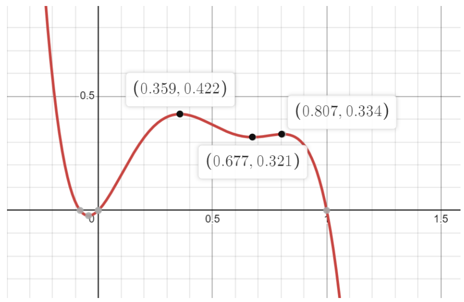

Figure 1: $P_j(q) = 24q^3 - 30q^2 + 10$