Equilibria and bifurcations of an elastic ring with interacting particles

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***Abstract*—Many-body systems appear in a diverse range of fields, such as microbiology, condensed matter physics, and chemistry. While some many-body systems only involve interactions between the bodies themselves, other systems involve interactions between both the bodies and the space on which they are constrained [1]. We focus on a canonical example of such a system — N interacting particles constrained to a deformable elastic ring. Using methods from optimal control theory, we derive conditions that the particle-ring system must satisfy to be in static equilibrium. We then consider the bifurcations that can occur as the interaction strength between the particles increases. Particular focus is given to the case of two and three particles. From these results, we are able to propose a general structure of the bifurcation behavior for $N > 3$ particles. Specifically, as the interaction strength increases, the N particles can bifurcate to form $M <= N$ clusters, which then behave similarly to the case of M individual particles.**

***Index Terms*—Optimization, Bifurcation theory**

I. Introduction

The study of a many-body system constrained to a surface dates back to the beginning of the XX century when J.J. Thomson studied equilibrium configurations of n charges confined to spheres [2]. It plays an important role in multiple subjects of study such as interaction molecules on elastic membranes [1], solid-state physics, and so on. This motivated our study on possible deformations of the simplest non-trivial elastic manifold, a ring, that undergoes when modifying the interaction between the particles. The theories of dynamics and optimization provide us with tools for approaching this problem. These permit us to find equilibrium conditions for a solution satisfying the (least action principle) dynamics of the corresponding system.

Our goal is to understand and simulate (using MATLAB) the possible deformations, this is the energy extrema, of an elastic ring on which there are n interacting particles on its surface. The use of bifurcation diagrams allows us to give a quantitative description of the range of possible equilibrium configurations.

II. Formulation

Consider a system of n interacting particles via a certain potential V_{ij} constrained to slide on an elastic ring of perimeter 1. We can think of this problem as dividing the ring into n segments of length l^i with the particles located at the beginning of each segment. The segment i is described by three parameters: x_1^i and x_2^i (the x and y coordinates of the segment at a particular point) and x_3^i (the angle of the segment at a point with respect to the x axis). By forcing the correct boundary conditions described later, we are faced to numerically solve a boundary value problem.

A. Optimization problem

The total potential energy of the system U is stored in the interaction between the particles and the deformation of the ring. The elastic potential energy for each segment is proportional to its curvature $u^i := \frac{dx_3^i}{ds^i}$. Thus integrate and sum up for the whole ring,

$$U = \sum_{\substack{i,j=1 \\ j>i}}^{n} V\left(x^i(0), x^j(0)\right) + \sum_{i=1}^{n} \int_0^{l^i} \frac{1}{2}\left(u^i\right)^2 ds^i$$

where $x^i(s^i)$ is the position of the i-th segment at arc-length $s^i \in [0, l^i]$ and $V\left(x^i(0)x^j(0)\right)$ is the potential energy between particles i and j. Without loss of generality, we can chose the frame of reference of one of the particles, i.e. $x^1(0) = (0,0,0)$ and $x^n(l^n) = (0,0,0)$. The idea now is to minimize the total energy U due to the constrains of the system. The problem is now reduced to the following,

$$\underset{x^i,u^i,l^i}{\text{minimize}} \sum_{\substack{i,j=1 \\ j>i}}^{n} V\left(x^i(0), x^j(0)\right) + \sum_{i=1}^{n} \int_0^{l^i} \frac{1}{2}\left(u^i\right)^2 ds^i \quad (1)$$

$$\text{s.t. } \frac{dx^i}{ds^i} = \begin{bmatrix} \cos\left(x_3^i\right) \\ \sin\left(x_3^i\right) \\ u^i \end{bmatrix}, \quad x^1(0) = x^n\left(l^n\right) = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix},$$

$$x^{i+1}(0) = x^i\left(l^i\right) \quad \text{for } i \in \{1, \ldots, n-1\}, \quad \sum_{i=1}^{n} l^i = 1.$$

B. Equilibrium conditions

We allude to optimal control theory tools to solve the latter minimization problem (refer to Appendix A for details). The idea relies on defining the auxiliary functions p^i (called the co-state) which simplifies the problem. We can deduce the equilibrium conditions and at the end we are faced to solve the following boundary value differential equations:

$$\dot{x}_1^i = l^i \cos(x_3^i) \qquad \dot{x}_2^i = l^i \sin(x_3^i) \qquad \dot{x}_3^i = l^i u^i$$
$$\dot{p}_1^i = 0 \qquad \dot{p}_2^i = 0 \qquad \dot{p}_3^i = l^i (p_1^i \sin(x_3^i) - p_2^i \cos(x_3^i)),$$

on the intervals $[0, l^i]$ and where the boundary conditions (a total of $7n-3$) that must be satisfied are:

$$x^1(0) = x^n(l^n) = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}, x^{i+1}(0) = x^i\left(l^i\right), \text{for } i \in \{1, \ldots, n-1\}$$

$$p_1^i(0) = p_1^{i-1}(l^{i-1}) + \sum_{\substack{j=1 \\ j \neq i}}^{n} V^{ij}_{x_1^i(0)}$$
$$p_2^i(0) = p_2^{i-1}(l^{i-1}) + \sum_{\substack{j=1 \\ j \neq i}}^{n} V^{ij}_{x_2^i(0)}$$
$$p_3^i(0) = p_3^{i-1}(l^{i-1}),$$

for $i \in \{2, \ldots, n\}$, and

$$(p_1^{i+1}(0) - p_1^i(l^i)) \cos(x_3^{i+1}(0)) + (p_2^{i+1}(0) - p_2^i(l^i)) \sin(x_3^{i+1}(0)) = 0$$

for $i \in \{1, \ldots, n-1\}$. Finally, we also have the constraint

$$\sum_{i=1}^{n} l^i = 1.$$

The next section will discuss some numerical solutions of the problem using MATLAB.

III. Analysis

To get some intuition on this problem, let us start with the simplest case. Consider we have two particles on the ring with a perimeter of 1. It is expected to have a pitchfork bifurcation (while decreasing R_{eq}) at a value of $R_{eq} = \frac{1}{\pi}$. These three branches that come out are: the particle on the top sliding to the left, symmetrically squeezing the ring, or sliding to the right as shown in Figure 1.

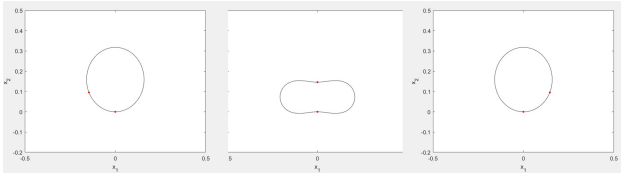

Fig. 1. Three equilibria branches that arise from the first pitchfork bifurcation that happens at $R_{eq} = \frac{1}{\pi}$ for the two-particle case.

Yet there is an unexpected behavior of the system on the symmetric branch. Continue to decrease R_{eq}, the middle branch undergoes another pitchfork bifurcation as shown in Figure 2.

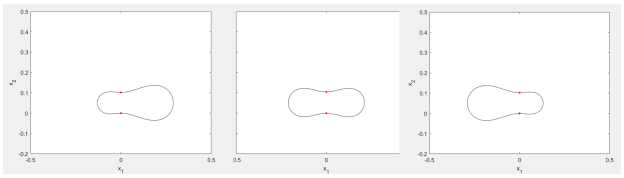

Fig. 2. Three equilibria branches that arise from the second pitchfork bifurcation that happens in the middle branch for the two-particle case.

Notice that this second bifurcation does not always occur (for example, when the force is very weak). The relations between V_0 vs R_{eq} and V_0 vs R_{12}(distance between two particles) can enhance our understanding of this phenomena. The key feature is captured in Figure 3, that is, this second bifurcation always occurs when the strength of interaction is not too weak and the two particles reach a particular distance ($R_{12} \approx 0.118$).

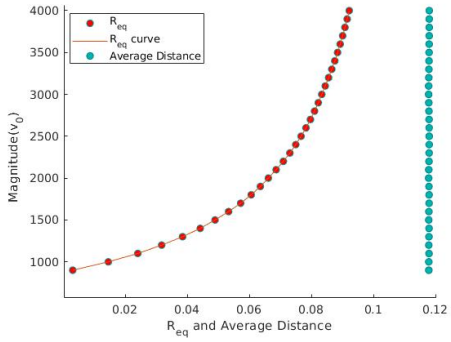

Fig. 3. Relation between V_0 (magnitude) and R_{eq} for which the second pitchfork bifurcation occurred on two particles.

The next case to consider is the three-particle case. Its behavior is similar to the two-particle case with the difference that there is a new branch where the three particles stay all separated when $R_{eq} = 0$ (Figure 4 middle branch). Aside from this, the other branches are the cases where there are one or two different clusters of particles. For the two-cluster case, a second bifurcation occurs like the one described in the two-particle case.

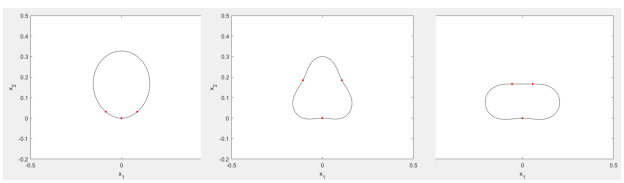

Fig. 4. Three equilibria branches that arise from the first pitchfork bifurcation at the equilibrium distance for the three-particle case.

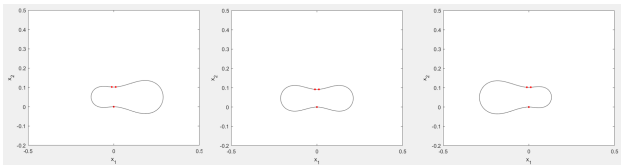

Fig. 5. Three equilibria branches that arise from a pitchfork bifurcation on the right branch of Figure 4 for the three-particle case.

An interesting pattern arises with the four-particle case (Figure 6) where the particles can bifurcate in multiple ways giving rise to clusters of particles that end up interacting with the other clusters on the ring. Whereby the study of the n-particle bifurcations reduces to understanding branches whose behavior is similar as the $n-1$ case, when there are less than n particle clusters, and one branch on which the configuration is a star-shaped ring consisting of n (independent) particle clusters.

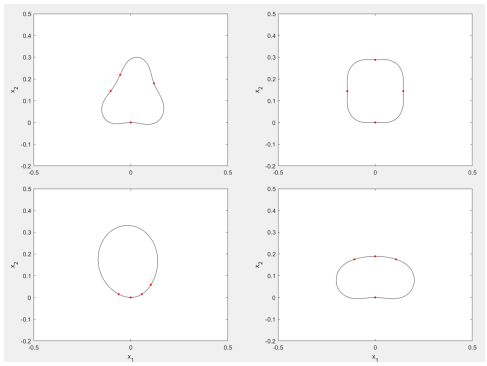

Fig. 6. Some equilibrium configurations for four particles with different numbers of particle clusters. Top left: 3 clusters, top right: 4 clusters, bottom left: 1 cluster, bottom right: 2 clusters.

For better visualization of these configurations, we project the ring and particle system on an average distance between the n particles axis. This will represent the possible bifurcations that could happen modulo symmetries[1]. For the two-particle case and three-particle case these diagrams are shown in Figure 7 and Figure 8.

[1]Since the particles never overlap, the symmetry is rotations on the particles $\mathbb{Z}_n$

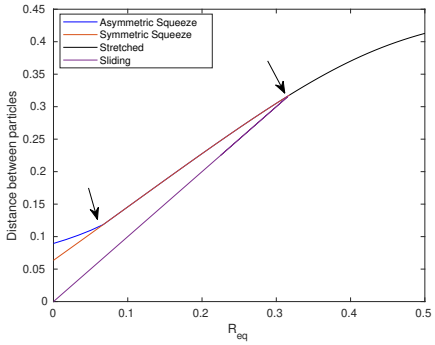

Fig. 7. Bifurcation diagram for the two particles case with $V_0 = 2000$. There are two pitchfork bifurcations indicated by the two arrows. The left arrow is visualized on Figure 2. The right arrow is visualized on Figure 1.

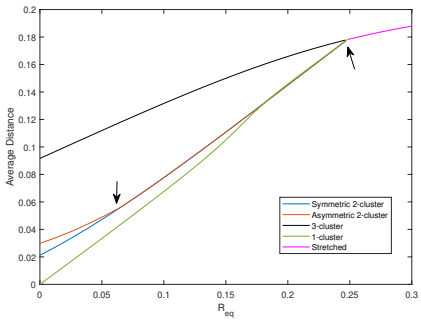

Fig. 8. Bifurcation diagram for the three particles case with $V_0 = 1000$. There are two pitchfork bifurcations (modulo symmetries) indicated by the two arrows. The left arrow is visualized on Figure 5. The right arrow is visualized on Figure 4.

IV. Conclusions

In this report we present a formulation for a n particle system constrained to an elastic ring and a way of finding equilibrium configurations. With the use of control theory and optimization techniques, the minimization of energy is reduced to a boundary valued problem which can be numerically solved. We studied the possible bifurcations the two and three particles systems can undergo by varying the strength of the interaction. The bifurcations found are of pitchfork type and occur on two or more clusters configurations and the new perpendicular branches are symmetrically equivalent under some rotation. Finally, we propose a general structure for the bifurcation diagram for the n particles case.

V. Acknowledgement

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VI. Appendix A: Deduction of equilibrium conditions

To numerically solve the minimization problem we can make use of control theory. Let us start defining the following augmented cost function

$$J = \sum_{\substack{i,j=1 \\ j>i}}^{n} V(x^i(0), x^j(0)) + \sum_{i=1}^{n-1} (\nu^i)^T \left(x^{i+1}(0) - x^i(l^i)\right) + \lambda \left(\sum_{i=1}^{n} l^i - 1\right) + \sum_{i=1}^{n} \int_0^{l^i} \left(\frac{1}{2}(u^i)^2 + (p^i)^T \left(\dot{x}^i - \left[\cos(x_3^i)\ \sin(x_3^i)\ u^i\right]^T\right)\right) ds^i$$

where v^i and λ are Lagrange multipliers associated with the constraints of segments matching at the boundary where the particles are and the perimeter of the ring being one respectively, and p^i are co-state functions associated with the remaining condition. The Hamiltonian in this case is defined as

$$H^i(x^i, u^i, p^i) = (p^i)^T \left[\cos(x_3^i)\ \sin(x_3^i)\ u^i\right]^T - \frac{1}{2}(u^i)^2.$$

Equilibrium conditions are found by considering the first variation of the augmented cost function and imposing it to be zero $dJ = 0$.

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