**ORIGINAL ARTICLE**

# Bifurcations of quasi-periodic solutions from relative equilibria in the Lennard–Jones 2-body problem

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## Abstract

We propose the general method of proving the bifurcation of new solutions from relative equilibria in $N$-body problems. The method is based on a symmetric version of Lyapunov center theorem. It is applied to study the Lennard–Jones 2-body problem, where we have proved the existence of new periodic or quasi-periodic solutions.

**Keywords** N-body problem · Lennard–Jones potential · Periodic solutions · Hamiltonian systems · Lyapunov center theorem

**Mathematics Subject Classification** 37J45 · 37G15

## 1 Introduction

$N$-body problems have been widely studied in celestial mechanics since Kepler and Newton. We study the motion of $N$ particles moving under the action of mutual potential forces. Denote by $q_1, \ldots, q_N \in \mathbb{R}^d$ the positions of the particles with the masses $m_1, \ldots, m_N$, respectively, by $U_{ij}(q_i, q_j) : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$ the potential between particles $q_i$ and $q_j$, and put $U(q_1, \ldots, q_N) = \sum\limits_{1 \le i < j \le N} U_{ij}(q_i, q_j)$. Then, denoting $q = (q_1, \ldots, q_N)$, the Newtonian equation of motion can be written as the system:

$$m_i \ddot{q}_i = -\nabla_{q_i} U(q) \qquad i = 1, \ldots, N.$$

A typical question for the N-body problem is the existence of relative equilibria, i.e., solutions where the system of particles behaves like a rigid body—the mutual distances of the particles remain constant during the motion. In other words, the system of particles moves under the action of rotation group (the center of mass of the system is fixed). Therefore, relative

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equilibria are special cases of periodic solutions. For the extend discussion about $N$-body problem, see Meyer et al. (2009).

In this paper, we show how to utilize the existence of relative equilibria to the demonstration of the existence of quasi-periodic solutions that are not relative equilibria. This method can be applied for a variety of problems like gravitational $N$-body problem, Lennard–Jones $N$-body problem or $N$-vortex problem. We apply this method to study the 2-body problem with Lennard–Jones potential.

Lennard–Jones potential describing the potential energy of a pair of molecules is given by

$$U_{LJ}(r) = \varepsilon \left[ \left( \frac{\sigma}{r} \right)^{12} - 2 \left( \frac{\sigma}{r} \right)^6 \right],$$

where $r$ is a distance of the molecules and the parameters $\varepsilon$ and $\sigma$ can be found experimentally for the specific model. The first term describes the Pauli repulsion (the molecules repel each other at a close distance), the second one—London forces (attraction at a moderate distance). Lennard–Jones potential is used frequently in a chemistry modeling. By the change of units and scale, we can assume $\varepsilon = \sigma = 1$. Then, the potential for the $N$-body problem is given by

$$U(q) = \sum_{1 \leq i < j \leq N} \left( \frac{1}{|q_i - q_j|^{12}} - \frac{2}{|q_i - q_j|^6} \right). \tag{1.1}$$

Lennard–Jones $N$-body problem has been studied in many ways, including more general class of potential. In Llibre and Long (2015), the authors have studied the circular periodic solutions and antiperiodic solutions of the generalized problem. The classical case studied here corresponds to the case $\gamma = 0$ in Llibre and Long (2015), where the authors have proved the existence of a circle of equilibria.

In Liu et al. (2018), the authors have used variational methods to study the structure of solutions of the generalized Lennard–Jones system. They have proved, among others, the existence of periodic non-circular solution with any period greater than the number $\tau_1^{\#}$, where $\tau_1^{\#} = \left( \frac{2 \cdot 11^7}{3^3 \cdot 5^4} \right)^{1/6}$ in the classical case. They have also studied the existence of periodic solutions in a rotating frame, giving the period of solution as an integral, see Proposition 5.2 in Liu et al. (2018).

Lennard–Jones $(N+2)$- and $(N+3)$-body problems with the generalized potential on $\mathbb{R}^3$ have been studied in Liu (2020) where the existence of circular and non-circular homographic solutions has been proven.

The 2-body problem with the potential (1.1) has been studied in Corbera et al. (2004) for the existence of equilibria and relative equilibria. In Pérez-Chavela et al. (2018), the existence of periodic solutions bifurcating from the stationary ones has been proven. Moreover, the detailed study of generalized 2-body Lennard–Jones potential was done in Bărbosu et al. (2011).

In this article, we study Lennard–Jones 2-body problem and we prove the existence of connected families of periodic or quasi-periodic solutions bifurcating from the relative equilibria with the moment of inertia in the given interval. The article is organized as follows. In Sect. 2, we reformulate the problem into Hamiltonian equation in rotating frame and we formulate the main tool of this work, Theorem 1. Section 3 is devoted to study the problem in a number of cases depending on the moment of inertia of the relative equilibrium.

## 2 The theoretical background

Consider a planar $N$-body problem with all masses equal to 1 described by the equation

$$\ddot{q}(t) = -\nabla U(q(t)), \tag{2.1}$$

where $q = (q_1, \ldots, q_N) : \mathbb{R} \to \Omega$, $\Omega = \{(q_1, \ldots, q_N) \in (\mathbb{R}^2)^N : q_i \neq q_j \text{ for } i \neq j\}$ is the configuration space and $U : \Omega \to \mathbb{R}$ is of the class $\mathcal{C}^2$. We treat $q$ and gradient as column vectors. Denote by $K(\theta)$ the matrix of planar rotation, i.e., $K(\theta) = \begin{bmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{bmatrix} \in SO(2)$ and by $R(\theta) = K(\theta) \oplus \ldots \oplus K(\theta)$ - the $2N \times 2N$ block matrix with $2 \times 2$ matrices $K(\theta)$ on its diagonal. We recall that the rotation group $SO(2)$ acts on $\mathbb{R}^{2N}$ as $SO(2) \times \mathbb{R}^{2N} \ni (K(\theta), q) \to R(\theta)q \in \mathbb{R}^{2N}$. Assume additionally that the potential $U$ is $SO(2)$-invariant, i.e., for any $\theta \in \mathbb{R}$, we have $U(R(\theta)q) = U(q)$. Then, the gradient $\nabla U$ is $SO(2)$-equivariant, i.e., $\nabla U(R(\theta)q) = R(\theta)\nabla U(q)$.

Suppose that for some $q_0 \in \Omega$, the map $\tilde{q}(t) = R(\omega t)q_0$, $q_0 \in \Omega$ is a solution of the equation (2.1). A solution of this form is called a relative equilibrium generated by $q_0$, and the point $q_0$ is called a central configuration. A relative equilibrium $\tilde{q}(t)$ can be viewed as an equilibrium point in a rotating frame with rotation rate $\omega$. One can show that $\tilde{q}(t)$ is a solution of (2.1) if and only if $\nabla U(q_0) = \omega^2 q_0$ (see also Corbera et al. (2004)).

We are going to put the system into a rotating frame. Firstly, we translate the Newtonian system (2.1) to the Hamiltonian one. Let's introduce the variable $p = (p_1, \ldots, p_N) = \dot{q}$. The problem can be written in the form

$$\begin{cases} \dot{q} = p = \nabla_p H(q, p) \\ \dot{p} = -\nabla U(q) = -\nabla_q H(q, p) \end{cases}, \tag{2.2}$$

for $H(q, p) = \frac{1}{2}\|p\|^2 + U(q)$. Now, we introduce the new variables in the frame rotating with velocity $\omega$: $Q(t) = R(-\omega t)q(t)$, $P(t) = R(-\omega t)p(t)$ and denote $J_N = R(\frac{\pi}{2}) = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix} \oplus \ldots \oplus \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix}$ - $N$-times. In these variables, the equation of motion can be written in the general form

$$\begin{bmatrix} \dot{Q} \\ \dot{P} \end{bmatrix} = J\nabla\mathcal{H}(Q, P), \tag{2.3}$$

where Hamiltonian function $\mathcal{H}$ is given by $\mathcal{H}(Q, P) = \frac{1}{2}\|P\|^2 + \omega Q^T J_N P + U(Q)$ and $J = \begin{bmatrix} 0 & I_{2N} \\ -I_{2N} & 0 \end{bmatrix}$ is a standard $4N$-dimensional symplectic matrix.

Since the potential $U$ is $SO(2)$-invariant and $R^T J_N R = J_N$, the Hamiltonian $\mathcal{H}$ is also $SO(2)$-invariant, where the action is given by $(\theta, (Q, P)) \to (R(\theta)Q, R(\theta)P)$. Recall that the block matrix $\begin{bmatrix} R(\theta) & 0 \\ 0 & R(\theta) \end{bmatrix}$ is a unitary one.

Note that $\nabla_P \mathcal{H}(Q, P) = P + \omega(Q^T J_N)^T = P - \omega J_N Q$ and $\nabla_Q \mathcal{H}(Q, P) = \nabla U(Q) + \omega J_N P$. Therefore, equilibria of the problem (2.3) are given by $P = \omega J_N Q$ and $0 = \nabla U(Q) + \omega J_N P = \nabla U(Q) - \omega^2 Q$. Hence, $(Q_0, P_0) = (q_0, \omega J_N q_0)$ is an equilibrium of the equation (2.3).

To prove the existence of family of solutions of the problem (2.3) emanating from the stationary solution $(Q_0, P_0)$, we can apply the following theorem. The theorem is a generalization of the famous Lyapunov center theorem, see Lyapunov (1895); Moser (1976);

Weinstein (1973). Since we are going to apply it to $2 \cdot (2N)$-dimensional system, it is given in this case.

**Theorem 1** *( Strzelecki (2020)) Assume that a compact Lie group $\Gamma$ acts unitary on $\mathbb{R}^{4N}$. Under the following assumptions:*

(A1)  *$\mathcal{H} : \mathbb{R}^{4N} \to \mathbb{R}$ is a $\Gamma$-invariant Hamiltonian of the class $C^2$,*

(A2)  *$z_0 \in \mathbb{R}^{4N}$ is a critical point of $\mathcal{H}$ such that the isotropy group $\Gamma_{z_0}$ is trivial,*

(A3)  *the orbit $\Gamma(z_0)$ is isolated in $(\nabla \mathcal{H})^{-1}(0)$,*

(A4)  *$\pm i\beta_1, \ldots, \pm i\beta_m$, $0 < \beta_m < \ldots < \beta_1$, $m \geq 1$ are the purely imaginary eigenvalues of $J\nabla^2 \mathcal{H}(z_0)$,*

(A5)  *$\deg \left( \nabla \left( \mathcal{H}_{|T_{z_0}^\perp \Gamma(z_0)} \right), B(z_0, \epsilon), 0 \right) \neq 0$ for sufficiently small $\epsilon$,*

(A6)  *$\beta_{j_0}$ is such that $\beta_j / \beta_{j_0} \notin \mathbb{N}$ for all $j \neq j_0$*

(A7)  *the Morse index $m^- \left( \begin{bmatrix} -\lambda \nabla^2 \mathcal{H}(z_0) & -J \\ J & -\lambda \nabla^2 \mathcal{H}(z_0) \end{bmatrix} \right)$ changes at $\lambda = \frac{1}{\beta_{j_0}}$ when $\lambda$ varies,*

*there exists a connected family of non-stationary periodic solutions of the system $\dot{z}(t) = J\nabla \mathcal{H}(z(t))$ emanating from the stationary solution $z_0$ (i.e., with amplitude tending to 0) such that minimal periods of solutions in a small neighborhood of $z_0$ are close to $2\pi/\beta_{j_0}$.*

**Remark 1** The assumption **(A6)** is needed to be studied if the period of the new solution has to be *minimal*. If we are interested in the existence of solutions only, we do not have to verify it.

**Remark 2** If $\dim \Gamma(z_0) = \dim \ker \nabla^2 \mathcal{H}(z_0)$, then $T_{z_0}\Gamma(z_0) = \ker \nabla^2 \mathcal{H}(z_0)$. Hence, $z_0$ is a non-degenerate critical point of $\mathcal{H}_{|T_{z_0}^\perp \Gamma(z_0)}$, and as a consequence, the Brouwer degree $\deg \left( \nabla \left( \mathcal{H}_{|T_{z_0}^\perp \Gamma(z_0)} \right), B(z_0, \epsilon), 0 \right)$ equals $\pm 1$ for sufficiently small $\epsilon$. Therefore, in this case the assumption **(A5)** is satisfied.

**Remark 3** The limit of $m^- \left( \begin{bmatrix} -\lambda \nabla^2 \mathcal{H}(z_0) & -J \\ J & -\lambda \nabla^2 \mathcal{H}(z_0) \end{bmatrix} \right)$ for $\lambda \to 0$ equals $4N$. The limit for $\lambda \to \infty$ is a singular matrix; however, for large values of $\lambda$ we can estimate

$$2m^+(\nabla^2 \mathcal{H}(z_0)) = 2m^-(-\nabla^2 \mathcal{H}(z_0)) \leq m^- \left( \begin{bmatrix} -\lambda \nabla^2 \mathcal{H}(z_0) & -J \\ J & -\lambda \nabla^2 \mathcal{H}(z_0) \end{bmatrix} \right) \leq$$

$$\leq 2(4N - m^+(-\nabla^2 \mathcal{H}(z_0))) = 2(4N - m^-(\nabla^2 \mathcal{H}(z_0))), \tag{2.4}$$

where $m^+(A)$ is a positive Morse index of a matrix $A$. Therefore, if $m^+(\nabla^2 \mathcal{H}(z_0)) > 2N$ or $m^-(\nabla^2 \mathcal{H}(z_0)) > 2N$, then the Morse index changes for some value of parameter $\lambda$.

Note that the only values of the parameter $\lambda$ where the Morse index from the assumption **(A7)** can change are $\lambda \in \{ \frac{1}{\beta_j} : j = 1, \ldots, m \}$. Therefore, $m^+(\nabla^2 \mathcal{H}(z_0)) > 2N$ or $m^-(\nabla^2 \mathcal{H}(z_0)) > 2N$ implies the existence of a purely imaginary eigenvalues of $J\nabla^2 \mathcal{H}(z_0)$ (the assumption **(A4)**). To summarize, when we are able to verify the stronger assumption

**(A7.1)** $m^+(\nabla^2 \mathcal{H}(z_0)) > 2N$ or $m^-(\nabla^2 \mathcal{H}(z_0)) > 2N$

then the assumptions **(A4)** and **(A7)** are satisfied. However, then we do not know the level $\lambda$ where the assumption **(A7)** holds true, and therefore, we cannot give the minimal period of new solutions. The assumption **(A6)** has not to be verified.

See Strzelecki (2020) for more details.

Theorem 1 provides the existence of *periodic* solutions of the problem in the *rotating frame* whose trajectories lie arbitrarily close to the stationary solution $(Q_0, P_0)$. In the original frame these solutions, we call *quasi-periodic* as a composition of two periodic motions with not necessarily resonant frequencies. Their trajectories lie arbitrarily close to the trajectory of the relative equilibrium $R(\omega t)q_0$.

One can ask whether we can apply classical Lyapunov center theorem to study the problem. Note that in the rotating frame, the Hamiltonian function $\mathcal{H}$ still has symmetries of the group $SO(2)$. It implies that critical points of $\mathcal{H}$ (i.e., stationary solutions of the problem in the rotating frame) are not isolated and therefore they are degenerate—Lyapunov theorem cannot be applied. It is possible to reduce the system to the space of orbits of the $SO(2)$-action (reduced Hamiltonian system). However, if $\dim \ker \nabla^2 \mathcal{H}(z_0) \geq 2$, the relative equilibrium is degenerate stationary solution of the reduced system and Lyapunov theorem is not applicable, while Theorem 1 could be applied.

Even when we research non-degenerate case, an application of Theorem 1 is direct and does not require the study of the properties of the orbit space which is a manifold. Note that in the case of general unitary action of the compact Lie group on the problem (as is stated in Theorem 1), the orbit space does not have to have a structure of manifold, while Theorem 1 is still applicable.

## 3 The results for the Lennard–Jones 2-body problem

In the paper Corbera et al. (2004) Corbera, Llibre and Pérez-Chavela have described equilibria and central configurations for Lennard–Jones 2- and 3-body problems with equal masses. We focus on 2-body problem where for each value of the moment of inertia $I \in (\frac{1}{4}, \infty)$ there exists a relative equilibrium generated by the central configurations in the set $CC = \{(q_1, q_2) \in \mathbb{R}^2 \times \mathbb{R}^2 : q_2 = -q_1, |q_1 - q_2| = 2\sqrt{I}\}$—a closed trajectory of this relative equilibrium. The period of this relative equilibrium equals $T = 2\pi/\omega_I$, where $\omega_I = \frac{\sqrt{384I^3-6}}{64\sqrt{I^7}}$. Moreover, the period function $T(I)$ has a minimum at the point $I_0 = \frac{1}{4}\left(\frac{7}{4}\right)^{1/3}$, see Corbera et al. (2004).

Applying the method described in the previous section and Theorem 1, we are going to prove the bifurcation of periodic solutions from this relative equilibrium for various values of the moment of inertia.

The symbolic computations in this section were performed by using Maple. One can find the Maple file under the following link: https://mat.umk.pl/~danio/LJ2BP.html.

Fix $I > \frac{1}{4}$. We consider the problem in the frame rotating with the angular velocity $\omega_I$ as described in the previous section. In this frame, the Hamiltonian of the motion has the form

$$\mathcal{H}(Q_{1x}, Q_{1y}, Q_{2x}, Q_{2y}, P_{1x}, P_{1y}, P_{2x}, P_{2y})$$
$$= \frac{1}{((Q_{1x} - Q_{2x})^2 + (Q_{1y} - Q_{2y})^2)^6} - \frac{2}{((Q_{1x} - Q_{2x})^2 + (Q_{1y} - Q_{2y})^2)^3}$$
$$+ \frac{1}{2}\left(P_{1x}^2 + P_{1y}^2 + P_{2x}^2 + P_{2y}^2\right) + \omega_I\left(-Q_{1x}P_{1y} + Q_{1y}P_{1x} - Q_{2x}P_{2y} + Q_{2y}P_{2x}\right).$$
$$(3.1)$$

Since the Lennard–Jones potential is $SO(2)$-invariant, the Hamiltonian $\mathcal{H}$ is invariant under the diagonal action of $SO(2)$. Note that for any point $z \neq 0 \in \mathbb{R}^8$, the isotropy group $SO(2)_z$ is trivial.

Put $a = \sqrt{I} > \frac{1}{2}$. The point $z_0 = (a, 0, -a, 0, 0, \omega_I a, 0, -\omega_I a)$ of the form $(q_0, \omega_I J_2 q_0)$, where $q_0 = (a, 0, -a, 0) \in CC$ comes from the central configuration and is a critical point of the Hamiltonian $\mathcal{H}$. The assumption **(A2)** is satisfied. Since there is only one relative equilibrium of Lennard–Jones 2-body problem rotating with frequency $\omega_I$, there is only one $SO(2)$-orbit of critical points of $\mathcal{H}$, i.e., $(\nabla\mathcal{H})^{-1}(0) = SO(2)(z_0)$ and the assumption **(A3)** is satisfied.

We begin with the study of the assumptions **(A4)** and **(A6)**, i.e., we calculate the eigenvalues of the matrix $J\nabla^2\mathcal{H}(z_0)$. These are: $\alpha_1 = 0$ with multiplicity 2, $\alpha_2 = \frac{\sqrt{-15+384a^6}}{32a^7}$, $\alpha_3 = -\alpha_2$, $\alpha_4 = i \cdot \frac{\sqrt{384a^6-6}}{64a^7}$ with multiplicity 2 and $\alpha_5 = -\alpha_4$ with multiplicity 2. Since $a > \frac{1}{2}$, the conjugate eigenvalues $\alpha_4$ and $\alpha_5$ are always purely imaginary. The number $-15 + 384a^6$ is negative for $a < \sqrt[6]{\frac{5}{128}} =: \delta$; therefore, we consider two cases:

1. $a < \delta$ when the matrix $J\nabla^2\mathcal{H}(z_0)$ possess two pairs of purely imaginary eigenvalues: $\pm i \cdot \frac{\sqrt{384a^6-6}}{64a^7} =: \pm i\beta_1$ and $\pm i \cdot \frac{\sqrt{15-384a^6}}{32a^7} =: \pm i\beta_2$,

2. $a \geq \delta$ when there is only one pair of imaginary eigenvalues $\pm i \cdot \frac{\sqrt{384a^6-6}}{64a^7} = \pm i\beta_1$.

Note that $\beta_1 < \beta_2 \Leftrightarrow a < \sqrt[6]{\frac{11}{320}} =: \gamma$, for $a = \gamma$ these numbers are equal and $\gamma < \delta$.

**Remark 4** $\beta_1 = \omega_{a^2}$.

To verify the assumption **(A7)** by its stronger version **(A7.1)** from Remark 3, we study the Hessian $\nabla^2\mathcal{H}(z_0)$. The eigenvalues of $\nabla^2\mathcal{H}(z_0)$ are:

$$\lambda_1 = 0, \qquad \lambda_2 = \frac{2048\,a^{14} + 192\,a^6 - 3}{2048\,a^{14}},$$

$$\lambda_3 = \frac{2048\,a^{14} - 1344\,a^6 + 39 + \sqrt{r(a)}}{4096\,a^{14}},$$

$$\lambda_4 = \frac{2048\,a^{14} - 1344\,a^6 + 39 - \sqrt{r(a)}}{4096\,a^{14}},$$

$$\lambda_5 = \frac{16\,a^7 + \frac{1}{2}\sqrt{1024\,a^{14} + 384\,a^6 - 6}}{32\,a^7},$$

$$\lambda_6 = \frac{16\,a^7 - \frac{1}{2}\sqrt{1024\,a^{14} + 384\,a^6 - 6}}{32\,a^7},$$

where $r(a) = 4194304\,a^{28} + 7077888\,a^{20} - 184320\,a^{14} + 1806336\,a^{12} - 104832\,a^6 + 1521$ and multiplicities of $\lambda_5$ and $\lambda_6$ equal 2. Since a Hessian is a symmetric matrix, its eigenvalues are real numbers. Since $a > \frac{1}{2}$, we can easily see that $\lambda_2, \lambda_5 > 0$ and $\lambda_6 < 0$. Moreover,

$$\lambda_3 \cdot \lambda_4 = \frac{1}{2^{24}a^{28}}\left((2048a^{14} - 1344a^6 + 39)^2 - r(a)\right)$$

$$= \frac{1}{2^{24}a^{28}}(-12582912a^{20} + 344064a^{14}),$$

this product equals 0 if and only if $a = a_0 := \sqrt{I_0} = \frac{1}{2}\left(\frac{7}{4}\right)^{1/6}$ for $a > 1/2$, is positive for $1/2 < a < a_0$ and negative for $a > a_0$. It is easy to verify that $\lambda_4 = 0$ for $a = a_0$. Since $\lambda_3 > \lambda_4$, we conclude $\lambda_3 > 0$ and $\lambda_4$ changes its sign at $a = a_0$. It means that for $a < a_0$ the positive Morse index $m^+(\nabla^2\mathcal{H}(z_0))$ equals 5 and the assumption **(A7.1)** is satisfied, while for $a > a_0$ $m^+(\nabla^2\mathcal{H}(z_0)) = 4$ and $m^-(\nabla^2\mathcal{H}(z_0)) = 3$.

Since $\frac{1}{2} < a_0 < \gamma < \delta$, we will study the cases as follows.

### 3.1 The case $a < a_0$

By the results above, in this case the stronger assumption **(A7.1)** is satisfied, and therefore, we do not have to verify the assumptions **(A4)**, **(A6)** and **(A7)**, but we will obtain a weaker theorem—without an information about the minimal period, see Remark 3. Moreover, in this case dim ker $\nabla^2 \mathcal{H}(z_0) = 1 = \dim SO(2)$, i.e., the assumption **(A5)** is satisfied, see Remark 2.

To summarize, we can formulate the following result as a consequence of Theorem 1.

**Theorem 2** *For $1/2 < a < \frac{1}{2}\left(\frac{7}{4}\right)^{1/6}$, there exists a connected family of quasi-periodic solutions of the Lennard–Jones 2-body problem bifurcating from the relative equilibrium generated by the central configuration from the set $\{(q_1, q_2) \in \mathbb{R}^2 \times \mathbb{R}^2 : q_2 = -q_1, |q_1 - q_2| = 2a\}$.*

When we are interested in the minimal period of solutions in this case, we might study the assumption **(A7)** in its general formulation as it is done in the next cases where the assumption **(A7.1)** is not satisfied. However, in the next sections the proofs are much complicated. Therefore, we utilized the condition **(A7.1)** in the case $a < a_0$.

### 3.2 The case $a = a_0$

The case $a = a_0 = \sqrt{I_0}$ is a critical one, where the assumption **(A5)** has to be studied in its general version and it is more complicated; therefore, the problem is far from being solved. However, in this case it is not hard to verify the assumption **(A7)**.

### 3.3 The case $a_0 < a < \gamma \Rightarrow 0 < \beta_1 < \beta_2$.

In this case and the following ones, dim ker $\nabla^2 \mathcal{H}(z_0) = 1 = \dim SO(2)$, $m^+(\nabla^2 \mathcal{H}(z_0)) = 4$ and $m^-(\nabla^2 \mathcal{H}(z_0)) = 3$. Thanks to Remark 2, the assumption **(A5)** is satisfied. Since $\beta_2 > \beta_1$, the assumption **(A6)** is satisfied for $\beta_{j_0} = \beta_2$. The assumption **(A7)** we will study in its general formulation. We denote

$$K_\lambda = \begin{bmatrix} -\lambda \nabla^2 H(z_0) & -J \\ J & -\lambda \nabla^2 H(z_0) \end{bmatrix}$$

for simplicity.
We will study the change of $m^-(K_\lambda)$ at $\lambda_0 = \frac{1}{\beta_2}$. Since $\lim_{\lambda \to 0} m^-(K_\lambda) = 2N = 8$ and $\lambda_0$ is the smallest value of parameter where this Morse index can change (see Remark 3), we have to verify whether $m^-(K_\lambda) \neq 8$ for some $\frac{1}{\beta_2} < \lambda < \frac{1}{\beta_1}$, i.e.,

$$\frac{64a^7}{\sqrt{-1536a^6 + 60}} < \lambda < \frac{64a^7}{\sqrt{384a^6 - 6}}.$$

Let's take $\lambda^* = \frac{64a^7}{\sqrt{-576a^6+27}}$, where the denominator is a quadratic mean of the two denominators. We are going to apply Descartes' rule of signs, i.e., for any $a \in (a_0, \gamma)$ we have to study the number of changes of signs of the coefficients of the characteristic polynomial $w_{K_{\lambda^*}}(r)$ of the matrix $K_{\lambda^*}$. The coefficients of $w_{K_{\lambda^*}}(r)$ are rational functions of $a$; hence, we are going to bring them into polynomials. Denote by $w_i(a)$, $i = 0, \ldots, 16$, the coefficient of $r^i$ in the polynomial $w_{K_{\lambda^*}}(r)$ and put $v_i(a) = w_i(a) \cdot (-64a^6+3)^{\alpha_{i,1}} \cdot a^{\alpha_{i,2}} : (11-320a^6)^{\alpha_{i,3}}$,

where the table $(\alpha_{i,j})_{i=0,\dots,16;\ j=1,2,3}^{T}$ is given by

$$\begin{bmatrix} 6 & 13/2 & 7 & 13/2 & 6 & 11/2 & 5 & 9/2 & 4 & 7/2 & 3 & 5/2 & 2 & 3/2 & 1 & 1/2 & 0 \\ 0 & 7 & 14 & 21 & 28 & 21 & 28 & 21 & 28 & 21 & 28 & 21 & 28 & 21 & 14 & 7 & 0 \\ 6 & 4 & 2 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}.$$

Note that $-64a^6 + 3$ and $11 - 320a^6$ are positive on the interval $(a_0, \gamma)$. Therefore, the polynomial $v_i(a)$ has the same zeros and the same sign on this interval as $w_i(a)$ function, for $i = 0, \dots, 16$.

We are interested in the signs of the values of $v_i(a)$; therefore, using Sturm method we verify how many distinct roots in the interval $(a_0, \gamma)$ they have.

| $v_0$ | $v_1$ | $v_2$ | $v_3$ | $v_4$ | $v_5$ | $v_6$ | $v_7$ | $v_8$ | $v_9$ | $v_{10}$ | $v_{11}$ | $v_{12}$ | $v_{13}$ | $v_{14}$ | $v_{15}$ | $v_{16}$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 0 | 1 | 1 | 1 | 0 | 0 | 0 | 1 | 1 | 1 | 1 | 1 | 1 | 0 | 1 | 1 | 0 |

Denote the root of $v_i(a)$ in the given interval as $r_i$ (if it exists). We can perform the Sturm method on smaller intervals to order the roots $r_i$:

$$r_{11} < r_9 < r_{14} < r_7 < r_{12} < r_{10} < r_1 < r_3 < r_8 < r_2 < r_{15}.$$

In the next table, we test the signs of the polynomials on the intervals determined by their roots. For example, the symbol $+ \rightarrow -$ denotes that a polynomial with a root $\zeta$ is positive for $a \in (a_0, \zeta)$ and negative for $(\zeta, \delta)$.

Now, we are well prepared to study the sequence of signs of $(v_0(a), v_1(a), \dots, v_{15}(a), v_{16}(a))$ on the subintervals of $(a_0, \gamma)$:

| | $v_0$ | $v_1$ | $v_2$ | $v_3$ | $v_4$ | $v_5$ | $v_6$ | $v_7$ |
|---|---|---|---|---|---|---|---|---|
| sign | $+$ | $+ \rightarrow -$ | $- \rightarrow +$ | $- \rightarrow +$ | $+$ | $+$ | $+$ | $- \rightarrow +$ |

| | $v_8$ | $v_9$ | $v_{10}$ | $v_{11}$ | $v_{12}$ | $v_{13}$ | $v_{14}$ | $v_{15}$ | $v_{16}$ |
|---|---|---|---|---|---|---|---|---|---|
| sign | $- \rightarrow +$ | $+ \rightarrow -$ | $+ \rightarrow -$ | $- \rightarrow +$ | $- \rightarrow +$ | $-$ | $+ \rightarrow -$ | $+ \rightarrow -$ | $+$ |

Note that in the endpoint $r_i$ the sign of $v_i$ equals 0, but 0 has no effect on the number of changes of signs, therefore, this number of changes in $r_i$ is the same as on the interval $(r_j, r_i)$; therefore, we study right-closed intervals.

To summarize, we have proved that for any $a \in (a_0, \gamma)$, there are 6 changes of signs in the sequence of coefficients of the characteristic polynomial of the matrix $K_{\lambda*}$. Hence, there are at most 6 positive roots of the characteristic polynomial. Moreover, the matrix $K_{\lambda*}$ is symmetric and non-singular. Therefore, $m^-(K_{\lambda*}) \geq 10$ and the assumption **(A7)** holds true. In fact, $m^-(K_{\lambda*}) = 10$, by the study of characteristic polynomial of the negative variable.

To summarize, in this case the assumptions of Theorem 1 with $\beta_{j_0} = \beta_2$ are satisfied and we can formulate the following result.

| Interval | Sequence of signs | Number of changes |
|---|---|---|
| $(a_0, r_{11}]$ | $+, +, -, -, +, +, +, -, -, +, +, -, -, -, +, +, +$ | 6 |
| $(r_{11}, r_9]$ | $+, +, -, -, +, +, +, -, -, +, +, +, -, -, +, +, +$ | 6 |
| $(r_9, r_{14}]$ | $+, +, -, -, +, +, +, -, -, -, +, +, -, -, +, +, +$ | 6 |
| $(r_{14}, r_7]$ | $+, +, -, -, +, +, +, -, -, -, +, +, -, -, -, +, +$ | 6 |
| $(r_7, r_{12}]$ | $+, +, -, -, +, +, +, +, -, -, +, +, -, -, -, +, +$ | 6 |
| $(r_{12}, r_{10}]$ | $+, +, -, -, +, +, +, +, -, -, +, +, -, -, -, +, +$ | 6 |
| $(r_{10}, r_1]$ | $+, +, -, -, +, +, +, -, -, -, +, +, -, -, -, +, +$ | 6 |
| $(r_1, r_3]$ | $+, -, -, -, +, +, +, +, -, -, -, +, +, -, -, +, +$ | 6 |
| $(r_3, r_8]$ | $+, -, -, +, +, +, +, +, -, -, -, +, +, -, -, +, +$ | 6 |
| $(r_8, r_2]$ | $+, -, -, +, +, +, +, +, +, -, -, +, +, -, -, +, +$ | 6 |
| $(r_2, r_{15}]$ | $+, -, +, +, +, +, +, +, +, -, -, +, +, -, -, +, +$ | 6 |
| $(r_{15}, \gamma)$ | $+, -, +, +, +, +, +, +, +, -, -, +, +, -, -, -, +$ | 6 |

**Theorem 3** *For $a_0 < a < \sqrt[6]{\frac{11}{320}}$, there exists a connected family of quasi-periodic solutions of the Lennard–Jones 2-body problem bifurcating from the relative equilibrium generated by the central configuration from the set $\{(q_1, q_2) \in \mathbb{R}^2 \times \mathbb{R}^2 : q_2 = -q_1, |q_1 - q_2| = 2a\}$. These solutions are compositions of two periodic motions: with minimal period $\frac{2\pi}{\omega_{a^2}} =$*
$\frac{128\pi a^7}{\sqrt{384a^6-6}}$ *and with minimal period close to $\frac{2\pi}{\beta_2} = \frac{64\pi a^7}{\sqrt{-384a^6+15}}$.*

One can ask whether there is a change of $m^-(K_\lambda)$ when $\lambda$ crosses the second possible value $\frac{1}{\beta_1}$. Performing the same study as above, we can verify that for some $\lambda^* > \frac{1}{\beta_1}$, for example, $\lambda^* = 1$, there is $m^-(K_{\lambda^*}) = 10$ and the assumption **(A7)** is not satisfied.

### 3.4 The case $a_0 = \gamma$.

$\pm i\beta_1$ is the only pair of purely imaginary eigenvalues of $J\nabla^2 H(z_0)$; therefore, it is sufficient to prove that $m^-(K_\lambda) \neq 8$ for some $\lambda > \frac{1}{\beta_1} \approx 0,47$. Put $\lambda^* = 1$. Denote by $w_i$ the coefficient of $r^i$, $i = 0, \dots, 16$ in the characteristic polynomial of $K_{\lambda^*}$. In the list below, we round the values of these coefficients to integers.

$$\begin{bmatrix} w_0 \approx 2088, & w_1 \approx 82739, & w_2 \approx 812352, & w_3 \approx -270347, & w_4 \approx -2561758, \\ w_5 \approx -688334, & w_6 \approx 2355090, & w_7 \approx 1532645, & w_8 \approx -255042, & w_9 \approx -400090, \\ w_{10} \approx -46706, & w_{11} \approx 29922, & w_{12} \approx 7077, & w_{13} \approx -275, & w_{14} \approx -153, \\ w_{15} \approx -1, & w_{16} \approx 1. & & & \end{bmatrix}$$

In the sequence of coefficients of the characteristic polynomial of $K_{\lambda^*}$, there are 6 changes of signs; therefore, by Descartes' rule of signs there are at most 6 positive eigenvalues. Since $K_{\lambda^*}$ is a non-singular matrix, we obtain $m^-(K_{\lambda^*}) \geq 10$ and the assumptions of Theorem 1 are satisfied. Moreover, $\omega_{a_0^2} = \beta_1 = 12 \cdot 5^{2/3} 11^{-7/6}$.

**Theorem 4** *There exists a connected family of* periodic *solutions of the Lennard–Jones 2-body problem bifurcating from the relative equilibrium generated by the central configuration from the set $\{(q_1, q_2) \in \mathbb{R}^2 \times \mathbb{R}^2 : q_2 = -q_1, |q_1 - q_2| = 2\sqrt[6]{\frac{11}{320}}\}$ with minimal periods close to $\frac{11^{7/6}\pi}{6 \cdot 5^{2/3}}$.*

## 3.5 The case $\gamma < a < \delta$ and $0 < \beta_2 < \beta_1$

This case we study similarly as $a_0 < a < \gamma$ for $\lambda_0 = \frac{1}{\beta_1}$, so we compute the Morse index of $K_{\lambda^*}$ for $\lambda^* = \frac{64a^7}{\sqrt{-576a^6+27}}$, $\frac{1}{\beta_1} < \lambda_* < \frac{1}{\beta_2}$. Unfortunately, by Descartes' rule of signs we compute $m^-(K_{\lambda^*}) = 8$ and the assumption **(A7)** is *not* satisfied for $\lambda_0 = \frac{1}{\beta_1}$. We are going to verify that $m^-(K_\lambda)$ changes at $\lambda_0 = \frac{1}{\beta_2}$. In order to do it, we will follow the same way as in the case $a_0 < a < \gamma$ to show that for $\lambda^* = \frac{2}{\beta_2}$, the Morse index of $K_{\lambda^*}$ equals 10, i.e., we apply Descartes' rule of signs to prove that there are at most six positive eigenvalues of symmetric non-singular matrix $K_{\lambda^*}$.

Denote by $w_i(a)$, $i = 0, \ldots, 16$, the coefficient of $r^i$ in the polynomial $w_{K_{\lambda^*}}(r)$, and put $v_i(a) = w_i(a) \cdot (-128a^6 + 5)^{\alpha_{i,1}} \cdot a^{\alpha_{i,2}} : (256a^6 - 7)^{\alpha_{i,3}}$, where the table $(\alpha_{i,j})_{i=0,\ldots,16; \, j=1,2,3}^T$ is given by

$$\begin{bmatrix} 4 & 11/2 & 7 & 13/2 & 6 & 11/2 & 5 & 9/2 & 4 & 7/2 & 3 & 5/2 & 2 & 3/2 & 1 & 1/2 & 0 \\ 0 & 7 & 14 & 21 & 28 & 21 & 28 & 21 & 28 & 21 & 28 & 21 & 28 & 21 & 14 & 7 & 0 \\ 4 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}.$$

Note that $-128a^6 + 5$ and $256a^6 - 7$ are positive on the interval $(\gamma, \delta)$. Therefore, the polynomial $v_i(a)$ has the same zeros and the same sign on this interval as $w_i(a)$ function, for $i = 0, \ldots, 16$.

By the Sturm method, we verify that there are only single roots of the polynomials $v_3(a)$ (denote the root by $r_3$) and $v_{13}(a)$ (with a root $r_{13}$). Moreover, $r_3 < r_{13}$.

In the next table, we test the signs of the polynomials on the intervals determined by their roots. For example, the symbol $+ \to -$ denotes that a polynomial with a root $\zeta$ is positive for $a \in (\gamma, \zeta)$ and negative for $(\zeta, \delta)$.

| | $v_0$ | $v_1$ | $v_2$ | $v_3$ | $v_4$ | $v_5$ | $v_6$ | $v_7$ | $v_8$ |
|---|---|---|---|---|---|---|---|---|---|
| sign | $+$ | $+$ | $+$ | $- \to +$ | $-$ | $-$ | $+$ | $+$ | $-$ |

| | $v_9$ | $v_{10}$ | $v_{11}$ | $v_{12}$ | $v_{13}$ | $v_{14}$ | $v_{15}$ | $v_{16}$ |
|---|---|---|---|---|---|---|---|---|
| sign | $-$ | $-$ | $+$ | $+$ | $- \to +$ | $-$ | $-$ | $+$ |

Now, we are well prepared to study the sequence of signs of $(v_0(a), v_1(a), \ldots, v_{15}(a), v_{16}(a))$ on the intervals $(\gamma, r_3]$, $(r_3, r_{13}]$, $(r_{13}, \delta)$.

| Interval | Sequence of signs | Number of changes |
|---|---|---|
| $(\gamma, r_3]$ | $+, +, +, -, -, -, +, +, -, -, -, +, +, -, -, -, +$ | 6 |
| $(r_3, r_{13}]$ | $+, +, +, +, -, -, +, +, -, -, -, +, +, -, -, -, +$ | 6 |
| $(r_{13}, \delta)$ | $+, +, +, +, -, -, +, +, -, -, -, +, +, +, -, -, +$ | 6 |

We have verified that for any $a \in (\gamma, \delta)$, there are 6 changes of signs in the sequence of coefficients of the characteristic polynomial of $K_{\lambda^*}$. Therefore, by Descartes' rule of signs there are at most 6 positive eigenvalues of this matrix, and at least 10 negative roots. The assumption **(A7)** of Theorem 1 is satisfied with $\beta_{j_0} = \beta_2 < \beta_1$. It remains to check the assumption **(A6)**.

Note that $\frac{\beta_1}{\beta_2} = k \in \mathbb{N} \Leftrightarrow a = \sqrt[6]{\frac{10k^2+1}{256k^2+64}} = \sqrt[6]{\frac{5}{128} - \frac{\frac{6}{4}}{256k^2+64}} =: \theta(k)$. The function $\theta(k) : \mathbb{N} \to \mathbb{R}$ is increasing, so $\theta(k) > \theta(1) = \gamma$, and moreover, $\theta(k) < \sqrt[6]{\frac{5}{128}} = \delta$. The assumption **(A6)** is satisfied when $a \in (\gamma, \delta) \setminus \{\sqrt[6]{\frac{10k^2+1}{256k^2+64}} : k \in \mathbb{N}\}$. However, this assumption does not have to be satisfied when we do not study the minimal period, see Remark 1.

To summarize, we can formulate the following result.

**Theorem 5** *For $\sqrt[6]{\frac{11}{320}} < a < \sqrt[6]{\frac{5}{128}}$, there exists a connected family of quasi-periodic solutions of the Lennard–Jones 2-body problem bifurcating from the relative equilibrium generated by the central configuration from the family $\{(q_1, q_2) \in \mathbb{R}^2 \times \mathbb{R}^2 : q_2 = -q_1, |q_1 - q_2| = 2a\}$. These solutions are compositions of two periodic motions: with period $\frac{2\pi}{\omega_{a^2}} = \frac{128\pi a^7}{\sqrt{384a^6-6}}$ and with period close to $\frac{2\pi}{\beta_2} = \frac{64\pi a^7}{\sqrt{-384a^6+15}}$. The period of the second motion is minimal for $a \neq \sqrt[6]{\frac{10k^2+1}{256k^2+64}}, k \in \mathbb{N}$.*

### 3.6 The case $\delta \leq a$

In this unbounded case, there is no way to find a general behavior of the Morse index $m^-(K_\lambda)$. It could be possible to study small intervals of $a$ or specific values of $a$ by Descartes' rule of signs. For example, for $\delta \leq a < 1$ the Morse index equals 8 and the assumption **(A7)** is not satisfied. But we are not able to formulate any general result.

### 3.7 Summary

We have proved that for any $a \in (1/2, \sqrt[6]{\frac{5}{128}}) \setminus \{\sqrt[6]{\frac{7}{256}}\}$, there is a bifurcation of families of quasi-periodic solutions from the family of central configurations $\{(x_1, x_2) \in \mathbb{R}^2 \times \mathbb{R}^2 : x_2 = -x_1, |x_1 - x_2| = 2a\}$ of the Lennard–Jones 2-body problem.

The case $a = \sqrt[6]{\frac{7}{256}}$, where it is hard to verify the assumption **(A5)**, remains to be solved.

The method proposed in this paper could be used to a variety of $N$-body problems where the relative equilibria exist.

## Declarations

**Conflict of interest** The authors declare that they have no conflict of interest.

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