EQUILIBRIUM POINTS IN A BUCKINGHAM TYPE PROBLEM

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Abstract. In this paper, we go deeper into the study of the two-body problem associated to a Buckingham type potential (Popescu, 2014). We consider the McGehee-type transformations to write the basic equations of motion and the integrals of energy and angular momentum. Then we investigate the equilibria for all possible situations by varying the parameters of the field and the angular momentum constant in the three cases: negative, zero, and positive energy. We find the number of equilibria for each such case.

Key words: celestial mechanics – two-body problem – Buckingham potential – equilibrium point.

1. INTRODUCTION

The Buckingham potential (Buckingham, 1938) was used in many studies for the simulations of both attractive and repulsive intermolecular and gravitational forces. It is considered a simplification of the Lennard-Jones potential (for Lennard-Jones potential see, for example, Mioc *et al.* (2008a), Mioc *et al.* (2008b)). The Buckingham potential describes the Pauli repulsion energy (the repulsive part is exponential) and van der Waals energy for the interaction of two atoms that are not directly bonded, as a function of the interatomic distance r,

$$U(r) = A\exp(-Br) - \frac{M}{r^6}, \tag{1}$$

where A, B and M are parameters. The Buckingham potential being an empirical approximation, the parameters can be fitted to reproduce experimental data in several phenomena from physics, astrophysics, astronomy and chemistry.

In Popescu (2014), we considered the two-body problem associated to the Buckingham potential. We described two limit situations of motion, collision and escape, and provided the symmetries that characterize the problem.

In this paper, our goal is to find the equilibria of the corresponding central-force problem. This is not so simple as for other potentials encountered in many problems of mechanics, because Buckingham's potential has an exponential part. Also, the

Seeliger's potential has such an exponential part (see Popescu *et al.*, 2010). Section 2 resume the basic equations of the problem after a sequence of McGehee-type transformations to remove the singularity, regularizing all these equations. Section 3 tackles the equilibria of the problem. We leave aside the equilibria corresponding to the collision manifold and infinity manifold (already studied in Popescu, 2014), dealing only with those for which $0 < r < +\infty$. Section 4 formulates some concluding remarks.

2. EQUATIONS OF MOTION

The Buckingham potential being a central one, the associated two-body problem can be reduced to a central-force problem. We fix one particle as centre at the origin of the plane $\mathbf{R}^2$ and we study the relative motion of the other particle. The position (or configuration) vector of this particle is denoted by $\mathbf{q} = (q_1, q_2)$ and the momentum vector by $\mathbf{p} = \dot{\mathbf{q}}$, $\mathbf{p} = (p_1, p_2)$. Then, the Buckingham potential is

$$U(\mathbf{q}) = A\exp(-B|\mathbf{q}|) - \frac{M}{|\mathbf{q}|^6}, \tag{2}$$

where $A > 0,\ B > 0,\ M > 0$ are constants and the kinetic energy of the unit-mass particle is $T(\mathbf{p}) = \frac{|\mathbf{p}|^2}{2}$. The following equations describe the motion:

$$\dot{\mathbf{q}} = \frac{\partial H}{\partial \mathbf{p}}, \qquad \dot{\mathbf{p}} = -\frac{\partial H}{\partial \mathbf{q}}, \tag{3}$$

where H is the Hamiltonian

$$H(\mathbf{q},\mathbf{p}) := T(\mathbf{p}) - U(\mathbf{q}) = \frac{|\mathbf{p}|^2}{2} - A\exp(-B|\mathbf{q}|) + \frac{M}{|\mathbf{q}|^6}. \tag{4}$$

It results that

$$\begin{aligned}
\dot{q_1} &= p_1\\
\dot{q_2} &= p_2\\
\dot{p_1} &= -AB\frac{q_1}{\sqrt{q_1^2+q_2^2}}\exp\left(-B\sqrt{q_1^2+q_2^2}\right) + 6M\frac{q_1}{\left(q_1^2+q_2^2\right)^4}\\
\dot{p_2} &= -AB\frac{q_2}{\sqrt{q_1^2+q_2^2}}\exp\left(-B\sqrt{q_1^2+q_2^2}\right) + 6M\frac{q_2}{\left(q_1^2+q_2^2\right)^4}.
\end{aligned} \tag{5}$$

The phase space is $\mathbf{Q} \times \mathbf{P}$, where $\mathbf{Q} = \mathbf{R}^2 \setminus \{(0,0)\}$ is the configuration space and $\mathbf{P} = \mathbf{R}^2$ is the momentum space. The problem admits two integrals in involution, energy and angular momentum:

$$H(\mathbf{q},\mathbf{p}) = \frac{h}{2} = \text{const.}, \quad L(\mathbf{q},\mathbf{p}) = q_1p_2 - q_2p_1 = C = \text{const.}, \tag{6}$$

where h is the energy constant and C stands for the constant of angular momentum.

The potential, the motion equations and the energy integral have an isolated singularity at the origin, which corresponds to a collision particle-centre. To regularize equations (5), we apply a sequence of McGehee-type transformations of the second kind (McGehee, 1974).

It follows (see Popescu, 2014):

$$\begin{aligned}
&r = |\mathbf{q}|,\\
&\theta = \arctan\left(\frac{q_2}{q_1}\right),\\
&\xi = \dot{r} = \frac{q_1p_1 + q_2p_2}{|\mathbf{q}|},\\
&\eta = r\dot{\theta} = \frac{q_1p_2 - q_2p_1}{|\mathbf{q}|},\\
&x = r^3\xi,\\
&y = r^3\eta.
\end{aligned} \tag{7}$$

Rescaling the time through $ds = r^{-4}dt$ and writing $' = d/ds$, the equations of motion become:

$$\begin{aligned}
&r' = rx\\
&\theta' = y\\
&x' = 3x^2 + y^2 - ABr^7\exp(-Br) + 6M\\
&y' = 2xy.
\end{aligned} \tag{8}$$

The first integrals now read respectively

$$x^2 + y^2 = hr^6 + 2Ar^6\exp(-Br) - 2M, \quad y = Cr^2. \tag{9}$$

3. EQUILIBRIA

For finding the equilibrium points for the two-body problem associated to Buckingham potential, we will use the motion equations given by the system (8) and the integrals (9). We observe that θ does not explicitly appear in either the right-hand side of motion equations or first integrals. So, we may discard the equation corresponding to θ. Thus, we are interested only in the system formed by

$$\begin{aligned}
&r' = rx\\
&x' = 3x^2 + y^2 - ABr^7\exp(-Br) + 6M\\
&y' = 2xy.
\end{aligned} \tag{10}$$

and the integrals (9). We obtain

$$x^2 = hr^6 + 2Ar^6\exp(-Br) - C^2r^4 - 2M. \tag{11}$$

The left-hand side is nonnegative. So, for every fixed values of h and C, the regions where real motion is allowed are given by

$$hr^6+2Ar^6\exp(-Br)-C^2r^4-2M\geq 0. \tag{12}$$

The effective potential is defined by

$$V_{eff}(r;C)=\frac{C^2}{r^2}-2A\exp(-Br)+2\frac{M}{r^6}. \tag{13}$$

For a fixed energy level h, the regions of possible motion are featured by the condition $V_{eff}(r;C)\leq h$.

The equilibria of the problem are of the form (r,x,y) with $r>0$, $x=0$ and must be solutions of the system

$$\begin{gathered} y^2-ABr^7\exp(-Br)+6M=0, \\ y^2=hr^6+2Ar^6\exp(-Br)-2M, \\ y=Cr^2. \end{gathered} \tag{14}$$

Eliminating y between these equations, compatibility relations have to be verified:

$$ABr^7\exp(-Br)-6M=hr^6+2Ar^6\exp(-Br)-2M=C^2r^4. \tag{15}$$

We consider two cases according to the values of the angular momentum C, namely $C=0$ and $C\neq 0$.

Case I. For $C=0$ (rectilinear motion), eliminating the terms that contain exponentials between the relations (15), we obtain

$$hBr^7-2MBr+12M=0. \tag{16}$$

We shall discuss its positive roots using Descartes' rule of signs.

Let $f(r):=ABr^7\exp(-Br)-6M$ and $g(r):=hBr^7-2MBr+12M$.

The equilibria have to verify both equations: $f(r)=0$ and $g(r)=0$.

We observe that:

- $f'(r)=0$ if and only if $r=\frac{7}{B}$;
- f is strictly increasing for $r<\frac{7}{B}$;
- f is strictly decreasing for $r>\frac{7}{B}$;
- $f''(r)=0$ if and only if $r=\frac{7\pm\sqrt{7}}{B}$;
- f is convex if $r<\frac{7-\sqrt{7}}{B}$ or $r>\frac{7+\sqrt{7}}{B}$;
- f is concave if $r\in\left(\frac{7-\sqrt{7}}{B},\frac{7+\sqrt{7}}{B}\right)$.

There are several cases and we investigate them according to the energy level.

1. **Negative-energy**.

If $h<0$, then $g(r)$ has one positive root, $\widetilde{r}$, using Descartes' rule of signs. We denote $f\left(\frac{7}{B}\right)$ by E,

$$E := \frac{A}{B^6}\left(\frac{7}{e}\right)^7 - 6M.$$

1.1. If $E < 0$, then $f(r)$ has no positive root, hence no equilibrium.

1.2. If $E = 0$, then $f(r)$ has one positive double root, $r = \frac{7}{B}$, but $g\left(\frac{7}{B}\right) < 0$. This means that there is no equilibrium.

1.3. If $E > 0$, then $f(r)$ has two positive roots, r_1 and r_2. If $r_1 = \widetilde{r}$ or $r_2 = \widetilde{r}$, then we have an equilibrium. If r_1 and r_2 are different of $\widetilde{r}$, hence there is no equilibrium.

2. **Zero-energy**.

If $h = 0$, then $g(r)$ has one positive root $\widetilde{r}_1 = \frac{6}{B}$. Since $f\left(\frac{6}{B}\right) = 0$, it follows that the problem admits one equilibrium, $r = \frac{6}{B}$.

3. **Positive-energy**.

If $h > 0$, $g(r)$ has two positive roots or no positive root at all, using the same Descartes' rule of signs.

3.1. If $E < 0$, then $f(r)$ has no positive root, hence no equilibrium.

3.2. If $E = 0$, then $f(r)$ has one positive double root, $r = \frac{7}{B}$.

3.2.1. If $h = \frac{A}{3e^7}$, $g(r)$ has the positive double root $r = \frac{7}{B}$, and we have an equilibrium.

3.2.2. If $h \neq \frac{A}{3e^7}$, $r = \frac{7}{B}$ is not the root of $g(r)$, thus there is no equilibrium.

3.3. If $E > 0$, then $f(r)$ has two positive roots, r_1 and r_2.

3.3.1. If $g(r_1) = 0$ and $g(r_2) \neq 0$, or $g(r_1) \neq 0$ and $g(r_2) = 0$, then we have a positive root, hence an equilibrium.

3.3.2. If $g(r_1) = 0$ and $g(r_2) = 0$, then we have two different positive roots, thus two equilibria.

3.3.3. If $g(r_1) \neq 0$ and $g(r_2) \neq 0$, then there is no positive root at all, therefore no equilibrium.

Case II. For $C \neq 0$, eliminating the terms which contain exponentials between the relations (15), we obtain

$$hBr^7 - C^2Br^5 + 2C^2r^4 - 2MBr + 12M = 0. \tag{17}$$

1. **Negative or zero-energy**.

If $h \leq 0$, denoting $f(r) := ABr^7 \exp(-Br) - C^2r^4 - 6M$ and $g(r) := hBr^7 - C^2Br^5 + 2C^2r^4 - 2MBr + 12M$ for $r > 0$, the equilibria must verify both equations: $f(r) = 0$ and $g(r) = 0$. We write the first equation as

$$\exp(-Br) = \frac{C^2}{AB}\frac{1}{r^3} + \frac{6M}{AB}\frac{1}{r^7} \tag{18}$$

and we denote by $u(r)$ and $v(r)$ the left, respectively the right member. We observe that

$$u'(r) < 0, \quad u''(r) > 0, \quad v'(r) < 0, \quad v''(r) > 0. \tag{19}$$

We deduce that the function $u(r)$ is strictly decreasing, convex and

$$\lim_{r \to 0, r > o} u(r) = 1, \quad \lim_{r \to +\infty} u(r) = 0. \tag{20}$$

Analogous, the function v is strictly decreasing, convex and

$$\lim_{r \to 0, r > 0} v(r) = +\infty, \quad \lim_{r \to +\infty} v(r) = 0. \tag{21}$$

It follows that the equation (18) and, as a consequence, the equation $f(r) = 0$ can have two or one positive roots, or no positive root at all.

On the other hand, by Descarte's rule of signs, the equation $g(r) = 0$ has three positive roots or one positive root.

Taking into account these two observations, we can analyse the equilibria of the problem:

1.1. $f(r)$ has two positive roots, r_1 and r_2, and $g(r)$ has three positive roots.

1.1.1. If $g(r_1) = 0$ and $g(r_2) = 0$, then we have two different positive roots, hence two equilibria.

1.1.2. If $g(r_1) = 0$ or $g(r_2) = 0$, then we have a positive root, thus an equilibrium.

1.1.3. If $g(r_1) \neq 0$ and $g(r_2) \neq 0$, then we have not positive root at all, hence no equilibrium.

1.2. $f(r)$ has two positive roots, r_1 and r_2, and $g(r)$ has one positive root.

1.2.1. If $g(r_1) = 0$ or $g(r_2) = 0$, then we have a positive root, thus an equilibrium.

1.2.2. If $g(r_1) \neq 0$ and $g(r_2) \neq 0$, then we have not positive root at all, hence no equilibrium.

1.3. $f(r)$ has one positive root, r, and $g(r)$ has three positive roots or one positive root.

1.3.1. If $g(r) = 0$, then we have a positive root, thus an equilibrium.

1.3.2. If $g(r) \neq 0$, there is no positive root at all, hence no equilibrium.

1.4. $f(r)$ has no positive root at all, and $g(r)$ has three positive roots or one positive root. Therefore there is no equilibrium at all.

2. **Positive-energy**.

For $h > 0$, using the same Descartes' rule of signs, (17) has four changes of sign, therefore four positive roots, two positive roots, or no positive root at all. From the above discussion concerning (18), we deduce that we can have the following cases:

2.1. $f(r)$ has two positive roots, r_1 and r_2, and $g(r)$ has four or two positive roots.

2.1.1. If $g(r_1) = 0$ and $g(r_2) = 0$, then we have two different positive roots, hence two equilibria.

2.1.2. If $g(r_1) = 0$ or $g(r_2) = 0$, then we have a positive root, thus an equilibrium.

2.1.3. If $g(r_1) \neq 0$ and $g(r_2) \neq 0$, then there is no positive root at all, therefore no equilibrium.

2.2. $f(r)$ has two positive roots, r_1 and r_2, and $g(r)$ has no positive root at all, then no equilibrium at all.

2.3. $f(r)$ has only one positive root, r, and $g(r)$ has four or two positive roots.

2.3.1. If $g(r) = 0$, we have a positive root, hence an equilibrium.

2.3.2. If $g(r) \neq 0$, we have no positive root at all, thus no equilibrium.

2.4. $f(r)$ has one positive root, r, and $g(r)$ has no positive root at all. Then, there is no equilibrium at all.

2.5. $f(r)$ has no positive root at all, and $g(r)$ has four or two positive roots, or no positive root at all. Therefore there is no equilibrium at all.

In physical terms, this discussion respectively means: two equilibria, one equilibrium or no equilibrium at all.

Remark. We want to emphasize that there are the situations described for the equation $f(r) = 0$.

a) Let $f(r) = 0$ for $A = 1$, $B = 1$, $C = 1$, $M = 1$:

$$r^7 \exp(-r) - r^4 - 6 = 0. \tag{22}$$

We have two positive solutions: $r_1 = 2.2926$ and $r_2 = 4.4928$ (see Fig. 1).

For $h \leq 0$, $g(r_1) \neq 0$ and $g(r_2) \neq 0$, hence there is no equilibrium. For $h = 2.7406 \times 10^{-2}$, we have $g(r_1) = 0$, hence an equilibrium.

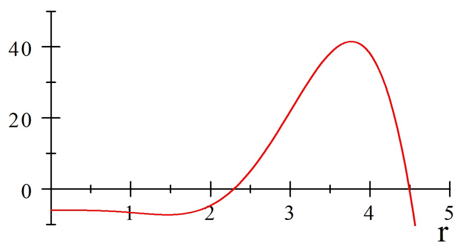

Fig. 1 – The equation $f(r) = 0$ has two positive roots

b) Let $f(r) = 0$ for $A = 1$, $B = 0.001$, $C = 0.01$, $M = 0.0001$:

$$0.001r^7 \exp(-0.001r) - 0.0001r^4 - 0.0006 = 0. \tag{23}$$

We have a single positive solution $r = 0.94658$ (see Fig. 2a).

For $h = -16.085$, we have $g(r) = 0$ and therefore an equilibrium. If $h > 0$, $g(r) \neq 0$ and there is no equilibrium at all.

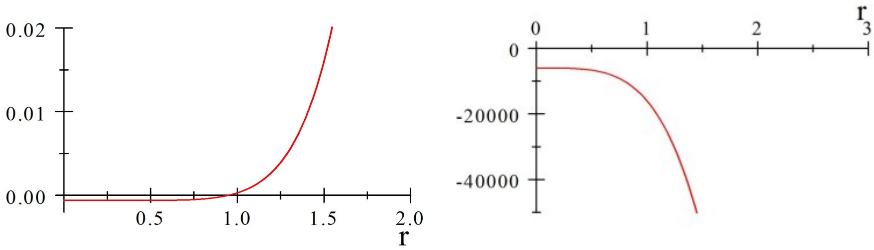

Fig. 2 – The equation $f(r) = 0$ has a) one positive root; b) no positive root at all

c) Let $f(r) = 0$ for $A = 1$, $B = 1$, $C = 100$, $M = 1000$:

$$r^7 \exp(-r) - 10000r^4 - 6000 = 0. \tag{24}$$

This equation has no positive root at all (see Fig. 2b). In this case there is no equilibrium at all.

4. CONCLUDING REMARKS

To find equilibria of the two-body problem associated to a Buckingham type potential is complicated because the potential has an exponential part. Nevertheless, we removed the exponential from the compatibility relations, obtaining a starting algebraic equation, which permits a disscution for all possible values of parameters of the field and the angular momentum constant in the three cases: negative, zero, and positive energy. We found the number of equilibria for each such case. Our problem admits equilibria even in the case of nonnegative energy. This situation is not encountered within the two-body problem in the Newtonian field, where equilibria occur only for negative-energy levels.

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