TWO-BODY PROBLEM ASSOCIATED TO BUCKINGHAM POTENTIAL. COLLISION AND ESCAPE DYNAMICS

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Abstract. We consider a first insight into the two-body problem associated to the potential proposed by Richard Buckingham in 1938. We describe two limit situations of motion, collision and escape, and provide the symmetries that characterize the problem. First, we use the McGehee transformations to remove the collision singularity and the escape singularity, and to replace them by manifolds pasted on the phase space. We study the flows on these manifolds and we provide information on the behavior of nearby orbits. Finally, we present the symmetries that characterize the vector field in cartesian and polar coordinates. These symmetries form isomorphic Abelian groups endowed with an idempotent structure.

Key words: celestial mechanics, two-body problem, Buckingham potential, collision, escape, symmetries.

1. INTRODUCTION

The Buckingham potential is a function proposed by Richard Buckingham in a theoretical study of the equation of state for gaseous helium, neon and argon (Buckingham, 1938). It describes the Pauli repulsion energy 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 constants. The Buckingham potential is a simplification of the Lennard-Jones potential (for Lennard-Jones potential and its astronomical connotations see Mioc *et al.*, 2008a, Mioc *et al.*, 2008b). In this paper, we approach some aspects of the two-body problem associated to a Buckingham potential of the form (1). This type of potential covers many physical situations, similar to the Lennard-Jones potential, but here we are interested only in some mathematical aspects of the dynamics in this framework.

In Section 2 we present the basic equations of the problem, reduced to a central-force problem. We write the equations of motion and the Hamiltonian with the Buckingham potential. Then we have the first integrals that characterize the problem: the energy integral and the angular momentum integral. In Section 3, the McGehee transformations are used to remove the collision singularity and to obtain regularized equations of motion. In Section 4, the collision singularity is replaced by the collision manifold, which is homeomorphic to a 2D torus. We describe the flow on this manifold and emphasize some properties of this limit situation. In the escape dynamics, exactly as in the previous limit case, we define the infinity manifold (that replaces the singularity given by infinite distance) and describe the flow on it. In Section 5 we show that the corresponding vector fields (in cartesian and polar coordinates) exhibit symmetries that form eight-element Abelian groups endowed with an idempotent structure.

2. BASIC EQUATIONS OF MOTION

Because the Buckingham potential is central, the associated two-body problem can be reduced to a central-force problem. The motion is confined to a plane, where we fix one particle as centre at the origin of this plane $\mathbf{R}^2$ and study the relative motion of the other particle. We denote the position (or configuration) vector of this particle by $\mathbf{q}=(q_1,q_2)\in\mathbf{R}^2$ 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, B and M are constants and the kinetic energy of the unit-mass particle is

$$T(\mathbf{p}) = \frac{|\mathbf{p}|^2}{2}. \tag{3}$$

The motion is described by the equations

$$\dot{\mathbf{q}} = \frac{\partial H}{\partial \mathbf{p}}, \qquad \dot{\mathbf{p}} = -\frac{\partial H}{\partial \mathbf{q}} \tag{4}$$

for the Hamiltonian

$$H(\mathbf{q},\mathbf{p}) = T(\mathbf{p}) - U(\mathbf{q}) = \frac{|\mathbf{p}|^2}{2} - A\exp(-B|\mathbf{q}|) + \frac{M}{|\mathbf{q}|^6}. \tag{5}$$

It follows that

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

These are the basic equations for our research. 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. For given initial conditions $(q_1,q_2,p_1,p_2)(0)\in\mathbf{Q}\times\mathbf{P}$, the existence and uniqueness of a real analytic solution (q_1,q_2,p_1,p_2) of the system (6) are ensured by classical results of the theory of differential equations. This solution is defined locally on some interval (t^-,t^+), where $t^-<0<t^+$ and can be analytically extended to a maximal interval$-\infty\leq\widetilde{t}^-<t^-<t^+<\widetilde{t}^+\leq+\infty$. Due to the symmetry (time-reversibility of motion equations), we may study, without loss of generality, the properties of the solution only on $(\widetilde{t}^-,0]$ namely in the past, or only on $[0,\widetilde{t}^+)$, namely in the future (see Mioc and Stavinschi, 2002; Mioc and Barbosu, 2003). Therefore we may confine our study to the interval $[0,\widetilde{t}^+)$. We denote $t^*=\widetilde{t}^+$. If $t^*<\infty$, one says that the solution encounters a singularity. In our case the equations of motion have an isolated singularity at the origin, which corresponds to a collision.

Using a standard technique, we find that the Hamiltonian function (5) is a first integral of the system (6), called the integral of energy:

$$H(\mathbf{q},\mathbf{p})=\frac{h}{2}=\text{const.} \tag{7}$$

where h is the energy constant.

The field $U(\mathbf{q})$ being central, the angular momentum is conserved, hence we obtain another first integral

$$L(\mathbf{q},\mathbf{p})=q_1p_2-q_2p_1=C=\text{const.} \tag{8}$$

where C stands for the constant of angular momentum.

3. McGEHEE - TYPE TRANSFORMATIONS

We observe that the potential (2), the motion equations (6) and the energy integral (7) have an isolated singularity for $t=t^*$, at the origin $\mathbf{q}=(0,0)$. This singularity corresponds to a collision particle-centre (see Mioc and Stavinschi, 2000). In what follows we will apply a sequence of McGehee-type transformations of the second kind (McGehee, 1974) to remove and to regularize the equations (6). Thus, we obtain the equations of motion and the first integrals into a simple form, which allows a qualitative analysis.

The first step is the introduction of standard polar coordinates (r,θ) and polar components of the velocity (ξ,η) using the real analytic diffeomorphism

$$\mathbf{Q}\times\mathbf{P}\times[0,t^*)\to(0,\infty)\times[0,2\pi]\times\mathbf{R}\times\mathbf{R}\times[0,t^*)$$

$$((q_1,q_2),(p_1,p_2),t)\mapsto(r,\theta,\xi,\eta,t)$$

$$\begin{aligned} r&=|\mathbf{q}|\\ \theta&=\arctan\left(\frac{q_2}{q_1}\right)\\ \xi&=\dot r=\frac{q_1p_1+q_2p_2}{|\mathbf{q}|}\\ \eta&=r\dot\theta=\frac{q_1p_2-q_2p_1}{|\mathbf{q}|}. \end{aligned} \tag{9}$$

We obtain

$$\begin{aligned} \dot r&=\xi\\ \dot\theta&=\frac{\eta}{r}\\ \dot\xi&=\frac{\eta^2}{r}-AB\exp(-Br)+6M\frac{1}{r^7}\\ \dot\eta&=-\frac{\xi\eta}{r}, \end{aligned} \tag{10}$$

while the first integrals (7) and (8) become respectively

$$\begin{gathered} \xi^2+\eta^2-2A\exp(-Br)+2M\frac{1}{r^6}=h\\ r\eta=C. \end{gathered} \tag{11}$$

The second step is to scale down the velocity components via the real analytic diffeomorphism:

$$(0,\infty)\times[0,2\pi]\times\mathbf{R}\times\mathbf{R}\times[0,t^*)\to(0,\infty)\times[0,2\pi]\times\mathbf{R}\times\mathbf{R}\times[0,t^*)$$

$$\begin{gathered} (r,\theta,\xi,\eta,t)\mapsto(r,\theta,x,y,t)\\ x=r^3\xi\\ y=r^3\eta. \end{gathered}$$

The equations of motion (10) become

$$\begin{aligned} \dot r&=\frac{x}{r^3}\\ \dot\theta&=\frac{y}{r^4}\\ \dot x&=\frac{3x^2+y^2}{r^4}-ABr^3\exp(-Br)+6M\frac{1}{r^4}\\ \dot y&=\frac{2xy}{r^4}. \end{aligned} \tag{12}$$

The first integrals (11) now read respectively

$$x^2+y^2=hr^6+2Ar^6\exp(-Br)-2M \tag{13}$$

$$y=Cr^2. \tag{14}$$

We observe that the singularity at $r=0$ still persists in (12). To remove it, we rescale the time through the real analytic diffeomorphism

$$(0,\infty)\times[0,2\pi]\times\mathbf{R}\times\mathbf{R}\times[0,t^*)\to(0,\infty)\times[0,2\pi]\times\mathbf{R}\times\mathbf{R}\times[0,\infty)$$

$$(r,\theta,x,y,t)\mapsto(r,\theta,x,y,s),$$

defined by

$$ds=r^{-4}dt.$$

Keeping by abuse the same notation for the new functions of the timelike variable s and $'=d/ds$, the equations of motion (12) become:

$$\begin{aligned} r' &= rx\\ \theta' &= y\\ x' &= 3x^2+y^2-ABr^7\exp(-Br)+6M\\ y' &= 2xy. \end{aligned} \tag{15}$$

The first integrals (13) and (14) keep the same expressions.

4. COLLISION AND ESCAPE

In this section, we want to study the flow in McGehee-type coordinates. We observe that both the equations of motion (15) and the first integrals (13) and (14) are well defined for the boundary $r=0$. Thus the phase space of the McGehee-type coordinates can be analytically extended to contain the manifold

$$E_{col}=\{(r,\theta,x,y)\,|r=0\},$$

which is invariant to the flow because $r'=0$ for $r=0$. The integrals (13) and (14) also extend smoothly to this boundary. Now, let us consider h to be a parameter, and define the constant-energy manifold

$$E_h=\left\{(r,\theta,x,y)\,|x^2+y^2=hr^6+2Ar^6\exp(-Br)-2M\right\},$$

which corresponds to a fixed level of energy. Then the *collision manifold* is

$$E_0=E_{col}\cap E_h=\left\{(r,\theta,x,y)\,|r=0,\ \theta\in S^1,\ x^2+y^2=-2M\right\}, \tag{16}$$

where S^1 is the segment $[0,2\pi]$ with the end points $\theta=0$ and $\theta=2\pi$ identified. We will understand the flow on this invariant manifold E_0 as the behavior of the flow near collision. The continuity of solutions with respect to initial data allows us to study the near-collisional orbits.

For $M > 0$, E_0 is the empty set. In this situation, the particle can approach the centre no matter how close, but cannot collide with it.

For $M = 0$, E_0 reduces to a circle.

For $M < 0$, E_0 is homeomorphic to a 2D cylinder in 3D space of the coordinates $(\theta, x, y) \in S^1 \times \mathbf{R}^2$. The cylinder E_0 may also be considered homeomorphic to a 2D torus, both actually imbedded in the 4D full phase space of the McGehee-type coordinates (r, θ, x, y). In what follows, we shall describe the flow on E_0. Using (15) and (13), the vector field on E_0 is

$$\begin{aligned} \theta' &= y \\ x' &= -2y^2 \\ y' &= 2xy. \end{aligned} \tag{17}$$

From (17) we observe that the flow on E_0 (in the torus representation) admits two circles of degenerate equilibria: the upper circle

$$UC = \left\{ (\theta_0, x, y) \mid x = \sqrt{-2M},\ y = 0 \right\}$$

and the lower circle

$$LC = \left\{ (\theta_0, x, y) \mid x = -\sqrt{-2M},\ y = 0 \right\},$$

with arbitrary $\theta_0 \in S^1$. Thus, the flow on E_0 consists of periodic orbits if $y \neq 0$, and of circles formed by degenerate equilibria if $y = 0$, in which case $x = \pm\sqrt{-2M}$. From the second equation of (17) we observe that the flow on E_0 is gradientlike with respect to the x-coordinate and $x' < 0$ for $y \neq 0$, hence the orbits on E_0 are heteroclinic and move from UC to LC. We can deduce the slope of these trajectories by putting

$$x = \sqrt{-2M}\sin\alpha, \qquad y = -\sqrt{-2M}\cos\alpha.$$

We have

$$\theta' = -\sqrt{-2M}\cos\alpha, \qquad \alpha' = -2\sqrt{-2M}\cos\alpha.$$

It follows that $\dfrac{d\alpha}{d\theta} = 2$. Fig.1 illustrates the flow on E_0.

All orbits on E_0 tend asymptotically, in infinite (fictitious) time, to the stationary solutions LC. By (14), we observe that collisions occur for $C = 0$, when we have rectilinear, radial motion. The collisions correspond to the halfplane $(x > 0,\ y = 0)$, whereas ejections correspond to the half-plane $(x < 0,\ y = 0)$.

On the other hand, since the variable θ does not appear explicitly in the equations (15) and in the relations (13) and (14), it means that the flow is invariant to rotations, so we can factorize it by S^1. Thus, we reduce the dimension of the phase space from 4 to 3. After this factorization, the collision manifold E_0 becomes a circle in the three-dimensional reduced phase space of the coordinates $(r, x, y) \in [0, \infty) \times \mathbf{R}^2$,

$$\widetilde{E_0} = \left\{ (r, x, y) \,|\, r = 0,\ x^2 + y^2 = -2M \right\}. \tag{18}$$

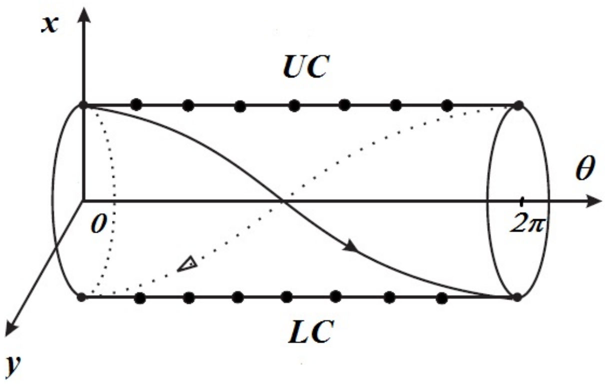

Fig. 1 – The flow on E_0.

The circles of equilibria on the torus are represented by two points on this circle. The other points on the collision-manifold circle correspond to the periodic orbits on the torus. In general, in the unreduced phase space, all orbits are manifolds consisting of the product between an orbit and S^1.

Now, we approach the escape dynamics. We consider $B > 0$. We shall use a new sequence of McGehee-type transformations for the equations of motion (15) and the first integrals (13) and (14). These transformations are real analytic diffeomorphisms. The first step is the McGehee-type transformation of the first kind (McGehee, 1973)

$$\rho = \frac{1}{r},$$

which brings the infinity at origin making it turn to the singularity $\rho = 0$. To remove this singularity, we resort to

$$u = \rho^3 x$$
$$y = \rho^3 y,$$

which rescale the velocity components, and

$$\mathrm{d}\tau = \rho^{-4} ds,$$

which rescales the time. We obtain the following equations of motion:

$$\begin{aligned}\frac{\mathrm{d}\rho}{\mathrm{d}\tau} &= -u\rho^2 \\ \frac{\mathrm{d}\theta}{\mathrm{d}\tau} &= \rho v \\ \frac{\mathrm{d}u}{\mathrm{d}\tau} &= \rho v^2 - AB\exp(-B/\rho) + 6C\rho^7 \\ \frac{\mathrm{d}v}{\mathrm{d}\tau} &= -\rho u v.\end{aligned} \tag{19}$$

The first integrals (13) and (14) become

$$u^2+v^2=-2C\rho^6+2A\exp\left(-B/\rho\right)+h \tag{20}$$

and

$$v=C\rho. \tag{21}$$

We remark that the equations of motion and first integrals make sense when $\rho\to 0$. So, the phase space of the McGehee-type coordinates can be analytically extended to include the manifold

$$E_{esc}=\left\{(\rho,\theta,u,v)\,|\rho=0\right\},$$

which is invariant to the flow, because $\dfrac{\mathrm{d}\rho}{\mathrm{d}\tau}=0$ for $\rho=0$. The integrals (20) and (21) also extend to this manifold. Let us define:

$$\begin{aligned}\widetilde{E}_h &= \left\{(\rho,\theta,u,v)\,|\rho\neq 0,\ u^2+v^2=-2C\rho^6+2A\exp\left(-B/\rho\right)+h\right\}\cup\\ &\cup\left\{(\rho,\theta,u,v)\,|\rho=0,\ u^2+v^2=h\right\},\end{aligned}$$

which corresponds to a fixed level of energy. The intersection $E_\infty=E_{esc}\cap\widetilde{E}_h$ is

$$E_\infty=\left\{(\rho,\theta,u,v)\,|\rho=0,\ \ \theta\in S^1,\ u^2+v^2=h\right\},$$

will be called the *infinity manifold*. For $h<0$, E_∞ is the empty set (in other words, for negative energy levels, the particle cannot escape). For $h=0$, E_∞ reduces to a circle

$$E_\infty=\left\{(\rho,\theta,u,v)\,|\rho=0,\ \ \theta\in S^1,\ u=0,\ v=0\right\}.$$

For $h>0$, E_∞ is homeomorphic to a 2D cylinder in the 3D space of the coordinates $(\theta,u,v)\in S^1\times\mathbf{R}^2$. This cylinder may also be considered homeomorphic to a 2D torus (see Section 4), both actually imbedded in the 4D full phase space of the coordinates (ρ,θ,u,v). There are two circles of degenerate equilibria: the upper circle

$$UC=\left\{(\theta_0,u,v)\mid u=\sqrt{h},\ v=0\right\}$$

and the lower circle

$$LC=\left\{(\theta_0,u,v)\mid u=-\sqrt{h},\ v=0\right\},$$

with arbitrary $\theta_0\in S^1$. We can deduce the slope of these trajectories by putting

$$u=\sqrt{h}\sin\alpha,\qquad v=-\sqrt{h}\cos\alpha.$$

We have

$$\theta'=-\sqrt{h}\cos\alpha,\qquad \alpha'=0.$$

It follows that $\dfrac{\mathrm{d}\alpha}{\mathrm{d}\theta}=0$. Fig. 2 illustrates the flow on E_∞.

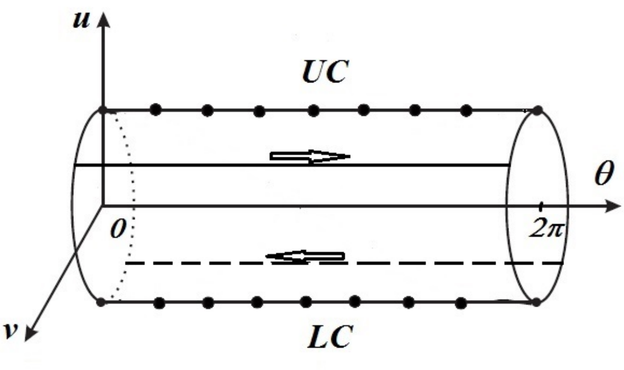

Fig. 2 – The flow on E_∞.

5. SYMMETRIES

In this section we approach the symmetries characteristic to our model based on the Buckingham potential. We show that the corresponding vector fields present symmetries that form isomorphic Abelian groups endowed with an idempotent structure. This approach was used for various fields in Mioc *et al.* (2008b), Mioc (2002a), Mioc (2002b), Mioc and Barbosu (2003), and is also valid for the Buckingham potential. Here we will follow the cited papers.

Explicitly, the vector field (4) corresponding to cartesian coordinates is given by (6).

These equations exhibit eight symmetries $S_i = S_i\,(q_1, q_2, p_1, p_2, t)$, $i = 0, 1, ..., 7$, as follows:

$$\begin{aligned}
S_0 &= (q_1, q_2, p_1, p_2, t) = I \\
S_1 &= (q_1, q_2, -p_1, -p_2, -t) \\
S_2 &= (q_1, -q_2, p_1, -p_2, t) \\
S_3 &= (-q_1, q_2, -p_1, p_2, t) \\
S_4 &= (q_1, -q_2, -p_1, p_2, -t) \\
S_5 &= (-q_1, q_2, p_1, -p_2, -t) \\
S_6 &= (-q_1, -q_2, -p_1, -p_2, t) \\
S_7 &= (-q_1, -q_2, p_1, p_2, -t)\,,
\end{aligned}$$

that map solution onto solution. Moreover, we observe that S_1, S_2, S_3 are independent and they generate the other four symmetries:

$$\begin{aligned}
S_4 &= S_1 \circ S_2 \\
S_5 &= S_1 \circ S_3 \\
S_6 &= S_2 \circ S_3 \\
S_7 &= S_1 \circ S_2 \circ S_3.
\end{aligned}$$

A similar structure is obtained for any three symmetries considered as independent of each other.

The set $G = \{S_i | i = \overline{0,7}\}$ (where $S_0 = I$ is the identity), endowed with the composition law "$\circ$", forms a symmetric Abelian group. To prove this, it is easy to construct the composition table, observing that every element of G is its own inverse. $(G, \circ)$ is an Abelian group of order eight with three generators of order two. Thus, G is isomorphic to $\mathbf{Z}_2 \times \mathbf{Z}_2 \times \mathbf{Z}_2$.

The results obtained for cartesian coordinates can be transposed to standard polar coordinates. The corresponding vector field (10) has eight symmetries $S_i^{pol} = S_i^{pol}(r, \theta, \xi, \eta, t)$, $i \in \{0, 1, ..., 7\}$, as follows:

$$\begin{aligned}
S_0^{pol} &= (r, \theta, \xi, \eta, t) = I^{pol} \\
S_1^{pol} &= (r, \theta, -\xi, -\eta, -t) \\
S_2^{pol} &= (r, -\theta, \xi, -\eta, t) \\
S_3^{pol} &= (r, \pi - \theta, \xi, -\eta, t) \\
S_4^{pol} &= (r, -\theta, -\xi, \eta, -t) \\
S_5^{pol} &= (r, \pi - \theta, -\xi, \eta, -t) \\
S_6^{pol} &= (r, \pi + \theta, \xi, \eta, t) \\
S_7^{pol} &= (r, \pi + \theta, -\xi, -\eta, -t) .
\end{aligned}$$

The set $G^{pol} = \{S_i^{pol} | i = \overline{0,7}\}$ (where $S_0^{pol} = I^{pol}$ is the identity), endowed with the composition law "$\circ$", forms a symmetric Abelian group, noting that every element of G is its own inverse. G^{pol} is isomorphic to $\mathbf{Z}_2 \times \mathbf{Z}_2 \times \mathbf{Z}_2$.

The groups G and G^{pol} are diffeomorphic to each other, considering the real analytic diffeomorphism

$$\begin{gathered}
\left(\mathbf{R}^2 \setminus \{(0,0)\}\right) \times \mathbf{R}^3 \to (0, \infty) \times S^1 \times \mathbf{R}^3, \\
(q_1, q_2, p_1, p_2, t) \mapsto (r, \theta, \xi, \eta, t) .
\end{gathered}$$

The symmetries revealed above show the existence of many other solutions, for each solution proved to exist. In terms of the physical motion, the transformations corresponding to each variable have the following meaning (for more details see Mioc and Barbosu, 2003; Mioc *et al.*, 2008b):

– $(t \to -t)$ corresponds to motion in the future/past;

– $(\xi \to -\xi)$ means motion performed outwards/inwards;

– $(\eta \to -\eta)$ means clockwise/counterclockwise motion;

– $(\theta \to -\theta)$, $(\theta \to \pi - \theta)$, $(\theta \to \pi + \theta)$ correspond to positions shifted each other by 2θ, $\pi - 2\theta$ and π, respectively.

6. CONCLUSIONS

The two-body problem associated to the Buckingham potential has similarities with problems associated to different potentials. The collision manifold does not depend on the energy constant h (so every energy level shares this manifold), but it depends on the field parameter M, such that collisions are possible only for non-positive values of M. The infinity manifold essentially depends on h and escape is possible only for nonnegative energy levels. Collisions occur only for zero angular momentum (radial motion), whereas escape is also possible for nonzero angular momentum (spiral motion). Both collision and infinity manifolds constitute manifolds of equilibria for the global flow in full phase space (each one on its own time scale). The equations of motion, expressed in cartesian or polar coordinates present symmetries that form eight-element Abelian groups endowed with an idempotent structure, which are isomorphic.

This paper represents the first part of a study concerning the dynamics which corresponds to the Buckingham potential.

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