Complete Description of the Static Level Sets for the System of Two Particles under a Van der Waals Potential

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***Abstract*— We study the orbits around of a two particle system under a pairwise good potential like the one of Van der Waals. We show that the levels sets are completely determined by polynomials at most four degree that can be factorized by means of standard algebraic procedures, such as the methods of Cardan and Ferrari. The distribution of real positive roots determine the level curves and provides a complete description of the map of the equipotential zones. We show that our methods can be generalized to a family of polynomials with degree multiple of 2, 3, and 4. We carry out a comparison with numerical simulations, with the true orbits, and 2-d and 3-d pictures depicting the true isopotential zones.**

Keywords: Pairwise good potential, solubility by radicals, Levels set, Equipotential Surfaces.

I. Introduction

The study of clusters of massless non-interactive particles under a potential fields has been approached, roughly speaking, under two view points: the one that considers the dynamics given by Newton's equations associated to the potential, and the one that considers static particles. The latter is related among others, to theoretical and experimental research in crystal formation, plasticity and swarming phenomena, whereas the former is connected with research in control theory, astrophysics and celestial mechanics. Another line of research involving pairwise good potentials and control of chaos concerns to the dynamical analysis and control of micro cantilevers as single mode approximation for tackling interactions under Van der Waals potential, see for instance [?].

In the study of the N-body problem, several pairwise good potential have been utilized for describing relative equilibria and central configurations, see for instance [?], the methods there include classical dynamical systems as well as non-linear geometric control techniques [?]. In finite elastoplasticity, Lie groups and algebras have been recently applied, for instance in [?], A. Mielke associates to the plastic tensor a certain element of a Lie group, and to the plastic dissipation a Finsler metric of the same Lie group. Following this approach, D. Mittenhuber [?], has solved the problem of 4-slip system in the plane with orthogonal slip directions by computing the associated dissipation metric as the solution of an optimal control problem.

We are interested in clusters of non-interactive particles under pairwise good potentials, our research points to the optimal control problems of optimal path planning, collision free navigation and crystal formation on equipotential zones of clusters. In this paper, we restrict ourselves to the study of the equipotential zones for a system of two static non interactive particles, as the preliminary step for continuing the control theoretic approach of the aforementioned problems.

In the literature, numerical methods of mathematical numerical software is commonly used to generate graphics of levels set or orbits. However, there are few algebraic methods and techniques for determining the shape of the surfaces or curves or dots of the potential energy surface (PES) even for small clusters. The novelty of our approach is to solve the implicit function problem of the determination of the levels sets using the algebraic methods for solving polynomials by radicals. With our methods, the exact solution of an orbit is obtained as a function. We also show that a numerical approximation could give a "good" numerical approximation to the solution that is visually similar to the true orbit.

To the best of our knowledge, most of the reported research on clusters of particles under a well pair potential is focused on methods for the problem of search of optimal clusters, see for instance [?], [?], [?], [?], [?], and the references therein. In this paper we take a different approach from numerics, although we include some for the purpose of comparison.

As we mentioned before, this is a first step of a general research program that pretends to tackle optimal control problems on clusters under pairwise good potentials.

The paper is organized as follows, in section II, we depict the notation of the problem, the general description of our approach, and our main result. Section III contains the description of algebraic procedures along with brief historical recount. In section IV we present a comparison of numerical and algebraic results. At the end in section V, we derive some conclusions and generally describe some of the future lines of research.

II. Notation and Problems

For a given metric d in $\mathbb{R}^3$, a smooth function $P : \mathbb{R}^+ \to \mathbb{R}$ is well pairwise good potential if satisfies the following conditions:

1) Infinite reject to avoid destroying or collapsing particles $\lim_{d\to 0} P(d) = \infty$.
2) A negative basin around a minima distance $d^\star = \arg\min_{d\in(0,\infty)} P(d)$.
3) Asymptotic attraction, $\lim_{d\to\infty} P(d) = 0^-$.

An elementary model of the Van der Waals that complies the previous properties is the following

$$B\left(d\right) = \frac{1}{d^4} - \frac{2}{d^2}.$$

This function has its minima at $d^\star = 1$, $B\left(d^\star\right) = -1$.

For a group of three particles $p_i = (x_i, y_i, z_i) \in \mathbb{R}^3$, $i = 1, 2, 3$, with the Euclidian metric $\sqrt{d_{ij}} = \sqrt{(x_i - x_j)^2 + (y_i - y_j)^2 + (z_i - z_j)^2}$ one has

$$B\left(p_1, p_2, p_3\right) = \sum_{1\le i<j\le 3} \frac{1}{\left(d_{ij}\right)^2} - \frac{2}{d_{ij}}.$$

The well know Lennard-Jones potential (LJ 12-6) is the following

$$J(d) = \frac{1}{d^{12}} - \frac{2}{d^6},$$

which has its minima at $d^\star = 1$, $J\left(d^\star\right) = -1$. For three particles with the Euclidian metric one has

$$J_E\left(p_1, p_2, p_3\right) = \sum_{1\le i<j\le 3} \frac{1}{\left(d_{ij}\right)^6} - \frac{2}{\left(d_{ij}\right)^3}.$$

But using the metric

$$\sqrt[6]{(x_i - x_j)^2 + (y_i - y_j)^2 + (z_i - z_j)^2}$$

the potential LJ(12-6) yields B, i.e.,

$$J_{\sqrt[6]{\cdot}}\left(p_1, p_2, p_3\right) = B\left(p_1, p_2, p_3\right).$$

We consider the problem of determining the orbits of a system of two given particles and one free under potential B, hereafter shall be called B_2.

Without lost of generality, we can assume $p_1 = (-\frac{l}{2}, 0, 0), p_2 = (\frac{l}{2}, 0, 0)$ where the distance $l > 0$ between them is fixed. Let be $p = (x, y, z) \in \mathbb{R}^3$ a free particle, then the complete potential of this system is the following

$$\begin{aligned} B_2\left(x, y, z\right) = \; & \frac{1}{\left((x+\frac{l}{2})^2+y^2+z^2\right)^2} - \frac{2}{(x+\frac{l}{2})^2+y^2+z^2} + \\ & \frac{1}{\left((x-\frac{l}{2})^2+y^2+z^2\right)^2} - \frac{2}{(x-\frac{l}{2})^2+y^2+z^2} + \\ & K_l. \end{aligned}$$

where $K_l = \frac{1}{l^4} - \frac{2}{l^2}$ is the corresponding potential between p_1 and p_2, which is constant.

An orbit of B_2 of value G is the set $\{(x, y, z) \in \mathbb{R}^3 \,|\, B_2\left(x, y, z\right) = G\}$. The values of G correspond to the range of B_2. Therefore, $G \in [m_l, \infty)$ where $l > 0$ is distance for a given system of two particles and

$$m_l = \min_{(x,y,z)\in\mathbb{R}^3} B_2(x, y, z).$$

The symmetry of $B_2\left(x, y, z\right)$ with respect to the third coordinate allow us to reduce the problem to $\mathbb{R}^2$. Moreover,

$$B_2\left(x, y\right) = B_2\left(x, -y\right) = B_2\left(-x, -y\right) = B_2\left(-x, y\right).$$

Therefore, it is only necessary to consider the orbits of B_2 of value G as the sets $O(l, G) = \{(x, y) \in \mathbb{R}^{+2} \,|\, B_2\left(x, y\right) = G\}$, where $R^+ = [0, \infty)$, $l > 0$ is the distance between the given system of two particles, $G \in [m_l, \infty)$. The corresponding 3D model can be constructed by appropriate rotations.

Our methodology is based on:

- The algebraic methods of Cardan and Ferrari.
- For a given $G = G_x$, the equation
$$B_2(x, y) = G$$
yields a third or fourth degree polynomial with coefficients in the ring $\mathbb{R}[x]$, that we solve to obtain an exact root $r(x, G, l)$.
- If $r(x, G, l) \ge 0$ is a root, then the orbit $O(l, G)$ is given as follows $\{(x, y) \,|\, x > 0, y = \sqrt{r(x, G, l)}\}$.

Let state our the main proposition

Proposition 2.1: Given a system of two particles, $p_1 = (-\frac{l}{2}, 0, 0), p_2 = (\frac{l}{2}, 0, 0)$ at distance l. The orbits $O(l, G)$ of B_2, for $G \in [m_l, \infty)$, correspond to the positive roots of the third and fourth degree polynomial obtained from the equation:

$$B_2\left(x, y\right) - G_l = 0. \tag{II.1}$$

Proof:

The equation II.1 gives:

$$\begin{aligned} &\left(\left(x - \tfrac{l}{2}\right)^2 + y^2\right)^2 - \\ &2\left(\left(x + \tfrac{l}{2}\right)^2 + y^2\right)\left(\left(x - \tfrac{l}{2}\right)^2 + y^2\right)^2 + \\ &\left(\left(x + \tfrac{l}{2}\right)^2 + y^2\right)^2 - \\ &2\left(\left(x - \tfrac{l}{2}\right)^2 + y^2\right)\left(\left(x + \tfrac{l}{2}\right)^2 + y^2\right)^2 - \\ &\left(K\left(l\right) + G\right) \\ &\left(\left(x + \tfrac{l}{2}\right)^2 + y^2\right)^2\left(\left(x - \tfrac{l}{2}\right)^2 + y^2\right)^2) = 0. \end{aligned}$$

It has power on x or y as $8, 6, 4, 2$ when $(K_l + G) \neq 0$ and it has power on x or y as $6, 4, 2$ when $(K_l + G) = 0$.

We let now $u = y^2$ the following third and fourth degree equations are obtained:

$$\begin{aligned} \left(1024Gx^2 + 256G + 1280 + 1024x^2\right)u^3 &\;+ \\ 352 + 256Gx^2 + 3328x^2 &\;+ \\ 1536Gx^4 + 1536x^4 + 96G)u^2 &\;+ \\ (-256Gx^4 + 1024Gx^6 - 576x^2 - 48 &\;- \\ 64Gx^2 + 2816x^4 + 16G + 1024x^6)u &\;- \\ 15 + G - 16Gx^2 + 96Gx^4 &\;- \\ 256Gx^6 + 256Gx^8 &\;- \\ 848x^2 - 672x^4 + 768x^6 + 256x^8 &\;= \;0, \end{aligned} \tag{II.2}$$

$$
\begin{aligned}
(256G + 256K_l)\, u^4 &\quad + \\
\left(1024Gx^2 + 256G + 1280 + 1024x^2\right) u^3 &\quad + \\
352 + 256Gx^2 + 3328x^2 &\quad + \\
1536Gx^4 + 1536x^4 + 96G)u^2 &\quad + \\
(-256Gx^4 + 1024Gx^6 - 576x^2 - 48 &\quad - \\
64Gx^2 + 2816x^4 + 16G + 1024x^6)u &\quad - \\
15 + G - 16Gx^2 + 96Gx^4 &\quad - \\
256Gx^6 + 256Gx^8 &\quad - \\
848x^2 - 672x^4 + 768x^6 + 256x^8 &\quad = \quad 0 \quad \text{(II.3)}
\end{aligned}
$$

The roots of them are constructed by the methods of Cardan and Ferrari in the complex numbers, $\mathbb{C}$. Therefore, $O(l, G) = \{(x, y) \,|\, x > 0, y = \sqrt{r(x, G, l)}, r(x, G, l) \geq 0\}$. ■

Remark 2.2: The construction of the roots is not done by mathematical software, but it is done by finding and replacing the parameters of the formulas of the methods of Cardan and Ferrari with the coefficients of the polynomials of the equations II.2 and II.3.

Proposition 2.3: For the system of the previous proposition, when $l = 1$, we have

1) $m_1 = -3$.
2) $O(1, -3) = \{(0, \frac{\sqrt{3}}{2})\}$, i.e., it is a point the root of fourth degree equation for $G_1 = -3$.
3) There are two orbits from the roots of fourth degree equation with $G_1 \in [m, -1)$.
4) There is one orbit from the roots of fourth degree equation with $G_1 \in (-1, \infty)$.

Proof: It follows by direct substitution of $l = 1$ in the resulting roots of the previous proposition. ■

Remark 2.4: Also for $l = 1$ the figure 3 depicts some examples of the orbits. The free point and the other two particles form an equilateral triangle of size 1, and minimum is $B_2(0, \frac{\sqrt{3}}{2}) = -3 = m_1$. There is one orbit from the roots of third degree equation with $G_1 = -1$, the details are given in section IV.

Also, this result follows:

Proposition 2.5: The Polynomials $Ax^{2k} + Bx^k + C$, $Ax^{3k} + Bx^{2k} + Cx^k + D$, $Ax^{4k} + Bx^{3k} + Cx^{2k} + Dx^k + E$ $k > 1$ are solvable by radicals.

Proof: Let be $u = x^k$. ■

III. Solving Polynomial by radicals

The Galois theory is the algebraic framework for the study of roots of polynomials. It is not focus in numerical estimations but in the construction of formulæ using radicals. For numerical estimation there is for instance the well know method of Newton–Raphson. Instead, the Galois theory is about the structure and characteristics of the groups of polynomials that can be solved by a formula using radicals. In this work, we are interested in applying the known methods for polynomials which are solvable by radicals. That is, for a polynomial, we want to write its roots by means formulæ involving its coefficients, arithmetic operations, and radicals.

It is known that there is not a general method or formula to find the polynomial's roots with degree $n \geq 5$. However, there are general formulas for polynomials with coefficient in $\mathbb{R}$ when $n \leq 4$.

The Babylonians at 1600 AC knew that the quadratic polynomial $f(x) = x^2 + 2px + q$ is solvable by the completing squares, by writing $f(x) = (x + p)^2 + q - p^2$, the roots are given by $-p \pm \sqrt{p^2 - q}$.

The cubic polynomial $f(x) = x^3 + ax^2 + bx + c$, was solved at the 16th century by more complicated formula found simultaneously by Ferro and Tartaglia. For the fourth degree polynomial $f(x) = x^4 + ax^3 + bx^2 + cx + d$, Ferrari provided a procedure. These methods were published by Cardano in the *Ars Magna* at 1545. In 18th century, Lagrange unified these methods for a polynomial with degree $n \leq 4$ using what now is know as the Lagrange's resolvent. This method involves an auxiliary equation with a polynomial with degree less than one, i.e., it uses, for example, a third degree polynomial to solve the fourth degree polynomial. In fact, this is the procedure for solving the quadratic polynomial. However, this method fails for the polynomials of degree 5, because the auxiliary polynomial is of degree 6. Ruffini at 1799, and Abel at 1824 proved that there is not a general formula using radicals for finding the roots of quintic polynomial. Galois by 1832 showed how to associate to each polynomial $f(x)$ a subgroup $Gal(f)$ of the symmetric group, call the Galois group of $f(x)$, and established the following result, for details see for instance [?]

Theorem 3.1: (Galois) A polynomial f is soluble by radicals if and only if its group $Gal(f)$ is soluble.

As an application of these algebraic techniques we have the following result.

Proposition 3.2: Given a system of two particles, $p_1 = (-\frac{l}{2}, 0, 0), p_2 = (\frac{l}{2}, 0, 0)$, at distance l, the critical points of $B_2(x, y)$ are the following

1) $(0, 0)\ \forall l \geq 0$.
2) $(\pm x^\star, 0)$, $x^\star$ is a positive root of the polynomial obtained from substituting $y = 0$ in $\frac{\partial}{\partial x} B_2(x, y)$ with $l > 2$. The points $(\pm x^\star, 0)$ are collinear with p_1, p_2.
3) $(0, \pm y^\star)$ where $y^\star$ is a positive root of the polynomial obtained from substituting $x = 0$ in $\frac{\partial}{\partial y} B_2(x, y)$. The points $(0, \pm y^\star)$ correspond to the oppositive vertex of an isosceles triangle of the side with vertices p_1, p_2.

Proof: The polynomial to solve come from the first optimality condition: $\frac{\partial}{\partial x} B_2(x, y) = 0$ and $\frac{\partial}{\partial y} B_2(x, y) = 0$, where

$$\frac{\partial}{\partial x} B_2(x, y) = -4 \frac{(x \pm \frac{l}{2})}{\left((x \pm \frac{l}{2})^2 + y^2\right)^3} + \frac{4(x \pm \frac{l}{2})}{\left((x \pm \frac{l}{2})^2 + y^2\right)^2}$$

and

$$\frac{\partial}{\partial y}B_2\left(x,y\right)=-4\frac{y}{\left((x\pm\frac{l}{2})^2+y^2\right)^3}+\frac{4y}{\left((x\pm\frac{l}{2})^2+y^2\right)^2}.$$

Note that from the previous equations, we have that $\nabla B_2(0,0)=0$, for all $l>0$.
Using that $y=0$ gives $\frac{\partial}{\partial y}B_2(x,0)=0$, the equation for $\frac{\partial}{\partial x}B_2(u^{\frac{1}{2}},0)=0$ ($x=u^2$ is changed) is

$$\begin{aligned}-64u^3+\left(64-16l^2\right)u^2 &+ \\ \left(20l^4+160l^2\right)u+\left(20l^4-3l^6\right) &= 0. \qquad \text{(III.1)}\end{aligned}$$

The positive roots of the previous third degree equation give the optimal points.

In a similar way, using that $x=0$ gives $\frac{\partial}{\partial x}B_2(0,u^{\frac{1}{2}})=0$, the equation for $\frac{\partial}{\partial x}B_2(0,u^{\frac{1}{2}})=0$ gives

$$4y^2+l^2-4=0 \qquad \text{(III.2)}$$

The real roots of the previous second degree equation give the optimal points for $l\in[0,2)$. The interval of l come from the restriction of the discriminant of the quadratic equation. ■

In the following paragraphs we summarizes the methods of solubility by radicals on which are based our results.

Quadratic equation

For the quadratic equation $Ax^2+Bx+C=0$ with $A\neq 0$ the roots are given by $x_1=(-B+\sqrt{B^2-4AC})(2A)^{-1}$ and $x_2=(-B-\sqrt{B^2-4AC})(2A)^{-1}$. It is clear that $(x-x_1)(x-x_2)=x^2+(-x_1-x_2)x+x_1x_2$ and $(-x_1-x_2)=BA^{-1}$, $x_1x_2=CA^{-1}$.

For the equation III.2 the roots are $y_1=\frac{1}{2}\sqrt{2^2-l^2}$ and $y_2=-\frac{1}{2}\sqrt{2^2-l^2}$. The real roots are constrained by $2^2-l^2>0$, it is $l\in(0,2]$.

Method of Cardan

For the cubic polynomial $x^3+ax^2+bx+c=0$, we eliminate the quadratic term by writing $x=y-\dfrac{a}{3}$, to obtain $y^3+py+q=0$, where $p=b-\dfrac{a^2}{3}$ and $q=c-\dfrac{ba}{3}+\dfrac{2a^3}{27}$.

We now introduce new variables u and v such that $y=u+v$ and $3uv=-p$ to get $u^3+v^3=-q$. For then, u^3 and v^3 are roots of $(t-u^3)(t-v^3)=0$, which is equivalent to $t^2+qt-\dfrac{p^3}{27}=0$. For these equation the roots are

$$A,B=\frac{-q}{2}\pm\sqrt{\frac{q^2}{4}+\frac{4p^3}{27}}.$$

We take now, $u^3=A$ and $v^3=B$, and extracting the cubic root to get $u=\sqrt[3]{A}$, $\omega\sqrt[3]{A}$, $\omega^2\sqrt[3]{A}$ where 1, ω, ω^2 are the unit cubic roots. We chose $\sqrt[3]{B}$ in such a way that $\sqrt[3]{A}\sqrt[3]{B}=uv=-\frac{p}{3}$ to obtain the following solutions for y

$$\begin{aligned}y_1 &= \sqrt[3]{A}+\sqrt[3]{B}\\ y_2 &= \omega\sqrt[3]{A}+\omega^2\sqrt[3]{B}\\ y_3 &= \omega^2\sqrt[3]{A}+\omega\sqrt[3]{B}\end{aligned}$$

Finally, we write $x=y-\dfrac{a}{3}$ for finding the corresponding solutions x_1, x_2, x_3.

For the general cubic equation $Ax^3+Bx^2+Cx+D=0, A\neq 0$. One gets $x^3+a_1x^2+a_2x+a_3=0$ with $a_1=BA^{-1}$, $a_2=CA^{-1}$, and $a_3=DA^{-1}$. And the above expressions apply.

Equation III.1. $-64u^3+\left(64-16l^2\right)u^2+\left(20l^4+160l^2\right)u+\left(20l^4-3l^6\right)=0$. The coefficients for the Cardan's formulas are the following $A=-64$, $B=\left(64-16l^2\right)$, $C=\left(20l^4+160l^2\right)$, and $D=\left(20l^4-3l^6\right)$.

The first root $x_1(l)=$

$$((-\tfrac{1}{2}(\tfrac{2}{27}(((64-16l^2))(-64)^{-1})^3-\tfrac{1}{3}(((64-16l^2))(-64)^{-1})(((20l^4+160l^2))(-64)^{-1})+(((20l^4-3l^6))(-64)^{-1}))+(\tfrac{1}{27}(((20l^4+160l^2))(-64)^{-1}-\tfrac{1}{3}(((64-16l^2))(-64)^{-1})^2)^3+\tfrac{1}{4}(\tfrac{2}{27}(((64-16l^2))(-64)^{-1})^3-\tfrac{1}{3}(((64-16l^2))(-64)^{-1})(((20l^4+160l^2))(-64)^{-1})+(((20l^4-3l^6))(-64)^{-1}))^2)^{\frac{1}{2}})^{\frac{1}{3}})+((-\tfrac{1}{2}(\tfrac{2}{27}(((64-16l^2))(-64)^{-1})^3-\tfrac{1}{3}(((64-16l^2))(-64)^{-1})(((20l^4+160l^2))(-64)^{-1})+(((20l^4-3l^6))(-64)^{-1}))-(\tfrac{1}{27}(((20l^4+160l^2))(-64)^{-1}-\tfrac{1}{3}(((64-16l^2))(-64)^{-1})^2)^3+\tfrac{1}{4}(\tfrac{2}{27}(((64-16l^2))(-64)^{-1})^3-\tfrac{1}{3}(((64-16l^2))(-64)^{-1})(((20l^4+160l^2))(-64)^{-1})+(((20l^4-3l^6))(-64)^{-1}))^2)^{\frac{1}{2}})^{\frac{1}{3}})-\tfrac{1}{3}(((64-16l^2))(-64)^{-1}).$$

The previous equation gives the optimal points on $(x_1(l),0)$ for $l\geq 2$.

As an example $s(2)=3.938\,003\,500$
$\sqrt{s(2)}=1.984\,4$ $B_2\left(0,0,2\right)=-\frac{39}{16}$.

Equation II.2 We have $1024u^3+\left(3072x^2+256\right)u^2+\left(3072x^4-512x^2-64\right)u+\left(1024x^6-768x^4-832x^2-16\right)=0$, we have $B_2\left(x,\sqrt{v_{-1}\left(x\right)}\right)=-1$.

Method of Ferrari

For the quartic $x^4+ax^3+bx^2+cx+d=0$, we eliminate first the quadratic term by mean of $x=y-\dfrac{a}{4}$, to obtain $y^4+py^2+qy+r=0$, where $p=b-\dfrac{3a^2}{2}$, $q=c+\dfrac{a^3-ba}{2}$, and $r=d-\dfrac{3a^4+64ac}{256}$. Writing the equation as $y^4+py^2=-qy-r$ and adding py^2+p^2 in both sides, we get $(y^2+p)^2=-qy-r+py^2+p^2$. By introducing a new variable for completing the square $(y^2+p+z)^2=(p+2z)y^2-qy+(p^2-r+2pz+z^2)$, the right side is a perfect square in y if and only if z satisfies $q^2=8z^3+20pz^2+(16p^2-8r)z+(4p^3-4pr)$, which is cubic and can be solved by Cardan's method.

For the general case the fourth degree equation is $x^4+\frac{B}{A}x^3+\frac{C}{A}x^2+\frac{D}{A}x+\frac{E}{A}=0, A\neq 0$. And the Ferrari's formulas are the following

$\alpha=-\frac{3B^2}{8A^2}+\frac{C}{A}$
$\beta=\frac{B^3}{8A^3}-\frac{BC}{2A^2}+\frac{D}{A}$
$\gamma=-\frac{3B^4}{256A^4}+\frac{CB^2}{16A^3}-\frac{BD}{4A^2}+\frac{E}{A}$
$P=-\frac{\alpha^2}{12}-\gamma$
$Q=-\frac{\alpha^3}{108}+\frac{\alpha\gamma}{3}-\frac{\beta^2}{8}$

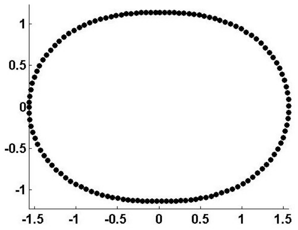

Fig. 1: The dots depict the numerical approximation of the orbit $O(1, -1.9305)$.

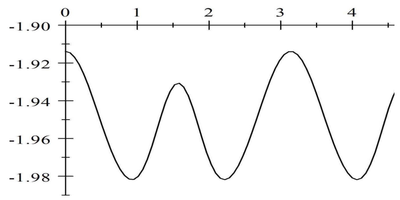

Fig. 2: The Potential of the numerical approximation of the orbit $O(1, -1.9305)$.

$R = -\frac{Q}{2} + \sqrt{\frac{Q^2}{4} + \frac{P^3}{27}}$
$U = \sqrt[3]{R}$, $y = -\frac{5}{6}\alpha + U - \frac{P}{3U}$, and
$W = (\alpha + 2y)^{\frac{1}{2}}$,
the roots are

$x_1 = -\frac{B}{4A} + \frac{W - \sqrt{-\left(3\alpha + 2y + \frac{2\beta}{W}\right)}}{2}$
$x_2 = -\frac{B}{4A} + \frac{W + \sqrt{-\left(3\alpha + 2y + \frac{2\beta}{W}\right)}}{2}$
$x_3 = -\frac{B}{4A} + \frac{-W - \sqrt{-\left(3\alpha + 2y - \frac{2\beta}{W}\right)}}{2}$
$x_4 = -\frac{B}{4A} + \frac{-W + \sqrt{-\left(3\alpha + 2y - \frac{2\beta}{W}\right)}}{2}$.

For the equation II.3, the formulas of the four roots have an extension of four pages each. The formulas are syntactically correct and allow to compute by symbolic mathematical software(SMS) the orbits. This is not efficient because the SMS replaces symbols and estimates the result each time. Compare with a compiled numerical routine, this is slower but nevertheless an orbit can be visualized or simplified in few minutes.

The next section shows the results for the orbits of the proposition 2.1.

IV. Levels set of the potential B_2

A. Numerical Results

Here the configuration of the fixed particles correspond to $l = 1$. For $G = -1.9305$ the figure 1 depicts a numerical approximation for the orbit $O(1, -1.9305)$. Figure 2 illustrates the corresponding values of the potential. The expected result is not the constant line at $G = -1.9305$.

B. Results

The proposition 3.2 gives similar results for B_2 instead of LJ 12-6 to the triangular and collinear choreographes of the 3-body system discussed in [?]. We remark that our approach is done by basic analysis and algebraic techniques for the static case.

The next proposition provides the asymptotics for the isosceles triangular configurations.

Proposition 4.1: Given a system of two particles of the proposition 3.2, and $l \in (2, 0)$. If a free particle is at $(0, y)$, where $y = \pm\frac{1}{2}\sqrt{2^2 - l^2}$. Then the free particle is on a local point. Moreover, from the free particle's point of view, the two particles act as one virtual particle of double B potential when $l \to 0$.

Proof: Without loss of generality, let be $y_1 = \frac{1}{2}\sqrt{2^2 - l^2}$. The free particle is perpendicular to middle point of the side with vertices (p_1, p_2). The result follows immediately from proposition 3.2 and the equation III.2, which corresponds to the condition $\nabla B_2(0, y_1) = 0$. Also, the free particle position goes to $(0, 2)$ when $l \to 0$, which is the double of the optimal distance ($d^\star = 1$) of the function B. ■

Proposition 4.2: Given a system of two particles of the proposition 3.2, with $l = 1$. Then the minimal points of a free particle is at $(0, y)$, where $y = \pm\frac{\sqrt{3}}{2}$. The particles are the vertices of an equilateral triangle.

Proof: Without loss of generality, let be $y_1 = \frac{1}{2}\sqrt{3}$, then the distance between the three particles is 1. The determinant of Hessian matrix of the system at $(0, y_1)$ is

$$|\nabla^2 B_2(0, \frac{\sqrt{3}}{2})| = -64\,(-3)\,.$$

The optimality follows from proposition 3.2 and $|\nabla^2 B_2(0, y_1)| > 0$. ■

Proposition 4.3: Given a system of two particles of the proposition 3.2, and $l \in (2, 0)$. Then the orbit of B_2 of value $G_y = B_2(0, y)$ is the pointed set $O(l, G_y) = \{(0, y) \in \mathbb{R}^{+2}\}$ where $y = \frac{1}{2}\sqrt{2^2 - l^2}$.

Proof: By the symmetry the space is restricted to $\mathbb{R}^{+2}$. The determinant of Hessian matrix of the system at $(0, y)$ is

$$|\nabla^2 B_2(0, \frac{1}{2}\sqrt{2^2 - l^2})| = -64 l^2 \left(l^2 - 4\right).$$

The polynomial $-64l^2\left(l^2 - 4\right)$ is strictly positive for $l \in (0, 2)$. This means that the positive root of the equation III.2 corresponds to the optimality conditions $\nabla B_2(0, y) = 0$ and $|\nabla^2 B_2(0, y)| > 0$. Therefore $O(l, G_y)$ is the minimal point $(0, y)$. ■

For $G = -3$ the four roots of fourth degree equation II.3 (with $l = 1$) are

$r_1(x) = \frac{1}{4} - x^2 - \frac{1}{2}\sqrt{4x^2 - 4ix + 1}$
$r_2(x) = \frac{1}{2}\sqrt{4x^2 - 4ix + 1} - x^2 + \frac{1}{4}$
$r_3(x) = \frac{1}{4} - x^2 - \frac{1}{2}\sqrt{4x^2 + 4ix + 1}$
$r_4(x) = \frac{1}{2}\sqrt{4x^2 + 4ix + 1} - x^2 + \frac{1}{4}$.

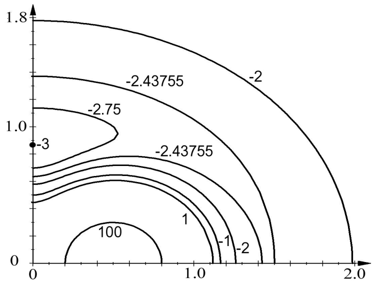

Fig. 3: The true orbits for $O(1,-3)$, $O(1,-2.75)$, $O(1,-2.43755)$, $O(1,-2)$, $O(1,-1)$, $O(1,0)$, and $O(1,100)$

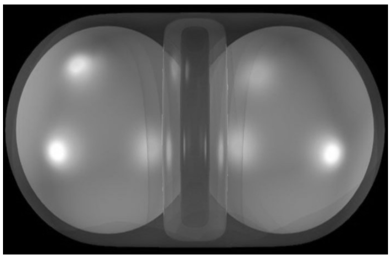

Fig. 4: 3D model of the levels set of $B_2(x,y,z) = G$, where $G \in [3,\infty)$.

Only for $x = 0$, $r_2(0) = \frac{3}{4} > 0$, therefore the orbit of $O(1,-3)$ is the point set $\{(0, \sqrt{\frac{3}{4}})\}$. Which is the optimal point of the equilateral triangle of size = 1. Here, our method gives the result without appealing to the optimal conditions as in proposition 4.2 and in proposition 4.3.

The detailed analysis of the third and fourth degree equations of proposition 2.1 for $l = 1$ was done to verify

1) $m_1 = -3$.
2) $O(1,-3) = \{(0, \frac{\sqrt{3}}{2})\}$, i.e., it is a point the root of fourth degree equation for $G_1 = -3$.
3) There are two orbits from the roots of fourth degree equation with $G_1 \in [m,-1)$
4) There is one orbit from the roots of third degree equation with $G_1 = -1$.
5) There is one orbit from the roots of fourth degree equation with $G_1 \in (-1,\infty)$.

Figure 3 depicts some examples of the orbits that comply the previous statements. Figure 4 depicts a 3D model of the PES for $l = 1$ and $G \in [-3,\infty)$.

V. Conclusions and future work

To our knowledge this is the first totally complete description of the level sets of a system of two particles under a Van der Waals Potential. The application of the research on solvable polynomial for a Galois Groups is promising [?] to apply as here.

We have presented a novel approach for the study of orbits of systems of non interactive particles. We tackle the problem by reducing the analysis of the equipotential zones to the one of finding the roots of certain polynomials. The structure of such polynomial allows the use of algebraic methods based on the solvability of the associated Galois group. A constructive method provided by the methods of Cardan and Ferrari, yields a complete factorization of the polynomials and consequently an analytical description of equipotential zones, we compare our results with the standard numerical routines of MATLAB$^{\text{TM}}$ reported in the literature. A complete description of the orbits of clusters, provides a good knowledge for tackling the optimal control problems of optimal path planning, collision free navigation and crystal formation.