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Volume LVI

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The paper for BULLETIN DE LA SOCIÉTÉ DES SCIENCES ET DES LETTRES DE ŁÓDŹ should be written in LaTeX, preferably in LaTeX 2e, using the style (the file **bull.cls**).

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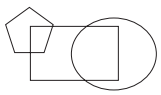

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References

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Recherches sur les déformations Vol. LVI

pp. 7–16

Maciej Skwarczyński

DISSECTIONS IN HOLOMORPHIC GEOMETRY

Summary

Holomorphic geometry centers around biholomorphic equivalence and biholomorphic invariants in $\mathbb{C}^N$. This contribution deals mainly with one-dimensional case (conformal mappings). We study Riemann mappings onto the unit disc Δ. A catalog of conformal mappings resembles the Mendeleev table: it reveals general regularities.

1. General context

Ideas of Newton are not forgotten neither in physics, nor in mathematics. Everybody knows that gravitational potential is harmonic outside masses. And harmonic functions are of importance for complex analysis in one variable. Consider a domain $D \subset \mathbb{C}$. Let $G_D(z,t)$ $z \in D$ be classical Green function of D. It is harmonic with exception of logarithmic singularity at t. By Schiffer-Suszczyński identity [12] the mixed derivative of G_D yields the Bergman function of D

$$K_D(z,t) = -\frac{2}{\pi}\,\frac{\partial^2}{\partial z \partial \bar{t}} G_D(z,t) \quad (z,t) \in D \times D. \tag{1}$$

Singularity is destroyed in the process of differentiation and the right side is holomorphic in z and antiholomorphic in t.

Example 1. For the unit disc Δ

$$G_\Delta(z,t) = \ln \left| \frac{1 - z\bar{t}}{z - t} \right|, \qquad K_\Delta(z,t) = \frac{1}{\pi(1 - z\bar{t})^2}. \tag{2}$$

Remark 1. Original definition of K_D given by S. Bergman [2] is valid for *all domains* $D \subset \mathbb{C}^N$ $N \geq 1$. Namely

$$K_D(z,t) := \sum_\nu \varphi_\nu(z)\overline{\varphi_\nu(t)}, \tag{3}$$

where the right side does not depend on particular choice of othonormal basis in the Hilbert space $L^2H(D) := L^2(D) \cap \mathrm{Hol}(D)$. For $n \geq 2$ an analog of (1) is not available.

For $D \subset \mathbb{C}$ the classical results of Myrberg, Carleson, Ramadanov imply that the following conditions are equivalent:

(i) D admits no Green function,
(ii) D has polar complement,
(iii) $K_D(z,t) = 0$ for all $z, t \in D$,
(iv) $L^2H(d) = \{0\}$.

For $N \geq 2$ a characterization of domains $D \subset \mathbb{C}^N$ such that $L^2H(D) = 0$ is unknown.

2. Relation with conformal mappings

For conformal mapping $\varphi : D \to W$ one verifies easily the transformation rule

$$K_D(z,t) = K_W\left(\varphi(z), \varphi(t)\right) \varphi'(z)\overline{\varphi'(t)}. \tag{4}$$

With $W = \Delta$ one can use (4) to compute K_D. Conversely, knowing K_D for simply connected D one can use (4) to determine the Riemann mapping φ. Briefly: φ and K_D contain the same information.

From (4) follows that the expression

$$\rho_D(z,t) := \left(1 - \left(\frac{K_D(z,t)K_D(t,z)}{K_D(z,z)K_D(t,t)}\right)^{1/2}\right)^{1/2} \tag{5}$$

is invariant under conformal mapping. In fact, ρ_D defines an invariant distance in every $D \subset \mathbb{C}$ with nonpolar complement. For the unit disc one finds

$$\rho_\Delta(z,t) = \left|\frac{z-t}{1-z\bar{t}}\right|. \tag{6}$$

When a smooth curve γ in D is divided into very small segments by points $A_1, A_2, \ldots, A_S$, the sum

$$\rho_D(A_1,A_2) + \rho_D(A_2,A_3) + \ldots + \rho_D(A_{s-1},A) \tag{7}$$

approaches (up to universal multiplicative constant) the Bergman length of γ. In principle one can always compute numerically K_D (and as a consequence ρ_D) via alternating projections. For details see [10].

Usually an explicit expression for the Riemann mapping $\varphi : D \to \Delta$ is determined in a finite number of steps, say $D \to D_s \to D_{s-1} \to \ldots \to D_1 \to \Delta$, and the same steps yield K_D. For convenience mapping catalog should include an expression for K_D along with φ. Such catalog (unpublished) was prepared in 1996 by Ms.

A. Kucharczyk, a student at UMCS, Lublin. We quote three formulae (to be used in the following).

1) The upper halfplane $H = \{z \in \mathbb{C}; \operatorname{Im} z > 0\}$

$$\boxed{K_H(z,t) = \frac{-1}{\pi(z-\bar{t})^2}}$$

2) The first quadrant $K_{Q_1} = \{z \in \mathbb{C}; \operatorname{Re} z > 0,\ \operatorname{Im} z > 0\}$

$$\boxed{K_{Q_1}(z,t) = \frac{-4z\bar{t}}{\pi(z^2-\bar{t}^2)^2}}$$

3) The lower strip $S = \{z \in \mathbb{C}; \pi < \operatorname{Im} z < 0\}$

$$\boxed{K_S(z,t) = \frac{-1}{4\pi}\left(\sinh\frac{z-\bar{t}}{2}\right)^{-2}}$$

It is easy to see that the Bergman functions for upper and lower halfplanes are "the same" like sparrows which sit at different places. Also the Bergman functions for left and right halfplanes are "the same"; see the diagram below.

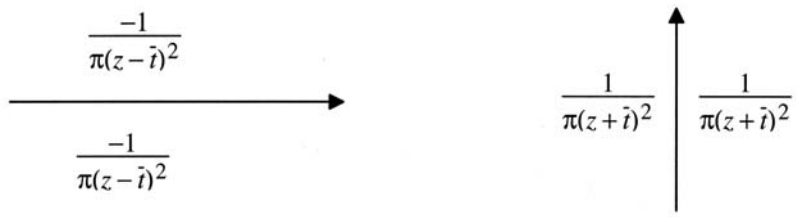

Fig. 1: Diagram 1. Halfplanes.

Four quadrants Q_1, Q_2, Q_3, Q_4 have "the same" Bergman functions; see below.

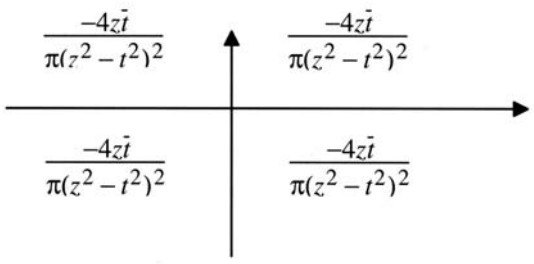

Fig. 2: Diagram 2. Quadrants.

Strips of width π are more like halfplanes; see below.

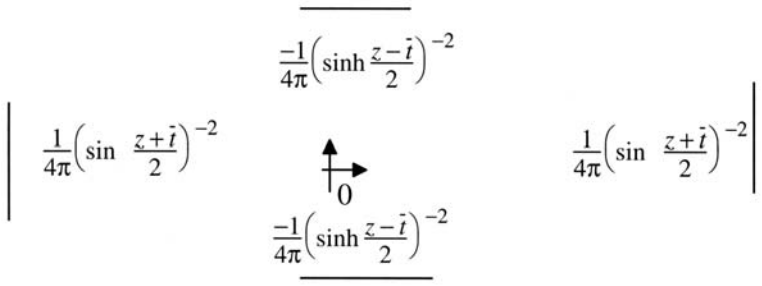

Fig. 3: Diagram 3. Strips of width π.

3. A theorem on dissections

One can remove from D an interval, or halfline to obtain so-called slit domain D'. Slit domains are important in the function theory. For example the Koebe function which maps Δ onto $\mathbb{C} \setminus (\infty, -1/4)$ appears in the uniformization problem and in coefficient problem. Extending the slit all the way results in dissection of D into a pair of domains, say A and B. By direct calculations (three subsequent sections) we establish the following

Theorem 1. *In a number of cases a dissection of D has the following properties:*
(a) $\lim K_{D'}(z,t) = K_A(z,t), \quad z,t \in A,$
(b) $\lim K_{D'}(z,t) = K_B(z,t), \quad z,t \in B.$

Remark 2. It is quite probable that conditions (a) and (b) are satisfied for each dissection in every domain $D \subset \mathbb{C}$. But no proof is known. Any progress in this direction would be of interest.

4. First case: two halfplanes

Consider $D = \mathbb{C}$. We shall dissect complex plane along the real axis. The slit plane $\mathbb{C}' := \mathbb{C} \setminus [0, +\infty)$ is mapped by $\Phi(z) = \sqrt{z}$ (with $\sqrt{-1} = i$) onto the upper halfplane. By transformation rule

$$K_{\mathbb{C}'}(z,t) = \frac{-1}{\pi\left(\sqrt{z} - \overline{\sqrt{t}}\right)^2} \, \frac{1}{4\sqrt{z}\overline{\sqrt{t}}}. \tag{8}$$

More generally, for $D' := \mathbb{C} \setminus [-d, +\infty)$ where $d > 0$:

$$K_{D'}(z,t) = \frac{-1}{\pi\left(\sqrt{z+d} - \overline{\sqrt{t+d}}\right)^2} \; \frac{1}{4\sqrt{z+d}\,\overline{\sqrt{t+d}}}. \tag{9}$$

We look for the limit when $d \to +\infty$. Symmetry of diagram 1 suggests that we prove (a) and (b) simultaneously. We remove irrationality in the denominator, then divide numerator and denominator by d. As a result

$$\begin{aligned} K_{D'}(z,t) &= \frac{-1}{\pi} \; \frac{\left(\sqrt{z+d} + \overline{\sqrt{t+d}}\right)^2}{(z-\overline{t})^2} \; \frac{1}{4\sqrt{z+d}\,\overline{\sqrt{t+d}}} \\ &= K_{\pm H}(z,t) \frac{\left(\sqrt{\frac{z}{d}+1} + \sqrt{\frac{t}{d}+1}\right)^2}{4\sqrt{\frac{z}{z}+1}\,\overline{\sqrt{\frac{t}{d}+1}}} \underset{d\to+\infty}{\longrightarrow} K_{\pm H}(z,t). \end{aligned} \tag{10}$$

□

Remark 3 (casual). It is well known that $K_{\mathbb{C}} \equiv 0$. In some sense, our calculation describes "creation out of nothing". Here a bounded slit is of no avail (it yields doubly connected domain). At every stage of described evolution the whole halfline is absent. In a way "the process has no beginning".

5. Second case: two quadrants

We shall consider the upper halfplane D. Recall that conformal mappings are useful in studying fluid flows. An elementary book by Janowski and Kaczmarski [6] gives convincing explanation. The authors present an example of flow over vertical obstacle which leads immediately to the idea of dissection. Take $D' := H \setminus (0, \mathrm{id}]$ where $d > 0$ and consider conformal mapping $\Phi : D' \to H$ given by

$$\Phi)z) = \sqrt{z^2 + d^2} \qquad \left(\sqrt{-1} = i\right). \tag{11}$$

In view of diagram 2 we may treat cases (a), (b) simultaneously. Applying transformation rule and arguing as in example 5 we find that

$$\begin{aligned} K_{D'}(z,t) &= \frac{-1}{\pi\left(\sqrt{z^2+d^2} - \overline{\sqrt{t^2+d^2}}\right)^2} \; \frac{z\bar{t}}{\sqrt{z^2+d^2}\,\overline{\sqrt{t^2+d}}} \\ &= \frac{-z\bar{t}}{\pi\left(z^2-\bar{t}^2\right)^2} \; \frac{\left(\sqrt{z^2+d^2} + \sqrt{t^2+d^2}\right)^2}{\sqrt{z^2+d^2}\,\overline{\sqrt{t^2+d^2}}} \underset{d\to+\infty}{\longrightarrow} \frac{-z\bar{t}}{\pi\left(z^2-\bar{t}^2\right)^2} 4 = K_Q(z,t). \end{aligned} \tag{12}$$

□

Remark 4. It is appropriate to indicate here the article *Witold Janowski 1912–1972*, published by prof. Z. Jakubowski in the Proceedings of II Conference Analytic Functions, Łódź 1973.

6. Third case: a halfplane and a strip

Consider $D = \tilde{H}$, where $\tilde{H} = \{z - \pi i;\ z \in H\}$. We make horizontal slit along negative reals, so that $D' = \tilde{H} \setminus (-\infty, 0]$; see diagram 4. The mapping $\Phi : H \to D'$ given explicitely by

$$\Phi(z) = z + \ln(1 - z), \qquad (\ln 1 = 0), \tag{13}$$

appears on p. 162 of the catalog [8] prepared by Ławrik and Sawienkow. Obviously

$$\Phi'(z) = 1 - \frac{1}{1 - z} = \frac{z}{z - 1}. \tag{14}$$

The mapping $\Phi : H \to D'$ goes in another direction then before; see the diagram 4. With $\zeta = \Phi(z),\ \tau = \Phi(t)$, we may write the transformation rule as

$$K_{D'}(\xi, \tau) = K_H(z, t)\frac{(z - 1)(\bar{t} - 1)}{z\bar{t}}. \tag{15}$$

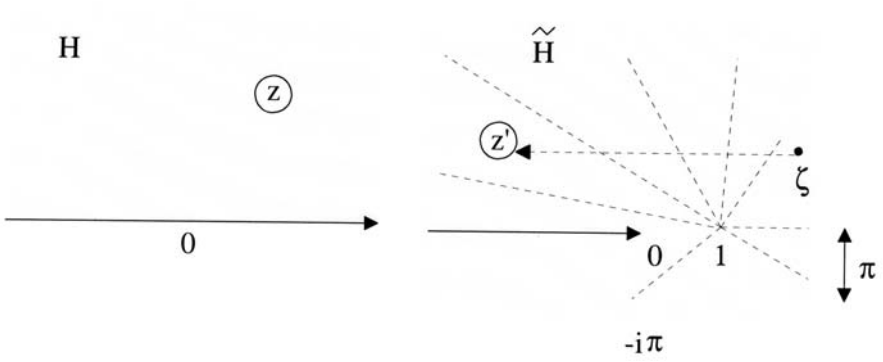

Fig. 4: Diagram 4. Halfplane $\tilde{H}$ is dissected into the halfplane H and strip S of width π.

Let us denote by $r,\ \varphi$ the absolute value and principal argument of the number $z - 1$. Hence $\varphi - \pi$ gives the principal argument of $1 - z$. We want to study how slit elongation affects $K_{D'}(\zeta, \tau)$. Or, equivalently, we can study $K_{D'}(z', t')$ where (z', t') results from horizontal translation of $\zeta, \tau)$ in the opposite direction. To this aim we shall consider in H two lines, determined by $z' = \Phi(z)$, which intersect at z:

$$\text{Re } \Phi(z) = c_{z'}, \qquad \text{Im } \Phi = d_{z'} = \text{Im}_\zeta \tag{16}$$

and two lines, determined by $t' = \Phi(t)$, which intersect t at

$$\text{Re } \Phi(t) = c_{t'}, \qquad \text{Im } \Phi(t) = d_{t'} = \text{Im } \tau. \tag{17}$$

We shall investigate the behavior of z, t when $c_{z'}, c_{\tau'} \to -\infty$. Note that $z' = \Phi(z)$ is the corresponding translation of ζ and $t' = \Phi(t)$ is the corresponding translation of τ. Hence $c_{z'} - c_{t'} = \mathrm{Re}(\zeta - \tau)$.

In the present example domains A, B are visibly different. We shall give separate proofs for conditions (a), (b) of Theorem 1. In case (a) we have $d \in (0, +\infty)$, $\varphi \in (0, \pi)$, $r > 0$. In case (b) we have $d \in (-\pi, 0)$, $\varphi \in (0, \pi)$, $r > 0$.

Proof of (a). We shall first consider equations (16), but analogous conclusions can be derived from equations (17). We may rewrite (16) in the form

$$1 + r\cos\varphi + \ln r = c_{z'}, \tag{18}$$

$$r\sin\varphi + \varphi - \pi = d_{z'}, \tag{19}$$

where $c_{z'} \in \mathbb{R}$, $d_{z'} \in (0, +\infty)$ and $\varphi \in (0, \pi)$. For $c_{z'} \to -\infty$ formula (18) implies $r \to +\infty$ or $r \to 0$. In the *second case* (19) implies that $\varphi \to \pi + d_{z'} > \pi$, a contradiction. Therefore $r \to +\infty$. By (18) $c_{z'} r^{-1}$ is close to $\cos\varphi$, and hence stays away from $+1$. By (19) $\sin\varphi \to 0$, and hence $\varphi \to \pi$. Now (19) yields $r\sin\varphi \to d_{z'}$. Also $\cos\varphi \to -1$ and $c_{z'} r^{-1} \to 1$.

Analogous reasoning applies to equations (17). Hence we have a pair of equations

$$\begin{gathered} 1 + r_{z'}\cos\varphi_{z'} + \ln r_{z'} = c_z, \\ 1 + r_{t'}\cos\varphi_{t'} + \ln r_{t'} = c_t \end{gathered} \tag{20}$$

and an identity

$$\lim \frac{r_{z'}}{r_{t'}} = \lim \frac{c_{z'}}{c_{t'}} = 1. \tag{21}$$

This yields, by subtracting equations (20):

$$\lim \left(r_{z'}\cos\varphi_{z'} - r_{t'}\cos\varphi_{t'}\right) : \mathrm{Re}(\xi - \tau) = \mathrm{Re}(\zeta - \bar{\tau}). \tag{22}$$

We know already that $r_{z'}\sin\varphi_{z'} \to d_{z'} = \mathrm{Im}\zeta$, $r_{t'}\sin\varphi_{t'} \to d_{t'} = \mathrm{Im}\tau$. Hence (22) implies that

$$\lim(z - \bar{t}) = \mathrm{Re}(\zeta - \bar{\tau}) + i\mathrm{Im}(\zeta - \bar{\tau}) = \zeta - \bar{\tau}. \tag{23}$$

Now we can pass to the limit in formula (15). Since $r_{z'} \to +\infty$, $r_{t'} \to +\infty$, the second factor converges to 1 and in view of (23):

$$\lim K_{D'}(\xi, \tau) = \lim K_H(z, t) = \lim \frac{-1}{\pi\left(z - \bar{t}\right)^2} = K_H(\zeta, \tau). \tag{24}$$

□

Proof of (b). Again, we consider first equations (16) and take for granted analogous results for equations (17). As before (18) leads to an alternative: $r \to +\infty$ or $r \to 0$. But the *first* case leads to contradiction. As before (19) yields $\sin\varphi \to 0$, $\varphi \to \pi$ and (again by (19)) $r\sin\varphi \to d$. But now the latter is impossible since $r\sin\varphi \geq 0$ while $d < 0$. Therefore $r \to 0$.

Now, in view of $r_{z'}, r_{t'} \to 0$, subtracting equations (20) yields

$$\lim(\ln r_{z'} - \ln r_{t'}) = \lim(c_{z'} - c_{t'}) = \mathrm{Re}(\zeta - \tau) = \mathrm{Re}(\zeta - \bar{\tau}). \tag{25}$$

Moreover (19) yields (now correct) limits

$$\lim \varphi_{z'} = d_{z'} = \mathrm{Im}\zeta, \qquad \lim \varphi_{t'} = d_{t'} = \mathrm{Im}\tau. \tag{26}$$

With abbreviations

$$\alpha := \ln r_{z'} + i\varphi_{z'} \quad \beta := \ln r_{t'} - i\varphi_{t'} \tag{27}$$

we find with (25), (26) the limits

$$\lim \mathrm{Re}\left(\alpha - \overline{\beta}\right) = \mathrm{Re}\left(\zeta - \overline{\tau}\right), \quad \lim \mathrm{Im}\left(\alpha - \overline{\beta}\right) = \mathrm{Im}\zeta + \mathrm{Im}\tau = \mathrm{Im}\left(\zeta - \overline{\tau}\right). \tag{28}$$

Moreover

$$(z-1)\,(\bar{t}-1) = e^{\alpha}e^{\bar{\beta}}, \qquad z - \bar{t} = e^{\alpha} - e^{\beta}. \tag{29}$$

With this results we consider the limit in formula (15). Obviously $z \to 1$, $t \to 1$. Hence

$$\lim K_{D'}(\zeta,\tau) = \lim K_H(z,t)(z-1)(\bar{t}_1) = \lim \frac{-\exp\alpha \exp\overline{\beta}}{\pi\left(\exp\alpha - \exp\overline{\beta}\right)^2}$$

$$= \lim \frac{-1}{\pi\left[\exp\left(\alpha/2 - \overline{\beta}/2\right) - \exp\left(\overline{\beta}/2 - \alpha/2\right)\right]^2} = \lim \frac{-1}{4\pi \sinh^2\left(\alpha/2 - \overline{\beta}/2\right)} \tag{30}$$

$$= \frac{-1}{4\pi}\sinh^{-2}; \quad \frac{\zeta - \overline{\tau}}{2} = K_S(\zeta,\tau).$$

□

Remark 5. Direct verification of general result with concrete examples is not complete without purpose (it fosters sideway observations). In the above calculations we have discovered a link between transcendental expressions $r + \ln r$, $\varphi + \sin\varphi$ and Bergman theory.

7. Rogowski condenser

In this section I would like to indicate related problems. Let us consider two parallel slits. By removing from $D = \mathbb{C}$ two halflines parallel to negative reals one obtains doubly slit domain D''. Such domain, with slits $(-\infty + \pi i, -1 + \pi i]$ and $(-\infty - \pi i, -1 - \pi i)$ appears on p. 217 in the catalog [8]. The function

$$\Phi(z) = z + e^z \tag{31}$$

maps conformally $T = \{-\pi < \mathrm{Im}z < \pi\}$ onto D''; see diagram 5. One expects that $K_{D''}$, under elongation of slits, would produce three Bergman functions: one for a strip and two for halfplanes.

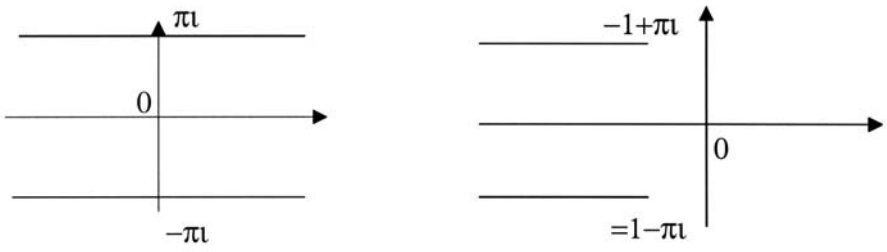

Fig. 5: Diagram 5. A strip is mapped onto a doubly slited plane.

The domain D'' appears as description of the condenser developed by Rogowski. His invention is widely used in precise measuring instruments; see the textbook by Fuks and Szabat [4] p. 353–357 (and the recent internet advertisements).

Of course, one can cosider domains with any finite number of slits, or even with infinitely many slits. Also there are reasons to study slited domains which are not simply connected. In the beginning of XX century an infinitely connected domains with periodic slits (Rus. *reshetka*, Eng. *grating*, Germ. *Gitter*) were studied within wing theory by Czapłygin [3], Grammel [5], König [7] , Achiezer [1]. Recently such domains may by of interest in connection with Kobayashi completeness conjecture [9, 11]. For general infinitely connected domains the best mathematical reference is Tsuji [13].

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ROZDZIELENIA W GEOMETRII HOLOMORFICZNEJ

S t r e s z c z e n i e

Geometria holomorficzna jest skoncentrowana wokół równoważności boholomorficznej i niezmienników biholomorficznych w przestrzeni $\mathbb{C}^N$. Obecny przyczynek dotyczy głównie przypadku jednowymiarowego (odwzorowań konforemnych). Badamy odwzorowania Riemanna na koło jednostkowe Δ. Uzyskany katalog odwzorowań konforemnych przypomina tablicę Mendelejewa: wykazuje on ogólną regularność.

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Dmytro Mierzejewski

INVESTIGATION OF QUATERNIONIC QUADRATIC EQUATIONS I

FACTORIZATION AND PASSING TO A SYSTEM OF REAL EQUATIONS

Summary

Sufficient conditions for a possibility to transform a quaternionic equation of the form $pxqxr-sxt-uxv+w=0$ to one of the form $(\alpha x\beta-a)(\gamma x\delta-b)=0$ are formulated. The shape of the set of solutions of any quaternionic equation of the form $x^2+\sum_{\ell=1}^{m}a^{(\ell)}xb^{(\ell)}+c=0$ is investigated.

1. Introduction

Since the system of quaternions is the most known extension of the system of complex numbers, it is natural to investigate solutions of quaternionic polynomial equations. But this task turns out to be so difficult. The work [2] contains a very beautiful theory about solutions of quaternionic equations of the form

$$\sum_{\ell=0}^{n}a_\ell x^\ell=0 \quad \text{or} \quad \sum_{\ell=0}^{n}x^\ell a_\ell=0$$

(here and below x is the unknown). But, since the system of quaternions is not commutative, the general form of a quaternionic polynomial equation is much more complicated, namely:

$$\sum_{p=1}^{n}\left(\sum_{\ell=1}^{m_p}a_{p,\ell,1}xa_{p,\ell,2}x\dots a_{p,\ell,p}xa_{p,\ell,p+1}\right)+c=0. \tag{1}$$

The problem about solutions of any such equation is far from being completely investigated.

As for now, a few particular cases of (1) are investigated in several works. Namely, [4] gives complete description of solutions of **linear** equations, in [3] and [1] only

several kinds of **quadratic** equations are investigated. This work is the next little step on this way. Here we investigate only **quadratic** equations (and again not all, but only some classes, though comparatively wide). In Section 3 we look for classes of quaternionic quadratic equations which can be easily solved by factorization of the left part into a product of linear polynomials. In Section 4 we investigate shape of the set of solutions of any quaternionic equation of the form

$$x^2 + \sum_{\ell=1}^{m} a^{(\ell)} x b^{(\ell)} + c = 0.$$

2. Notations of the paper

We use the standard notations i, j, k for the quaternionic imaginary units; recall that

$$\begin{aligned} i^2 = j^2 = k^2 = -1, \\ ij = -ji = k, \\ jk = -kj = i, \\ ki = -ik = j. \end{aligned}$$

We always use natural subindices to denote the components of a quaternion: $x = x_0 + x_1 i + x_2 j + x_3 k$, where $x_0, x_1, x_2, x_3 \in \mathbb{R}$. Note also that we deal only with **real** quaternions, i. e., their components are real; we use the word "quaternion" only for a real one and denote the system of all (real) quaternions by $\mathbb{H}$.

3. Factorisable quaternionic quadratic equations

Note that in the system $\mathbb{H}$ there is no such simple connection between roots of polynomials and factorization of polynomials by linear factors as in $\mathbb{C}$. For example, the equation $x^2 - i = 0$ has exactly two quaternionic solutions:

$$\frac{(1+i)}{\sqrt{2}} \quad \text{and} \quad -\frac{(1+i)}{\sqrt{2}}$$

(this fact can be checked by the theory from [2]). But the expressions

$$x^2 - i \quad \text{and} \quad \left(x - \frac{(1+i)}{\sqrt{2}}\right)\left(x + \frac{(1+i)}{\sqrt{2}}\right)$$

are not identically equal if x is any quaternion; the latter expression equals

$$x^2 + \frac{xi}{\sqrt{2}} - \frac{ix}{\sqrt{2}} - i$$

and cannot be reduced to the former expression due to non-commutativity of quaternions.

Nevertheless if a quaternionic polynomial can be written as $(x - a_1) \dots (x - a_n)$ then $\{a_1, \dots, a_n\}$ is the set of all its roots; this is obvious from the fact of absence of

zero divisors in $\mathbb{H}$. So, it is useful to know a method to determine whether a given quaternionic polynomial can be factored as above.

We will restrict our investigation to quadratic polynomials. Yet, we will take somewhat more general factors than above-mentioned ones, namely of the form $\alpha x\beta - a$, where $\alpha \neq 0$, $\beta \neq 0$. Really, the equation $\alpha x\beta - a = 0$ can be easily solved as follows: $\alpha x\beta = a$, $x = \alpha^{-1}a\beta^{-1}$. So, an arbitrary quadratic polynomial constructed as a product of such factors is

$$(\alpha x\beta - a)(\gamma x\delta - b).$$

By simple direct calculations we rewrite it as follows:

$$\alpha x\beta\gamma x\delta - \alpha x\beta b - a\gamma x\delta + ab. \tag{2}$$

We have obtained a polynomial of the form $pxqxr - sxt - uxv + w$.

Thus our aim is to describe conditions under which it is possible to reduce a quaternionic equation of the form

$$pxqxr - sxt - uxv + w = 0 \tag{3}$$

to one of the form

$$(\alpha x\beta - a)(\gamma x\delta - b) = 0 \tag{4}$$

(where x is the unknown, and every other letter denotes a known quaternion).

Comparing (3) and (2), we pass to the following system of quaternionic equations with known quaternions p, q, r, s, t, u, v, w and unknown quaternions α, β, γ, δ, a, b:

$$\begin{array}{ll} \alpha = p, & \beta b = t, \\ \beta\gamma = q, & a\gamma = u, \\ \delta = r, & \delta = v, \\ \alpha = s, & ab = w. \end{array} \tag{5}$$

Solvability of this system is a sufficient condition for (3) to be factorisable in the proper sense.

By simple equivalent transformation we rewrite (5) as follows:

$$\begin{array}{ll} p = s, & \beta\gamma = q, \\ r = v, & \beta b = t, \\ \alpha = p, & a\gamma = u, \\ \delta = r, & ab = w. \end{array} \tag{6}$$

Hence we have already obtained information that (5) can be solvable only if $p = s$ and $r = v$, and also we can see that α and δ are determined exactly.

According to the latter four equations of (6), conditions of the solvability essentially depend on whether q, t, u, or w equals 0. It is easy to conclude from these four equations that:

- if $q = 0$, then the system can be solved only if $t = 0$ or $u = 0$;
- if $t = 0$, then the system can be solved only if $q = 0$ or $w = 0$;

- if $u = 0$, then the system can be solved only if $q = 0$ or $w = 0$;
- if $w = 0$, then the system can be solved only if $t = 0$ or $u = 0$.

Hence if the system is solvable and at least one from the coefficients q, t, u, w equals 0 then in reality at least **two** from them equal 0. But since all these four coefficients are from different terms of (3), such situation means that there are **at most two non-zero terms** in the left part of (3) and thus the equation is much simpler than a typical equation of the form (3). If one wants to solve such an equation, we recommend to apply a direct method similar to one used in Section 4 rather than to try to factorize it. Therefore we will not describe the further theory concerning these cases of zeros, and we hope that the reader will forgive us for absence of the corresponding long and boring descriptions of different cases.

Thus in what follows we assume that $q \neq 0$, $t \neq 0$, $u \neq 0$, $w \neq 0$; note that this assumption implies that also $\gamma \neq 0$. Let us continue to look for equivalent transformations of (5):

$$\begin{array}{ll} p = s, & \beta = q\gamma^{-1}, \\ r = v, & b = \beta^{-1}t, \\ \alpha = p, & a = u\gamma^{-1}, \\ \delta = r, & a = wb^{-1}; \end{array}$$

$$\begin{array}{ll} p = s, & \beta = q\gamma^{-1}, \\ r = v, & b = \gamma q^{-1}t, \\ \alpha = p, & a = u\gamma^{-1}, \\ \delta = r, & u\gamma^{-1} = wt^{-1}q\gamma^{-1}; \end{array}$$

$$\begin{array}{ll} p = s, & \beta = q\gamma^{-1}, \\ r = v, & b = \gamma q^{-1}t, \\ \alpha = p, & a = u\gamma^{-1}, \\ \delta = r, & u = wt^{-1}q. \end{array}$$

Therefore we have obtained one more strict condition on the coefficients of (3) for (5) to be solvable: $u = wt^{-1}q$. But moreover we can see that it is possible to calculate exactly not only α and δ, but also β, a, and b if γ is given; moreover every non-zero quaternion can be taken as γ. This information implies that fulfilment of the relations $p = s$, $r = v$, and $u = wt^{-1}q$ is a necessary and sufficient condition for (5) to be solvable, and thus it is a sufficient condition for (3) to be factorisable in the sense described above.

Let us describe the obtained information as a proposition:

Proposition 1. *Let a quaternionic equation of the form* (3) *be given* (*the unknown is* x)*, where* $q \neq 0$*,* $t \neq 0$*,* $u \neq 0$*,* $w \neq 0$*. Let moreover*

$$p = s, \quad r = v, \quad u = wt^{-1}q. \tag{7}$$

Then it is possible to rewrite this equation as (4). *In order to calculate the coefficients of* (4) *it is sufficient to take any non-zero quaternion* γ *and to apply the formulae:*

$$\alpha = p, \quad \beta = q\gamma^{-1}, \quad \delta = r, \quad a = u\gamma^{-1}, \quad b = \gamma q^{-1}t.$$

In particular, it is possible to take $\gamma = 1$ *getting the formulae:*

$$\alpha = p, \quad \beta = q, \quad \gamma = 1, \quad \delta = r, \quad a = u, \quad b = q^{-1}t. \tag{8}$$

Then it is important to note the following: it is possible that an equation of the form (3) can be factored, but by a way somewhat different from one described above. First of all, it is possible to rearrange the second and third terms in (3). Then s will be instead of u, t will be instead of v, and vice versa. This gives a second interpretation of (7) and widens the set of equations known to be factorizable.

Then it is known that every real number commutes with every quaternion. Therefore we can consider a case where (3) can be factored as above after moving some real factors between coefficients. So, now we put

$$\tilde{s} = \frac{s}{\rho_1}, \quad \tilde{t} = \rho_1 t, \quad \tilde{u} = \frac{u}{\rho_2}, \quad \tilde{v} = \rho_2 v, \quad \tilde{p} = \frac{p}{\rho_3}, \quad \tilde{q} = \frac{q}{\rho_4}, \quad \tilde{r} = \rho_3\rho_4 r, \tag{9}$$

where ρ_1, ρ_2, ρ_3, ρ_4 are non-zero **real** numbers. Then (3) can be transformed into

$$\tilde{p}x\tilde{q}x\tilde{r} - \tilde{s}x\tilde{t} - \tilde{u}x\tilde{v} + w = 0,$$

and for the factorability it is sufficient to assume that

$$\tilde{p} = \tilde{s}, \quad \tilde{r} = \tilde{v}, \quad \tilde{u} = w\tilde{t}^{-1}\tilde{q},$$

or

$$\frac{p}{\rho_3} = \frac{s}{\rho_1}, \quad \rho_3\rho_4 r = \rho_2 v, \quad \frac{u}{\rho_2} = \frac{wt^{-1}q}{\rho_1\rho_4},$$

or

$$p = \frac{\rho_3}{\rho_1}s, \quad r = \frac{\rho_2}{\rho_3\rho_4}v, \quad u = \frac{\rho_2}{\rho_1\rho_4}wt^{-1}q.$$

Let us introduce the following real numbers:

$$\sigma_1 := \frac{\rho_3}{\rho_1}, \quad \sigma_2 := \frac{\rho_2}{\rho_3\rho_4}. \tag{10}$$

Since ρ_1, ρ_2, ρ_3, ρ_4 may be **arbitrary** non-zero real numbers, it is easy to see that σ_1 and σ_2 are also **arbitrary** non-zero real numbers. Then

$$p = \sigma_1 s, \quad r = \sigma_2 v, \quad u = \sigma_1\sigma_2 wt^{-1}q. \tag{11}$$

Hence (11) (with any $\sigma_1, \sigma_2 \in \mathbb{R} \setminus \{0\}$) is a sufficient condition for (3) to be factorizable in the proper sense.

Let us find out by which formulae should one calculate the coefficients α, β, γ, δ, a, b in the case of (11). From a given equation of the form (3) satisfying (11) one knows σ_1 and σ_2. One can choose any real ρ_1, ρ_2, ρ_3, ρ_4 satisfying (10). It is easy to see that the following values are appropriate:

$$\rho_1 = 1, \quad \rho_2 = \sigma_1\sigma_2, \quad \rho_3 = \sigma_1, \quad \rho_4 = 1. \tag{12}$$

Then, taking into attention (8), (9), and (12), it is easy to get the following formulae (note that we have to apply (8) with $\tilde{p}$, $\tilde{q}$, $\tilde{r}$, $\tilde{s}$, $\tilde{t}$, $\tilde{u}$, $\tilde{v}$ instead of p, q, r, s, t, u, v):

$$\alpha = \frac{p}{\sigma_1}, \qquad \beta = q, \qquad \gamma = 1, \qquad \delta = \sigma_1 r,$$
$$a = \frac{u}{\sigma_1\sigma_2}, \qquad b = q^{-1}t. \tag{13}$$

At last let us consider such a simple operation as multiplication of the equation by a quaternionic constant. If the factor is on the left, then p, s, u, w are multiplied on the left by the same quaternion and it is easy to see that (11) remains true. It is easy to carry out analogous consideration for right multiplication, taking into account that

$$(tc)^{-1} = c^{-1}t^{-1}.$$

So, this possibility of multiplication does not widen the set of equations known to be factorizable in the proper sense.

As a conclusion of the considerations above we formulate the following proposition:

Proposition 2. *Let a quaternionic equation of the form* (3) *be given* (*the unknown is* x)*, where* $q \neq 0$, $t \neq 0$, $u \neq 0$, $w \neq 0$. *Let moreover there exist such* $\sigma_1, \sigma_2 \in \mathbb{R}\backslash\{0\}$ *for which the relations* (11) *hold true. Then it is possible to rewrite this equation as* (4). *The coefficients of* (4) *can be calculated by* (13).

Moreover if the relations (11) *are not true then one should check whether they would be true after rearrangement of the second and third terms in* (3). *If yes, then the factorization is possible by the same way after this rearrangement.*

4. Sets of solutions of quaternionic equations of the form $x^2 + \sum_{\ell=1}^{m} a^{(\ell)} x b^{(\ell)} + c = 0$

Consider an equation

$$x^2 + \sum_{\ell=1}^{m} a^{(\ell)} x b^{(\ell)} + c = 0, \tag{14}$$

where x is an unknown quaternion, $a^{(1)}$, …, $a^{(m)}$, $b^{(1)}$, …, $b^{(m)}$, c are known quaternions. Our aim is to investigate the set of all solutions of (14). We shall do this reducing the quaternionic equation to a **system** of **real** equations.

Let us rewrite (14) decomposing every quaternion by the standard basis of $\mathbb{H}$:

$$(x_0 + x_1 i + x_2 j + x_3 k)^2 +$$
$$\sum_{\ell=1}^{m} (a_0^{(\ell)} + a_1^{(\ell)} i + a_2^{(\ell)} j + a_3^{(\ell)} k)(x_0 + x_1 i + x_2 j + x_3 k)(b_0^{(\ell)} + b_1^{(\ell)} i + b_2^{(\ell)} j + b_3^{(\ell)} k) +$$
$$(c_0 + c_1 i + c_2 j + c_3 k) = 0.$$

Opening all brackets and then moving each imaginary unit out of new brackets, we pass to the following equation:

$$
\begin{aligned}
&\Bigg(x_0^2 - x_1^2 - x_2^2 - x_3^2 + c_0 + \\
&\quad \sum_{\ell=1}^{m} \Big((a_0^{(\ell)}b_0^{(\ell)} - a_1^{(\ell)}b_1^{(\ell)} - a_2^{(\ell)}b_2^{(\ell)} - a_3^{(\ell)}b_3^{(\ell)})x_0 + \\
&\qquad (a_2^{(\ell)}b_3^{(\ell)} - a_1^{(\ell)}b_0^{(\ell)} - a_0^{(\ell)}b_1^{(\ell)} - a_3^{(\ell)}b_2^{(\ell)})x_1 + \\
&\qquad (a_3^{(\ell)}b_1^{(\ell)} - a_2^{(\ell)}b_0^{(\ell)} - a_0^{(\ell)}b_2^{(\ell)} - a_1^{(\ell)}b_3^{(\ell)})x_2 + \\
&\qquad (a_1^{(\ell)}b_2^{(\ell)} - a_3^{(\ell)}b_0^{(\ell)} - a_2^{(\ell)}b_1^{(\ell)} - a_0^{(\ell)}b_3^{(\ell)})x_3\Big)\Bigg) + \\
&\Bigg(2x_0x_1 + c_1 + \sum_{\ell=1}^{m} \Big((a_0^{(\ell)}b_1^{(\ell)} + a_1^{(\ell)}b_0^{(\ell)} + a_2^{(\ell)}b_3^{(\ell)} - a_3^{(\ell)}b_2^{(\ell)})x_0 + \\
&\qquad (a_0^{(\ell)}b_0^{(\ell)} - a_1^{(\ell)}b_1^{(\ell)} + a_2^{(\ell)}b_2^{(\ell)} + a_3^{(\ell)}b_3^{(\ell)})x_1 + \\
&\qquad (a_0^{(\ell)}b_3^{(\ell)} - a_2^{(\ell)}b_1^{(\ell)} - a_3^{(\ell)}b_0^{(\ell)} - a_1^{(\ell)}b_2^{(\ell)})x_2 + \\
&\qquad (a_2^{(\ell)}b_0^{(\ell)} - a_3^{(\ell)}b_1^{(\ell)} - a_1^{(\ell)}b_3^{(\ell)} - a_0^{(\ell)}b_2^{(\ell)})x_3\Big)\Bigg)i + \qquad (15)\\
&\Bigg(2x_0x_2 + c_2 + \sum_{\ell=1}^{m} \Big((a_0^{(\ell)}b_2^{(\ell)} - a_1^{(\ell)}b_3^{(\ell)} + a_2^{(\ell)}b_0^{(\ell)} + a_3^{(\ell)}b_1^{(\ell)})x_0 + \\
&\qquad (a_3^{(\ell)}b_0^{(\ell)} - a_1^{(\ell)}b_2^{(\ell)} - a_0^{(\ell)}b_3^{(\ell)} - a_2^{(\ell)}b_1^{(\ell)})x_1 + \\
&\qquad (a_0^{(\ell)}b_0^{(\ell)} + a_1^{(\ell)}b_1^{(\ell)} - a_2^{(\ell)}b_2^{(\ell)} + a_3^{(\ell)}b_3^{(\ell)})x_2 + \\
&\qquad (a_0^{(\ell)}b_1^{(\ell)} - a_3^{(\ell)}b_2^{(\ell)} - a_2^{(\ell)}b_3^{(\ell)} - a_1^{(\ell)}b_0^{(\ell)})x_3\Big)\Bigg)j + \\
&\Bigg(2x_0x_3 + c_3 + \sum_{\ell=1}^{m} \Big((a_0^{(\ell)}b_3^{(\ell)} + a_1^{(\ell)}b_2^{(\ell)} - a_2^{(\ell)}b_1^{(\ell)} + a_3^{(\ell)}b_0^{(\ell)})x_0 + \\
&\qquad (a_0^{(\ell)}b_2^{(\ell)} - a_1^{(\ell)}b_3^{(\ell)} - a_3^{(\ell)}b_1^{(\ell)} - a_2^{(\ell)}b_0^{(\ell)})x_1 + \\
&\qquad (a_1^{(\ell)}b_0^{(\ell)} - a_2^{(\ell)}b_3^{(\ell)} - a_3^{(\ell)}b_2^{(\ell)} - a_0^{(\ell)}b_1^{(\ell)})x_2 + \\
&\qquad (a_0^{(\ell)}b_0^{(\ell)} + a_1^{(\ell)}b_1^{(\ell)} + a_2^{(\ell)}b_2^{(\ell)} - a_3^{(\ell)}b_3^{(\ell)})x_3\Big)\Bigg)k = 0.
\end{aligned}
$$

Obviously, this equation is equivalent to the corresponding system of four equations with real coefficients and with four real unknowns x_0, x_1, x_2, x_3. Write down this system introducing new notations for some long expressions:

$$(16)\qquad \begin{cases} x_0^2 - x_1^2 - x_2^2 - x_3^2 + \alpha_0 x_0 + \alpha_1 x_1 + \alpha_2 x_2 + \alpha_3 x_3 + c_0 = 0, \\ 2x_0 x_1 + \beta_0 x_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + c_1 = 0, \\ 2x_0 x_2 + \gamma_0 x_0 + \gamma_1 x_1 + \gamma_2 x_2 + \gamma_3 x_3 + c_2 = 0, \\ 2x_0 x_3 + \delta_0 x_0 + \delta_1 x_1 + \delta_2 x_2 + \delta_3 x_3 + c_3 = 0. \end{cases}$$

The system (16) will be our main tool for investigations below. It is a system of the degree 2, and if one has to solve a **certain** equation of the form (14), then it is a good recommendation to pass to (16) and to solve it. But our aim is to investigate equations of such form in general.

Namely, we wish to investigate possible kinds of shape of the set of all solutions of (14). Let us do this by means of sections of this set by hyperplanes perpendicular to the real axis. So, let x_0 be fixed, and let us look at the equations of (16) which represent now sets of points in the usual tree-dimensional space. The first equation can represent a sphere, or a point, or the empty set. Secondly, one can represent a plane, or the empty set, or the whole three-dimensional space; it is possible to say just the same about third and fourth ones. The intersection of the corresponding four bodies is the section of the set of the solution by the hyperplane. Obviously, this intersection can be the empty set, or one point, or two points, or a circle, or a sphere. So, we have obtained the following result:

Proposition 3. *Let an equation of the form* (14) *be given. Let any $\xi_0 \in \mathbb{R}$ be fixed. Consider the section of the set of all solutions of* (14) *by a hyperplane $x_0 = \xi_0$. Then this section is or the empty set, or one point, or two points, or a circle, or a sphere.*

An interesting question arises whether every from these five possibilities can be realized for some equation and some section of the set of its solution. It is easy to get the positive answer for four cases from these five, namely:

Proposition 4. *For each from such four types of sets as empty set, one point, two points, and a sphere there exists an equation of the form* (14) *and a hyperplane perpendicular to the real axis, such that the section of the set of all solutions of this equation by this hyperplane is a set of just the given type.*

Proof. Note that a particular case of (14) is

$$(17)\qquad x^2 + xa + bx + c = 0.$$

Such equations were investigated in [1] and, according to Theorem 2 in [1], for every point, for every pair of points and for every sphere perpendicular to the real axis there exists an equation of the form (17) whose set of solutions is just this point, this pair of points, or this sphere, respectively. Concerning a pair of points, note also that since **every** pair is referred to, one can choose two points from the same hyperplane perpendicular to the real axis. Now it is understandable that taking a

corresponding equation and a hyperplane containing the set of its solutions, one proves the proposition for one point, two points and a sphere. Then taking the same equation and another hyperplane perpendicular to the real axis, one proves the proposition for the empty set. □

Therefore only the case of a circle remains unknown and up to now we do not know the answer.

Another interesting question is how many sections of the same kind can have the set of solutions of a certain equation of the form (14). We know the answer only about spheres, namely:

Proposition 5. *Let an equation of the form* (14) *be given, and suppose that there exists a hyperplane perpendicular to the real axis, such that the section of the set of all solutions of the equation by this hyperplane is a sphere. Then the section of this set by every other hyperplane perpendicular to the real axis is not a sphere. In other words, the number of spheres among our sections is not larger than 1 for each particular equation.*

Proof. Let us recall the system (16). Obviously, for a spherical section to appear it is necessary for whole the three-dimensional space to be the set of solutions of each from the latter three equations of the system (treating x_1, x_2, x_3 as the unknowns). Of course, it may occur only if all the coefficients of the equations equal 0. In particular, considering the coefficient at x_1 from the second equation of (16), we have:

$$2x_0 + \beta_1 = 0,$$

or, recalling from (15) what is β_1,

$$2x_0 + \sum_{\ell=1}^{m}(a_0^{(\ell)}b_0^{(\ell)} - a_1^{(\ell)}b_1^{(\ell)} + a_2^{(\ell)}b_2^{(\ell)} + a_3^{(\ell)}b_3^{(\ell)}) = 0.$$

Thus

$$x_0 = \frac{1}{2}\sum_{\ell=1}^{m}(a_0^{(\ell)}b_0^{(\ell)} - a_1^{(\ell)}b_1^{(\ell)} + a_2^{(\ell)}b_2^{(\ell)} + a_3^{(\ell)}b_3^{(\ell)}).$$

Thus x_0 is determined uniquely by the coefficients of the equation. But just x_0 determines a hyperplane. So, only one hyperplane can satisfy the necessary conditions of a spherical section, and the proposition is proved. □

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BADANIE KWADRATOWYCH RÓWNAŃ KWATERNIONOWYCH I

ROZKŁAD NA CZYNNIKI ORAZ PRZEJŚCIE DO UKŁADU RÓWNAŃ RZECZYWISTYCH

S t r e s z c z e n i e

Sformułowano warunki wystarczające dla możliwości przekształcenia równania kwaternionowego postaci $pxqxr - sxt - uxv + w = 0$ do postaci $(\alpha x\beta - a)(\gamma x\delta - b) = 0$. Badany jest kształt zbioru rozwiązań dowolnego równania kwaternionowego postaci $x^2 + \sum_{\ell=1}^{m} a^{(\ell)} x b^{(\ell)} + c = 0$.

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Paulius Miškinis

SPIN ALGEBRA IN THE FRACTION-DIMENSIONAL SPACE

Summary

The author shows that in the case when the effective dimension of space is not an integer and may acquire fractional values, the electron becomes a particle with spin projection $s_z = 1/2^\alpha$, where $0 \leqslant \alpha \leqslant 1$.

The mathematical model of the electron in the magnetic field, according to which the electron is a particle that has a spin, *i.e.* a moment of its own, was proposed in 1927 by W. Pauli. To the quantum value, spin s, corresponds the operator of spin $\hat{s}$ whose components are expressed by Pauli matrices [1]:

$$\hat{s}_i = \frac{1}{2}\sigma_i, \quad \sigma_i\sigma_k = -\sigma_k\sigma_i, \quad \sigma_i^2 = I. \tag{1}$$

Independently of a concrete representation, the spin algebra meets the following commutation relations [2]:

$$[\hat{s}_i, \hat{s}_j] = i\varepsilon_{ijk}\ \hat{s}_k, \quad [\hat{s}_i, \hat{s}^2] = 0. \tag{2}$$

Recently, in applications, geometrical objects with unusual properties have been gaining more and more attention. An explicit example may be fractals introduced by B. Mandelbrot [3]. What changes will undergo the properties of a particle with a spin, if it is moving in the spongy Menger space or on a fuzzy surface? The question seems reasonable because unusual electric or magnetic properties of a solid body may sometimes be explained exactly by changes of the effective dimensions of the space in which free carriers of charge are moving.

What will be the changes the commutation relations (2) undergo in a space of non-whole dimension?

In the fraction-dimensional space, let us make an infinitesimal turn at the angle $\delta\varphi$ round the axis z. The operator of such a turn is expressed through the fractional

spin operator in the form $I + i^{\alpha}(\delta\varphi)^{\alpha}\hat{s}^{\alpha}_{z\pm}$. We will distinguish between the right "+" and the left "−" turns. Therefore, as a result of the turn, the functions $\psi(\sigma)$ will become $\psi(\sigma) + \delta_{\pm}\psi(\sigma)$ where

$$\delta_{\pm}\psi(\sigma) = i^{\alpha}(\delta\varphi)^{\alpha}\hat{s}^{\alpha}_{z\pm}\psi(\sigma), \qquad 0 \leqslant \alpha \leqslant 1, \tag{3}$$

with $\alpha = 1$ corresponding to usual rotation round $\alpha = 0$ to the absence of rotation and the axis z.

First of all, let us establish the way in which the operator should be understood. The direct consideration of

$$\hat{s}^{\alpha}_{i+} = (\hat{s}_i)^{\alpha}$$

as a series does not work because this expansion is valid in the neighborhood of I. The analytical expansion from the region of whole numbers to the region of fractional values is multivalued. The representation in the form of the series

$$(\hat{s}_i)^{\alpha} = e^{\alpha \ln \hat{s}_i}$$

is indefinite because $\ln \hat{s}_i$ is a relatively convergent series. The best way to understand $(\hat{s}_i)^{\alpha}$ is to consider this expression in the sense of function analysis and to apply the so-called Balakrishnan formula. However, there is a natural and simplest physical approach.

We shall use the fact that the spin operator $\hat{s}_i$ is expressed through Pauli matrices (1). It is a well-known fact (see, *e.g.*, [2]) that *any* function from the linear combination of Pauli matrices in the form $a + \mathbf{b}\hat{\boldsymbol{\sigma}}$ where

$$\hat{\sigma} \equiv \{\sigma_x, \sigma_y, \sigma_z\} \quad \text{and} \quad \mathbf{b} \equiv \{b_x, b_y, b_z\}$$

is again a linear combination of Pauli matrices. From this fact and from the relations (1) it follows that *any* function from a linear combination of spin operators will also be a linear combination of spin operators:

$$f(a + \mathbf{b}\hat{\mathbf{s}}) = A + \mathbf{B}\hat{\mathbf{s}}, \tag{4}$$

where

$$A = \frac{1}{2}\left[f(a+b) + f(a-b)\right], \quad \mathbf{B} = \frac{\mathbf{b}}{2b}\left[f(a+b) - f(a-b)\right]$$

and $\pm b$ are the eigenvalues of the operator $\mathbf{b}\hat{\mathbf{s}}$. In the case of power function $f(\hat{s}_i) = (\hat{s}_i)^{\alpha}$ it is enough to apply a special case when $a = 0$ and $b = 1$. From the relation (4) it follows that

$$\hat{s}^{\alpha}_{k+} = \left(-\frac{i}{2}\right)^{\alpha}\left[\cos\left(\frac{\pi\alpha}{2}\right) + 2i\sin\left(\frac{\pi\alpha}{2}\right)\hat{s}_k\right], \quad \hat{s}^{\alpha}_{k-} \equiv \left(\hat{s}^{\alpha}_{k}\right)^{+}. \tag{5}$$

Note here that the physical sense is inherent not in the operators $\hat{s}^{\alpha}_{k\pm}$, but their symmetrized combinations

$$\hat{s}^{\alpha}_{i} = \frac{1}{2}\left(\hat{s}^{\alpha}_{i+} + \hat{s}^{\alpha}_{i-}\right) = \frac{1}{2^{\alpha}}\left[\cos^2\left(\frac{\pi\alpha}{2}\right)I + 2\sin^2\left(\frac{\pi\alpha}{2}\right)\hat{s}_i\right]. \tag{6}$$

The operators $\hat{s}^{\alpha}_{i}$ are Hermitian and their eigenvalues are real numbers.

The relation (6) allows an easy derivation of commutation relations for spin operators of fractional power:

$$[\hat{s}_i^\alpha, \hat{s}_j^\alpha] = \frac{i}{2^{2(\alpha-1)}} \sin^4\left(\frac{\pi\alpha}{2}\right) \varepsilon_{ijk}\ \hat{s}_k\,. \tag{7}$$

Does this proof depend on a particular matrix representation of spin algebra? The answer is negative: to proof the commutation relations of spin operators in the fraction-dimensional space, we did not use any particular representation.

The peculiarity of the spin operator $\hat{s}_i^\alpha$ is that its eigenvalue s_m exceeds 1/2:

$$\hat{s}_i^\alpha \psi(\sigma) = \frac{1}{2^\alpha}\psi(\sigma)\,, \quad s_m = \frac{1}{2^\alpha}\,. \tag{8}$$

Because the operator $\hat{s}_z^\alpha$ for any α has the form $aI + b\hat{s}_z$, the spin operator $\hat{s}_z^\alpha$ evidently commutes with the operator $\hat{s}^2$:

$$[\hat{s}_z^\alpha, \hat{s}^2] = 0\,, \quad \forall\alpha\,. \tag{9}$$

To find the eigenvalues of the square operator

$$(\hat{s}^\alpha)^2 = (\hat{s}_x^\alpha)^2 + (\hat{s}_y^\alpha)^2 + (\hat{s}_z^\alpha)^2,$$

let us consider the operators

$$\hat{s}_\pm^\alpha = \hat{s}_x^\alpha \pm i\hat{s}_y^\alpha.$$

Then the operator

$$\hat{s}_-^\alpha \hat{s}_+^\alpha = (\hat{s}^\alpha)^2 - (\hat{s}_z^\alpha)^2 + i[\hat{s}_x^\alpha, \hat{s}_y^\alpha] = (\hat{s}^\alpha)^2 - A\hat{s}_z - B\,, \tag{10}$$

where

$$A = \sin^2(\pi\alpha/2)/2^{2(\alpha-1)}, \qquad B = I/2^{2\alpha}.$$

The effect of operator (10) on the state function with the maximal projection of spin is trivial and thus allows determining the eigenvalues $(s^\alpha)^2$ of the square spin operator $(\hat{s}^\alpha)^2$:

$$(s^\alpha)^2 = \frac{A}{2} + B = \frac{1}{2^{2\alpha}}\left[1 + 2\sin^2\left(\frac{\pi\alpha}{2}\right)\right]\,. \tag{11}$$

Figure 1 presents the dependencies s_m and $(s^\alpha)^2$ as a function of the fractional dimension α. An essential feature is the region $\alpha \in [\alpha_1, \alpha_2]$ in which α_i corresponds to the solution of the equation

$$2^{2\alpha} - 2\sin^2\left(\frac{\pi\alpha}{2}\right) = 1 \qquad (\alpha_1 = 0.5, \quad \alpha_2 \approx 0.6348).$$

For these values of α, $(s^\alpha)^2 \geqslant 1$; *i.e.* the electron turns into a vectorial particle, which is equivalent to the appearance in the medium of an additional electromagnetic interaction. In all other cases the electron is not a pure fermion and may be considered as a particle in a mixed state, which has both fermionic and bosonic components. As follows from equation (11), the transformation rule under rotation is the same

$$\psi(\sigma)' = e^{i\sigma\varphi}\psi(\sigma),$$

but the value of spin σ in spaces $\mathbb{R}^3$ and $\mathbb{R}^{3\alpha}$ is different.

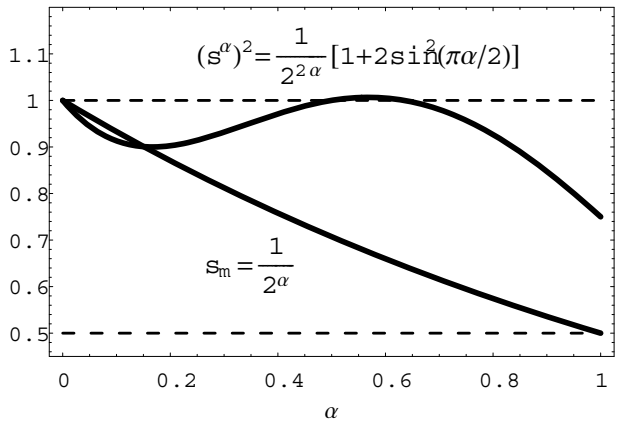

Fig. 1: The eigenvalues of $(s^\alpha)^2$ and s_m as a function of the fractional dimension α ($\hbar = 1$).

The above peculiarities of electrons in the fraction-dimensional space may contribute to theory of solid body, theory of superconductivity, the quantum Hall effect, theory of phase transitions.

Thus, the answer to the question formulated in the beginning of the paper regarding the electron spin in the fraction-dimensional space is as follows: the spin projection becomes large and the value of spin square has nonmonotonic growth. In particular, in the Menger sponge case (Hausdorff dimension $d_M = \ln 20/\ln 3 \approx 2.726833$) $\alpha = \ln 20/\ln 27 \approx 0.9089443$ and $s_m^\alpha = 1/2^\alpha \approx 0.5325747$, $(s^\alpha)^2 \approx 0.8393812$.

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ALGEBRA SPINÓW W PRZESTRZENI O WYMIARZE UŁAMKOWYM

S t r e s z c z e n i e

Autor wykazuje, że w przypadku, gdy efektywny wymiar przestrzeni nie jest całkowity i może przyjmować wartości ułamkowe, elektron staje się cząstką, dla której rzut spinu s_z wynosi $1/2^\alpha$, gdzie $0 \leq \alpha \leq 1$.

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Roman Stanisław Ingarden and Julian Ławrynowicz

RANDERS GEOMETRY AND GAUGE THEORIES I

SOLITONS AND COMPLEX GAUGE THEORIES

Summary

The gauge theorems play in physics a role of interpretation of the fundamental theorems of Emmy Noether concerning, in particular, invariance of action integrals with respect to some proper groups of transitions. The formalism related to Kałuża-Klein gauge theories, natural e.g. for theories unifying electrodynamics and thermodynamics, and the corresponding gauge transformation due to an external field leads, in general, to a Randers metric. Now, the Randers geometrical approach to gauge theories yields the theory containing solitons of field equations. It is then natural to distinguish static, dynamic, probabilistic, and quantum Randers spaces including, because of space-time, complex Randers structures. Finally, we outline the Hurwitz pair description of gauge theories related to solitons.

Introduction

For *Randers spaces* we refer to [AIM, T]. We also have to summarize some material of [Ł3B, Ł5.5] according [ILS].

Take two real numbers x and y. They satisfy

$$|xy| = |x|\ |y|.$$

Setting $f(x, y) = xy$, we have $|f(x, y)| = |x|\ |y|$. Taking account of the fact that f is a bilinear mapping $f : \mathbb{R} \times \mathbb{R} \to \mathbb{R}$, we proceed as follows. Let $\mathbb{E}^n$ denote the n-dimensional Euclidean space with the norm $\| \ \|_n$. If a bilinear mapping $f : \mathbb{E}^n \otimes \mathbb{E}^p \to \mathbb{E}^n$ satisfies

$$\|f(x, y)\|_n = \|x\|_p\ \|y\|_n,$$

f is said to satisfy the *Hurwitz condition*; cf. [H].

In the case of a pseudoeuclidean space $\mathbb{E}^{r,s}, r+s=p,\ \|x\|_p$ denotes the usual pseudonorm, but $\|y\|_n$ has to be replaced by the scalar product $\langle y,z\rangle_n = y\kappa z^T$, where z^T means z transposed, so that the condition becomes

$$\langle f(x,y), f(x,z)\rangle_n = \|x\|_p \langle y,z\rangle_n.$$

It appears that, if κ is diagonalized, it is sufficient to take it either $\kappa = I_n$, I_n being the unit matrix of dimension n (euclidean or, differently speaking, elliptic case), or

$$\kappa = \operatorname{diag}\left(I_{\frac{1}{2}n}, -I_{\frac{1}{2}n}\right) \equiv \begin{pmatrix} I_{\frac{1}{2}n} & 0 \\ 0 & -I_{\frac{1}{2}n} \end{pmatrix} \quad \text{(pseudoeuclidean hyperbolic case)}$$

– for $p>1$, the n-dimensional space in question is always even-dimensional. If κ cannot be diagonalized, it is sufficient to take it symplectic:

$$\kappa = \operatorname{diag}^*\left(I_{\frac{1}{2}n}, -I_{\frac{1}{2}n}\right) \equiv \begin{pmatrix} 0 & I_{\frac{1}{2}n} \\ -I_{\frac{1}{2}n} & 0 \end{pmatrix} \quad \text{(pseudoeuclidean symplectic case).}$$

On the other side, a symplectic κ represents also a complex structure.

If f is irreducible, i.e. there exist no subspaces V of $\mathbb{E}^n,\ V\neq\{0\},\ \mathbb{E}^n$, such that

$$f|\mathbb{E}^{r,s}\otimes V \to V,$$

the pair $(\mathbb{E}^n, \mathbb{E}^{r,s})$ is called *pseudoeclidean* (in particular, *Euclidean*) *Hurwitz pair* [ŁR2, ŁR3]. Since, for $p>1$, the n-dimensional space in question is even-dimensional, it can be complexified. If we suppose that

$$\kappa_{jm}\in\mathbb{C}, j,m=1,2,\dots,n, \quad \text{and} \quad \kappa = |\kappa_{jm}| \quad \text{is hermitian,}$$

then in the Hurwitz-type condition we have to replace n by $\frac{1}{2}n$ and suppose that $y,z\in\mathbb{C}^{\frac{1}{2}n}$. The corresponding pair is called *Hermitian Hurwitz pair* [FK, KS, Ł2].

The determination of a Hurwitz pair is equivalent to that of a special Clifford algebra with generators $\gamma_1,\gamma_2,\dots,\gamma_{p-1},I_n$. It appears [H, ŁR4] that

$$n = 2^{\left[\frac{1}{2}p+\frac{1}{2}\right]} \quad \text{for} \quad |r-s| \equiv 2,3,4,5,6 \ (\text{mod } 8),$$

$$n = 2^{\left[\frac{1}{2}p\right]} \quad \text{for} \quad |r-s| \equiv 7,0,1 \ (\text{mod } 8).$$

Moreover, with each Hurwitz pair we can associate a Dirac-type equation. For this purpose we define the *quantization mapping* as follows. By replacement of x_α by

$$\partial_\alpha = \frac{\partial}{\partial x_\alpha}, \qquad \alpha = 1,2,\dots,p,$$

in the mapping f, we obtain a Dirac-type operator

$$D_p^n = \sum_{\alpha=1}^{p-1} I\gamma_\alpha\partial_\alpha - I_\nu\partial_p \tag{1}$$

which, in the opposite way, can be used for determining the corresponding Hurwitz pair.

Finally, we introduce a special complex structure which is deeply connected with physics. Since

$$\gamma_\alpha^2 = -I_\alpha,\ \gamma_\alpha^T = -\gamma_\alpha,\ \alpha = 1, 2, \dots, p-1,$$

we get a graded complex structure

$$J_{\tilde{x}} = \sum_{\alpha=1}^{p-1} \tilde{x}_\alpha \gamma_\alpha$$

which we call *supercomplex structure* with the direction $\tilde{x}$ [LR2, SŁK]. If we interpret the mapping f as a multiplication

$$f(x, y) \equiv x \circ_f y,$$

then, clearly, the endomorphism $\hat{J}_{\tilde{x}}$ corresponding to $J_{\tilde{x}}$ plays the role of a Hamiltonian with eigenvalues or eigenfunctions $\tilde{x}$:

$$\hat{J}_{\tilde{x}} y = \tilde{x} \circ_f y. \tag{2}$$

Let us restrict $\tilde{x}$ to a $(p-1)$-dimensional sphere S^{p-1} in $\mathbb{E}^p$. Then, with the notation

$$\mathrm{Supcom}(\mathbb{E}^n, \mathbb{E}^p) = \{J_{\tilde{x}} : \tilde{x} \in S_{p-1}\},$$

we state what follows:

Remark 1. There exists an element S of $SO(p-1, \mathbb{R})$ such that

$$J_{\tilde{x}} = S J_0 S^{-1}, \quad \text{where} \quad J_0 = \mathrm{diag}^* \left(I_{\frac{1}{2}n}, -I_{\frac{1}{2}n} \right).$$

Example 1. $\mathrm{Supcom}(\mathbb{E}^2, \mathbb{E}^2) = \{J_0\}$, $\mathrm{Supcom}(\mathbb{E}^4, \mathbb{E}^3) \simeq S^2 \simeq \mathbb{P}^1$.

1. Solitons in the Randersian physics

We start with (cf. [IŁS], p. 84):

Theorem 1. *If $\mathcal{L}$, $\mathcal{L} \neq 0$, is a Lagrangian in the sense of Finsler, satisfying the condition:*

(α) *the function*

$$\mathcal{L} = \mathcal{L}(\varphi^A, \varphi^A_{|t}, \varphi^A_{|x^1}, \varphi^A_{|x^2}, \varphi^A_{|x^3}, \varphi^A_{|x^4})$$

is homogeneous of degree 1 with respect to $\varphi^A_{|t}$, $A = 1, 2, \dots, N$;

(β) $\det[(\partial^2 / \partial \varphi^A_{|t} \partial \varphi^B_{|t}) \mathcal{L}^2] \neq 0$ *for $A, B = 1, 2, \dots, N$,*

then the corresponding Euler-Lagrange equations imply

$$\sum_{A=1}^{N} \varphi^A_{|t} \frac{\partial \mathcal{L}}{\partial \varphi^A} \left(\mathcal{L} - \sum_{B=1}^{N} \frac{\partial \mathcal{L}}{\partial \varphi^B_{|t}} \varphi^B_{|t} \right) - \mathcal{L} \sum_{j=1}^{4} \frac{\partial}{\partial x^j} \sum_{A=1}^{N} \varphi^A_{|t} \frac{\partial \mathcal{L}}{\partial \varphi^A_{|x^j}} = 0.$$

Proof. Let us multiply the Euler-Lagrange equations for $\mathcal{L}$ by $\mathcal{L}$:

$$\mathcal{L}\frac{\partial}{\partial t}\left(\frac{\partial \mathcal{L}}{\partial \varphi^A_{|t}}\right)+\mathcal{L}\sum_{j=1}^{4}\frac{\partial}{\partial x^j}\left(\frac{\partial \mathcal{L}}{\partial \varphi^{A_j}_{|x}}\right)-\mathcal{L}\frac{\partial \mathcal{L}}{\partial \varphi^A}=0,\quad A=1,2,\dots,N.$$

Since

$$\frac{\partial}{\partial t}\left(\mathcal{L}\frac{\partial \mathcal{L}}{\partial \varphi^A_{|x_j}}\right)=\frac{\partial \mathcal{L}}{\partial t}\cdot\frac{\partial \mathcal{L}}{\partial \varphi^A_{|t}}+\mathcal{L}\frac{\partial}{\partial t}\left(\frac{\partial \mathcal{L}}{\partial \varphi^A_{|t}}\right),$$

we get

$$\frac{\partial}{\partial t}\left(\mathcal{L}\frac{\partial \mathcal{L}}{\partial \varphi_{|t^A}}\right)-\frac{\partial \mathcal{L}}{\partial t}\cdot\frac{\partial \mathcal{L}}{\partial \varphi^A_{|t}}+\mathcal{L}\sum_{j=1}^{4}\frac{\partial}{\partial x^j}\left(\frac{\partial \mathcal{L}}{\partial \varphi^A_{|x_j}}\right)-\mathcal{L}\frac{\partial \mathcal{L}}{\partial \varphi^A}=0,$$

(3)

$$A=1,2,\dots,N.$$

Introducing the *generalized momenta in the sense of Finsler*

$$p_A:=\frac{1}{2}\left(\partial/\partial\varphi^A_{|t}\right)\mathcal{L}^2\left(\varphi^A,\varphi^A_{|t},(\varphi^A_{|x^j})\right)\equiv\mathcal{L}\left(\partial/\partial\varphi^A_{|t}\right)\mathcal{L},\tag{4}$$

where

$$(\varphi^A_{|x^j})=(\varphi^A_{|x^1},\varphi^A_{|x^2},\varphi^A_{|x^3},\varphi^A_{|x^4}),$$

and the *Hamiltonian in the sense of Finsler*

$$\mathcal{H}(\varphi^A,\varphi^A_{|x^j},p_A):=\mathcal{L}(\varphi^A,\varphi^A_{|t},(\varphi^A_{|x^j}))\text{ with }\varphi^A_{|t}=\Lambda^A(\varphi^A,(\varphi^A_{|y^j}),p_A),\tag{5}$$

Λ^A being homogeneous of degree 1 with respect to p^A, we have

$$\frac{\partial \mathcal{L}}{\partial t}\cdot\frac{\partial \mathcal{L}}{\partial \varphi^A_{|t}}=\frac{\partial \mathcal{H}}{\partial t}\cdot\frac{p_A}{\mathcal{H}}.$$

In consequence, by (4) we can rewrite (3) in the form

$$\frac{\partial p_A}{\partial t}-\mathcal{L}\frac{\partial \mathcal{L}}{\partial \varphi^A}-\frac{p_A}{\mathcal{H}}\cdot\frac{\partial \mathcal{H}}{\partial t}+\mathcal{L}\sum_{j=1}^{4}\frac{\partial}{\partial x^j}\left(\frac{\partial \mathcal{L}}{\partial \varphi^A_{|x^j}}\right)=0.$$

Next, by

$$\frac{\partial \mathcal{H}}{\partial t}=\sum_{B=1}^{N}\left(\frac{\partial \mathcal{H}}{\partial \varphi^B}\varphi^B_{|t}+\frac{\partial \mathcal{H}}{\partial p_B}\cdot\frac{\partial p_B}{\partial t}+\frac{\partial \mathcal{H}}{\partial \varphi^B}\cdot\frac{\partial^2\varphi^B}{\partial x^j\partial t}\right),$$

we obtain

$$\frac{\partial p_A}{\partial t}=\frac{p_A}{\mathcal{H}}\sum_{B=1}^{N}\left(\frac{\partial \mathcal{H}}{\partial \varphi^B}\varphi^B_{|t}+\frac{\partial \mathcal{H}}{\partial p_B}\cdot\frac{\partial p_B}{\partial t}+\frac{\partial \mathcal{H}}{\partial \varphi^B_{|x^j}}\cdot\frac{\partial^2\varphi^B}{\partial x^j\partial t}\right)$$
$$+\mathcal{L}\frac{\partial \mathcal{L}}{\partial \varphi^A}-\mathcal{L}\sum_{j=1}^{4}\frac{\partial}{\partial x^j}\left(\frac{\partial \mathcal{L}}{\partial \varphi^A_{|x^j}}\right)=0,\quad A=1,2,\dots,N.$$

It is not difficult to check that

$$\left(\partial/\partial\varphi^A\right)\mathcal{L} = -\left(\partial/\partial\varphi^A\right)\mathcal{H}, \quad A = 1, 2, \dots, N. \tag{6}$$

Hence, by (4)

$$\frac{p_A}{\mathcal{H}}\sum_{B=1}^{N}\frac{\partial\mathcal{H}}{\partial\varphi^B}\varphi^B_{|t} = \frac{\mathcal{L}}{\mathcal{H}}\cdot\frac{\partial\mathcal{L}}{\partial\varphi^A_{|t}}\sum_{B=1}^{N}\frac{\partial\mathcal{H}}{\partial\varphi^A}\varphi^B_{|t} = -\frac{\partial\mathcal{L}}{\partial\varphi^A_{|t}}\sum_{B=1}^{N}\frac{\partial\mathcal{L}}{\partial\varphi^A}\varphi^B_{|t}.$$

Yet, the relations (6) have obvious analogues

$$\left(\partial/\partial\varphi^A_{|x^j}\right)\mathcal{L} = -\left(\partial/\partial\varphi^A_{|x^j}\right)\mathcal{H}, \quad A = 1, 2, \dots, N;\ j = 1, 2, 3, 4, \tag{7}$$

so

$$\begin{aligned}\frac{\partial P_A}{\partial t} = {}& \mathcal{L}\frac{\partial\mathcal{L}}{\partial\varphi^A} - \frac{\partial\mathcal{L}}{\partial\varphi^A_{|t}}\sum_{B=1}^{N}\frac{\partial\mathcal{H}}{\partial\varphi^B}\varphi^B_{|t} + \frac{p_A}{\mathcal{L}}\sum_{B=1}^{N}\left(\frac{\partial\mathcal{H}}{\partial p_B}\cdot\frac{\partial p_B}{\partial t} - \frac{\partial\mathcal{L}}{\partial\varphi^B_{|x^j}}\cdot\frac{\partial^2\varphi^B}{\partial x^j\partial t}\right)\\ & -\mathcal{L}\sum_{j=1}^{4}\frac{\partial}{\partial x^j}\left(\frac{\partial\mathcal{L}}{\partial\varphi^A_{|x^j}}\right),\ A = 1, 2, \dots, N.\end{aligned} \tag{8}$$

By the homogeneity of $\mathcal{L}$, we have

$$\sum_{A=1}^{N}\varphi^A_{|t}p_A = \sum_{A=1}^{N}\varphi^A_{|t}\mathcal{L}\frac{\partial L}{\partial\varphi^A_{|t}} = \mathcal{L}\sum_{A=1}^{N}\varphi^N_{|t}\frac{\partial\mathcal{L}}{\partial\varphi^A_{|t}} = \mathcal{L}\cdot\mathcal{L} = \mathcal{L}^2.$$

Multiplying both sides of (8) by $\mathcal{L}\varphi^A_t$, summing them with respect to A, and applying the latter relation, we get

$$\begin{aligned}\sum_{A=1}^{N}\left(\varphi^A_{|t}\frac{\partial p_A}{\partial t} - \mathcal{L}\frac{\partial\mathcal{H}}{\partial p_A}\cdot\frac{\partial p_A}{\partial t}\right) = {}& \sum_{A=1}^{N}\varphi^A_{|t}\frac{\partial\mathcal{L}}{\partial\varphi^A}\left(\mathcal{L} - \sum_{B=1}^{N}\frac{\partial\mathcal{L}}{\partial\varphi^B_{|t}}\varphi^B_{|t}\right)\\ & -\mathcal{L}\sum_{j=1}^{4}\sum_{A=1}^{N}\left[\frac{\partial\mathcal{L}}{\partial\varphi^A_{|x^j}}\cdot\frac{\partial^2\varphi^A}{\partial x^j\partial t} + \varphi^A_{|t}\frac{\partial}{\partial x^j}\left(\frac{\partial\mathcal{L}}{\partial\varphi^A_{|x^j}}\right)\right].\end{aligned}$$

It is not difficult to calculate the derivatives φ^A_t:

$$\begin{aligned}\varphi^A_{|t} &= \mathcal{H}\left(\varphi^A, (\varphi^A_{|x^j}), p_A\right)\frac{\partial}{\partial p_A}\mathcal{H}\left(\varphi^A, (\varphi^A_{|x^j}), p_A\right)\\ &\equiv \frac{1}{2}\frac{\partial}{\partial p_A}\mathcal{H}^2\left(\varphi^A, (\varphi^A_{|x_j}), p_A\right),\ A = 1, 2, \dots\\ &\equiv \frac{1}{2}\frac{\partial}{\partial p_A}\mathcal{H}^2\left(\varphi^A, (\varphi^A_{|x_j}), p_A\right),\ A = 1, 2, \dots, N.\end{aligned} \tag{9}$$

By this we observe that the preceding formula becomes

$$\sum_{A=1}^{N}\left(\varphi^A_{|t}\frac{\partial p_A}{\partial t}-\mathcal{L}\frac{\partial\mathcal{H}}{\partial p_A}\cdot\frac{\partial p_A}{\partial t}\right)=\sum_{A=1}^{N}\left(\varphi^A_{|t}\frac{\partial p_A}{\partial t}-\mathcal{H}\frac{\partial\mathcal{H}}{\partial p_A}\cdot\frac{\partial p_A}{\partial t}\right)$$
$$=\sum_{A=1}^{N}\left(\varphi^A_{|t}\frac{\partial p_A}{\partial t}-\varphi^A_{|t}\frac{\partial p_A}{\partial t}\right)=0.$$

Finally we notice that

$$\sum_{j=1}^{4}\sum_{A=1}^{N}\left[\frac{\partial\mathcal{L}}{\partial\varphi^A_{|x^j}}\cdot\frac{\partial^2\varphi^A}{\partial x^j\partial t}+\varphi^A_{|t}\frac{\partial}{\partial x^j}\left(\frac{\partial\mathcal{L}}{\partial\varphi^A_{|x^j}}\right)\right]=\sum_{j=1}^{4}\sum_{A=1}^{N}\frac{\partial}{\partial x^j}\left(\varphi^A_{|t}\frac{\partial\mathcal{L}}{\partial\varphi^A_{|x_j}}\right),$$

so, indeed we arrive at the assertion of Theorem 1.

Remark 3. In particular, Theorem 1 together with the Finsler version of Emmy Noether's theorem [M1] imply the first principle of thermodynamics in the extended form given, e.g., in [SS1], formula (3.1.8); cf. also [SS2].

Remark 4. Of course, the assertion of Theorem 1 remains true when $j=1,2,3,4$ is formally replaced by $j=1,2,\dots,n$ with $n=2,3,\dots$.

Remark 5. In the case $N=1$, i.e. when the field is described by only one function $\varphi=\varphi(t,(x^j))$, the equation given in Theorem 1 reduces to

$$\sum_{j=1}^{4}\frac{\partial}{\partial x^j}\left(\varphi_{|j}\frac{\partial\mathcal{L}}{\partial\varphi_{|x^j}}\right)=0$$

because, by the homogeneity of $\mathcal{L}$, its first term becomes 0.

Remark 6. If the number of space variables n is equal to 1, let us change the notation from φ to $u=u(x,t)$ and set

$$u_t=(\partial/\partial t)\,u(x,t),\quad u_x=(\partial/\partial x)\,u(x,t).$$

Then the equation of Remark 5 takes the form

$$\frac{\partial}{\partial x}\left(u_t\frac{\partial\mathcal{L}}{\partial u_x}\right)=0,\ \text{where}\ \mathcal{L}=\mathcal{L}(u,u_t,u_x). \tag{10}$$

The latter equation, equivalent in our case to the Euler-Lagrange equation, is the 1-*dimensional equation of motion in the sense of Finsler*.

It is natural to ask for which Lagrangian (in the sense of Finsler), the equation (9) is fulfilled by any function u of the form $f(x+\omega t)$ or $g(x-\omega t)$, where ω is a constant (physically, a phase). In this direction we have [SK]:

Theorem 2. *A function $u=u(x,t)$ of the form $f(x+\omega t)$ or $g(x-\omega t)$ with ω constant is a solution of the equation* (10) *if and only if the Lagrangian* (*in the sense of Finsler*) *has the form*

$$\mathcal{L}(u, u_t, u_x) = C(u_t/u_x) + u_t D(u),$$

where C is a constant and $D = D(u)$ is a function of the variable u, provided that $u_x \neq 0$ and $(\partial/\partial u_x)\mathcal{L} \neq 0$.

Proof and examples are given, following [DEG, E], in [Ł5.5].

2. Complex Randersian physics

Consider the eigenvalue problem $Ly = \lambda y$ for the differential operator

$$L = -(d^2/dx^2) + u(x, y).$$

For an arbitrary function u, λ may depend on t, a deformation parameter. As a special case we have a deformation which does not change λ, and is called *isospectral deformation*. We call λ an *isospectral parameter*.

Remark 7. Note a formal parallelism between the basic eigenvalue problems related to the operator L with the isospectral parameter λ and the endomorphism $\hat{J}_{\tilde{x}}$ corresponding to the supercomplex structure $J_{\tilde{x}}$ with the direction $\tilde{x}$, fixed whenever $\tilde{x}$ ranges over a Stiefel manifold being the $(p-1)$-dimensional hypersphere determined by $\tilde{x}$ [ŁR1]:

$$Ly = \lambda y \text{ vs. } \hat{J}_{\tilde{x}} y = \tilde{x} \circ_f y. \tag{11}$$

From now on, we restrict ourselves to isospectral deformations and obtain an equation of Heisenberg type. For this purpose we assume that a generator of the isospectral deformation is given by

$$y_t = Ay, \tag{12}$$

where A is a differential operator with respect to x. By differentiating the first relation in (11), we have $Ly_t + L_t y = \lambda y_t$. hence, by (12) we get $(L_t + [L, A])y = 0$. This holds for every eigenvalue λ, so we obtain

Lemma 1. *An isospectral deformation L with the generator* (11) *satisfies*

$$L_t + [L, A] = 0. \tag{13}$$

The left-hand side of (13) is called the *Lax representation* of the isospectral deformation in (11).

Now, let us note that that ordinary differential operators can be written as

$$B = \sum_{j=0}^{n} b_j D^{n-j}, \quad D^0 = 1,$$

where b_j are functions of x (say) and $D = d/dx$. We intend to consider pseudo-differential operators of the form

$$P = \sum_{j=-n}^{\infty} u_{-j} D^{-j}.$$

Operators in question constitute an algebra $\mathcal{A}$. We choose in it a collection of elements W that can be expressed as

$$W = \sum_{j=0}^{\infty} u_{-j} D^{-j}, \quad u_0 = \mathrm{id};$$

it forms a group $\mathcal{A}^*$ which makes elements of $\mathcal{A}$ invertible. If we choose a space H on which W operates as the linear envelope of $\{e^{kx} : k \in \mathcal{C}^*\}, \mathcal{C}^* = \mathcal{C} \cup \{\infty\}$, we can see that

$$D(e^{kx}) = e^{kx} \quad \text{and} \quad D^{-1}(e^{kx}) = \frac{1}{k} e^{kx}.$$

Let us specify L in (11) as a pseudo-differential operator of the form

$$L = D + \sum_{j=0}^{\infty} u_{-j} D^{-j}$$

and set $L^n := L^{n-1} L$. Then

$$L^n = \sum_{j=-n}^{\infty} b_{-j} D^{-j}, \quad b_n = 0.$$

We denote the part of non-negative orders and the part of negative orders by L^n_+ and L^n_-, respectively. If we choose an invertible operator $P : H \to H$, then L is transformed to $\tilde{L} = P^{-1} L P$. Hence, by choosing a suitable P, we may obtain some kind of the normal form of L. Explicitly, if we choose

$$P(f) = e^{\phi} f \quad \text{for} \quad f \in H,$$

where f is a C^∞-function, then we can see that

$$\tilde{L} = D + \sum_{j=1}^{\infty} u_{-j} D^{-j-1}$$

by choosing a suitable ϕ and, consequently, we may assume that L is of this form. Hence

Lemma 2. *There is an element $W \in A^*$ such that $W^{-1} L W = D$.*

Now, let $t = t_n)$ be a possibly infinite system of parameters. We set $L(t) = W D W^{-1}$; it determines an isospectral deformation of D.

Remark 8. Note a formal parallelism between the resolutions (cf. Remark 1):

$$\tilde{L} = P^{-1} L P, \; L(t) = W D W^{-1}, \quad \text{and} \quad J_{\tilde{x}} = S J_0 S^{-1}.$$

Lemma 1 may be completed by [DJK, L, Mo, SłK1]:

Theorem 3. *The isospectral deformation $L(t)$ of D has a generator of a differential operator for any t_n if and only if*

$$(\partial/\partial t_n)\psi = L_+^n\psi \quad \textit{for} \quad n = 1, 2, \ldots .$$

Proof and an example are given, following [DJK, SŁK1, SK], in [Ł5.4].

Theorem 3 motivates the following

Definition 1. $L(t)$ as given by $L(t) = WDW^{-1}$ is called the *Kadomtsev-Petviashvili system* whenever it satisfies the equations

$$(\partial/\partial t_n)\, L + [L, L_+^n] = 0 \quad \text{for} \quad n = 1, 2, \ldots . \tag{14}$$

Then $L = L(t)$ is called a *solution* of the associated Kadomtsev-Petviashvili system (14).

3. Complex gauge connections of interacted fields

We are going to show that the associated Kadomtsev-Petviashvili systems (14) include some Kodaira-Spencer equations [KSp] of complex structures and Wu-Kobayashi connections [Kb] as special cases. By use of these gauge connections we can treat the interacted fields with the Hurwitz- and Dirac-like equations in relation to the Fueter equation [F1, F2].

Let G be a finite- or infinite-dimensional Lie group and let $\mathcal{A}$ be a vector space which is a right *and* left G-module. The adjoint operator Ad_g, $g \in G$, sends $x \in \mathcal{A}$ to $gxg^{-1} \in \mathcal{A}$; it defines an *action* of G on $\mathcal{A}$. Clearly,

$$[x, g]x^{-1} = x = \mathrm{Ad}_g x,$$

where, as before, [,] denotes the commutator.

Definition 2. The pair $(\mathcal{A}, G)$ as above with the action $\{\mathrm{Ad}_g : g \in G\}$ is called a *gauge decomposition with the gauge group* G whenever there exists a decomposition $\mathcal{A} = \mathfrak{G} \oplus \mathfrak{M}$ which satisfies the following conditions:

$$\text{(I)} \qquad \mathrm{Ad}_g\mathfrak{G} \subseteq \mathfrak{G} \quad \text{for} \quad g \in G,$$

$$\text{(II)} \quad [x, g]g^{-1} \in \mathfrak{G} \quad \text{for} \quad x \in \mathfrak{M},\ g \in G.$$

Definition 3. Consider the pair $(\mathcal{A}, G)$ as above (as in Definition 2) with the action $\{\mathrm{Ad}_g : g \in G\}$ and let $\mathcal{A} = \mathfrak{G} \oplus \mathfrak{M}$ be an arbitrary decomposition of $\mathcal{A}$. Then we call

$$\mathfrak{M}_1(G) = \left\{x \in \mathfrak{M} : [x, g]g^{-1} \in \mathfrak{G} \quad \text{for} \quad g \in G\right\}$$

the *set of gauge elements of the gauge group* G.

For the examples of notions introduced in Definitions 2 and 3 we refer to [Ł5.5].

Denote next by $(z^\nu : \nu = 1, 2, \dots, n)$ a system of co-ordinates in the complex vector space $\mathbb{C}^n$, and by $\bar{z}^\nu : \nu 1, 2, \dots, n)$ – the system of complex conjugate co-ordinates. We set

$$\partial_\nu := \partial/\partial z^\nu,\ \bar{\partial}_\nu := \partial/\partial \bar{z}^\nu,\ \nu = 1, 2, \dots, n.$$

and, more generally,

$$\partial^\alpha \bar{\partial}^\beta := \prod_{\nu=1}^{n} \partial_\nu^{\alpha_\nu} \bar{\partial}_\nu^{\beta_\nu}, \quad \begin{matrix} \alpha = (\alpha_\nu, \nu = 1, 2, \dots, n), \\ \beta = (\bar{\beta}_\nu, \nu = 1, 2, \dots, n) \end{matrix}$$

with

$$|\alpha| = \sum_{\nu=1}^{n} \alpha_\nu, \quad |\beta| = \sum_{\nu=1}^{n} \bar{\beta}_\nu.$$

More simply, we may write the differential operator in question as

$$\partial^A, \quad \text{where} \quad A = (\alpha, \bar{\beta}),\ |A| = |\alpha| + |\beta|.$$

Then a pseudo-differential operator P can be written as

$$P = \sum_{|A| \geq 0} u_A(z, \bar{z}) \partial^A$$

and we set

$$\mathcal{P} = \left\{ P = \sum_{|A| \geq 0} u_A(z, \bar{z}) \partial^A \right\}.$$

In the following we assume that u_A are C^∞-functions or real-analytic functions of z and $\bar{z}$. Obviously, $\mathcal{P}$ is an associative algebra with respect to the usual composition of operators and a Lie algebra. In order to consider a gauge theory of $\mathcal{P}$ we set

$$\mathcal{P}_\partial := \left\{ \sum_{|A| \geq 0} u_A \partial^A \in \mathcal{P} : A = (\alpha, 0) \right\}, \quad \mathcal{P}_{\bar{\partial}}^c : \mathcal{P} \ominus \mathcal{P}_\partial.$$

Then we have $\mathcal{P} = \mathcal{P}_\partial \oplus \mathcal{P}_{\bar{\partial}}^c$ and distinguish the *analytic group of the first kind*:

$$G_\partial^1 := \{ g \in \mathcal{P}_\partial : u_0 = 1 \} \tag{15}$$

and the *analytic group of the second kind*:

$$G_\partial^2 := \{ g \in \mathcal{P}_\partial : u_0 \neq 0 \}. \tag{16}$$

Consider now the associated Kadomtsev-Petviashvili system (14) related to the decomposition in question. Thus we have to choose a commuting system of $\bar{\partial}_\nu : \nu = 1, 2, \dots, n$, namely $\bar{\partial}_\beta$, $\beta = (\bar{\beta}_\nu : \nu = 1, 2, \dots, n)$, and set

$$L_\beta(W) := W \bar{\partial}^\beta W^{-1}, \quad \text{where} \quad W = G_\partial^1 \otimes G_\partial^2. \tag{17}$$

Denote the part of orders in L_β corresponding to $\mathcal{P}_\partial$ and $\mathcal{P}_{\bar{\partial}}^c$ by L_∂^β and $L_{\bar{\partial}}^\beta$, respectively: $L^\beta = L_\partial^\beta + L_{\bar{\partial}}^\beta$. Therefore the associated Kadomtsev-Petviashvili system (14) becomes

$$(\partial/\partial t_\beta)\, L_\alpha + [L_\alpha, L^\beta_\partial] = 0 \quad \text{for} \quad \alpha, \beta = \left(\bar\alpha_\nu, \bar\beta_\nu : \nu = 1, 2, \dots, n\right)$$

or, equivalently,

$$(\partial/\partial t_\beta)\, L_\alpha + [L^\beta_{\bar\partial}, L_\alpha] = 0 \quad \text{for} \quad \alpha, \beta = \left(\bar\alpha_\nu, \bar\beta_\nu : \nu = 1, 2, \dots, n\right). \tag{18}$$

We conclude with

Theorem 4. *Any solution of the associated Kadomtsev-Petviashvili system* (18) *can be obtained from a solution of the system of equations*

$$(\partial/\partial t_\beta)U = \bar\partial_\beta U, \quad \textit{where} \quad \beta = (\bar\beta_\nu : \nu = 1, 2, \dots, n), \tag{19}$$

by use of the decomposition $U = W^{-1}V$*, where* $W \in G_\partial$ *and* $V \in G^c_{\bar\partial}$*, and by setting* (17)*.*

Proof is given, following [IŁS], in [Ł5.5].

Now, by (19), we may set $t_\alpha = \bar z_\alpha$ for $\alpha = (\bar\alpha_\nu : \nu = 1, 2, \dots, n)$. Hence (18) becomes

$$(\partial/\partial \bar z_\beta)\, L_\alpha + \left[L^\beta_{\bar\partial}, L^\alpha\right] = 0 \quad \text{for} \quad \alpha, \beta = (\bar\alpha_\nu, \bar\beta_\nu : \nu = 1, 2, \dots, n). \tag{20}$$

We are going to show that these equations lead to the Kodaira-Spencer equations [KSp]. In fact, The Schrödinger equation of (20) is

$$(\partial/\partial \bar z_\beta)\mathbf{\Psi} + L^\beta_{\bar\partial}\mathbf{\Psi} = 0 \quad \text{for} \quad \beta = \left(\bar\beta_\nu : \nu = 1, 2, \dots, n\right), \tag{21}$$

where the correspondence between L and $\mathbf{\Psi}$ is determined by the correspondence between (17) and a relation of the form $\mathbf{\Psi} = W\mathbf{\Psi}_0$.

Definition 3. A solution of the system of equations (20) is called its *k-reduction solution* whenever

$$L_\beta = \bar\partial^\beta + \sum_{j=0}^{k} \sum_{|\sigma|=j} u^\beta_\sigma \partial^\sigma, \text{ where } \beta, \sigma = \left(\bar\beta_\nu, \bar\sigma_\nu : \nu = 1, 2, \dots, n\right).$$

Definition 4. Let $\mathcal{A} = \mathfrak{G} \oplus \mathfrak{M}$ be a gauge decomposition related to the pairs $(\mathcal{A}, G)$. A mapping $\Omega : \mathfrak{M} \otimes G \to \mathfrak{G}$ is called a *gauge connection* whenever

(A) Ω is a linear mapping with respect to the variable $x \in \mathfrak{M}$ for a fixed $g \in G$.

(B) For a fixed $x \in \mathfrak{M}$ and $W, W' \in G$, we have

$$x - \Omega_x(W) = \mathbf{\Psi}(x - \Omega_x(W'))\mathbf{\Psi}^{-1},$$

where $\mathbf{\Psi} = WW'^{-1}$ and $\Omega_x(W)$ stays for $\Omega(x, W)$.

Definition 5. The mapping $\hat\Omega$ from $\mathfrak{M}$ to $\mathfrak{G}$, defined by

$$\hat\Omega(x) = W^{-1}\left([X, W]W^{-1} - \Omega_x(W)W\right),$$

is called the *connection form of the connection* Ω.

Definition 6. (a) Suppose that $\mathcal{A}$ and G in Definition 4 are operators on a Hilbert space $\boldsymbol{H}$. By the *covariant differentiations* of the connection Ω we mean the operator $\nabla_x^W := x - \Omega_x(W)$ acting from $\boldsymbol{H}$ to $\boldsymbol{H}$.

(b) Then, by the *G-invariant covariant differentiation* we mean the operator $\hat{\nabla}_x = W^{-1}\nabla_x W$ or, equivalently,

$$\hat{\nabla}_x \boldsymbol{\Psi} = \left[x + \hat{\Omega}(x)\right] \boldsymbol{\Psi} \quad \text{for} \quad \boldsymbol{\Psi} \in \boldsymbol{H}.$$

Now we are ready to state precisely the already announced correspondence theorem.

Theorem 5. *In case of the analytic group of the first kind* (15) *any one-reduction solution of the associated Kadomtsev-Petviashvili system* (20) *is a solution of the Kodaira-Spencer equations*

$$(\partial/\partial \bar{z}_\beta)\boldsymbol{\Psi} + \sum_{j=1}^{n} \sum_{|\sigma|=j} u_\sigma^\beta (\partial/\partial \bar{z}_\sigma)\boldsymbol{\Psi} = 0$$

(22)

$$\textit{for} \quad \beta, \sigma = \left(\bar{\beta}_\nu, \bar{\sigma}_\nu : \nu = 1, 2, \dots, n\right),$$

where the correspondence between L and $\boldsymbol{\Psi}$ is determined by the correspondence between (17) *and a relation of the form $\boldsymbol{\Psi} = W\boldsymbol{\Psi}_0$.*

Proof and an example are given, following [KSp], in [Ł5.5].

4. Hurwitz pair description of gauge theories

Theorem 5 shows that solutions of the associated Kadomtsev-Petviashvili system (20) may lead to a complex structure yielding holomorphic functions. When proceeding to supercomplex structures we can see, by Remark 1, that when setting

$$\mathcal{O}_\partial^1 = \{W \in \mathcal{P}_\partial : W^* W = \mathrm{id}\} \tag{23}$$

and restricting ourselves to the complex structure implied by (20), we can get the supercomplex structure

$$\Omega = [\bar{\partial}, W]W^{-1} \quad \text{with} \quad \Omega^* = -\Omega.$$

When applying the above procedure to the Hurwitz- and Dirac-like operators in question, we can obtain some interacting fields which are similar to anti-self dual Yang-Mills connections [SŁK1].

We are going to concentrate on the complex analytic gauge theory of the vector bundle over $\mathbb{C}^p$, $p = 2, 3, \dots$, and its application to Hurwitz pairs. Let $\pi : E \to \mathbb{C}^p$ be a vector bundle over $\mathbb{C}^p$ of rank n. It is assumed to be a G_0-bundle, $G_0 = \mathrm{GL}(n, \mathbb{C})$. Similarly, set $\mathfrak{G}_0 = \mathrm{gL}(n, \mathbb{C})$. Suppose that $\mathfrak{G}$ and G are of the class C^∞ and act

from $\mathbb{C}^p$ to $\mathfrak{G}_0$ and from $\mathbb{C}^p$ to G_0, respectively. Let $\mathcal{P}_\partial \oplus \mathcal{P}^c_\partial$ denote the complex analytic decomposition as introduced in the preceding section. Let us set

$$\mathfrak{G} = \mathfrak{H} \oplus \mathfrak{M}, \quad \text{where} \quad \mathfrak{H} = \mathcal{P}^c_\partial \otimes \mathfrak{G} \quad \text{and} \quad \mathfrak{M} = \mathcal{P}_\partial \otimes \mathfrak{G}. \tag{24}$$

Next let

$$\begin{aligned} G &= \left\{ g \in \mathfrak{G} : g^{-1} \in \mathfrak{G} \right\}, \\ G_+ &= \left\{ g \in \mathfrak{H} : g^{-1} \in \mathfrak{H} \right\}, \\ G_- &= \left\{ g \in \mathfrak{M} : g^{-1} \in \mathfrak{M} \right\}. \end{aligned} \tag{25}$$

We conclude with

Theorem 6. *A zero-reduction solution of the associated Kadomtsev-Petviashvili system subjected to the condition* $WW^* = \mathrm{id}$ *determines the Wu-Kobayashi connection* [At] *determined itself by*

$$\bar{\partial}\Omega = \frac{1}{2}[\Omega, \Omega].$$

Proof is given, following [At, SŁK2], in [Ł5.5].

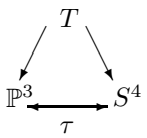
Corollary 1. *In the case of a Euclidean Hurwitz pair* $(\mathbb{E}^n, \mathbb{E}^p)$ *with an even* p *we take into account*

$$\mathcal{O}^1_G = \{W \in G : WW^* = \mathrm{id}\}$$

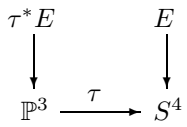
and hence $\Omega^* = -\Omega$. *Then a holomorphic mapping* $\mathbf{\Psi}$ *gives rise to an interacting field with a Hurwitz- or Dirac-type operator.*

Remark 8. The interacting field in question may be regarded as a realization of an anti-self dual connection.

Remark 9. A relationship with the Yang-Mills connections $[N, T]$ is clearly seen. Indeed, let S^4 be the 4-dimensional sphere and let $\pi : E \to S^4$ be an $SU(2)$-bundle over S^4. Consider an anti-self dual connection of E. Since S^4 admits no complex structure, the essential Penrose's idea is that these connections can be treated in terms of complex analysis as follows: We make the Penrose transformation



where T is the twistor space. Then in the diagram



τ^*E becomes an hermitian vector bundle when the connection is anti-self dual. In this case the complex structure is determined by a pullback of the connection via τ, which is the Wu-Kobayashi connection.

In analogy to Penrose twistors one of us discusses in [Ł3B], Section B3, eight types of similar structures introduced in [ŁS3-6]:

(i) Hurwitz twistors, determined by a system of $\binom{5}{4} = 5$ algebraic equations (Lemma B3 in [Ł3B], Case I of Theorem 3.3 in [Ł4.3]);

(ii) pseudotwistors and pseudobitwistors, determined by a system of $\binom{9}{4} = 126$ algebraic equations (Lemma B5 in [Ł3B], Case II of Theorem 3.3 in [Ł4.3]);

(iii) bitwistors, determined by a system of $\binom{13}{5} = 175$ algebraic equations (Lemma B.7 in [Ł3B], Case III of Theorem 3.3 in [Ł4.3]);

(iv) four types of the corresponding "anti-objects"; cf. Fig. B2 in [Ł3B] and Fig. 3.8 in [Ł4.3].

All the structures mentioned are related to some Hurwitz pairs. A particular case of Hurwitz pairs concerns Kałuża-Klein theories; cf. [Ł3.1], Section 1.2, and [ŁR4]. In connection with the Kałuża-Klein gauge theories, Beil [Be1, 2] has shown that *the $U(1)$-symmetry of the electromagnetic field yields the gauge transformation*

$$Y^{\mu}_{\nu} = \delta^{\mu}_{\nu} - B^{-2}[1 - (1 + kB^2)^{\frac{1}{2}}]B_{\mu}B_{\nu},$$

$$Y^{*\mu}_{\nu} = \delta^{\mu}_{\nu} - B^{-2}[1 - (1 + kB^2)^{-\frac{1}{2}}]B_{\mu}B_{\nu},$$

where

$$B^2 = \sum_{\alpha,\beta} \eta_{\alpha,\beta} B^{\alpha} B^{\beta},$$

$\eta_{\alpha\beta}$ is the initial base space metric in the Lorentz form, and k is, in general, velocity dependent. The resulting metric

$$g_{\mu\nu} = \eta_{\mu\nu} + kB_{\mu}B_{\nu}$$

is, in general, Finslerian, even in the case where k is a universal constant related to the gravitational constant.

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[AIM–Zy] See this issue, pp. 56-59.

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GEOMETRIA RANDERSA I TEORIE CECHOWANIA I

SOLITONY I ZESPOLONE TEORIE CECHOWANIA

S t r e s z c z e n i e

Twierdzenia o cechowaniu odgrywają w fizyce rolę interpretacyjną dla fundamentalnych twierdzeń Emmy Noether dotyczących, w szczególności, niezmienniczości całki działania ze względu na pewne właściwe grupy transformacji. Formalizm związany z teoriami cechowania Kałuży-Kleina, naturalny np. w teoriach unifikacji elektrodynamiki i termodynamiki oraz odpowiednia transformacja cechowania wynikająca z istnienia i postaci pola zewnętrznego, prowadzi na ogół do metryki Randersa. Z kolei geometryczne podejście Randersa do występujących teorii cechowania prowadzi do teorii pola zawierającej solitony jako rozwiązania równań pola. Jest zatem rzeczą naturalną wyróżnienie statycznych, dynamicznych, probabilistycznych i kwantowych przestrzeni Randersa włączających, z uwagi na czasoprzestrzeń, zespolone struktury Randersa. Wreszcie, szkicujemy przy użyciu par Hurwitza teorie cechowania związane z solitonami.

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RANDERS GEOMETRY AND GAUGE THEORIES II

RANDERS AND KAŁUŻA-KLEIN GAUGE THEORIES, SELF-DUALITY AND HOMOGENEITY

Summary

Continuing the first part of the paper (this issue, the preceding paper), especially the Hurwitz pair description of gauge theories related to solitons, the totality of dualities generated by the generalized Hurwitz problem is shown to contain five generations of the Kałuża-Klein dualities. Next, following G. Zet and V. Manta (2003), we observe that the gauge theories are usually formulated in terms of potentials $A^\alpha_\mu(x)$, where $\alpha = 1, 2, \ldots, m$ (m is the dimension of the gauge group) and $\mu = 0, 1, 2, 3$. In the Lagrangian formalism equations of the gauge fields $A^\alpha_\mu(x)$ are of second order. To simplify the search for solutions of the field equations it is useful to solve equations of the first order. The self-duality equations are differential equations of the first order and it is easier to investigate the solutions for different particular configurations of the gauge fields and of space-times. Here we have to remember that one of the most important properties of the self-duality equations is that they imply the Yang-Mills field equations. We conclude with A. Sandovici (2003) implications of homogeneity in R. Miron's sense in gauge theories of the second order.

5. Five generations of the Kałuża-Klein dualities

Following [ŁKS] we are going to show that the totality of dualities generated by the generalized Hurwitz problem contains exactly five generations of the Kałuża-Klein dualities.

Continuing considerations of [Ł3A, Ł3B] consider a pair (V, S) of real vector spaces V and S, equipped with scalar products $(a, b)_s \mapsto a\eta b^T$, $a, b \in S$, and $(\ ,\ )_V = (\ ,\ )$, and a multiplication

$$a \cdot f_k := \sum_\alpha \sum_j c^A_{j\alpha} a^\alpha f^j_k, \quad f_k \in V,\ k = 1, 2;\ n = \dim V,$$

$$\eta := \operatorname{diag}(\underbrace{1, \dots, 1}_{r+1 \text{ times}}, \underbrace{-1, \dots, -1}_{s \text{ times}}), \quad r + 1 + s = p = \dim S, \tag{26}$$

satisfying, for all $f_k \in V,\ k = 1, 2, 3;\ a, b \in S,\ \gamma \in \mathbb{R}$, the conditions

$$(f_1, f_2) \in \mathbb{R},\ (\gamma f_1, f_2) = \gamma(f_1, f_2), \quad (f_1, f_2 + f_3) = (f_1, f_2) + (f_2, f_3);$$

either $(f_2, f_1) = (f_1, f_2)$ for all f_1, f_2,
or $\quad = -(f_1, f_2)$ for all f_1, f_2;

$$\gamma a \cdot f_1 = a \cdot \gamma f_1 = \gamma(a \cdot f_1), \quad (a + b) \cdot f_1 = a \cdot f_1 + b f_2,$$
$$a \cdot (f_1 + f_2) = a \cdot f_1 + a \cdot f_2$$

$$(a \cdot f_1, a \cdot f_2) = \left[\sum_{\alpha=1}^{r} (a^\alpha)^2 - \sum_{\alpha=r+1}^{p} (a^\alpha)^2 \right] (f_1, f_2).$$

The pair (V, S) is said to be reducible whenever there are

1° real vector subspaces V_1 and V_2 of V, $\{0\} \neq V_1 \neq V_2 \neq V$, and
2° real vector subspaces V_3 and V_4 of V, $V_3 \cap V_4 \neq \{0\}$,

such that $[S \times V_1] \subset V_3$ and $[S \times V_2] \subset V_4$. The pair (V, S) is called *irreducible* whenever it is not reducible.

An irreducible pair (V, S) is called a *pseudo-euclidean Hurwitz pair* [ŁR1]. Consider now the real $n \times n$-matrices

$$C_\alpha := \left[c^A_{j\alpha} \right],\ \overline{C}_\alpha := \kappa C^T_\alpha \kappa^{P-1}, \quad \text{where} \quad f_1 \times f_2^T = (f_1, f_2),\ f_1, f_2 \in V.$$

We can define purely imaginary $n \times n$-matrices γ_α by

$$C_\alpha = I \gamma_\alpha C_t, \quad t \text{ fixed}, \quad t \in \{1, \dots, p\},\ \alpha \neq t, \tag{27}$$

where i denotes the imaginary unit. It appears that γ_α are generators of a real Clifford algebra $C^{(r,s)}$ chosen in the (imaginary) Maiorana representation. Recall that the real (resp. imaginary) *Maiorana representation* of a Clifford algebra $C^{(r,s)}$ is defined by the choice of its generators as real (resp. purely imaginary) matrices.

Let (V, S) be a pseudo-euclidean Hurwitz pair with the scalar product of S given by the matrix (26). Choose $t \in \{1, \dots, p\}$. It can be proved [ŁPoR] that then the equations (27) and

$$C_t\overline{C}_t = \eta_{tt}I_n, \quad t \text{ fixed}, \quad t \in \{1,\dots,p\};$$
$$\overline{\gamma}_\alpha = -\gamma_\alpha, \quad re\gamma_\alpha = 0, \quad \alpha = 1,\dots,p;\ \alpha \neq t;$$
$$\{\gamma_\alpha,\gamma_\beta\} := \gamma_\alpha\gamma_\beta + \gamma_\beta\gamma_\alpha = 2\hat{\eta}_{\alpha\beta}I_n, \quad \alpha,\beta = 1,\dots,p; \quad \alpha,\beta \neq t;$$
$$\hat{\eta}_{\alpha,\beta} := \eta_{\alpha\beta}/\eta_{tt}, \quad \eta_{tt} = 1 \quad \text{or} \quad -1, \quad \alpha,\beta = 1,\dots,p; \alpha,\beta \neq t,$$

where I_n stands for the identity $n\times n$-matrix, define a Clifford algebra $C^{(r,s)}$, chosen in the imaginary Maiorana representation.

(I.1) By a further change of basis these generators can be chosen as antisymmetric or symmetric according to $\hat{\eta} = 1$ or -1.

(I.2) The integers r, s satisfy (31) if $\eta_{tt} = 1$ and

$$\eta := \mathrm{diag}(\underbrace{1,\dots,1}_{s \text{ times}},\underbrace{-1,\dots,-1}_{r+1 \text{ times}}), \quad s + r + 1 = p = \dim S, \quad \text{if} \quad \eta_{tt} = -1.$$

Thus two Clifford algebras are obtained unless η is positive definite, in which case only one Clifford algebra is obtained.

(I.3) Further, if $\eta_{tt} = 1$, then via a change of basis one may assume $C_t = I_n$. If $\eta_{tt} = -1$, then via a change of basis one may assume $C_r = I_n$ for an arbitrary $r \neq t$ so that $C_t = -I\gamma_r$.

(II) Let $C^{(r,s)}$ be a Clifford algebra generated by the matrices in the imaginary Maiorana representation. Then there are exactly two pseudo-euclidean Hurwitz pairs (V_1, S_1) and (V_2, S_2) which give rise to $C^{(r,s)}$ via the process described above.

We are interested in determining all the *Kałuża-Klein dualities* defined as dualities, where at least one s_k is 1 or at least one r_k is 0, $k = 1, 2,$. Let (V, S) be a Hurwitz pair which will thereafter be denoted by $(r+1, s; \kappa)$. Consider the sequence of matrices

$$\check{\gamma}_\alpha = \gamma_\alpha,\ \alpha = 1,\dots,r;\ \hat{\gamma}_\beta = \gamma_{r+\beta},\ \beta = 1,\dots,s,$$

and, further, the real matrices

$$A = (-1)^r\check{\gamma}_1\check{\gamma}_2\dots\check{\gamma}_r, \quad B = (-1)^s\hat{\gamma}_1\hat{\gamma}_2\dots\hat{\gamma}_s.$$

If $r = -1, 0$, we set $A = I_n$; if $s = 0$ we set $B = I_n$.

Consider, in particular, the cases where each irreducible representation of $C^{(r,s)}$ can be embedded in an irreducible representation of either $C^{(r+1,s)}$ with generators $\gamma_1,\dots,\gamma_{r+1+s}$ or $C^{(r,s+1)}$ with $\gamma_1,\dots,\gamma_{r+s+1}$, or $C^{(r+1,s)}$ and then of $C^{(r+2,s)}$ with $\gamma_1,\dots,\gamma_{r+2+s}$. Then the corresponding sequences of matrices $\check{\gamma}_\alpha, \hat{\gamma}_\beta$ can naturally be modified as follows: either

$$\check{\gamma}_\alpha = \gamma_\alpha, \quad \alpha = 1,\dots,r+1; \quad \hat{\gamma}_\beta = \gamma_{r+1+\beta}, \quad \beta = 1,\dots,s;$$

or

$$\check{\gamma}_\alpha = \gamma_\alpha, \quad \alpha = 1,\dots,r; \quad \hat{\gamma}_\beta = \gamma_{s+\beta}, \quad \beta = 1,\dots,s+1;$$

or

$$\check{\gamma}_\alpha = \gamma_\alpha, \quad \alpha = 1, \dots, r+2; \quad \hat{\gamma}_\beta = \gamma_{r+2+\beta}, \quad \beta = 1, \dots, s;$$

or

$$\check{\gamma}_\alpha = \gamma_\alpha, \quad \alpha = 1, \dots, r; \quad \hat{\gamma}_\beta = \gamma_{r+\beta}, \quad \beta = 1, \dots, s+2,$$

respectively. We arrive [ŁKS] at the following result; cf. [ŁKW, KŁS, MY, S, GSW] for physical motivation: There are exactly five generations of the Kałuża-Klein dualities (s – symmetric, a – antisymmetric; $\ell = 0, 1, 2, \dots$):

I. Strict Kałuża-Klein generation

$$\begin{array}{rl} (8\ell+4,1;A)^s \rightleftharpoons (1,8\ell+4;iA\check{\gamma}_1)^a & \\ \uparrow\downarrow & \\ (8\ell+4,1;iB\hat{\gamma}_2)^a \rightleftharpoons (1,8\ell+4;B)^s & \\ (1,8\ell+4,1;iA\check{\gamma}_1)^a \leftrightharpoons (8\ell+4;A)^s & \\ \downarrow\uparrow & \\ (1,8\ell+4;B)^s \leftrightharpoons (8\ell+4,1;iB\check{\gamma}_2)^a & \end{array}$$

II. The exciton generation

$$\begin{array}{rl} (1,8\ell+6;B\hat{\gamma}_{8\ell+6}\hat{\gamma}_{8\ell+7})^s \rightleftharpoons (8\ell+6,1;A)^a & \\ \uparrow\downarrow & \\ (1,8\ell+6;B)^a \rightleftharpoons (8\ell+6,1;A\check{\gamma}_{8\ell+7}\check{\gamma}_{8\ell+8})^s & \\ (8\ell+6,1;A)^a \leftrightharpoons (1,8\ell+6;B\check{\gamma}_{8\ell+7}\check{\gamma}_{8\ell+8})^s & \\ \downarrow\uparrow & \\ (8\ell+6,1;A\check{\gamma}_{8\ell+6}\check{\gamma}_{8\ell+7})^s \leftrightharpoons (1,8\ell+6;B)^a & \end{array}$$

III. The Yang-Mills generation

$$\begin{array}{rl} (8\ell+4,0;A)^s \rightleftharpoons (1,8\ell+3;iA\check{\gamma}_1)^a & \\ \uparrow\downarrow & \\ (1,8\ell+3;iB\hat{\gamma}_1)^a \rightleftharpoons (8\ell+4,0;B)^s & \\ (8\ell+3,1;iA\check{\gamma}_2)^a \leftrightharpoons (0,8\ell+4;A)^s & \\ \downarrow\uparrow & \\ (0,8\ell+4;B)^s \leftrightharpoons (8\ell+3,1;iB\hat{\gamma}_2)^a & \end{array}$$

IV. The extended octonion generation

$$\begin{array}{rl}(1,8\ell+7;iA\check{\gamma}_{8\ell+7})^s \rightleftharpoons (8\ell+6,2;B)^a & \\ \uparrow\downarrow & \\ (8\ell+6,2;A)^a \rightleftharpoons & (1,8\ell+7;iB\check{\gamma}_{8\ell+8})^s \\ (2,8\ell+6;A)^a \leftrightharpoons & (8\ell+7;iB\hat{\gamma}_{8\ell+7})^s \\ \downarrow\uparrow & \\ (8\ell+7,1;iA\check{\gamma}_{8\ell+7})^s \leftrightharpoons (2,8\ell+6;B)^a & \end{array}$$

Va. The Neveu-Schwarz generation

$$\begin{array}{rl}(8\ell+4,3;A)^s \rightleftharpoons (1,8\ell+2;B)^a & \\ \uparrow\downarrow & \\ (8\ell+2,1;A)^a \rightleftharpoons & (3,8\ell+4;B)^s \end{array}$$

Vb. The Penorose generation

$$\begin{array}{rl} & (8\ell+10,3;A)^s \rightleftharpoons (1,8\ell+8;B)^s \\ & \downarrow\uparrow \\ (8\ell+8,1;A)^s \rightleftharpoons & (3,8\ell+10;B)^a. \end{array}$$

In all the cases listed with superscript s the solution to the problem is *hyperbolic* except for

$$(8\ell+4,0;A)^s,\ (8\ell+4,0;A)^s,\ (0,8\ell+4;A)^s,\ (0,8\ell+4;B)^s,$$

where the solution is *elliptic*. In all the cases listed with superscript a the solution is *symplectic*. The basis of the space V in any pseudo-euclidean Hurwitz pair in question can be chosen so that we have one of the following possibilities: $\kappa = I_n$ in the elliptic case,

$$\kappa = \begin{pmatrix} I_{\frac{1}{2}n} & 0_{\frac{1}{2}n} \\ 0_{\frac{1}{2}n} & -I_{\frac{1}{2}n} \end{pmatrix} \text{ in the hyperbolic case,}$$

$$\kappa = \begin{pmatrix} 0_{\frac{1}{2}n} & I_{\frac{1}{2}n} \\ -I_{\frac{1}{2}n} & 0_{\frac{1}{2}n} \end{pmatrix} \text{ in the symplectic case,}$$

where $0_{\frac{1}{2}n}$ and $I_{\frac{1}{2}n}$ stand for the zero and unit $\frac{1}{2}n \times \frac{1}{2}n$ matrices, respectively.

6. Self-duality equations for gauge theories

Following Zet and Manta [ZM] we consider a particular form of spherically gauge fields of the Poincaré group. For e^a_μ gauge fields interpreted as tetrads and ω^{ab}_μ being the spin connection (Ricci rotation coefficients) we may take

$$e^0_\mu = A(A,0,0,0),\ e^1_\mu = (0,1/r^2A,0,0),\ e^2_\mu = (0,0,rC,0),\ e^3_\mu = (0,0,0,rC\sin\vartheta)$$

and

$$\omega^{01}_\mu = (U,0,0,0),\ \omega^{02}_\mu = \omega^{03}_\mu = \omega^{12}_\mu = \omega^{13}_\mu = (0,0,0,0),\ \omega^{23}_\mu = (iV,0,0,\cos\vartheta),$$

where A, C, U and V are functions of the 3D radius r only. The non-zero components $F^a_{\mu\nu}$ of the torsion tensor and, respectively, $F^{ab}_{\mu\nu}$ of the curvature tensor are:

$$\begin{aligned} &F^0_{01} = -\frac{r^2AA' + U}{r^2A}, \quad F^2_{03} = -irCV\sin\vartheta, \qquad F^2_{12} = C + rC', \\ &F^3_{02} = irCV, \qquad\qquad F^3_{13} = (C + rC')\sin\vartheta, \\ &F^{01}_{01} = -U', \qquad\qquad F^{23}_{01} = -iV', \qquad\qquad F^{23}_{23} = -\sin\vartheta, \end{aligned} \tag{28}$$

where A', C', U', V' denote the derivatives with respect to the variable r.

In order to obtain a self-dual model, following [F], the dual tensor

$$*F_{\mu\nu} = \frac{1}{2}\sqrt{-g}\varepsilon_{\mu\nu\rho\sigma}F^{\rho\sigma}$$

is defined, where g is the metric, $F_{\mu\nu}$ is the tensor of gauge fields ($F_{\mu\nu} = F^A_{\mu\nu}X_A$), $*$ is the Hodge star, and $\varepsilon_{\mu\nu\rho\sigma}$ is the Levi-Civita symbol of rank 4 with $\varepsilon = 1$. One calculates:

$$*F^a_{\mu\nu} = \frac{1}{2}\sqrt{-g}\varepsilon_{\mu\nu\rho\sigma}F^{a\rho\sigma}, \quad *F^{ab}_{\mu\nu} = \frac{1}{2}\sqrt{-g}\varepsilon_{\mu\nu\rho\sigma}F^{ab\rho\sigma};$$

$$\begin{aligned} &*F^0_{23} = \frac{r^2AA' + U}{A}\sin\vartheta, \quad *F^2_{03} = (C + rC')\sin\vartheta, \quad *F^2_{12} = irCV, \\ &*F^3_{02} = -C - rC', \qquad\qquad *F^3_{13} = irCU\sin\vartheta, \\ &*F^{01}_{23} = r^2U'\sin\vartheta, \qquad\qquad *F^{23}_{01} = -1/r^2, \qquad\qquad *F^{23}_{23} = ir^2V'\sin\vartheta. \end{aligned} \tag{29}$$

The Yang-Mills equations are solved by gauge fields satisfying the self-duality condition $*F_{\mu\nu} = iF_{\mu\nu}$, and hence

$$*F^a_{\mu\nu} = iF^a_{\mu\nu}, \quad *F^{ab}_{\mu\nu} = iF^{ab}_{\mu\nu}. \tag{30}$$

From the system (28)–(30) one obtains four independent equations

$$A' + U/r^2A = 0, \quad rC' + (1 - rV)C = 0, \tag{31}$$

$$U' = 0, \quad V' = -1/r^2. \tag{32}$$

Equations (31) and (32) are self-duality equations on the Minkowski space-time endowed with spherical symmetry and with the Poincaré groups as gauge group. Zet and Manta [ZM] stress that *these equations are of the first order unlike the Yang-Mills equations which are of the second order*. Thus the search of solutions is

now easier especially because for the Minkowski space-time solutions to self-duality equations are automatically solutions to the Yang-Mills equations.

Example 1 [ZM]. We shall find exact solutions with spherical symmetry for the field equations (31) and (32). Integration of (32) gives

$$U = \alpha,\ V(r) = 1/r + \beta,\ \alpha \text{ and } \beta \text{ being constants of integration.}$$

Hence, by the second equation in (30),

$$A(r) = \sqrt{a + 2\alpha/r},\ C(r) = be^{\beta r},\ a \text{ and } b \text{ being constants of integration.}$$

The corresponding gauge potentials e^a_μ and $\omega^{ab}_{\mu\nu}$ read:

$$e^0_\mu = \left(\sqrt{a+2\alpha/r}, 0, 0, 0\right), \quad e^1_\mu = \left(0, 1/r^2\sqrt{a+2\alpha/r}, 0, 0\right),$$

$$e^2_\mu = \left(0, 0, bre^{\beta r}, 0\right), \qquad e^3_\mu = \left(0, 0, 0, bre^{\beta r}\sin\vartheta\right)$$

and

$$a^{01}_\mu = (\alpha, 0, 0, 0), \quad \omega^{02}_\mu = \omega^{03}_\mu = \omega^{12}_\mu = \omega^{13}_\mu = (0, 0, 0, 0),$$

$$\omega^{23}_\mu = (i(1/r + \beta), 0, 0, \cos\vartheta)\,.$$

Replacing the metric g by $\tilde{g}$ given by $\tilde{g}_{\mu\nu} = e^a_\mu e^b_\nu \eta_{\alpha\beta}$, we get the following non-zero metric coefficients:

$$\tilde{g}_{00} = a + \frac{2\alpha}{r}, \quad \tilde{g}_{11} = \frac{1}{r^4(a+2\alpha/r)},$$
$$\tilde{g}_{22} = b^2r^2e^{2\beta r}, \quad \tilde{g}_{33} = b^2r^2e^{3\beta r}\sin^2\vartheta.$$

For the corresponding line element $d\sigma$ we obtain

$$d\sigma^2 = \left(a + \frac{2\alpha}{r}\right)dt^2 - \frac{1}{r^4(a+2\alpha/r)}dr^2 - b^2r^2e^{2\beta r}\left(d\vartheta^2 + \sin^2\vartheta d\varphi^2\right).$$

7. Homogeneity vs. gauge theories of the second order

The role of homogeneity in gauge theories related to Randers metrics was recently brought to attention by Miron [M1, 2] in the form of studying the homogeneous lift to tangent bundle of a Finsler (in particular, Randers) metric. The implications of such homogeneity in gauge theories of the second order were studied in detail by Sandovici [Sa]. In order to deal with really generalized Einstein-Yang-Mills equations with a wide range of applicability he introduces the following complete gauge invariant Lagrangian:

$$L_0 = \sum_{j=1}^{17} n_j L_j, \quad \text{all} \quad n_j \in \mathbb{R},$$

where, in standard notation, the gauge invariant Lagrangians $L_1, L_2, \ldots, L_{17}$ read:

$$L_1 = \overset{(2)}{T}{}^i_{jk} \cdot \overset{(2)}{T}{}^{jk}_i, \qquad L_2 = \overset{(3)}{T}{}^i_{jk} \cdot \overset{(3)}{T}{}^{jk}_i, \qquad L_3 = \overset{(1)}{P}{}^i_{jk} \cdot \overset{(1)}{P}{}^{jk}_i,$$

$$L_4 = \overset{(2)}{P}{}^i_{jk} \cdot \overset{(2)}{P}{}^{jk}_i, \qquad L_5 = \overset{(3)}{P}{}^i_{jk} \cdot \overset{(3)}{P}{}^{j}_{ki}, \qquad L_6 = \overset{(2)}{Q}{}^i_{jk} \cdot \overset{(2)}{Q}{}^{j}_{ki},$$

$$L_7 = \overset{(3)}{Q}{}^i_{jk} \cdot \overset{(3)}{Q}{}^{jk}_i, \qquad L_8 = \overset{(3)}{S}{}^i_{jk} \cdot \overset{(3)}{P}{}^{jk}_i, \qquad L_9 = \overset{(3)}{V}{}^i_{jk} \cdot \overset{(3)}{V}{}^{jk}_i,$$

$$L_{10} = \overset{(1)}{R}{}^i_{hjk} \cdot \overset{(1)}{R}{}^{hjk}_i, \quad L_{11} = \overset{(2)}{R}{}^i_{hjk} \cdot \overset{(2)}{R}{}^{h}_{jki}, \quad L_{12} = \overset{(1)}{P}{}^i_{hjk} \cdot \overset{(1)}{P}{}^{h}_{jki},$$

$$L_{13} = \overset{(1)}{P}{}^i_{hjk} \cdot \overset{(1)}{P}{}^{hjk}_i, \quad L_{14} = \overset{(1)}{Q}{}^i_{hjk} \cdot \overset{(1)}{Q}{}^{hjk}_i, \quad L_{15} = \overset{(2)}{Q}{}^i_{hjk} \cdot \overset{(2)}{Q}{}^{hjk}_i,$$

$$L_{16} = \overset{(1)}{S}{}^i_{hjk} \cdot \overset{(1)}{S}{}^{h}_{jki}, \quad L_{17} = \overset{(2)}{S}{}^i_{hjk} \cdot \overset{(2)}{S}{}^{hjk}_i.$$

The quoted Author states that the generalized Einstein-Yang-Mills equations, corresponding to L_0 and to generalized gauge fields $Q \in \{X^j_i, Y^j_i, \gamma^i_{jk}, \theta^i_{jk}, \nabla^i_{jk}\}$, are expressed by the relation

$$\frac{\partial L_0}{\partial Q} - \overset{(h)i}{Q}{}_{|i} - \sum_{\alpha=1}^{2} \overset{(V_\alpha)_i}{Q}{}^{(\alpha)}_{|i} + \overset{(h)}{A}{}_m \cdot \overset{(h)^m}{Q} + \sum_{\alpha=1}^{2} \overset{(V_\alpha)}{A}{}_m \cdot \overset{(V_\alpha)m}{Q} = 0,$$

where

$$\overset{(h)}{A}{}_m = 3\gamma^i_{mi} - n\frac{\alpha'}{\alpha} X^t_m y^{(1)}_t + \frac{\delta X^t_m}{\delta y^{(1)i}} + \frac{\delta\left[(Y^t_p - \gamma^i_{p0})X^p_m\right]}{\delta y^{(2)i}} - \frac{1}{G} \cdot \frac{\delta G}{\delta X^m},$$

$$\overset{(V_1)}{A}{}_m = n\frac{\beta'}{\beta} y^{(1)}_m + \frac{\delta X^t_m}{\delta y^{(2)i}} - \frac{1}{G} \cdot \frac{\delta G}{\delta y^{(1)m}}, \qquad \overset{(V_2)}{A}{}_m = -\frac{1}{G} \cdot \frac{\delta G}{\delta y^{(2)m}}.$$

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GEOMETRIA RANDERSA I TEORIE CECHOWANIA II

TEORIE CECHOWANIA RANDERSA I KAŁUŻY-KLEINA, SAMODUALNOŚĆ I JEDNORODNOŚĆ

S t r e s z c z e n i e

W ramach kontynuacji pierwszej części pracy (obecny wolumen, poprzedni artykuł), a szczególnie w ramach opisu przy użyciu par Hurwitza teorii cechowania związanych z solitonami, wskazujemy na fakt, że zbiór dualności generowanych przez uogólnione zagadnienie Hurwitza zawiera pięć generacji dualności Kałuży-Kleina. Następnie, idąc za G. Zetem i V. Mantą (2003) zauważamy, że teorie cechowania są zwykle formułowane w terminach potencjałów $A^{\alpha}_{\mu}(x)$, gdzie $\alpha = 1, 2, \ldots, m$ (m jest wymiarem grupy cechowania) oraz $\mu = 0, 1, 2, 3$. W formalizmie lagranżianów równania pól cechowania $A^{\alpha}_{\mu}(x)$ są równaniami drugiego rzędu. Aby uprościć poszukiwanie rozwiązań równań pola, dogodne jest rozwiązywanie równań pierwszego rzędu. Właśnie równania samodualności są równaniami różniczkowymi pierwszego rzędu i w oparciu o nie łatwiej jest rozważać rozwiązania dla rozmaitych konfiguracji szczególnych pól cechowania i czasoprzestrzni. Musimy tu pamiętać, że jedną z najważniejszych własności równań samodualności jest wynikanie stąd równań pola Yanga-Millsa. Pracę kończy dyskusja wniosków A. Sandovivi (2003) z jednorodności w sensie Mirona teorii cechowania drugiego rzędu.

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ANALYSIS OF A FRICTIONAL CONTACT PROBLEM WITH ADHESION FOR NONLINEAR ELASTIC MATERIALS I

PROBLEM FORMULATION, EXISTENCE AND UNIQUENESS

Summary

We consider a mathematical model which describes a contact problem between a nonlinear elastic body and a foundation. The contact is frictional and is modelled with Signorini's conditions and the associated nonlocal friction law in which the adhesion of contact surfaces is taken into account. The evolution of the bonding field is discribed by a first order differential equation. We provide a variational formulation of the mechanical problem and prove an existence and uniqueness result of the weak solution if the coefficient of friction is sufficiently small. The proofs are based on arguments of time-dependent variational inequalities, differential equations and the Banach fixed point theorems.

1. Introduction

Contact problems involving deformable bodies are quite frequent in industry as well as in daily life and play an important role in structural and mechanical systems. Because of the importance of this process a considerable effort has been made in its modelling and numerical simulations. A first study of frictional contact problems within the framework of variational inequalities was made in [7]. The mathematical, mechanical and numerical state of the art can be found in [15]. The frictionless contact problem with adhesion for nonlinear elastic materials was studied in [21]. In this paper we deal with the study of a quasistatic unilateral contact problem with nonlocal friction law in which the adhesion of contact surfaces is taken into account between a nonlinear elastic body and a foundation. Models for dynamic or quasistatic process of frictionless adhesive contact between a deformable body and a foundation have been studied in [3, 4, 11, 19]. In [2] the unilateral quasistatic contact

problem with friction and adhesion was studied and an existence result for a friction coefficient small enough was established. As in [10, 11] we use the bonding field as an additional state variable β, defined on the contact surface of the boundary. The variable is restricted to values $0 \leq \beta \leq 1$, when $\beta = 0$ all the bonds are severed and there are no active bonds; when $\beta = 1$ all the bonds are active; when $0 < \beta < 1$ it measures the fraction of active bonds and partial adhesion takes place. We refer the reader to the extensive bibliography on the subject in [14–18]. In this work we provide the variational formulation of the mechanical problem for which we prove the existence of a unique weak solution if the coefficient of friction is sufficiently small, and obtain a partial regularity result for the solution.

The paper is structured as follows. In Section 2 we present some notations and give the variational formulation. In Section 3 we state and prove our main existence and uniqueness result, Theorem 2.1. In Section 4 we consider a sequence of penalized and regularized problems which have at least one solution. The proofs are based on a result on pseudomonotone operators. Using compactness properties, the solution of the original model is obtained by passing to the limit as the penalization and regularization parameter converges to zero.

2. Problem statement and variational formulation

Let $\Omega \subset \mathbf{R}^d; (d = 2, 3)$, be the domain initially occupied by an elastic body. Ω is supposed to be open, bounded, with a sufficiently regular boundary Γ. Γ is partitioned into three parts $\Gamma = \bar{\Gamma}_1 \cup \bar{\Gamma}_2 \cup \bar{\Gamma}_3$ where $\Gamma_1, \Gamma_2, \Gamma_3$ are disjoint open sets and *meas* $\Gamma_1 > 0$. The body is acted upon by a volume force of density φ_1 on Ω and a surface traction of density φ_2 on Γ_2. On Γ_3 the body is in adhesive frictional contact with a foundation.

Thus, the classical formulation of the mechanical problem is written as follows.

Problem P_1. Find a displacement field

$$u : \Omega \times [0, T] \to \mathbf{R}^d$$

and a bonding field

$$\beta : \Gamma_3 \times [0, T] \to [0, 1]$$

such that

$$\operatorname{div} \sigma + \varphi_1 = 0 \text{ in } \Omega \times (0, T), \tag{2.1}$$

$$\sigma = F\varepsilon(u) \quad \text{in } \Omega \times (0, T), \tag{2.2}$$

$$u = 0 \quad \text{on } \Gamma_1 \times (0, T), \tag{2.3}$$

$$\sigma\nu = \varphi_2 \quad \text{on } \Gamma_2 \times (0, T), \tag{2.4}$$

$$u_\nu \leq 0, \sigma_\nu - c_\nu \beta^2 R_\nu(u_\nu) \leq 0, \left(\sigma_\nu - c_\nu \beta^2 R_\nu(u_\nu)\right) u_\nu = 0 \quad \text{on } \Gamma_3 \times (0, T), \tag{2.5}$$

$$
\left\{
\begin{array}{l}
\left|\sigma_\tau + c_\tau \beta^2 R_\tau\left(u_\tau\right)\right| \leq \mu \left|R^*\left(\sigma_\nu\left(u\right)\right)\right|, \\
\\
\left|\sigma_\tau + c_\tau \beta^2 R_\tau\left(u_\tau\right)\right| < \mu \left|R^*\left(\sigma_\nu\left(u\right)\right)\right| \Longrightarrow u_\tau = 0, \\
\\
\left|\sigma_\tau + c_\tau \beta^2 R_\tau\left(u_\tau\right)\right| = \mu \left|R^*\left(\sigma_\nu\left(u\right)\right)\right| \Longrightarrow \\
\\
\exists \lambda \geq 0 \text{ s.t. } u_\tau = -\lambda\left(\sigma_\tau + c_\tau \beta^2 R_\tau\left(u_\tau\right)\right),
\end{array}
\right. \quad \text{on } \Gamma_3 \times (0,T), \tag{2.6}
$$

$$
\dot{\beta} = -\left[\beta\left(c_\nu\left(R_\nu\left(u_\nu\right)\right)^2 + c_\tau\left(\left|R_\tau\left(u_\tau\right)\right|\right)^2\right) - \varepsilon_a\right]_+ \quad \text{on } \Gamma_3 \times (0,T), \tag{2.7}
$$

$$
\beta\left(0\right) = \beta_0 \quad \text{on } \Gamma_3. \tag{2.8}
$$

Equation (2.1) represents the equilibrium equation. Equation (2.2) represents the elastic constitutive law of the material in which F is a given function and $\varepsilon\left(u\right)$ denotes the small strain tensor; (2.3) and (2.4) are the displacement and traction boundary conditions, respectively, in which ν denotes the unit outward normal vector on Γ and $\sigma\nu$ represents the Cauchy stress vector. Condition (2.5) represents the unilateral contact with adhesion. Conditions (2.6) represent a nonlocal frictional contact with adhesion and u_τ is the tangential displacement on the boundary. The tangential shear cannot exceed the maximal frictional resistance $\mu\left|R^*\left(\sigma_\nu\left(u\right)\right)\right|$. Then, if the strict inequality is satisfied, the surface adheres to the foundation and is in the so-called stick state, and when equality is satisfied there is relative sliding, the so-called slip state. Here R^* is a compact regularization operator (see [6]) and the parameters c_ν, c_τ and ε_a are given adhesion coefficients which may depend on $x \in \Gamma_3$. As in [20], R_ν, R_τ are truncation operators defined by

$$
R_\nu\left(s\right) = \left\{
\begin{array}{l}
L \text{ if } s < -L, \\
-s \text{ if } -L \leq s \leq 0, \\
0 \text{ if } s > 0
\end{array}
\right. \quad R_\tau\left(v\right) = \left\{
\begin{array}{ll}
v & \text{if } |v| \leq L, \\
L\dfrac{v}{|v|} & \text{if } |v| > L
\end{array}
\right. ,
$$

where $L > 0$ is a characteristic length of the bonds. Equation (2.7) represents the ordinary differential equation which describes the evolution of the bonding field and it was already used in [20] where $[s]_+ = \max\left(s, 0\right) \forall s \in \mathbf{R}$. Since $\dot{\beta} \leq 0$ on $\Gamma_3 \times (0,T)$, once debonding occurs, bonding cannot be reestablished. Also we wish to make it clear that from [13] it follows that the model does not allow for complete debonding field in finite time. Finally, (2.8) is the initial condition, in which β_0 denotes the initial bonding field. In (2.7) a dot above a variable represents its derivative with respect to time.

We recall that the inner products and the corresponding norms on $\mathbf{R}^d$ and S_d are given by

$$
\begin{array}{l}
u.v = u_i v_i, \quad |v| = (v.v)^{\frac{1}{2}} \quad \forall u, v \in \mathbf{R}^d, \\
\sigma.\tau = \sigma_{ij}\tau_{ij}, \ |\tau| = (\tau.\tau)^{\frac{1}{2}} \quad \forall \sigma, \tau \in S_d,
\end{array}
$$

where S_d is the space of second order symmetric tensors on $\mathbf{R}^d$ $(d = 2, 3)$. Hereafter, the indices i and j run between 1 and d and the summation convention over repeated

indices is adopted. Now, to proceed with the variational formulation, we need the following function spaces:

$$H = \left(L^2(\Omega)\right)^d,\ H_1 = \left(H^1(\Omega)\right)^d,\ Q = \left\{\tau = (\tau_{ij});\tau_{ij} = \tau_{ji} \in L^2(\Omega)\right\},$$

$$Q_1 = \{\sigma \in Q; \text{div } \sigma \in H\}.$$

Note that H and Q are real Hilbert spaces endowed with the respective canonical inner products

$$\langle u, v\rangle_H = \int_\Omega u_i v_i dx, \quad \langle \sigma, \tau\rangle_Q = \int_\Omega \sigma_{ij}\tau_{ij} dx.$$

The small strain tensor is

$$\varepsilon(u) = (\varepsilon_{ij}(u)) = \frac{1}{2}(u_{i,j} + u_{j,i}),\ i,j = \{1,...,d\};$$

div $\sigma = (\sigma_{ij,j})$ is the divergence of σ. For every element $v \in H_1$ we denote by v_ν and v_τ the normal and the tangential components of v on the boundary Γ given by

$$v_\nu = v.\nu,\ \ v_\tau = v - v_\nu\nu.$$

Similary, for a regular tensor field $\sigma \in Q_1$, we define its normal and tangential components by

$$\sigma_\nu = (\sigma\nu).\nu, \quad \sigma_\tau = \sigma\nu - \sigma_\nu\nu$$

and we recall that the following Green's formula holds:

$$\langle \sigma, \varepsilon(v)\rangle_Q + \langle \text{div } \sigma, v\rangle_H = \int_\Gamma \sigma\nu.v da \ \ \forall v \in H_1,$$

where da is the surface measure element. Let V be the closed subspace of H_1 defined by

$$V = \{v \in H_1 : v = 0 \text{ on } \Gamma_1\},$$

and let K the set of admissible displacements of V defined by

$$K = \{v \in V : v_\nu \le 0 \ a.e. \text{ on } \Gamma_3\}.$$

Since meas $\Gamma_1 > 0$, the following Korn's inequality holds [7]:

$$\|\varepsilon(v)\|_Q \ge c_\Omega \|v\|_{H_1} \quad \forall v \in V, \tag{2.7}$$

where the constant $c_\Omega > 0$ depends only on Ω and Γ_1. We equip V with the inner product

$$\langle u, v\rangle_V = \langle \varepsilon(u), \varepsilon(v)\rangle_Q$$

and $\|.\|_V$ is the associated norm. It follows from Korn's inequality (2.9) that the norms $\|.\|_{H_1}$and $\|.\|_V$ are equivalent on V. Then $(V, \|.\|_V)$ is a real Hilbert space. Moreover by Sobolev's trace theorem, there exists $d_\Omega > 0$ which depends only on the domain Ω, Γ_1 and Γ_3 such that

$$\|v\|_{(L^2(\Gamma_3))^d} \le d_\Omega \|v\|_V \quad \forall v \in V. \tag{2.8}$$

For $p \in [1,\infty]$, we use the standard norm of $L^p(0,T;V)$. We also use the Sobolev space $W^{1,\infty}(0,T;V)$ equipped with the norm

$$\|v\|_{W^{1,\infty}(0,T;V)} = \|v\|_{L^\infty(0,T;V)} + \|\dot{v}\|_{L^\infty(0,T;V)}.$$

For every real Banach space $(X, \|.\|_X)$ and $T > 0$ we use the notation $C([0,T];X)$ for the space of continuous functions from $[0,T]$ to X; recall that $C([0,T];X)$ is a real Banach space with the norm

$$\|x\|_{C([0,T];X)} = \max_{t\in[0,T]} \|x(t)\|_X.$$

We suppose that the body forces and surface tractions have the regularity

$$\varphi_1 \in W^{1,\infty}(0,T;H), \quad \varphi_2 \in W^{1,\infty}\left(0,T;\left(L^2(\Gamma_2)\right)^d\right) \tag{2.9}$$

and we denote by $f(t)$ the element of V defined by

$$\langle f(t), v\rangle_V = \int_\Omega \varphi_1(t).v dx + \int_{\Gamma_2} \varphi_2(t).v da \quad \forall v \in V, \text{ for } t \in [0,T]. \tag{2.10}$$

Using (2.11) and (2.12) yield

$$f \in W^{1,\infty}(0,T;V).$$

Let

$$H^{\frac{1}{2}}(\Gamma_3) = \left\{ w|_{\Gamma_3} : w \in H^{\frac{1}{2}}(\Gamma),\ w = 0 \text{ on } \Gamma_1 \right\}$$

equipped with the norm of $H^{\frac{1}{2}}(\Gamma)$. $\langle .,. \rangle$ shall denote the duality pairing on $H^{\frac{1}{2}}(\Gamma_3) \times H^{-\frac{1}{2}}(\Gamma_3)$. Before we start with the variational formulation of problem P_1 let us state in which sense the duality pairing $\langle .,. \rangle$ is taken.

For $\sigma \in Q_1$, if $\sigma\nu \in \left(L^2(\Gamma_2)\right)^d$ in the sense of distributions, i-e. $\exists s \in \left(L^2(\Gamma_2)\right)^d$ such that

$$\langle \sigma\nu, \varphi\rangle_{H'(\Gamma)\times H(\Gamma)} = \int_{\Gamma_2} s.\varphi da \quad \forall \varphi \in (C_0^\infty(\Gamma_2))^d,$$

where

$$H(\Gamma) = \left(H^{\frac{1}{2}}(\Gamma)\right)^d \quad \text{and} \quad H'(\Gamma) = \left(H^{-\frac{1}{2}}(\Gamma)\right)^d,$$

we define the normal stress σ_ν on Γ_3 as follows:

$$\begin{cases} \forall w \in H^{\frac{1}{2}}(\Gamma_3): \\ \langle \sigma_\nu, w\rangle = \langle \sigma, \varepsilon(v)\rangle_Q + \langle \text{div } \sigma, v\rangle_H - \int_{\Gamma_2} s.v da \\ \forall v \in V;\ v_\nu = w \text{ and } v_\tau = 0 \text{ on } \Gamma_3. \end{cases} \tag{2.11}$$

We assume that $R^* : H^{-\frac{1}{2}}(\Gamma_3) \to L^2(\Gamma_3)$ is a linear compact mapping. Now, in the study of the mechanical problem P_1 we suppose that the operator F satisfies the following assumptions:

$$
\left.
\begin{array}{l}
(a) \text{ there exists } M > 0 \text{ such that} \\
\qquad |F(x,\varepsilon_1) - F(x,\varepsilon_2)| \le M\,|\varepsilon_1 - \varepsilon_2|\,, \\
\qquad \text{for all } \varepsilon_1, \varepsilon_2 \text{ in } S_d, \text{ for a.e. } x \text{ in } \Omega; \\
\\
(b) \text{ there exists } m > 0 \text{ such that} \\
\qquad (F(x,\varepsilon_1) - F(x,\varepsilon_2)) \cdot (\varepsilon_1 - \varepsilon_2) \ge m\,|\varepsilon_1 - \varepsilon_2|^2\,, \\
\qquad \text{for all } \varepsilon_1, \varepsilon_2 \text{ in } S_d, \text{ for a.e. } x \text{ in } \Omega; \\
\\
(c) \text{ the mapping } x \to F(x,\varepsilon) \text{ is Lebesgue measurable on } \Omega, \\
\qquad \text{for any } \varepsilon \text{ in } S_d; \\
\\
(d)\ F(x,0) = 0 \text{ for a.e. } x \text{ in } \Omega.
\end{array}
\right\} \tag{2.12}
$$

As in [18] we suppose that the adhesion coefficients c_ν, c_τ and ε_a satisfy the conditions

$$
c_\nu, c_\tau \in L^\infty(\Gamma_3)\,,\ \varepsilon_a \in L^\infty(\Gamma_3)\,,\ \ c_\nu,\ c_\tau,\ \varepsilon_a \ge 0 \text{ a.e. on } \Gamma_3. \tag{2.13}
$$

μ is a coefficient of friction and it satisfies

$$
\mu \in L^\infty(\Gamma_3) \text{ and } \mu \ge 0 \text{ a.e. on } \Gamma_3. \tag{2.14}
$$

We need the following set for the bonding fields,

$$
B = \left\{\beta \in L^\infty\left(0,T;L^2(\Gamma_3)\right);\ 0 \le \beta(t) \le 1\ \forall t \in [0,T],\ \text{a.e. on } \Gamma_3\right\},
$$

and, finally we assume that the initial bonding field satisfies

$$
\beta_0 \in L^2(\Gamma_3);\ 0 \le \beta_0 \le 1 \text{ a.e. on } \Gamma_3. \tag{2.15}
$$

Now by assuming the solution to be sufficiently regular, we obtain by using Green's formula that the problem P_1 has the following variational formulation.

Problem P_2. Find a displacement field $u \in W^{1,\infty}(0,T;V)$ and a bonding field $\beta \in W^{1,\infty}\left(0,T;L^2(\Gamma_3)\right) \cap B$ such that

$$
\begin{array}{l}
u(t) \in K,\ \langle F\varepsilon(u(t)), \varepsilon(v - u(t))\rangle_Q + j(u(t), v) - j(u(t), u(t)) + \\
r(\beta(t), u(t), v - u(t)) \ge \langle f(t), v - u(t)\rangle_V\ \ \forall\, v \in K,\ t \in [0,T]\,,
\end{array} \tag{2.16}
$$

$$
\dot\beta(t) = -\left[\beta(t)\left(c_\nu\left(R_\nu(u_\nu(t))\right)^2 + c_\tau\left(|R_\tau(u_\tau(t))|\right)^2\right) - \varepsilon_a\right]_+ \text{ for a.e. } t \in (0,T)\,, \tag{2.17}
$$

$$
\beta(0) = \beta_0 \text{ on } \Gamma_3, \tag{2.18}
$$

where

$$r_\nu(\beta,u,v) = -\int_{\Gamma_3} c_\nu \beta^2 R_\nu(u_\nu)\, v_\nu da,\ r_\tau(\beta,u,v) = \int_{\Gamma_3} c_\tau \beta^2 R_\tau(u_\tau).v_\tau da,$$

$$j(u,v) = \int_{\Gamma_3} \mu\,|R^*(\sigma_\nu(u))|\,|v_\tau|\,da,\ r = r_\nu + r_\tau.$$

Our main result of this section, which will be established in the next is the following theorem.

Theorem 2.1. *Let $T > 0$ and assume that* (2.11), (2.14), (2.15), (2.16) *and* (2.17) *hold. Then there exists a constant $c > 0$ such that Problem P_2 has a unique solution if*

$$cd_\Omega^2 \|\mu\|_{L^\infty(\Gamma_3)} < m.$$

3. Existence and uniqueness result

The proof of Theorem 2.1 is carried out in several steps. In the first step, for a given $\beta \in C\left([0,T];L^2(\Gamma_3)\right) \cap B$, we consider the following variational problem.

Problem $P_{1\beta}$. Find $u_\beta : [0,T] \to K$ such that

$$\begin{aligned} &\langle F\varepsilon(u_\beta(t)), \varepsilon(v-u_\beta(t))\rangle_Q + j(u_\beta(t),v) - j(u_\beta(t),u_\beta(t)) + \\ &r(\beta(t),u_\beta(t),v-u_\beta(t)) \geq \langle f(t), v-u_\beta(t)\rangle_V \ \ \forall\, v \in K,\, t \in [0,T]. \end{aligned} \tag{3.1}$$

We show the following result.

Proposition 3.1. *There exists a constant $c > 0$ such that Problem $P_{1\beta}$ admits a unique solution $u_\beta \in C([0,T];K)$ if*

$$cd_\Omega^2 \|\mu\|_{L^\infty(\Gamma_3)} < m.$$

Proof. For the proof of this proposition we consider an intermediate problem. Indeed, for $g \in C_+^*$, where

$$C_+^* = \left\{k \in C\left([0,T];L^2(\Gamma_3)\right);\ k(t) \geq 0\ \forall t \in [0,T],\ a.e.\ \text{on}\ \Gamma_3\right\},$$

we define the auxiliary problem $P_{1\beta}^g$ as:

Problem $P_{1\beta}^g$. Find $u_g : [0,T] \to K$ such that

$$\begin{aligned} &\langle F\varepsilon(u_g(t)), \varepsilon(v-u_g(t))\rangle_Q + j_{g(t)}(v) - j_{g(t)}(u_g(t)) + \\ &r(\beta(t),u_g(t),v-u_g(t)) \geq \langle f(t), v-u_g(t)\rangle_V \ \ \forall\, v \in K,\, t \in [0,T], \end{aligned} \tag{3.2}$$

where

$$j_{g(t)}(v) = \int_{\Gamma_3} \mu g(t)\,|v_\tau|\,da.$$

We have the following result.

Lemma 3.2. *There exists a unique solution to Problem $P_{1\beta}^{g}$ and it satisfies*

$$u_g \in C\left([0,T];K\right).$$

Proof. Let $t \in [0,T]$ and let $A_t : V \to V$ be the operator given by

$$(A_t u, v)_V = \langle F\varepsilon(u), \varepsilon(v)\rangle_Q + \int_{\Gamma_3} (-c_\nu \beta^2 R_\nu(u_\nu) v_\nu + c_\tau \beta^2 R_\tau(u_\tau).v_\tau) da.$$

We use (2.14) (a), (2.10), (2.15), $|\beta| \leq 1$ and the properties (see [18]) of the operators R_ν and R_τ such that

$$\text{(3.3)} \qquad \begin{cases} |R_\nu(a) - R_\nu(b)| \leq |a-b|, \ \forall a,b \in \mathbf{R}, \\ \\ |R_\tau(a) - R_\tau(b)| \leq |a-b|, \ \forall a,b \in \mathbf{R}^d. \end{cases}$$

It follows that A_t satisfies

$$|(A_t u - A_t v, w)_V| \leq \left[M + \left(\|c_\nu\|_{L^\infty(\Gamma_3)} + \|c_\tau\|_{L^\infty(\Gamma_3)}\right) d_\Omega^2\right] \|u-v\|_V \|w\|_V.$$

Also, we use (2.14) (b) to see that

$$(A_t u - A_t v, u-v)_V \geq m\|u-v\|_V^2 - \int_{\Gamma_3} \beta^2 c_\nu \left(R_\nu(u_\nu) - R_\nu(v_\nu)\right)(u_\nu - v_\nu)\, da$$

$$+ \int_{\Gamma_3} \beta^2 c_\tau \left(R_\tau(u_\tau) - R_\tau(v_\tau)\right).(u_\tau - v_\tau)\, da.$$

Since

$$\left(R_\nu(u_\nu) - R_\nu(v_\nu)\right)(u_\nu - v_\nu) \leq 0 \text{ a.e. on } \Gamma_3,$$

$$\left(R_\tau(u_\tau) - R_\tau(v_\tau)\right).(u_\tau - v_\tau) \geq 0 \text{ a.e. on } \Gamma_3,$$

we get

$$(A_t u - A_t v, u-v)_V \geq m\|u-v\|_V^2,$$

which implies that A_t is strongly monotone. Therefore A_t is an operator strongly monotone and Lipschitz continuous. On the other hand $j_{g(t)}$ is a continuous seminorm, then by a classical argument of elliptic variational inequalities [1], we deduce that the problem $P_{1\beta}^{g}$ has a unique solution $u_g(t)$. Now, we shall prove that $u_g \in C\left([0,T];K\right)$. Indeed, write the inequality (3.2) for $t = t_i$ and take $v = u_g(t_j)$, $i,j = 1,2$, we have by adding the two inequalities

$$\langle F\varepsilon\left(u_g\left(t_1\right)\right)-F\varepsilon\left(u_g\left(t_2\right)\right),\varepsilon\left(u_g\left(t_2\right)-u_g\left(t_1\right)\right)\rangle_Q+$$

$$j_{g(t_1)}\left(u_g\left(t_2\right)\right)-j_{g(t_1)}\left(u_g\left(t_1\right)\right)+j_{g(t_2)}\left(u_g\left(t_1\right)\right)-j_{g(t_2)}\left(u_g\left(t_2\right)\right)+$$

$$r\left(\beta\left(t_1\right),u_g\left(t_1\right),u_g\left(t_2\right)-u_g\left(t_1\right)\right)+r\left(\beta\left(t_2\right),u_g\left(t_2\right),u_g\left(t_1\right)-u_g\left(t_2\right)\right)\geq$$

$$\langle f\left(t_1\right)-f\left(t_2\right),u_g\left(t_2\right)-u_g\left(t_1\right)\rangle_V.$$

Using (2.14) (b), (3.3), $|R_\nu\left(u_\nu\right)|\leq L$ and $|R_\tau\left(u_\tau\right)|\leq L$, it follows that there exists a constant $C>0$ such that

$$\left\|u_g\left(t_1\right)-u_g\left(t_2\right)\right\|_V\leq$$

$$C\left(\left\|\beta\left(t_1\right)-\beta\left(t_2\right)\right\|_{L^2(\Gamma_3)}+\left\|f\left(t_1\right)-f\left(t_2\right)\right\|_V+\left\|g\left(t_1\right)-g\left(t_2\right)\right\|_{L^2(\Gamma_3)}\right)$$

$$\forall t_1,t_2\in[0,T].$$

As β, $g\in C\left([0,T];L^2\left(\Gamma_3\right)\right)$ and $f\in C\left([0,T];V\right)$, we conclude from the previous inequality that $u_g\in C\left([0,T];K\right)$. Now, in the second step we consider the folowing mapping defined by

$$\Phi:C_+^*\to C_+^*$$

$$g\to\Phi\left(g\right)=\left|R^*\left(\sigma_\nu\left(u_g\right)\right)\right|.$$

We have the following result.

Lemma 3.3. *For every $g\in C_+^*$, $\Phi\left(g\right)$ belongs to C_+^* and there exists a constant $c>0$ such that if*

$$cd_\Omega^2\left\|\mu\right\|_{L^\infty(\Gamma_3)}<m,$$

then the mapping Φ admits a unique fixed point g_* and u_{g_*} is a unique solution tothe Problem $P_{1\beta}$.

Proof. Let t_1, $t_2\in[0,T]$ and $g\in C_+^*$. Using the continuity of R^* and (2.13), there exists a constant $C>0$ such that

$$\left\|\Phi\left(g\left(t_1\right)\right)-\Phi\left(g\left(t_2\right)\right)\right\|_{L^2(\Gamma_3)}\leq$$

$$C\left(\left\|u_g\left(t_1\right)-u_g\left(t_2\right)\right\|_{L^2(\Gamma_3)}+\left\|f\left(t_1\right)-f\left(t_2\right)\right\|_V\right).$$

Therefore as $u_g\in C\left([0,T];K\right)$ and $f\in C\left([0,T];V\right)$, the previous inequality implies that $\Phi\left(g\right)\in C\left([0,T];L^2\left(\Gamma_3\right)\right)$. Moreover $\Phi\left(g\left(t\right)\right)\geq 0$ $\forall t\in[0,T]$ *a.e.* on Γ_3, so we deduce that $\Phi\left(g\right)\in C_+^*$. Now, let g_1, $g_2\in C_+^*$, then

$$\left\|\Phi\left(g_1\left(t\right)\right)-\Phi\left(g_2\left(t\right)\right)\right\|_{L^2(\Gamma_3)}=\left\|R^*\left(\sigma_\nu\left(u_{g_1}\left(t\right)\right)\right)-R^*\left(\sigma_\nu\left(u_{g_2}\left(t\right)\right)\right)\right\|_{L^2(\Gamma_3)}.$$

Using (2.13), the continuity of R^* and (2.10), we deduce that there exists a constant $c > 0$ such that

$$\|\Phi(g_1(t)) - \Phi(g_2(t))\|_{L^2(\Gamma_3)} \leq c \|u_{g_1}(t) - u_{g_2}(t)\|_V .$$

Let $g_j(t)$, $j = 1, 2$ and $u_{g_j}(t)$ the corresponding solutions. Take $v = u_{g_2}(t)$ in the equivalent inequality to relation (3.2) with $g = g_1(t)$ and take $v = u_{g_1}(t)$ in the equivalent inequality to relation (3.2) with $g(t) = g_2(t)$, we get:

$$\|u_{g_1}(t) - u_{g_2}(t)\|_V \leq \frac{d_\Omega}{m} \|\mu\|_{L^\infty(\Gamma_3)} \|g_1(t) - g_2(t)\|_{L^2(\Gamma_3)} .$$

It follows that

$$\|\Phi(g_1(t)) - \Phi(g_2(t))\|_{L^2(\Gamma_3)} \leq c\frac{d_\Omega^2}{m} \|\mu\|_{L^\infty(\Gamma_3)} \|g_1(t) - g_2(t)\|_{L^2(\Gamma_3)} ,$$

and thus,

$$\|\Phi(g_1) - \Phi(g_2)\|_{C([0,T];L^2(\Gamma_3))} \leq c\frac{d_\Omega^2}{m} \|\mu\|_{L^\infty(\Gamma_3)} \|g_1 - g_2\|_{C([0,T];L^2(\Gamma_3))} .$$

This last inequality implies such that if

$$cd_\Omega^2 \|\mu\|_{L^\infty(\Gamma_3)} < m,$$

the mapping Φ is a contraction and then it admits a unique fixed point g_* and u_{g_*} is a unique solution to Problem $P_{1\beta}$. □

In the second step we consider the following problem.

Problem $P_{2\beta}$. Find a bonding field $\beta_a : [0,T] \to L^\infty(\Gamma_3)$ such that

$$\dot{\beta}_a(t) = -\left[\beta_a(t)\left(c_\nu\left(R_\nu\left(u_{\beta_a \nu}(t)\right)\right)^2 + c_\tau\left(\left|R_\tau\left(u_{\beta_a \tau}(t)\right)\right|\right)^2\right) - \varepsilon_a\right]_+$$

(3.4)

$$a.e.\ t \in (0,T),$$

$$\beta_a(0) = \beta_0 \text{ on } \Gamma_3. \tag{3.5}$$

We obtain the following result.

Proposition 3.4. *There exists a unique solution to Problem* $P_{2\beta}$ *and it satisfies*

$$\beta_a \in W^{1,\infty}\left(0,T;L^2(\Gamma_3)\right) \cap B.$$

Proof. Let $k > 0$ and let

$$X = \left\{\beta \in C\left([0,T];L^2(\Gamma_3)\right);\ \sup_{t\in[0,T]}\left[\exp(-kt)\|\beta(t)\|_{L^2(\Gamma_3)}\right] < +\infty\right\}.$$

X is a Banach space for the norm

$$\|\beta\|_X = \sup_{t\in[0,T]}\left[\exp(-kt)\|\beta(t)\|_{L^2(\Gamma_3)}\right],$$

and consider the mapping $T : X \to X$ given by

$$T\beta(t) = \beta_0 - \int_0^t \left[\beta(s)\left(c_\nu\left(R_\nu\left(u_{\beta\nu}(s)\right)\right)^2 + c_\tau\left(\left|R_\tau\left(u_{\beta\tau}(s)\right)\right|\right)^2\right) - \varepsilon_a\right]_+ ds.$$

Then there exists a constant $c_1 > 0$ such that

$$\|T\beta_1(t) - T\beta_2(t)\|_{L^2(\Gamma_3)}$$

$$\leq c_1 \int_0^t \left\|(\beta_1(s))\left(R_\nu\left(u_{\beta_1\nu}(s)\right)\right)^2 - (\beta_2(s))\left(R_\nu\left(u_{\beta_2\nu}(s)\right)\right)^2\right\|_{L^2(\Gamma_3)} ds$$

$$+c_1 \int_0^t \left\|(\beta_1(s))\left(\left|R_\tau\left(u_{\beta_1\tau}(s)\right)\right|\right)^2 - (\beta_2(s))\left(\left|R_\tau\left(u_{\beta_2\tau}(s)\right)\right|\right)^2\right\|_{L^2(\Gamma_3)} ds.$$

We use the definition of the truncation operators R_ν and R_τ and write

$$\beta_1(s) = \beta_1(s) - \beta_2(s) + \beta_2(s).$$

After some elementary calculation we find that there exists a constant $c_2 > 0$ such that

$$\|T\beta_1(t) - T\beta_2(t)\|_{L^2(\Gamma_3)} \leq$$

$$c_2 \int_0^t \|\beta_1(s) - \beta_2(s)\|_{L^2(\Gamma_3)} ds + c_2 \int_0^t \|u_{\beta_1}(s) - u_{\beta_2}(s)\|_{L^2(\Gamma_3)} ds.$$

Now, we still need to show the following result.

Lemma 3.5. *For*

$$cd_\Omega^2 \|\mu\|_{L^\infty(\Gamma_3)} < m,$$

there exists a constant $c_3 > 0$ such that

$$\|u_{\beta_1}(t) - u_{\beta_2}(t)\|_V \leq c_3 \|\beta_1(t) - \beta_2(t)\|_{L^2(\Gamma_3)}.$$

Proof. We take $v = u_{\beta_j}(t)$ in the inequality (3.1) written for $\beta(t) = \beta_i(t)$ $i, j = 1, 2$ and adding the two inequalities, we get

$$\langle F\varepsilon(u_{\beta_1}(t)) - F\varepsilon(u_{\beta_2}(t)), \varepsilon(u_{\beta_2}(t) - u_{\beta_1}(t))\rangle_Q + j(u_{\beta_1}(t), u_{\beta_2}(t)) -$$

$$j(u_{\beta_1}(t), u_{\beta_1}(t)) + j(u_{\beta_2}(t), u_{\beta_1}(t)) - j(u_{\beta_2}(t), u_{\beta_2}(t)) + \tag{3.6}$$

$$r(\beta_1(t), u_{\beta_1}(t), u_{\beta_2}(t) - u_{\beta_1}(t)) + r(\beta_2(t), u_{\beta_2}(t), u_{\beta_1}(t) - u_{\beta_2}(t)) \geq 0.$$

We have

$$j(u_{\beta_1}(t), u_{\beta_2}(t)) - j(u_{\beta_1}(t), u_{\beta_1}(t)) +$$

$$j(u_{\beta_2}(t), u_{\beta_1}(t)) - j(u_{\beta_2}(t), u_{\beta_2}(t)) =$$

$$\int_{\Gamma_3} \mu(|R^*(\sigma_\nu(u_{\beta_1\nu}(t)))| - |R^*(\sigma_\nu(u_{\beta_2\nu}(t)))|)(|u_{\beta_2\tau}(t)| - |u_{\beta_1\tau}(t)|) da.$$

Using the continuity of R^*, (2.10) and (2.13), we deduce that there exists a constant $c > 0$ such that

$$\left|\int_{\Gamma_3} \mu(|R^*(\sigma_\nu(u_{\beta_1\nu}(t)))| - |R^*(\sigma_\nu(u_{\beta_2\nu}(t)))|)(|u_{\beta_2\tau}(t)| - |u_{\beta_1\tau}(t)|)\,da\right|$$

$$\leq c\,\|\mu\|_{L^\infty(\Gamma_3)}\, d_\Omega^2\, \|u_{\beta_1}(t) - u_{\beta_2}(t)\|_V^2$$

On the other hand, we have

$$r(\beta_1(t), u_{\beta_1}(t), u_{\beta_2}(t) - u_{\beta_1}(t)) + r(\beta_2(t), u_{\beta_2}(t), u_{\beta_1}(t) - u_{\beta_2}(t)) =$$

$$-\int_{\Gamma_3} c_\nu \left(\beta_1(t)^2 R_\nu(u_{\beta_1\nu}(t)) - \beta_2(t)^2 R_\nu(u_{\beta_2\nu}(t))\right)(u_{\beta_2\nu}(t) - u_{\beta_1\nu}(t))\,da +$$

$$\int_{\Gamma_3} c_\tau(\beta_1(t)^2 R_\tau(u_{\beta_1\tau}(t)) - \beta_2(t)^2 R_\tau(u_{\beta_2\tau}(t))).(u_{\beta_2\tau}(t) - u_{\beta_1\tau}(t))\,da,$$

and write

$$\int_{\Gamma_3} c_\nu \left(\beta_1(t)^2 R_\nu(u_{\beta_1\nu}(t)) - \beta_2(t)^2 R_\nu(u_{\beta_2\nu}(t))\right)(u_{\beta_2\nu}(t) - u_{\beta_1\nu}(t))\,da =$$

$$\int_{\Gamma_3} c_\nu \left(\beta_1(t)^2 - \beta_2(t)^2\right) R_\nu(u_{\beta_1\nu}(t))(u_{\beta_2\nu}(t) - u_{\beta_1\nu}(t))\,da +$$

$$\int_{\Gamma_3} c_\nu \beta_2(t)^2 (R_\nu(u_{\beta_1\nu}(t)) - R_\nu(u_{\beta_2\nu}(t)))(u_{\beta_2\nu}(t) - u_{\beta_1\nu}(t))\,da,$$

$$\int_{\Gamma_3} c_\tau(\beta_1(t)^2 R_\tau(u_{\beta_1\tau}(t)) - \beta_2(t)^2 R_\tau(u_{\beta_2\tau}(t))).(u_{\beta_2\tau}(t) - u_{\beta_1\tau}(t))\,da =$$

$$\int_{\Gamma_3} c_\tau \left(\beta_1(t)^2 - \beta_2(t)^2\right) R_\tau(u_{\beta_1\tau}(t)).(u_{\beta_2\tau}(t) - u_{\beta_1\tau}(t))\,da +$$

$$\int_{\Gamma_3} c_\tau \beta_2(t)^2 (R_\tau(u_{\beta_1\tau}(t) - R_\tau(u_{\beta_2\tau}(t))).(u_{\beta_2\tau}(t) - u_{\beta_1\tau}(t))\,da.$$

Since we have

$$\int_{\Gamma_3} c_\nu \beta_2(t)^2 (R_\nu(u_{\beta_1\nu}(t)) - R_\nu(u_{\beta_2\nu}(t)))(u_{\beta_2\nu}(t) - u_{\beta_1\nu}(t))\,da \geq 0,$$

$$\int_{\Gamma_3} c_\tau \beta_2(t)^2 (R_\tau(u_{\beta_1\tau}(t) - R_\tau(u_{\beta_2\tau}(t))).(u_{\beta_2\tau}(t) - u_{\beta_1\tau}(t))\,da \leq 0,$$

so by using (3.6), (2.14) (b), (2.10), $|R(u_\nu)| \leq L$ and $|R(u_\tau)| \leq L$, we get the estimate

$$m\,\|u_{\beta_1}(t) - u_{\beta_2}(t)\|_V^2 \leq c d_\Omega^2\, \|\mu\|_{L^\infty(\Gamma_3)}\, \|u_{\beta_1}(t) - u_{\beta_2}(t)\|_V^2 +$$

$$\left(\|c_\nu\|_{L^\infty(\Gamma_3)} + \|c_\tau\|_{L^\infty(\Gamma_3)}\right) L d_\Omega\, \|\beta_1(t) - \beta_2(t)\|_{L^2(\Gamma_3)}\, \|u_{\beta_1}(t) - u_{\beta_2}(t)\|_V.$$

Therefore if

$$cd_{\Omega}^{2} \|\mu\|_{L^{\infty}(\Gamma_3)} < m,$$

we obtain

$$\|u_{\beta_1}(t) - u_{\beta_2}(t)\|_{V} \leq c_3 \|\beta_1(t) - \beta_2(t)\|_{L^2(\Gamma_3)}, \tag{3.7}$$

for some constant $c_3 > 0$, and so the lemma is proved. Now, to end the proof of Proposition 3.4, we use (2.10) to see that there exists a constant $c_4 > 0$ such that

$$\|T\beta_1(t) - T\beta_2(t)\|_{L^2(\Gamma_3)} \leq$$

$$c_4 \int_0^t \|\beta_1(s) - \beta_2(s)\|_{L^2(\Gamma_3)} ds + c_4 \int_0^t \|u_{\beta_1}(s) - u_{\beta_2}(s)\|_{V} ds,$$

and therefore (3.7) implies that for some constant $c_5 > 0$:

$$\|T\beta_1(t) - T\beta_2(t)\|_{L^2(\Gamma_3)} \leq c_5 \int_0^t \|\beta_1(s) - \beta_2(s)\|_{L^2(\Gamma_3)} ds,$$

and then,

$$\|T\beta_1 - T\beta_2\|_{X} \leq \frac{c_5}{k} \|\beta_1 - \beta_2\|_{X}. \tag{3.8}$$

The inequality (3.8) shows that for k sufficiently large T is a contraction. Hence we deduce, by using the fixed point theorem that T has a unique fixed point β_a which satisfies (3.4) and (3.5). The regularity $\beta_a \in B$ is a consequence of (3.4) and (2.17); see [19] for details. □

Now, we provide the existence of the solution of Theorem 2.1. Indeed, let β_a be the fixed point of T and let u_a be the solution of the Problem $P_{1\beta}$ for $\beta = \beta_a$, i-e., $u_a = u_{\beta_a}$. Take $v = u_a(t_j)$ in the inequality (3.1) written for $t = t_i$, $i, j = 1, 2$ and adding the two inequalities, as in Proposition 3.1, there exists a constant $c_6 > 0$ such that

$$\|u_a(t_1) - u_a(t_2)\|_{V} \leq$$

$$c_6 \left(\|\beta_a(t_1) - \beta_a(t_2)\|_{L^2(\Gamma_3)} + \|f(t_1) - f(t_2)\|_{V} \right) \quad \forall t_1, t_2 \in [0, T]. \tag{3.9}$$

Now, as $T\beta_a = \beta_a$ we deduce from Proposition 3.4 that $\beta_a \in W^{1,\infty}\left(0, T; L^2(\Gamma_3)\right)$ and moreover as $f \in W^{1,\infty}(0, T; V)$, then (3.9) implies that $u_a \in W^{1,\infty}(0, T; V)$. Thus, we conclude by (3.1), (3.4) and (3.5) that (u_a, β_a) is a solution to the Problem P_2. To prove the uniqueness of the solution, suppose that (u, β) is a solution of the Problem P_2 which satisfies

$$(u, \beta) \in W^{1,\infty}(0, T; V) \times W^{1,\infty}\left(0, T; L^2(\Gamma_3)\right) \cap B,$$

it follows that $\beta \in B$. Moreover we deduce from (3.1) that u is a solution to problem $P_{1\beta}$, and as by Proposition 3.1 this problem has a unique solution denoted by u_β, we get $u = u_\beta$. Take $u = u_\beta$ in (2.19) and use the initial condition (2.21), we deduce that β is a solution of the Problem $P_{2\beta}$. Therefore, we obtain from Proposition 3.4 that $\beta = \beta_a$ and we conclude that (u_a, β_a) is a unique solution to the Problem P_2.

References

[1]–[22] See this issue, pp. 81–82.

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ANALIZA ZAGADNIENIA SZORSTKIEGO STYKU WRAZ Z PRZYLEGANIEM DLA NIELINIOWYCH CIAŁ SPRĘŻYSTYCH I

SFORMUŁOWANIE ZAGADNIENIA, ISTNIENIE I JEDNOZNACZNOŚĆ

S t r e s z c z e n i e

Rozpatrujemy model matematyczny, który opisuje zagadnienie styku nieliniowego ciała sprężystego z podłożem. Zetknięcie się jest szorstkie i jest modelowane przez warunki Signoriniego i przyporządkowane prawo tarcia, w którym uwzględnia się przyleganie stykających się powierzchni. Ewolucja pola wiążącego jest opisana przez równanie różniczkowe pierwszego rzędu. Przedstawiamy sformułowanie wariacyjne zagadnienia mechanicznego i dowodzimy wyniku o istnieniu i jednoznaczności rozwiązania słabego, o ile współczynnik tarcia jest dostatecznie mały. Dowody są oparte na wykorzystaniu nierówności wariacyjnych zależnych od czasu, równań różniczkowych i twierdzeń Banacha o punkcie stałym.

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ANALYSIS OF A FRICTIONAL CONTACT PROBLEM WITH ADHESION FOR NONLINEAR ELASTIC MATERIALS II

THE PENALIZED AND REGULARIZED PROBLEM

Summary

In this part II we consider a sequence of penalized and regularized problems which have at least one solution by using a result on pseudomonotone operators. Using compactness properties we obtain a solution of the original model by passing to the limit as the penalization and regularization parameter converges to zero.

4. The penalized and regularized problem

Let us define for $\delta > 0$ the penalized and regularized problems with frictional contact and adhesion as:

Problem $P_{1\delta}$. Find $(u_\delta, \beta_\delta) \in W^{1,\infty}(0,T;V) \times W^{1,\infty}(0,T;L^\infty(\Gamma_3))) \cap B$ such that

$$\begin{aligned} &\langle F\varepsilon(u_\delta(t)), \varepsilon(v)\rangle_Q + \frac{1}{\delta}\left((u_{\delta\nu}(t))_+, v_\nu\right)_{L^2(\Gamma_3)} + j_\delta(u_\delta(t), v) + \\ &r(\beta_\delta(t), u_\delta(t), v) = \langle f(t), v\rangle_V \quad \forall v \in V,\ t \in [0,T], \end{aligned} \tag{4.1}$$

$$\dot{\beta}_\delta(t) = -\left[\beta(t)\left(c_\nu\left(R_\nu\left(u_{_\delta\nu}(t)\right)\right)^2 + c_\tau\left(\left|R_\tau\left(u_{\delta\tau}(t)\right)\right|\right)^2\right) - \varepsilon_a\right]_+ \tag{4.2}$$

$$\text{for a.e. } t \in (0,T),$$

$$\beta_\delta(0) = \beta_0 \text{ on } \Gamma_3, \tag{4.3}$$

where

$$j_\delta\left(u_\delta\left(t\right),v\right)=\int_{\Gamma_3}\mu\left|R^*\left(\sigma_{\delta\nu}\left(t\right)\right)\right|\frac{u_{\delta\tau}\left(t\right)}{\sqrt{u_{\delta\tau}^2\left(t\right)+\delta^2}}v_\tau da,\ \sigma_{\delta\nu}=-\frac{1}{\delta}\left(u_{\delta\nu}\right)_+.$$

We have the following result.

Theorem 4.1. *There exists at least one solution to the Problem $P_{1\delta}$.*

Proof. The proof of Theorem 4.1 is similar to that of Theorem 2.1 and is carried out in several steps. For thus, we omit the details of the proof. The steps are the following:

i) For any $\beta\in C\left(\left[0,T\right];L^2\left(\Gamma_3\right)\right)\cap B$, we prove that there exists at least one solution $u_\delta\in L^\infty\left(0,T;V\right)$ such that

$$\begin{aligned}&\left\langle F\varepsilon\left(u_\delta\left(t\right)\right),\varepsilon\left(v\right)\right\rangle_Q+\frac{1}{\delta}\left(\left(u_{\delta\nu}\left(t\right)\right)_+,v_\nu\right)_{L^2(\Gamma_3)}+j_\delta\left(u_\delta\left(t\right),v\right)+\\&r\left(\beta_\delta\left(t\right),u_\delta\left(t\right),v\right)=\left\langle f\left(t\right),v\right\rangle_V\quad\forall v\in V,\,t\in\left[0,T\right].\end{aligned}\tag{4.4}$$

To provide this step for all $t\in\left[0,T\right]$, we define the operator $T_t:V\to V^{'}$ by

$$\left(T_tu,v\right)_{V'\times V}=\left\langle F\varepsilon\left(u\right),\varepsilon\left(v\right)\right\rangle_Q+\frac{1}{\delta}\left(\left(u_\nu\right)_+,v_\nu\right)_{L^2(\Gamma_3)}+r\left(\beta,u,v\right)$$

$$\forall u,v\in V,$$

where $V^{'}$ is the dual of V. In the study of the operator T_t we need to recall that for $a,b\in\mathbf{R}$, we have

$$\begin{aligned}&\left(a_+-b_+\right)\left(a-b\right)\geq\left(a_+-b_+\right)^2,\\&\left|a_+-b_+\right|\leq\left|a-b\right|.\end{aligned}\tag{4.5}$$

Using (4.5) we see as in the proof of Lemma 3.2 that the operator T_t is strongly monotone as for all $u,v\in V$,

$$\left(T_tu-T_tv,u-v\right)_{V'\times V}\geq m\left\|u-v\right\|_V^2,$$

bounded and elliptic for each $\delta>0$, as also for all $u,v\in V$, the following holds:

$$\left|\left(T_tu,v\right)_{V'\times V}\right|\leq\left[M+\left(\left\|c_\nu\right\|_{L^\infty(\Gamma_3)}+\left\|c_\tau\right\|_{L^\infty(\Gamma_3)}+\frac{1}{\delta}\right)d_\Omega^2\right]\left\|u\right\|_V\left\|v\right\|_V,$$

$$\left(T_tv,v\right)_{V'\times V}\geq m\left\|v\right\|_V^2$$

On the other hand, we define the operator $P_t:V\to V^{'}$ by

$$\left(P_tu,v\right)_{V'\times V}=\int_{\Gamma_3}\mu\left|R^*\left(\sigma_{\delta\nu}\right)\right|\frac{u_\tau}{\sqrt{u_\tau^2+\delta^2}}v_\tau da.$$

We notice as in [22], by using (2.13) and the compactness of R^*, that there exists a constant $c_0>0$ such that

$$\left|\left(P_tu,v\right)_{V'\times V}\right|\leq\frac{c_0}{\delta}\left\|u\right\|_V\left\|v\right\|_V,\ \forall u,v\in V.$$

Using the compact embedding $H^{\frac{1}{2}}(\Gamma_3) \hookrightarrow L^2(\Gamma_3)$ and the Lebesgue dominated convergence, we get that the operator P_t is completely continuous for each $\delta > 0$. Moreover it satisfies $(P_t v, v)_{V' \times V} \geq 0 \ \forall v \in V$. Therefore, using the result on pseudomonotone operators obtained in [8], we conclude that the operator $T_t + P_t$ is pseudomonotone, bounded and coercif for each $\delta > 0$. So, there exists at least one solution $u_\delta(t)$ of (4.4). Take $v = u_\delta(t)$ in (4.4), it follows that

$$\sup_{t\in(0,T)} \|u_\delta(t)\|_V \leq \frac{1}{m} \|f\|_{L^\infty(0,T;V)},$$

which implies $u_\delta \in L^\infty(0,T;V)$.

ii) There exists a unique β_δ such that

$$\beta_\delta \in W^{1,\infty}\left(0,T;L^2(\Gamma_3)\right), \tag{4.6}$$

$$\dot{\beta}_\delta(t) = -\left[\beta_\delta(t)\left(c_\nu\left(R_\nu\left(u_{\beta_\delta\nu}(t)\right)\right)^2 + c_\tau\left(\left|R_\tau\left(u_{\beta_\delta\tau}(t)\right)\right|\right)^2\right) - \varepsilon_a\right]_+ \tag{4.7}$$

$$\text{for a.e. } t \in (0,T),$$

$$\beta_\delta(0) = \beta_0. \tag{4.8}$$

iii) Let β_δ defined in ii) and denote again by u_δ the function obtained in step i) for $\beta = \beta_\delta$. Then, by using (4.6)–(4.8) it is easy to see that β_δ is the unique solution to Problem $P_{2\delta}$ such that

$$(u_\delta, \beta_\delta) \in W^{1,\infty}\left(0,T;L^2(\Gamma_3)\right) \times W^{1,\infty}\left(0,T;L^2(\Gamma_3)\right) \cap B,$$

and (u_δ, β_δ) is a solution to the Problem $P_{1\delta}$.

Now, in the following theorem we shall prove the convergence of the solution (u_δ, β_δ) as $\delta \to 0$ to the solution (u, β) of thr Problem P_2 as follows.

Theorem 4.2. *Assume that* (2.14), (2.15) *and* (2.17) *hold. Then we have the following convergences:*

$$\lim_{\delta\to 0} \|u_\delta(t) - u(t)\|_V = 0 \text{ for all } t \in [0,T], \tag{4.9}$$

$$\lim_{\delta\to 0} \|\beta_\delta(t) - \beta(t)\|_{L^2(\Gamma_3)} = 0 \text{ for all } t \in [0,T]. \tag{4.10}$$

The proof is carried out in several steps. In the first step, we show the following lemma.

Lemma 4.3. *There exists a function* $\bar{u}(t) \in V$ *such that after passing to a subsequence still denoted* $(u_\delta(t))$ *we have*

$$u_\delta(t) \to \bar{u}(t) \quad \text{weakly in } V \text{ for all } t \in [0,T]. \tag{4.11}$$

Proof. Take in (4.9) $v = u_\delta(t)$. Then we get

$$\begin{aligned} &\langle F\varepsilon(u_\delta(t)), \varepsilon(u_\delta(t))\rangle_Q + \frac{1}{\delta}\left((u_{\delta\nu}(t))_+, (u_\delta(t))\right)_{L^2(\Gamma_3)} + \\ &r(\beta_\delta(t), u_\delta(t), u_\delta(t)) + j_\delta(u_\delta(t), u_\delta(t)) = \langle f(t), u_\delta(t)\rangle_V. \end{aligned} \tag{4.12}$$

Using (4.5), we have

$$\left((u_{\delta\nu}(t))_+, (u_{\delta\nu}(t))\right)_{L^2(\Gamma_3)} \geq \left((u_{\delta\nu}(t))_+, (u_{\delta\nu}(t))_+\right)_{L^2(\Gamma_3)} \geq 0,$$

and since

$$r(\beta_\delta(t), u_\delta(t), u_\delta(t)) + j_\delta(u_\delta(t), u_\delta(t)) \geq 0,$$

then we get from (4.12) that

$$\langle F\varepsilon(u_\delta(t)), \varepsilon(u_\delta(t))\rangle_Q \leq \langle f(t), u_\delta(t)\rangle_V$$

Keeping in mind (2.14) (b), we deduce that there exists a constant $C > 0$ such that

$$\|u_\delta(t)\|_V \leq C\|f(t)\|_V.$$

It follows that the sequence $(u_\delta(t))$ is bounded in V, so there exists a function $\bar{u}(t) \in V$ and a subsequence again denoted $(u_\delta(t))$ such that (4.11) holds. Now, consider the following auxiliary problem.

Problem P_3. Find $\beta \in W^{1,\infty}\left(0, T; L^2(\Gamma_3)\right)$, such that

$$\dot{\beta}(t) = -\left[\beta(t)\left(c_\nu\left(R_\nu\left(\bar{u}_{\beta\nu}(t)\right)\right)^2 + c_\tau\left(\left|R_\tau\left(\bar{u}_{\beta\tau}(t)\right)\right|\right)^2\right) - \varepsilon_a\right]_+ \quad a.e.\ t \in (0,T),$$

$$\beta(0) = \beta_0.$$

Using the same proof as in Proposition 3.4, we have the following result.

Lemma 4.4. *Problem* P_3 *has a unique solution* $\beta \in W^{1,\infty}\left(0, T; L^2(\Gamma_3)\right) \cap B$.

Now, we show the following convergence result.

Lemma 4.5. *Let* β *be the solution to the Problem* P_3. *Then we have*

$$\lim_{\delta\to 0}\|\beta_\delta(t) - \beta(t)\|_{L^2(\Gamma_3)} = 0 \text{ for all } t \in [0,T]. \tag{4.13}$$

Proof. Similarly as in the proof of Proposition 3.4, using Gronwall-type argument and the properties of R_ν and R_τ, we can seethere exists a constant $C > 0$ such that

$$\|\beta_\delta(t) - \beta(t)\|_{L^2(\Gamma_3)} \leq C\int_0^t \|u_\delta(s) - \bar{u}(s)\|_{L^2(\Gamma_3)}\, ds. \tag{4.14}$$

Using (4.11) and the compact imbedding $H^{\frac{1}{2}}(\Gamma_3) \hookrightarrow L^2(\Gamma_3)$, we deduce that $u_\delta(t) \to \bar{u}(t)$ strongly in $L^2(\Gamma_3)$, as $\delta \to 0$. On the other hand, there exists a constant $C_2 > 0$ such that

$$\|u_\delta(t)-\bar{u}(t)\|_{L^2(\Gamma_3)} \le d_\Omega \|u_\delta(t)-\bar{u}(t)\|_V$$

$$\le C_2\left(\|f(t)\|_V+\|\bar{u}(t)\|_V\right),$$

which implies that there exists a constant $C_3>0$ depending on f and $\bar{u}$ such that

$$\|u_\delta(t)-\bar{u}(t)\|_{L^2(\Gamma_3)} \le C_3.$$

It follows from the Lebesgue convergence theorem that

$$\lim_{\delta\to 0}\int_0^t \|u_\delta(s)-\bar{u}(s)\|_{L^2(\Gamma_3)}\,ds=0, \tag{4.15}$$

and so from (4.14) we get

$$\|\beta_\delta(t)-\beta(t)\|_{L^2(\Gamma_3)}\to 0 \text{ for all } t\in[0,T].$$

Lemma 4.6. *We have* $\bar{u}(t)=u(t)$ *for all* $t\in[0,T]$.

Proof. From (4.12) it follows that there exists a constant $C_1>0$ such that

$$\left((u_{\delta\nu}(t))_+,(u_{\delta\nu}(t))\right)_{L^2(\Gamma_3)}\le \delta C_1,$$

and then

$$\left((u_{\delta\nu}(t))_+,(u_{\delta\nu}(t))_+\right)_{L^2(\Gamma_3)}\le \delta C_1. \tag{4.16}$$

Since

$$(u_{\delta\nu}(t))_+\to(\bar{u}_\nu(t))_+ \text{ strongly in } L^2(\Gamma_3), \text{ as } \delta\to 0, \tag{4.17}$$

we deduce from (4.16) and (4.17) that

$$\left\|(\bar{u}_\nu(t))_+\right\|_{L^2(\Gamma_3)}\le \liminf_{\delta\to 0}\left\|(u_{\delta\nu}(t))_+\right\|_{L^2(\Gamma_3)}=0, \tag{4.18}$$

and it follows from (4.18) that $(\bar{u}_\nu(t))_+=0$, i-e. $\bar{u}_\nu(t)\le 0$ *a.e.* on Γ_3 which shows that $\bar{u}(t)\in K$. Now, testing with $v-u_\delta(t)$ in (4.4) and keeping in mind that

$$\left((u_{\delta\nu}(t))_+,v_\nu-u_{\delta\nu}(t)\right)_{L^2(\Gamma_3)}=\left((u_{\delta\nu}(t))_+-v_{\nu+},v_\nu-u_{\delta\nu}(t)\right)_{L^2(\Gamma_3)}$$

$$\le 0 \quad \forall v\in K,$$

we get

$$\begin{aligned}&\langle F\varepsilon(u_\delta(t)),\varepsilon(v-u_\delta(t))\rangle_Q+j_\delta(u_\delta(t),v-u_\delta(t))+\\ &r(\beta_\delta(t),u_\delta(t),v-u_\delta(t))\ge\langle f(t),v-u_\delta(t)\rangle_V \quad \forall v\in K.\end{aligned} \tag{4.19}$$

Now, we pass to the limit, as $\delta\to 0$, in (4.19). We have as in [22], $\sigma_{\delta\nu}(t)\to\sigma_\nu(\bar{u}(t))$ weakly in $H^{-\frac{1}{2}}(\Gamma_3)$ $\forall t\in[0,T]$. Then, using (2.13) and the compacity of R^*, we get

$$R^*(\sigma_{\delta\nu}(t))\to R^*(\sigma_\nu(\bar{u}(t))) \text{ strongly in } L^2(\Gamma_3).$$

Hence, we obtain

$$\lim_{\delta\to 0}\int_{\Gamma_3}\mu\left|R^*\left(\sigma_{\delta\nu}\left(t\right)\right)\right|\frac{u_{\delta\tau}\left(t\right)}{\sqrt{u_{\delta\tau}^2\left(t\right)+\delta^2}}\left(v_\tau-u_{\delta\tau}\left(t\right)\right)da\leq$$

$$\int_{\Gamma_3}\mu\left|R^*\left(\sigma_\nu\left(\bar{u}\left(t\right)\right)\right)\right|\left(\left|v_\tau\right|-\left|\bar{u}_\tau\left(t\right)\right|\right)da=j\left(\bar{u}\left(t\right),v\right)-j\left(\bar{u}\left(t\right),\bar{u}\left(t\right)\right).$$

Now write

$$r\left(\beta_\delta\left(t\right),u_\delta\left(t\right),v-u_\delta\left(t\right)\right)=r\left(\beta_\delta\left(t\right),u_\delta\left(t\right),v-u_\delta\left(t\right)\right)-$$

$$r\left(\beta\left(t\right),u_\delta\left(t\right),v-u_\delta\left(t\right)\right)+r\left(\beta\left(t\right),u_\delta\left(t\right),v-u_\delta\left(t\right)\right).$$

Since

$$\left|r\left(\beta_\delta\left(t\right),u_\delta\left(t\right),v-u_\delta\left(t\right)\right)-r\left(\beta\left(t\right),u_\delta\left(t\right),v-u_\delta\left(t\right)\right)\right|\leq$$

$$C\left\|\beta_\delta\left(t\right)-\beta\left(t\right)\right\|_{L^2(\Gamma_3)}\left\|v-u_\delta\left(t\right)\right\|_V,$$

it follows by using (4.13) that

$$r\left(\beta_\delta\left(t\right),u_\delta\left(t\right),v-u_\delta\left(t\right)\right)-r\left(\beta\left(t\right),u_\delta\left(t\right),v-u_\delta\left(t\right)\right)\to 0,\text{ as }\delta\to 0.$$

Moreover, using the proprieties (3.3) of R_ν and R_τ, it is clear that

$$r\left(\beta\left(t\right),u_\delta\left(t\right),v-u_\delta\left(t\right)\right)\to r\left(\beta\left(t\right),u\left(t\right),v-u\left(t\right)\right),\text{ as }\delta\to 0.$$

Therefore, passing to the limit in (4.19) as $\delta\to 0$, we obtain

$$\bar{u}\left(t\right)\in K,$$

$$\left\langle F\varepsilon(\bar{u}\left(t\right)),\varepsilon\left(v-\bar{u}\left(t\right)\right)\right\rangle_Q+j\left(\bar{u}\left(t\right),v\right)-j\left(\bar{u}\left(t\right),\bar{u}\left(t\right)\right)+ \tag{4.20}$$

$$r\left(\beta\left(t\right),\bar{u}\left(t\right),v-\bar{u}\left(t\right)\right)\geq\left\langle f\left(t\right),v-\bar{u}\left(t\right)\right\rangle_V\quad\forall v\in K.$$

Now, taking $v=u\left(t\right)$ in (4.20) and $v=\bar{u}\left(t\right)$ in (2.19) and adding the two inequalities, we get by using the assumption (2.14) (b) on F that

$$m\left\|\bar{u}\left(t\right)-u\left(t\right)\right\|_V^2$$

$$\leq\left|j\left(\bar{u}\left(t\right),u\left(t\right)\right)+j\left(u\left(t\right),\bar{u}\left(t\right)\right)-j\left(\bar{u}\left(t\right),\bar{u}\left(t\right)\right)-j\left(u\left(t\right),u\left(t\right)\right)\right|$$

$$+r\left(\beta\left(t\right),\bar{u}\left(t\right),u\left(t\right)-\bar{u}\left(t\right)\right)+r\left(\beta\left(t\right),u\left(t\right),\bar{u}\left(t\right)-u\left(t\right)\right),$$

and using the estimate

$$r\left(\beta\left(t\right),\bar{u}\left(t\right),u\left(t\right)-\bar{u}\left(t\right)\right)+r\left(\beta\left(t\right),u\left(t\right),\bar{u}\left(t\right)-u\left(t\right)\right)\leq 0$$

we get

$$m\left\|\bar{u}\left(t\right)-u\left(t\right)\right\|_V^2$$

$$\leq\left|j\left(\bar{u}\left(t\right),u\left(t\right)\right)+j\left(u\left(t\right),\bar{u}\left(t\right)\right)-j\left(\bar{u}\left(t\right),\bar{u}\left(t\right)\right)-j\left(u\left(t\right),u\left(t\right)\right)\right|,$$

which implies

$$m \left\| \bar{u}\left(t\right) - u\left(t\right) \right\|_V^2 \leq c d_\Omega^2 \left\| \mu \right\|_{L^\infty(\Gamma_3)} \left\| \bar{u}\left(t\right) - u\left(t\right) \right\|_V^2 .$$

This previous inequality enables us to obtain that, as $c\, d_\Omega^2 \left\| \mu \right\|_{L^\infty(\Gamma_3)} < m$,

$$\bar{u}\left(t\right) = u\left(t\right).$$

Now, we have all the ingredients to prove Theorem 4.2. Indeed, take $v = u\left(t\right)$ in (4.19). By using the assumption (2.14) (b) on F we get

$$\begin{aligned} & m \left\| u_\delta\left(t\right) - u\left(t\right) \right\|_V^2 \leq \\ & j_\delta\left(u_\delta\left(t\right), u\left(t\right) - u_\delta\left(t\right)\right) + r\left(\beta_\delta\left(t\right), u_\delta\left(t\right), u\left(t\right) - u_\delta\left(t\right)\right) \\ & + \left\langle F\varepsilon\left(u\left(t\right)\right), \varepsilon\left(u\left(t\right) - u_\delta\left(t\right)\right)\right\rangle_Q + \left\langle f\left(t\right), u_\delta\left(t\right) - u\left(t\right)\right\rangle_V . \end{aligned} \tag{4.21}$$

Using the convergences, as $\delta \to 0$:

$$j_\delta\left(u_\delta\left(t\right), u\left(t\right) - u_\delta\left(t\right)\right) + r\left(\beta_\delta\left(t\right), u_\delta\left(t\right), u\left(t\right) - u_\delta\left(t\right)\right) \to 0,$$

$$\left\langle F\varepsilon\left(u\left(t\right)\right), \varepsilon\left(u\left(t\right) - u_\delta\left(t\right)\right)\right\rangle_Q + \left\langle f\left(t\right), u_\delta\left(t\right) - u\left(t\right)\right\rangle_V \to 0,$$

we obtain by passing to the limit in (4.21) that

$$\left\| u_\delta\left(t\right) - u\left(t\right) \right\|_V \to 0 \text{ for all } t \in \left[0, T\right],$$

and so, (4.9) is proved.

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ANALIZA ZAGADNIENIA SZORSTKIEGO STYKU WRAZ Z PRZYLEGANIEM DLA NIELINIOWYCH CIAŁ SPRĘŻYSTYCH II

ZREGULARYZOWANE ZAGADNIENIE Z FUNKCJĄ KARY

S t r e s z c z e n i e

Rozpatrujemy model matematyczny, który opisuje zagadnienie styku nieliniowego ciała sprężystego z podłożem. W obecnej części II rozważamy ciąg zregularyzowanych zagadnień z funkcją kary, posiadających co najmniej jedno rozwiązanie, przy użyciu pewnego wyniku o operatorach pseudomonotonicznych. Stosując z kolei własności zwartości uzyskujemy rozwiązanie dla pierwotnego modelu przez przejście do granicy przy parametrze penalizacji (kary) i regularyzacji dążącym do zera.

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Stanisław Bednarek

AN INSTRUMENT FOR MODELLING ENERGY LEVELS OF PARTICLES AND THEIR NATURAL TRANSITIONS

Summary

In this article wes describe a construction and an operation principle of a simple instrument co-operating with a centrifuge and consisting of two transparent, coaxial, respectively profiled funnels. After setting the instrument in rotary motion, the device allows modelling the continuous and discrete distribution of particles energy by using globules located inside the funnels.

An understanding of ideas of energy distribution and energy levels of particles is crucial for explanation of many phenomena in classic and quantum physics. It is also important to notice differences between continuous and discrete energy distribution and transitions between the energy levels [1, 2]. In order to achieve these aims, a simple instrument was constructed allowing a demonstration of the energy levels of particles and transitions between them in a model manner.

The construction of the instrument is shown in a cross-axial section in Fig. 1. The instrument consists of two transparent funnels 1, 2, placed coaxially on a vertical rod 3. The bottom end of the rod is fixed in a spindle centrifuge 4 using the screw 5. The lateral surface of upper funnel 1 has a stepped form. The heights of the steps are well matched and increase together with their radii. The bottom funnel 2 is in shape similar to that of rotary paraboloid. The upper edges of both funnels are inclined towards their centres. Several small globules 6 are placed in both funnels.

A principle of operation of the instrument is as follows. When the instrument remains immovable, the globules 6 are in the bottoms of both funnels. After setting the instrument in a rotary motion, a centrifugal force of inertia F_r acts on each of the globules. Together with the increase of angular velocity of motion ω the value

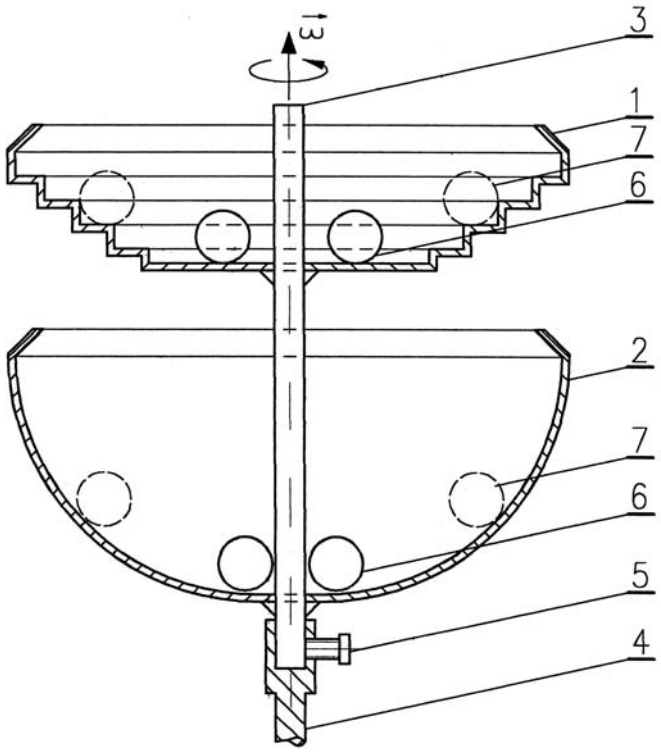

Fig. 1: Construction of the instrument shown in cross-axial section.

of F_r force also rises [3]. In the lower funnel the force causes continuous climbing of the globules to the position 7 and increasing their distance from rotation axis. This situation corresponds to continuous energy distribution of the particles. In the upper funnel the globules can increase the distance from the rotation axis and transit to higher positions 7 by rolling in the consecutive steps. It can occur only when the angular velocity ω achieves strictly defined values. This situation corresponds to non-continuous energy distribution of particles and occurring the energetic levels.

In order to ensure a correct operation of the instrument, the globules should roll in the consecutive steps when angular velocity becomes higher and higher, hence the height of the steps must meet a certain condition. In order to calculate this condition, there should be compared the momentum of forces acting on the globule: centrifugal force of inertia F_{rn} to the force of weight of the globule Q acting on the globule being in n step of h_n height and moving in the circle of r_n radius (Fig. 2). Both the moments calculated in respect to upper edge of the step (point A in Fig. 2) fulfil the following equation:

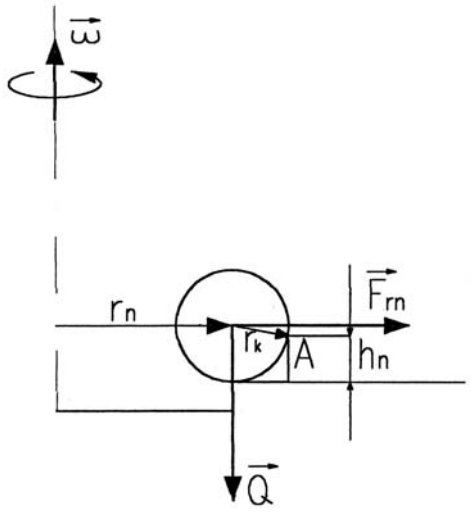

Fig. 2: Forces acting on the globule located on the step.

$$F_{rn}(r_k - h_n) = Q\sqrt{r_k^2 - (r_k - h_n)^2}, \tag{1}$$

where r_k denotes the globule radius. Let m denote the globule mass, then forces F_{rn} and Q appearing in equation (1) are expressed by the following formulas:

$$F_{rn} = m\omega^2 r_n, \tag{2}$$

$$Q = mg. \tag{3}$$

After substitution of formulas (2) and (3) to (1) and solving the resulting quadratic equation, one achieves the following formula for h_n:

$$h_n = r_k\left(1 - \frac{1}{\sqrt{\omega^4 r_n^2 + g^2}}\right). \tag{4}$$

In the constructed model of the instrument, the widths of the steps were equal to the radius of the globules r_k. (An advantage of this approach is a self-acting returning of the globules to the bottom of the funnel after the rotary motion is stopped.) In this situation the radius of the circle r_n, in which the globules were moving was also the internal radius of the n step.

In the lower funnel, a globule remains in the equilibrium position in a distance r from the axis of rotation, if the result of forces F_r and Q is perpendicular to the surface of the funnel (Fig. 3). This condition can be expressed by following equation:

$$\tan\alpha = \frac{F_r}{Q} = \frac{\omega^2 r}{g}. \tag{5}$$

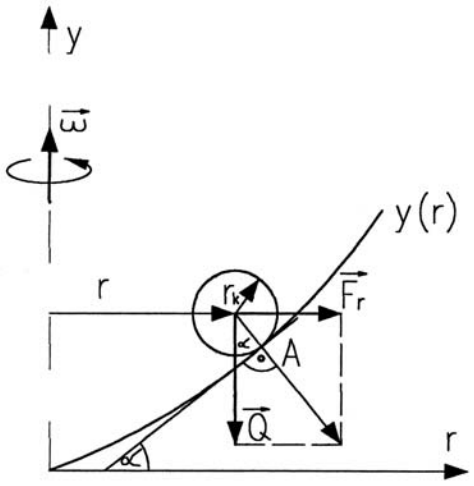

Fig. 3: Forces acting on the globule located in the lower funnel.

After substitution the formula known from geometry $\tan\alpha = dy/dr$ to equation (5) and the elementary integration, we achieve equation of curve describing cross-axial section of the bottom funnel as follows:

$$y(r) = \left(\frac{\omega^2}{2g}\right) r^2. \tag{6}$$

The results of the formula (6) suggest that the curve should be a parabola. Using equation (6) we can also easily show that a potential energy of the globule E_p being on the height $h = y(r)$ changes continuously and equals to its kinetic energy E_k. Indeed:

$$E_p = mgy(r) = \frac{m\omega^2 r^2}{2} = \frac{m\nu^2}{2} = E_k. \tag{7}$$

The described instrument can be self-made using easily accessible materials. It is reasonable to adjust a dimension of the instrument to the dimensions of the globules. Plastic or wooden globules are recommended. In the model described in this article, there were used the plastic globules having diameter of 16 mm. Upper funnel having stepped form was made of rings cut out of Plexiglas. The rings constituted the horizontal surface of steps and the bottom of the funnel. The upper edge and vertical surface of the funnel were made of strips of thin and transparent polyester. The strips were cut out of smooth walls of plastic bottles. The width of strips should be calculated by using the formula (4), taking into consideration radius of the globules used r_k, radiuses of the steps and an angular velocity ω required for rolling the globules. The calculated value should be increased by adding the thickness of the rings made of Plexiglas.

The bottom funnel was made of the cut off upper part of large plastic bottle having parabolic shape. In order to assemble all the parts of the instrument, it was used the transparent epoxy glue. The dimensions of the instrument are not critical and can be changed in a relatively broad range. The instrument used in this study, for example, had a diameter of 100 mm and its total height was 250 mm. The transitions of globules to the highest location was achieved at 5 rotation per second (31.4 rad/s). The most convenient way to set the instrument in motion was the use of electrical centrifuge with a rotation counter, however a normal centrifuge propelled by a crank could also be applied.

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PRZYRZĄD DO MODELOWANIA POZIOMÓW ENERGETYCZNYCH CZĄSTEK I PRZEJŚĆ MIĘDZY NIMI

S t r e s z c z e n i e

W artykule opisano budowę i zasadę działania prostego przyrządu, współpracującego z wirownicą i stanowiącego dwa współśrodkowe, odpowiednio wyprofilowane lejki. Po wprawieniu przyrządu w ruch obrotowy, umożliwia on modelowanie ciągłego albo dyskretnego rozkładu energii kulek umieszczonych w lejku.

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Piotr Matczak and Stanisław Romanowski

ADSORPTION OF ATOMIC OXYGEN ON Pt(001). A DENSITY-FUNCTIONAL THEORY STUDY

Summary

In this paper the preliminary results of the density-functional theory (DFT) calculations for the atomic oxygen adsorption on Pt(001) are reported. The Pt(001) surface is modelled by means of two five-atom clusters of planar and pyramidal geometries. Some structural, energetic and electronic properties of the adsorbed O atom have been determined to probe the interactions between the atomic adsorbate and the Pt(001) surface.

1. Introduction

Gas adsorption on transition-metal surfaces constitutes undoubtedly the central pillar of heterogeneous catalysis [1–3]. Oxygen adsorption on platinum is one of the most important heterogeneous processes due to its practical application for the further catalytic oxidation of carbon oxide (CO).

Gas-surface interactions and subsequent reactions of the adsorbed species may be complex and in many cases the fundamental mechanisms of adsorption and catalytic reactions on surfaces are hard to discern. Two major mechanisms have been proposed for catalytic reactions between two reactants on a surface so far [4, 5]. The first one called the Eley-Rideal mechanism assumes that one reactant adsorbs on a surface first, and then another species reacts with the adsorbed reactant directly from the gas phase. As a result of the reaction a product is formed. In the second one, called the Langmuir-Hinshelwood mechanism, both reactants adsorb on a surface, and then they diffuse towards each other or one to the other along the surface. If they are close enough, they can react to form a product. Most catalytic reactions follow the Langmuir-Hinshelwood mechanism.

Platinum is probably the most versatile transition metal because it catalyzes many oxidation, reduction and reforming processes [1, 6]. In particular, the oxidation reactions are of considerable interest and the oxidation of automotive exhaust gases has become the most visible recent application of Pt. In this application, platinum forms the so-called three-way catalyst which converts simultaneously two reducing pollutants (CO and uncombusted hydrocarbons) and one oxidizing pollutant (NO) to nontoxic products. Platinum is also employed in the industrial oxidation of ammonia (the Ostwald process), ethylene epoxidation and partial oxidation of methane into some useful derivatives such as methanol and formaldehyde. However, there are a few obstacles to the use of platinum as a universal oxidation catalyst. Pt exhibits the lack of selectivity for NO oxidation in the presence of sulphur dioxide (SO_2). It leads to the formation of SO_3 and the poisoning of active sites on the surface of Pt. Moreover, in partial oxidation reactions it is difficult to limit combustion to CO_2 and H_2O. These products are favoured because of the large thermodynamic driving force for combustion and the high temperatures required for partial oxidation. In the course of the Ostwald process a considerable loss of Pt catalyst is observed due to the generation of volatile platinum oxide (PtO_2) at the temperatures above 1000 K. A subsurface oxygen species may be a precursor of PtO_2. For the understanding of all the above-mentioned applications, as well as the obstacles, the in-depth elucidation of the nature of the interactions between oxygen and platinum surface is crucial.

The adsorption of oxygen has been mainly examined experimentally for the Pt(111) surface [7–12]. At low temperatures oxygen adsorption is molecular. The physisorbed state of O_2 is present below 25 K and identified as a precursor to a molecular chemisorbed state. In the temperature range 90–135 K, two molecular chemisorbed states are observed, namely the superoxo- (O_2^-) and peroxo-like (O_2^{2-}) configurations. Molecular oxygen can either desorb at ca. 170 K with an estimated desorption barrier of ca. 0.4 eV or dissociate into atoms. Atomic oxygen dominates on Pt(111) for a wide range of temperatures between 150 and 500 K. After the dissociation, the oxygen atoms form islands which remain stable up to temperatures 450–500 K, and then they desorb. The exact desorption temperature of the O atoms is difficult to measure because of the strong coverage dependence. Campbell et al. have determined desorption barriers of 1.82 eV at high coverage and of 2.21 eV at low coverage [13]. The bond dissociation energy of free O_2 is 5.12 eV, thus the estimated heat of adsorption of an oxygen atom is 3.66 eV. At room temperature, oxygen forms a (2×2) ordered overlayer with atoms in threefold sites on Pt(111) [14]. The oxygen-surface vertical and Pt-O distances are of 1.36 [15] and 2.02 Å [16] respectively.

Pt(111) is a rather simple surface, where there is no lateral reconstruction and surface layer relaxation is extremely small. On the contrary, Pt(001) exhibits two different structures of distinguished chemical reactivities. One is the unreconstructed (1×1) phase which is 0.21 eV less stable than the other which is a reconstructed quasihexagonal structure [17]. At 123 K, O_2 adsorbs dissociatively on the (1×1)

surface whereas the dissociation does not occur on the reconstructed surface [18]. Oxygen adsorption lifts the surface reconstruction, but the detailed structure of atomic oxygen on Pt(001) is not known.

Atomic-scale knowledge of adsorbate-surface interactions, adsorption positions and energetics of individual reactants on the catalyst surface is required for the precise understanding of the mechanisms of catalytic processes. A large amount of information can be provided by various computational methods based on the first principles. In particular, the methods using DFT have progressed in recent years due to advances in computational speed along with the development of new algorithms [19], and thus they have become indispensable for the investigations of heterogeneous-catalysis processes [20]. The adsorption of oxygen on the Pt(111) surface has been extensively studied by means of DFT [12, 21–29 and references therein]. By contrast, the oxygen adsorption on Pt(001) has been the subject of only a small number of theoretical studies [30–32]. Ge et al. [32] performed total-energy pseudopotential calculations within the framework of DFT using the basis set which consisted of plane waves. The Pt(001) surface was modelled by a slab inside a supercell. The authors found that the bridge site was the most stable for the atomic oxygen adsorption, followed by the fourfold hollow site. The atop site turned out the least stable.

The objective of this paper is to increase the knowledge of the Pt(001) surface by providing a detailed description of the O-atom adsorption on this surface. The description includes some structural, energetic and electronic properties of the O atom adsorbed on Pt(001).

2. Computational details

DFT, as implemented in the Gaussian 98 code [33], has been used for all of the calculations. The calculations are carried out by means of the B3LYP hybrid functional [34], which combines exact Hartree-Fock exchange, the Slater local [5] and Becke gradient-corrected [36] exchange functionals, together with the Vosko-Wilk-Nusair III local [37] and Lee-Yang-Parr nonlocal [38] correlation functionals. B3LYP is used because of its established accuracy for the thermochemistry of organic reactions. This will be important for the future investigations of catalyzed organic reactions on the Pt(001) surface. The spin-unrestricted scheme has been employed, together with the quadratically-convergent self-consistent field (QCSCF) procedure [39]. For Pt, the electrons from the $5s^2$, $5p^6$, $5d^9$ and $6s^1$ shells are treated explicitly using the Gaussian $(3s3p2d)$ basis set [40–42]. For the O atom, the D95++$(3df)$ basis set is applied [43].

The Pt(001) surface is modelled by two five-atom clusters of different structures. The clusters with the O atom adsorbed in an exemplary position are presented in Fig. 1. The first cluster contains all the Pt atoms put in the same plane, whereas the second one exhibits a pyramidal structure. Distances between the Pt atoms in

both clusters are characteristic of the face-centred cubic (fcc) Pt lattice and of the (001) crystal plane. The planar and pyramidal platinum clusters are denoted further in the paper as $Pt_5(001)$ and $Pt_{4+1}(001)$ respectively. Each of the clusters models reliably one adsorption site of high symmetry, which is placed in the centre of the cluster. In the case of $Pt_5(001)$ such a characteristic site on the central Pt atom is called the atop site, while for $Pt_{4+1}(001)$ on the subsurface Pt atom – the hollow site.

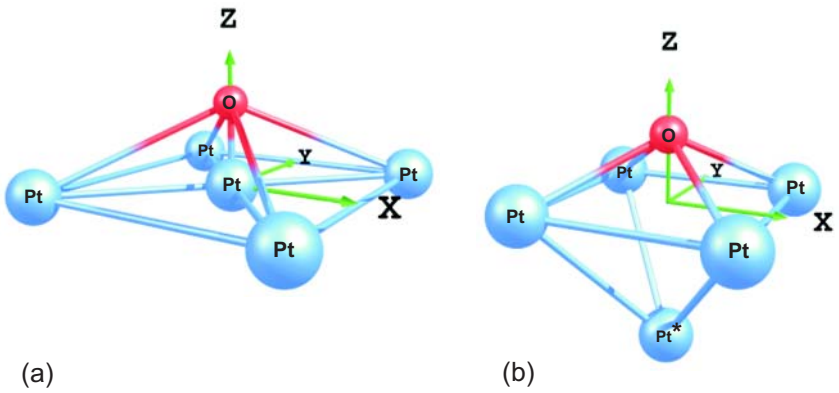

Fig. 1: Cluster models of the Pt(001) surface with the adsorbed O atom. (a) O on the planar $Pt_5(001)$ cluster. (b) O on the pyramidal $Pt_{4+1}(001)$ cluster. The Pt atom of the second crystal layer (the subsurface atom) is marked with an asterisk in (b).

The O atom has been adsorbed in a great deal of points above the plane of the platinum clusters (in the case of $Pt_{4+1}(001)$ above the plane containing four surface Pt atoms). For each point the height between the O atom and the plane of the platinum clusters is optimized to obtain the lowest total energy $E_{OPt_x(001)}$ of the $OPt_x(001)$ system, where $x = 5$ or $4 + 1$. The optimization is carried out using the Berny algorithm [44], which calculates the derivatives of total energy with respect to the coordinates of all atoms. The height which refers to $E_{OPt_x(001)}$ is denoted as z_{opt}. In the course of the optimization, the geometry of $Pt_x(001)$ stays "frozen". The binding energy (BE) of the O atom on $Pt_x(001)$ is calculated as the difference between $E_{OPt_x(001)}$ and the sum of the energies of the free O atom and the isolated $Pt_x(001)$ cluster. The ground state of both clusters is a quintet and the O atom has a triplet multiplicity. For some adsorption sites, the basis-set superposition error (BSSE) correction as proposed by Boys and Bernardi [45] has been also incorporated into the BE values. The atomic electronic charge on the adsorbed O atom is determined with the help of the electron population analysis according to Mulliken [46].

3. Results and discussion

Fig. 2 shows plots of three properties of the O atom adsorbed on the $Pt_5(001)$ cluster. The multiplicity of the $OPt_5(001)$ system has been established as a singlet. There is a plot of the height z_{opt} of the O atom above the cluster plane in Fig. 2a. z_{opt} exhibits the highest values directly above the Pt atoms. The central Pt atom represents the atop adsorption position, whose z_{opt} value is equal to 1.758 Å. The surface of the O-atom BE is depicted in Fig. 2b. All the BE values are negative, thus the atomic oxygen adsorption is energetically favourable. The adsorption in the atop position is the least exoenergetic with $BE = -0.97\,\mathrm{eV}$ (BSSE-corrected $BE = -0.80\,\mathrm{eV}$). The adsorption in sites between two Pt atoms is much more probable.

Intuitively, when an oxygen atom is close to a metal surface, one expects metal electrons to flow to the electronegative oxygen creating a negative charge on it. It is confirmed by the Mulliken's electron population analysis as presented in Fig. 2c. This figure shows that electronic charge is transferred from the $Pt_5(001)$ cluster to the adsorbate. The same behaviour was observed by Li and Balbuena [48] for the small platinum clusters of gas-phase geometries which interacted with oxygen. The electronic charge is moved from the platinum d orbitals to the oxygen p orbitals. As displayed in Fig. 2c, $q_m(\mathrm{O}) = -0.646\,\mathrm{e}$ on the O-atom adsorbed in the atop site.

The electronic charge of the O atom can be connected with the catalytic reactivity of platinum in some organic processes which occur in the presence of oxygen. According to the Brönsted acid-base formalism, the adsorbed O atom which exhibits a negative atomic charge acts as a strong Brönsted base. Therefore, it can abstract easily a proton from other reactant molecule on the catalyst surface, as it is observed for the dehydrogenation of cyclohexane [49].

The z_{opt}, BE and $q_m(\mathrm{O})$ of the O atom on the $Pt_{4+1}(001)$ cluster are presented in Figs. 3a, 3b and 3c respectively. The adsorption position in the centre of the cluster corresponds to the hollow site and the atomic oxygen is bound in this site at $z_{\mathrm{opt}} = 0.896\,\text{Å}$. The calculations of the O-atom BE have been performed for the singlet multiplicity of the $OPt_{4+1}(001)$ system. In the hollow site, the BE value is equal to $-0.78\,\mathrm{eV}$ (BSSE-corrected $BE = -0.62\,\mathrm{eV}$), which is rather far from the experimental result of ca. $-2.40\,\mathrm{eV}$ for Pt(001) [50]. The transfer of electronic charge in this site exceeds one electron, $q_m(\mathrm{O}) = -1.131\,\mathrm{e}$.

It is interesting to investigate the influence of the $OPt_{4+1}(001)$ multiplicity on the O atom properties. A variety of possible multiplicities originates from the complex electronic structure of Pt. The properties of the O atom adsorbed on the $Pt_{4+1}(001)$ cluster and obtained for five different multiplicities of $OPt_{4+1}(001)$ are collected in Tab. 1. For all the multiplicities, high spin contamination has not been detected. The multiplicities affect strongly the z_{opt} values. The nonet exhibits the z_{opt} value quite close to the experimental oxygen-surface distance for Pt(111); there is no referential result for Pt(001). The higher the O atom adsorbs, the smaller electronic-charge transfer from the cluster to the adsorbate is observed. For all the multiplicities, the

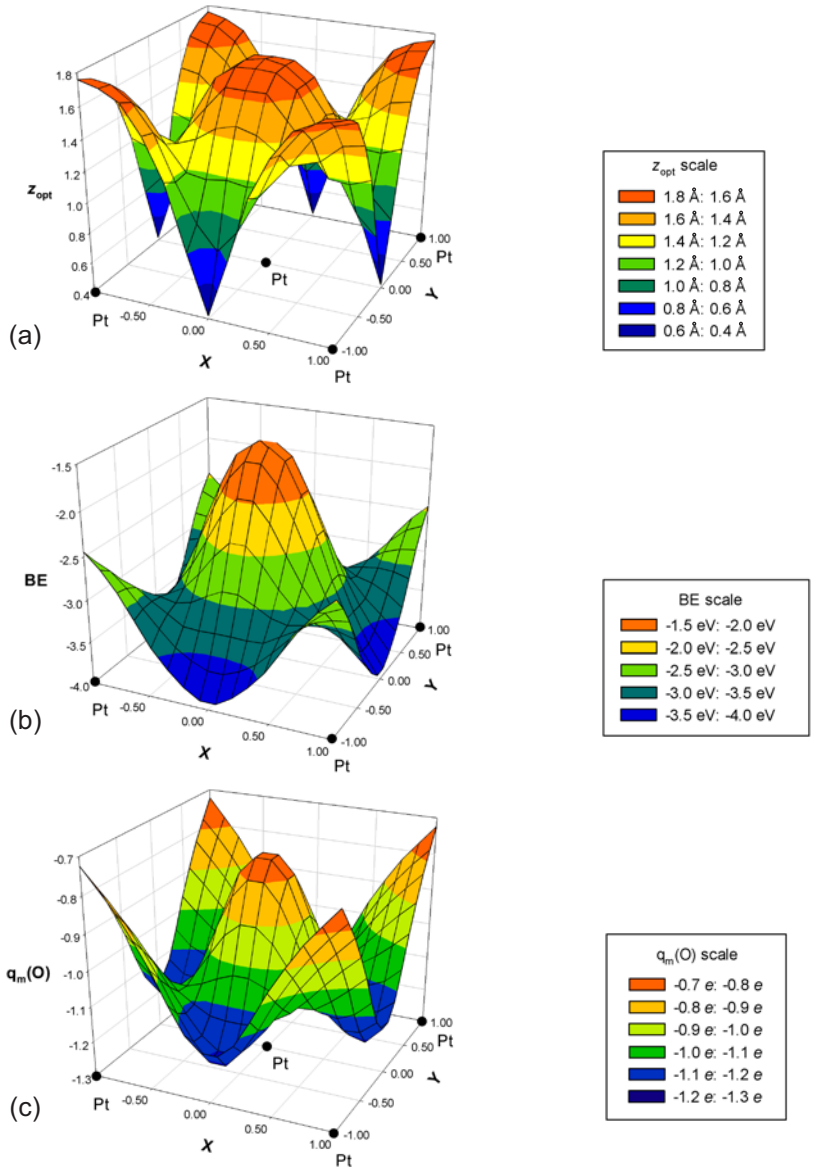

Fig. 2: Properties of the O atom adsorbed on the $Pt_5(001)$ cluster. Surface plots of the values of the O atom: (a) height z_{opt} above the cluster plane, (b) binding energy BE on the cluster and (c) Mulliken's electronic charge $q_m(\mathrm{O})$. For the sake of simplicity, the scale on the OX and OY axes of all the plots have the range of two units (they are equal to the Pt lattice constant, 3.9242 Å [47]).

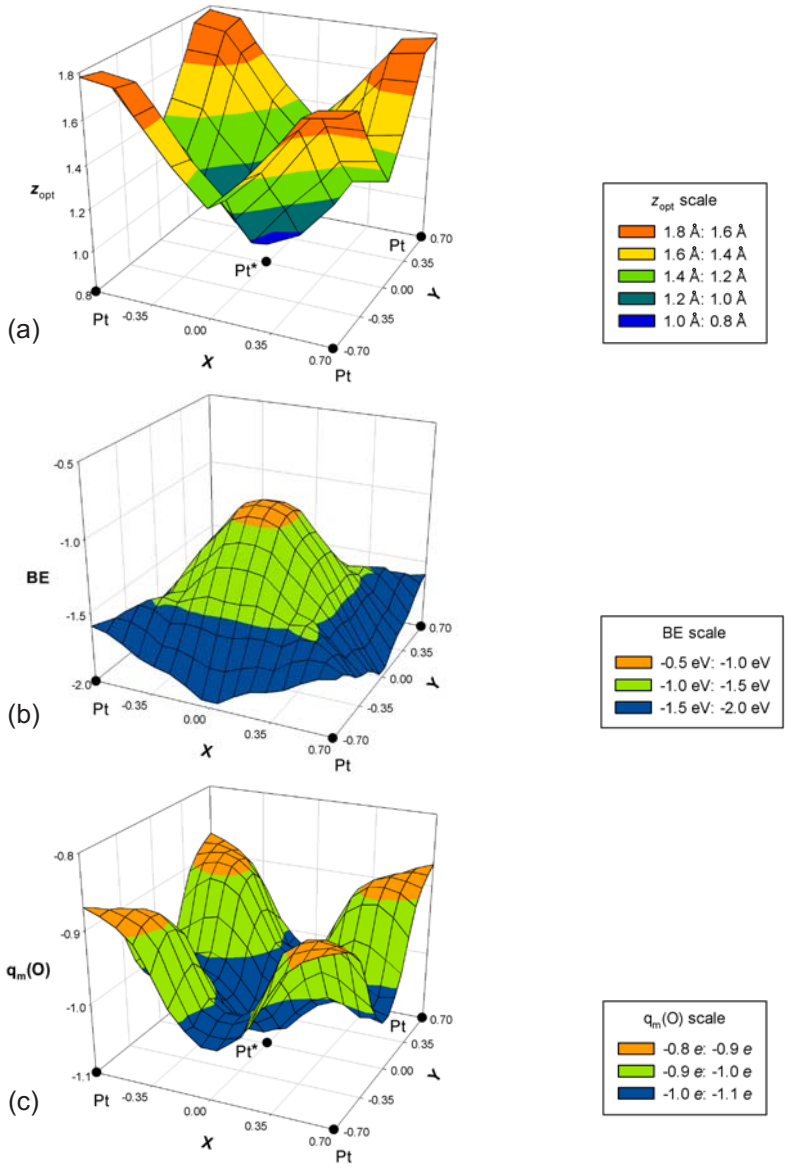

Fig. 3: Properties of the O atom adsorbed on the $Pt_{4+1}(001)$ cluster. Surface plots of the values of the O atom: (a) height $z_{\rm opt}$ above the cluster plane, (b) binding energy BE on the cluster and (c) Mulliken's electronic charge $q_m(\mathrm{O})$. For the sake of simplicity, the scale on the OX and OY axes of all the plots have the range of $[-0.70, 0.70]$ proportionally to the range used in Fig. 2. The subsurface Pt atom is marked with an asterisk.

Tab. 1: Height z_{opt}, BSSE-corrected binding energy BE, and electronic charge $q_m(\mathrm{O})$ of the O atom adsorbed on the $\mathrm{Pt}_{4+1}(001)$ cluster for five multiplicities of the $\mathrm{OPt}_{4+1}(001)$ system.

Multiplicity	z_{opt} [Å]	BSSE-corrected BE [eV]	$q_m(\mathrm{O})$ [e]
1	0.896	−0.62	−1.131
3	0.902	−1.28	−1.163
5	0.997	−0.77	−0.999
7	1.155	−1.21	−0.768
9	1.337	−1.06	−0.467

calculated BSSE-corrected BE of the O atom remains far from the experimental value. It unambiguously results from the small number of Pt atoms used in the cluster. A significant variation of the BE values, as a function of cluster size, was found by Lin et al. [26].

4. Conclusions

The adsorption of atomic oxygen on Pt(001) has been investigated by means of the B3LYP hybrid functional. The Pt(001) surface has been modelled by two five-atom clusters of planar and pyramidal geometries. The adsorption of the O atom on the clusters is exoenergetic both for the hollow site and the atop position. The Mulliken's electron population analysis reveals a significant electronic-charge transfer from the cluster to the adsorbate. It indicates that the adsorbed O atom acts as a strong Brönsted base in the catalytic reactions on the Pt(001) surface.

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ADSORPCJA ATOMOWEGO TLENU NA Pt(001). BADANIA W RAMACH TEORII FUNKCJONAŁÓW GĘSTOŚCI

S t r e s z c z e n i e

W pracy prezentowane są wstępne wyniki obliczeń prowadzonych w ramach teorii funkcjonałów gęstości (DFT) dla adsorpcji atomowego tlenu na Pt(001). Powierzchnia Pt(001) modelowana jest za pomocą dwóch pięcioatomowych klasterów o planarnej i piramidalnej geometrii. Własności strukturalne, energetyczne i elektronowe zaadsorbowanego atomu tlenu zostały określone w celu zbadania oddziaływania między atomowym adsorbatem i powierzchnią Pt(001).

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Piotr Matczak

GEOMETRIES AND ENERGETICS OF Pd_2, Pt_2, Ag_2, AND Au_2 DIMERS. A BENCHMARK OF NONLOCAL AND HYBRID DENSITY FUNCTIONALS

Summary

In this work the comparison of the calculated bond lengths, dissociation energies and harmonic vibrational frequencies of four dimers (Pd_2, Pt_2, Ag_2, Au_2), together with the experimental data is presented. All calculations have been performed by means of a series of nonlocal and hybrid density functionals combined with the LANL2DZ basis set. The comparison leads to the conclusion that the BP86, G96P86, B3P86 and BH&H functionals, in conjunction with LANL2DZ, are superior to the other functionals. The G96P86 and B3P86 functionals are recommended for the reliable predictions of both geometric as well as energetic properties of the Pd-, Pt-, Ag- and Au-containing systems, while BP86 rather for energetic properties and BH&H only for the extremely accurate determination of the geometries. The geometries and energetics of some excited states of the dimers have also been computed using these four selected functionals.

1. Introduction

Palladium and platinum are considered to be two of the most important metals in heterogeneous catalysis because of their rich catalytic power [1, 2]. These metals are particularly useful for the reactions involving H_2. They also find an application as efficient catalysts in automotive exhaust systems where they reduce toxic pollutants such as CO, NO and hydrocarbons. On the contrary, silver and gold are stable and inactive in the reactions with H_2, although they are located next to Pd and Pt in the Periodic Table [3–6]. In the last two decades, bimetallic catalysts have attracted much attention [7–9] despite the fact that they have been known since the 1960s [10–12]. The combination of neighbouring metals, e.g. PdAg, PdAu, PtAg and PtAu, leads to the catalysts which have new properties different from pure Pd, Pt,

Ag and Au metals alone. The bimetallic catalysts exhibit unique selectivity in the reactions involving H_2.

Among various forms of metallic heterogeneous catalysts, clusters have been in the centre of considerable attention in recent years because they offer the improvement in catalytic activity, selectivity and stability in comparison with the corresponding metallic bulk [13–15]. Moreover, the clusters which consist of only a few metal atoms exhibit extreme reactivity due to their non-saturated valence. Clusters of various sizes can be generated in a molecular beam using laser-vaporization techniques. However, detailed spectroscopic investigations are possible mostly for the smallest metallic clusters such as dimers and trimers. A few experimental works have been addressed to the investigations on the Pd_2 [16, 17], Pt_2 [18–21], Ag_2 [22–24] and Au_2 [25] dimers. Some older works on these dimers have been presented in the review by Morse [26].

A large number of theoretical studies have been devoted to Pd_2 [27–32], Pt_2 [28, 31, 33–37], Ag_2 [31, 38–46] and Au_2 [28, 31, 36, 37, 39, 45–51]. On the quantum-chemical side, metallic dimers are quite interesting since they are the simplest systems with a metal-metal bond. The description of the interaction between the atoms of the dimers seems to be particularly challenging due to:

- the large number of electrons,
- correlation effects,
- relativistic effects,
- the existence of several electronic molecular states with different spin multiplicities and geometries.

The relativistic effects such as mass-velocity, Darwin and spin-orbit corrections make substantial contributions to the interaction in the heavy-metal dimers, Pt_2 and Au_2.

The Pd_2, Pt_2, Ag_2 and Au_2 dimers have been investigated by means of a variety of computational methods. Examples of the methods used in recent studies include embedded-atom model (EAM) [35], tight-binding molecular dynamics (TBMD) [43], Möller-Plesset (MP) perturbation theory [31], Douglas-Kroll-Hess (DKH) coupled-cluster method [51] and density functional theory (DFT) within the relativistic [46] as well as nonrelativistic [31, 32, 36, 37, 44, 45] schemes. Nonrelativistic DFT generally provides a very good balance between accuracy and computational cost and, as a consequence, the majority of the studies have been carried out within the framework of this method, spanning various nonlocal [32, 36, 37, 44, 45] and hybrid [31] density functionals. However, it is not clear which combination of the exchange and correlation components of nonlocal and hybrid functionals is most appropriate for the investigation of the metallic dimers.

In this work the Pd_2, Pt_2, Ag_2 and Au_2 dimers are examined within twelve nonlocal and seven hybrid density functionals to establish the best ones for the calculations of the geometric and energetic properties of these dimers. In particular, a proper and careful choice of the functionals is needed for the future study of

bimetallic molecules (PdAg, PdAu, PtAg and PtAu) to elucidate their catalytic activity, selectivity and stability. The search for the best combinations of the exchange and correlation components in the density functionals is based on the comparison of the calculated bond lengths, r_e, dissociation energies, D_0, and harmonic vibrational frequencies, ω_e, with the corresponding experimental data.

2. Method

DFT methods, as implemented in Gaussian 98 package [52], have been used for the calculations of r_e, D_0 and ω_e for the Pd_2, Pt_2, Ag_2 and Au_2 dimers. The nonlocal density functionals included in this work are: BLYP, BP86, BPW91, PW91LYP, PW91P86, PW91PW91, MPWLYP, MPWP86, MPWPW91, G96LYP, G96P86 and G96PW91. The list of hybrid density functionals encompasses seven representatives, which are the functionals pre-defined in Gaussian 98: B1LYP, B3LYP, B3P86, B3PW91, BH&H, BH&HLYP and MPW1PW91. All the abbreviations above are explained in the Gaussian 98 help files [52], also available via the Internet [53].

In regards to basis set, the effective core potential (ECP) of Hay and Wadt in conjunction with the valence double-zeta Gaussian-type orbitals (GTO) has been employed [54–56]. This basis set is commonly denoted as the Los Alamos National Laboratory double-zeta (LANL2DZ). ECPs are often used to describe heavy atoms such as Pd, Pt, Ag and Au [36, 37]. The replacement of core electrons with an energy potential, termed as a pseudopotential, reduces significantly computational cost. In the case of the LANL2DZ basis set only the innermost core electrons are assigned to the ECP. Forty-six and sixty innermost core electrons are replaced by the ECP for the fourth-row (Pd, Ag) and fifth-row (Pt, Au) metals respectively. The mass-velocity and Darwin relativistic effects are also incorporated into the ECP. The outer core electrons, ns^2np^6, and the valence electrons, $nd^q(n+1)s^r$, are treated explicitly.

The r_e values of the dimers are obtained by gas-phase geometry optimizations using a standard gradient technique with a tight convergence criterion. For the optimized bond lengths the harmonic vibrational frequencies are calculated as the second-order derivatives of total energy with respect to the atomic coordinates (Hessian). Later, for Pd_2, Pt_2, Ag_2 and Au_2, the dissociation energies are determined and the following dissociation limits are taken into account: ^1S for palladium (^1S arises from the $4d^{10}$ electronic configuration), ^3D for platinum ($5d^96s^1$), and ^2S for silver ($4d^{10}5s^1$) as well as gold ($5d^{10}6s^1$). The basis-set superposition error (BSSE) correction [57] and the zero-point energy (ZPE) are incorporated into the D_0 values.

3. Results and discussion

In order to assess the ability of various nonlocal and hybrid density functionals (combined with the LANL2DZ basis set) to predict the geometries and energetics of the Pd_2, Pt_2, Ag_2 and Au_2 dimers accurately, the calculated r_e, D_0 and ω_e have

been compared with the corresponding experimental data (see Table 1). The r_e, D_0 and ω_e values that are used for the comparison have been calculated for the dimers in their electronic ground states. For Pd_2 and Pt_2, four electronic molecular states have been taken into consideration, while for Ag_2 and Au_2 only two due to their relatively simple electronic configurations (the occupied d shells). The investigated electronic states of the dimers, together with the corresponding configurations of the valence electrons, are presented in Table 2. All the molecular states shown in this table have been examined by means of a series of the nineteen density functionals (twelve nonlocal plus seven hybrid). For the sake of brevity, only the results which have been computed by some selected density functionals are reported further in the text and tables. For each dimer the ground state is ascribed to the state of the lowest total electronic energy whose value has been obtained from the geometry optimization. The $^3\sum_u^+$ state is predicted to be the ground state of the Pd_2 dimer. In the case of Pt_2, all the functionals establish the ground state as $^3\sum_g^-(\pi\pi)$. Ag_2 and Au_2 exhibit the same singlet ground state, namely the $^1\sum_g^+$ one.

Tab. 1: Experimental bond lengths, r_e, dissociation energies, D_0, and harmonic vibrational frequencies, ω_e, of Pd_2, Pt_2, Ag_2 and Au_2.

Dimer	r_e [Å]	D_0 [eV]	ω_e [cm^{-1}]
Pd_2	2.48 [58]	1.03 [16]	210.0 [17]
Pt_2	2.333 [18]	3.14 [19]	222.5 [20]
Ag_2	2.530 [22]	1.65 [26]	192.4 [58]
Au_2	2.472 [58]	2.29 [58]	190.9 [58]

It is desirable to focus on some details of the statistical approach used to assess the precision of the functionals. To compare the calculated r_e, D_0 and ω_e with the corresponding experimental values, the standard deviations in the bond lengths, $\sigma(r_e)$, the dissociation energies, $\sigma(D_0)$, and the harmonic vibrational frequencies, $\sigma(\omega_e)$, have been determined for each functional. The standard deviations are defined below:

$$\sigma(r_e) = \sqrt{\frac{\sum_{i=1}^{n}\left(r_{e,i}^{\mathrm{calcd}} - r_{e,i}^{\mathrm{exptl}}\right)^2}{(n-1)}}, \tag{1}$$

$$\sigma(D_0) = \sqrt{\frac{\sum_{i=1}^{n}\left(D_{0,i}^{\mathrm{calcd}} - D_{0,i}^{\mathrm{exptl}}\right)^2}{(n-1)}}, \tag{2}$$

$$\sigma(\omega_e) = \sqrt{\frac{\sum_{i=1}^{n}\left(\omega_{e,i}^{\mathrm{calcd}} - \omega_{e,i}^{\mathrm{exptl}}\right)^2}{(n-1)}}, \tag{3}$$

Tab. 2: Electronic configurations of the investigated molecular states of Pd_2, Pt_2, Ag_2 and Au_2.

Dimer	State	Configuration[(1)]
Pd_2	$^1\sum_g^+$	$1\sigma_g^2 1\sigma_u^2 2\sigma_g^2 2\sigma_u^2 3\sigma_g^2 3\sigma_u^2 1\pi_u^4 1\pi_g^4 2\pi_u^4 2\pi_g^4 1\delta_g^4 1\delta_u^4$
	$^3\sum_u^+$	$1\sigma_g^2 1\sigma_u^2 2\sigma_g^2 2\sigma_u^2 3\sigma_g^2 3\sigma_u^1 4\sigma_g^1 1\pi_u^4 1\pi_g^4 2\pi_u^4 2\pi_g^4 1\delta_g^4 1\delta_u^4$
	$^3\sum_g^-(\pi\pi)$	$1\sigma_g^2 1\sigma_u^2 2\sigma_g^2 2\sigma_u^2 3\sigma_g^2 3\sigma_u^2 4\sigma_g^2 1\pi_u^4 1\pi_g^4 2\pi_u^4 2\pi_g^2 1\delta_g^4 1\delta_u^4$
	$^3\sum_g^-(\delta\delta)$	$1\sigma_g^2 1\sigma_u^2 2\sigma_g^2 2\sigma_u^2 3\sigma_g^2 3\sigma_u^2 4\sigma_g^2 1\pi_u^4 1\pi_g^4 2\pi_u^4 2\pi_g^4 1\delta_g^4 1\delta_u^2$
Pt_2	$^1\sum_g^+$	$1\sigma_g^2 1\sigma_u^2 2\sigma_g^2 2\sigma_u^2 3\sigma_g^2 3\sigma_u^2 1\pi_u^4 1\pi_g^4 2\pi_u^4 2\pi_g^4 1\delta_g^4 1\delta_u^4$
	$^3\sum_u^+$	$1\sigma_g^2 1\sigma_u^2 2\sigma_g^2 2\sigma_u^2 3\sigma_g^2 3\sigma_u^1 4\sigma_g^1 1\pi_u^4 1\pi_g^4 2\pi_u^4 2\pi_g^4 1\delta_g^4 1\delta_u^4$
	$^3\sum_g^-(\pi\pi)$	$1\sigma_g^2 1\sigma_u^2 2\sigma_g^2 2\sigma_u^2 3\sigma_g^2 3\sigma_u^2 4\sigma_g^2 1\pi_u^4 1\pi_g^4 2\pi_u^4 2\pi_g^2 1\delta_g^4 1\delta_u^4$
	$^3\sum_g^-(\delta\delta)$	$1\sigma_g^2 1\sigma_u^2 2\sigma_g^2 2\sigma_u^2 3\sigma_g^2 3\sigma_u^2 4\sigma_g^2 1\pi_u^4 1\pi_g^4 2\pi_u^4 2\pi_g^4 1\delta_g^4 1\delta_u^2$
Ag_2	$^1\sum_g^+$	$1\sigma_g^2 1\sigma_u^2 2\sigma_g^2 2\sigma_u^2 3\sigma_g^2 3\sigma_u^2 4\sigma_g^2 1\pi_u^4 1\pi_g^4 2\pi_u^4 2\pi_g^4 1\delta_g^4 1\delta_u^4$
	$^3\sum_u^+$	$1\sigma_g^2 1\sigma_u^2 2\sigma_g^2 2\sigma_u^2 3\sigma_g^2 3\sigma_u^2 4\sigma_g^1 4\sigma_u^1 1\pi_u^4 1\pi_g^4 2\pi_u^4 2\pi_g^4 1\delta_g^4 1\delta_u^4$
Au_2	$^1\sum_g^+$	$1\sigma_g^2 1\sigma_u^2 2\sigma_g^2 2\sigma_u^2 3\sigma_g^2 3\sigma_u^2 4\sigma_g^2 1\pi_u^4 1\pi_g^4 2\pi_u^4 2\pi_g^4 1\delta_g^4 1\delta_u^4$
	$^3\sum_u^+$	$1\sigma_g^2 1\sigma_u^2 2\sigma_g^2 2\sigma_u^2 3\sigma_g^2 3\sigma_u^2 4\sigma_g^1 4\sigma_u^1 1\pi_u^4 1\pi_g^4 2\pi_u^4 2\pi_g^4 1\delta_g^4 1\delta_u^4$

[(1)] configurations of the valence electrons, which are not incorporated into the ECP.

where n denotes the number of the dimers, $n = 4$, and the upper right indices, namely "calcd" and "exptl", stand for the calculated and experimental values respectively. Table 3 lists the standard deviations in r_e, D_0 and ω_e for the twelve nonlocal and seven hybrid density functionals.

As shown in Table 3, $\sigma(r_e)$ ranges from 0.029 to 0.098 Å. The minimal $\sigma(r_e)$ is assigned to the BH&H hybrid functional. Considering only the nonlocal functionals, the G96P86 one turns out most accurate for the prediction of the geometries of Pd_2, Pt_2, Ag_2 and Au_2. In the case of $\sigma(D_0)$, the nonlocal functionals yield results closer to the experiment than those of the hybrid functionals. For the nonlocal density functionals, the majority of the $\sigma(D_0)$ values is clustered around 0.24 eV. The same lowest value of $\sigma(D_0)$ is given by three nonlocal functionals, namely BP86, MPWLYP and MPWPW91. Among the hybrid functionals, B3P86 exhibits the best accuracy (the smallest value of the $\sigma(D_0)$). BH&H, which has described excellently the geometries of the dimers, is less appropriate for the prediction of energetics. The $\sigma(D_0)$ obtained by means of this functional exceeds the $\sigma(D_0)$ of BP86 by over 150 %. For the nonlocal functionals the standard deviations of ω_e range from 13.6 to 23.5 cm^{-1}, with most around 14 cm^{-1}. The hybrid density functionals provide

Tab. 3: Standard deviations in bond lengths, $\sigma(r_e)$, dissociation energies, $\sigma(D_0)$, and harmonic vibrational frequencies, $\sigma(\omega_e)$, of Pd_2, Pt_2, Ag_2 and Au_2.

Functional	$\sigma(r_e)$ [Å]	$\sigma(D_0)$ [eV]	$\sigma(\omega_e)$ [cm^{-1}]
BLYP	0.098	0.24	23.5
BP86	0.059	0.22	14.4
BPW91	0.063	0.24	15.6
PW91LYP	0.093	0.23	21.8
PW91P86	0.055	0.32	13.6
PW91PW91	0.059	0.25	14.5
MPWLYP	0.096	0.22	22.8
MPWP86	0.058	0.25	14.0
MPWPW91	0.062	0.22	15.2
G96LYP	0.082	0.32	20.0
G96P86	0.045	0.24	14.1
G96PW91	0.048	0.31	14.4
B1LYP	0.090	0.65	21.8
B3LYP	0.083	0.51	20.3
B3P86	0.049	0.36	17.4
B3PW91	0.058	0.48	17.8
BH&H	0.029	0.56	27.8
BH&HLYP	0.087	1.15	24.4
MPW1PW91	0.057	0.53	18.9

Tab. 4: Electronic transition energies, T_e, bond lengths, r_e, and harmonic vibrational frequencies, ω_e, for the low-lying molecular states of Pd_2 at the BP86, G96P86, B3P86 and BH&H levels. For the ground state, dissociation energies, D_0, also displayed.

Functional	$^3\sum_u^+$				$^1\sum_g^+$		
	T_e [cm^{-1}]	r_e [Å]	ω_e [cm^{-1}]	D_0 [eV]	T_e [cm^{-1}]	r_e [Å]	ω_e [cm^{-1}]
BP86	0	2.504	208.7	1.22	3023	2.700	154.5
G96P86	0	2.492	212.4	1.09	2895	2.690	155.5
B3P86	0	2.494	215.4	0.83	2524	2.725	138.6
BH&H	0	2.477	226.4	0.81	2727	2.720	135.8
	$^3\sum_g^-(\pi\pi)$				$^3\sum_g^-(\delta\delta)$		
BP86	5028	2.387	254.0	–	13458	2.517	207.5
G96P86	5663	2.375	259.4	–	14359	2.502	212.1
B3P86	8776	2.357	271.2	–	19349	2.491	219.5
BH&H	11700	2.311	302.1	–	25332	2.441	246.9

the worse accuracy of the calculated ω_e values than the nonlocal functionals. Such a behaviour is similar to that observed for the $\sigma(D_0)$ values. B3P86 exhibits one more time the lowest $\sigma(\omega_e)$ among the seven hybrid functionals. Taking all the nineteen density functionals into account, one can notice that the use of the Lee-Yang-Parr's formulation of electronic correlation causes an increase of $\sigma(\omega_e)$.

Tab. 5: The same as in Table 4 but for Pt_2.

Functional	$^3\sum_g^-(\pi\pi)$				$^3\sum_g^-(\delta\delta)$		
	T_e [cm^{-1}]	r_e [Å]	ω_e [cm^{-1}]	D_0 [eV]	T_e [cm^{-1}]	r_e [Å]	ω_e [cm^{-1}]
BP86	0	2.372	232.3	3.33	6781	2.465	202.4
G96P86	0	2.362	237.5	3.28	7026	2.453	206.3
B3P86	0	2.352	246.4	2.70	9408	2.445	212.0
BH&H	0	2.325	267.3	2.22	12587	2.413	231.3
	$^3\sum_u^+$				$^1\sum_g^+$		
BP86	7646	2.523	187.3	–	16767	2.670	153.5
G96P86	7583	2.511	191.6	–	16851	2.656	156.2
B3P86	4388	2.520	189.3	–	17400	2.654	157.1
BH&H	1042	2.515	193.4	–	19280	2.648	154.9

Tab. 6: The same as in Table 4 but for Ag_2.

Functional	$^1\sum_g^+$				$^3\sum_u^+$		
	T_e [cm^{-1}]	r_e [Å]	ω_e [cm^{-1}]	D_0 [eV]	T_e [cm^{-1}]	r_e [Å]	ω_e [cm^{-1}]
BP86	0	2.578	188.4	1.65	13298	3.056	64.6
G96P86	0	2.562	193.7	1.52	12720	3.070	61.2
B3P86	0	2.576	189.7	1.54	12487	3.145	49.3
BH&H	0	2.556	197.9	1.63	12699	3.052	60.0
CI [40]	0	2.620	187.3	1.67	–	3.251	54.6

Tab. 7: The same as in Table 4 but for Au_2.

Functional	$^1\sum_g^+$				$^3\sum_u^+$		
	T_e [cm^{-1}]	r_e [Å]	ω_e [cm^{-1}]	D_0 [eV]	T_e [cm^{-1}]	r_e [Å]	ω_e [cm^{-1}]
BP86	0	2.549	168.4	2.03	14351	2.862	86.3
G96P86	0	2.536	171.9	1.92	14190	2.846	86.8
B3P86	0	2.539	173.5	1.91	14519	2.931	70.9
BH&H	0	2.515	186.9	2.07	15107	2.913	71.5
B3PW91 [49]	0	2.547	–	1.90	14180	2.961	–

To sum up the paragraph above, it is deduced from the statistical approach that, among the nonlocal functionals, the BP86 and G96P86 ones are recommended for the prediction of the geometries and energetics of the Pd_2, Pt_2, Ag_2 and Au_2 dimers. BP86 together with MPWLYP and MPWPW91 exhibit the smallest $\sigma(D_0)$ but, in addition, BP86 yields smaller standard deviations of the geometric and vibrational properties than MPWLYP and MPWPW91. The G96P86 functional reproduces the bond lengths of the dimers very well. In the case of the hybrid functionals, the B3P86

one should be employed for the calculations of D_0 and ω_e. The $\sigma(r_e)$ value obtained by this functional remains only slightly greater than that of G96P86. The BH&H functional computes the bond lengths in excellent agreement with the experiment. However, its $\sigma(D_0)$ and $\sigma(\omega_e)$ indicate a rather poor performance.

The properties of all the investigated electronic molecular states calculated by means of the four selected functionals are presented in Tables 4–7. The dissociation energies have been determined only for the ground states of the dimers. The transition energies, T_e, from the ground state to the excited ones are also displayed in the tables. In the cases of Ag_2 and Au_2, the results are compared with some earlier theoretical investigations [40, 49].

To conclude, the comparison of the standard deviations of the calculated bond lengths, dissociation energies and harmonic vibrational frequencies with respect to the corresponding experimental values shows that the G96P86 and B3P86 density functionals are recommended for the accurate predictions of all these three properties for the Pd_2, Pt_2, Ag_2 and Au_2 dimers. BP86 should be employed for the reliable determination of D_0 and ω_e rather than for r_e, whereas the use of BH&H is limited to extremely accurate calculations of the geometries. These four functionals will be used in the future study of bimetallic molecules such as PdAg, PdAu, PtAg and PtAu.

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GEOMETRIA I WŁASNOŚCI ENERGETYCZNE DIMERÓW Pd_2, Pt_2, Ag_2 I Au_2. TEST PORÓWNAWCZY FUNKCJONAŁÓW NIELOKALNYCH ORAZ HYBRYDOWYCH

S t r e s z c z e n i e

W pracy prezentowane jest porównanie obliczonych długości wiązania, energii dysocjacji oraz harmonicznej częstości drgań czterech dimerów (Pd_2, Pt_2, Ag_2, Au_2) z danymi eksperymentalnymi. Wszystkie obliczenia wykonano za pomocą szeregu funkcjonałów nielokalnych oraz hybrydowych w połączeniu z bazą funkcyjną LANL2DZ. Przeprowadzone porównanie prowadzi do wniosku, że funkcjonały BP86, G96P86, B3P86 i BH&H w połączeniu z bazą LANL2DZ okazują się dokładniejsze od innych. Funkcjonały G96P86 i B3P86 są polecane do dokładnego przewidywania własności geometrycznych i energetycznych układów zawierających Pd, Pt, Ag i Au. Funkcjonał BP86 stosować można raczej tylko do dokładnych obliczeń własności energetycznych a funkcjonał BH&H wyłącznie do określania geometrii z bardzo wysoką dokładnością. Przy pomocy czterech powyższych funkcjonałów wyznaczona została geometria i energetyka niektórych stanów wzbudzonych badanych dimerów.

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