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APPLICATIONS OF THE CATASTROPHE THEORY (CT) IN THE STUDY OF THE SCF THEORY AND METHOD

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abstract: The energetic SCF(selfconsistent field) functionals (the SCF energy(I), the rotational increment of the SCF energy(II) and the rotational gradient of of SCF Lagrange multipliers(III)) are fitted by the catastrophe structures(CSs), allowing applications of the of the catastrophe theory(CT) in the study of the SCF theory and method. Through (I)-(II), in the SCF theory, rise qualitatively distinct problems by CT. They reduce themselves to a unique general problem with the stages: (a) the finding of the polynomial form (I)-(III) possibly to be approximated by the catastrophe potentials(CPs) (or the unfoldings of the catastrophe); (b) the identification of the parameter α of the behaviour(or state) for (a); (c) the inducing of the k-jets and the corresponding CPs; (d) the research of the extremum (minimum) of the critical points of CSs that fit the hypersurfaces (I)-(III); (e) the computation and analysis of the integral quadratic error as a measure of the degree of the fitting of (I)-(III) by the CSs; (f) the interpretation of the general results (a)-(e) by the peculiarity of the SCF problem risen by (I)-(III).

key words: scf theory and method; catastrophe theory; catastrophe structures; catastrophe potentials; scf energy; rotational increment of scf energy; rotational gradient of scf Lagrange multipliers; scf functionals fitted by CSs; parameter α of behaviour (or state); parameters of control; k-jets; hipersurfaces in $S_\alpha \otimes S_c$; integral quadratic error

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1. Introduction

The principal physical-mathematical problems of the **SCF theory (and the method)** applied to the multielectronic quantum systems (atomic, molecular etc.)[1-3,17] are treated by (or connected to) the functionals: the **SCF energy(E_{SCF}) (I)**, the **rotational increment of the SCF energy (ΔE_{SCF}) (II)** and the **rotational gradient of the SCF Lagrange multipliers [$(\Delta e_{ij})_{SCF}$] (III),** the last, at hermiticity, leading to the orbital energies ($\{e_i=-e_{ii}; i=j\}$). The **SCF energetic functionals (I)-(III),** all being dependent on the set of the basic monoelectronic functions (2) (corresponding to the treated quantum electronic system), may be prepared for their approaching by the **Catastrophe Theory(CT)** [9-11]. The structure of this approach is (a)-(f) (see the abstract of this paper) and solves a **unique general**

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problem. The SCF problem as: the computation of the SCF energy and of the the orbital energies $\{e_i\}$, the SCF convergeance [22], the SCF stability and instability, the number of the SCF solutions, the hermiticity of the SCF Lagrange multipliers etc are directly connected to (I)-(III). The approach by the CT will take into account the classic SCF result [1-8,23] and the nonclassic result too, obtained by the first author [18-22].

2. The general polynomial form F_J of the functionals (I)-(III)

The all energetic SCF functionals (I)-(III), in the SCF theory (and the method) [1-4,8,12,13,17] being dependent on the set (2) of the basic monoelectronic functions corresponding to a quantum system with N electrons, may be transformed in polynomial dependences of the type:

$$F_J=f(\alpha,\{c_m^J;\ m=1,2,\ldots n_J\}) \qquad (J\in\{I,II,III\}\equiv J) \tag{1}$$

In (1) α represents the unique parameter of the behaviour (or state) defining the monodimensional space of the behaviour (or state) S_α, and $\{c_m^J\}$ a number n_J ($J\in J$) of the control parameters defining the multidimensional space of the control S_c. The control parameters are dependent on the basic monoelectronic functions:

$$\{|\varphi_i\rangle,\ i=1,2,\ldots N\} \tag{2}$$

In the SCF general and peculiar cases $\{c_m^J\}$ representing the combinations both of atomic and molecular integrals [18-22]. The parameter α is obtained: or (A) after a localisation of the representative quantum state point $\Psi(\{|\varphi_i\rangle\})$ (Ψ – the wave function of the quantum system) on the sphere of the normalization [7,18], if J=I; or (B) after a unitary transformation of the type 2x2 [5,6] plane rotation [16] of the pairs of the functions (2), if J=II and J=III [19-21].

2.1. The polynomial form F_I

The SCF functional of the energy, $E_{SCF}(I)$, dependent on (2), by Ψ, we consider it of the same form [7,18]:

$$E_{SCF}=E_1\sin 2\alpha+E_2\cos 2\alpha+E_3\sin\alpha+E_4\cos\alpha+E_5 \tag{1´}$$

Corresponding to a helium-like quantum system treated in the multiconfigurational SCF(MC-SCF) variant. The parameter α, in the case (A), allows the rewriting of (1´):

$$F_I\equiv E_{SCF}=c_1^I x^2+c_2^I xy+c_3^I x+c_4^I y+c_5^I \tag{1$_I$}$$

with $\{c_m^I;\ m=1,2,\ldots 5\}$ combinations of the SCF energy coefficients ($\{E_i;\ i=1,2,\ldots 5\}$) [18] and

$$x=\sin\alpha;\ y=(1-x^2)^2\ (\alpha\in[-\pi;\pi]\text{ or }x\in[-1;1]) \tag{3}$$

2.2. The polynomial form F_{II}

The SCF energy rotational increment, ΔE_{SCF} (II), dependent also on (2) may be obtained applying the pairs of the functions $\{|\varphi_i\rangle, |\varphi_j\rangle\}$ a 2x2 [5,6] plane rotation [16] of the angle α. The general form of ΔE_{SCF} is formally obtained the same: either by generalising [19,20] the

peculiar expressions ΔE_{SCF} (atomic [4,8] and molecular [14,15]), or by starting from the general expression of the SCF functional (I) [21]. For a multielectronic system of the closed shell type in the MC-SCF variant, (II) has the condensed form:

$$F_{II}\equiv\Delta E_{SCF}=c_1^{II}x^4+c_2^{II}x^3y+c_3^{II}x^2+c_4^{II}xy+c_5^{II} \qquad (1_{II})$$

with $\{c_m^{II};\ m=1,2,\ldots5\}$ specified in [19,20], x and y defined by (3), but with α newly specified (B). The formal difference between (1_{II}) obtained in [18] and the one obtained in [19,20] is $c_5^{II}=0$ in [18], nonsignificant in the general treating by the CT of (1_{II}).

2.3. The polynomial form F_{III}

The rotational gradient of the SCF Lagrange multipliers, $(\Delta e_{ij})_{SCF}$(III), obtained as (II) also by a 2x2 plane rotation of α angle (B), according to [12], has a complicated mathematical expression that in the condensed form is the simple polynomial [21]:

$$F_{III}\equiv(\Delta e_{ij})_{SCF}=c_1^{III}x^2+c_2^{III}xy+c_3^{III}x+c_4^{III}y+c_5^{III} \qquad (1_{III})$$

The coefficients $\{c_m^{III};\ m=1,2,\ldots5\}$ from (1_{III}) have the explicit expressions given in [21], x and y defined by (3) and α newly specified for J=III. From (1_I) and (1_{III}) we notice the formal identity of the polynomial dependences E_{SCF} and $(\Delta e_{ij})_{SCF}$ a significant fact for (I) and (III) which represent SCF energies: (I) the SCF total energy, respectively (III) the SCF orbital energies (at the accomplishment of the hermitian condition of the SCF lagrange multipliers). This formal identity makes (1_I) and (1_{III}), in this application of the CT, to appear directly as a unique problem. For the increment ΔE_{SCF}, the appearance of the terms of 3rd degree, respectively 4th degree in x is significant, contributing to the qualitative separation of (II) from (I) and (III), even when we will apply the CT at the fitting of the hypersurfaces (1_J) $(J\in J)$ by the CSs.

2.4. The general polynomial form F_J

The dependences, formally identical (1_I) and (1_{III}), may appear in fact as the peculiar cases of a polynomial dependence generalising (1_{II}):

$$F_J=f(\alpha,\{C_m^J;\ m=1,2,\ldots7\})=C_1^Jx^4+C_2^Jx^3y+C_3^Jx^2+C_4^Jxy+C_5^Jx+C_6^Jy+C_7^J \qquad (4)$$

from which (1_I) and (1_{III}) are easily obtained by:

$$C_1^J=C_2^J=0\ (J=I,\ III) \qquad (4')$$

and for (1_{II}):

$$C_6^J=C_7^J=0\ (J=II) \qquad (4'')$$

In a multidimensional space $S_\alpha\otimes S_c$, (4) represents a hypersurface whose topological behaviour may be fitted by the CSs, if (4) (or (1_J) $(J\in J)$) is approximated by the catastrophe potentials (CPs) (or the unfoldings of the catastrophe). Because the behaviour (or α state) parameter α defined by (3) and (A) or (B) is unique,

$$\mathrm{Corank}(F_J)=1\ (J\in J) \qquad (4''')$$

all the CSs which will fit (4) (or (1_J) $(J\in J)$) will be of the cuspoid type [9-11] (see index).

3. The application of the CT through the fitting of the energetic SCF functionals (I)-(III) by the CSs

Aiming the application of the CT [9-11] at the nonclassic study of the classic SCF theory and method, one will proceed to the fitting of the functionals (I)-(III) (with analytical explicit forms (1_J) ($J \in J$)) of the generalized form by eliminating the upper index "J" from (4), resulting:

$$F_J=f(\alpha,\{C_m;\ m=1,2,\ldots 7\})=C_1x^4+C_2x^3y+C_3x^2+C_4xy+C_5x+C_6y+C_7 \quad (5)$$

3.1. The induction of k-jets $F_J^{(k)}$ ((k)=2n(n=0; 1,2,3))

If we take into account the definition (3) of the behaviour (or state) parameter α and we develop y in the Taylor series [9-11]:

$$y=(1-x^2)^{1/2}=1-(0.5x^2+2^{-3}x^4+2^{-4}x^6+\ldots) \quad (6)$$

then (5) leads to the k-jets of the orders (k)=2n(n=0; 1,2,3), if we cut off the expression (6) from the term in x^8:

$$F_J^{(0)}=a_J^{(0)}x^4+b_J^{(0)}x^3+c_J^{(0)}x^2+d_J^{(0)}x+e_J^{(0)} \quad (7)$$

where $$a_J^{(0)}=C_1,\ b_J^{(0)}=C_2,\ c_J^{(0)}=C_3,\ d_J^{(0)}=C_4+C_5,\ e_J^{(0)}=C_6+C_7 \quad (7')$$

$$F_J^{(2)}=a_J^{(2)}x^5+b_J^{(2)}x^4+c_J^{(2)}x^3+d_J^{(2)}x^2+e_J^{(2)}x+f_J^{(2)} \quad (8)$$

where $a_J^{(2)}=-0.5\ b_J^{(0)}$, $b_J^{(2)}=a_J^{(0)}$, $c_J^{(2)}=C_2-0.5C_4$, $d_J^{(2)}=C_3-0.5C_6$, $e_J^{(2)}=d_J^{(0)}$ and $f_J^{(2)}=e_J^{(0)}$ (8′)

$$F_J^{(4)}=a_J^{(4)}x^7+b_J^{(4)}x^5+c_J^{(4)}x^4+d_J^{(4)}x^3+e_J^{(4)}x^2+f_J^{(4)}x+g_J^{(4)} \quad (9)$$

where $$a_J^{(4)}=-2^{-3}b_J^{(0)},\ b_J^{(4)}=-0.5(C_2+2^{-2}C_4),\ c_J^{(4)}=C_1-2^{-3}C_6,$$

$$d_J^{(4)}=c_J^{(2)},\ e_J^{(4)}=d_J^{(2)},\ f_J^{(4)}=d_J^{(0)} \text{ and } g_J^{(4)}=e_J^{(0)} \quad (9')$$

and $$F_J^{(6)}=a_J^{(6)}x^9+b_J^{(6)}x^7+c_J^{(6)}x^6+d_J^{(6)}x^5+e_J^{(6)}x^4+f_J^{(6)}x^3+g_J^{(6)}x^2+h_J^{(6)}x+i_J^{(6)} \quad (10)$$

where $$a_J^{(6)}=-2^{-4}b_J^{(0)},\ b_J^{(6)}=2^{-2}b_J^{(4)},\ c_J^{(6)}=-2^{-4}C_6,\ d_J^{(6)}=b_J^{(4)},$$

$$e_J^{(6)}=c_J^{(4)},\ f_J^{(6)}=c_J^{(2)},\ g_J^{(6)}=d_J^{(2)},\ h_J^{(6)}=d_J^{(0)} \text{ and } i_J^{(6)}=e_J^{(0)} \quad (10')$$

3.2. The catastrophe potentials (CPs) corresponding to the k-jets $F_J^{(k)}$

In order to put into evidence the catastrophe potentials (CPs) (or the unfoldings of the catastrophe), the k-jets of the zero order (7) and the two order (8) need a change of the variable, while the fourth order k-jets (9) and the sixth order (10) lead directly to the CPs searched through the fitting of the hypersurface (5) (or (4)) by the CSs.

3.2.1. The simple cusp CP

By performing the change of the variable:

$$x=z-b_J^{(0)}/4a_J^{(0)}=-z-C_2/4C_1 \quad (11)$$

the k-jet of the zero order (7) leads to the simple cusp CP [9] (see index):

$$V_{sc}=a_{sc}z^4+b_{sc}z^2+c_{sc}z+d_{sc} \quad (12)$$

where the control parameters a_{sc}, b_{sc}, c_{sc} and d_{sc} could be easily identified if one substitutes (11) in (7) and identifies, respectively z-the behaviour (or state) parameter.

3.2.2. The swallowtail CP

By the change of t he variable:

$$x=z-b_J^{(2)}/5a_J^{(2)}=z+(2/5)C_1/C_2 \quad (13)$$

in (8), the k-jet of the second order (8) takes into evidence the swallowtail CP [10] (see index):

$$V_s=a_sz^5+b_sz^3+c_sz^2+d_sz+e_s \quad (14)$$

where the control parameters a_s, b_s, c_s, d_s and e_s could be easily identified by (13) in (8), respectively z-the behaviour (or state) parameter.

3.2.3. The Wigwam CP

For k-jet of the fourth order, (9) represents just the wigwam CP [11] (see index):

$$V_w=a_wx^7+b_wx^5+c_wx^4+d_wx^3+e_wx^2+f_wx+g_w \quad (15)$$

with the control parameters a_w, b_w, c_w, d_w, e_w, f_w and g_w identical to those of (9) (not being necessary the change of the variable), respectively x-the behaviour (or state) parameter.

3.2.4. The fold $\otimes$ butterfly product CP

By (10) we have, directly, the fold $\otimes$ butterfly product CP (or simple cusp $\otimes$ swallowtail) [10,11] (see index): $V_{fb}=a_{fb}x^9+b_{fb}x^7+c_{fb}x^6+d_{fb}x^5+e_{fb}x^4+f_{fb}x^3+g_{fb}x^2+h_{fb}x+i_{fb}$ (16)

with the the control parameters identical to those of (10), respectively x-the behaviour (or state) parameter.

3.2.5. Conclusion

The hypersurface (5) (or (4)-the generalization of the hypersurfaces ((1_J) ($J\in J$)) representing the energetic SCF functionals (I)-(III) may be fitted by the CSs whose CPs are of the cuspoid type: simple cusp (12), swallowtail (14), wigwam (15), and fold $\otimes$ butterfly product (16), if the expansion in the Taylor series (6) cuts itself off from the term in x^8.

3.3. The catastrophe Manifolds corresponding to the CPs (12), (14)-(16)

The catastrophe manifolds (with the help of which the extremum points will be identified) corresponding to the CPs identified in the paragraph 3.2 are obtained, in turn by

$$V_i^n(n)=\partial V_i(n)/\partial n=0 \text{ (n=z or x), as:} \quad (17)$$

$$V_{sc}^{\ z}(z)=4a_{sc}z^3+2b_{sc}z+c_{sc}=0 \text{ (simple cusp)} \quad (18)$$

$$V_s^{\ z}(z)=5a_sz^4+3b_sz^2+2c_sz+d_s=0 \text{ (swallowtail)} \quad (19)$$

$$V_w^{\ x}(x)=7a_wx^6+5b_wx^4+4c_wx^3+3d_wx^2+2e_wx+f_w=0 \text{ (wigwam)} \quad (20)$$

and

$$V_{fb}^{\ x}(x)=9a_{fb}x^8+7b_{fb}x^6+6c_{fb}x^5+5d_{fb}x^4+4e_{fb}x^3+3f_{fb}x^2+2g_{fb}x+h_{fb}=0 \text{ (fold } \otimes \text{ butterfly)} \quad (21)$$

The nature of the extremum points of the catastrophe surfaces is detected by the sign of the hessian:

$$V_i^{nn}(n)=\partial^2 V_i(n)/\partial n^2 \ (n=z \text{ or } x) \tag{22}$$

in the extremum points obtained by (17) through (18)-(21), respectively the critical points obtained by the annulment of the hessian (22). In the effective computations, the results of this paragraph will be used mostly for (II). For (I) and (III), (18)-(21) will be particularized in the following.

3.4. The CSs which fit (I) and (III)

According to the relation (4´), the hyper surface (5) (or (4)) is particularized to (I) and (III), if the terms of the 3rd and 4th degree in x are annulled. In this case, (1_I) and (1_{III}) are reduced to the hypersurface:

$$F_{I,III}=ax^2+bxy+cx+dy+e \tag{23}$$

with {a,b,c,d,e} explained in [18, 21], x and y given by (3). Applying (6) in (23) we obtain the k-jets peculiar to the k-jets (7)-(10):

$$F_{I,III}^{(0)}=a^{(0)}x^2+b^{(0)}x+c^{(0)} \tag{24}$$

$$F_{I,III}^{(2)}=a^{(2)}x^3+b^{(2)}x^2+c^{(2)}x+d^{(2)} \tag{25}$$

$$F_{I,III}^{(4)}=a^{(4)}x^5+b^{(4)}x^4+c^{(4)}x^3+d^{(4)}x^2+e^{(4)}x+f^{(4)} \tag{26}$$

$$F_{I,III}^{(6)}=a^{(6)}x^6+b^{(6)}x^5+c^{(6)}x^4+d^{(6)}x^3+e^{(6)}x^2+f^{(6)}x+g^{(6)} \tag{27}$$

with the control parameters specified in [18] for (I), respectively in [21] for (III).

By a change of the variable of the type:

$$x=z-b^{(k)}/(k+1)a^{(k)} \ (k=2,4,6,) \tag{28}$$

(25)-(27) lead to the CSs: fold (k=2), swallowtail (k=4), respectively (k=6), the fold CP being given by [9-11,18,21] as :

$$V_f=a_f z^3+b_f z+cf \tag{29}$$

Table 1 The CSs which fit the Functionals (I)-(III) (1_I)-(1_{III}).

k-jet	E_{SCF}(I) and $(\Delta e_{ij})_{SCF}$(III)	ΔE_{SCF}(II)
(0)	noncatastrophe structure (nonCS)	simple cusp
(2)	fold	swallowtail
(4)	swallowtail	wigwam
(6)	wigwam	fold ⊗ butterfly
(8)*	fold ⊗ butterfly	fold ⊗ star
(10)*	fold ⊗ star	swallow ⊗ star

*CSs not icluded in the text, which are obtained with (6) containing the term in x^8 (k=8), respectively in x^8 and x^{10} (k=10)

For k=0, the fitting of the hypersurface (23) is done by a nonCS (24). These results are obtained directly too, from (7)-(10), by taking into account (4´). The table 1 synthesizes the

results from subparagraphs 3.3 and 3.4 on the CSs which fit (I)-(III) comprising the CSs too for k=8 and k=10 nonincluded in the text (see table1).

4. The integral quadratic error

The degree of the fitting of the hypersurfaces (I)-(III) ((1_I)-(1_{III})) by the CSs taken into evidence in the paragraph 3, my be measured by the integral quadratic error [18-21]:

$$\varepsilon_J^{(k)}=\int_{-1}^{1}|F_J-F_J^{(k)}|dx,\ (k=2n(n=0;\ 1,2,3);\ (J\in J)) \tag{30}$$

if we take into account that $x\in[-1,1]$, when $\alpha\in[-\pi,\pi]$. Appealing to the relations which define F_J and $F_J^{(k)}$ respectively, (30) is transformed into:

$$\varepsilon_J^{(k)}=\varepsilon_{1J}^{(k)}[C_2^J]^2+\varepsilon_{2J}^{(k)}[C_4^J]+\varepsilon_{3J}^{(k)}C_2^JC_4^J\ \ (k=2n(n=0;\ 1,2,3)\ (J\in J)) \tag{31}$$

in which C_2^J and C_4^J are the coefficients of the terms in y from (1_I)-(1_{III}), $\varepsilon_{iJ}^{(k)}$ (i=1,2,3) being computed and tabled in [18-21]. It is significant that, for J=I and J=III we have:

$$\varepsilon_{3J}^{(k)}=0 \tag{32}$$

and that in the integral quadratic error (31) interfere those coefficients of the functionals (I)-(III) explained, which contain cosα (according to the relations (1_I)-(1_{III}) and (3)). The analysis of the integral quadratic error (30) made in [18-21] shows that $\varepsilon_J^{(k)}$ diminishes while the order (k) of the k-jets that fit the hypersurfaces (1_I)-(1_{III}) rises setting approximatively at k=6. It shows that the optimum fitting is achieved for (I) and (III) by the wigwam CS and for (II) by the fold$\otimes$butterfly CS. The same analysis shows that satisfactory results are obtained even for the fitting by the CSs corresponding to k=2 for (I) and (III), respectively to k=0 for (II). The best results are obtained at the highest k, with a lot of quantity of computation and time, but not greater than in the classic SCF procedure.

5. Discussions

A debating of the nonclassic results which are obtained for (I)-(III) ((1_I)-(1_{III})), by the application of the CT, with classic results existing in the literature, may be realized with a less quantity of computation and time, in the case k=2 for (I) and (III) [18,21], and k=0 for (II) respectively [19,20]. For k=2, according to the table 1, the hypersurface $E_{SCF}(I)$ (1_I) may be fitted by the fold CS (29). If (17) is applied to (29) and the obtained equation is solved in the case of the quantum system He, two values of α [18] occur which minimize (29), according to the number of the SCF solutions obtained classically in [7]. Additionally, the minimum values $E_{SCF}^{(2)}$ computed by the CT are in accordance with the classic values obtained in [7].

With k=0, according to the Table 1, the hypersurface $\Delta E_{SCF}(II)$ (1_I) may be fitted by the simple cusp CS (12). By the simple cusp catastrophe manifold (18), and by taking into account the definitions of the control parameters and solving (18), value α_{min} are obtained through which one may obtained the nonclassic values $\Delta E_{SCF}^{(0)}\ll\varepsilon$ [19,20], with ε as order of

magnitude in accordance with that classically obtained (or pre—established) for the atomic and molecular closed shell systems [8,14,15]. We can thus approach nonclassically the MC-SCF convergence, by the possibility of the establishment of the convergence criteria.

The non classical study of the hypersurface $(\Delta e_{ij})_{SCF}(III)$ $((1_I)$, for k=2), by the fold CS, refinds [21] the algebraic conditions [12] of the approximation of the hermiticity of the SCF Lagrange multipliers, as a peculiar case of the topological conditions [21] of the approximation of the hermiticity. It also allows the nonclassic finding of a $[(\Delta e_{ij})_{SCF}]_{min} \sim 10^{-4}$ Hartree a. u., for the quantum systems methylene and ethylene, in accordance with the order of the magnitude from [12,13]. Quantitatively, better results may be obtained by fitting (I)-(III) by CSs corresponding to k higher [22] with the disadvantage of the increase of the quantity of the necessary computation and time.

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