MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **57** (2007) 69-104

ISSN 0340 - 6253

ERROR PROPAGATION IN THE ESTIMATE OF SURFACE FREE ENERGY COMPONENTS BY NONLINEAR BEST-FITTING

C. Della Volpe and S. Siboni(^{o})
Dept. of Materials Engineering and Industrial Technologies
University of Trento
Mesiano di Povo 38050 Povo, Trento - Italy
e-mail: stefano.siboni@ing.unitn.it Fax: I-0461 881977

(^{o}) to whom correspondence should be addressed

(Received May 22, 2006)

Abstract

The problem of error propagation in the estimate of material components for quadratic multicomponent surface free energy theories is addressed. It is shown that invariance properties of the model equations, through an appropriate group of linear transformations, imply a very peculiar structure of any merit function used for general best-fit estimates of surface free energy components in quadratic multicomponent models. Such a structure is reflected in the distribution of merit-function minima, involved in the calculation of best-fit estimates to surface free energy components, according to the nonlinear method. A simple and reasonable stategy allows to describe the displacement of minima due to uncertainties on experimental data, and therefore to evaluate the consequent error propagation on the final results.

1. Introduction

The multicomponent approach plays an important role in the description of the interfacial interactions of many materials and, more specifically, in the prediction of the solid-liquid work of adhesion and surface free energy of solid surfaces. The idea of modeling the surface interaction of two materials by means of a certain number of "components" concerning contributions of different physico-chemical nature is shared my many theories proposed in different years. Although not free from problems, multicomponent models are widely applied in common practice as a pragmatic way to characterize the surface energetics of various materials. Certainly one of the most famous and succesful multicomponent models is van Oss-Chaudhury-Good (vOCG) theory[1−6], which expresses the work of adhesion of a liquid l on a solid s as

$$W^{\mathrm{adh}} = 2\Big[\sqrt{\gamma_s^{LW}\gamma_l^{LW}} + \sqrt{\gamma_s^{+}\gamma_l^{-}} + \sqrt{\gamma_s^{-}\gamma_l^{+}}\Big] \tag{1.1}$$

while the surface tension of the liquid and the surface free energy of the solid take the form

$$\gamma_l = \gamma_l^{LW} + 2\sqrt{\gamma_l^{+}\gamma_l^{-}} \qquad \gamma_s = \gamma_s^{LW} + 2\sqrt{\gamma_s^{+}\gamma_s^{-}} \tag{1.2}$$

respectively. In (1.1) and (1.2) the superscript LW labels the Lifshizt-van del Waals components of the materials, related to dispersive interactions, while $+$ and $-$ denote the acidic and the basic components, which account for the acid-base interactions between electron-donor (basic) and electron-acceptor (acidic) sites of the interacting molecules — so that acidity and basicity must be understood in a Lewis' sense. All the model equations reflect the complementary nature of acid-base interactions. vOCG may provide very satisfactory informations provided that some cares are taken in performing calculations and in the interpretation of the final results[7,8]. Equations (1.1) and (1.2) can be rewritten into the equivalent matrix form

$$W^{\mathrm{adh}} = 2\,X^TTY \qquad \gamma_l = X^TTX \qquad \gamma_s = Y^TTY \tag{1.3}$$

by introducing the column vectors X and Y of square roots of components for the liquid and solid, along with a suitable "structure matrix" T

$$X = \begin{pmatrix} \sqrt{\gamma_l^{LW}} \\ \sqrt{\gamma_l^+} \\ \sqrt{\gamma_l^-} \end{pmatrix} \qquad Y = \begin{pmatrix} \sqrt{\gamma_s^{LW}} \\ \sqrt{\gamma_s^+} \\ \sqrt{\gamma_s^-} \end{pmatrix} \qquad T = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}. \tag{1.4}$$

In order to calculate the acid-base components of materials it is necessary to measure: (i) the surface tensions $\gamma_{l,i}$, $i = 1, \ldots, L$, of a given set of L liquids and (ii) the adhesion works $W_{i,j}^{\mathrm{adh}}$ of the same liquids on an appropriate set of S solids, each denoted by the index $j = 1, \ldots, S$. Typically, adhesion work is estimated by measuring equilibrium contact angle $\theta_{i,j}$ of liquid i on solid j and using Young-Dupré equation

$$W_{i,j}^{\mathrm{adh}} = \frac{1}{2}(1 + \cos\theta_{i,j})\gamma_{l,i}. \tag{1.5}$$

Reckon strategies can be subdivided into two categories:

(i) determined linear and overdetermined linear (best-fit) methods, which assume the components of a given set of test liquids to be known in some way;

(ii) nonlinear best-fit method, which does not rely on any assumption, since it consists in the determination of a best-fit solution for the available equations of surface tension and adhesion work, with respect to the components of all the liquids and the solids involved.

Uncertainties in contact angle and surface tension measurements imply that the left-handed sides of equations (1.3) are affected by an error, whose influence is to be found in the final estimates of components. Error propagation in linear methods can be easily discussed by the classical tools of vector/matrix norm and condition number[8−10]. The nonlinear method requires a much more delicate investigation, further complicated by the problem of scale multiplicity[7], that will be briefly illustrated in Section 2. The same troubles extend also to all the multicomponent theories with quadratic structure (Quadratic Multicomponent Models), of which vOCG model constitutes a sort of prototype. The latter theories share a similar mathematical formulation, with model equations of the same form of (1.3) but an eventually different number and/or definition of components per each material and a peculiar structure matrix T: therefore, columns vectors X and Y may have any number c of entries and T may be any $c \times c$ nonsingular matrix.

This work is devoted to a detailed analysis of the problem of error propagation in the estimate of surface free energy components of quadratic multicomponent models. The plan of the paper is as follows: Section 2 concerns the mathematical setup of the nonlinear best-fit problem, also putting into evidence the aspects of invariance-group symmetry and scale multiplicity; Section 3 is devoted to a detailed analysis of the geometrical structure of the critical point set, containing all the minima of any merit function used for best-fitting, due to symmetry of the model equations. Finally, Section 4 specifically tackles the problem of error propagation and Section 5 contains conclusions.

2. Mathematical formulation of the problem

The research of any best-fit solution implies the optimization of some merit function V dependent on the residuals

$$\begin{aligned} \Delta_{l,i} &= X_i^T T X_i - \gamma_{l,i} \qquad \Delta_{s,j} = Y_j^T T Y_j - \gamma_{s,j} \\ \Delta_{i,j} &= X_i^T T Y_j - \frac{1}{2}(1 + \cos\theta_{i,j})\gamma_{l,i} \ , \end{aligned} \tag{2.1}$$

with $1 \leq i \leq L$, the number of liquids, and $1 \leq j \leq S$, that of solids. The merit function is in principle arbitrary, but it is certainly preferable to adopt smooth functions like the usual weighted sum of squared residuals

$$V_w(X, Y, \Gamma; \lambda) = \sum_{i=1}^{L} w_{l,i} \big[X_i^T T X_i - \gamma_{l,i}\big]^2 + \sum_{j=1}^{S} w_{s,j} \big[Y_j^T T Y_j - \Gamma_j\big]^2 +$$

$$+\sum_{i=1}^{L}\sum_{j=1}^{S} w_{\mathrm{adh},ij}\Big[X_i^T T Y_j - \frac{1}{2}(1+\cos\theta_{i,j})\gamma_{l,i}\Big]^2 \tag{2.2}$$

where the constant weights $w_{l,i}$, $w_{s,j}$, $w_{\mathrm{adh},ij} > 0$ accounts for relevance of liquid surface tension, solid surface tension and liquid-solid adhesion work equations, respectively — depending for instance on the availability or on the level of accuracy of the single equations. The variables of function (2.2) are denoted with

$$X = (X_1, X_2, \ldots, X_L) \qquad Y = (Y_1, Y_2, \ldots, Y_S) \qquad \Gamma = (\gamma_{s,1}, \ldots, \gamma_{s,S}).$$

Notice that unlike liquid surface tensions $\gamma_{l,i}$, $1 \le i \le L$, which can be measured independently, the total surface free energies $\gamma_{s,j}$, $1 \le j \le S$, of the solids must be taken as unknowns of the merit functions, since no direct experimental method exists for their measurement. The parameter λ collectively indicates all the constant data

$$\gamma_{l,i} \in \mathbb{R}_+ \qquad \theta_{i,j} \in [0,\pi]\,, \quad 1 \le i \le L\,,\ 1 \le j \le S\,,$$

which are affected by a certain amount of uncertainty due to experimental errors. The weights are assumed to be *a priori* fixed.

It is easy to show that the previous choice of the merit function can be appreciably simplified. Indeed, if $(X, Y, \Gamma) = (\overline{X}, \overline{Y}, \overline{\Gamma})$ is a best-fit solution for V_w, then necessarily

$$\overline{\Gamma}_j = \overline{Y}_j^T T \overline{Y}_j \qquad 1 \le j \le S\,.$$

If not, the term

$$\sum_{j=1}^{S} w_{s,j}\,[\overline{Y}_j^T T \overline{Y}_j - \overline{\Gamma}_j]^2$$

in (2.2) would be strisctly positive and the substitution

$$\overline{\Gamma}_j \longrightarrow \Gamma_j^\star = \overline{Y}_j^T T \overline{Y}_j \qquad 1 \le j \le S$$

would lead to $(X, Y, \Gamma) = (\overline{X}, \overline{Y}, \Gamma^\star)$ as a better best-fit solution than $(X, Y, \Gamma) = (\overline{X}, \overline{Y}, \overline{\Gamma})$, a clear contradiction. We can then replace V_w with the simplified merit function

$$V(X, Y; \lambda) = \sum_{i=1}^{L} w_{l,i} \big[X_i^T T X_i - \gamma_{l,i}\big]^2 + \sum_{i=1}^{L}\sum_{j=1}^{S} w_{\mathrm{adh},ij} \Big[X_i^T T Y_j - \frac{1}{2}(1 + \cos\theta_{i,j})\gamma_{l,i}\Big]^2 . \tag{2.3}$$

Existence of best-fit solutions for V is highly nontrivial, since no general argument can be easily invoked. All we can generally claim is that the best-fit solution, if defined, is never unique owing to the invariance property

$$V(X, Y; \lambda) = V(R(\alpha)X, R(\alpha)Y; \lambda) \qquad \forall\, \alpha \in \mathbb{R}^3,\ X \in \mathbb{R}^{3L},\ Y \in \mathbb{R}^{3S},\ \lambda ,$$

where $\alpha = (\omega_1, \omega_2, \omega_3) \in \mathbb{R}^3$,

$$R(\alpha)X = \begin{pmatrix} E(\alpha)X_1 \\ \vdots \\ E(\alpha)X_L \end{pmatrix} \qquad R(\alpha)Y = \begin{pmatrix} E(\alpha)Y_1 \\ \vdots \\ E(\alpha)Y_S \end{pmatrix}$$

and $E(\alpha)$ is an arbitrary 3×3 real matrix of the form[7–8]

$$\exp[\omega_1 E_1 + \omega_2 E_2 + \omega_3 E_3] ,$$

with

$$E_1 = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{pmatrix} \qquad E_2 = \begin{pmatrix} 0 & 0 & 1 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \qquad E_3 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix} .$$

More generally, it has been shown that each residual — and therefore the whole merit function — is invariant through a linear transformation described by a 3×3 real matrix C satisfying $C^T T C = T$. These matrices form a group with respect to the usual matrix product — the group is isomorphic to the $O(2, 1; \mathbb{R})$ group.

By assuming that a best-fit solution exists for each choice of λ in a neighborhood of an appropriate $\lambda = \overline{\lambda}$, it is reasonable to describe the errors affecting such a solution as due to the parameter uncertainty, since any variation of λ results in a displacement of the minimum of V. Some problems arise from the invariance properties and deserve an accurate analytical discussion. Although the previous analysis has been sketched in the case of vOCG theory, it is important to point out that:

(i) similar invariance properties hold for all the quadratic multicomponent models;

(ii) it is convenient to state and tackle the problem in the most general n-dimensional case, by considering vectors X and Y of whatever dimension c — the number of components characteristic of each material — and by posing then $(X,Y) = x \in \mathbb{R}^n$, with $n = (L+S)c$. Here T can be any structure matrix (e.g. real, symmetrical and nonsingular, as typically happens) and the matrix representations of the invariance transformations will take the form $R(\alpha)$, being dependent on a set of g scalar parameters $(\alpha_1, \ldots, \alpha_g) = \alpha \in \mathbb{R}^g$.

3. Analytical results

A useful estimate to error propagation due to parameter uncertainty comes from the following result.

Theorem 1. Local structure of the critical point s et.

Let $V : (x,\lambda) \in (\Omega \times \Lambda) \longrightarrow V(x,\lambda) \in \mathbb{R}$ *be a real* C^k *function,* $k \geq 2$*, of the set* $\Omega \times \Lambda$*, where both* $\Omega \subseteq \mathbb{R}^n$ *and* $\Lambda \subseteq \mathbb{R}^p$ *are open — and* n, p *appropriate natural numbers.*

Denoted with $M_n(\mathbb{R})$ *the linear space of* $n \times n$ *real matrices, let* $R : \alpha \in U \longrightarrow R(\alpha) \in M_n(\mathbb{R})$ *a* C^k *function defined on an open set* $U \subseteq \mathbb{R}^g$*,* $g \in \mathbb{N}$*, such that* $0 \in U$ *and* $R(0) = \mathbb{I}$*, the identity* $n \times n$ *matrix.*

Suppose that:

- $R(\alpha)x \in \Omega \ \forall x \in \Omega$ *and* $\alpha \in U$*;*

- $\forall \alpha \in U,\ x \in \Omega,\ \lambda \in \Lambda$ *there holds* $V(R(\alpha)x, \lambda) = V(x, \lambda)$*;*

- *a point* $(\overline{x}, \overline{\lambda}) \in \Omega \times \Lambda$ *exists such that*

$$\frac{\partial V}{\partial x}(\overline{x}, \overline{\lambda}) \;=\; 0$$

  namely, $\overline{x} \in \Omega$ *is a critical point of the function* $V_{\overline{\lambda}} \,:\, x \in \Omega \longrightarrow V(x, \overline{\lambda}) \in \mathbb{R}$*;*

- *the following equality holds*

$$\operatorname{Rank} H_V(\overline{x}, \overline{\lambda}) \;=\; n - g' \ ,$$

  being $H_V(\overline{x}, \overline{\lambda}) = \dfrac{\partial^2 V}{\partial x^2}(\overline{x}, \overline{\lambda})$ *the Hessian matrix of* $V_{\overline{\lambda}}$ *in* $\overline{x}$ *and* $g' \leq g$ *the maximum number of linearly independent vectors of the set* $P := \left\{ \dfrac{\partial R}{\partial \alpha_i}(0)\,\overline{x}\,,\ 1 \leq i \leq g \right\}$*, with* $g' < n$*.*

Then if $\left\{ \dfrac{\partial R}{\partial \alpha_i}(0)\,\overline{x}\,,\ 1 \leq i \leq g' \right\}$ *is the maximal linearly independent subset of* P(°) *and the vectors* $h_j \in \mathbb{R}^n$*,* $1 \leq j \leq n - g'$*, are fixed in such a way that*

$$\left\{ \frac{\partial R}{\partial \alpha_i}(0)\,\overline{x}\,,\ 1 \leq i \leq g' \right\} \cup \{ h_j\,,\ 1 \leq j \leq n - g' \} \tag{3.1}$$

is a base of $\mathbb{R}^n$*, open neighborhoods* $B_0 \subset \Omega \times \Lambda$ *of* $(x, \lambda) = (\overline{x}, \overline{\lambda})$*,* $E_0 \subset \mathbb{R}^{g'}$ *of* $(\alpha_1, \ldots, \alpha_{g'})$ $= (0, \ldots, 0)$ *and* $E_0' \subset \Lambda - \overline{\lambda} = \{\mu = \lambda - \overline{\lambda} \,:\, \lambda \in \Lambda\}$ *of* $\mu = 0$ *exist such that all the critical points of* $V_\lambda \,:\, x \longrightarrow V(x, \lambda)$ *for which* $(x, \lambda) \in B_0$ *are individuated by*

$$x \;=\; R(\alpha_1, \ldots, \alpha_{g'}, \underbrace{0, \ldots, 0}_{g - g'}) \left(\overline{x} + \sum_{j=1}^{n-g'} \xi_j(\mu)\, h_j \right) \ , \tag{3.2}$$

with $(\alpha_1, \ldots, \alpha_{g'}) \in E_0\,,\ \mu \longrightarrow \xi_j(\mu)$ *real* C^{k-1} *functions of* E_0' *and* $\xi_j(0) = 0,\ 1 \leq j \leq n - g'$*.* $\square$

(°) We suppose the linear independency of the first g' vectors of P, without loss of generality. If necessary, this condition can always be fulfilled by an appropriate permutation of the variables α_i, $1 \leq i \leq g$.

We subdivide the proof into several lemmas, by assuming $0 < g' < g$. The particular cases $g' = g$ and $g' = 0$ will be treated separately. Throughout the paper we will pose

$$\alpha = (\alpha_1, \dots, \alpha_g),\ \alpha_i \in \mathbb{R},\ 1 \le i \le g, \qquad \alpha' = (\alpha_1, \dots, \alpha_{g'}),\ \alpha_i \in \mathbb{R},\ 1 \le i \le g',$$

$$\mu = (\mu_1, \dots, \mu_p),\ \mu_k \in \mathbb{R},\ 1 \le k \le p, \qquad \xi = (\xi_1, \dots, \xi_{n-g'}),\ \xi_j \in \mathbb{R},\ 1 \le j \le n-g',$$

and $(\alpha', 0)$ will denote a vector α of the form $(\alpha_1, \dots, \alpha_{g'}, 0, \dots, 0)$, the last $g - g'$ components being equal to zero.

Lemma 1. Local change of variables.

An open neighborhood $A = \operatorname{int}(A) \subset \mathbb{R}^{g'} \times \mathbb{R}^{n-g'} \times \mathbb{R}^p$ *of the point* $(\alpha', \xi, \mu) = (0,0,0)$ *and an open neighborhood* $B = \operatorname{int}(B) \subset \mathbb{R}^n \times \mathbb{R}^p$ *of* $(x, \lambda) = (\overline{x}, \overline{\lambda})$ *exist such that the application* $\Phi : (\alpha', \xi, \mu) \in A \longrightarrow (x, \lambda) \in B$ *defined by*

$$x = R(\alpha', 0)\Big[\overline{x} + \sum_{j=1}^{n-g'} \xi_j h_j\Big] \qquad \lambda = \overline{\lambda} + \mu$$

is a C^k *diffeomorphism of* A *onto* B. $\square$

Proof

The vectors $\dfrac{\partial R}{\partial \alpha_i}(0)\,\overline{x}$, $i = 1, \dots, g'$, are linearly independent and the set (3.1) constitutes a base of $\mathbb{R}^n$. Our goal is to introduce a regular change of variables in a neighborhood of $(\overline{x}, \overline{\lambda}) \in \Omega \times \Lambda$ by means of the transformation

$$\begin{cases} x \,=\, X(\alpha', \xi) \,=\, R(\alpha', 0)\Big[\overline{x} + \displaystyle\sum_{j=1}^{n-g'} \xi_j h_j\Big] \\ \lambda \,=\, L(\mu) \,=\, \overline{\lambda} + \mu \end{cases} \tag{3.3}$$

The transformation can be assumed to be be defined in the open rectangle $D_1 \times D_2$, where

$$D_1 = \big\{(\alpha', \xi) \ :\ |\alpha_i| < d_1\,,\ 1 \le i \le g'\,,\ |\xi_j| < d_1\,,\ 1 \le j \le n - g'\big\} \subset \mathbb{R}^{g'} \times \mathbb{R}^{n-g'}$$

and

$$D_2 = \{\mu \ :\ |\mu_k| < d_2\,,\ 1 \le k \le p\}$$

with $d_1 > 0$ such that $\{\alpha \in \mathbb{R}^g \,:\, |\alpha_i| < d_1\,,\ 1 \le i \le g\} \subset U$ — always possible since $0 \in U$ and U is open — and $d_2 > 0$ chosen in such a way that $\overline{\lambda} + D_2 \subset \Lambda$ — Λ is open. In $D_1 \times D_2$ the function (3.3) is C^k.

The only nonzero partial derivatives are the following

$$
\begin{aligned}
\frac{\partial X}{\partial \alpha_i}(\alpha',\xi) &= \frac{\partial R}{\partial \alpha_i}(\alpha',0)\Big[\overline{x} + \sum_{j=1}^{n-g'} \xi_j h_j\Big] && 1 \le i \le g' \\
\frac{\partial X}{\partial \xi_k}(\alpha',\xi) &= R(\alpha',0) h_k && 1 \le k \le n-g' \\
\frac{\partial L_i}{\partial \mu_j}(\mu) &= \delta_{ij} && 1 \le i,j \le p
\end{aligned}
$$

on having denoted with δ_{ij} the usual Kronecker delta. For $(\alpha',\xi,\mu) = (0,0,0)$ the previous expressions become

$$
\begin{aligned}
\frac{\partial X}{\partial \alpha_i}(0,0) &= \frac{\partial R}{\partial \alpha_i}(0)\,\overline{x} && 1 \le i \le g' \\
\frac{\partial X}{\partial \xi_k}(0,0) &= R(0)h_k \;=\; h_k && 1 \le k \le n-g' \\
\frac{\partial L_i}{\partial \mu_j}(0) &= \delta_{ij} && 1 \le i,j \le p
\end{aligned}
$$

and the jacobian matrix is written as

$$
\frac{\partial(x,\lambda)}{\partial(\alpha',\xi,\mu)}(0,0,0) = \left(\begin{array}{c|c|c}
\begin{matrix}\dfrac{\partial R}{\partial \alpha_i}(0)\,\overline{x} \\ n \times g'\end{matrix} & \begin{matrix} h_k \\ n \times (n-g')\end{matrix} & \begin{matrix}\mathbb{O} \\ n \times p\end{matrix} \\
\hline
\multicolumn{2}{c|}{\begin{matrix}\mathbb{O} \\ p \times n\end{matrix}} & \begin{matrix}\mathbb{I} \\ p \times p\end{matrix}
\end{array}\right)
$$

with determinant

$$
\det \frac{\partial(x,\lambda)}{\partial(\alpha',\xi,\mu)}(0,0,0) = \det \left(\begin{array}{c|c}
\begin{matrix}\dfrac{\partial R}{\partial \alpha_i}(0)\,\overline{x} \\ n \times g'\end{matrix} & \begin{matrix} h_k \\ n \times (n-g')\end{matrix}
\end{array}\right)
$$

different from zero since the set (3.1) is a base of $\mathbb{R}^n$. Moreover

$$\begin{cases} X(0,0) \;=\; R(0)\Big[\overline{x} + \sum_{j=1}^{n-g'} 0\, h_j\Big] \;=\; \overline{x} \\ L(0) \;=\; \overline{\lambda} + 0 \;=\; \overline{\lambda} \end{cases}$$

and by the Implicit Function Theorem there exist an open neighborhood $A = \mathrm{int}(A) \subset D_1 \times D_2$ of the point $(\alpha', \xi, \mu) = (0,0,0)$ and an open neighborhood of $B = \mathrm{int}(B) \subset \mathbb{R}^n \times \mathbb{R}^p$ of $(x, \lambda) = (\overline{x}, \overline{\lambda})$, such that (3.3) defines a C^k diffeomorphism of A onto B. $\square$

Remark

Owing to the particular form of (3.3), we can always assume that

$$A \;=\; A_1 \times A_2$$

with A_1 open neighborhood of $(\alpha', \xi) = (0,0)$ and A_2 open neighborhood of $\mu = 0$. In an analogous way, we can always write

$$B \;=\; \Phi(A) \;=\; B_1 \times B_2$$

being $B_1 \subset \mathbb{R}^n$ an open neighborhood of $x = \overline{x}$ and B_2 an open neighborhood of $\lambda = \overline{\lambda}$.

Lemma 2. Local characterization of critical points.

An open neighborhood $B'' \subseteq B$ of $(x, \lambda) = (\overline{x}, \overline{\lambda})$ exists such that

$$\frac{\partial V}{\partial x}(x, \lambda) \;=\; 0\;, \quad (x, \lambda) \in B''$$

if and only if $(x, \lambda) = \Phi(\alpha', \xi, \mu)$ with

$$\frac{\partial \tilde{V}}{d\xi_k}(\alpha', \xi, \mu) \;=\; 0 \quad \forall\, k = 1, \ldots, n - g' \quad , \qquad (\alpha', \xi, \mu) \in A''\;,$$

where $A'' = \Phi^{-1}(B'') \subseteq A$ and $\tilde{V} = V \circ \Phi$. $\square$

Proof

On the open set A consider the C^k function

$$\tilde V(\alpha',\xi,\mu) = (V\circ\Phi)(\alpha',\xi,\mu) = V\Big[R(\alpha',0)\Big(\overline{x}+\sum_{j=1}^{n-g'}\xi_j h_j\Big),\overline{\lambda}+\mu\Big] = V\Big(\overline{x}+\sum_{j=1}^{n-g'}\xi_j h_j,\overline{\lambda}+\mu\Big)$$

whose partial derivatives are easily calculated

$$\frac{\partial\tilde V}{\partial\alpha_i}(\alpha',\xi,\mu) = 0 \qquad 1\le i\le g'$$

$$\frac{\partial\tilde V}{\partial\xi_k}(\alpha',\xi,\mu) = \frac{\partial V}{\partial x}\Big(\overline{x}+\sum_{j=1}^{n-g'}\xi_j h_j,\overline{\lambda}+\mu\Big)\,h_k \qquad 1\le k\le n-g'$$

$$\frac{\partial\tilde V}{\partial\mu_\ell}(\alpha',\xi,\mu) = \frac{\partial V}{\partial\lambda_\ell}\Big(\overline{x}+\sum_{j=1}^{n-g'}\xi_j h_j,\overline{\lambda}+\mu\Big) \qquad 1\le \ell\le p\,.$$

By using the diffeomorphism Φ, which defines a regular change of coordinates, we firstly have that

$$\frac{\partial V}{\partial x}(x,\lambda) = 0\,, \quad (x,\lambda)\in B$$

if and only if $(x,\lambda)=\Phi(\alpha',\xi,\mu)$ with $(\alpha',\xi,\mu)\in A$ satisfying

$$\frac{\partial V}{\partial x}\Big[R(\alpha',0)\Big(\overline{x}+\sum_{j=1}^{n-g'}\xi_j h_j\Big),\overline{\lambda}+\mu\Big] = 0\,.$$

Moreover, the invariance property $V[R(\alpha)x,\lambda]=V(x,\lambda)$ implies

$$\frac{\partial V}{\partial x_i}(x,\lambda) = \sum_{j=1}^{n}\frac{\partial V}{\partial x_j}[R(\alpha)x,\lambda]\,\frac{\partial}{\partial x_i}[R(\alpha)x]_j = \sum_{j=1}^{n}\frac{\partial V}{\partial x_j}[R(\alpha)x,\lambda]\,\frac{\partial}{\partial x_i}\sum_{k=1}^{n}R_{jk}(\alpha)\,x_k =$$

$$\sum_{j=1}^{n}\frac{\partial V}{\partial x_j}[R(\alpha)x,\lambda]\sum_{k=1}^{n}R_{jk}(\alpha)\,\delta_{ik} = \sum_{j=1}^{n}\frac{\partial V}{\partial x_j}[R(\alpha)x,\lambda]R_{ji}(\alpha) = \sum_{j=1}^{n}[R(\alpha)^\dagger]_{ij}\frac{\partial V}{\partial x_j}[R(\alpha)x,\lambda]$$

so that

$$\frac{\partial V}{\partial x}(x,\lambda) = R(\alpha)^\dagger\frac{\partial V}{\partial x}[R(\alpha)x,\lambda] \qquad \forall\, x\in\Omega,\ \alpha\in U,\ \lambda\in\Lambda\,, \tag{3.4}$$

on having denoted with $R(\alpha)^\dagger$ the adjoint of the matrix $R(\alpha)$. Therefore

$$\frac{\partial V}{\partial x}\Big(\overline{x}+\sum_{j=1}^{n-g'}\xi_j h_j,\overline{\lambda}+\mu\Big) = R(\alpha',0)^\dagger\frac{\partial V}{\partial x}\Big[R(\alpha',0)\Big(\overline{x}+\sum_{j=1}^{n-g'}\xi_j h_j\Big),\overline{\lambda}+\mu\Big]\ \forall(\alpha',\xi,\mu)\in A\,.$$

On the other hand, for $(\alpha', \xi, \mu) \in A$ we have

$$R(\alpha',0)^{\dagger}\frac{\partial V}{\partial x}\left[R(\alpha',0)\Big(\overline{x}+\sum_{j=1}^{n-g'}\xi_j h_j\Big),\overline{\lambda}+\mu\right] = 0$$

if and only if

$$\frac{\partial V}{\partial x}\left[R(\alpha',0)\Big(\overline{x}+\sum_{j=1}^{n-g'}\xi_j h_j\Big),\overline{\lambda}+\mu\right] = 0$$

provided that $R(\alpha',0)^{\dagger}$ is invertible. This is certainly true if we *a priori* assume $R(\alpha)$ nonsingular $\forall\, \alpha \in U$, or if we require that $|\alpha_i| < \varepsilon$, $1 \le i \le g'$, with ε positive and sufficiently small — remember that $R(0) = \mathbb{I}$ and that $R(\alpha)$ is C^k, thus continuous. In the present case, according to our hypotheses, the second condition is verified by replacing the open set A with the neighborhood of $(\alpha', \xi, \mu) = (0,0,0)$

$$A' = A \cap \{(\alpha', \xi, \mu) \in \mathbb{R}^{g'} \times \mathbb{R}^{n-g'} \times \mathbb{R}^p \,:\, |\alpha_i| < \varepsilon,\, 1 \le i \le g'\} \subseteq A$$

open as intersection of a finite number of open sets, and the neighborhood B of $(x, \lambda) = (\overline{x}, \overline{\lambda})$ with the neighborhood

$$B' = \Phi(A') \subseteq B$$

— it is clear that B' is open, since $\Phi(A') = (\Phi^{-1})^{-1}(A')$, Φ^{-1} is continuous and therefore B' is the continuous preimage of an open set. It is also evident that $(\overline{x}, \overline{\lambda}) \in B'$.

As a conclusion

$$\frac{\partial V}{\partial x}(x,\lambda) = 0 \quad , \qquad (x,\lambda) \in B'$$

if and only if $(x, \lambda) = \Phi(\alpha', \xi, \mu)$ with (α', ξ, μ) such that

$$\frac{\partial V}{\partial x}\left[R(\alpha',0)\Big(\overline{x}+\sum_{j=1}^{n-g'}\xi_j\, h_j\Big),\overline{\lambda}+\mu\right] = 0 \qquad (\alpha', \xi, \mu) \in A'$$

which is equivalent to the condition

$$R(\alpha',0)^{\dagger}\frac{\partial V}{\partial x}\left[R(\alpha',0)\Big(\overline{x}+\sum_{j=1}^{n-g'}\xi_j\, h_j\Big),\overline{\lambda}+\mu\right] = 0 \qquad (\alpha', \xi, \mu) \in A'$$

and owing to the invariance property reduces to the relationship

$$\frac{\partial V}{\partial x}\Big(\overline{x} + \sum_{j=1}^{n-g'} \xi_j\, h_j, \overline{\lambda} + \mu\Big) \;=\; 0 \qquad (\alpha', \xi, \mu) \in A'$$

— notice that there is no actual dependence on the vector parameter α'. We now have only to prove the equivalence of the latter condition with

$$\frac{\partial \tilde{V}}{\partial \xi_k}(\alpha', \xi, \mu) \;=\; 0\;, \quad 1 \leq k \leq n - g'\;, \qquad (\alpha', \xi, \mu) \in A'\;.$$

If $(\alpha', \xi, \mu) \in A'$ obeys

$$\frac{\partial V}{\partial x}\Big(\overline{x} + \sum_{j=1}^{n-g'} \xi_j\, h_j, \overline{\lambda} + \mu\Big) \;=\; 0$$

then, as already remarked,

$$\frac{\partial \tilde{V}}{\partial \xi_k}(\alpha', \xi, \mu) \;=\; \frac{\partial V}{\partial x}\Big(\overline{x} + \sum_{j=1}^{n-g'} \xi_j\, h_j, \overline{\lambda} + \mu\Big)\, h_k \;=\; 0\, h_k \;=\; 0 \qquad 1 \leq k \leq n - g'\;.$$

Vice versa, let $(\alpha', \xi, \mu) \in A'$ and

$$\frac{\partial \tilde{V}}{\partial \xi_k}(\alpha', \xi, \mu) \;=\; 0\;, \quad 1 \leq k \leq n - g'\;.$$

This implies that

$$\frac{\partial V}{\partial x}\Big(\overline{x} + \sum_{j=1}^{n-g'} \xi_j\, h_j, \overline{\lambda} + \mu\Big)\, h_k \;=\; 0 \qquad 1 \leq k \leq n - g'$$

while there always holds

$$\frac{\partial V}{\partial x}\Big(\overline{x} + \sum_{j=1}^{n-g'} \xi_j\, h_j, \overline{\lambda} + \mu\Big)\, \frac{\partial R}{\partial \alpha_i}(0)\, \Big(\overline{x} + \sum_{j'=1}^{n-g'} \xi_{j'}\, h_{j'}\Big) \;=\; 0 \qquad 1 \leq i \leq g'$$

since $\dfrac{\partial V}{\partial x}[R(\alpha)x, \lambda]\dfrac{\partial R}{\partial \alpha_i}(\alpha)\, x = 0\ \forall x \in \Omega,\ \lambda \in \Lambda,\ \alpha \in U,\ 1 \leq i \leq g$. On the other hand, the set of n vectors of $\mathbb{R}^n$

$$\Big\{\frac{\partial R}{\partial \alpha_i}(0)\Big(\overline{x} + \sum_{j'=1}^{n-g'} \xi_{j'}\, h_{j'}\Big)\,,\ 1 \leq i \leq g'\Big\} \cup \{h_k\,,\ 1 \leq k \leq n - g'\} \tag{3.5}$$

is as linearly indipendent as

$$\left\{\frac{\partial R}{\partial \alpha_i}(0)\,\overline{x}\,,\ 1 \le i \le g'\right\} \cup \{h_k\,,\ 1 \le k \le n-g'\} \tag{3.6}$$

provided we consider $|\xi_{j'}| < \varepsilon$ small enough, $1 \le j' \le n-g'$. There holds indeed

$$\frac{\partial R}{\partial \alpha_i}(0)\Big(\overline{x} + \sum_{j'=1}^{n-g'} \xi_{j'} h_{j'}\Big) \;=\; \frac{\partial R}{\partial \alpha_i}(0)\,\overline{x} + \sum_{j'=1}^{n-g'} \xi_{j'}\,\frac{\partial R}{\partial \alpha_i}(0)\,h_{j'} \qquad 1 \le i \le g'$$

where

$$\frac{\partial R}{\partial \alpha_i}(0)\,h_{j'} \;=\; \sum_{k=1}^{g'} b_k^{(i,j')}\,\frac{\partial R}{\partial \alpha_i}(0)\,\overline{x} + \sum_{k=1}^{n-g'} b_{k+g'}^{(i,j')} h_k$$

with suitable scalar coefficients $b_k^{(i,j')}$, $1 \le i \le g'$, $1 \le j' \le n-g'$, $1 \le k \le n$, so that

$$\sum_{j'=1}^{n-g'} \xi_{j'}\left[\sum_{k=1}^{g'} b_k^{(i,j')}\,\frac{\partial R}{\partial \alpha_i}(0)\,\overline{x} + \sum_{k=1}^{n-g'} b_{k+g'}^{(i,j')} h_k\right] \;=\; \sum_{k=1}^{g'} \varepsilon_{k,i}\,\frac{\partial R}{\partial \alpha_i}(0)\,\overline{x} + \sum_{k=1}^{n-g'} \varepsilon_{k+g',i} h_k\ ,$$

upon having

$$|\varepsilon_{k,i}| = \Big|\sum_{j'=1}^{n-g'} b_k^{(i,j')}\xi_{j'}\Big| \le \sum_{j'=1}^{n-g'} \big|b_k^{(i,j')}\big|\,|\xi_{j'}| \le \sum_{j'=1}^{n-g'} \big|b_k^{(i,j')}\big|\,\varepsilon \le \max_{\substack{1\le k\le n\\ 1\le i\le g'}} \sum_{j'=1}^{n-g'} \big|b_k^{(i,j')}\big|\,\varepsilon = K\,\varepsilon$$

for every $i = 1, \dots, g'$ and $k = 1, \dots, n$. The transformation matrix from the n-tuple (3.6) to (3.5) is therefore written as

$$\begin{pmatrix} 1+\varepsilon_{1,1} & \cdots & \varepsilon_{1,g'} & \multirow{3}{*}{$\boxed{\begin{matrix}\mathbb{O}\\ g'\times(n-g')\end{matrix}}$} \\ \vdots & \ddots & \vdots & \\ \varepsilon_{g',1} & \cdots & 1+\varepsilon_{g',g'} & \\ \varepsilon_{g'+1,1} & \cdots & \varepsilon_{g'+1,g'} & \multirow{3}{*}{$\boxed{\begin{matrix}\mathbb{I}\\ (n-g')\times(n-g')\end{matrix}}$} \\ \vdots & & \vdots & \\ \varepsilon_{n,1} & \cdots & \varepsilon_{n,g'} & \end{pmatrix} \tag{3.7}$$

and its determinant coincides with

$$\det\begin{pmatrix} 1+\varepsilon_{1,1} & \cdots & \varepsilon_{1,g'} \\ \vdots & \ddots & \vdots \\ \varepsilon_{g',1} & \cdots & 1+\varepsilon_{g',g'} \end{pmatrix}$$

which is certainly different from zero for ε sufficiently small, since $|\varepsilon_{k,i}| \leq K\varepsilon$, $1 \leq k \leq n$, $1 \leq i \leq g'$. Under this condition we conclude that the gradient operator $\mathbb{R}^n \longrightarrow \mathbb{R}$

$$\frac{\partial V}{\partial x}\Big(\overline{x} + \sum_{j=1}^{n-g'} \xi_j h_j, \overline{\lambda} + \mu\Big)$$

admits a kernel of dimension n and it must be thus identified with the identically zero linear functional

$$\frac{\partial V}{\partial x}\Big(\overline{x} + \sum_{j=1}^{n-g'} \xi_j h_j, \overline{\lambda} + \mu\Big) \;=\; 0\ .$$

The possible replacement of the set A with the open set

$$A'' \;=\; A' \cap \{(\alpha', \xi, \mu) \in \mathbb{R}^{g'} \times \mathbb{R}^{n-g'} \times \mathbb{R}^p \;:\; |\xi_j| < \varepsilon\,,\; 1 \leq j \leq n - g'\} \subseteq A' \subseteq A$$

and of B with the open set $B'' \;=\; \Phi^{-1}(A'') \subseteq \Phi^{-1}(A') \;=\; B' \subseteq B$ completes the proof of Lemma 2. $\square$

According to the previous result, in the neighborhood B'' of $(\overline{x}, \overline{\lambda})$ we have $\dfrac{\partial V}{\partial x}(x, \lambda) = 0$ if and only if

$$x \;=\; R(\alpha', 0)\Big(\overline{x} + \sum_{j=1}^{n-g'} \xi_j h_j\Big) \quad , \qquad \lambda \;=\; \overline{\lambda} + \mu \tag{3.8}$$

with $(\alpha', \xi, \mu) \in A''$ such that

$$\frac{\partial \tilde{V}}{\partial \xi_k}(\alpha', \xi, \mu) \;=\; 0 \qquad 1 \leq k \leq n - g'\ ,$$

or, equivalently,

$$\frac{\partial V}{\partial x}\Big(\overline{x} + \sum_{j=1}^{n-g'} \xi_j h_j, \overline{\lambda} + \mu\Big)\, h_k \;=\; 0 \qquad 1 \leq k \leq n - g'\ . \tag{3.9}$$

In order to simplify the subsequent discussion, it is convenient to consider instead of A'' the open neighborhood of $(\alpha', \xi, \mu) = (0, 0, 0)$

$$E_1 \times E_2 \times E_3 \;\subset\; A''$$

where $E_1 \subset \mathbb{R}^{g'}$, $E_2 \subset \mathbb{R}^{n-g'}$, $E_3 \subset \Lambda - \overline{\lambda} \subset \mathbb{R}^p$ are open neighborhoods of $\alpha' = 0$, $\xi = 0$ and $\mu = 0$ respectively. The possibility of introducing the open sets E_1, E_2, E_3 is assured by the fact that A'' is an open neighborhood of $(\alpha', \xi, \mu) = (0, 0, 0)$. By means of the transformation (3.8), the condition

$$\frac{\partial V}{\partial x}\Big(\overline{x} + \sum_{j=1}^{n-g'} \xi_j h_j, \overline{\lambda} + \mu\Big)\, h_k \;=\; 0 \quad 1 \leq k \leq n - g' \;, \quad (\alpha', \xi, \mu) \in E_1 \times E_2 \times E_3 \qquad (3.10)$$

will characterize all and only the solutions of $\dfrac{\partial V}{\partial x}(x, \lambda) = 0$ in the neighborhood $\Phi(E_1 \times E_2 \times E_3) \subset B''$ of $(\overline{x}, \overline{\lambda})$. We have the further result illustrated below.

Lemma 3. Local characterization of nondegenerate critical points.

Let $H_V(\overline{x}, \overline{\lambda}) = \dfrac{\partial^2 V}{\partial x^2}(\overline{x}, \overline{\lambda})$ denote the Hessian matrix of $V(\cdot, \overline{\lambda})$ calculated in the critical point $\overline{x}$, and suppose that the real symmetric $(n - g') \times (n - g')$ matrix

$$M_{ij} \;=\; h_i^{\dagger}\, H_V(\overline{x}, \overline{\lambda})\, h_j \qquad 1 \leq i, j \leq n - g'$$

is nonsingular. Then there are two neighborhoods $E_2' \subseteq E_2$ and $E_3' \subseteq E_3$ of $\xi = 0$ and $\mu = 0$ respectively, such that all the critical points of $V_\lambda \,:\, x \longrightarrow V(x, \lambda)$ in the neighborhood $\Phi(E_1 \times E_2' \times E_3') \subseteq B''$ of $(x, \lambda) = (\overline{x}, \overline{\lambda})$ are individuated by

$$x \;=\; R(\alpha', 0)\Big(\overline{x} + \sum_{j=1}^{n-g'} \xi_j(\mu)\, h_j\Big)$$

with $\mu \longrightarrow \xi_j(\mu)$ C^{k-1}-functions of the open set E_3' to E_2', $\xi_j(0) = 0 \;\forall j = 1, \ldots, n - g'$ and $\alpha' \in E_1$. $\square$

Proof

Equations (3.10) constitute a set of $n - g'$ scalar equations in the variables (ξ, μ). By hypothesis, the functions on the left-hand side

$$F_k(\xi, \mu) \;=\; \frac{\partial V}{\partial x}\Big(\overline{x} + \sum_{j=1}^{n-g'} \xi_j h_j, \overline{\lambda} + \mu\Big)\, h_k \quad 1 \leq k \leq n - g'$$

are C^{k-1} in $E_2 \times E_3$ and satisfy

$$F_k(0,0) \;=\; \frac{\partial V}{\partial x}(\overline{x},\overline{\lambda})\, h_k \;=\; 0\, h_k \;=\; 0 \qquad 1 \le k \le n-g' \;.$$

Their partial derivatives with respect to the ξ_ℓ's take the form

$$\frac{\partial F_k}{\partial \xi_\ell}(\xi,\mu) \;=\; \frac{\partial}{\partial \xi_\ell}\left[\frac{\partial V}{\partial x}\Big(\overline{x}+\sum_{j=1}^{n-g'}\xi_j h_j, \overline{\lambda}+\mu\Big)\, h_k\right] \;=\; h_\ell^\dagger\, \frac{\partial^2 V}{\partial x^2}\Big(\overline{x}+\sum_{j=1}^{n-g'}\xi_j h_j, \overline{\lambda}+\mu\Big)\, h_k$$

with $1 \le \ell, k \le n-g'$, and for $(\xi,\mu)=(0,0)$ become

$$\frac{\partial F_k}{\partial \xi_\ell}(0,0) \;=\; h_\ell^\dagger\, H_V(\overline{x},\overline{\lambda})\, h_k \;=\; M_{\ell k} \qquad 1 \le \ell, k \le n-g' \;.$$

As a consequence, if the matrix M is nonsingular, by the Implicit Function Theorem we have that there exist some — uniquely determined — C^{k-1}-functions of an open neighborhood $E_3' \subseteq E_3$ of $\mu = 0$ with range in an open neighborhood $E_2' \subseteq E_2$ of $\xi = 0$:

$$\xi_k \;=\; \xi_k(\mu) \qquad 1 \le k \le n-g'$$

such that $\xi_k(0) = 0 \;\forall\, k = 1,\ldots,n-g'$ and the set of equations (3.9) is satisfied $\forall \mu \in E_3'$:

$$\frac{\partial V}{\partial x}\Big(\overline{x}+\sum_{j=1}^{n-g'}\xi_j(\mu) h_j, \overline{\lambda}+\mu\Big)\, h_k \;=\; 0 \qquad 1 \le k \le n-g' \;. \qquad \forall\, \mu \in E_3' \;,$$

Recalling the transformation (3.8), the proof of Lemma 3 is complete. $\square$

The central point is now to provide conditions in order that the matrix M is actually nonsingular, as required by Lemma 3. To this end the statement below is helpful .

Lemma 4. Rank of the Hessian matrix $H_V(\overline{x},\overline{\lambda})$.

The following upper bound is always satisfied

$$\mathrm{Rank} H_V(\overline{x},\overline{\lambda}) \;\le\; n-g' \;. \qquad \square$$

Proof

From $V(x,\lambda) = V[R(\alpha)\,x,\lambda]\ \forall\,\alpha,\xi,\lambda$, by calculating the partial derivative with respect to α_i, $1 \le i \le g$, we obtain

$$0 \;=\; \frac{\partial V}{\partial x}[R(\alpha)\,x,\lambda]\frac{\partial R}{\partial \alpha_i}(\alpha)\,x \;=\; \sum_{r,s=1}^{n} \frac{\partial V}{\partial x_r}[R(\alpha)\,x,\lambda]\left(\frac{\partial R}{\partial \alpha_i}(\alpha)\right)_{rs} x_s$$

and a further partial derivative with respect to x_t provides

$$0 = \sum_{r,s=1}^{n} \frac{\partial V}{\partial x_r}[R(\alpha)\,x,\lambda]\left(\frac{\partial R}{\partial \alpha_i}(\alpha)\right)_{rs}\delta_{st} + \sum_{r,s=1}^{n}\sum_{u=1}^{n} \frac{\partial^2 V}{\partial x_u \partial x_r}[R(\alpha)\,x,\lambda]\,R(\alpha)_{ut}\left(\frac{\partial R}{\partial \alpha_i}(\alpha)\right)_{rs} x_s$$

In particular, in the point $(x,\lambda) = (\overline{x},\overline{\lambda})$ we get for $\alpha = 0$,

$$0 = \sum_{r,s=1}^{n} \frac{\partial V}{\partial x_r}(\overline{x},\overline{\lambda})\left(\frac{\partial R}{\partial \alpha_i}(0)\right)_{rs}\delta_{st} + \sum_{r,s=1}^{n}\sum_{u=1}^{n} \frac{\partial^2 V}{\partial x_u \partial x_r}(\overline{x},\overline{\lambda})\,\delta_{ut}\left(\frac{\partial R}{\partial \alpha_i}(0)\right)_{rs} \overline{x}_s$$

and since $\dfrac{\partial V}{\partial x_r}(\overline{x},\overline{\lambda}) = 0\ \forall\, r = 1,\ldots,n$, it follows that

$$\sum_{r=1}^{n} \frac{\partial^2 V}{\partial x_t \partial x_r}(\overline{x},\overline{\lambda}) \sum_{s=1}^{n}\left(\frac{\partial R}{\partial \alpha_i}(0)\right)_{rs} \overline{x}_s \;=\; 0 \qquad 1 \le t \le n\;, \quad 1 \le i \le g$$

and finally

$$H_V(\overline{x},\overline{\lambda})\,\frac{\partial R}{\partial \alpha_i}(0)\,\overline{x} \;=\; 0 \qquad 1 \le i \le g\;. \tag{3.11}$$

The latter relation implies that the g' linearly independent vectors $\dfrac{\partial R}{\partial \alpha_i}(0)\,\overline{x}$, $1 \le i \le g'$, belong to the kernel of the Hessian matrix $H_V(\overline{x},\overline{\lambda})$. This is equivalent to claim that $\dim \operatorname{Ker} H_V(\overline{x},\overline{\lambda}) \;\ge\; g'$ and therefore $\operatorname{Rank} H_V(\overline{x},\overline{\lambda}) \;\le\; n - g'$. $\square$

Lemma 5. Nonsingular matrix M.

A necessary and sufficient condition for M to be nonsingular is that

$$\operatorname{Rank} H_V(\overline{x},\overline{\lambda}) \;=\; n - g'\;. \qquad \square$$

Proof

We show that $\mathrm{Rank}\, H_V(\overline{x},\overline{\lambda}) = n - g'$ if and only if $\{z \in \mathbb{R}^n \,:\, Mz = 0\} = \{0\}$.

(i) Let $Mz = 0$ only if $z = 0$. We want to prove that in such a case $\mathrm{Rank}\, H_V(\overline{x},\overline{\lambda}) = n - g'$. If it were $\mathrm{Rank}\, H_V(\overline{x},\overline{\lambda}) < n - g'$, then $\dim \mathrm{Ker}\, H_V(\overline{x},\overline{\lambda}) > g'$ and there would exist a vector $h_0 \in \mathbb{R}^n \backslash \{0\}$ linearly independent on $\dfrac{\partial R}{\partial \alpha_i}(0)\,\overline{x}$, $1 \le i \le g'$, such that $H_V(\overline{x},\overline{\lambda})\, h_0 = 0$. But since $\left\{\dfrac{\partial R}{\partial \alpha_i}(0)\,\overline{x}\,,\ 1 \le i \le g'\right\} \cup \{h_k\,,\ 1 \le k \le n - g'\}$ is a base of $\mathbb{R}^n$, there must hold

$$h_0 \,=\, \sum_{i=1}^{g'} \eta_i \,\frac{\partial R}{\partial \alpha_i}(0)\,\overline{x} \,+\, \sum_{j=1}^{n-g'} \nu_j\, h_j$$

with at least one scalar coefficient ν_j different from zero — if not, h_0 would be linearly dependent of $\dfrac{\partial R}{\partial \alpha_i}(0)\,\overline{x}$, $1 \le i \le g'$. Then, owing to (3.11),

$$0 \,=\, H_V(\overline{x},\overline{\lambda})\, h_0 \,=\, \sum_{j=1}^{n-g'} \nu_j\, H_V(\overline{x},\overline{\lambda})\, h_j$$

and left-multiplying both sides by $h_i^\dagger$ we get

$$\sum_{j=1}^{n-g'} h_i^\dagger\, H_V(\overline{x},\overline{\lambda})\, h_j\, \nu_j \,=\, 0 \qquad 1 \le i \le n - g' \tag{3.12}$$

namely

$$\sum_{j=1}^{n-g'} M_{ij}\nu_j \,=\, 0 \qquad 1 \le i \le n - g'$$

and therefore $Mz_0 = 0$ with $z_0^\dagger = (\nu_1 \ldots \nu_{n-g'}) \neq 0$ since not all the ν_i's are zero. This contradicts the hypothesis.

(ii) Let $\mathrm{Rank}\, H_V(\overline{x},\overline{\lambda}) = n - g'$. We claim that $Mz = 0$ only for $z = 0$. If a $z_0 \neq 0$ existed such that $Mz_0 = 0$, then by posing $z_0^\dagger = (\nu_1 \ldots \nu_{n-g'})$ we would have

$$\sum_{j=1}^{n-g'} M_{ij}\nu_j \,=\, 0 \qquad 1 \le i \le n - g'$$

and therefore (3.12) would hold. Notice that for every $w \in \mathbb{R}^n$ we can write, with appropriate $w_k \in \mathbb{R}$, $1 \le k \le n$,

$$w = \sum_{k=1}^{g'} w_k \, \frac{\partial R}{\partial \alpha_k}(0)\, \overline{x} + \sum_{i=1}^{n-g'} w_{g'+i}\, h_i$$

and therefore

$$w^\dagger = \sum_{k=1}^{g'} w_k \left(\frac{\partial R}{\partial \alpha_k}(0)\, \overline{x} \right)^\dagger + \sum_{i=1}^{n-g'} w_{g'+i}\, h_i^\dagger$$

so that

$$w^\dagger \, H_V(\overline{x}, \overline{\lambda}) \Big(\sum_{j=1}^{n-g'} \nu_j h_j \Big) =$$

$$= \sum_{k=1}^{g'} w_k \left(\frac{\partial R}{\partial \alpha_k}(0)\, \overline{x} \right)^\dagger H_V(\overline{x}, \overline{\lambda}) \Big(\sum_{j=1}^{n-g'} \nu_j h_j \Big) + \sum_{i=1}^{n-g'} w_{g'+i}\, h_i^\dagger \, H_V(\overline{x}, \overline{\lambda}) \Big(\sum_{j=1}^{n-g'} \nu_j h_j \Big)$$

where, owing to (3.12),

$$h_i^\dagger \, H_V(\overline{x}, \overline{\lambda}) \Big(\sum_{j=1}^{n-g'} \nu_j h_j \Big) = 0 \qquad 1 \le i \le n - g' \, ,$$

while

$$\left(\frac{\partial R}{\partial \alpha_k}(0)\, \overline{x} \right)^\dagger H_V(\overline{x}, \overline{\lambda}) = \left(H_V(\overline{x}, \overline{\lambda}) \, \frac{\partial R}{\partial \alpha_k}(0)\, \overline{x} \right)^\dagger = 0 \qquad 1 \le k \le g' \, .$$

Thus

$$w^\dagger \, H_V(\overline{x}, \overline{\lambda}) \Big(\sum_{j=1}^{n-g'} \nu_j h_j \Big) = 0 \qquad \forall \, w \in \mathbb{R}^n$$

and finally

$$H_V(\overline{x}, \overline{\lambda}) \Big(\sum_{j=1}^{n-g'} \nu_j h_j \Big) = 0 \, .$$

As a consequence, the vector $h_0 = \sum_{j=1}^{n-g'} \nu_j h_j \ne 0$ satisfies $H_V(\overline{x}, \overline{\lambda})\, h_0 = 0$. In other words, $h_0 = \sum_{j=1}^{n-g'} \nu_j h_j \ne 0$ belongs to $\operatorname{Ker} H_V(\overline{x}, \overline{\lambda})$. However, since h_0 is linearly independent on $\dfrac{\partial R}{\partial \alpha_i}(0)\, \overline{x} \in \operatorname{Ker} H_V(\overline{x}, \overline{\lambda})$, $1 \le i \le g'$ — if not, $\Big\{ \dfrac{\partial R}{\partial \alpha_i}(0)\, \overline{x} \, , \; 1 \le i \le g' \Big\} \cup$

$\{h_k\,,\ 1 \le k \le n-g'\}$ would not be a base of $\mathbb{R}^n$ —, we deduce that $\dim \operatorname{Ker} H_V(\overline{x},\overline{\lambda}) > g'$, i.e., the contradictory statement that $\operatorname{Rank} H_V(\overline{x},\overline{\lambda}) < n - g'$. $\square$

Proof of Theorem 1

The proof of Theorem 1 for $0 < g' < g$ is now an immediate application of the previous Lemmas 1 to 5. We simply have to identify the open sets E_1, E_3' and $\Phi(E_1 \times E_2' \times E_3')$ in Lemma 3 with the sets E_0, E_0', B_0 of the main statement, respectively.

All the previous lemmas trivially extend to the case $g' = g$, by observing that $\alpha' = \alpha$ and that therefore the matrix $R(\alpha', 0)$ must be replaced with $R(\alpha)$ everywhere.

Finally, whenever $g' = 0$ we have that all the vectors $\dfrac{\partial R}{\partial \alpha_i}(0)\,\overline{x}$, $1 \le i \le g$ are zero and the invariance properties of V cannot be used in the same way as in the previous discussion. In particular, Lemma 1 becomes trivial since the local change of coordinates (3.3) is simply an arbitrary invertible linear transformation defined in a neighborhood of $(x,\lambda) = (\overline{x},\overline{\lambda})$ with respect to an arbitrary base $\{h_i\,,\ 1 \le i \le n\}$ of $\mathbb{R}^n$. Correspondingly, Lemmas 2, 3 and 4 become trivial as well, although the matrix M can certainly be defined. Lemma 5 is applicable, but it takes the straightforward form that M is nonsingular if and only if $H_V(\overline{x},\overline{\lambda})$ is, no more than an observation. Theorem 1 holds, but it comes from an immediate application of the Implicit Function Theorem. We have indeed that the C^{k-1}-function $(x,\lambda) \in \Omega \times \Lambda \longrightarrow \dfrac{\partial V}{\partial x}(x,\lambda) \in \mathbb{R}^n$, $k \ge 2$, satisfies the conditions

$$\frac{\partial V}{\partial x}(\overline{x},\overline{\lambda}) = 0 \qquad \det \frac{\partial^2 V}{\partial x^2}(\overline{x},\overline{\lambda}) = \det H_V(\overline{x},\overline{\lambda}) \ne 0$$

so that Implicit Function Theorem ensures the existence of open neighborhoods $\Omega' \subseteq \Omega$ of $\overline{x}$ and $\Lambda' \subseteq \Lambda$ of $\overline{\lambda}$, together with an application $\varphi : \Lambda' \longrightarrow \Omega'$, such that:

φ is a C^{k-1}-function in Λ'

$\varphi(\overline{\lambda}) = \overline{x}$

$$\frac{\partial V}{\partial x}(\varphi(\lambda), \lambda) = 0 \;\forall\, \lambda \in \Lambda'.$$

We can then pose $B_0 = \Omega' \times \Lambda'$ and $E_0' = \Lambda' - \overline{\lambda}$, and claim that all the solutions in B_0 of $\dfrac{\partial V}{\partial x}(x, \lambda) = 0$ can be characterized as

$$x = \varphi(\lambda) = \overline{x} + \varphi(\overline{\lambda} + \mu) - \overline{x} = \overline{x} + \sum_{j=1}^{n} \xi_j(\mu)\, h_j$$

being $\xi_j(\mu)$ the j-th component of $\varphi(\overline{\lambda} + \mu) - \overline{x}$ with respect to the base $\{h_i\,,\ 1 \le i \le n\}$. Since $\xi_j(\mu)$ is obviously as C^{k-1} as $\varphi(\lambda)$ and $\xi_j(0) = 0$ owing to $\varphi(\overline{\lambda}) - \overline{x} = 0$, we conclude that the statement of Theorem 1 is verified. $\square$

Remark

The case $g' = n$ has been explicitly excluded in the statement of Theorem 1. This is due to a sort of degeneracy which occurs and makes the structure of the critical point set very trivial, in some sense. It is clear that Lemma 1 still holds, even if the introduction of the auxiliary vectors h_j is no more necessary. Lemma 1 takes now the particular form stated below, whose proof is exactly the same previously illustrated.

Lemma 1.a Local change of variables for $g' = n$.

An open neighborhood $A = \mathrm{int}(A)$ of the point $(\alpha', \mu) = (0, 0)$ and an open neighborhood $B = \mathrm{int}(B) \subset \mathbb{R}^n \times \mathbb{R}^p$ of $(x, \lambda) = (\overline{x}, \overline{\lambda})$ exist such that the application $\Phi : (\alpha', \mu) \in A \longrightarrow (x, \lambda) \in B$ defined by

$$x = R(\alpha', 0)\, \overline{x} \qquad \lambda = \overline{\lambda} + \mu \tag{3.13}$$

is a C^k diffeomorphism of A onto B. $\square$

Of course the same result also extends to the case of $g' = g$, with the replacement of α and $R(\alpha)$ to α' and $R(\alpha', 0)$ respectively.

For any $(x,\lambda) \in B$ we have then, by applying (3.13) and the invariance property of V,

$$V(x,\lambda) \;=\; V[R(\alpha',0)\,\overline{x},\overline{\lambda}+\mu] \;=\; V(\overline{x},\overline{\lambda}+\mu)$$

which means that the restriction of V to B is constant at fixed λ. As a consequence,

$$\frac{\partial V}{\partial x}(x,\lambda) \;=\; 0 \qquad \forall\,(x,\lambda) \in B$$

so that the whole set B consists of critical points of V_λ.

The previous Theorem 1 admits a very simple geometrical interpretation. Equation (3.4) implies that if x is a solution of $\dfrac{\partial V}{\partial x}(x,\lambda) = 0$, then $R(\alpha)\,x$ also is, provided that $R(\alpha)$ is nonsingular. This means that at a fixed $\lambda \in \Lambda$ the global set of the critical points of V_λ in Ω is a union of "fibers" like $F_y = \{x = R(\alpha)\,y\,,\ \alpha \in U\}$, with y critical. Generally speaking, fibers are not disjoint subsets of Ω, but it is anyway possible to detect some trivially nonintersecting fibers by means of the invariance property on V, without further hypotheses on the matrices $R(\alpha)$. Indeed, since $V[R(\alpha)x,\lambda] = V(x,\lambda)\ \forall x \in \Omega$, $\alpha \in U$, $\lambda \in \Lambda$, the fibers

$$F_{y_1} = \{x = R(\alpha)\,y_1\,,\ \alpha \in U\} \qquad F_{y_2} = \{x = R(\alpha)\,y_2\,,\ \alpha \in U\}$$

are certainly disjoint whenever the critical points $y_1, y_2 \in \Omega$ satisfy $V(y_1) \neq V(y_2)$. The local structure of the critical point set described by Theorem 1 provides more specific informations about fiber distribution — see Figure 1.

We firstly notice that we can always assume, without loss of generality, $B_0 = B_0' \times \Lambda_0$, being $B_0' = \mathrm{int}(B_0') \subset \Omega$ and $\Lambda_0 = \mathrm{int}(\Lambda_0) \subset \Lambda$ appropriate neighborhoods of $\overline{x}$ and $\overline{\lambda}$ respectively. Denoted with $\mathcal{L}$ the linear subspace spanned by $\{h_j\,,\ 1 \leq j \leq n-g'\}$ and with $\overline{x}+\mathcal{L}$ the relative linear maniforld passing through $\overline{x}$, Theorem 1 implies that for any fixed $\lambda \in \Lambda_0$ the only critical point of V_λ in $B'_0 \cap (\overline{x}+\mathcal{L})$ is

$$x_0 \;=\; \overline{x} + \sum_{j=1}^{n-g'} \xi_j(\lambda - \overline{\lambda})\, h_j \;.$$

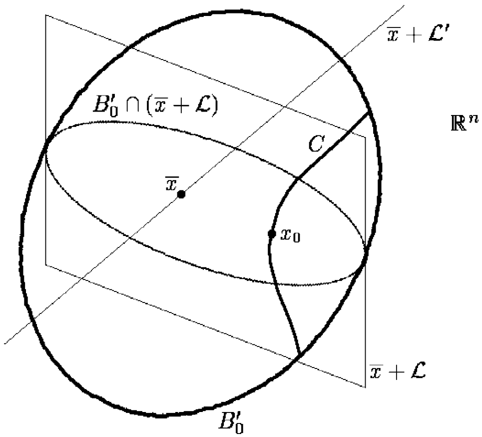

Figure 1: Local distribution of the critical points. Here $\mathcal{L}'$ stands for the linear subspace spanned by $\{\partial R/\partial\alpha_i(0)\,\overline{x}\,,\ 1 \le i \le g'\}$. Obviously, $\mathcal{L}\oplus\mathcal{L}' = \mathbb{R}^n$.

Moreover, there is a unique fiber F_{x_0} which intersects B'_0, and the intersection $C = B'_0 \cap F_{x_0}$ — set of all the critical point of V_λ in B'_0 — is given by

$$C \;=\; \big\{ x = R(\alpha', 0)\, x_0 \,,\ \alpha' \in E_0 \big\} \;.$$

Theorem 1 can be used to stem a simple estimate to the displacement of critical points as the parameter λ is slightly varied. A straightforward application of Taylor's approximation formula leads to the result below.

Corollary 1

Under the same hypotheses and with the same notations of Theorem 1, the solutions of $\dfrac{\partial V}{\partial x}(x,\lambda) = 0$ *in* B_0 *are individuated by the relationship*

$$x \;=\; R(\alpha', \underbrace{0,\ldots,0}_{g-g'}) \Big[\overline{x} - \sum_{q=1}^{p} \mu_q \sum_{j=1}^{n-g'} h_j \sum_{i=1}^{n-g'} (M^{-1})_{ji} \Big[\frac{\partial}{\partial \lambda_q}\Big(\frac{\partial V}{\partial x}\Big)\Big](\overline{x},\overline{\lambda})\, h_i + o(\|\mu\|)\Big] \quad (3.14)$$

where $\|\;\|$ *denotes the usual Euclidean norm of* $\mathbb{R}^p$, $\mu \in E_0'$, $\lim_{\mu\to 0} o(\|\mu\|)/\|\mu\| = 0$ *and* $M_{ij} = h_i^\dagger H_V(\overline{x},\overline{\lambda}) h_j$, $1 \le i,j \le n-g'$. □

Proof

We have to calculate the first partial derivatives of the functions $\xi_j(\mu)$ in $\mu = 0$, by applying then a first order Taylor's approximation to equation (3.2). By means of Lemma 3 we have the relationships

$$\frac{\partial V}{\partial x}\Big[\overline{x} + \sum_{j=1}^{n-g'} \xi_j(\mu)\, h_j, \overline{\lambda} + \mu\Big]\, h_i \;=\; 0 \qquad \forall\, \mu \in E_3' \equiv E_0' \quad 1 \le k \le n-g' \;. \qquad (3.15)$$

The partial derivatives of the left-hand side functions in (3.15) with respect to the variables μ_q, $1 \le q \le p$, are then identically zero and lead to the equations

$$\sum_{k=1}^{n-g'} h_k^\dagger \,\frac{\partial^2 V}{\partial x^2}\Big(\overline{x} + \sum_{j=1}^{n-g'} \xi_j(\mu)\, h_j, \overline{\lambda}+\mu\Big)\, h_i\, \frac{\partial \xi_k}{\partial \mu_q}(\mu) + \frac{\partial}{\partial \mu_q}\Big(\frac{\partial V}{\partial x}\Big)\Big(\overline{x} + \sum_{j=1}^{n-g'} \xi_j(\mu)\, h_j, \overline{\lambda}+\mu\Big)\, h_i = 0$$

verified $\forall\, \mu \in E_0'$, $1 \le i \le n-g'$ and $1 \le q \le p$. In $\mu = 0$ there holds, in particular,

$$\sum_{k=1}^{n-g'} h_k^\dagger\, H_V(\overline{x},\overline{\lambda})\, h_i\, \frac{\partial \xi_k}{\partial \mu_q}(0) \;+\; \Big[\frac{\partial}{\partial \lambda_q}\Big(\frac{\partial V}{\partial x}\Big)\Big](\overline{x},\overline{\lambda})\, h_i \;=\; 0 \qquad 1 \le i \le n-g' \quad 1 \le q \le p$$

which, once the nonsingular matrix M is introduced, takes the equivalent form

$$\sum_{k=1}^{n-g'} M_{ki}\, \frac{\partial \xi_k}{\partial \mu_q}(0) \;+\; \Big[\frac{\partial}{\partial \lambda_q}\Big(\frac{\partial V}{\partial x}\Big)\Big](\overline{x},\overline{\lambda})\, h_i \;=\; 0 \qquad 1 \le i \le n-g' \quad 1 \le q \le p$$

namely, owing to the symmetry of M,

$$\sum_{k=1}^{n-g'} M_{ik}\, \frac{\partial \xi_k}{\partial \mu_q}(0) \;+\; \Big[\frac{\partial}{\partial \lambda_q}\Big(\frac{\partial V}{\partial x}\Big)\Big](\overline{x},\overline{\lambda})\, h_i \;=\; 0 \qquad 1 \le i \le n-g' \quad 1 \le q \le p \;.$$

If now both sides are multiplied by $(M^{-1})_{ji}$ and a sum over the index i is performed, we deduce

$$\sum_{i,k=1}^{n-g'} (M^{-1})_{ji} M_{ik} \frac{\partial \xi_k}{\partial \mu_q}(0) + \sum_{i=1}^{n-g'} (M^{-1})_{ji} \Big[\frac{\partial}{\partial \lambda_q}\Big(\frac{\partial V}{\partial x}\Big)\Big](\overline{x},\overline{\lambda})\, h_i = 0$$

and finally

$$\frac{\partial \xi_j}{\partial \mu_q}(0) = -\sum_{i=1}^{n-g'} (M^{-1})_{ji} \Big[\frac{\partial}{\partial \lambda_q}\Big(\frac{\partial V}{\partial x}\Big)\Big](\overline{x},\overline{\lambda})\, h_i \qquad 1 \le j \le n-g' \quad 1 \le q \le p\,. \tag{3.16}$$

The first order Taylor's approximation of (3.2) in $\mu = 0$ provides therefore

$$x = R(\alpha_1, \dots, \alpha_{g'}, \underbrace{0, \dots, 0}_{g-g'}) \Big[\overline{x} + \sum_{q=1}^{p} \mu_q \sum_{j=1}^{n-g'} \frac{\partial \xi_j}{\partial \mu_q}(0)\, h_j + o(\|\mu\|)\Big]$$

where $\dfrac{\partial \xi_j}{\partial \mu_q}(0)$ is determined by (3.16). $\square$

Remark

Formulas (3.2) and (3.14) explicitly contain the vectors h_j's and may suggest the idea that such a dependence is real. Obviously this is not the case. The possible, different choice of the complementary vectors h_j's in (3.2) or (3.14) simply provides a different local representation of the same critical point set, whenever (3.1) constitutes a base of $\mathbb{R}^n$ — apart from this requirement, the set of h_j's is completely arbitrary.

We have in particular the two corollaries below.

Corollary 2

Under the same hypotheses and with the same notations of Theorem 1, let $\{h'_j\,,\ 1 \le j \le n-g'\}$ be a set of linearly independent vectors beloging to the linear space spanned by $\{h_i\,,\ 1 \le i \le n-g'\}$. Then the local representation (3.14) of the critical point set is equivalent to

$$x = R(\alpha', \underbrace{0, \dots, 0}_{g-g'}) \Big[\overline{x} - \sum_{q=1}^{p} \mu_q \sum_{j=1}^{n-g'} h'_j \sum_{i=1}^{n-g'} (M'^{-1})_{ji} \Big[\frac{\partial}{\partial \lambda_q}\Big(\frac{\partial V}{\partial x}\Big)\Big](\overline{x},\overline{\lambda})\, h'_i + o(\|\mu\|)\Big] \tag{3.17}$$

where M' is the $(n-g')\times(n-g')$ matrix of entries $M'_{\ell j} = {h'}_{\ell}^{\dagger} H_V(\overline{x},\overline{\lambda})\, h'_j$, $1 \le \ell, j \le n-g'$.

□

Proof

The vectors h'_j's and h_i's are related by

$$h_i = \sum_{j=1}^{n-g'} c_{ij} h'_j \tag{3.18}$$

and the matrix C of entries c_{ij}, $1 \le i, j \le n-g'$, is obviously nonsingular owing to the linear independency of both sets. We show that equation (3.17) stems from (3.14) by inserting (3.18). We firstly notice that

$$M_{ki} = \Big[\sum_{\ell=1}^{n-g'} c_{k\ell} h'_\ell\Big]^{\dagger} H_V(\overline{x},\overline{\lambda}) \sum_{j=1}^{n-g'} c_{ij} h'_j = \sum_{\ell,j=1}^{n-g'} c_{k\ell} {h'}_{\ell}^{\dagger} H_V(\overline{x},\overline{\lambda})\, h'_j c_{ij} = \sum_{\ell,j=1}^{n-g'} c_{k\ell} M'_{\ell j} (C^{\dagger})_{ji}$$

or, equivalently, that $C\, M'\, C^{\dagger} = M$. M' is nonsingular if and only if M is. Under the hypothesis of nonsingular M we can write $M^{-1} = (C^{\dagger})^{-1} {M'}^{-1} C^{-1}$ and the expression

$$\overline{x} - \sum_{q=1}^{p} \mu_q \sum_{j=1}^{n-g'} h_j \sum_{i=1}^{n-g'} (M^{-1})_{ji} \Big[\frac{\partial}{\partial \lambda_q}\Big(\frac{\partial V}{\partial x}\Big)\Big](\overline{x},\overline{\lambda})\, h_i + o(\|\mu\|) \tag{3.19}$$

becomes

$$\overline{x} - \sum_{q=1}^{p} \mu_q \sum_{j,j'=1}^{n-g'} c_{jj'} h'_{j'} \sum_{i=1}^{n-g'} \big[(C^{\dagger})^{-1} {M'}^{-1} C^{-1}\big]_{ji} \Big[\frac{\partial}{\partial \lambda_q}\Big(\frac{\partial V}{\partial x}\Big)\Big](\overline{x},\overline{\lambda}) \sum_{i'=1}^{n-g'} c_{ii'} h'_{i'} + o(\|\mu\|) =$$

$$= \overline{x} - \sum_{q=1}^{p} \mu_q \sum_{j'=1}^{n-g'} h'_{j'} \sum_{i'=1}^{n-g'} ({M'}^{-1})_{j'i'} \Big[\frac{\partial}{\partial \lambda_q}\Big(\frac{\partial V}{\partial x}\Big)\Big](\overline{x},\overline{\lambda})\, h'_{i'} + o(\|\mu\|)$$

which after left-multiplication by $R(\alpha', 0)$ takes precisely the same form of (3.17). □

Corollary 3

Under the same hypotheses and with the same notations of Theorem 1, let $\{h'_j\,,\ 1 \le j \le n-g'\} \subset \mathbb{R}^n$ be a set of linearly independent vectors such that

$$\Big\{\frac{\partial R}{\partial \alpha_i}(0)\,\overline{x}\,,\ 1 \le i \le g'\Big\} \cup \{h'_j\,,\ 1 \le j \le n-g'\}$$

is a base of $\mathbb{R}^n$*. Then the relationships*

$$x \;=\; R(\alpha',\underbrace{0,\ldots,0}_{g-g'})\Big[\overline{x} - \sum_{q=1}^{p}\mu_q \sum_{j=1}^{n-g'} h_j \sum_{i=1}^{n-g'}(M^{-1})_{ji}\Big[\frac{\partial}{\partial\lambda_q}\Big(\frac{\partial V}{\partial x}\Big)\Big](\overline{x},\overline{\lambda})\,h_i + o(\|\mu\|)\Big] \quad (3.20)$$

and

$$x \;=\; \overline{x} - \sum_{q=1}^{p}\mu_q \sum_{j=1}^{n-g'} h'_j \sum_{i=1}^{n-g'}({M'}^{-1})_{ji}\Big[\frac{\partial}{\partial\lambda_q}\Big(\frac{\partial V}{\partial x}\Big)\Big](\overline{x},\overline{\lambda})\,h'_i + o(\|\mu\|) \qquad (3.21)$$

coincide for a suitable choice of the vector parameter $\alpha' = \Pi\mu + o(\|\mu\|)$*, being* Π *a constant* $g' \times p$ *real matrix.* $\square$

Proof

If, as assumed, $\Big\{\dfrac{\partial R}{\partial\alpha_i}(0)\,\overline{x}\,,\; 1 \le i \le g'\Big\} \cup \{h_j\,,\; 1 \le j \le n-g'\}$ constitutes a base of $\mathbb{R}^n$, any other base of the form

$$\Big\{\frac{\partial R}{\partial\alpha_i}(0)\,\overline{x}\,,\; 1 \le i \le g'\Big\} \cup \{h'_j\,,\; 1 \le j \le n-g'\}$$

is characterized by the relationships

$$h_i \;=\; \sum_{j=1}^{n-g'} c_{ij}h'_j + \sum_{k=1}^{g'} d_{ik}\frac{\partial R}{\partial\alpha_k}(0)\,\overline{x} \qquad 1 \le i \le n-g'$$

in terms of appropriate real coefficients c_{ij} and d_{ik}, $1 \le i,j \le n-g'$, $1 \le k \le g'$. The matrix C of entries $C_{ij} = c_{ij}$, $1 \le i,j \le n-g'$ is nonsingular. Indeed, the matrix T of the base transformation comes from

$$\begin{cases} \dfrac{\partial R}{\partial\alpha_\ell}(0)\,\overline{x} \;=\; \dfrac{\partial R}{\partial\alpha_\ell}(0)\,\overline{x} & 1 \le \ell \le g' \\[2ex] h_i \;=\; \displaystyle\sum_{k=1}^{g'} d_{ik}\frac{\partial R}{\partial\alpha_k}(0)\,\overline{x} + \sum_{j=1}^{n-g'} c_{ij}h'_j & 1 \le i \le n-g' \end{cases}$$

and is written as

$$T \;=\; \begin{pmatrix} \boxed{\begin{matrix}\mathbb{I} \\ g' \times g'\end{matrix}} & \boxed{\begin{matrix}d_{ki}\;\; 1\le k\le g'\;\; 1\le i\le n-g' \\ g' \times (n-g')\end{matrix}} \\[2ex] \boxed{\begin{matrix}\mathbb{O} \\ (n-g') \times g'\end{matrix}} & \boxed{\begin{matrix}c_{ji}\;\; 1\le i,j\le n-g' \\ (n-g') \times (n-g')\end{matrix}} \end{pmatrix}$$

with determinant $\det T = \det C^\dagger = \det C$. Since $\det T \neq 0$, we deduce that also $\det C \neq 0$ so that C is nonsingular.

The entries of the matrix M can be calculated in terms of the new base according to the expression

$$M_{ki} = \Big[\sum_{k'=1}^{g'} d_{kk'} \frac{\partial R}{\partial \alpha_{k'}}(0)\,\overline{x} + \sum_{\ell=1}^{n-g'} c_{k\ell} h'_\ell\Big]^\dagger H_V(\overline{x},\overline{\lambda}) \Big[\sum_{i'=1}^{g'} d_{ii'} \frac{\partial R}{\partial \alpha_{i'}}(0)\,\overline{x} + \sum_{j=1}^{n-g'} c_{ij} h'_j\Big] =$$

$$= \sum_{j=1}^{n-g'} c_{ij} \Big[\sum_{k'=1}^{g'} d_{kk'} \frac{\partial R}{\partial \alpha_{k'}}(0)\,\overline{x} + \sum_{\ell=1}^{n-g'} c_{k\ell} h'_\ell\Big]^\dagger H_V(\overline{x},\overline{\lambda})\, h'_j$$

because $H_V(\overline{x},\overline{\lambda}) \dfrac{\partial R}{\partial \alpha_{i'}}(0)\,\overline{x} = 0$, $1 \leq i' \leq g'$, for any critical point $\overline{x}$ of $V_{\overline{\lambda}}$. Moreover, the symmetry of $H_V(\overline{x},\overline{\lambda})$ implies

$$\Big[\frac{\partial R}{\partial \alpha_{k'}}(0)\,\overline{x}\Big]^\dagger H_V(\overline{x},\overline{\lambda}) = \Big[H_V(\overline{x},\overline{\lambda})\, \frac{\partial R}{\partial \alpha_{k'}}(0)\,\overline{x}\Big]^\dagger = 0 \qquad 1 \leq k' \leq g'$$

and therefore the further simplification

$$M_{ki} = \sum_{j,\ell=1}^{n-g'} c_{ij}\, c_{k\ell}\, h'_\ell\, H_V(\overline{x},\overline{\lambda})\, h'_j = \sum_{j,\ell=1}^{n-g'} c_{k\ell} M'_{\ell j} (C^\dagger)_{ji} = (CM'C^\dagger)_{ki}$$

which is equivalent to the matrix expression $M = CM'C^\dagger$. We deduce that $M^{-1} = (C^\dagger)^{-1} {M'}^{-1} C^{-1}$ and that the sum

$$\sum_{i,j=1}^{n-g'} h_j\,(M^{-1})_{ji} \Big[\frac{\partial}{\partial \lambda_q}\Big(\frac{\partial V}{\partial x}\Big)\Big](\overline{x},\overline{\lambda})\, h_i$$

in (3.20) becomes

$$\sum_{i,j=1}^{n-g'} [(C^\dagger)^{-1} {M'}^{-1} C^{-1}]_{ji} \Big(\sum_{k'=1}^{g'} d_{jk'} \frac{\partial R}{\partial \alpha_{k'}}(0)\,\overline{x} + \sum_{j'=1}^{n-g'} c_{jj'} h'_{j'}\Big) \cdot$$

$$\cdot \Big[\frac{\partial}{\partial \lambda_q}\Big(\frac{\partial V}{\partial x}\Big)\Big](\overline{x},\overline{\lambda}) \Big(\sum_{k=1}^{g'} d_{ik} \frac{\partial R}{\partial \alpha_k}(0)\,\overline{x} + \sum_{\ell=1}^{n-g'} c_{i\ell} h'_\ell\Big) =$$

$$= \sum_{i,j=1}^{n-g'} [(C^\dagger)^{-1} {M'}^{-1} C^{-1}]_{ji} \Big(\sum_{k'=1}^{g'} d_{jk'} \frac{\partial R}{\partial \alpha_{k'}}(0)\,\overline{x} + \sum_{j'=1}^{n-g'} c_{jj'} h'_{j'}\Big) \cdot$$

$$\cdot \Big(\sum_{k=1}^{g'} d_{ik} \Big[\frac{\partial}{\partial \lambda_q}\Big(\frac{\partial V}{\partial x}\Big)\Big](\overline{x},\overline{\lambda})\, \frac{\partial R}{\partial \alpha_k}(0)\,\overline{x} + \sum_{\ell=1}^{n-g'} c_{i\ell} \Big[\frac{\partial}{\partial \lambda_q}\Big(\frac{\partial V}{\partial x}\Big)\Big](\overline{x},\overline{\lambda})\, h'_\ell\Big) =$$

$$= \sum_{i,j=1}^{n-g'} [(C^\dagger)^{-1} {M'}^{-1} C^{-1}]_{ji} \sum_{k,k'=1}^{g'} d_{jk'} d_{ik} \frac{\partial R}{\partial \alpha_{k'}}(0)\, \overline{x}\ \Big[\frac{\partial}{\partial \lambda_q}\Big(\frac{\partial V}{\partial x}\Big)\Big](\overline{x},\overline{\lambda})\, \frac{\partial R}{\partial \alpha_k}(0)\, \overline{x} +$$
$$+ \sum_{i,j=1}^{n-g'} [(C^\dagger)^{-1} {M'}^{-1} C^{-1}]_{ji} \sum_{k'=1}^{g'} \sum_{\ell=1}^{n-g'} d_{jk'} c_{i\ell} \frac{\partial R}{\partial \alpha_{k'}}(0)\, \overline{x}\ \Big[\frac{\partial}{\partial \lambda_q}\Big(\frac{\partial V}{\partial x}\Big)\Big](\overline{x},\overline{\lambda})\, h'_\ell +$$
$$+ \sum_{i,j=1}^{n-g'} [(C^\dagger)^{-1} {M'}^{-1} C^{-1}]_{ji} \sum_{j'=1}^{n-g'} \sum_{k=1}^{g'} c_{jj'} d_{ik} h'_{j'}\ \Big[\frac{\partial}{\partial \lambda_q}\Big(\frac{\partial V}{\partial x}\Big)\Big](\overline{x},\overline{\lambda})\, \frac{\partial R}{\partial \alpha_k}(0)\, \overline{x} +$$
$$+ \sum_{i,j=1}^{n-g'} [(C^\dagger)^{-1} {M'}^{-1} C^{-1}]_{ji} \sum_{j',\ell=1}^{n-g'} c_{jj'} c_{i\ell} h'_{j'}\ \Big[\frac{\partial}{\partial \lambda_q}\Big(\frac{\partial V}{\partial x}\Big)\Big](\overline{x},\overline{\lambda})\, h'_\ell$$

and finally

$$\begin{aligned}
&\sum_{k,k'=1}^{g'} \frac{\partial R}{\partial \alpha_{k'}}(0)\, \overline{x}\ \big[D^\dagger (C^\dagger)^{-1} {M'}^{-1} C^{-1} D\big]_{k'k} \Big[\frac{\partial}{\partial \lambda_q}\Big(\frac{\partial V}{\partial x}\Big)\Big](\overline{x},\overline{\lambda})\, \frac{\partial R}{\partial \alpha_k}(0)\, \overline{x} + \\
&+ \sum_{k'=1}^{g'} \sum_{\ell=1}^{n-g'} \frac{\partial R}{\partial \alpha_{k'}}(0)\, \overline{x}\ \big[D^\dagger (C^\dagger)^{-1} {M'}^{-1}\big]_{k'\ell} \Big[\frac{\partial}{\partial \lambda_q}\Big(\frac{\partial V}{\partial x}\Big)\Big](\overline{x},\overline{\lambda})\, h'_\ell + \\
&+ \sum_{j'=1}^{n-g'} \sum_{k=1}^{g'} h'_{j'}\ \big[{M'}^{-1} C^{-1} D\big]_{j'k} \Big[\frac{\partial}{\partial \lambda_q}\Big(\frac{\partial V}{\partial x}\Big)\Big](\overline{x},\overline{\lambda})\, \frac{\partial R}{\partial \alpha_k}(0)\, \overline{x} + \\
&+ \sum_{j',\ell=1}^{n-g'} h'_{j'}\ \big[{M'}^{-1}\big]_{j'\ell} \Big[\frac{\partial}{\partial \lambda_q}\Big(\frac{\partial V}{\partial x}\Big)\Big](\overline{x},\overline{\lambda})\, h'_\ell
\end{aligned} \tag{3.22}$$

on having introduced the matrix D such that $D_{ij} = d_{ij}$, $1 \leq i \leq n-g'$, $1 \leq j \leq g'$. A slight simplification of (3.22) is possible by observing that the equality

$$\frac{\partial V}{\partial x}(R(\alpha)x,\lambda)\, \frac{\partial R}{\partial \alpha_i}(\alpha)\, x \;=\; 0 \qquad \forall\, \alpha \in U\,,\ x \in \Omega\,,\ \lambda \in \Lambda\,, \quad 1 \leq i \leq g\,,$$

implies the vanishing of all the partial derivatives with respect to λ_q, $1 \leq q \leq p$,

$$\Big[\frac{\partial}{\partial \lambda_q}\Big(\frac{\partial V}{\partial x}\Big)\Big](R(\alpha)x,\lambda)\, \frac{\partial R}{\partial \alpha_i}(\alpha)\, x \;=\; 0 \qquad \forall\, \alpha \in U\,,\ x \in \Omega\,,\ \lambda \in \Lambda\,, \quad 1 \leq i \leq g\,,$$

and for $x = \overline{x}$, $\lambda = \overline{\lambda}$, $\alpha = 0$ provides

$$\Big[\frac{\partial}{\partial \lambda_q}\Big(\frac{\partial V}{\partial x}\Big)\Big](\overline{x},\overline{\lambda})\frac{\partial R}{\partial \alpha_i}(0)\, \overline{x} \;=\; 0\,, \quad 1 \leq i \leq g\,,$$

so that (3.22) can be put in the shorter form

$$\sum_{k'=1}^{g'} \sum_{\ell=1}^{n-g'} \frac{\partial R}{\partial \alpha_{k'}}(0)\,\overline{x}\;\big[D^{\dagger}(C^{\dagger})^{-1}{M'}^{-1}\big]_{k'\ell}\Big[\frac{\partial}{\partial\lambda_q}\Big(\frac{\partial V}{\partial x}\Big)\Big](\overline{x},\overline{\lambda})\,h'_\ell +$$

$$+\sum_{j',\ell=1}^{n-g'} h'_{j'}\,\big[{M'}^{-1}\big]_{j'\ell}\Big[\frac{\partial}{\partial\lambda_q}\Big(\frac{\partial V}{\partial x}\Big)\Big](\overline{x},\overline{\lambda})\,h'_\ell\,.$$

By inserting the latter result into equation (3.20), we obtain now

$$\begin{aligned} x \;=\; R(\alpha',0)\Big[&\overline{x} - \sum_{q=1}^{p}\mu_q \sum_{j',\ell=1}^{n-g'} h'_{j'}\,\big[{M'}^{-1}\big]_{j'\ell}\Big[\frac{\partial}{\partial\lambda_q}\Big(\frac{\partial V}{\partial x}\Big)\Big](\overline{x},\overline{\lambda})\,h'_\ell - \\ &- \sum_{q=1}^{p}\mu_q \sum_{k'=1}^{g'} \sum_{\ell=1}^{n-g'} \frac{\partial R}{\partial \alpha_{k'}}(0)\,\overline{x}\;\big[D^{\dagger}(C^{\dagger})^{-1}{M'}^{-1}\big]_{k'\ell}\Big[\frac{\partial}{\partial\lambda_q}\Big(\frac{\partial V}{\partial x}\Big)\Big](\overline{x},\overline{\lambda})\,h'_\ell + o(\|\mu\|)\Big] \end{aligned}$$

where the smoothness of $\alpha \to R(\alpha)$ allows us to introduce the matrix equality

$$\begin{aligned} R(\alpha',0) \;&=\; R(0) + \sum_{k'=1}^{g'} \alpha_{k'}\,\frac{\partial R}{\partial \alpha_{k'}}(0) + o(\|(\alpha',0)\|) \;= \\ &= \mathbb{I} + \sum_{q=1}^{p}\sum_{k'=1}^{g'} \Pi_{k'q}\mu_q\,\frac{\partial R}{\partial \alpha_{k'}}(0) + o(\|\mu\|) + o\big(\big\|(\Pi\mu + o(\|\mu\|),0)\big\|\big)\;. \end{aligned} \tag{3.23}$$

It is evident that $\forall\,\mu \neq 0$, $\|\mu\|$ small enough, there holds $o\big(\big\|(\Pi\mu + o(\|\mu\|),0)\big\|\big)\,/\,\|\mu\| \;=\; 0$ if $\Pi\mu + o(\|\mu\|) = 0$, and

$$\frac{o\big(\big\|(\Pi\mu + o(\|\mu\|),0)\big\|\big)}{\|\mu\|} \;=\; \frac{o\big(\big\|(\Pi\mu + o(\|\mu\|),0)\big\|\big)}{\big\|(\Pi\mu + o(\|\mu\|),0)\big\|}\;\frac{\big\|(\Pi\mu + o(\|\mu\|),0)\big\|}{\|\mu\|} \tag{3.24}$$

if not. As a consequence, since the last factor in the right-hand side of (3.24) is bounded we conclude that $o\big(\big\|(\Pi\mu + o(\|\mu\|),0)\big\|\big) \;=\; o(\|\mu\|)$ and that (3.23) reduces to

$$R(\alpha',0) \;=\; \mathbb{I} + \sum_{q=1}^{p}\mu_q \sum_{k'=1}^{g'} \Pi_{k'q}\,\frac{\partial R}{\partial \alpha_{k'}}(0) + o(\|\mu\|)\;.$$

The further expression follows

$$\begin{aligned} x \;=\; \overline{x} &+ \sum_{q=1}^{p}\mu_q \sum_{k'=1}^{g'} \Pi_{k'q}\,\frac{\partial R}{\partial \alpha_{k'}}(0)\,\overline{x} - \sum_{q=1}^{p}\mu_q \sum_{j',\ell=1}^{n-g'} h'_{j'}\,\big[{M'}^{-1}\big]_{j'\ell}\Big[\frac{\partial}{\partial\lambda_q}\Big(\frac{\partial V}{\partial x}\Big)\Big](\overline{x},\overline{\lambda})\,h'_\ell - \\ &- \sum_{q=1}^{p}\mu_q \sum_{k'=1}^{g'} \sum_{\ell=1}^{n-g'} \frac{\partial R}{\partial \alpha_{k'}}(0)\,\overline{x}\;\big[D^{\dagger}(C^{\dagger})^{-1}{M'}^{-1}\big]_{k'\ell}\Big[\frac{\partial}{\partial\lambda_q}\Big(\frac{\partial V}{\partial x}\Big)\Big](\overline{x},\overline{\lambda})\,h'_\ell + o(\|\mu\|) \end{aligned}$$

which coincides with (3.21) by posing

$$\Pi_{k'q} = \sum_{\ell=1}^{n-g'} \left[D^\dagger (C^\dagger)^{-1} M'^{-1}\right]_{k'\ell} \Big[\frac{\partial}{\partial \lambda_q}\Big(\frac{\partial V}{\partial x}\Big)\Big](\overline{x}, \overline{\lambda})\, h'_\ell$$

for $1 \le k' \le g'$ and $1 \le q \le p$. $\square$

4. Estimate of errors

For each fixed λ in a neighborhood of $\overline{\lambda}$ the function V_λ admits a set of critical points in a neighborhood of $\overline{x}$ which is locally described by (3.14).

A reasonable way to represent the changement of the critical points of V_λ when λ varies may be to consider the only point $x(\lambda)$ of intersection between the critical point set and the linear manifold individuated by $\overline{x}$ and $\{h_j\,,\ 1 \le j \le n-g'\}$ — the other critical points are individuated by applying an appropriate invariance transformation $R(\alpha', 0)$ of the function V. Such a point is obtained by posing $\alpha' = 0$ within (3.14)

$$x(\lambda) = \overline{x} - \sum_{q=1}^{p} (\lambda_q - \overline{\lambda}_q) \sum_{j=1}^{n-g'} h_j \sum_{i=1}^{n-g'} (M^{-1})_{ji} \Big[\frac{\partial}{\partial \lambda_q}\Big(\frac{\partial V}{\partial x}\Big)\Big](\overline{x}, \overline{\lambda})\, h_i + o(\|\lambda - \overline{\lambda}\|) \tag{4.1}$$

and obviously depends on the choice of the vectors $\{h_j\,,\ 1 \le j \le n-g'\}$ or, more precisely, of the linear subspace $L\{h_j\,,\ 1 \le j \le n-g'\}$ spanned by $\{h_j\,,\ 1 \le j \le n-g'\}$. Owing to Corollary 2, the possible replacement of $\{h_j\,,\ 1 \le j \le n-g'\}$ by a set of $n-g'$ linearly independent vectors beloging to the same linear space $L\{h_j\,,\ 1 \le j \le n-g'\}$ does not affect (4.1).

A convenient strategy consists in introducing the h_j's in such a way that the spanned space $L\{h_j\,,\ 1 \le j \le n-g'\}$ is orthogonal to

$$L\Big\{\frac{\partial R}{\partial \alpha_i}(0)\,\overline{x}\,,\ 1 \le i \le g'\Big\}$$

with respect to the usual scalar product in $\mathbb{R}^n$ — which induces the correspondent Euclidean norm $\| \ \|$. The correcting terms due to the matrix $R(\alpha', 0)$ in (3.14), for small $\|(\alpha', 0)\|$, are written

$$\sum_{k=1}^{g'} \alpha_k \frac{\partial R}{\partial \alpha_k}(0)\,\overline{x} + o(\|(\alpha',0)\|) + o(\|\lambda - \overline{\lambda}\|)$$

and thus turn out to be orthogonal to the main contribution

$$x_0(\lambda) \;=\; \overline{x} - \sum_{q=1}^{p}(\lambda_q - \overline{\lambda}_q) \sum_{j=1}^{n-g'} h_j \sum_{i=1}^{n-g'} (M^{-1})_{ji} \Big[\frac{\partial}{\partial \lambda_q}\Big(\frac{\partial V}{\partial x}\Big)\Big](\overline{x}, \overline{\lambda})\, h_i$$

up to the terms $o(\|(\alpha',0)\|)$ and $o(\|\lambda - \overline{\lambda}\|)$. We are then led to conclude that

$$\|R(\alpha',0)x_0(\lambda) \;-\; \overline{x}\| \;\gtrsim\; \|x_0(\lambda) \;-\; \overline{x}\|$$

so that the selected points are, for varying λ, the nearest to $\overline{x}$.

A set of h_j's satisfying the previous condition can be easily determined. We can apply the Gram-Schmidt orthonormalization method to any base of $\mathbb{R}^n$ of the form

$$\Big\{\frac{\partial R}{\partial \alpha_i}(0)\,\overline{x}\,,\ 1 \le i \le g'\Big\} \cup \{\overline{h}_k\,,\ 1 \le k \le n - g'\}$$

by processing the base vectors *in the same order as above.* If $\{e_j\,,\ 1 \le j \le n\}$ is the orthonormal base we obtain, the linear space $L\{e_j\,,\ 1 \le j \le g'\}$ coincides with $L\Big\{\frac{\partial R}{\partial \alpha_i}(0)\,\overline{x}\,,\ 1 \le i \le g'\Big\}$, whereas $L\{e_j\,,\ g'+1 \le j \le n\}$ is orthogonal to it:

$$\mathbb{R}^n \;=\; L\Big\{\frac{\partial R}{\partial \alpha_i}(0)\,\overline{x}\,,\ 1 \le i \le g'\Big\} \oplus L\{e_j\,,\ g'+1 \le j \le n\}\,.$$

We will simply have to pose $h_i = e_{g'+i}$ for $1 \le i \le n - g'$.

Thus we have determined a simple and reasonable way to characterize the critical point (minimum) displacement due to parameter uncertainty.

5. Conclusions

It has been shown as invariance properties of the model equations, through an appropriate group of linear transformations, imply a very peculiar structure of any merit function used for best-fit estimates of surface free energy components in quadratic multicomponent models. Such a structure is reflected in the distribution of merit-function minima, involved in the calculation of best-fit estimates to surface free energy components, according to the nonlinear method. A simple and reasonable stategy allows us to describe the displacement of minima due to uncertainties on experimental data, and therefore to estimate the related error propagation on the final results.

References

[1] C.J. van Oss, R.J. Good, M.K. Chaudhury, J. Protein Chem. **5**, 385-402 (1986)

[2] C.J. van Oss, M.K. Chaudhury, R.J. Good, Adv. Coll. Interf. Sci. **28**, 35-60 (1987)

[3] C.J. van Oss, R.J. Good, M.K. Chaudhury, Langmuir **4**, 884-891 (1988)

[4] R.J. Good, M.K. Chaudhury, in Fundamentals of Adhesion, L.H. Lee Ed., Plenum Press, New York (1991), Chapt. 3

[5] R.J. Good, C.J. van Oss, in Modern Approach to Wettability: Theory and Application, M.E. Schrader, G Loed Eds., Plenum Press, New York (1991), Chapt. 1

[6] C.J. van Oss. Interfacial Forces in Aqueous Media, Marcel Dekker, New York (1994)

[7] C. Della Volpe, S. Siboni, Acid-base surface free energies of solids and the definition of scales in van Oss-Good theory, J. Adhesion Sci. Technol. **14**, 235-272 (2000). Reprinted in Apparent and Microscopic Contact Angles, J. Drelich, J.S. Laskowsky and K.L. Mittal Eds., VSP, New York (2000)

[8] C. Della Volpe, S. Siboni, Troubleshooting of surface free energy acid-base theory applied to solid surfaces: The case of Good, van-Oss and Chaudhury theory, Acid-base reactions: relevance to adhesion science and technology, K.L. Mittal Ed., Volume 2, VSP, New York, 55-90, (2000)

[9] A.N. Tikhonov and A.V. Goncharsky Eds., Ill-Posed Problems in the Natural Sciences MIR, Moscow (1987)

[10] A. Deif, in Sensitivity Analysis in Linear Systems, SpringerVerlag, Berlin (1986)