The Orbit Space Approach to the Theory of Phase Transitions: The Non-Coregular Case

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Abstract

We consider the problem of the determination of the isotropy classes of the orbit spaces of all the real linear groups, with three independent basic invariants satisfying only one independent relation. The results are obtained in the $P$-matrix approach solving a universal differential equation (master equation) which involves as free parameters only the degrees $d_i$ of the invariants. We begin with some remarks which show how the $P$-matrix approach may be relevant in physical contexts where the study of invariant functions is important, like in the analysis of phase spaces and structural phase transitions (Landau’s theory).

1 The Orbit Space (OS) Approach

Invariant functions under the transformations of a Compact Linear Group (CLG) acting in $\mathbb{R}^n$ can be expressed in terms of functions defined in the OS of the group, i.e. as functions of a finite set of basic invariant polynomials $p(x) \equiv (p_1(x), \ldots, p_q(x))$, $x \in \mathbb{R}^n$, which may be chosen to form a Minimal Integrity Basis (MIB) for the group $G$. Such an observation, originally due to Gufan (1971), simplifies the determination of the patterns of spontaneous symmetry breaking (SSB) in theories in which the ground state is determined by the minimum of an invariant potential $V(x)$. When $p$ ranges in the domain spanned by $p(x)$, $x \in \mathbb{R}^n$, the function $\hat{V}(p)$ has the same range as $V(x)$, but is not plagued by the same degeneracies. A correct exploitation of this idea required, however, the determination of the ranges of the functions $p_i(x)$, a problem which was completely solved only using
the powerful tools of geometric invariant theory. An excellent review with motivations and references was written by G. Sartori [1]. He discovered a simple recipe allowing to determine the structure of the OS of any CLG (the $\hat{P}$-matrix approach). The OSs admit an analytical image in terms of connected semi-algebraic varieties, whose defining relations can be expressed from (semi)positivity conditions of matrices $\hat{P}(p)$, which are constructed only through the knowledge of a MIB for the group. In solid state physics, the OS approach was applied to the Landau theory of phase transitions, but it was mainly reduced to a naive numerical technique. Since the free energy expansion is commonly considered up to the 6th degree in the order parameter, the OS was realized through a “projection” onto the subspace of $\mathbb{R}^q$ corresponding to invariants $p_a(x)$ such that $\deg p_a(x) \leq 6$. On the contrary, using the $\hat{P}$-matrix-approach, it is possible to get an exact, complete analytical determination of the primary stratification of the OS, as it was shown for the “classical” example of Ba Ti O$_3$ transitions [2]. Nevertheless the complete MIB’s are at disposal only for finite groups generated by reflections, and for simple Lie groups [2, 3]. A way to obtain the matrices $\hat{P}(p)$ generated by CLG’s, bypassing the problem, is to use an axiomatic approach, which is based on the notion of MIB transformations [4]. An equivalence relation is defined on the set of $\hat{P}$-matrix, consequently on the set of OSs. Thus, universality properties of the schemes of SSB are pointed out; here, we shall examine the non-coregular case.

2 Non-Coregular Compact Linear Groups

Given a MIB $p(x) \equiv (p_1(x), \ldots, p_q(x))$, if polynomial functions $\hat{F}$ exist such that $\hat{F}(p_1(x), \ldots, p_q(x)) \equiv 0$, then $G$ is said to be non-coregular. 

Examples: Consider the 2-dimensional point groups $C_n$, $n \geq 2$ and the 3-dimensional point groups $Y, O, T_h, T$.

Let $\{\hat{F}_A(p)\}_{1 \leq A \leq K}$ be a complete set of basic homogeneous relations among the elements of a MIB. The polynomials $\hat{F}_A(p)$ can be chosen to be $w$-homogeneous and irreducible on $\mathfrak{C}$. The associated equations $\hat{F}_A(p) = 0$, define an irreducible algebraic variety in $\mathbb{R}^q$ (and in $\mathfrak{C}^q$ for $p \in \mathfrak{C}^q$), the variety $\mathcal{Z}$ of the relations among the elements of the MIB.

The variety $\mathcal{Z}$ has a singularity in $p = 0$. In fact, for all $A$, $\hat{F}_A(p)$ cannot be solved polynomially with respect to anyone of the basic invariants $p_a$. The absence of linear terms in any $p_a$ implies the vanishing of $\hat{F}_A(0)$ and $\partial \hat{F}_A(0)$ for all $A = 1, \ldots, K$. For $k = \dim(\mathcal{Z})$, the couple $(q, k)$ will define the regularity type (called $r$-type) of $G$. 

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3 Characterizing the matrices $\hat{P}(p)$

The $\hat{P}$-matrices associated to CLG’s will be characterized through a set of structural properties that can be put in the form of differential relations. Therefore, forgetting altogether the original definition of the matrices $\hat{P}(p)$, we shall be able to determine the $\hat{P}$-matrices as solutions of a system of differential equations obeying convenient initial conditions.

Although we cannot enter the details of the generalization of the coregular approach [1], we shall point out the new initial conditions which fit the non-coregular case [5]. We shall show the striking results obtained for groups of r-type $(q, q - 1)$ in the simplest case of MIBs having cardinality $q = 3$.

Let $\sigma$ be a general primary stratum of $\mathfrak{S} \equiv p(\mathbb{R}^n)$, and $\mathcal{I}(\sigma)$ the ideal formed by all the polynomials in $p \in \mathbb{R}^q$ vanishing on $\sigma$. Every $\hat{f}(p) \in \mathcal{I}(\sigma)$ defines in $\mathbb{R}^q$ an invariant polynomial function $f(x) = \hat{f}(p(x))$, and $f(x) = 0$ for all $x \in \Sigma_f = p^{-1}(\sigma)$. As in the coregular case, the gradient $\partial f(x)$ is obviously orthogonal to $\Sigma_f$ at every $x \in \Sigma_f$, but, it must also be tangent to $\Sigma_f$ since $f(x)$ is a $G$–invariant function [4]. Consequently, it has to vanish on $\Sigma_f$:

$$0 = \partial f(x) = \frac{\partial_b \hat{f}(p) \partial p_b(x) \bigg|_{p=p(x)}}{\partial p_a(x)}, \quad \forall x \in \Sigma_f.$$  \hspace{1cm} (1)

By taking the scalar product of (1) with $\partial p_a(x)$, we end up with the following boundary conditions:

$$\sum_b^{q} \hat{P}_{ab}(p) \partial_b \hat{f}(p) \in \mathcal{I}(\sigma), \quad \forall \hat{f} \in \mathcal{I}(\sigma) \text{ and } \forall \sigma \subseteq \mathfrak{S}. \hspace{1cm} (2)$$

Relation (2) can be re-proposed in the form of a differential relation involving only polynomial functions of $p$. According to the Hilbert basis theorem, the ideal $\mathcal{I}(\sigma)$ is finitely generated. Let $\{f^{(1)}(p), f^{(2)}(p), \ldots, f^{(m)}(p)\}$ be a $w$-homogeneous basis for $\mathcal{I}(\sigma)$, then (2) is equivalent to the following relations:

$$\sum_b^{q} \hat{P}_{ab}(p) \partial_b f^{(r)}(p) = \sum_s^{m} \lambda_a^{(rs)}(p) f^{(s)}(p), \quad a = 1, \ldots, q; \ r = 1, \ldots, m,$$ \hspace{1cm} (3)

where the $\lambda^{(rs)}$’s are $w$-homogeneous polynomial functions of $p$. 

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If, in particular, \( \sigma \) is a \((q - 1)\)-dimensional primary stratum, the ideal \( \mathcal{I}(\sigma) \) has a unique \emph{irreducible} generator, \( a(p) \), and (3) reduces to the simpler form

\[
\sum_{b} \hat{P}_{ab}(p) \partial_b a(p) = \lambda_a(p) a(p), \quad a = 1, \ldots, q.
\]

Equation (4) will be quoted as \emph{master relation}. It is valid for the principal stratum of the OS of a group of \( r \)-type \((q, q - 1)\).

The structure of (4) has been completely analyzed \cite{6}. We just recall that, like in the coregular case, \( a(p) \) is a polynomial factor of \( \det \hat{P}(p) \); besides, there exist particular MIB’s, which we shall call \( A \)-bases, in which the master relation takes the following \emph{canonical} form:

\[
\sum_{b} \hat{P}_{ab}(p) \partial_b A(p) = 2\delta_{aq} w(A) A(p), \quad a = 1, \ldots, q.
\]

But there are further properties which are \emph{peculiar to the coregular case}. They play the role of \emph{initial conditions}, because they are so restrictive to select among the solutions of the canonical equation just the ones which may correspond to (images) of OSs of coregular CLGs \( (allowable\ solutions)\).

i) Consider the hyperplane \( \Pi = \{p \equiv (p_1, \ldots, p_q) \mid p_q = 1\} \) of \( \mathbb{R}^q \). The restriction \( A(p)|_{\Pi} \) of \( A(p) \) to \( \Pi \) has a unique local non degenerate maximum lying at \( p^{(0)} = (0, \ldots, 0, 1) \).

ii) The matrix \( \hat{P}(p^{(0)}) \) is block diagonal and, for \emph{standard} \( A \)-bases, it is diagonal: \( \hat{P}_{ab}(p^{(0)}) = d_a d_b \delta_{ab} \), \( (a, b = 1, \ldots, q) \).

3.1 Second order boundary conditions

The \( \hat{P} \)-matrices generated by non-coregular groups do not satisfy the set of “initial conditions” specified above, but the presence of relations connecting the elements of any MIB gives rise to interesting constraints.

Let us consider a compact non-coregular group \( G \), whose OS is realized as a semi-algebraic subset \( \mathcal{S} \) of the variety \( \mathcal{Z} \) of the relations. Let \( \mathcal{I}(\mathcal{Z}) \) be the ideal of the polynomial functions of \( p \) vanishing on \( \mathcal{Z} \). Any polynomial \( \hat{F}(p) \in \mathcal{I}(\mathcal{Z}) \) defines an identity in \( \mathbb{R}^n \):

\[
F(x) = \hat{F}(p(x)) = 0, \quad \forall x \in \mathbb{R}^n,
\]

which, after differentiating twice with respect to \( x_i \) and summing over \( i \), gives rise to the following condition, valid \( \forall x \in \mathbb{R}^n \):

\[
\]
\[ \sum_{i=1}^{n} \left\{ \sum_{a,b} q \partial_{ab} \tilde{F}(p(x)) \partial_{i} p_{b}(x) \partial_{i} p_{a}(x) + \sum_{a} \partial_{a} \tilde{F}(p(x)) \partial_{i}^{2} p_{a}(x) \right\} = 0. \] (7)

Since \( G \) is a matrix subgroup of \( O_{n}(\mathbb{R}) \), the \( n \)-dimensional Laplacian of any invariant polynomial function of \( x \) is a \( G \)-invariant polynomial. Thus Hilbert’s theorem ensures the existence of a set \( \{ \hat{l}_{a}(p) \}_{a=1,2,\ldots,q} \) of \( w \)-homogeneous polynomials in \( p \in \mathbb{R}^{q} \) with weights \( w(\hat{l}_{a}) = d_{a} - 2 \), such that:

\[ l_{a}(x) = \sum_{i=1}^{n} \partial_{i}^{2} p_{a}(x) = \hat{l}_{a}(p(x)), \quad a = 1, 2, \ldots, q. \] (8)

The identity expressed in (7) induces, through the orbit map, the following polynomial relation, valid for all \( p \in \mathbb{R}^{q} \), and consequently, for all \( p \in Z \), as \( p(\mathbb{R}^{n}) \) is a semi-algebraic subset of \( Z \) of the same dimension as \( Z \):

\[ \sum_{a,b} q \hat{P}_{ab}(p) \partial_{a} \partial_{b} \tilde{F}(p) + \sum_{a} q \hat{l}_{a}(p) \partial_{a} \tilde{F}(p) = 0, \quad p \in Z. \] (9)

We stress that, owing to the convention \( p_{q} = \sum_{j=1}^{n} x_{j}^{2} \), we get \( l_{q} = 2n \). Even if in our approach the explicit form of the polynomials of a MIB is not specified, we have a clue of the power of relation (9), since it is linked with the effective group action. The parameter \( n \) interprets the role of the dimension of the real space in which \( G \) acts. Therefore (9) will be considered as a sort of second order boundary condition in which \( l_{q} = 2n \geq 4 \). (10)

If the group \( G \) is of \( r \)-type \( (q, q-1) \), the ideal \( \mathcal{I}(Z) \) has a unique generator \( \hat{F}(p) \), which fulfills the canonical equation (5). It may be proved that (9) holds identically \( \forall p \in \mathbb{R}^{q} \), essentially for weight reasons (5). The solution procedure consists in expressing all the polynomials involved in (5) and (9) in the most general form in agreement with their structural properties. For groups \( G \) of \( r \)-type \( (3,2) \) we get a complicated system of coupled algebro-differential equations. Some simplifications are obtained replacing (9) with a form in which it appears only the first order derivative of \( \hat{F}(p) \). The \( \partial_{3} \hat{F}(p) \) term can be eliminated using the \( w \)-homogeneity conditions on \( \hat{F}(p) \).

### 3.2 Allowable \( \hat{P} \)-matrices: the non-coregular case

A proper solution is a couple \((\hat{P}(p), \hat{F}(p))\), where \( \hat{F}(p) \) is the factor of \( \det \hat{P}(p) \), which defines the variety \( Z \). Consider the semialgebraic variety
\( \mathcal{R}(\geq) = \{ p \in \mathbb{Z} \mid \hat{P}(p) \geq 0 \} \). In our approach for non-coregular groups, \( \mathcal{R}(\geq) \) and its algebraic stratification may potentially be identified with (the image of) the OS of an actual group only if the following conditions hold:

i) On \( \mathbb{Z} \), rank \((\hat{P}(p)) \leq k \) and the set \( \mathcal{R} = \{ p \in \mathbb{Z} \mid \hat{P}(p) \geq 0 \} \) is \( k \)-dimensional and connected; its closure \( \overline{\mathcal{R}} \equiv \mathcal{R}(\geq) \).

ii) \( \hat{P}(p) \) satisfies the boundary conditions (8), for each primary stratum \( \sigma^{(\alpha)} \) of \( \overline{\mathcal{R}} \), and the second order boundary condition (9) for each \( \hat{F}(p) \in \mathcal{I}(\mathbb{Z}) \).

If that is the case, we speak of allowable non-coregular solution \((\hat{P}(p), \hat{F}(p))\).

### 4 The results

We proved that Eq. 3 with Eq. 4 as initial condition admits only 3 families of proper solutions [5].

**Solution family S1:** It is found in correspondence with the degrees \( d_1 = k(1 + 2m) \), \( d_2 = 2k \), for \( k, m \in \mathbb{N}_+ \). It depends on the parameter \( \epsilon = \pm 1 \). For \( \epsilon = +1 \), the set \( \mathcal{R}(\geq) \) is not connected, neither the boundary conditions are satisfied at the peripherical strata. For \( \epsilon = -1 \), the set \( \mathcal{R}(\geq) \cap \Pi \) is 0-dimensional. Thus, this family does not determine allowable \( \hat{P} \)-matrices.

**Solution family S2:** The degrees are \( d_1 = 6k \), \( d_2 = 4k \), for \( k \in \mathbb{N}_+ \). It is a one-parameter collection of distinct classes of equivalent \( \hat{P} \)-matrices, which defines an allowable solution only for the value \( z = 0 \) of the parameter. Nevertheless, the generator of \( \mathcal{Z} \) is \( \hat{F}(p) = p_1^2 + p_2^3 \). Thus, the existence of a generating group can be excluded on the basis of a general proposition [5].

**Solution family S3:** Among the 4 distinct classes of proper solutions, we get only 1 class of allowable \( \hat{P} \)-matrices which exactly coincides with the coregular solution of \( r \)-type \((3,3)\) for the class \( I(1,1) \) [6]. Generating coregular groups of the first element of the family are, for instance, the linear groups \( \text{SO}(n, \mathbb{R}) \) acting in \( \mathbb{R}^n \oplus \mathbb{R}^n \) for \( n \geq 3 \).

Thus we can assert that coregular and non-coregular groups may share the same \( \hat{P} \)-matrix. The non-coregular solution for degrees \( d_1 = d_2 = k \geq 2 \), \( k \in \mathbb{N} \) corresponds for instance to the action of a 2-dimensional representation of the point group \( C_n \), \( n \geq 2 \), that is the cyclic group of rotations about an axis of the \( n \)-th order. The variety \( \mathcal{Z} \) is determined by the relation \( p_1(x)^2 = p_3(x) - p_2(x)^2 \); the image of the OS \( \overline{\mathcal{Z}} \cap \Pi \) is the unit circumference.
Finally, if the action of $G$ is restricted to the unit sphere ($p_3 = 1$), all the orbit spaces of groups of r-type $(3, 2)$ turn out to be isomorphic.

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