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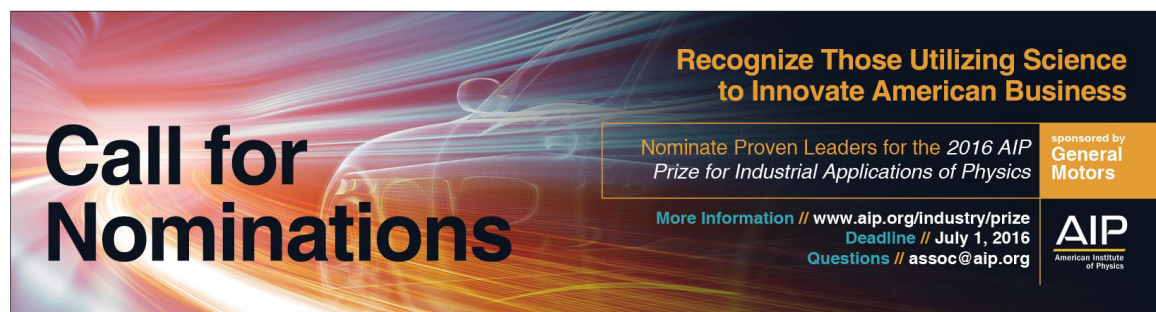
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Poincaré-like approach to Landau theory. I. General theory

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We discuss a procedure to simplify the Landau potential, based on Michel's reduction to orbit space and Poincaré normalization procedure, and illustrate it by concrete examples. The method makes use, as in Poincaré theory, of a chain of near-identity coordinate transformations with homogeneous generating functions; using Michel's insight, one can work in orbit space. It is shown that it is possible to control the choice of generating functions so to obtain a (in many cases, substantial) simplification of the Landau polynomial, including a reduction of the parameters it depends on. Several examples are considered in detail. © 2015 AIP Publishing LLC. [<http://dx.doi.org/10.1063/1.4927425>]

I. INTRODUCTION

Landau theory^{1,2} is a standard tool in analyzing phase transition; it describes the state of a physical system in terms of the minima of a certain (Landau) potential. The Landau potential can however be very complicated, and it is thus essential to be able to simplify it in concrete applications.

Our motivation here is mainly in applications to liquid crystals; these will be treated more specifically in a companion paper,⁸ while the present one deals with the general theory.

We will assume the order N at which the expansion can be truncated is determined (we will then disregard all terms of degree higher than N); this is usually done by requiring thermodynamic stability of the resulting model. We focus then on the problem of identifying the terms of order smaller than or equal to N which are “inessential,” i.e., that can be dropped without changing the qualitative properties of the Landau potential Φ . More precisely, we discuss which terms can be eliminated by a careful choice of the coordinates in the order parameter space; our procedure is thus fully algorithmic, requires only to solve linear equations, and can easily be computer-implemented via an algebraic manipulation language.

It should be stressed that our procedure, while simplifying terms of order lower than N , will at the same time generate terms of higher orders. Coherently with the general framework of Landau theory, which considers truncated series expansions, we will not consider these. In other words, all of our series will be truncated at the same order N .

Our approach will be through application of Poincaré normalization technique (see, e.g., Refs. 3–6); we generalize previous work⁷ in which we gave full justification to a criterion stated by Gufan^{9,10} and extended it to consider a full range of order parameters, in particular, near a phase transition.

In this paper, a more detailed analysis (compared to Ref. 7) of the relevant operators acting in the reduction process allows for a more complete characterization of the reduction procedure and of the reduced potential obtained in this way. In a companion paper,⁸ as already mentioned, we apply our method to nematic liquid crystals.

It should be stressed that in the present paper we will work at first nontrivial order, in particular, when describing the effects of the change of variables to be considered; this corresponds to classical Poincaré-Birkhoff theory.^{3–6} In the framework of Dynamical Systems, extensions of this

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classical theory have been considered in order to take into account higher order effects; this goes under the name of “further normalization”⁶ and would require some more delicate discussion. This approach—and its possible extension to Landau theory—will not be discussed here; for the application of the Poincaré approach to Landau-deGennes theory of nematic liquid crystals considered in the companion paper,⁸ it would be rather convenient to take into account these higher order effects as well.³¹

The main result of the paper will be the formulation of an algorithmic method (requiring only the solution of linear equations) to simplify the Landau potential. It should be stressed that this will be just based on mathematical manipulations, and more specifically on the choice of adapted coordinates (which are built through a perturbation approach), that is, we will not introduce any physical considerations. Introducing the latter could of course result, in principle, in a further reduction of the Landau potential. Thus, our procedure should be seen as a first step eliminating unnecessary complications through the choice of convenient coordinates; it leaves room for further reduction based on the Physics of the specific system under study.

We also anticipate that in many cases the resulting simplified potential will still be quite complex, despite a substantial reduction. For example, in Examples 5 and 6 below, we will have to consider a potential depending in principle on 22 parameters, and will be able to eliminate 16 of them, but the simplified potential will still depend on 6 parameters and thus be very hard to study.

The *plan of the paper* is as follows. In Sec. II, we will recall some basic notions, to be used in the following, also in order to set down our general notation. In Sec. III, we will start applying the Poincaré approach: we will identify a class of changes of coordinates which is convenient for our purposes; these are identified by generating functions which are the gradients of invariant functions. We also discuss how invariant polynomials are transformed under these. In Sec. IV, we will apply this discussion to Landau polynomials, and see how one can choose the generating functions mentioned above in order to obtain a simpler Landau polynomial. Section V is then devoted to illustrate the different steps analyzed theoretically in previous sections by means of a number of case studies. In Sec. VI, we discuss how the analysis can be simplified by passing to adapted coordinates, and in Sec. VII how the reduction procedure can be of help in analyzing the behavior of physical systems, i.e., in performing an—quantitative and qualitative—analysis of Landau polynomials. Finally, in Sec. VIII, we discuss the advantages and the limitations of our methods, as well as possible direction of further extension of the present results, and in brief Sec. IX, we draw some conclusions.

II. PRELIMINARIES

We will briefly recall some notions from Landau theory, mainly to set the notation to be used below; see also Ref. 7 for details and for further references (in particular, on invariants theory). Summation over repeated indices is understood.

A. Generalities

We denote by $x \in M \subseteq \mathbf{R}^m$ the order parameter, and by G the group acting in M to describe symmetry of the system in the order parameters space; this acts through a real representation, i.e., a set of matrices $\{T_g, g \in G\}$; as this is fixed and in order to avoid cumbersome notation, we also just write g for T_g as well. We assume G is compact, and it acts linearly and orthogonally in \mathbf{R}^m , mapping the order parameter space M to itself.³²

The effective potential $\widehat{\Phi}(x) \in \mathbf{R}$ is a G -invariant polynomial, so we should preliminarily determine the most general G -invariant polynomial in the x^i ; the Landau potential $\Phi(x)$ will be a truncation of $\widehat{\Phi}$ to a suitable order N . We would then like to omit some “unessential” terms of order $n \leq N$ in Φ (see below).

The polynomials $\widehat{\Phi}$ and Φ have coefficients depending on external (control) parameters $\lambda \in \Lambda \subseteq \mathbf{R}^L$, so that we will also write $\widehat{\Phi}(x; \lambda)$, $\Phi(x; \lambda)$; the equilibrium state of the system is described by the minima of $\Phi(x; \lambda)$, which we denote as $x_\alpha(\lambda)$. In general, there will be different minima for a given value of λ : in particular, if $x(\lambda)$ is not a fixed point for the G -action, then the whole G orbit

through $x(\lambda)$ will be an orbit of minima. Moreover, there can be different G -orbits of minima for a given value of λ .

The symmetry of the state corresponding to $x(\lambda)$ will correspond to $G_{x(\lambda)}$, the isotropy group of $x(\lambda)$; we recall that by definition $G_x := \{g \in G : T_g x = x\}$.

If x and y are on the same G -orbit, $y = gx$, then $G_y = gG_xg^{-1}$; the conjugacy class of isotropy subgroups associated to any G -orbit in M is called the *orbit type* $[Gx]$. A *phase* will be described by an orbit type.

A necessary condition to have a phase transition at $\lambda = \lambda_0$ is that the orbit type $[Gx(\lambda)]$ is not constant in a neighborhood of λ_0 , no matter how small.

We stress again that it is inherent to Landau theory to consider a truncated series expansion; thus, all of our computations and theoretical considerations will disregard higher order terms. In particular, when our change of variables would generate terms of order higher than N , these will simply be dropped.

B. Invariant polynomials

By the *Hilbert basis theorem*,^{12,13} there is a set $\{J_1(x), \dots, J_r(x)\}$ (with our hypotheses on G , r is guaranteed to be finite¹²) of G -invariant homogeneous polynomials of degrees $\{d_1, \dots, d_r\}$ (we can and will always order these so that $d_1 \leq d_2 \leq \dots \leq d_r$) such that any G -invariant polynomial $\widehat{\Phi}(x)$ can be written as a polynomial in the $\{J_1, \dots, J_r\}$, i.e.,

$$\widehat{\Phi}(x) = \widehat{\Psi}[J_1(x), \dots, J_r(x)], \quad (1)$$

with $\widehat{\Psi}$ a polynomial in (J_1, \dots, J_r) .

When the J_a are chosen so that none of them can be written as a polynomial of the others and r has the smallest possible value, we say that they are a *minimal integrity basis (MIB)*, and that the $\{J_a\}$ are a set of *basic invariants* for G .

When the elements of a MIB for G are algebraically independent, we say that the MIB is *regular*; not all groups G admit a regular MIB (see Example 2 below).

We will from now on assume we have chosen a MIB, with elements $\{J_1, \dots, J_r\}$ (of degrees $\{d_1, \dots, d_r\}$ in x , with $d_1 \leq d_2 \leq \dots \leq d_r$).

C. The (Sartori) \mathcal{P} -matrix

In the following, we will need to consider a matrix built with the gradients of basic invariants, which we call the Sartori \mathcal{P} -matrix.¹⁴ This is defined, with $\langle \cdot, \cdot \rangle$ the standard scalar product in $M = \mathbf{R}^m$, as

$$\mathcal{P}_{ih}(x) := \langle \nabla J_i(x), \nabla J_h(x) \rangle. \quad (2)$$

The gradient of an invariant is necessarily a covariant quantity; the scalar product of two covariant quantities is an invariant one, and thus can be expressed again in terms of the basic invariants. Moreover, we always deal with polynomials. Thus, *the \mathcal{P} -matrix can always be written in terms of the J themselves.*

D. Orbit space and the Michel principle

Let us come back to $\widehat{\Phi}$; this is G -invariant and thus can be written in terms of the basic invariants. The evaluation of $\widehat{\Phi} : M \rightarrow \mathbf{R}$ is in principle substituted by evaluation of $\mathbf{J} : M \rightarrow \Omega$ and $\widehat{\pi} : \Omega \rightarrow \mathbf{R}$; here, we have denoted by $\Omega \subseteq \mathbf{R}^r$ the target space for $\mathbf{J} = (J_1, \dots, J_r)$.

If—as in Landau theory—we have to consider the most general G -invariant polynomial on M , we only have to deal with the map $\pi : \Omega \rightarrow \mathbf{R}$. In general, Ω is a semi-algebraic submanifold (i.e., it is defined by polynomial equalities and inequalities) of \mathbf{R}^r , possibly of dimension smaller than r ; if the MIB is regular, then Ω has dimension r .

The space Ω is also known as the *orbit space* for the G action on M ; indeed, its points are in one-to-one correspondence with the G -orbits in M , $\Omega \simeq M/G$. The geometry of orbit space is discussed, e.g., in Refs. 12 and 14–16; for applications to Dynamics, see, e.g., Ref. 17.

The *Landau-Michel principle* states that *Landau theory can be worked out in the G -orbit space* $\Omega := M/G$.

E. Thermodynamic stability and convexity

Let us now briefly discuss how the request of thermodynamic stability,² i.e., convexity, is reflected in the polynomial $\widehat{\pi}(J)$.

Consider first the regular case; now $\widehat{\pi} : \mathbf{R}^r \rightarrow \mathbf{R}$, and the J_a can be considered as independent variables. The minimal Landau polynomial $\Phi(x) = \pi(J)$ will be quadratic in the J , and the stability is ensured by requiring that the matrix $D_{ih} = \partial^2\Phi/(\partial x^i \partial x^h)$ is positive definite for $|x|$ sufficiently large.

So the prescription in this case will be to *consider a polynomial of order (at least) $N = 2 \max(d_1, \dots, d_r) = 2d_r$* , and of course choose coefficients so that the matrix D is positive definite for large $|x|$.

If we deal with a non-regular case, this prescription also works: maybe it would also be possible to stop at a lower order, as we have to care only about the submanifold of Ω allowed by the relations between the J_a , but if we require stability in all of Ω we are on the safe side.

Some remarks are in order here:

- (i) The prescription is *not* to write π as a quadratic polynomial in the J_a and then express Φ in terms of this; rather it is to *consider the most general G -invariant polynomial of order $2d_r$* , (this can contain quite high powers in some of the J_a 's, see examples below).
- (ii) The requirement to have D positive definite for large $|x|$ is surely satisfied if the largest order term in $\Phi(x)$ is a power of $\rho = |x|^2$.
- (iii) The coefficients of (at least some of) the polynomials will depend on the external parameters; in particular, this will be the case for $J_1 = |x|^2$, whose coefficient controls the loss of stability of the critical point $x = 0$ and thus the onset of the phase transition.

III. TRANSFORMATION OF INVARIANT POLYNOMIALS

We will apply to Landau theory the technique of *Poincaré transformations*. These are the fundamental tool of the theory of Poincaré-Birkhoff normal forms;³⁻⁵ see Ref. 7 for a more complete discussion of the relation of these with Landau theory.

Let us consider G -invariant polynomials $\Phi(x) = \Psi[J(x)]$. We write

$$\Phi(x) = \sum_{k=0}^{\infty} \Phi_k(x), \quad (3)$$

where $\Phi_k(ax) = a^{k+2}\Phi_k(x)$.

We want to consider changes of coordinates of the form

$$x^i \rightarrow x^i + h_m^i(x), \quad (4)$$

with $h_m(ax) = a^{m+1}h_m(x)$; moreover, we want to preserve the symmetry properties of Φ . Thus, the function $h : M \rightarrow M$ has to transform in the same way as x under the G -action, i.e., we have to require

$$h(T_g x) = T_g h(x)$$

for all $x \in M$ and all $g \in G$. We will choose h_m to be the gradient of a G -invariant function $H_m(x)$, i.e.,

$$h_m^i(x) = g^{ij}(\partial H_m / \partial x^j),$$

with g the metric in M ; note $H_m(ax) = a^{m+2}H_m(x)$.

As H_m is G -invariant, it is also possible to write it as a function of the basic invariants: $H_m(x) = \chi_m[J_1(x), \dots, J_r(x)]$. This yields

$$(\partial H_m / \partial x^i) = (\partial \chi_m / \partial J_\alpha) \cdot (\partial J_\alpha / \partial x^i). \quad (5)$$

In order to know how (4) acts on (3), it suffices to know how it acts on the basic invariants J_a , and how this is reflected in the action on Φ . The computations are straightforward, but the resulting formulas can be considerably involved.

Luckily, we will only need the first order terms; dropping higher order terms, recalling the expression for h^i , and using (5), we get

$$\begin{aligned} J_a(x) &\rightarrow J_a(x) + (\partial J_a / \partial x^i) \delta x^i \\ &= J_a(x) + (\partial J_a / \partial x^i) g^{ij} (\partial H_m / \partial x^j) \\ &= J_a(x) + (\partial J_a / \partial x^i) g^{ij} (\partial \chi_m / \partial J_b) (\partial J_b / \partial x^j) \\ &= J_a(x) + \mathcal{P}_{ab} (\partial \chi_m / \partial J_b). \end{aligned} \quad (6)$$

IV. REDUCTION OF LANDAU POLYNOMIALS

Let us now apply the above discussion to the reduction of an invariant polynomial $\Phi(x) = \Psi(J_1, \dots, J_r)$. That is, we want to choose the χ_m so to obtain a convenient (reduced) form of the polynomials Ψ_k , hence of the Φ_k as well.

A. General reduction scheme

We have in general, dropping h.o.t. as usual,

$$\Psi(J) \rightarrow \Psi(J + \delta J) = \Psi(J) + \sum_{\alpha=1}^r \frac{\partial \Psi(J)}{\partial J_\alpha} \delta J_\alpha. \quad (7)$$

We have seen that under (4) the $J_a(x)$ change according to (6); hence, we readily obtain at first order

$$\delta \Psi = \frac{\partial \Psi}{\partial J_\alpha} \mathcal{P}_{\alpha\beta} \frac{\partial \chi_m}{\partial J_\beta}. \quad (8)$$

Let us now consider expansion (3) for Φ , and write correspondingly $\Psi = \sum_k \Psi_k$, where $\Phi_k(x) = \Psi_k[J(x)]$. We will also expand the \mathcal{P} -matrix in homogeneous terms, $\mathcal{P} = \sum_k \mathcal{P}^{(k)}$, again with $\mathcal{P}^{(k)}$ homogeneous of degree $(k+2)$ in the x . Note that \mathcal{P}_{ih} is homogeneous of degree $(d_i + d_h - 2)$; in particular, $\mathcal{P}^{(0)}$ corresponds to the sub-matrix relating quadratic invariants only.

It follows from our discussion that the terms Ψ_k with $k < m$ are not changed, while the term Ψ_m changes as

$$\Psi_m \rightarrow \Psi_m + \frac{\partial \Psi_0}{\partial J_\alpha} \mathcal{P}_{\alpha\beta}^{(0)} \frac{\partial \chi_m}{\partial J_\beta}. \quad (9)$$

Terms of higher order change in a more complex way.³³

We can thus operate sequentially with H_1, H_2, H_3, \dots ; at each stage (generator H_m), we are not affecting the terms Ψ_k with $k < m$. Moreover, we can just consider the first order correction; higher order terms will be changed in some complex way but they were generic, hence will continue being such, and (those of degree not higher than the truncation order N) will be taken care of in subsequent steps.

It should be stressed that in (9) it is *not* the full \mathcal{P} -matrix which appears, but only its quadratic (in x) part $\mathcal{P}^{(0)}$; this in turn only depends (linearly) on the quadratic invariants.

B. Analysis of the reduction procedure

Let us now consider (9) in more detail; we are interested in the case where $x = 0$ is always a critical point for the Landau polynomial (albeit not necessarily a minimum); then there will be

invariants J_1, \dots, J_s (with $s \leq r$) quadratic in the x , and only these will appear in Ψ_0 , which will be of the form

$$\Psi_0 = \sum_{\alpha=1}^s c^\alpha J_\alpha, \tag{10}$$

with c^α some real constants. Thus, (9) can be rewritten as $\Psi_m \rightarrow \Psi_m + \delta\Psi_m$ with

$$\delta\Psi_m = c^\alpha \mathcal{P}_{\alpha\beta}^{(0)} \frac{\partial \chi_m}{\partial J_\beta} := -\mathcal{L}_0(\chi_m). \tag{11}$$

It is quite clear that any term in Ψ_m which lies in the range of the linear differential operator

$$\mathcal{L}_0 := -c^\alpha \mathcal{P}_{\alpha\beta}^{(0)} \frac{\partial}{\partial J_\beta} \tag{12}$$

can be eliminated by a suitable choice of χ_m . On the other hand, we can always add to χ_m some term in the kernel of \mathcal{L}_0 without affecting $\delta\Psi_m$.

More precisely, let us denote by S_m the set of smooth functions $F : M \rightarrow \mathbf{R}$ which are G -invariant and homogeneous of degree $(m + 2)$ in the x , and by π_m the operator of projection to $\text{Ran}(\mathcal{L}_0) \cap S_m$. Then, any term $\Psi_m \in \pi_m(S_m)$ can be eliminated via the step- m Poincaré transformation by choosing the generating function as $H_m(x) = \chi_m[J(x)]$ with χ_m a solution to the equation

$$\mathcal{L}_0(\chi_m) = \pi_m \Psi_m; \tag{13}$$

we will refer to this as the *homological equation*, like in standard Poincaré normal forms theory.^{3,4}

It should be noted that if $\pi_m \Psi_m = \Psi_m$ homological equation (13) determines the generating function to completely cancel the Ψ_m term; but when we deal with the highest order terms in the Landau polynomial ($m = N$), we do not want to completely cancel these. In fact, we should be careful to preserve the thermodynamical stability (i.e., the convexity at large $|x|$, as discussed in Sec. II E), see below.

Remark 1. It should be stressed that the whole procedure is based on a non-degeneration hypothesis, i.e., on the assumption to have a non-zero quadratic part Ψ_0 . If this is not the case, i.e., if the c^α in (10) are all zero, the homological operator \mathcal{L}_0 is trivial, and the theory simply vanishes.³⁴ Thus, the reader should not be surprised if later on, in concrete examples, he/she will always find that results depend on conditions amounting indeed to the non-vanishing of the quadratic part of the potential.

C. The operator \mathcal{L}_0

Let us consider in more detail the operator \mathcal{L}_0 . As remarked above, $\mathcal{P}^{(0)}$ necessarily depends only on the quadratic invariants J_1, \dots, J_s (with $1 \leq s \leq r$) and is linear in these. Thus, we can always write $\mathcal{P}^{(0)} = \kappa^\gamma J_\gamma$ with κ^γ a constant real matrix (with numerical entries $K_{\alpha\beta}^\gamma$), i.e.,

$$\mathcal{P}_{\alpha\beta}^{(0)} = K_{\alpha\beta}^\gamma J_\gamma; \tag{14}$$

the real coefficients $K_{\alpha\beta}^\gamma$ (and the matrices κ^γ) are identically zero for $\gamma > s$.

With this notation, the operator \mathcal{L}_0 reads

$$\mathcal{L}_0 = -[(c^\alpha K_{\alpha\beta}^\gamma) J_\gamma] \frac{\partial}{\partial J_\beta} := -(Q_\beta^\gamma J_\gamma) \frac{\partial}{\partial J_\beta}. \tag{15}$$

Note that we can reach the same expression in a slightly different way; indeed, (12) can be rewritten as

$$\mathcal{L}_0 = -\Theta_\beta (\partial/\partial J_\beta), \tag{16}$$

with of course $\Theta_\beta = c^\alpha \mathcal{P}_{\alpha\beta}^{(0)}$; as we know that $\mathcal{P}^{(0)}$ is linear in the J , necessarily $\Theta_\beta = Q_\beta^\gamma J_\gamma$ for some constant matrix Q , and we arrive again at (15).

D. Normalized versus original coordinates

It should be stressed that the simplification (or normalization, *à la Poincaré*) procedure is based on passing from the original coordinates—which in this case are the order parameters—to new coordinates which are expressed as *non-homogeneous* functions of the old ones.

This means, in particular, that albeit one may have at first sight the impression that the reduced Landau polynomial supports phase transitions of order different from the original one (e.g., in the case where the next to lowest order terms are fully canceled), when the predictions obtained on the basis of the reduced polynomial are mapped back to the original coordinates, one does of course go back to the original phase transition order.

More generally, as what we do here is just a sequence of changes of coordinates, it is clear that no physical predictions can be altered—albeit obtaining such predictions may be simpler in the new coordinates.

V. EXAMPLES

In order to fix ideas, let us consider explicitly some concrete (simple) example. We will follow our theoretical discussion, and consider “in parallel” the different steps for various examples, in different subsections; we trust this will better help the reader to familiarize with the present approach. We will also deal with some of the examples considered in Ref. 7, in order to make easier comparison with the methods used in previous work.

Note that the symmetry considered in Example 1 is the one of bent-core (or chevron-shaped) nematic liquid crystals, that in Example 4 is the one of isotropic nematics, and those of Examples 5 and 6 are relevant to anisotropic nematics.^{19,20}

Here, all the indices will be written as lower ones, in order to avoid any possible confusion with exponents.

A. The \mathcal{P} and \mathcal{Q} matrices

Example 1. Consider $M = \mathbf{R}^2 = \{x, y\}$ with group $G = Z_2 \times Z_2$ generated by

$$g_x : (x, y) \rightarrow (-x, y), \quad g_y : (x, y) \rightarrow (x, -y);$$

in this case, the MIB is given by two invariants, both of them quadratic,

$$J_1 = x^2, \quad J_2 = y^2.$$

Note that here $\rho := |x|^2$ is written in terms of the chosen basic invariants as $\rho = J_1 + J_2$.

We have $\mathcal{P}^{(0)} = \mathcal{P}$, and we get immediately

$$\mathcal{P} = \mathcal{P}^{(0)} = \begin{pmatrix} 4J_1 & 0 \\ 0 & 4J_2 \end{pmatrix}; \quad \Theta = \underline{c} \mathcal{P}^{(0)} = \begin{pmatrix} 4c_1 J_1 \\ 4c_2 J_2 \end{pmatrix}.$$

In other words, now the matrix \mathcal{Q} is diagonal,

$$\mathcal{Q} = \begin{pmatrix} 4c_1 & 0 \\ 0 & 4c_2 \end{pmatrix}.$$

Example 2. Consider $M = \mathbf{R}^2$, and $G = Z_2$ is the group generated by inversion (simultaneous reflections in x and in y), i.e., by

$$g : (x, y) \rightarrow (-x, -y).$$

Now the MIB is given by three invariants, all of them quadratic,

$$J_1 = x^2, \quad J_2 = y^2, \quad J_3 = xy.$$

Again $\rho = J_1 + J_2$. Note that the basis is *not* regular: we have $J_1 J_2 = J_3^2$.

Again $\mathcal{P}^{(0)} = \mathcal{P}$, and in this case we get

$$\mathcal{P}(x, y) = \begin{pmatrix} 4x^2 & 0 & 2xy \\ 0 & 4y^2 & 2xy \\ 2xy & 2xy & x^2 + y^2 \end{pmatrix} = \begin{pmatrix} 4J_1 & 0 & 2J_3 \\ 0 & 4J_2 & 2J_3 \\ 2J_3 & 2J_3 & J_1 + J_2 \end{pmatrix}.$$

It follows that

$$\Theta = \begin{pmatrix} 4c_1J_1 + 2c_3J_3 \\ 4c_2J_2 + 2c_3J_3 \\ c_3(J_1 + J_2) + 2c_1J_3 + 2c_2J_3 \end{pmatrix},$$

and hence

$$Q = \begin{pmatrix} 4c_1 & 0 & 2c_3 \\ 0 & 4c_2 & 2c_3 \\ c_3 & c_3 & 2(c_1 + c_2) \end{pmatrix}.$$

Example 3. Consider now the group generated by rotation of an angle $\vartheta = (2\pi/3)$ in the plane (x, y) ; with R , the rotation matrix

$$R = \begin{pmatrix} \cos(\vartheta) & -\sin(\vartheta) \\ \sin(\vartheta) & \cos(\vartheta) \end{pmatrix},$$

the group consists simply of $G = \{I, R, R^2\}$. The basic invariants are

$$J_1 = x^2 + y^2, \quad J_2 = x^3 - 3xy^2, \quad J_3 = y^3 - 3x^2y;$$

only the first one is quadratic.³⁵ In this case, $\rho = J_1$. The \mathcal{P} -matrix is

$$\mathcal{P} = \begin{pmatrix} 4J_1 & 6J_2 & 6J_3 \\ 6J_2 & 9J_1^2 & 0 \\ 6J_3 & 0 & 9J_1^2 \end{pmatrix},$$

and $\mathcal{P}^{(0)}$ is just the \mathcal{P}_{11} entry, hence

$$\Theta = 4c_1J_1, \quad Q = 4c_1.$$

Example 4. Consider $M = \mathbf{R}^3$ and $G = SO(2) \times Z_2$, with $SO(2)$ acting as rotations in the (x, y) plane, i.e., with the same R as in Example 3, and with Z_2 acting as reflections in the z variable, $z \rightarrow -z$ (this is met in studying isotropic nematic liquid crystal). Here, we have two basic invariants,

$$J_1 = (x^2 + y^2), \quad J_2 = z^2;$$

both of them are quadratic and they have no algebraic relation. Here, again $\rho = J_1 + J_2$. Now

$$\mathcal{P} = \mathcal{P}^{(0)} = \begin{pmatrix} 4J_1 & 0 \\ 0 & 4J_2 \end{pmatrix}$$

and of course

$$\Theta = \begin{pmatrix} 4c_1J_1 \\ 4c_2J_2 \end{pmatrix}; \quad Q = \begin{pmatrix} 4c_1 & 0 \\ 0 & 4c_2 \end{pmatrix}.$$

Note that the dimension of the MIB and the expression of Q (and ρ as well) are the same as in Example 1; thus, the two examples will be dealt with in a similar manner for what concerns the orbit space analysis, albeit the interpretation in the original (order parameters) space will be different due to the different expressions for J_1, J_2 in terms of the order parameters.

Example 5. Consider now $M = \mathbf{R}^3$ and the group $G = Z_2 \times Z_2 \times Z_2 \times S_3$ generated by reflections in each of the coordinates, i.e., by

$$g_x : (x, y, z) \rightarrow (-x, y, z), \quad g_y : (x, y, z) \rightarrow (x, -y, z), \quad g_z : (x, y, z) \rightarrow (x, y, -z)$$

and by permutations in the (x, y, z) coordinates. This is the situation studied by Sergienko, Gufan, and Urazhdin.¹⁰ (More precisely, they considered the crystallographic group $Pm3m$;¹¹ this includes the reflections in each of the coordinate planes (xy) , (yz) , (xz) mentioned above as well as inversion across an axis ($i_x : (x, y, z) \rightarrow (x, -y, -z)$ and the like for i_y and i_z), reflections in planes through the diagonal of the unit cube, i.e., in the planes $y = \pm x$, $z = \pm x$, $z = \pm y$, and rotations around the coordinate axes. All these elements are also generated by the g_x, g_y, g_z elements plus the full permutation group in three elements.) The MIB consists of three invariants,

$$J_1 = x^2 + y^2 + z^2, \quad J_2 = x^2 y^2 + y^2 z^2 + x^2 z^2, \quad J_3 = x^2 y^2 z^2;$$

only one of these is quadratic, and $\rho = J_1$. In this case,

$$\mathcal{P} = 4 \begin{pmatrix} J_1 & 2J_2 & 3J_3 \\ 2J_2 & (J_1 J_2 + 3J_3) & 2J_1 J_3 \\ 3J_3 & 2J_1 J_3 & J_2 J_3 \end{pmatrix};$$

the quadratic part reduces to \mathcal{P}_{11} and is hence scalar, i.e., $\mathcal{P}^{(0)} = 4J_1$. In this case, $\Theta = 4c_1 J_1$, $Q = 4c_1$.

Example 6. Consider now $M = \mathbf{R}^3$ and G the crystallographic group $G = D_{2h}$ (this is also met in studying anisotropic nematic liquid crystals); this acts in \mathbf{R}^3 via

- (i) inversion through the center,

$$I : (x, y, z) \rightarrow (-x, -y, -z);$$

- (ii) reflections in each of the coordinate planes,

$$\sigma_{xy} : (x, y, z) \rightarrow (x, y, -z), \quad \sigma_{yz} : (x, y, z) \rightarrow (-x, y, z), \quad \sigma_{xz} : (x, y, z) \rightarrow (x, -y, z);$$

- (iii) rotations (by an angle π) around each coordinate axis,

$$R_x : (x, y, z) \rightarrow (x, -z, y), \quad R_y : (x, y, z) \rightarrow (z, y, -x), \quad R_z : (x, y, z) \rightarrow (-y, x, z);$$

- (iv) and, of course, the identity.

It follows immediately from (i) and (ii) that functions $f(x, y, z)$ can be invariant under $G = D_{2h}$ only if they are actually functions of x^2, y^2, z^2 ; it is then easy to check that, in view of (iii), they must actually be also symmetric under any permutation of the coordinates.

We conclude that the MIB is provided by

$$J_1 = x^2 + y^2 + z^2, \quad J_2 = x^2 y^2 + x^2 z^2 + y^2 z^2, \quad J_3 = x^2 y^2 z^2.$$

This is the same set of invariants met in Example 5 above, and the discussion for that case (above and in the following) also applies here; we will thus not further discuss this example. This illustrates an important point, i.e., different groups can give raise to the same set of invariants and can hence be dealt with, from our point of view, in exactly the same way (see also the note at the end of Example 4).

B. Straightforward reduction—non-maximal order

We can apply the general reduction scheme discussed earlier on to the examples considered above, which we will do now for what concerns non-maximal order terms. Note that in Examples 1, 2, and 4, we would have a polynomial of order four and no terms of non-maximal order to simplify. Thus, for these examples, we will consider a Landau polynomial of order six, and discuss the simplification of the terms of order four. In Examples 5 and 6, on the other hand, the lowest possible truncation of the Landau polynomial is at order 12, and there is no need to artificially increase it.

The main purpose of this subsection is to show that one can obtain very explicit formulas for the generating functions appearing in our reduction procedure.

For terms of the non-maximal orders, the strategy is simple: simplify them as much as possible. Terms of maximal order will be dealt with—taking care of thermodynamic stability—in Subsection V C.

Remark 2. The reader should be warned that we are using a simplified notation. In fact, each change of variables at order m will affect the terms of higher orders, hence will change the coefficients k_q (with $q > m$) appearing in the Landau potential. In the explicit formulas below for a_m , the k_m should be understood as the coefficients appearing in the potential after all the previous steps have been performed. This should be taken into account when working concrete applications, as in the companion paper devoted to application of this method to liquid crystals.⁸

Example 1 (continued). In this case, the quadratic part of the Landau polynomial will be written as

$$\Phi_0 = c_1 J_1 + c_2 J_2;$$

the general invariant polynomial of order four is

$$\Phi_2 = k_1 J_1^2 + k_2 J_2^2 + k_3 J_1 J_2.$$

A similar general expression also holds for the invariant generating function of order four,³⁶

$$H_2 = - (a_1 J_1^2 + a_2 J_2^2 + a_3 J_1 J_2).$$

Acting with \mathcal{L}_0 on H_2 , we obtain

$$\begin{aligned} \mathcal{L}_0(H_2) &= [(4c_1 J_1)(2a_1 J_1 + a_3 J_2) + (4c_2 J_2)(2a_2 J_2 + a_3 J_1)] \\ &= 8a_1 c_1 J_1^2 + 8a_2 c_2 J_2^2 + 4a_3(c_1 + c_2) J_1 J_2. \end{aligned}$$

In order to eliminate the term Φ_2 , we should solve the homological equation $\mathcal{L}_0(H_2) = \Phi_2$, which is now an equation for the unknown coefficients (a_1, a_2, a_3) appearing in the generating function. Actually, the homological equation is promptly recast in terms of the coefficients—and of the parameters c_i —as

$$8a_1 c_1 = k_1, \quad 8a_2 c_2 = k_2, \quad 4a_3(c_1 + c_2) = k_3;$$

thus, it suffices to choose

$$a_1 = \frac{k_1}{8c_1}, \quad a_2 = \frac{k_2}{8c_2}, \quad a_3 = \frac{k_3}{4(c_1 + c_2)}$$

in order to eliminate completely the Φ_2 term. Needless to say, this is possible provided $c_1 \neq 0$, $c_2 \neq 0$, $(c_1 + c_2) \neq 0$; if some of these non-degeneracy conditions (involving only the quadratic part of the Landau polynomial) fails, we correspondingly have to retain the associated quartic term(s).

Example 2 (continued). In this case, the quadratic part of the Landau polynomial will be written as

$$\Phi_0 = c_1 J_1 + c_2 J_2 + c_3 J_3;$$

the general invariant polynomial of order four is

$$\Phi_2 = k_1 J_1^2 + k_2 J_2^2 + k_3 J_3^2 + k_4 J_1 J_3 + k_5 J_2 J_3$$

(note we have not written any $J_1 J_2$ term; as $J_1 J_2 = J_3^2$, this would be redundant). A similar general expression also holds for the invariant generating function of order four,

$$H_2 = - (a_1 J_1^2 + a_2 J_2^2 + a_3 J_3^2 + a_4 J_1 J_3 + a_5 J_2 J_3).$$

Acting with \mathcal{L}_0 on H_2 , we obtain

$$\begin{aligned} \mathcal{L}_0(H_2) &= 4a_1 c_1 J_1^2 + 4a_2 c_2 J_2^2 + [(a_4 + a_5)c_3 + 2a_3(c_1 + c_2 + 2c_3)] J_3^2 \\ &\quad + [2a_1 c_3 + a_4(3c_1 + c_2 + 2c_3)] J_1 J_3 + [2a_2 c_3 + a_5(c_1 + 3c_2 + 2c_3)] J_2 J_3. \end{aligned}$$

The homological equation $\mathcal{L}_0(H_2) = \Phi_2$ is now recast as

$$\begin{aligned} k_1 &= 4a_1 c_1, \quad k_2 = 4a_2 c_2, \quad k_3 = (a_4 + a_5)c_3 + 2a_3(c_1 + c_2 + 2c_3), \\ k_4 &= 2a_1 c_3 + a_4(3c_1 + c_2 + 2c_3), \quad k_5 = 2a_2 c_3 + a_5(c_1 + 3c_2 + 2c_3). \end{aligned}$$

Its solution is provided by

$$a_1 = \frac{k_1}{4c_1}, \quad a_2 = \frac{k_2}{4c_2}, \quad a_3 = \left[2k_3 + \frac{c_3(c_3k_1 - 2c_1k_4)}{c_1(3c_1 + c_2 + 2c_3)} + \frac{c_3(c_3k_2 - 2c_2k_5)}{c_2(c_1 + 3c_2 + 2c_3)} \right] \left[\frac{1}{4(c_1 + c_2 + 2c_3)} \right],$$

$$a_4 = \frac{2c_1k_4 - c_3k_1}{2c_1(3c_1 + c_2 + 2c_3)}, \quad a_5 = \frac{2c_2k_5 - c_3k_2}{2c_2(c_1 + 3c_2 + 2c_3)}.$$

Here, again one should impose non-degeneracy conditions corresponding to the requirement that the fractions appearing in the explicit expressions for the a_i are well defined; if these fail, some (or all) of the fourth-order terms cannot be eliminated.

Example 3 (continued). The situation in Example 3 is different from the one of previous examples; indeed, now we have third order invariants. We write as usual

$$\Phi_0 = c_1 J_1^2,$$

and the third order invariant term will be

$$\Phi_1 = k_1 J_2 + k_2 J_3;$$

correspondingly, the third order generating functions will be written as

$$H_1 = -(a_1 J_2 + a_2 J_3)$$

and does not depend on J_1 . Thus, any third order invariant is in the kernel of \mathcal{L}_0 , and it does not produce any effect (at the first order level). At order four, the invariant term and the generating functions will be written as

$$\Phi_2 = k_3 J_1^2, \quad H_2 = -a_3 J_1^2.$$

We immediately have

$$\mathcal{L}_0(H_2) = 8 c_1 a_3 J_1^2,$$

and the homological equation is solved by choosing

$$a_3 = \frac{k_3}{8c_1}.$$

We also have invariants (and generating functions) of order five; these are

$$\Phi_3 = k_4 J_1 J_2 + k_5 J_1 J_3; \quad H_3 = -(a_4 J_1 J_2 + a_5 J_1 J_3).$$

Now we have

$$\mathcal{L}_0(H_3) = 4c_1 a_4 J_1 J_2 + 4c_1 a_5 J_1 J_3;$$

hence, in order to solve the homological equation, we just choose

$$a_4 = \frac{k_4}{4c_1}, \quad a_5 = \frac{k_5}{4c_1}.$$

Needless to say, the elimination of terms of both order four and five is possible only under the condition $c_1 \neq 0$.

Example 4 (continued). As remarked above, once we set our problem in orbit space this is the same as Example 1 (albeit with a different interpretation when we want to go back to the order parameters space). We can thus just reproduce the computations seen in dealing with Example 1 above. We write the quadratic term in the form

$$\Phi_0 = c_1 J_1 + c_2 J_2;$$

the quartic term and generating functions will read

$$\Phi_2 = k_1 J_1^2 + k_2 J_2^2 + k_3 J_1 J_2; \quad H_2 = -(a_1 J_1^2 + a_2 J_2^2 + a_3 J_1 J_2).$$

Thus, we readily get

$$\mathcal{L}_0(H_2) = 8a_1 c_1 J_1^2 + 8a_2 c_2 J_2^2 + 4a_3(c_1 + c_2) J_1 J_2;$$

the homological equation is solved by choosing

$$a_1 = \frac{k_1}{8c_1}, \quad a_2 = \frac{k_2}{8c_2}, \quad a_3 = \frac{k_3}{4(c_1 + c_2)}.$$

In this case, the non-degeneracy conditions are of course $c_1 \neq 0, c_2 \neq 0, (c_1 + c_2) \neq 0$.

Examples 5 and 6 (continued). We will as usual write $\Phi_0 = c_1 J_1$. In this case, no terms of odd order are allowed by the symmetry, and we should eliminate as many terms as possible at orders 4,6,8,10.

The different invariant terms of order not higher than ten are written as

$$\begin{aligned} \Phi_2 &= k_1 J_1^2 + k_2 J_2, \\ \Phi_4 &= k_3 J_1^3 + k_4 J_1 J_2 + k_5 J_3, \\ \Phi_6 &= k_6 J_1^4 + k_7 J_1^2 J_2 + k_8 J_1 J_3 + k_9 J_2^2, \\ \Phi_8 &= k_{10} J_1^5 + k_{11} J_1^3 J_2 + k_{12} J_1^2 J_3 + k_{13} J_1 J_2^2 + k_{14} J_2 J_3; \end{aligned}$$

the expressions for the H_k are obtained from these by replacing the k_i coefficients with a_i ones and changing sign. As we have seen above,

$$\Theta = 4 c_1 J_1, \quad Q = 4 c_1.$$

This means that, as easy to compute,

$$\begin{aligned} \mathcal{L}_0(H_2) &= 8a_1 c_1 J_1^2, \\ \mathcal{L}_0(H_4) &= 12a_3 c_1 J_1^3 + 4a_4 c_1 J_1 J_2, \\ \mathcal{L}_0(H_6) &= 16a_6 c_1 J_1^4 + 8a_7 c_1 J_1^2 J_2 + 4a_8 c_1 J_1 J_3, \\ \mathcal{L}_0(H_8) &= 20a_{10} c_1 J_1^5 + 12a_{11} c_1 J_1^3 J_2 + 8a_{12} c_1 J_1^2 J_3 + 4a_{13} c_1 J_1 J_2^2. \end{aligned}$$

Note that in this case several terms appearing in Φ are *not* in the range of \mathcal{L}_0 , and hence cannot be eliminated. At the same time, some terms in the H_k are in the kernel of \mathcal{L}_0 and thus inessential to our procedure.

In particular, by choosing

$$\begin{aligned} a_1 &= \frac{k_1}{8c_1}, \quad a_3 = \frac{k_3}{12c_1}, \quad a_4 = \frac{k_4}{4c_1}, \quad a_6 = \frac{k_6}{16c_1}, \quad a_7 = \frac{k_7}{8c_1}, \\ a_8 &= \frac{k_8}{4c_1}, \quad a_{10} = \frac{k_{10}}{20c_1}, \quad a_{11} = \frac{k_{11}}{12c_1}, \quad a_{12} = \frac{k_{12}}{8c_1}, \quad a_{13} = \frac{k_{13}}{4c_1}, \end{aligned}$$

the Landau potential is reduced to one of the form

$$\widehat{\Phi} = \beta_1 J_2 + \beta_2 J_3 + \beta_3 J_2^2 + \beta_4 J_2 J_3.$$

Needless to say, this is possible provided $c_1 \neq 0$. It would be possible (but not of interest here) to compute explicitly the coefficients β_i in terms of the k_i and a_i . Note that the coefficients a_2, a_5, a_9, a_{14} are not determined by our procedure.

C. Straightforward reduction—maximal order

For terms of maximal order, our strategy should *not* be to eliminate whatever can be eliminated through our procedure. We should instead take care to guarantee the thermodynamic stability (i.e., convexity for large $|x|$, see Section II E) of the simplified (truncated) Landau polynomial.

A simple way to guarantee this, if all terms could be eliminated, is by arranging things so that $\Phi_N = |x|^{N+2}$. (Note this is surely possible: all terms which can be eliminated are in the range of \mathcal{L}_0 , so we can also arrange things so that a specific term appears as result of applying \mathcal{L}_0 on a suitable generating function.) In practice, we should express $\rho = |x|^2$ in terms of the basic polynomials J_i , and then keep the term ρ^m (with $m = N/2 + 1$) in Φ_N .³⁷

Example 1 (continued). In this case $N = 4$, and

$$\Psi_4 = k_4 J_1^3 + k_5 J_1^2 J_2 + k_6 J_1 J_2^2 + k_7 J_2^3;$$

the general generating function at this order can be written as

$$\chi_4 = b_1 J_1^3 + b_2 J_1^2 J_2 + b_3 J_1 J_2^2 + b_4 J_2^3.$$

Acting on this with \mathcal{L}_0 , we obtain

$$\mathcal{L}_0(\chi_4) = 12b_1c_1J_1^3 + 4J_2[b_2(2c_1 + c_2)J_1^2 + J_2(b_3(c_1 + 2c_2)J_1 + 3b_4c_2J_2)].$$

Recalling that the transformed term will be

$$\tilde{\Psi}_4 = \Psi_4 + \delta\Psi_4 = \Psi_4 - \mathcal{L}_0(\chi_4),$$

and that in this case $\rho = J_1 + J_2$, it is possible to get $\tilde{\Psi}_4 = \beta\rho^3$ by choosing (provided $c_2 \neq 0$, $c_1 + c_2 \neq 0$)

$$b_2 = \frac{36b_1c_1 - 3k_4 + k_5}{4(2c_1 + c_2)}, \quad b_3 = \frac{36b_1c_1 - 3k_4 + k_6}{4(2c_1 + c_2)}, \quad b_4 = \frac{12b_1c_1 - k_4 + k_7}{12c_2}.$$

With this choice, we have

$$\tilde{\Psi}_4 = (k_4 - 12b_1c_1)\rho^3;$$

thus, by choosing (as usual, under the assumption $c_1 \neq 0$)

$$b_1 = \frac{k_4 - 1}{12c_1},$$

we always obtain $\tilde{\Psi}_4 = \rho^3$.

Summarizing, in this case ($G = Z_2 \times Z_2$, Landau polynomial of order six), under the assumptions $c_1 \neq 0$, $c_2 \neq 0$, $(c_1 + c_2) \neq 0$ we can always reduce to consider a Landau polynomial of the form

$$\Psi = c_1J_1 + c_2J_2 + (J_1 + J_2)^3,$$

thus getting rid of the seven additional parameters k_1, \dots, k_7 .

Example 1B. In Example 1, we have considered the case where one considers a Landau polynomial of order six (this was in order to avoid a trivial case at non-maximal orders, i.e., in Sec. VB). We can now also consider the case where the Landau polynomial is of order four (thus, $N = 2$), i.e., $\Phi = \Phi_0 + \Phi_2$. The quadratic part Φ_0 is not modified, so we only have to modify the quartic—and maximal—term Φ_2 . We know from Example 1 that it could be fully eliminated, but in order to preserve stability we should actually leave a term of the type ρ^2 , i.e., $(J_1 + J_2)^2$. In view of the expressions for Ψ_2 and χ_2 (see again Example 1 in Sec. VB), this is obtained by choosing

$$a_1 = \frac{k_1 - 1}{8c_1}, \quad a_2 = \frac{k_2 - 2}{4(c_1 + c_2)}, \quad a_3 = \frac{k_3 - 1}{8c_2}.$$

Thus, for $G = Z_2 \times Z_2$, and Landau polynomial of order four, under the assumption $c_1 \neq 0$, $c_2 \neq 0$, $(c_1 + c_2) \neq 0$, we can always reduce to consider a Landau polynomial of the form

$$\Psi = c_1J_1 + c_2J_2 + (J_1 + J_2)^2,$$

thus getting rid of the three additional parameters $\{k_1, k_2, k_3\}$.

Example 2 (continued). In this case, also $N = 4$, but we should take into account that $J_1J_2 = J_3^2$; we can thus write the general Ψ_4 term and the generating function χ_4 as

$$\begin{aligned} \Psi_4 &= k_6J_1^3 + k_7J_1^2J_3 + k_8J_1J_3^2 + k_9J_2^2J_3 + k_{10}J_2J_3^2 + k_{11}J_2^3 + k_{12}J_3^3, \\ \chi_4 &= b_1J_1^3 + b_2J_1^2J_3 + b_3J_1J_3^2 + b_4J_2^2J_3 + b_5J_2J_3^2 + b_6J_2^3 + b_7J_3^3. \end{aligned}$$

The explicit expressions (which can be readily obtained with a symbolic manipulation language, e.g., in Mathematica) are in this case rather involved and we will not report them. However, one obtains that by a suitable choice of the coefficients appearing in χ_4 , it is possible to obtain

$$\tilde{\Psi}_4 := \Psi_4 - \mathcal{L}_0(\chi_4) = \rho^3 = (J_1 + J_2)^3.$$

The suitable choices for the b_i have a denominator d_i of the form $d_i = r_i(c_1 + c_2)R$ where r_i are some positive integers and

$$R = (5c_1^2 + 26c_1c_2 + 5c_2^2 - 4c_3^2)(4c_1c_2 - c_3^2)(8c_1^2 + 20c_1c_2 + 8c_2^2 - c_3^2).$$

The non-degeneracy conditions allowing for such a reduction of the Landau polynomial (besides those met at order four, see Sec. **V B**) are then just the non-vanishing of the above denominators, i.e., $(c_1 + c_2) \neq 0, R \neq 0$.

Summarizing, in this case ($G = Z_2$, Landau polynomial of order six), under the assumption $c_1 \neq 0, c_2 \neq 0, (c_1 + c_2) \neq 0, (c_1 + c_2 + 2c_3) \neq 0, (3c_1 + c_2 + 2c_3) \neq 0, (c_1 + 3c_2 + 2c_3) \neq 0, R \neq 0$, we can always reduce to consider a Landau polynomial of the form

$$\Psi = c_1 J_1 + c_2 J_2 + c_3 J_3 + (J_1 + J_2)^3,$$

thus getting rid of the 12 additional parameters k_1, \dots, k_{12} .

Example 2B. In this case as well we can consider a variant of the above example, namely, the case where the Landau polynomial is of order four ($N = 2$), $\Phi = \Phi_0 + \Phi_2$ and hence the discussion in the framework of Sec. **V B** would have been trivial.

In this case,

$$\begin{aligned} \Psi_2 &= k_1 J_1^2 + k_2 J_1 J_3 + k_3 J_2 J_3 + k_4 J_2^2 + k_5 J_3^2, \\ \chi_2 &= a_1 J_1^2 + a_2 J_1 J_3 + a_3 J_2 J_3 + a_4 J_2^2 + a_5 J_3^2. \end{aligned}$$

Explicit formulas are still rather involved; in fact now $\tilde{\Psi}_2 = \Psi_2 - \mathcal{L}_0(\chi_2)$ results to be simply $\tilde{\Psi}_2 = \rho^2$ with the choice

$$a_i = \frac{\alpha_i}{r_i A}$$

where α_i are some rather involved polynomial in the c_i and k_i , the r_i are positive integers, and

$$A = (c_1 + c_2) [12c_1^3 c_2 - 3c_2^2 c_3^2 + c_3^4 + c_1^2 (40c_2^2 - 3c_3^2) + 2c_1 (6c_2^3 - 7c_2 c_3^2)].$$

This allows to explicitly identify the non-degeneracy conditions under which such a reduction is possible.

Example 3 (continued). In this case, the general term Ψ_4 and the generating function χ_4 of order six read

$$\begin{aligned} \Psi_4 &= k_6 J_1^3 + k_7 J_2^2 + k_8 J_3^2 + k_9 J_2 J_3, \\ \chi_4 &= b_1 J_1^3 + b_2 J_2^2 + b_3 J_3^2 + b_4 J_2 J_3. \end{aligned}$$

We have

$$\mathcal{L}_0(\chi_4) = 12 b_1 J_1^3;$$

thus, the terms other than J_1^3 cannot be eliminated. On the other hand, in this case $\rho = J_1$, so this is precisely the term which we do not want to cancel (the reader can easily check that setting this to zero produces direction in which the potential is not convex for large $|\mathbf{x}|$); we can however set this to unity, which is obtained by setting

$$b_1 = \frac{k_6 - 1}{12}.$$

Summarizing, in this case, i.e., for $G = Z_3$, the sixth order Landau polynomial can always (provided $c_1 \neq 0$) be reduced to

$$\Phi = c_1 J_1 + k_1 J_2 + k_2 J_3 + k_7 J_2^2 + k_8 J_3^2 + k_9 J_2 J_3 + J_1^3$$

(recall k_7, k_8, k_9 are in general different from the initial ones), thus getting rid of the four additional parameters $\{k_3, \dots, k_6\}$.

Example 4 (continued). In orbit space, this is the same as Example 1; the computations and results would just reproduce those seen in dealing with Example 1 above and are thus omitted.

Examples 5 and 6 (continued). In this case, the general term Ψ_{10} and the generating function χ_{10} of order 12 are written as

$$\begin{aligned} \Psi_{10} &= k_{15} J_1^6 + k_{16} J_1^4 J_2 + k_{17} J_1^3 J_3 + k_{18} J_1^2 J_2^2 + k_{19} J_1 J_2 J_3 + k_{20} J_2^3 + k_{21} J_3^2, \\ \chi_{10} &= b_1 J_1^6 + b_2 J_1^4 J_2 + b_3 J_1^3 J_3 + b_4 J_1^2 J_2^2 + b_5 J_1 J_2 J_3 + b_6 J_2^3 + b_7 J_3^2. \end{aligned}$$

We obtain immediately

$$\begin{aligned} \mathcal{L}_0(\chi_{10}) = & (k_{15} - 24b_1c_1) J_1^6 + (k_{16} - 16b_2c_1) J_1^4 J_2 + (k_{17} - 12b_3c_1) J_1^3 J_3 \\ & + (k_{18} - 8b_4c_1) J_1^2 J_2^2 + (k_{19} - 4b_5c_1) J_1 J_2 J_3 + k_{20} J_2^3 + k_{21} J_3^2. \end{aligned}$$

It is thus clear that we could cancel the J_1^6 term (which we do not actually want to cancel) and we can cancel all the other terms at the exception of the J_2^3 and the J_3^2 ones, just by choosing, under the assumption $c_1 \neq 0$,

$$b_1 = \frac{k_{15}}{24c_1}, b_2 = \frac{k_{16}}{16c_1}, b_3 = \frac{k_{17}}{12c_1}, b_4 = \frac{k_{18}}{8c_1}, b_5 = \frac{k_{19}}{4c_1}.$$

On the other hand, the coefficients b_6 and b_7 are inessential (the corresponding terms are in the kernel of \mathcal{L}_0). As for b_1 , with the choice

$$b_1 = \frac{k_{15} - 1}{24c_1},$$

we will have a term ρ^6 in $\tilde{\Psi}_6$.

In fact, with these choices (and those considered in Sec. V B for lower order generating functions, all of them valid under $c_1 \neq 0$), the Landau polynomial of order 12 is reduced to

$$\widehat{\Phi} = c_1 J_1 + \beta_1 J_2 + \beta_2 J_3 + \beta_3 J_2^2 + \beta_4 J_2 J_3 + \beta_5 J_2^3 + \beta_6 J_3^2 + J_1^6;$$

this depends on 6 parameters, while the original one depended on 22 parameters.

Note also that the convexity for large $|\mathbf{x}|$ is guaranteed, precisely by the presence of the J_1^6 term.

VI. ADAPTED COORDINATES

Let us go back to considering (15); in that formula, $Q_\alpha^\beta = c_\gamma K_{\gamma\alpha}^\beta$ is by construction a numerical matrix. It is quite clear that we would be better off using a set of quadratic invariants such that the matrix Q characterizing the homological operator \mathcal{L}_0 had diagonal form; if this is not possible, one could at least set Q in Jordan normal form.

Let us denote a set of new quadratic invariants as

$$Z_\mu = A_{\mu\nu} J_\nu; \tag{17}$$

here, A is a constant matrix; correspondingly, we have

$$J_\alpha = A_{\alpha\beta}^{-1} Z_\beta, \quad (\partial/\partial J_\alpha) = A_{\alpha\beta}^T (\partial/\partial Z_\beta).$$

The operator \mathcal{L}_0 defined in (15) reads, with these basis invariants,

$$\mathcal{L}_0 = \left[(A_{\mu\alpha} Q_{\alpha\beta} A_{\beta\nu}^{-1}) Z_\nu \right] \frac{\partial}{\partial Z_\mu} := (P_{\mu\nu} Z_\nu) \frac{\partial}{\partial Z_\mu}; \tag{18}$$

here, the matrix P is given by

$$P = A Q A^{-1}. \tag{19}$$

We also write $P = P_s + P_n$, with P_s and P_n the semisimple and nilpotent parts³⁸ of P , with

$$P_s = \text{diag}(\lambda_1, \dots, \lambda_s). \tag{20}$$

Needless to say, to reach this form, the matrix A in (17) should be chosen precisely as the matrix taking Q into Jordan normal form, which we assume below.

In the following, we will use the set Z_α ($\alpha = 1, \dots, s$) of quadratic invariants, and write $\zeta_i = J_{s+i}$ ($i = 1, \dots, q = r - s$; if $s = r$ then no ζ is present) for basic invariants of higher order.

A. Semisimple P

Let us consider the case where $P_n = 0$. In this case, we can consider the monomials (in the invariants)

$$\Gamma_{\mathbf{kh}} := Z_1^{k_1} \dots Z_s^{k_s} \zeta_1^{h_1} \dots \zeta_q^{h_q}; \tag{21}$$

note that χ_m can be written as

$$\chi_m = \gamma_{k_1, \dots, k_s; h_1, \dots, h_q} \Gamma_{\mathbf{k}\mathbf{h}}, \tag{22}$$

where the sum extends on all the sets \mathbf{k}, \mathbf{h} such that

$$\sum_{\alpha=1}^s 2k_\alpha + \sum_{i=1}^q d_{r+i} h_i = m + 2. \tag{23}$$

It follows immediately from (19) and (20) that

$$\mathcal{L}_0(\Gamma_{\mathbf{k}\mathbf{h}}) = (\lambda_\alpha \cdot k_\alpha) \Gamma_{\mathbf{k}\mathbf{h}}. \tag{24}$$

Thus, the kernel of \mathcal{L}_0 restricted to S_m is spanned by all the Γ —among those satisfying (23)—such that

$$\sum_{\alpha=1}^s \lambda_\alpha \cdot k_\alpha = 0. \tag{25}$$

This is the equivalent of the Poincaré resonance condition in our case; thus, we will call terms $\Gamma_{\mathbf{k}\mathbf{h}}$ satisfying it, *resonant*, and (25) will be said to be the *resonance condition*.

Similarly, the range of \mathcal{L}_0 (applied to S_m) is the subspace of S_m spanned by the $\Gamma_{\mathbf{k}\mathbf{h}}$ —among those satisfying (23)—which do *not* satisfy (25).

We conclude that in this case one can always eliminate—as usual, by a careful choice of the generating functions H_1, H_2, \dots , see below—all terms of higher order which are not resonant.³⁹ In other words, we can always reduce—at least in principle—to consider Landau polynomials in which *the terms of higher (but not maximal) order which are allowed by the symmetry but are non-resonant, are absent*.

In more detail, we can always write the generating function as $H_m = -\xi_{\mathbf{k}\mathbf{h}} \Gamma_{\mathbf{k}\mathbf{h}}$; if the term of order $m + 2$ is written as $\Phi_m = c_{\mathbf{k}\mathbf{h}} \Gamma_{\mathbf{k}\mathbf{h}}$, then the homological equation is solved by choosing

$$\xi_{\mathbf{k}\mathbf{h}} = \frac{c_{\mathbf{k}\mathbf{h}}}{(\lambda_\alpha \cdot k_\alpha)}, \tag{26}$$

for the \mathbf{k} satisfying $(\lambda_\alpha \cdot k_\alpha) \neq 0$, while $\xi_{\mathbf{k}\mathbf{h}}$ is undetermined (we can, e.g., set it to zero) for \mathbf{k} satisfying (25).

Note that our procedure produces hence some (possibly small) denominators; this will make that the procedure is well defined only in a small neighborhood of the origin in the M space. Physically, this is not a problem provided this neighborhood is large enough to include the symmetry-breaking minima of the theory; if this is not the case, the procedure described here is only formal and not helpful in practice. This problem is well known in the applications of Poincaré-Birkhoff normal forms in dynamical and Hamiltonian systems (see also Sec. VIII).

B. Non-semisimple P

In the case where P is not semisimple, i.e., $P_n \neq 0$, one does actually proceeds in the same way, dealing with P_s rather than the full P . That is, the system is set in normal form with respect to the semisimple part of P , and resonant terms are defined with reference to the semisimple part of P alone (i.e., as above); this is completely analogous to what is done in the Poincaré approach to dynamical systems.³⁻⁵

As a result, the Landau polynomial can be reduced to include only resonant higher order terms Φ_k , while the quadratic one is $\Phi_0 = \Phi_s + \Phi_n$, where of course Φ_s, Φ_n are associated, respectively, to P_s and P_n .

In terms of the operator \mathcal{L}_0 , this amounts to saying that our previous results (nonlinear terms can be reduced to those not in the range of \mathcal{L}_0 , etc.) remain true, with a difference: now the operator \mathcal{L}_0 is not associated to the full quadratic part Φ_0 , but instead to its semisimple part Φ_s only.

C. Example

By looking at Section V A, one sees that in Example 1, the Q matrix is diagonal, and in Examples 3–6, it actually reduces to a scalar. Thus, the only example, among those considered above, in which the coordinates are not already adapted is Example 2; we are now going to consider this.

Note that the matrix Q for this case (see Section V A) is diagonal when $c_3 = 0$; we will thus assume $c_3 \neq 0$, and simplify our notation by setting $k_1 = c_1/c_3$, $k_2 = c_2/c_3$, $\gamma = k_1 + k_2$. Then, Q reads

$$Q = c_3 \begin{pmatrix} 4k_1 & 0 & 2 \\ 0 & 4k_2 & 2 \\ 1 & 1 & 2(k_1 + k_2) \end{pmatrix}.$$

This is taken into Jordan normal form by the map

$$A = \frac{1}{4\beta^2} \begin{pmatrix} -2\delta & 2\delta & 4\delta^2 \\ \delta - \beta & -(\delta + \beta) & 2 \\ \delta + \beta & -(\delta - \beta) & 2 \end{pmatrix},$$

where we have defined

$$\delta := k_1 - k_2; \quad \beta = \sqrt{1 + \delta^2}.$$

The inverse matrix is given by

$$A^{-1} = \begin{pmatrix} -\delta^{-1} & (1 + 2\beta\delta - 2\beta^2)(\beta - \delta)^{-1} & (-1 + 2\beta\delta + 2\beta^2)(\beta + \delta)^{-1} \\ \delta^{-1} & -(\beta - \delta)^{-1} & (\beta + \delta)^{-1} \\ 1 & 1 & 1 \end{pmatrix};$$

the corresponding (diagonal) Jordan form for Q is

$$\tilde{P} = 2c_3 \begin{pmatrix} \gamma & 0 & 0 \\ 0 & \gamma - \beta & 0 \\ 0 & 0 & \gamma + \beta \end{pmatrix}.$$

In order to check that our construction is working correctly, one can reach the same result in a different way. The new invariants $Z_\alpha = A_{\alpha\beta} J_\beta$ are given by

$$\begin{aligned} Z_1 &= [\delta/(2\beta^2)] (-x^2 + 2\delta xy + y^2), \\ Z_2 &= [(\delta - \beta)/(4\beta^2)] [x^2 - 2(\delta + \beta)xy + (\delta + \beta)^2 y^2], \\ Z_3 &= [(\delta + \beta)/(4\beta^2)] [x^2 + 2(\beta - \delta)xy + (\beta - \delta)^2 y^2]. \end{aligned}$$

From these expressions, one easily computes the \mathcal{P} -matrix in terms of the Z , which we denote by $\tilde{\mathcal{P}}$. On the other hand, we should now express the quadratic part of the Landau polynomial in terms of the Z_α , i.e., writes

$$\Phi_0 = c_\alpha J_\alpha = c_\alpha A_{\alpha\beta}^{-1} Z_\beta := \tilde{c}_\beta Z_\beta.$$

Finally, we can write $\mathcal{L}_0 = -\tilde{c}_\alpha \tilde{\mathcal{P}}_{\alpha\beta} (\partial/\partial Z_\beta)$; doing this explicitly, with standard (and boring) algebra, we obtain $\mathcal{L}_0 = (\tilde{P}_{\alpha\beta} Z_\beta) (\partial/\partial Z_\alpha)$ with the same \tilde{P} given above.

VII. REDUCTION AND ANALYSIS OF LANDAU POTENTIALS

In this section, we will discuss how the reduction studied here can be used to analyze—both quantitatively and qualitatively—the behavior of concrete physical systems in the framework of Landau theory, i.e., the critical points of Landau potentials. We will again refer to the examples considered in Sec. V.

A. Quantitative analysis of Landau polynomials

In this subsection, we consider the simplest of the examples presented above—i.e., Example 1 (recall all computations will also immediately apply to Example 4), albeit with a sixth order Landau polynomial—and show how the method depicted here can be concretely used to study the problem. We will give a complete—qualitative and quantitative—analysis of this simple problem.

In concrete cases, one would be satisfied in discussing the qualitative behavior, as will be done in Subsection VII B, and the simple case at hand here is just to be meant as an illustration of the method.

The analysis of a concrete problem requires to obtain definite expressions for the coefficients appearing in the generating functions, i.e., to describe exactly the change of variables to be considered. A discussion of how to obtain these in a computationally efficient way is contained in the companion paper,⁸ and here we will just provide the resulting formulas for the normalizing change of coordinates, see below.

Examples 1 and 4 (continued). The general sixth order G -invariant Landau polynomial for the G action considered in Example 1 (and also applying to Example 4) is given, in terms of the original (x, y) coordinates, by

$$\Phi = (c_1x^2 + c_2y^2) + (k_1x^4 + k_2x^2y^2 + k_3y^4) + (k_4x^6 + k_5x^4y^2 + k_6x^2y^4 + k_7y^6);$$

note this depends on eight parameters, and analyzing its behavior in terms of these parameters would be quite a substantial task.

By the (nonunique, see above) change of coordinates

$$\begin{aligned} x \rightarrow \tilde{x} &= x \left[1 - \left(\frac{(k_1x^2 + k_2y^2)}{2c_1} \right) + \left(\frac{(1 - k_4)x^4 + (3 - k_6)y^4}{2c_1} + \frac{7k_1^2x^4 + 3k_2^2y^4}{8c_1^2} + \frac{k_2k_3y^4}{2c_1c_2} \right) \right], \\ y \rightarrow \tilde{y} &= y \left[1 - \left(\frac{k_3y^2}{2c_2} \right) \left(\frac{(3 - k_5)x^4 + (1 - k_7)y^4}{2c_2} + \frac{5k_1k_2x^4}{4c_1c_2} + \frac{7k_3^2y^4}{8c_2^2} \right) \right], \end{aligned}$$

and truncating the resulting polynomial again at order six, the Landau potential is transformed into

$$\tilde{\Phi} = c_1\tilde{x}^2 + c_2\tilde{y}^2 + (\tilde{x}^2 + \tilde{y}^2)^3.$$

This depends only on the two parameters associated to the quadratic terms, and the analysis of its critical points is simple enough.

In fact, there is the trivial critical point

$$p_0 = (0, 0),$$

always present and stable for $c_1 > 0$ and $c_2 > 0$; this is invariant under the full G group. Then, there are some solutions with both x and y nonzero (the explicit expressions for these are extremely involved and will not be reported), which are therefore invariant only under the trivial subgroup made of the identity alone. Moreover, there are four families of nontrivial critical points (\tilde{x}, \tilde{y}) , whose existence is limited to ranges of the parameters c_1 and c_2 . The latter are given by

$$\begin{aligned} p_1^\pm &= (\pm(-c_1/3)^{1/4}, 0), \\ p_2^\pm &= (0, \pm(-c_2/3)^{1/4}). \end{aligned}$$

The family p_1^\pm exists for $c_1 < 0$, the family p_2^\pm for $c_2 < 0$. As for their stability, by explicit computations, we obtain that the eigenvalues of the Hessian matrix on p_1^\pm are given by $\{-8c_1, -2c_1 + 2c_2\}$. Thus, in their range of existence, these solutions are stable provided $(c_2 - c_1) > 0$; given that $c_1 < 0$, this is always the case for $c_2 > 0$, while for $c_2 < 0$, it amounts to the condition $|c_1| > |c_2|$. Solutions in this family are invariant under g_y .

Similarly, by explicit computations, the eigenvalues of the Hessian matrix on p_2^\pm are given by $\{2(c_1 - c_2), -8c_2\}$. In their range of existence, these solutions are stable provided $(c_1 - c_2) > 0$; given that $c_2 < 0$, this is always the case for $c_1 > 0$, while for $c_1 < 0$, it amounts to the condition $|c_2| > |c_1|$. Solutions in this family are invariant under g_x .

Thus, qualitative information can be obtained by the reduced Landau potential $\tilde{\Phi}$. Should we require to obtain the exact dependence of the solutions on all the control parameters, we should

invert the change of coordinates $(x, y) \rightarrow (\tilde{x}, \tilde{y})$; this inversion should be sought for working by series.

In this case, such an inversion (again nonunique) is obtained by setting

$$\begin{aligned} x &= \tilde{x} \left[1 - (a_1\tilde{x}^2 + a_2\tilde{y}^2) + ((3a_1^2 - a_3)\tilde{x}^4 + (4a_1a_2 - a_4 + 2a_2b_1)\tilde{x}^2\tilde{y}^2 + (a_2^2 - a_5 + 2a_2b_2)\tilde{y}^4) \right], \\ y &= \tilde{y} \left[1 - (b_1\tilde{x}^2 + b_2\tilde{y}^2) + ((2a_1b_1 + b_1^2 - b_3)\tilde{x}^4 + (2a_2b_1 + 4b_1b_2 - b_4)\tilde{x}^2\tilde{y}^2 + (3b_2^2 - b_5)\tilde{y}^4) \right]. \end{aligned}$$

With these, and writing

$$\begin{aligned} \alpha &= 3^{3/2}, \quad \beta_1 = \frac{3k_1}{2|c_1|}, \quad \beta_2 = \frac{3k_3}{2|c_2|}, \\ \gamma_1 &= \sqrt{3} \left(\frac{4|c_1|(1 - k_4) - k_1^2}{8|c_1|^2} \right), \quad \gamma_2 = \sqrt{3} \left(\frac{4|c_2|(1 - k_7) - k_3^2}{8|c_2|^2} \right), \end{aligned}$$

the solutions in the family p_1^\pm are given by

$$(x, y) = \left(\pm \frac{|c_1|^{1/4}}{3^{7/4}} \left[\alpha - \beta_1\sqrt{|c_1|} + \gamma_1|c_1| \right], 0 \right),$$

and those in the family p_2^\pm by

$$(x, y) = \left(0, \pm \frac{|c_2|^{1/4}}{3^{7/4}} \left[\alpha - \beta_2\sqrt{|c_2|} + \gamma_2|c_2| \right] \right).$$

B. Qualitative analysis of Landau polynomials

The concrete computational problem in Sec. VII A was the determination of the explicit changes of coordinates, i.e., the expression of (\tilde{x}, \tilde{y}) in terms of (x, y) , and the inverse transformation expressing (x, y) in terms of (\tilde{x}, \tilde{y}) . This can be obtained through the method presented in the main body of the paper, and would easily produce for the other examples considered here explicit (and rather lengthy) formulas.

However, as mentioned above, in many cases one would be satisfied with a qualitative analysis of the Landau potential, that is, determine which phases are possible and how these change with the parameters.

Note that it is true that the explicit relation between parameters in the reduced and in the original Landau potential requires to explicitly determine the change of variables relating (x, y) and (\tilde{x}, \tilde{y}) , but it is also true that in a wealth of physical applications, the parameters entering in the (original) Landau potential are effective ones, determined phenomenologically by fitting data. So the same approach can be followed directly on the reduced Landau potential, and we can work directly at this level.

Needless to say, an analysis of the reduced Landau potential is much simpler than that of the full (original) one. In this section, we will shortly indicate how such an analysis can be performed in the examples considered above; we will omit Example 1 (and 4), considered in Section VII A.

Example 2 (continued). In Example 2, we started from a potential depending on three parameters associated to the quadratic part, plus twelve additional ones. All of them can be eliminated by Poincaré changes of coordinates, and recalling the explicit expression for the J_a we arrive at the reduced potential

$$\tilde{\Phi} = c_1 x^2 + c_2 y^2 + c_3 xy + (x^2 + y^2)^3. \quad (27)$$

The trivial critical point $(0, 0)$ is always present; there are several branches of nontrivial critical points (x_*, y_*) , and we omit the explicit expressions for these in terms of the c_i parameters. These are invariant under a nontrivial subgroup only for $c_3 = 0$, in which case potential (27) reduces to

$$\tilde{\Phi} = c_1 x^2 + c_2 y^2 + (x^2 + y^2)^3,$$

and we have (i) solutions with $y_* = 0$ and hence invariant under the y reflection (for such solutions $x_* = \pm(-c_1/3)^{1/4}$) and (ii) solutions with $x_* = 0$ and hence invariant under the x reflection (for such

solutions $y_* = \pm(-c_2/3)^{1/4}$. Solutions (i) are stable for $c_1 > 0$ and $c_2 < c_1$, while solutions (ii) are stable for $c_2 > 0$ and $c_1 < c_2$. Thus, there is a phase transition semi-infinite line at $c_1 = c_2$, for both parameters being positive.

Note that $c_3 = 0$ implies that actually the potential is invariant not only under the simultaneous reflection in x and y but also separately under reflection in each variable, so that we are in the frame of Example 1.

Example 3 (continued). In this case, as seen above (but with a small change of notation), the reduced potential is written as

$$\Phi = c_1 J_1 + k_1 J_2 + k_2 J_3 + k_3 J_2^2 + k_4 J_3^2 + k_5 J_2 J_3 + J_1^3.$$

By considering the gradient of this in the orbit space—that is, with respect to the J_i variables—we get immediately that critical points exist for $c_1 < 0$ and

$$J_1 = \pm \sqrt{\frac{-c_1}{3}}, \quad J_2 = \frac{2k_1 k_4 - k_2 k_5}{k_5^2 - 4k_3 k_4}, \quad J_3 = \frac{2k_2 k_3 - k_1 k_5}{k_5^2 - 4k_3 k_4}.$$

However, it should be recalled that the three invariants J_1, J_2, J_3 depend on two variables (x, y) (or one complex variable $z = x + iy$) so that the ∇J_i are surely not independent at each point.

Moreover, in this case, the symmetry group does not admit any nontrivial subgroup; it is easily checked that solutions with other symmetries—such as reflections in x or y —only exist for special values of the parameters and hence do not form a branch.

Examples 5 and 6 (continued). The reduced Landau polynomial is in this case

$$\Phi = c_1 J_1 + \beta_1 J_2 + \beta_2 J_3 + \beta_3 J_2^2 + \beta_4 J_2 J_3 + \beta_5 J_2^3 + \beta_6 J_3^2 + J_1^6.$$

By looking at the gradients in terms of the J_i variables, we have two branches of critical points, i.e.,

$$\begin{aligned} J_1 &= (-c_1/6)^{1/5}, \\ J_2 &= \frac{\beta_4^2 - 4\beta_3\beta_6 \pm \sqrt{\Theta_2}}{12\beta_5\beta_6}, \\ J_3 &= -\frac{\beta_4^3 + 12\beta_2\beta_5\beta_6 - \beta_4(4\beta_3\beta_6 \mp \sqrt{\Theta_3})}{24\beta_5\beta_6^2}; \\ \Theta_2 &= 24\beta_5\beta_6(\beta_2\beta_4 - 2\beta_1\beta_6) + (\beta_4^2 - 4\beta_3\beta_6)^2, \\ \Theta_3 &= \beta_4^4 - 8\beta_3\beta_4^2\beta_6 + 24\beta_2\beta_4\beta_5\beta_6 + 16\beta_3^2\beta_6^2 - 48\beta_1\beta_5\beta_6^2. \end{aligned}$$

We can have other solutions at points where the gradients ∇J_i are not independent. The matrix built with the gradients of the three invariants is

$$M = 2 \begin{pmatrix} x & y & z \\ x(y^2 + z^2) & y(x^2 + z^2) & z(x^2 + y^2) \\ xy^2z^2 & x^2yz^2 & x^2y^2z \end{pmatrix}$$

with determinant

$$\text{Det}(M) = 8xyz(x^2 - y^2)(y^2 - z^2)(x^2 - z^2).$$

Thus, the singular sets where gradients of the basic invariants are not independent are made of the three coordinate axes and of the six lines bisecting (the positive or negative quadrants of) the three coordinate planes. One should then consider restrictions of Φ to these singular sets; actually due to the inherent symmetry of the potential, it would suffice to consider just one case for each type, e.g., just the sets $z = 0$ and $z = y$. The solutions obtained on these singular sets will have a transparent symmetry and will provide symmetry-breaking solutions.

It should be stressed that these reductions would provide simpler systems for determination of critical points, i.e., two polynomial equations in two variables (e.g., choosing the cases mentioned above, in x and y). However, these equations would be of high degree, degree 10 for the reduction to coordinate axes and degree 11 for reduction to lines bisecting coordinate planes.

We will not analyze these high degree systems; the symmetry breakings for this group have been studied in detail in Ref. 10 (and also reconsidered in Ref. 6); in particular, Sergienko, Gufan, and Urazhdin considered in detail the different types of phase transitions occurring in this case, and the reader is referred to their work for a detailed (quantitative and not just qualitative) analysis.

VIII. DISCUSSION

We have so far shown that all terms in the range of the homological operator \mathcal{L}_0 can be eliminated by a suitable sequence of Poincaré transformations, and shown how one can proceed in practice to obtain this.

We will now briefly discuss the advantages, together with the limitations and some possible extensions of our approach.

A. Advantages of the method

In studying the behavior of (the extremal points of) the Landau polynomial Φ when the parameters appearing in it are varied, one is usually faced with a formidable task, just due to the high number of these parameters. In fact, the general approach should go through a study (often possible only via a numerical approach, in particular, for high N) of the critical point of Φ , exploring a high dimensional parameter space.

The advantage of the method proposed here, which is just a reformulation of the Poincaré approach to the study of dynamical systems around an equilibrium point (or other known solutions), lies in that the number of parameters, and thus the dimension of the space to be explored, is reduced. This reduction can in fact be quite substantial, as we have seen in some of the examples considered through Section V. In fact, in Example 1 (and Example 4), we passed from nine to two parameters, in Example 2 from fifteen to three parameters, in Example 3 from ten to six parameters, and in Examples 5 and 6 from twenty-two to six parameters.

Thus, the effectiveness of the method depends on the group (representation) one is considering. Moreover, while a problem depending on two parameters can be analyzed, a problem depending say on six parameters is still extremely hard to analyze; so obviously the present method provides in general a step forward, but not a full solution.

We will now pass to consider several other limitations of the method

B. Varying parameters

First of all it should be stressed that we have worked with a given Landau polynomial, i.e., with *fixed* values of the parameters entering in it (the coefficients of the Landau polynomial). These parameters—or at least some of them—will in general depend on the external “control” parameter, i.e., the physical ones: temperature, pressure, and magnetic field, and indeed the Landau parameters *have* to change with the physical ones for a phase transition to take place. Thus, some extra care is needed if we want to work on a full interval of values of the control parameter(s).

In particular, one is often interested in (the vicinity of) phase transitions; in this case, the coefficients of the polynomial $\Phi(x)$ not only depend on external control parameters λ but also at phase transition necessarily pass through critical values.

The discussion given so far should be modified if we want to consider not just given fixed values of the parameter(s) but a full range of values, including, in particular, critical ones.

Let us consider, for ease of discussion, a single control parameter $\lambda \in \Lambda \subseteq \mathbf{R}$, and let $\lambda_0 \in \Lambda$ be a critical value. If we want to describe a small but finite interval $\Lambda_0 \subset \Lambda$, we have to require that the near-identity changes of variables considered in Secs. I–VII are defined uniformly in Λ_0 . In particular, if we want to consider an interval which includes the critical point, e.g., $\Lambda_0 = [\lambda_0 - \varepsilon, \lambda_0 + \varepsilon]$, this would mean requiring that these changes of variables are well defined also at $\lambda = 0$. Note that the changes of variables considered in Section V B do not in general pass this criterion: e.g., many of them are not allowed when $c_1 = 0$.

It should be stressed that, as mentioned in Remark 1 above, this is just inherent to the method. In fact, the vanishing of c_1 means the vanishing of the quadratic part of the Landau potential, on which all of the Poincaré procedure is based. Note also that this makes perfect physical sense: we cannot expect to have results uniform in λ over an interval which includes a phase transition.

The conclusion is that special care must be taken (as also rather obvious physically) if we want to consider reduction of the Landau polynomial over a full range of parameters, and in particular the allowed reduction is (in general, severely) limited if this range includes critical values (actually, one should avoid these). On the other hand, our method can give a simplified description of the outcome of a phase transition, analyzing the simplified potential for values of the parameters higher or lower than the critical ones.

C. Small denominators

The generating functions for the Poincaré near-identity changes of variables are obtained as solutions of the homological equation. As seen quite clearly in the examples, and as is specially clear once the Q matrix (or its semisimple part) has been set in diagonal form, this involves inversion of a matrix and thus introduces some denominators.

When the latter vanish, the transformation is not defined and hence the reduction turns out to be impossible. But even when the denominators are nonzero, some care should be taken if they are small.

In fact, our approach is based on a series expansion; for this to make sense, it is needed that the terms of different orders have a size which correspond to their order (that is, that the series is well ordered). If the expansion parameter (roughly speaking, the distance from the critical point) is ε and we perform a change of variables in which the involved denominator is larger than ε^{-1} , then terms which are apparently of order ε^k will actually be of lower orders, and the series is not well ordered any more. In other words, the series expansion gets not justified in this case.

Thus, one should check the appearance of these small denominators; they will in general make that the resulting change of coordinates is well defined only within a certain radius of convergence, and the computation will have physical relevance only if the minima of the Landau polynomial (i.e., the physical state) lie within this convergence region.

It should be mentioned that some way to partially escape this problem is well known in dynamical systems. In fact, the small denominators will appear only when attempting to eliminate terms which correspond to near-resonances, i.e., such that $\lambda_\alpha \cdot k_\alpha \simeq 0$, see Eq. (25). It is thus possible to circumvent them by simply renouncing to eliminate near-resonant terms.

In more formal terms, this is obtained by “detuning the resonance”:²¹ we write $\lambda_\alpha = \sigma_\alpha + \varepsilon^2 \eta_\alpha$, and consider σ_α as the eigenvalues of P , while the difference $\lambda_\alpha - \sigma_\alpha$ is considered as a perturbation term⁴⁰ to be included between higher order terms in the Landau expansion.

We will not discuss this approach here (see Ref. 22 for a recent overview), but it is worth mentioning that it gave extremely satisfactory results in explicitly computing quantum levels of molecules up to near the dissociation threshold.^{23,24}

D. Non-orthogonal action

We have assumed the group G acts in $M = \mathbf{R}^n$ by an orthogonal action. Unfortunately, this is not always the case in concrete applications; albeit in principle (by Palais-Mostow theorem, see, e.g., Refs. 12 and 16), one can always reduce to an orthogonal action, this goes through dimension increase and/or modification of the metric. This means that in practice the method can become much more involved and less computationally convenient.

In particular, it is known that Landau theory for liquid crystals^{25,26} requires a description in terms of a tensorial order parameter of second order; the natural group action on this is not fitting simply in the framework considered here, and will be discussed elsewhere.

E. Further reduction

In our discussion, we have considered the result of changes of variable on terms of the same order as the generating function, without describing in detail the higher order effects.

Actually, the reduction procedure can be iterated—restricting to generating functions in the kernel of \mathcal{L}_0 , so not to change terms which have already been reduced—using higher order effects; the latter are basically controlled by using the Baker-Campbell-Hausdorff formula. This is known (under different approaches) in the framework of dynamical systems as “further normalization,” and we will just refer the interested reader to, e.g., Refs. 5, 6, and 27 and references therein.

F. Dynamics and Landau-Ginzburg

In standard Landau theory, the equilibrium state x of the physical system is described by the minima of the Landau potential $\Phi(x)$; this description is inherently static. One can also provide, in nearly the same terms, a dynamical description; the time evolution of the state $x(t)$ of the system is then described by $\dot{x} = -\nabla\Phi(x)$. Needless to say this agrees with standard Landau theory if we look at asymptotic solutions.

In this case, the equations of motion also include a \dot{x} term, and our computations for the effect of a change of variables on the equations have to be changed accordingly. Once again we will defer a detailed account of this modification of our approach, and just refer the reader to the equivalent treatment given in the dynamical systems framework (by construction, one would be interested only in the time evolution of invariants); see, e.g., Ref. 28.

A well known extension of Landau theory is provided by Ginzburg-Landau theory; here, the order parameter is a local function on spacetime, and the theory is described by an (gauge) invariant functional. Michel theory can be extended to this framework,²⁹ and it has thus to be expected that our approach works also here. (There will be a severe reduction of the regularity of the functional upon reduction to the orbit space;³⁰ luckily this reduction does not take place if one works with C^∞ , or analytic, functionals. I am grateful to Professor Ball for pointing out these facts.)

IX. CONCLUSIONS

In the Landau theory of phase transitions, one considers an effective potential Φ whose symmetry group G and degree d depend on the Physics of the system under consideration.

One should consider as Φ the most general G -invariant polynomial of a certain degree d . When such a Φ turns out to be too complicated for a direct analysis, it is essential to be able to consider a simplified potential $\hat{\Phi}$ giving rise to the same behavior as the original one.

Here, we have described in detail a reduction procedure based on classical Lie-Poincaré theory; this just considers changes of variables, defined locally. Thus, it expresses the *same* potential Φ in *different* coordinates.

In many cases, one is satisfied with analyzing the behavior of the Landau potential for fixed values (near the transition point) of the control parameter(s); in these cases, our method is specially effective. In other cases, one wants to be able to “follow” the critical points of the Landau potential as the control parameter(s) is (are) changed over a range Λ ; in this case, one has to require the change of variables required by our method is uniformly defined in all of Λ , which poses serious limitations on the applicability of the method.

We stress that our discussion does not just provide a proof of the fact one can consider a reduced potential of the form described in detail in Secs. I–VIII; it also gives a constructive algorithm to make completely explicit computations.

We have shown this by a number of explicit examples; these included, in particular, groups describing the symmetry of isotropic, non-isotropic, and chevron-shaped nematics.

Finally, we would like to stress that in this paper we consider just changes of coordinates: we eliminate terms by choosing suitable coordinates, but we are *not* changing the physical potential. On the other hand, in Landau theory, one allows changes of the potential, provided these do not alter its qualitative behavior.

Thus, we are *not* considering the most general transformation of Φ allowed by Landau theory. On the other hand, our reduction amounts to a change of variables, requires only to solve linear equations, and is completely algorithmic; it can thus be easily implemented, maybe resorting to a symbolic manipulation language in order to perform the algebraically complex (albeit conceptually

simple) required computations. Further analysis—maybe with an actual change of the physical potential, and based on physical considerations rather than on mathematical manipulations—can then be applied on the simplified form of the potential thus obtained.

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- ³¹ In that paper, they will however be considered via a “brute force” approach; this will avoid to enter into the mathematical details needed for further normalization, which are therefore not discussed here.
- ³² Note that if G is a continuous group, some of the x variables will actually be inessential physically, as can be quotiented out; in the present note, we only consider discrete groups, while in the companion paper⁸ we will meet this situation.
- ³³ Actually, their transformation can be described by means of the Baker-Campbell-Hausdorff formula;⁵ but this is inessential here.
- ³⁴ One could actually consider a “higher order normalization,” e.g., following the steps of Ref. 6, but we prefer not to enter into such details.
- ³⁵ With $z = x + iy$, these correspond to $J_1 = |z|^2$, $J_2 = \text{Re}[z^3]$, $J_3 = -\text{Im}[z^3]$.
- ³⁶ Here and in the other examples, the generating function has a minus sign for convenience in writing the homological equation and the final results.
- ³⁷ If some term in Φ_N is resonant and cannot be eliminated, then we should enter into details of the term, and see how we can guarantee convexity for large $|x|$.
- ³⁸ The nilpotent part could (and will most often) vanish, but we are not guaranteed this will be the case in general.
- ³⁹ Note again here we should not attempt to eliminate the maximal order terms as these are needed to guarantee the thermodynamic stability.
- ⁴⁰ It is necessary to consider this as being second order in ε for the method to be viable.^{21,22}