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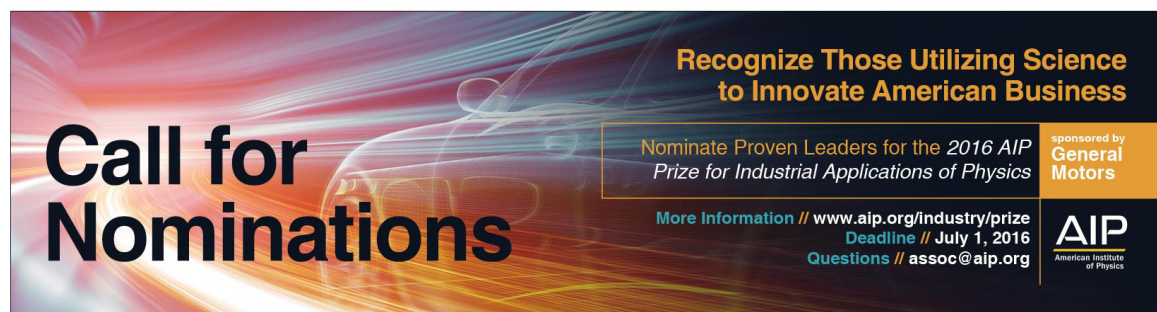
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Poincaré-like approach to Landau theory. II. Simplifying the Landau-deGennes potential for nematic liquid crystals

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In a previous paper, we have discussed how the Landau potential (entering in Landau theory of phase transitions) can be simplified using the Poincaré normalization procedure. Here, we apply this approach to the Landau-deGennes functional for the isotropic-nematic transitions, and transitions between different nematic phases, in liquid crystals. We give special attention to applying our method in the region near the main transition point, showing in full detail how this can be done via a suitable simple modification of our Poincaré-like method. We also consider the question if biaxial phases can branch directly off the fully symmetric state; some partial results in this direction are presented. © *2015 AIP Publishing LLC.*
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I. INTRODUCTION

In the Landau theory of phase transitions,[1,2] the state of a system is described by minima of a group-invariant potential $\Phi(x)$, depending on the order parameters x and on external physical parameters (temperature, pressure, etc.) which control the phase transition. As these are varied, the minima of the Landau potential change location and assume different invariance properties, so corresponding to different phases.

The Landau potential is a polynomial one, and the order[33] N of this is sometimes not so low; moreover, all possible terms (that is, invariant monomials) of order up to N should be included. Thus, in concrete applications, the Landau potential can be rather complex, and the study of its minima depending on parameters can result quite difficult.

It would of course be convenient to have a criterion for simplifying the Landau potential, i.e., to be able to drop certain of the invariant monomials. Different criteria to this effect have been proposed in the literature, and among these we mention, in particular, the one by Gufan,[3,4] then recast in an earlier paper by the present author.[5]

In the companion paper,[6] we have provided a simple discussion of how the technique created by Poincaré in the framework of dynamical systems to simplify nonlinear terms[7–14] could be adapted to the framework of Landau theory; note that in this context one should most often refrain from a complete simplification of the highest order terms, as the requirement of thermodynamic stability—that is, convexity at large distances from the origin—should be taken into account, as discussed in Ref. 6 and recalled here in Sec. IV B.

This Poincaré-like approach is completely algorithmic and quite general; in particular, it can be pushed up to any desired order (albeit some convergence issues should be controlled; these are related to small denominators and will be completely explicit in any concrete computation; see the remarks at the end of Sec. IV).[34]

In the present note, we want to proceed along the same lines to analyze a concrete problem, i.e., the Landau-deGennes (LdG in the following) theory for the isotropic-nematic transitions in liquid crystals;[15–18] this also describes transitions between different nematic phases (biaxial, and

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different uniaxial ones, in particular, oblate and prolate uniaxial). In this respect, we will devote special attention to the possible direct transition between the isotropic and a biaxial phase.[19]

More generally, we consider how our method can be applied near the main transition point; at this point, the linear (homological) operator on which the Poincaré procedure is based is degenerate, so that the standard method does not apply; however, our general method[6] is formulated in such a way to be readily applicable in this more general case. We show in full detail how this is done operationally; this implicitly makes use of the "further normalization" technique developed for dynamical systems,[13,14] but we will not need to discuss it here.

It should be stressed that in this note, at difference with the general discussion given in Ref. 6, we do not aim at mathematical generality, but have a very concrete case—i.e., a given Landau potential, the LdG one—at hand. Also we know the order of the LdG potential. This means that some of the issues in the general approach proposed in Ref. 6 can be substantially streamlined (see Appendix B for a comparison); in particular, we do not need to proceed order by order but can proceed by a direct computation[35] taking into account the main ideas behind the Poincaré approach.

As well known, in the LdG theory,[15–18] the order parameter is a tensorial one (this corresponds to the general situation in liquid crystals[16]), i.e., a three-dimensional symmetric traceless matrix Q, and the symmetry group, which in this case is the three-dimensional rotation group $SO(3)$, acts on it by conjugations, i.e., $Q \to RQR^{-1}$.[36]

The *plan of the paper* is as follows. We will first analyze in detail this $SO(3)$ action (Sec. II) and the LdG functional (Sec. III) and then pass to implement the Poincaré approach on the LdG functional. We will first report on the results of computations up to order six (Sec. IV), as it would follow from the fact the two basic invariants are of order two and three (see Secs. II and III), but in subsequent analysis, it will result that working at this order we find a non-physical degeneration (which also leads to non-physical results), so that we will extend our computations and analysis to order eight (Sec. V); this will eliminate the degeneracy met at order six and give agreement with classical results.[18] Sec. VI is devoted to the analysis of the reduced LdG obtained through our method. Here, we will find out that, as mentioned above, the computations at order six yield a non-physical degeneration, which in turn gives results in disagreement with the widely accepted ones.[18] On the other hand, going at the next order in our expansion, i.e., order eight (a functional of order seven is forbidden by the request of thermodynamic stability), we remove the degeneracy, and it turns out the results obtained via the reduced functional are then in agreement with those of the full theory.[18] These computations are performed under a nondegeneracy assumption for the quadratic term of the LdG potential, which fails precisely at the main transition point; so they do not apply in the vicinity of the main phase transition. This region of the parameter space is studied in Sec. VII; here, we will, in particular, look for biaxial solutions and conclude that under some non-degeneracy assumptions (involving only coefficients of higher order terms in the LdG potential), the branches identified in Sec. VI are unstable at the main bifurcation. We conclude our work by summarizing and discussing our results in Sec. VIII. Two brief Appendices are devoted to the Molien function (Appendix A) and to comparison with previous work (Appendix B). Two other Appendices collect some involved formulas related to the discussion in Sec. V (Appendix C) and in Sec. VII B (Appendix D).

We would like to mention that in our computations, several of the "intermediate" terms can be eliminated from the LdG potential by a suitable change of coordinates;[37] the relevant point here is that the change of coordinates needed to reach this simpler form can, and will, be *explicitly* computed.

We also mention that our work here follows the same approach as in the companion paper;[6] however, there we considered only effects of changes of coordinates at first significant order, while here higher orders effects are considered and are actually relevant in obtaining a more radical simplification of the LdG functional. In terms of the Poincaré theory, this would correspond to a "further normalization" of Poincaré normal forms (see also Appendix B in this respect). We avoid entering in a discussion of the fine details of this procedure, thanks to the fact our computations are completely explicit, and our "brute force" approach—made possible by dealing with a concrete case rather than with a general theory (and the use of symbolic manipulation programs)—allows to

avoid mathematical subtleties (see Refs. 13 and 14 for a discussion of these in terms of dynamical systems).

II. THE SO(3) ADJOINT REPRESENTATION

In this section, we give some algebraic details on the SO(3) adjoint representation and its invariants and covariants of low order. These will be of use in our subsequent computations.

A. Definition and generators

Let us consider the action of $G = SO(3)$ on the space $\mathcal{M}$ of 3×3 symmetric traceless matrices

$$Q = \begin{pmatrix} x_1 & x_2 & x_3 \\ x_2 & x_4 & x_5 \\ x_3 & x_5 & -(x_1 + x_4) \end{pmatrix} ; \tag{1}$$

we recall that if Q is such a matrix, the element $R \in G$ acts on it by $Q \to RQR^{-1}$. As for the infinitesimal $SO(3)$ action, this is generated by

$$L_1 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix}, \, L_2 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{pmatrix}, \, L_3 = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}. \tag{2}$$

These satisfy of course the $so(3)$ Lie algebra relations

$$[L_i, L_j] = \epsilon_{ijk} L_k . \tag{3}$$

B. Invariants

The orbits of this G-action are three-dimensional and are indexed by

$$T_2 = \text{Tr}(Q^2), \, T_3 = \text{Tr}(Q^3) ; \tag{4}$$

the trace of Q is also an invariant, but in this case a trivial one, as by definition $Q \in \mathcal{M}$ implies $\text{Tr}(Q) = 0$.[38]

We also recall that in this case all orbits pass through the set of diagonal matrices, and of course traces are invariant under conjugation. This helps in checking identities or inequalities among invariants, e.g., the basic relation[17,18]

$$(T_2)^3 - 6(T_3)^2 = 2(\lambda_1 - \lambda_2)^2(2\lambda_1 + \lambda_2)^2(\lambda_1 + 2\lambda_2)^2 \geq 0, \tag{5}$$

where λ_1, λ_2 are the eigenvalues of Q. Note that for $\lambda_1 = \lambda_2$, i.e., in the uniaxial case, we have an equality, and conversely the equality holds only in the uniaxial case.

It may be useful to have explicit expressions for the invariants in terms of the x_i; with trivial computations, these turn out to be

$$T_2 = x_1^2 + x_2^2 + x_3^2 + x_4^2 + x_5^2 + x_1 x_4, \tag{6}$$

$$T_3 = x_1(x_2^2 - x_4^2 - x_5^2) - x_4(x_1^2 - x_2^2 + x_3^2) + 2 x_2 x_3 x_5 . \tag{7}$$

It should be noted that, by definition, the invariants and hence the LdG functional are invariant under conjugation by SO(3) matrices; thus, one could aim at working with matrices in diagonal form. In this context, a particularly convenient parametrization is provided by (q, ω), where $q \geq 0$ is the amplitude of the tensorial order parameter

$$q = |Q| = \sqrt{T_2} \tag{8}$$

(see Eq. (11) below), and $\omega \in [0, 1]$ is a measure of the biaxiality,[17,18] defined in the present notation by

$$\omega = 1 - \sqrt{\frac{6\,T_3^2}{T_2^3}}\ . \tag{9}$$

Thus, the other three variables needed to complete a coordinate system besides (q,ω) could be seen as irrelevant ones (being coordinates along the group orbits); note that relation (5) just requires $q \geq 0, 0 \leq \omega \leq 1$.

For our approach, it is however convenient to operate with the x_i variables, as degrees (orders) are defined in terms of these. Any result given in terms of T_2, T_3 is promptly mapped to the (q,ω) variables formulation by recalling that

$$T_2 = q^2\,,\ \ T_3 = \frac{(1-\omega)\,q^3}{\sqrt{6}}\ . \tag{10}$$

Remark 1. Finally, we note that besides the $SO(3)$ invariance mentioned above, the functions T_2 and T_3 are also invariant under the discrete transformations

$$(x_1, x_2, x_3, x_4, x_5) \rightarrow (x_4, x_2, \pm x_5, x_1, \pm x_3)\,,$$
$$(x_1, x_2, x_3, x_4, x_5) \rightarrow (x_1, -x_2, -x_3, x_4, x_5)\,,$$
$$(x_1, x_2, x_3, x_4, x_5) \rightarrow (x_1, -x_2, x_3, x_4, -x_5)\,.$$

Correspondingly, we have subspaces which are invariant under the gradient dynamics of any invariant potential (that is, the gradient at points of the subspace is granted to be tangent to the subspace), given by $\{x_1 = x_4, x_3 = \pm x_5\}$, by $\{x_2 = 0, x_3 = 0\}$, and by $\{x_2 = 0, x_5 = 0\}$. The intersection $\{x_2 = x_3 = x_5 = 0, x_4 = x_1\}$ of these is also an invariant (one-dimensional) subspace.

C. Five-dimensional representation

The adjoint $SO(3)$ action can be described by a linear (vector) representation on the space $\widehat{\mathcal{M}} = \mathbf{R}^5 = \{x_1, x_2, x_3, x_4, x_5\}$; the matrices corresponding to the adjoint action of the $SO(3)$ generators L_i are

$$J_1 = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -2 \\ 1 & 0 & 0 & 2 & 0 \end{pmatrix},\ J_2 = \begin{pmatrix} 0 & 0 & 2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ -2 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 \end{pmatrix},\ J_3 = \begin{pmatrix} 0 & -2 & 0 & 0 & 0 \\ 1 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & -1 \\ 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \end{pmatrix}.$$

It is immediate to check these are not orthogonal with respect to the standard metric in $\mathbf{R}^5$. They are, however, orthogonal with respect to the natural metric in the space of n-dimensional matrices (here $n = 5$), identified by

$$\langle A, B \rangle = \frac{1}{n}\ \mathtt{Tr}(A^+ B)\,;$$

note that with this metric,

$$|Q|^2 = \langle Q, Q \rangle = T_2(x) = \sum_{i,j} Q_{ij}^2\,. \tag{11}$$

It would thus be possible, at least in principles,[39] to use the general approach provided in Ref. 6; we will, however, prefer to operate by direct explicit computations.

D. Covariants

We are interested in explicitly determining the nonlinear covariants for this action, that is, five-dimensional vectors $\mathbf{F}_k(x)$, homogeneous of degree k in the x_i—hence $\mathbf{F}_k(ax) = a^k \mathbf{F}_k(x)$—which transform in the same way as $\mathbf{x}$, i.e., according to the same five-dimensional representation of $SO(3)$.[40]

This means satisfying at first order in ε the condition

$$(I + \varepsilon\, J_\alpha)\, \mathbf{F}_k(\mathbf{x}) = \mathbf{F}_k(\mathbf{x} + \varepsilon J_\alpha \mathbf{x}) \tag{12}$$

for $\alpha = 1, 2, 3$, i.e., $(I + \varepsilon L)\mathbf{F}_k(\mathbf{x}) = \mathbf{F}_k(\mathbf{x} + \varepsilon L\mathbf{x})$ for any $L \in so(3)$. This is of course equivalent to

$$g[\mathbf{F}(x)] \;=\; \mathbf{F}(gx) \quad \forall g \in G = SO(3)\,. \tag{13}$$

The multiplicity of these can be determined using Molien functions,[20–25] see Appendix A. Here, it is not enough to know the number of covariants (and invariants), but we need their explicit expressions; they can be determined in several ways, including by direct explicit computations.

It turns out that there is a single covariant for each of the orders $k = 1$, $k = 2$, and $k = 3$, while there are two covariants for each of the orders $k = 4$, $k = 5$, and $k = 6$; there are three covariants at each of the orders $k = 7$ and $k = 8$.[41]

Some of these covariants are rather obvious, e.g., the (only) covariant of order one coincides with $\mathbf{x}$, and there are covariants of order k given by the product of an invariant of order $(k - 1)$ with $\mathbf{x}$. That is, we have

$$\mathbf{F}_1 = \mathbf{x}\,, \;\; \mathbf{F}_3 = T_2\, \mathbf{x}\,, \;\; \mathbf{F}_4^{(1)} = T_3\, \mathbf{x}\,, \;\; \mathbf{F}_5^{(1)} = (T_2)^2\, \mathbf{x}\,,$$
$$\mathbf{F}_6^{(1)} = T_2 T_3\, \mathbf{x}\,, \;\; \mathbf{F}_7^{(1)} \;=\; T_2^3\, \mathbf{x}\,, \;\; \mathbf{F}_7^{(2)} = T_3^2\, \mathbf{x}\,, \;\; \mathbf{F}_8^{(1)} = T_2^2 T_3\, \mathbf{x}\,. \tag{14}$$

Then, one can check by explicit computations that the second order covariant (whose existence is guaranteed by Molien function computations) is given by

$$\mathbf{F}_2 = \begin{pmatrix} (x_1^2 + x_2^2 + x_3^2) - 2\,(x_1 x_4 + x_4^2 + x_5^2) \\ 3(x_1 x_2 + x_2 x_4 + x_3 x_5) \\ 3(x_2 x_5 - x_3 x_4) \\ (x_2^2 + x_4^2 + x_5^2) - 2\,(x_1^2 + x_3^2 + x_1 x_4) \\ 3(x_2 x_3 - x_1 x_5) \end{pmatrix}. \tag{15}$$

This entails that we also have the covariants

$$\mathbf{F}_4^{(2)} = T_2\, \mathbf{F}_2\,, \;\; \mathbf{F}_5^{(2)} = T_3\, \mathbf{F}_2\,, \;\; \mathbf{F}_6^{(2)} = T_2^2\, \mathbf{F}_2\,,$$
$$\mathbf{F}_7^{(3)} = T_2 T_3\, \mathbf{F}_2; \;\; \mathbf{F}_8^{(2)} \;=\; T_2^3\, \mathbf{F}_2\,, \;\; \mathbf{F}_8^{(3)} = T_3^2\, \mathbf{F}_2\,. \tag{16}$$

No other covariant exists at these orders, as guaranteed by the Molien function approach,[22–24] or by explicit computation.[42]

III. THE LANDAU-DEGENNES FUNCTIONAL AND ITS REDUCTION. ORDER SIX

It follows from our discussion in Section II, see, in particular, Eqs. (6) and (7), that the most general invariant polynomial of order six can henceforth be written (with c_i arbitrary constants) as

$$\Phi = c_1 T_2 + c_2 T_3 + c_3 T_2^2 \;+\; c_4 T_2 T_3 + c_5 T_2^3 + c_6 T_3^2\,. \tag{17}$$

In the following, we will suppose to be *not* at exactly the transition point, i.e., we will (until Sec. VII) assume

$$c_1 \neq 0\,. \tag{18}$$

Note this means we are requiring the quadratic part of the potential to be non-degenerate. As discussed and emphasized in Ref. 6, this is an essential (and natural) condition for the standard Poincaré approach to work.[43]

It is sometimes convenient to write Φ as

$$\Phi = \sum_{k=0}^{4} \Phi_k\,, \tag{19}$$

where Φ_k is homogeneous of order $(k + 2)$; needless to say for the Φ of (17), we have

$$\Phi_0 = c_1 T_2, \ \Phi_1 = c_2 T_3, \ \Phi_2 = c_3 T_2^2, \ \Phi_3 = c_4 T_2 T_3, \ \Phi_4 = c_5 T_2^3 + c_6 T_3^2. \tag{20}$$

The central idea in the Poincaré approach[7,8,10] is to perform near-identity changes of variables $x \to y = x + \varepsilon h(x)$. Note that here the small parameter ε does not need to be explicit; actually, it should be seen as the size of the region in which we operate. In other words, we want to consider changes of variables of the form

$$\mathbf{x} \ \to \ \mathbf{y} = \mathbf{x} \ + \ \mathbf{h(x)}, \tag{21}$$

where $\mathbf{h}$ is at least quadratic in the x_i.

As we want to deal with polynomials, $\mathbf{h}$ should itself be a polynomial; moreover, in Landau theory, symmetry is a central ingredient of the theory, and hence we should make sure that the change of variables preserves the symmetry.

All in all, this means that we should look for changes of variables of form (21) with $\mathbf{h}$ a linear combination of the higher order covariants identified above. That is, we set

$$\mathbf{h} = k_1 \mathbf{F}_2 + k_2 \mathbf{F}_3 + k_3 \mathbf{F}_4^{(1)} + k_4 \mathbf{F}_4^{(2)} + k_5 \mathbf{F}_5^{(1)} + k_6 \mathbf{F}_5^{(2)}. \tag{22}$$

Note that, contrary to what is discussed in our general approach described in Ref. 6, here we are *not* working step by step, but just proceed by a brute force comprehensive computation; this is possible in that we know *a priori* we just want to go to order six (or order eight in Sec. V), and this order is not too high.

IV. POINCARÉ TRANSFORMATIONS ON THE LDG FUNCTIONAL OF ORDER SIX

We will thus consider the general Landau polynomial $\Phi(\mathbf{x})$ and operate on it via the change of variables (21) and (22). This will produce a new Landau polynomial $\widehat{\Phi}$, which can again be written (with truncation at order six in the x_i variables) in form (19), i.e., as

$$\widehat{\Phi} = \sum_{k=0}^{4} \widehat{\Phi}_k. \tag{23}$$

A. Generalities

The expression of the $\widehat{\Phi}_k$ will depend both on the expression of the original homogeneous polynomials Φ_m, hence on the coefficients c_j, and on the coefficients k_i appearing in (22). Note that the former have physical significance and are given (at least for given values of the external physical parameters) in our theory, but the latter are just indexing the change of variables and we can choose them.

We will thus try to choose these in such a way to simplify as much as possible the resulting Landau polynomial $\widehat{\Phi}$. In particular, we will see that a suitable choice of the k_i leads to $\widehat{\Phi}_k(x) = 0$ for $k = 1, \ldots, 4$; our simplification should, however, preserve the stability of the theory, see Subsection IV B.

We write

$$\Phi(\mathbf{y}) = \Phi[\mathbf{x} + \mathbf{h(x)}] \ := \ \widehat{\Phi}(\mathbf{x})$$

in terms of the explicit form of $\mathbf{h}$ provided by (22) and by the explicit expressions for the $\mathbf{F}_k$; this produces explicit expressions for the $\widehat{\Phi}_k(\mathbf{x})$.

By construction, we will get

$$\widehat{\Phi}_0(\mathbf{x}) = \Phi_0(\mathbf{x}),$$

as follows from the change of variables being a near-identity one; higher order terms will be affected by our change of variables. In any case, having chosen a covariant change of coordinates (21) guarantees the $\widehat{\Phi}_k(\mathbf{x})$ will be invariant; hence, written in the same form as in (20) (obviously with different coefficients), that is, we have necessarily

$$\widehat{\Phi}_1 = \gamma_3 T_3, \ \ \widehat{\Phi}_2 = \gamma_4 T_2^2, \ \ \widehat{\Phi}_3 = \gamma_5 T_2 T_3, \ \ \widehat{\Phi}_4 = \gamma_6 T_2^3 + \gamma_7 T_3^2 . \tag{24}$$

The expressions for the coefficients γ_k can be computed explicitly by simple albeit increasingly involved algebra; it is convenient to perform these on a computer using a symbolic manipulation language.

B. Maximal order terms and convexity

In dealing with the maximal order terms—that is, the terms of the order N at which we truncate the Landau polynomial—some care should be taken. In fact, these terms control the thermodynamical stability of the theory.[1,2] The criterion to ensure such a stability is that the Landau polynomial should be convex for large (absolute) values of the order parameter; in our case, this means large $|Q|$. In our case, and more generally when the Poincaré transformations would be able to completely cancel terms of this order and N is even, a simple way to guarantee the criterion is satisfied is by having a highest order term of the type $\Phi_N = |Q|^{2q} = \rho^q$, where $q = (N + 2)$, and of course $\rho = |Q|^2$. See also Ref. 6.

C. The simplifying transformation. I: Non-maximal orders

We will now implement the procedure described above. Thus, at first order, we get

$$\widehat{\Phi}_1 = (c_2 + 9 \, c_1 \, k_1) \, T_3(x) . \tag{25}$$

Obviously, it suffices to choose

$$k_1 = - \frac{c_2}{9 \, c_1} , \tag{26}$$

which is possible, thanks to (18), in order to get $\widehat{\Phi}_1 = 0$, i.e., eliminate the cubic terms from the Landau potential.

The quartic term reads

$$\widehat{\Phi}_2 = (1/3) \, (c_3 + 2c_2 k_1 + 3c_1 k_1^2 + 2c_1 k_2) \, [T_2(x)]^2 ; \tag{27}$$

by choosing k_1 according to (26), this reduces to

$$\widehat{\Phi}_2 = \left(3c_3 - \frac{5c_2^2}{27c_1} + 2c_1 k_2 \right) [T_2(x)]^2 . \tag{28}$$

It thus suffices to choose

$$k_2 = \frac{5 \, c_2^2 - 27 \, c_1 \, c_3}{54 \, c_1^2} \tag{29}$$

to get $\widehat{\Phi}_2(x) = 0$ as well. Note we are again using (18); this will also be true in the next steps, but we will not remark it any more.

The term of order five turns out to be

$$\widehat{\Phi}_3 = (c_4 + 18c_3 k_1 + 9c_2 k_1^2 + 3c_2 k_2 + 9c_1 k_1 k_2 + 2c_1 k_3 + 9c_1 k_4) \, T_2(x) \, T_3(x) ; \tag{30}$$

choosing k_1 and k_2 as in (26) and (29), this reduces to

$$\widehat{\Phi}_3 = \frac{1}{27 \, c_1^2} \, \left[8c_2^3 - 81c_1 c_2 c_3 + 27c_1^2(c_4 + c_1(2k_3 + 9k_4)) \right] \, T_2(x) \, T_3(x) . \tag{31}$$

Here, we have two parameters, k_3 and k_4, which are not yet determined. By choosing, e.g.,

$$k_3 = \frac{-8c_2^3 + 81c_1 c_2 c_3 - 27c_1^2 c_4 - 243c_1^3 k_4}{54 \, c_1^3} \tag{32}$$

(note we are free to set $k_4 = 0$ if desired), or however k_3 and k_4 satisfying

$$2\,k_3 + 9\,k_4 = \frac{-8c_2^3 + 81c_1c_2c_3 - 27c_1^2c_4}{27\,c_1^3}\,,$$

we get $\widehat{\Phi}_3 = 0$.

In this way, under the assumption $c_1 \neq 0$, we have reduced original Landau potential (17) to the simpler form

$$\widehat{\Phi}(x) = c_1\,T_2(x) + \alpha\,[T_2(x)]^3 + \beta\,[T_3(x)]^2\,; \tag{33}$$

here, c_1 is the same coefficient as in the original potential, while α and β are coefficients depending on the original coefficients c_i as well as on the coefficients k_i entering in the function $\mathbf{h}(\mathbf{x})$ identifying the transformation, see (22).

By explicit computations, these are (recall k_4 is undetermined and can be set to zero if desired)

$$\alpha = [-29c_2^4 + 558c_1c_2^2c_3 - 1701c_1^2c_3^2 - 216c_1^2c_2c_4 + 972c_1^3c_5 + 1296c_1^3c_2k_4]\,/\,[972\,c_1^3], \tag{34}$$

$$\beta = [-c_2^4 + 12c_1c_2^2c_3 - 6c_1^2c_2c_4 + 3c_1^3c_6 - 27c_1^3c_2k_4]\,/\,[3\,c_1^3]\,. \tag{35}$$

D. The simplifying transformation. II: Maximal order

We have now to deal with terms of maximal order. Thus, we should *not* try to set $\alpha = \beta = 0$, and hence $\widehat{\Phi}_4 = 0$, but rather try to simplify this term while being guaranteed it remains convex for large $|Q|$.

It should be noted that the natural norm for the tensorial order parameter Q is just the one induced by the natural scalar product in $\mathcal{M} = GL(3)$, i.e.,

$$|Q|^2 = \langle Q, Q \rangle = \frac{1}{3}\,\mathtt{Tr}(Q^+Q)\,; \tag{36}$$

thus, we have simply

$$|Q|^2 = \frac{1}{3}\,T_2(x)\,. \tag{37}$$

In other words, convexity is guaranteed if we have $\Phi_4 = a^2[T_2(x)]^3$ for any nonzero real number a; we will just set $a = 1$. This means looking for a transformation, i.e., for coefficients k_5 and k_6 identifying the transformation, which maps (α, β) above into $\widetilde{\alpha} = 1$, $\widetilde{\beta} = 0$.

This is obtained by choosing (the formulas can be slightly simplified by a suitable choice of the value of the undetermined parameter k_4)

$$k_5 = \left[29c_2^4 - 558c_1c_2^2c_3 + 27c_1^2(63c_3^2 + 8c_2c_4) + 324c_1^3(3 - 3c_5 - 4c_2k_4)\right]\left[1944c_1^4\right]^{-1}, \tag{38}$$

$$k_6 = \left[c_2^4 - 12c_1c_2^2c_3 - 3c_1^3c_6 + 3c_1^2c_2(2c_4 + 9c_1k_4)\right]\left[27c_1^4\right]^{-1}\,. \tag{39}$$

We have thus reduced the Landau polynomial of order six to the form

$$\widehat{\Phi}(x) = c_1\,T_2(x)\ +\ [T_2(x)]^3\,. \tag{40}$$

The transformation producing this simplification has been made completely explicit, being encoded in the coefficients $k_1, \ldots, k_6$.

Finally, we note that, as discussed in Ref. 6, we should pay some attention to the requirement that the resulting series is a well ordered one; as the denominators δ_m appearing in the formula for k_m grow as c_1^m, we should require $c_1 > \varepsilon$. In other words, the radius of convergence of our transformation (acting on the order parameters $\mathbf{x}$) is estimated by $|c_1|$, i.e., by the distance from the transition point $c_1 = 0$: the transformation allow to deal with the Landau polynomial in a simpler form provided we do not get too near to the transition point.

Thus, we can use it to analyze the possible phases at a given nonzero value of the leading parameter c_1 (and possibly secondary phase transitions), but not to analyze the situation

(e.g., compute the critical exponents) at the primary transition point $c_1 = 0$. This problem will be tackled in Sec. VII.

V. SIMPLIFICATION OF THE LDG FUNCTIONAL AT ORDER EIGHT

We will now consider what happens if we have to deal with a higher order, i.e., order eight, functional; one purpose of this section is to show that even in this case one can obtain completely explicit formulas.[44]

More relevantly, when in Sec. VI we will discuss the physical implications of our computations, we will find that going to order eight does remove an un-physical degeneration obtained at order six and gives results in agreement with those obtained (through different methods) in the literature.[18]

In this case, we can still attempt a full cancellation of the terms of order six and seven while the highest (eight) order terms should not be fully eliminated but just simplified, for the same reason as discussed above.

A. Invariants, covariants, generating functions

We have now to consider also higher order polynomials, so that (17) will be replaced by

$$\Phi = c_1 T_2 + c_2 T_3 + c_3 T_2^2 + c_4 T_2 T_3 + c_5 T_2^3 + c_6 T_3^2 + c_7 T_2^2 T_3 + c_8 T_2 T_3^2 + c_9 T_2^4. \tag{41}$$

Correspondingly, we will still consider a change of variables of form (21) but (22) will now be replaced by

$$\mathbf{h} = k_1 \mathbf{F}_2 + k_2 \mathbf{F}_3 + k_3 \mathbf{F}_4^{(1)} + k_4 \mathbf{F}_4^{(2)} + k_5 \mathbf{F}_5^{(1)} + k_6 \mathbf{F}_5^{(2)}$$
$$+ k_7 \mathbf{F}_6^{(1)} + k_8 \mathbf{F}_6^{(2)} + k_9 \mathbf{F}_7^{(1)} + k_{10} \mathbf{F}_7^{(2)} + k_{11} \mathbf{F}_7^{(3)}. \tag{42}$$

B. Terms of order six

Needless to say, up to order five, we get the same results as above. The order six is not any more, in this framework, the maximal one; hence, we can attempt to fully eliminate it without harming thermodynamical stability.

We know *a priori* that the invariant polynomial will be of the form

$$\widehat{\Phi}_4(x) = \alpha \, [T_2(x)]^3 + \beta \, [T_3(x)]^2 ; \tag{43}$$

the values of the coefficients α and β—provided k_1, k_2, and k_3 are chosen according to (26), (29), and (32)—are given by (34) and (35). It is possible to make both α and β—and hence $\widehat{\Phi}_4$—vanish by choosing (these formulas can also be slightly simplified by a suitable choice of the undetermined parameter k_4)

$$k_5 = [29c_2^4 - 558c_1c_2^2c_3 + 243c_1^2(7c_3^2 - 4c_1c_5) - 216c_1^2c_2(-c_4 + 6c_1k_4)] \, [1944 \, c_1^4]^{-1} , \tag{44}$$

$$k_6 = [c_2^4 - 12c_1c_2^2c_3 - 3c_1^3c_6 + 3c_1^2c_2(2c_4 + 9c_1k_4)] \, [27 \, c_1^4]^{-1} . \tag{45}$$

C. Terms of order seven

At order seven, we have only one invariant, i.e., we know that

$$\widehat{\Phi}_5 = \gamma \, T_2^2 T_3 . \tag{46}$$

Setting $k_1, \ldots, k_6$ as determined at lower orders, we get an explicit expression for γ which depends moreover on the two parameters k_7 and k_8; these can be chosen—and actually one of these can be chosen at will—so to obtain $\gamma = 0$; details are given in Appendix C. In other words, we can obtain

$$\widehat{\Phi}_5 = 0 .$$

D. Terms of order eight

At order eight, we are at maximal order and we should not fully eliminate terms of this order; with the same discussion as in the $N = 4$ case of Sec. IV, we see that they should instead be reduced, if possible, to $\widehat{\Phi}_6 = [T_2(x)]^4$.

Now we have two invariants of order eight, i.e., T_2^4 and $T_2 T_3^2$; thus, we know *a priori* that, for whatever choice of the k_i, we will have

$$\widehat{\Phi}_6(x) = \xi \, [T_2(x)]^4 \; + \; \eta \, T_2(x) \, [T_3(x)]^2$$

for some ξ, η; thus, we should aim at

$$\xi = 1 \, , \; \eta = 0 \, .$$

Explicit forms for ξ and η are easily computed (and reported in Appendix C). The requirements $\xi = 1$, $\eta = 0$ can be satisfied by a suitable choice of the parameters k_8 and k_9 (explicit for of these choices are given again in Appendix C).

These present a new feature: while so far all the denominators only depended on c_1, at this stage we will have denominators of the parameters (and also of the resulting coefficients for $\widehat{\Phi}_6$) which also depend on c_2.

Thus, for the results to make sense, we should require not only $|c_1|$ large enough (which, as we remarked several time, is inherent to the very spirit of the standard Poincaré approach) but also $|c_2|$ large enough as well.

On the other hand, if we only require $\xi = 1$ (without requiring also $\eta = 0$), this can be satisfied with parameters—and resulting coefficients—which do not see the appearance of c_2 in the denominator (see Appendix C).

With the choices described above, and with the same cautionary notes about the need to have $|c_1|$ and $|c_2|$ large enough, we can reduce the Landau polynomial to the form

$$\widehat{\Phi}(x) = c_1 \, T_2(x) + [T_2(x)]^4 \; ; \tag{47}$$

needless to say what matters here are not the explicit (and rather involved) expressions obtained for $k_1, \ldots, k_9$, but the fact such expressions *can* be explicitly determined and yield (47).

If we assume $|c_1|$ large enough, but are not ready to make any assumption regarding c_2, we can still reduce the Landau polynomial to the form

$$\widehat{\Phi}(x) \; = \; c_1 \, T_2(x) + [T_2(x)]^4 + \eta \, T_2(x) \, [T_3(x)]^2 \, . \tag{48}$$

VI. BIAXIAL AND UNIAXIAL NEMATIC PHASES. I: ANALYSIS OF THE SIMPLIFIED POTENTIAL AWAY FROM THE MAIN TRANSITION POINT

A physically relevant question is whether the theory allows for direct transitions to biaxial phases, or if only transitions to uniaxial ones are allowed directly from the fully isotropic phase;[19] see, e.g., the discussion in Ref. 18. This section is devoted to applying our approach in this context. As already mentioned, our method cannot (without modifications, see Sec. VII) deal with the degeneration corresponding to the phase transitions. On the other hand, our method provides some hint, consisting in the form of the would-be bifurcating branch after the phase transition; this information will allow (see Sec. VII C) to identify an ansatz for the would-be biaxial bifurcating solution and effectively run computations to provide the first term in the series expansion of a biaxial branch bifurcating directly from the fully symmetric solutions, and determine its stability.

It should be recalled that in the present notation, anisotropy is measured by the parameter $\omega \in [0, 1]$, defined in terms of T_2 and T_3 by (9); see also Fig. 1. The biaxial phase has $\omega > 0$, while the uniaxial one is characterized by $\omega = 0$.

Remark 2. A good deal of the discussion about this problem present in the literature has been conducted using either the (q, ω) coordinates or the orbit space ones, i.e., (T_2, T_3). It should be stressed that from the point of view of perturbation theory this causes troubles, in that one is
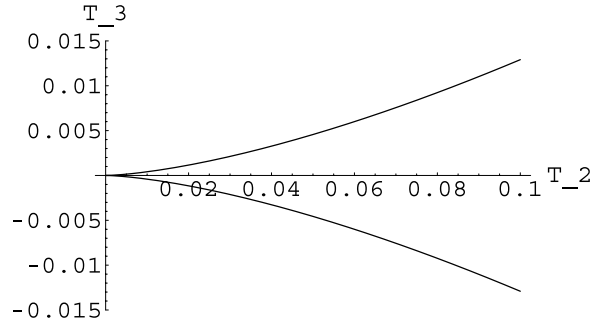
FIG. 1. The allowed phase space in terms of invariants. Inequality (5) implies the state of the system belongs to the region between the two curves $T_3 = \pm\sqrt{T_2^3/6}$. The borders of this region correspond to $\omega = 0$, i.e., to the uniaxial phase, the interior to $0 < \omega < 1$ to the biaxial phase.

destroying the grading present in the x coordinates; moreover, the branching point $(q,\omega) = (0,0)$ or $(T_2,T_3) = (0,0)$ is lying on the border of the domain of definition. We will thus work in the x coordinates in order to reduce the LdG potential; once this is done, working in the (q,ω) or (T_2,T_3) variables is legitimate.

A. Sixth order potential

The result of the computations with a sixth order LdG potential is that we can always reduce to a potential of form (40). When we look for critical points, these are identified by

$$\nabla\widehat{\Phi} = \left[c_1 + 3[T_2(x)]^2\right] \nabla T_2(x) = 0 . \tag{49}$$

Thus, all (and only, apart from the trivial one $x = 0$) the points satisfying

$$T_2(x) = |Q(x)|^2 = \sqrt{-c_1/3} \tag{50}$$

are critical ones. Needless to say, this is possible only for $c_1 < 0$; for $c_1 > 0$, the fully isotropic phase is stable.

The point is that (50) does not depend at all on T_3; thus, the outcome of our computations at order six is that all values of $T_3(x)$ compatible with the value of $T_2(x)$ in view of (5) would be allowed.

This makes little sense physically, and is in contrast with well established results in the literature.[18] As we are dealing with a perturbation approach and the situation obtained at order six is degenerate (no selection on T_3), it is natural to try to remove the degeneration by going at higher orders.

B. Eight order potential

Going at order eight, the situation is indeed different. If we are ready to make assumptions on c_2—besides those on c_1—then the situation is similar to the one described above, except that $\widehat{\Phi}$ will be of form (47) and hence the critical points identified by

$$\nabla\widehat{\Phi} = \left[c_1 + 4[T_2(x)]^3\right] \nabla T_2(x) = 0 . \tag{51}$$

Thus, all (and only, apart from the trivial one $x = 0$) the points satisfying

$$T_2(x) = 3 |Q(x)|^2 = (-c_1/4)^{1/3} \tag{52}$$

are critical ones. Note that now symmetry breaking phases again are possible only for $c_1 < 0$, as expected.

On the other hand, if we want to deal with a generic c_2, we only get to $\widehat{\Phi}$ given by (48); we assume $\eta \neq 0$ (or we would be reduced to the previous case).

In the following, we will also write

$$c_1 = -\lambda$$

to emphasize this is a varying parameter (we will consider the other ones as given) and that we are interested in the case $c_1 < 0$ (so that the origin is not a minimum). Thus, (48) reads now

$$\widehat{\Phi}(x) = -\lambda\, T_2(x) + \eta\, T_2(x)\, [T_3(x)]^2 + [T_2(x)]^4 . \tag{53}$$

An explicit expression for η is computed in Appendix C.

C. Analysis of the reduced potential

With (53), critical points are identified by

$$\nabla\widehat{\Phi} = \big[-\lambda + 4\,[T_2(x)]^3 + \eta\,[T_3(x)]^2\big]\,\nabla T_2(x) + [2\,\eta\,T_2(x)\,T_3(x)]\,\nabla T_3(x) = 0 . \tag{54}$$

Writing this explicitly in terms of the x would produce a quite involved equation, which cannot be easily handled; it is convenient to analyze the problem in form (54).

This equation requires the vanishing of a vector, which is expressed as the sum of the two gradients ∇T_2 and ∇T_3 with certain x-dependent coefficients. If the two gradients are not collinear, the coefficients must vanish separately (the gradients themselves are nowhere zero outside the origin), while in case of collinearity, the two vectors can combine to give a zero sum. Thus, in order to discuss solutions to (54), we should distinguish two cases, i.e., points such that $\nabla T_3(x) = \mu \nabla T_2(x)$ for some real constant μ and points such that $\nabla T_3(x) \neq \mu \nabla T_2(x)$ for any μ.

Let us first consider the case where the two gradients are nowhere collinear. In this case, we must have

$$\begin{cases} c_1 + 4\,T_2^3 + \eta\,T_3^2 = 0 \quad , \\ 2\,\eta\,T_2\,T_3 = 0 \quad\quad\quad ; \end{cases} \tag{55}$$

recalling that by hypothesis $\eta \neq 0$,[45] we have either $T_2 = 0$ or $T_3 = 0$. The first case implies $|Q|^2 = 0$ and is thus not relevant.

In the second case, $T_3 = 0$, which implies $\omega = 1$ and hence a biaxial phase, the other equation yields

$$T_2 = -(-c_1/4)^{1/3} = -(\lambda/4)^{1/3} ; \tag{56}$$

for $\lambda > 0$, this entails $q^2 < 0$ and is thus not acceptable.

We can now pass to consider the case where there are points $\mathbf{x} \in \mathbf{R}^5$ such that the two gradients are collinear. The explicit expressions for the gradients are easily obtained. With lengthy explicit computations (performed with Mathematica and not to be reported here), it turns out that when we require $\nabla T_3 = \mu\, \nabla T_2$, there are four possibilities for μ, i.e. (here and in the following, we write $\theta := \sqrt{(x_1 - x_4)^2 + 4\,x_2^2}$)

$$\begin{aligned} (a) \quad & \mu = -x_1 , \\ (b) \quad & \mu = -x_4 , \\ (c) \quad & \mu = -(1/2)\,[x_1 + x_4 + \theta] , \\ (d) \quad & \mu = -(1/2)\,[x_1 + x_4 - \theta] . \end{aligned} \tag{57}$$

Each of the μ values given in (57) allows for two (multi-dimensional) branches of nontrivial critical points of the LdG potential. We will now briefly discuss their features and identify one-parameter families of solutions embedded in such branches. It should be stressed that such one-parameter families fall within the scope of Remark 1; thus, the restriction to these is legitimate independently of the normalization procedure.

(a) Case (a) gives two two-dimensional branches,

$$x_2 = x_3 = 0, \ x_5 = \pm\sqrt{2x_1^2 - x_1 x_4 - x_4^2} . \tag{58}$$

Note these are acceptable only for $-2x_1 \le x_4 \le x_1$. With (58), we get immediately

$$T_2 = 3\, x_1^2, \; T_3 = -2\, x_1^3; \; \omega = 1 - \frac{2\sqrt{2}}{3} \approx 0.057\,191. \tag{59}$$

Simpler formulas are obtained by choosing special values for x_4, e.g., we can choose $x_4 = 0$ and get the one-dimensional representative branch $x_2 = x_3 = x_4 = 0$, $x_5 = \pm\sqrt{2}x_1$ or choose $x_4 = x_1$, with also $x_2 = x_3 = x_5 = 0$.

Inserting conditions (58) into the equation $\nabla\widehat{\Phi} = 0$, we get immediately that the latter yields

$$x_1 = \pm\left(\frac{\lambda}{4\,(27 + 4\eta)}\right)^{1/6}, \tag{60}$$

which is of course acceptable only for either one of

$$\{\lambda \ge 0 \text{ and } \eta > -27/4, \; \lambda \le 0 \text{ and } \eta < -27/4\}. \tag{61}$$

(b) Similarly, case (*b*) also gives two two-dimensional branches,

$$x_2 = x_5 = 0, \; x_3 = \pm\sqrt{2x_4^2 - x_1 x_4 - x_1^2}. \tag{62}$$

These are acceptable only for $x_4 \le -x_1/2$ or $x_4 \ge x_1$. With (62), we get immediately

$$T_2 = 3\, x_4^2, \; T_3 = -2\, x_4^3; \; \omega = 1 - \frac{2\sqrt{2}}{3}. \tag{63}$$

Simpler formulas are obtained choosing special values for x_4, e.g., choosing $x_4 = x_1$, we get the one-dimensional branch representative $x_2 = x_3 = x_5 = 0$, $x_4 = x_1$.

Inserting conditions (58) into the equation $\nabla\widehat{\Phi} = 0$, we get immediately that the latter yields again (60); conditions (61) do still apply. Actually, the one-dimensional representatives obtained for (*a*) and (*b*) are just the same.

(c) As for (*c*), in this case, we get two three-dimensional branches,

$$
\begin{aligned}
x_3 &= \pm\frac{1}{\sqrt{2}}\sqrt{2x_2^2 + 2x_4(x_4 + \theta) - x_1(x_1 + x_4 - \theta)}, \\
x_5 &= \pm\frac{-\theta - x_1 + x_4}{4x_2}\sqrt{4[x_2^2 + x_4(x_4 + \theta)] + 2x_1(\theta - x_4 - x_1)}.
\end{aligned} \tag{64}
$$

These are acceptable provided all the arguments of the roots are positive; we will not analyze this condition in detail. The expressions for T_2 and T_3 are readily obtained.

Formulas become simpler if we set $x_4 = x_1$, which implies $\theta = 2x_2$; in this case, we get

$$T_2 = 3(x_1 + x_2)^2, \; T_3 = -2(x_1 + x_2)^3; \; \omega = 1 - \frac{2\sqrt{2}}{3}. \tag{65}$$

The resulting two-dimensional branch is identified by $x_3 = \pm\sqrt{x_2(3x_1 + x_2)}$, $x_5 = -x_3$; for $x_1 > 0$, this is acceptable for $x_2 \le -3x_1$ or $x_2 \ge 0$, while for $x_1 < 0$, we require either $x_2 \le 0$ or $x_2 \ge -3x_1$.

In both cases, we can set $x_2 = x_1$, which gives a one dimensional representative for this branch, $x_2 = x_1$, $x_3 = \pm 2x_1$, $x_4 = x_1$, $x_5 = \mp 2x_1$. Inserting these into the equation $\nabla\widehat{\Phi} = 0$, the latter yields again (60); conditions (61) do again apply.

(d) Finally, case (*d*) gives two three-dimensional branches as well (again we will not discuss in detail the bounds on the admissible values),

$$
\begin{aligned}
x_3 &= \pm\frac{1}{\sqrt{2}}\sqrt{2x_2^2 + 2x_4(x_4 - \theta) - x_1(x_1 + x_4 + \theta)}, \\
x_5 &= \pm\frac{\theta - x_1 + x_4}{4x_2}\sqrt{4[x_2^2 + x_4(x_4 - \theta)] - 2x_1(\theta + x_4 + x_1)}.
\end{aligned} \tag{66}
$$

Here, again we get simpler formulas by choosing $x_4 = x_1$, which yields

$$T_2 = 3\,(x_1 - x_2)^2\,,\ T_3 = -\,2\,(x_1 - x_2)^3\,;\ \ \omega = 1 - \frac{2\,\sqrt{2}}{3}\,. \tag{67}$$

The two-dimensional branch is identified by $x_3 = \pm\sqrt{x_2(x_2 - 3x_1)}$, $x_5 = x_3$. For $x_1 > 0$, this requires either $x_2 < 0$ or $x_2 > 3x_1$; for $x_1 < 0$, it requires either $x_2 \geq 0$ or $x_2 \leq 3x_1$.

In both cases, we can set $x_2 = -x_1$ and have a one-dimensional representative of the branch, $x_2 = -x_1$, $x_3 = \pm 2x_1$, $x_4 = x_1$, $x_5 = \pm 2x_1$. Inserting these into the equation $\nabla\widehat{\Phi} = 0$, the latter yields again (60); conditions (61) do again apply.

We have thus discussed the properties of these branches of solutions but not yet investigated their stability. In order to do so, we can consider the Hessian $H_{ij} = (\partial^2 \widehat{\Phi}/\partial x^i \partial x^j)$ along the solution branches. In this computation, it will be convenient to consider the one-dimensional representative identified above.

Note that due to the dimensionality of the branches, we will always have two zero eigenvalues. Thus, the condition of stability is that the other three eigenvalues are positive.

((a)and(b))   In case (a), we easily obtain the Hessian, which is rather simple; its eigenvalues are

$$\sigma_{(a)} = \{0\,,\, 0\,,\, 18\,\lambda\,,\, -\,\frac{18\,\eta\,\lambda}{27 + 4\eta}\,,\, -\,\frac{18\,\eta\,\lambda}{27 + 4\eta}\}\,. \tag{68}$$

Recalling (61), the denominator is always positive for $\lambda \geq 0$; thus, the condition for (existence and) local stability of this branch is

$$\lambda > 0\,,\ \ -27/4 < \eta < 0\,. \tag{69}$$

With our choice of the one-dimensional representative, case (b) is identical to (a); hence, we get the same formulas and results.

((c)and(d))   In case (c), we get a quite more complex Hessian; its eigenvalues can still be computed and we get

$$\sigma_{(b)} = \{0\,,\, 0\,,\, -\,\frac{12\,\eta\,\lambda}{27 + 4\eta}\,,\, \frac{3\,(486 + 47\eta - \gamma)\,\lambda}{8\,(27 + 4\eta)}\,,\, \frac{3\,(486 + 47\eta + \gamma)\,\lambda}{8\,(27 + 4\eta)}\}\,, \tag{70}$$

where we have written

$$\gamma = \sqrt{236\,196 + 94\,068\,\eta + 9377\eta^2}\,;$$

the argument of the square root is always positive. The last two eigenvalues do always have the same sign as λ; thus, again for $\lambda > 0$, this is a stable branch for $-27/4 < \eta < 0$. Computations and results are just the same in case (d) as for case (c).

The present discussion suffices to conclude that in cases (a)–(d), we have branches of critical points with non-zero ω, i.e., biaxial ones, and that they are stable[46] for $\lambda > 0$ provided $-27/3 < \eta < 0$. Note that these are quite weakly biaxial, as shown by the value of $\omega = [1 - 2\sqrt{2}/3] \approx 0.057\,191$ (such a low value can pose serious problem for experimentally distinguishing this biaxial solution from a uniaxial one).

It should be stressed that our discussion does *not* give a proof of the possibility of direct transition from the fully isotropic phase to biaxial phases (actually, in Sec. VII, we will see things are quite different). In fact, our reduction procedure fails precisely at the $c_1 = 0$ point.

The present analysis identifies branches of biaxial solutions existing near—but not "too near"—to the critical point. If there is a branch of biaxial solutions stemming directly from the critical point, it must be of the same form, and thus our analysis gives a hint for the form of the critical branch to be sought for in this subsequent analysis, developed in Sec. VII.[47]

VII. BIAXIAL AND UNIAXIAL NEMATIC PHASES. II: THE MAIN TRANSITION REGION

In Section VI, we have implemented our method under the assumption $-c_1 = \lambda \neq 0$. If we want to consider the parameter region near the main phase transition at $\lambda = 0$, that discussion does simply not apply.

In this section, we will apply again our method keeping in mind we want to analyze exactly the region near $c_1 = 0$. This will produce some different results than for c_1 bounded away from zero, and these results *can* be used to analyze the biaxial phase problem.

On the other hand, it is known that the analysis of the biaxial phase problem leads to consider an intricate situation as parameters are varied; in our case, we will have less parameters (after the simplification), but as the Physics has not changed we should expect an equally intricate situation. The analysis of this lies outside the limits of the present paper, so we will be satisfied with showing that our method allows to identify a simpler LdG potential via a change of variables which is admissible in a full neighborhood (whose size will depend on $|c_2| \neq 0$, see below) of the main transition point.

In simplifying the LdG potential, we will work under the assumption that the next-to-leading order term is nonzero, i.e.,

$$c_2 \neq 0 ; \tag{71}$$

this condition takes the place of (18).

A. Simplified potential—order six

In order to analyze the phase transition taking place at $\lambda = 0$, we can implement the simplification procedure paying attention to the fact that *no division by a factor c_1 should take place*.

We will first conduct our discussion based on the order six LdG potential. We will thus write Φ and $\mathbf{h}$ as in Sec. IV, see (17) and (22) (actually we only need generators up to order four, i.e., in (22) we can set $k_5 = k_6 = 0$), that is, we have (repeating here these formula for convenience of the reader)

$$\Phi = c_1 T_2 + c_2 T_3 + c_3 T_2^2 + c_4 T_2 T_3 + c_5 T_2^3 + c_6 T_3^2 ; \quad \mathbf{h} = k_1 \mathbf{F}_2 + k_2 \mathbf{F}_3 + k_3 \mathbf{F}_{41} + k_4 \mathbf{F}_{42} .$$

With these, we obtain a transformed potential $\widehat{\Phi}$ written in the same way but with γ_i taking the place of c_i (for $i \neq 1$). By explicit computations, we easily get the detailed form of the γ_i. These become simpler if we set, as we do in the following, $k_1 = 0$; the reader will easily observe that no further reduction would be possible by considering a nonzero k_1 (as we cannot divide by factors containing c_1). With this, we get

$$
\begin{aligned}
\gamma_2 &= c_2 , \\
\gamma_3 &= c_3 + 2c_1 k_2 , \\
\gamma_4 &= c_4 + 3c_2 k_2 + 2c_1 k_3 + 9c_1 k_4 , \\
\gamma_5 &= c_5 + c_1 k_2^2 + 4c_3 k_2 + 2c_2 k_4 , \\
\gamma_6 &= c_6 + 3c_2 k_3 .
\end{aligned}
$$

It is now easy to choose the k_i so to get a simpler form for the LdG potential; in particular, we want to set either one of

$$
\begin{cases}
\gamma_5 = 0 , \ \gamma_6 = 1 & (a) , \\
\gamma_5 = 1 , \ \gamma_6 = 0 & (b) , \\
\gamma_5 = 1 , \ \gamma_6 = 1 & (c) ;
\end{cases} \tag{72}
$$

actually in all cases, one can also set $\gamma_4 = 0$, see below.

The reader can check that in all cases explicit solutions for the critical points of the simplified potential $\widehat{\Phi}$ can be explicitly obtained.

Case (a) is obtained by choosing

$$k_2 = \frac{18c_2^2 - 108c_1c_3 - \sqrt{(108c_1c_3 - 18c_2^2)^2 - 108c_1^2(27c_5c_1 + 4c_6c_1 - 4c_1 - 6c_2c_4)}}{54c_1^2}$$

$$= -\frac{c_4}{3c_2} + \left(-\frac{2c_3c_4}{c_2^3} + \frac{3c_5}{2c_2^2} + \frac{2c_6}{9c_2^2} - \frac{2}{9c_2^2}\right)c_1 + O\left(c_1^2\right) ;$$

$$k_3 = \frac{1 - c_6}{3c_2} ;$$

$$k_4 = \frac{-c_1k_2^2 - 4c_3k_2 - c_5}{2c_2}$$

$$= \left(\frac{2c_3c_4}{3c_2^2} - \frac{c_5}{2c_2}\right) + \left(\frac{4c_4c_3^2}{c_2^4} - \frac{3c_5c_3}{c_2^3} - \frac{4c_6c_3}{9c_2^3} + \frac{4c_3}{9c_2^3} - \frac{c_4^2}{18c_2^3}\right)c_1 + O\left(c_1^2\right) .$$

With these, we obtain

$$\widehat{\Phi} = -\lambda\, T_2 + \gamma_2\, T_3 + T_3^2 . \tag{73}$$

The remaining coefficients are given in terms of the original ones by

$$\gamma_2 = c_2 , \quad \gamma_3 = c_3 + 2c_1k_2 = c_3 + \frac{2c_4}{3c_2}\lambda + O(\lambda^2) . \tag{74}$$

We obtain case (b) by choosing

$$k_2 = \frac{18c_2^2 - 108c_1c_3 - \sqrt{(108c_1c_3 - 18c_2^2)^2 - 108c_1^2(27c_5c_1 + 4c_6c_1 - 27c_1 - 6c_2c_4)}}{54c_1^2}$$

$$= -\frac{c_4}{3c_2} + \left(-\frac{2c_3c_4}{c_2^3} + \frac{3c_5}{2c_2^2} + \frac{2c_6}{9c_2^2} - \frac{3}{2c_2^2}\right)c_1 + O\left(c_1^2\right) ;$$

$$k_3 = -\frac{c_6}{3c_2} ;$$

$$k_4 = \frac{1 - c_1k_2^2 - 4c_3k_2 - c_5}{2c_2} .$$

With these, we obtain

$$\widehat{\Phi} = -\lambda\, T_2 + \gamma_2\, T_3 + \gamma_3\, T_2^2 + T_2^3 . \tag{75}$$

The remaining coefficients are again given in terms of the original ones by (74).

Finally, we note that case (c) is obtained for

$$k_2 = \frac{18c_2^2 - 108c_1c_3 - \sqrt{(108c_1c_3 - 18c_2^2)^2 - 108c_1^2(27c_5c_1 + 4c_6c_1 - 31c_1 - 6c_2c_4)}}{54c_1^2}$$

$$= -\frac{c_4}{3c_2} + \left(-\frac{2c_3c_4}{c_2^3} + \frac{3c_5}{2c_2^2} + \frac{2c_6}{9c_2^2} - \frac{31}{18c_2^2}\right)c_1 + O\left(c_1^2\right) ;$$

$$k_3 = \frac{1 - c_6}{3c_2} ;$$

$$k_4 = \frac{-3c_2^4 + 18c_1c_3c_2^2 + \sqrt{3}\sqrt{3c_2^4 - 36c_1c_3c_2^2 + 6c_1^2\left(18c_3^2 + c_2c_4\right) + c_1^3(-27c_5 - 4c_6 + 31)}c_2^2 - 3c_1^2c_4c_2 + 2c_1^3(c_6 - 1)}{27c_1^3c_2}$$

$$= \left(\frac{2c_3c_4}{3c_2^2} - \frac{c_5}{2c_2} + \frac{1}{2c_2}\right) + \left(\frac{4c_4c_3^2}{c_2^4} - \frac{3c_5c_3}{c_2^3} - \frac{4c_6c_3}{9c_2^3} + \frac{31c_3}{9c_2^3} - \frac{c_4^2}{18c_2^3}\right)c_1 + O\left(c_1^2\right) .$$

In this case, the potential reads

$$\widehat{\Phi} = -\lambda\, T_2 + \gamma_2\, T_3 + \gamma_3\, T_2^2 + T_3^2 + T_2^3 , \tag{76}$$

with the remaining coefficients given explicitly by (74) once again.

It is maybe worth remarking that having kept both terms of order six but having fixed their coefficients to one, we are guaranteed of convexity at large $|x|$; in fact, in terms of (q, ω) variables, we have

$$T_2^3 + T_3^2 = \left[1 + \frac{(1 - \omega)^2}{6} \right] q^6 .$$

The reader can note that γ_2 and γ_3, and actually also k_2, are the same in the three cases; both facts are natural, in that the three cases differ only for order six terms.

We have thus shown that, with explicit computations, the Landau-deGennes potential can be reduced, *uniformly in a neighborhood of the transition point* $c_1 = -\lambda = 0$ (again, the size of this neighborhood being controlled by $c_2 \neq 0$) to a simpler form, i.e., to either (73) or (75) or (76). Retaining the γ_2 and γ_3 terms was unavoidable due to the requirement to avoid any division by a c_1 factor.

B. Simplified potential—order eight

A similar analysis can be performed for the LdG potential of degree eight, as suggested by the discussion of Sec. VI, see (41): in this case, we obtain more involved formulas, and several options are possible concerning the simplification of the highest order term (i.e., retaining the T_2^4 or the $T_2 T_3^2$ one; equivalently, setting $\gamma_8 = 0$, $\gamma_9 = 1$ or $\gamma_8 = 1$, $\gamma_9 = 0$) and some of the sub-maximal ones. It should be stressed that we can again arrive at a reduced eight order potential for which explicit (albeit rather involved) expressions for the critical points can be obtained.

Here, we will consider two possible forms of the reduced potential, which correspond to the maximal possible simplification (in the sense of eliminating as many terms as possible), i.e.,

$$\begin{cases} \widehat{\Phi} = -\lambda\, T_2 \ + \ \gamma_2 T_3 + \gamma_3 T_2^2 + \gamma_5 T_2^3 + T_2 T_3^2 & (a) \, , \\ \widehat{\Phi} = -\lambda\, T_2 + \gamma_2 T_3 + \gamma_3 T_2^2 \ + \ \gamma_6 T_3^2 + T_2^4 & (b) \, . \end{cases} \tag{77}$$

In case (a), the remaining coefficients are given in terms of the original ones by

$$\begin{aligned} \gamma_2 &= c_2 \, , \\ \gamma_3 &= c_3 + \frac{2c_4}{3c_2}\, \lambda + \frac{4c_6}{9c_2^2}\, \lambda^2 \, , \\ \gamma_5 &= \left(c_5 - \frac{4c_3 c_4}{3c_2} \right) - \left(\frac{c_4^2}{c_2^2} + \frac{16c_3 c_6}{9c_2^2} - \frac{2c_7}{3c_2} \right) \lambda + O\left(\lambda^2 \right) \, . \end{aligned} \tag{78}$$

In case (b), the remaining coefficients are given in terms of the original ones by

$$\begin{aligned} \gamma_2 &= c_2 \, , \\ \gamma_3 &= c_3 + \frac{2c_4}{3c_2}\, \lambda \, , \\ \gamma_6 &= \left(c_6 - \frac{9c_3 c_4}{c_2} + \frac{27c_5}{4} \right) - \left(\frac{27c_4^2}{4c_2^2} - \frac{9c_7}{2c_2} \right) \lambda + O\left(\lambda^2 \right) \, . \end{aligned} \tag{79}$$

The coefficients of the change of coordinates taking us to these expressions are rather involved and are given in Appendix D.

C. Branching unstable biaxial solutions

It would be natural to attempt to use these results to analyze the biaxial phase problem; this would have led us too far, but we present here some computations based on the simplified potential and related to the one-dimensional weakly biaxial branches determined (outside the transition region) in Sec. VI. We will show here that these branches are unstable at the transition point.

It will suffice to consider the LdG potential at order six, i.e., (17), with **h** of form (22); we will consider the reduced potential of form (75), i.e.,

$$\widehat{\Phi} = -\lambda\, T_2 + \gamma_2\, T_3 + \gamma_3\, T_2^2 + T_2^3 \, , \tag{80}$$

with actually

$$\gamma_2 = c_2; \quad \lim_{\lambda \to 0} \gamma_3 = c_3 \, .$$

The discussion of Sec. VI suggests to focus on the one-dimensional manifold

$$M = \{x_1 = x, \ x_2 = 0, \ x_3 = 0, \ x_4 = x, \ x_5 = 0\} \, .$$

Doing this, we are reduced to study a one-dimensional problem, described by the effective potential

$$\Psi = -3\,\lambda\, x^2 - 2\,\gamma_2\, x^3 + 9\,\gamma_3\, x^4 + x^6 \, . \tag{81}$$

We will write $\lambda = \varepsilon$, and look for a solution as a power series in ε, i.e., as

$$x = \sum_k z_k\, \varepsilon^k \, .$$

With standard computations, we obtain at first orders

$$z_1 = -\frac{1}{\gamma_2} \ ; \quad z_2 = 6\, \frac{\gamma_3}{\gamma_2^3} \ ; \quad z_3 = -72\, \frac{\gamma_3^2}{\gamma_2^5} \ ; \quad z_4 = 4\left(\frac{\gamma_2^2 + 270\gamma_3^3}{\gamma_2^7}\right) \ ; \quad z_5 = -144\,\gamma_3\left(\frac{\gamma_2^2 + 126\gamma_3^3}{\gamma_2^9}\right) \, .$$

In order to study the stability of this solutions, we consider the Hessian H_b computed on the solutions branch so determined. This will also be written as a series expansion, and we get

$$H_b = H_1\, \varepsilon + H_2\, \varepsilon^2 + O(\varepsilon^3) \ ; \quad H_1 = \begin{pmatrix} 0 & 0 & 0 & 3 & 0 \\ 0 & -6 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 3 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix} \ ; \quad H_2 = \frac{18\gamma_3}{\gamma_2^2}\begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix} \, .$$

As for the eigenvalues, we have a double zero eigenvalue (which corresponds to the degeneracy of the problem, as discussed in Sec. VI), and three nonzero ones, which are

$$\mu_1 = -6\left(1 - 6\frac{\gamma_3}{\gamma_2^2}\varepsilon\right)\varepsilon \ ; \quad \mu_2 = -3\left(1 - 6\frac{\gamma_3}{\gamma_2^2}\varepsilon\right)\varepsilon \ ; \quad \mu_3 = 3\left(1 + 6\frac{\gamma_3}{\gamma_2^2}\varepsilon\right)\varepsilon \, . \tag{82}$$

Thus, for small ε (that is, small λ), we have an unstable branch. For $\gamma_3 > 0$, this becomes stable for

$$\lambda > \lambda_s \simeq \frac{\gamma_2^2}{6\gamma_3} \, . \tag{83}$$

Some numerical experiments, conducted assigning random values to γ_2 and γ_3, confirm this description. Moreover, they show we always have a stable solution on the manifold M, but this is *not* branching off from the origin.

VIII. DISCUSSION AND CONCLUSIONS

The Landau-deGennes potential describing the isotropic-nematic phase transition (and those between different nematic phases) in liquid crystals is a sixth order polynomial, depending on six parameters, see (17); going to the next order, we have an eight order parameter, depending on nine parameters, see (41). We have shown that passing to suitable non-homogeneous new variables, see (21) and (42), the potential is written in a simpler form, see (48), depending only on two parameters. The transformation to reach this simpler form has been explicitly determined in terms of the coefficients c_i appearing in the original potential.

This allows to study the equilibrium points of the potential in the new variables, i.e., using the simplified form $\widehat{\Phi}(x)$. Albeit going back to the original variables requires to invert the nonlinear change of variables (21) and (42) and is thus a nontrivial task (but see below); qualitative information obtained from the simplified potential remains true in whatever coordinates.

The quantitative aspect would concern the value of the parameters at which phase transitions occur, and the relation between the value of the parameters c_i and those assumed by the order parameters x_i. As mentioned above, in order to pass from the new variables x_i to the old ones, one should invert the nonlinear change of variables (21) and (42); note that it suffices to work at a finite order in $\varepsilon = |\mathbf{x}|$, so that the inversion is obtained by a series expansion. Explicit formulas could be obtained for the case at hand, but they are very complex and not significant.[48]

A significant weakness of our standard method, built in the basic idea behind the Poincaré normalization approach, is that it cannot be applied when the quadratic part of the Landau potential vanishes. Or, this is precisely the situation met at the main transition point, and one would be specially interested in analyzing the transition region. Our method is however flexible enough so that by a small modification—consisting in avoiding to operate division by factor which vanishes at the transition point—it can be also applied around critical points (this makes that low order terms cannot be eliminated, but several among the higher order terms are anyway erased), as shown explicitly in Sec. VII.

We have moreover considered a concrete open problem, i.e., that of possible direct transition from the fully isotropic phase to the biaxial one.[18,19] The implementation of the method in the singular region as in Sec. VII can be used to analyze in simpler terms the possibility of having a stable biaxial phase branching directly off the fully symmetric state, and we hope to be able to tackle this problem in the near future. Some partial results, concerning the special one-dimensional branches identified by Remark 1 and studied in Sec. VI, are presented in Sec. VII C.

In conclusion, we have shown by explicit computations that the Poincaré approach, devised to study critical points of dynamical systems, can also be profitably adopted to simplify computations in Landau theory of phase transitions. We have here considered a concrete and relevant application, i.e., the Landau-deGennes theory for the isotropic-nematic transition in liquid crystals, but it is clear that the validity of the Poincaré approach is much more general.

It should also be mentioned that the LdG theory considered here did *not* satisfy the simple hypotheses considered in Ref. 6 (under which quite general results were obtained) for the standard metric in $\mathbf{R}^5$, but did for standard metric in $GL(3)$. Rather than discussing things with this metric, here we have implemented the essential of Poincaré ideas, i.e., looked for a near-identity change of variables which does preserve the symmetry of the problem at hand and depends on arbitrary parameters; the latter can be chosen to obtain a simpler form of the function under study (in this case the LdG potential) in the new variables.

This also shows that the method proposed in Ref. 6 can be applied avoiding the (mild) mathematical sophistication which would be needed to take into account the non-standard metric to be introduced in the orbit space, see Appendix B. The direct approach pursued here has also another advantage, also discussed in Appendix B, i.e., that in this way we are able to take into account the higher order effects which were not considered in previous work.[6]

APPENDIX A: THE MOLIEN FUNCTION

The Molien function[49] is a generating function; given a ("source") representation T of a group G, acting on a vector space with variables x_i, the coefficients of its expansion in series of the parameter yield the number of independent tensors (with components being polynomials in the x_i) which transforms under a possibly different ("target") representation $\widetilde{T}$ of G.

In the case of interest here, $G = SO(3)$, vector representations are indexed by an integer number ℓ and have odd dimension $(2\ell + 1)$ [spinor representations are indexed by half-integer numbers $m/2$, with m odd, and have even dimension $(m + 1)$]; thus, the trivial representation $\ell = 0$ has dimension 1, the defining representation $\ell = 1$ has dimension 3, and the $\ell = 2$ representation we are considering here has dimension 5. The Molien function will then be denoted as $F_{\ell, \lambda}(t)$, where t is the parameter and ℓ, λ refer to the "source" and the "target" representations, respectively.

Here, we are interested in $F_{2,0}(t)$ and in $F_{2,2}(t)$, providing, respectively, the number of invariants and of covariants for the $\ell = 2$ representation at different orders. These turn out to be

$$F_{2,0} = \frac{1}{(1 - t^2)\,(1 - t^3)} \; ; \;\; F_{2,2} = \frac{t + t^2}{(1 - t^2)\,(1 - t^3)} \; .$$

Expanding these in series up to the order of interest here, we easily obtain

$$F_{2,0}(t) = 1 + t^2 + t^3 + t^4 + t^5 + 2t^6 + t^7 + 2t^8 + O\left(t^9\right) \, ,$$
$$F_{2,2}(t) = t + t^2 + t^3 + 2t^4 + 2t^5 + 2t^6 + 3t^7 + 3t^8 + O\left(t^9\right) \, .$$

We refer, e.g., to Refs. 20–25 for details on the Molien function, both in the specific case $G = SO(3)$ and in general.

APPENDIX B: COMPARISON WITH PREVIOUS WORK

We will now sketch how the same problem could be tackled following strictly the procedure given in Ref. 6. We will just follow this procedure, referring to Ref. 6 for its justification and detail; the understanding of the main body of the present work does not depend in any way on this appendix.

As mentioned above, the $SO(3)$ representation given by the J_a is not orthogonal with respect to the standard scalar product in $\mathbf{R}^5$, and thus we have to introduce a suitable scalar product for the procedure described in Ref. 6 to work, in particular, for the Sartori $\mathcal{P}$-matrix[26,27] to be properly defined. This turns out to be the one associated to the matrix

$$M = \begin{pmatrix} 4/3 & 0 & 0 & -2/3 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ -2/3 & 0 & 0 & 4/3 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix} \; .$$

The gradients $\nabla T_i(x)$ of the two basic invariants are easily computed. The $\mathcal{P}$-matrix, defined by $\mathcal{P}_{\alpha\beta} = (\nabla I_\alpha, \nabla I_\beta)$ with I_α the invariants, is

$$\mathcal{P} = \begin{pmatrix} 4\,T_2 & 6\,T_3 \\ 6\,T_3 & (4/3)\,T_2^2 \end{pmatrix} \; .$$

Proceeding as in Ref. 6, the homological operator $\mathcal{L}_0$ is therefore

$$\mathcal{L}_0 = 4\,c_1\,T_2\,(\partial/\partial T_2) \; .$$

This is discussed in Ref. 6; here, it suffices to say that under a change of variables generated by a function H_m (homogeneous of degree $m + 2$), the terms Φ_k with $m < k$ are not changed, while the term Φ_m is changed into $\widetilde{\Phi}_m = \Phi_m - \mathcal{L}_0(H_m)$. (The terms Φ_k with $k > m$ are changed in a more complex way; this could be described in precise terms[14] but is not relevant here.)

We should then apply this on homogeneous invariant generating functions of order up to five or seven (depending if we are in the framework of Section IV or V), i.e.,

$$H_1 = k_1 T_3 , \qquad H_2 = k_2 T_2^2 , \qquad H_3 = k_3 T_2 T_3 ,$$
$$H_4 = k_4 T_2^3 + k_5 T_3^2 , \qquad H_5 = k_6 T_2^2 T_3 .$$

This yields immediately

$$\mathcal{L}_0(H_1) = 0 , \qquad \mathcal{L}_0(H_2) = 8 c_1 k_2 T_2^2 = 8 c_1 H_2 , \qquad \mathcal{L}_0(H_3) = 4 c_1 k_3 T_2 T_3 = 4 c_1 H_3 ,$$
$$\mathcal{L}_0(H_4) = 12 c_1 k_4 T_2^3 , \qquad \mathcal{L}_0(H_5) = 8 c_1 k_6 T_2^2 T_3 = 8 c_1 H_5 .$$

Thus, the terms Φ_2, Φ_3, Φ_5 and the term proportional to T_2^3 in Φ_4, see (41), are in the range of $\mathcal{L}_0$ and by the discussion of Ref. 6 can be eliminated from the LdG functional.

Note that, on the other hand, the general results of Ref. 6 do not imply the elimination of Φ_1 and of the other term in Φ_4; this point will be discussed in a moment.

Moreover, as discussed in Ref. 6, while we can conclude that in the first effective step (assuming we just choose $k_1 = 0$, i.e., do not perform any change with cubic generating function), one should choose $k_2 = c_2/(8c_1)$, the actual determination of generating functions at higher orders, hence of k_i with $i > 2$, requires to consider in detail the effect of the previous transformation(s) on the coefficient c_i.

The procedure discussed in the present paper does instead provide a simultaneous computation of the modified coefficients in the potential and of those identifying the generating function; we recall this is possible because we know *a priori* at which order we want to stop, while the procedure given in Ref. 6 can in principles be pursued up to any order.

Finally, let us come back to the terms which are eliminated in the present approach but seemingly not in the general one discussed in Ref. 6. It was mentioned in there that the method only considered first order effects, and that one could take into account also higher order ones, mimicking what is done in dynamical systems,[10,13,14] thus obtaining a "further reduction." The procedure proposed here does take these higher order effects into account and hence obtains the further reduction, avoiding at the same time the relatively sophisticated mathematical tools which would be needed to obtain a comprehensive theory (valid at all orders) of it.[14]

APPENDIX C: REDUCTION OF TERMS OF ORDER SEVEN AND EIGHT

Here, we give explicit formulas for the reduction of terms of order seven and eight, considered in Section V.

1. Terms of order seven

As mentioned in the text, at order seven, we have only one invariant,

$$\widehat{\Phi}_5 = \gamma T_2^2 T_3 ;$$

by explicit computations, it results that

$$\gamma = c_7 + 27c_5k_1 + 4c_6k_1 + 30c_4k_1^2 + 54c_3k_1^3 + 5c_4k^2 + 54c_3k_1k_2 + 9c_2k_1^2k_2 + 3c_2k_2^2 + 4c_3k_3 + 4c_2k_1k_3$$
$$+2c_1k_2k_3 + 18c_3k_4 + 18c_2k_1k_4 + 9c_1k_2k_4 + 3c_2k_5 + 9c_1k_1k_5 + 2c_2k_6 + 6c_1k_1k_6 + 2c_1k_7 + 9c_1k_8 .$$

Setting $k_1, \ldots, k_6$ as determined at lower orders, we get

$$\gamma = [112c_2^5 - 2160c_1c_2^3c_3 + 1080c_1^2c_2^2c_4 - 54c_1^2c_2(-135c_3^2 + 54c_1c_5 + 8c_1c_6)$$
$$+729c_1^3(-4c_3c_4 + c_1(c_7 + 2c_1k_7 + 9c_1k_8))] / [729c_1^4] .$$

Note this depends on the two parameters k_7 and k_8; thus, one of these will remain undetermined (and can, e.g., be set to zero, or to some other convenient value).

If we choose, e.g.,

$$k_7 = [-112c_2^5 + 2160c_1c_2^3c_3 - 1080c_1^2c_2^2c_4 + 54c_1^2c_2(-135c_3^2 + 54c_1c_5 + 8c_1c_6)$$
$$-729c_1^3(-4c_3c_4 + c_1(c_7 + 9c_1k_8))] [1458\,c_1^5]^{-1},$$

then γ vanishes, and $\widehat{\Phi}_5$ with it.

2. Terms of order eight

We will refer to the formulas and notation of Sec. V D.

In general terms, with $k_1, \ldots, k_7$ taking the values determined at lower orders (apart from the undetermined k_4), we have

$$\xi = \Big[3609c_1c_2^4c_3 + 27c_1^2c_2^2(516c_1c_5 + 32c_1c_6 - 1149c_3^2) + 24c_1^2c_2^3(342c_1k_4 - 85c_4)$$
$$+1944c_1^3c_2(7c_3c_4 - 2c_1c_7 - 48c_1c_3k_4 + 12c_1^2k_8) + 2187c_1^3(33c_3^3 - 36c_1c_3c_5 + 8c_1^2(c_9 + 2c_4k_4 + 3c_1k_4^2$$
$$+2c_1k_9)) - 101c_2^6\Big] \Big[17\,496c_1^5\Big]^{-1},$$

$$\eta = \Big[5886c_1c_2^4c_3 - 266c_2^6 + 243c_1^2c_2^2(28c_1c_5 + 6c_1c_6 - 113c_3^2) - 18c_1^2c_2^3(172c_4 + 171c_1k_4)$$
$$+243c_1^4(-9c_4^2 - 18c_3c_6 - 54c_1c_4k_4 + c_1(4c_8 - 81c_1k_4^2)) + 1458c_1^3c_2(c_3(13c_4 + 24c_1k_4) - 2c_1(c_7 + 3c_1k_8))\Big]$$
$$\times \Big[971c_1^5\Big]^{-1}.$$

The requirements $\xi = 1$, $\eta = 0$ are satisfied by setting

$$k_8 = \Big[5886c_1c_2^4c_3 - c_1^2c_2^2(27\,459c_3^2 + 3096c_2c_4) + c_1^3c_2(18\,954c_3c_4 + 6804c_2c_5 + 1458c_2c_6 - 3078c_2^2k_4)$$
$$-c_1^4(2187c_4^2 + 4374c_3c_6 + 2916c_2c_7 - 34\,992c_2c_3k_4) + c_1^5(972c_8 - 13\,122c_4k_4) - 19\,683c_1^6k_4^2 - 266c_2^6\Big]$$
$$\times \Big[8748c_1^5c_2\Big]^{-1},$$

$$k_9 = \Big[-57\,915c_1c_2^4c_3 + c_1^2c_2^2(312\,741c_3^2 + 30\,888c_2c_4) - c_1^3(216\,513c_3^3 + 192\,456c_2c_3c_4 + 96\,228c_2^2c_5 + 14\,256c_2^2c_6)$$
$$+c_1^4(17\,496c_4^2 + 236\,196c_3c_5 + 34\,992(c_3c_6 + c_2c_7)) + c_1^5(52\,488(1 - c_9) - 7776c_8) + 2431c_2^6\Big]$$
$$\times \Big[104\,976c_1^6\Big]^{-1}.$$

As remarked in Sec. V D, these see the appearance of c_2 factors in the denominator, so are valid under the assumption—besides that $|c_1|$ is large enough—that $|c_2|$ is large enough as well. Note that even if we require only $\eta = 0$, we would however get denominators depending on c_2 as well.

On the other hand, the condition $\xi = 1$ (without requiring $\eta = 0$) can be satisfied by choosing

$$k_9 = \Big[101c_2^6 - 3609c_1c_2^4c_3 + 3c_1^2c_2^2(10\,341c_3^2 + 680c_2c_4) + 972c_1^4(81c_3c_5 + 4c_2c_7 + 96c_2c_3k_4)$$
$$-27c_1^3(2673c_3^3 + 504c_2c_3c_4 + 4c_2^2(129c_5 + 8c_6 + 76c_2k_4)) - 52\,488c_1^6k_4^2 - 5832c_1^5(-3 + 3c_9 + 6c_4k_4 + 4c_2k_8)\Big]$$
$$\times [34\,992\,c_1^6]^{-1}.$$

In this case, we obtain (as usual, these formulas would be slightly simplified by a suitable choice for the undetermined parameters k_4 and k_8)

$$\eta = \Big[-266c_2^6 + 5886c_1c_2^4c_3 + 243c_1^2c_2^2(-113c_3^2 + 28c_1c_5 + 6c_1c_6) - 18c_1^2c_2^3(172c_4 + 171c_1k_4)$$
$$+243c_1^4(-9c_4^2 - 18c_3c_6 - 54c_1c_4k_4 + c_1(4c_8 - 81c_1k_4^2)) - 1458c_1^3c_2(-c_3(13c_4 + 24c_1k_4)$$
$$+2c_1(c_7 + 3c_1k_8))\Big] \times [972\,c_1^5]^{-1}.$$

APPENDIX D: THE TRANSFORMATION FOR THE LdG POTENTIAL OF DEGREE EIGHT NEAR THE MAIN TRANSITION POINT

In this appendix, we provide explicit expressions for the coefficients k_i appearing in **h**, see (42), used to obtain simplified potentials (77). For the more involved expressions, we will just give the series expansion in c_1. Higher order coefficients appearing in (42), i.e., $k_9, k_{10}, \ldots$ have no role in this computation and can be set to zero.

The potential of case (a) is obtained by choosing

$$k_2 = \frac{2c_1c_6 - 3c_2c_4}{9c_2^2} \; ;$$

$$k_3 = -\frac{c_6}{3c_2} \; ;$$

$$k_4 = 0 \; ;$$

$$k_5 = \frac{4c_4^2 + 4c_3c_6 - 3c_2c_7}{9c_2^2}$$
$$+ \frac{\left(3(4c_8 + 27c_9 - 4)c_2^2 - 2(81c_4c_5 + 26c_4c_6 + 54c_3c_7)c_2 + 18c_3\left(11c_4^2 + 8c_3c_6\right)\right)}{54c_2^4} c_1 + O\left(c_1^2\right) \; ;$$

$$k_6 = 0 \; ;$$

$$k_7 = -\frac{(c_8 - 1)c_2^2 - 3c_4c_6c_2 + c_1c_6^2}{3c_2^3} \; ;$$

$$k_8 = -\frac{9c_9c_2^2 - 18c_4c_5c_2 - 12c_3c_7c_2 + 22c_3c_4^2 + 16c_3^2c_6}{18c_2^3}$$
$$+ \frac{\left(-3(6c_5c_6 + c_4c_7 + c_3(4c_8 + 27c_9 - 4))c_2^2 + 2\left(2c_4^3 + c_3(81c_5 + 34c_6)c_4 + 54c_3^2c_7\right)c_2 - 18c_3^2\left(11c_4^2 + 8c_3c_6\right)\right)}{27c_2^5} c_1$$
$$+ O\left(c_1^2\right) \; .$$

As for the potential of case (b), this is obtained by choosing

$$k_2 = -\frac{c_4}{3c_2} \; ;$$

$$k_3 = \frac{9c_5c_2^2 - 12c_3c_4c_2 + c_1c_4^2}{4c_2^3} \; ;$$

$$k_4 = -\frac{9c_5c_2^2 - 12c_3c_4c_2 + c_1c_4^2}{18c_2^3} \; ;$$

$$k_5 = 0 \; ;$$

$$k_6 = \frac{-6c_7c_2^3 + 8c_4^2c_2^2 + c_1\left((4c_8 + 27c_9 - 27)c_2^2 - 2c_4(27c_5 + 4c_6)c_2 + 18c_3c_4^2\right)}{12c_2\left(c_2^3 - 6c_1c_3c_2 + c_1^2c_4\right)} \; ;$$

$$k_7 = \frac{c_2(-9c_4c_5 + 8c_4c_6 - 4c_2c_8) - 36c_3\left(c_4^2 - c_2c_7\right)}{12c_2^3}$$
$$+ \frac{\left(-3\left(-27c_5^2 + 8c_4c_7 + 8c_3(4c_8 + 27c_9 - 27)\right)c_2^2 + 4\left(7c_4^3 + 6c_3(45c_5 + 8c_6)c_4 + 216c_3^2c_7\right)c_2 - 1440c_3^2c_4^2\right)}{48c_2^5} c_1$$
$$+ O\left(c_1^2\right) \; ;$$

$$k_8 = \frac{-9(c_9 - 1)c_2^2 + 21c_4c_5c_2 - 10c_3c_4^2}{18c_2^3} + \frac{\left(-144c_3^2c_4^2 + 216c_2c_3c_5c_4 + c_2\left(4c_4^3 - 81c_2c_5^2\right)\right)c_1}{216c_2^5} + O\left(c_1^2\right) \; .$$

[1] L. D. Landau, Nature **138**, 840-841 (1936); Zh. Exsp. Teor. Fiz. **7**, 19-32 & 627-637 (1937), http://www.ujp.bitp.kiev.ua/files/journals/53/si/53SI08p.pdf.
[2] L. D. Landau and E. M. Lifshitz, *Statistical Physics* (Pergamon Press, 1958).
[3] Yu. M. Gufan, *Structural Phase Transitions* (Nauka, 1982).
[4] I. A. Sergienko, Yu. M. Gufan, and S. Urazhdin, Phys. Rev. B **65**, 144104 (2002).
[5] G. Gaeta, Ann. Phys. **312**, 511-540 (2004).
[6] G. Gaeta, "Poincaré-like approach to Landau theory. I. General theory," J. Math. Phys. **56**, 083504 (2015).
[7] V. I. Arnold, *Geometrical Methods in the Theory of Ordinary Differential Equations* (Springer, 1983).
[8] C. Elphick *et al.*, Physica D **29**, 95-127 (1987); **32**, 488 (1988).
[9] S. Walcher, Math. Ann. **291**, 293-314 (1991); J. Math. Anal. Appl. **180**, 617-632 (1993).
[10] G. Cicogna and G. Gaeta, *Symmetry and Perturbation Theory in Nonlinear Dynamics* (Springer, 1999).
[11] G. Cicogna and S. Walcher, Acta Appl. Math. **70**, 95-111 (2002).

[12] S. Walcher, "Convergence of perturbative expansions," in *Encyclopedia of Complexity and Systems Science* (Springer, 2009), pp. 6760-6771; reprinted in *Mathematics of Complexity and Dynamical Systems* (Springer, 2012), pp. 1389-1399.

[13] G. Gaeta, Acta Appl. Math. **70**, 113-131 (2002).

[14] G. Gaeta, Ann. I.H.P.: Phys. Theor. **70**, 461-514 (1999), http://archive.numdam.org/ARCHIVE/AIHPA/AIHPA_1999 __70_6/AIHPA_1999__70_6_461_0/AIHPA_1999__70_6_461_0.pdf; Lett. Math. Phys. **42**, 103-114 (1997); **57**, 41-60 (2001).

[15] P. G. de Gennes and J. Prost, *The Physics of Liquid Crystals* (Oxford UP, 1993).

[16] E. Virga, *Variational Theories for Liquid Crystals* (Chapman & Hall, 1995).

[17] E. F. Gramsbergen, L. Longa, and W. H. de Jeu, Phys. Rep. **135**, 195-257 (1986).

[18] D. Allender and L. Longa, Phys. Rev. E **78**, 011704 (2008).

[19] M. J. Freiser, Phys. Rev. Lett. **24**, 1041-1043 (1970).

[20] M. V. Jaric and J. L. Birman, J. Math. Phys. **18**, 1459-1465 (1977), 2085.

[21] D. H. Sattinger, J. Math. Phys. **19**, 1720-1732 (1978).

[22] L. Michel, Rev. Mod. Phys. **52**, 617-651 (1980).

[23] L. Michel, J. S. Kim, J. Zak, and B. Zhilinskii, Phys. Rep. **341**, 1-395 (2001), http://www.sciencedirect.com/science/article/pii/S0370157300000880.

[24] P. Chossat and R. Lauterbach, *Methods in Equivariant Bifurcation Theory and Dynamical Systems* (World Scientific, 2000).

[25] P. Chossat, Acta Appl. Math. **70**, 71-94 (2002).

[26] M. Abud and G. Sartori, Ann. Phys. **150**, 307-372 (1983).

[27] G. Sartori, La Rivista del Nuovo Cimento **14**, 1 (1991); Acta Appl. Math. **70**, 183-207 (2002).

[28] H. Broer, in *Lecture Notes in Mathematics* (Springer, 1981), Vol. 898.

[29] G. Benettin, L. Galgani, A. Giorgilli, and J. M. Strelcyn, Nuovo Cimento B **79**, 201-223 (1984).

[30] A. Giorgilli, "On the representation of maps by Lie transforms," Itstituto Lombardo (Rend. Scienze) **146**, 251-277 (2012); preprint arXiv:1211.5674 (2012).

[31] M. Joyeux, J. Chem. Phys. **109**, 2111-2122 (1998).

[32] D. Sugny and M. Joyeux, J. Chem. Phys. **112**, 31-39 (2000).

[33] By this we mean of course the degree of the polynomial; it is customary to use the word "order" in this context since the degree of the Landau polynomial corresponds to the order in perturbation theory we are considering.

[34] It should also be recalled that Poincaré-Birkhoff normal forms have been used to compute quantum spectra with a remarkable level of accuracy up to near dissociation threshold, see, e.g., Refs. 31 and 32.

[35] Which is implemented by an algebraic manipulation language, given the considerable complexity of the algebra involved.

[36] Note the effective order parameters reduce to the two independent eigenvalues λ_1, λ_2 of Q, as different Q's related by a similarity transformation are equivalent.

[37] It should be noted this will be non-homogeneous; thus, the disappearing terms are actually just recombined to a simpler expression in the new coordinates.

[38] As for the determinant of Q and its iterates, these are of course also invariant but are expressed as a polynomial in terms of the traces, e.g., for a three-dimensional matrix A, one has $\mathtt{Det}(A) = (1/3)\mathtt{Tr}(A^3) - (1/2)\mathtt{Tr}(A^2)\mathtt{Tr}(A) + (1/6)[\mathtt{Tr}(A)]^3$.

[39] This would actually find some relevant obstacles when dealing with the physically significant problem discussed in Secs. VI and VII; what we actually (implicitly) use there is a more refined version of the normalization algorithm,[14] and resorting to explicit allows to avoid discussing the general mathematical theory, for which the reader is referred to Refs. 10, 13, and 14.

[40] In the mathematical literature, these are also mentioned as 2-covariants, where the "2" specifies the SO(3) representation they follow; we recall vector SO(3) representations have dimension $d = 2\ell + 1$ with $\ell \in \mathbf{Z}_+$, and in this case $\ell = 2$.

[41] Homogeneous covariants are determined up to linear combinations; thus, one could choose expressions with different overall constants and, in the case where more covariants of the same order exist, different linear combinations of them.

[42] It should be noted that, albeit we computed all the low order covariants, such a complete knowledge is not always needed: in fact, covariants index the (covariant) changes of variables, and knowing only some of them means that the considered changes of variable would not be the most general ones. E.g., in the following, we will see that disregarding one of the fourth order covariants, e.g., $\mathbf{F}_4^{(2)}$, would not harm our procedure.

[43] In mathematically more precise terms, we should actually require that $|c_1|$ is large enough, with $|c_1| > \varepsilon_*$ with ε_* depending on the region of the phase space we want to study.

[44] Dealing with still higher orders does not present any new conceptual difficulty, but the algebraic manipulations become rapidly quite involved.

[45] Note however that $\eta = 0$ leaves us with T_3 fully undetermined (in fact, in (55) η and T_3 always appear together), and $T_2^2 = q^2 = \lambda/4$.

[46] We stress we have only studied *local* stability, determined by the Hessian; our analysis does not exclude the possibility that Φ has also different local minima, maybe with a lower value.

[47] It should be stressed again that the x_i appearing above are those obtained *after* the normalization steps have been carried out; this has to be taken into account in trying to compute this solution branch in explicit terms. However, our choice of one-dimensional representative has been guided by Remark 1, so that these are embedded in invariant subspaces for the full Landau theory.

[48] The conceptual problems related to inversion are radically solved by considering more refined changes of variables, corresponding to *Lie series*.[10,28–30] In this way, the map $y \mapsto x$ corresponds to the time-one flow of a vector field $X = h^i(x)(\partial/\partial x^i)$, and inversion corresponds to time-reversed flow. The computational details to actually obtain the inversion at finite orders are however essentially the same. See Refs. 11 and 12 for other details on convergence issues.

[49] So called after the Latvian-born Russian mathematician Theodor Molien (Riga 1861–Tomsk 1941), the relevant work for our topic dates back to 1897.