Free energy according to Poincaré and Landau

Giuseppe Gaeta
Dipartimento di Matematica, Università degli Studi di Milano
via Saldini 50, I–20133 Milano (Italy)
giuseppe.gaeta@unimi.it

Summary. I discuss how – and how much – the Landau free energy functional can be simplified following the (normal forms) approach by Poincaré.

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Outline

In the Landau theory of phase transitions one considers an effective potential Φ (Landau polynomial). When Φ is too complicate, it is essential to be able to drop unessential terms, i.e. to apply a simplifying criterion.

Criteria based on singularity theory exist and have a rigorous foundation, but are often very difficult to apply in practice.

Here we consider a simplifying criterion and justify it on the basis of classical Poincaré theory. When one considers a range of values near a phase transition, the criterion has to be partially modified, as we discuss.

1. Landau

2. Poincaré

3. Extensions

4. Invariant potentials

5. Reduction of invariant potentials

6. Varying parameters

7. Conclusions & references

1. LANDAU

In Landau Theory one has to determine minima of an effective potential (Landau potential) depending on parameters.

The Landau potential is characterized by its symmetry.

Roughly speaking, one represents the state of the system by certain order parameters $(x_1, ..., x_n)$, $\mathbf{x} \in B \subseteq R^n$, and considers the most general potential $\Phi = \Phi(\mathbf{x})$ of order N which is invariant under the action of a Lie group G (acting through a representation) in B.

The order N is usually chosen as the minimal one guaranteeing thermodynamic stability (that is, Φ should be convex for large $|\mathbf{x}|$) and allowing spontaneous symmetry breaking.
But it might be higher.

The **Landau problem** is that of finding the minima of the Landau potential (functional), and the dependence of these on the parameters appearing in the potential.

Trouble with this program: outside textbook examples, Φ can be very complicated, and its study can be very hard.

It would be nice to simplify the potential. Two ways:

(1) Physical: drop "irrelevant" terms;

(2) Mathematical: change coordinates so that in the new ones things are simpler.

The first way is an art* (but working in proper space can help); the second way can be made algorithmic, and I will discuss this.

* *"The art of throwing away inessential terms of Taylor series, retaining the higher order but physically important terms"*; quoted from V.I. Arnold, "Catastrophe theory", in *Dynamical Systems V* (EMS – Vol. 5), sect. 5.5.

2. POINCARE'

Poincaré considered a problem which turns out to be related.

2.1. The Poincaré problem.

Consider a vector ODE

$$dx^i/dt \;=\; f^i(\mathbf{x}) \qquad f(0) = 0 \;.$$

Expanding in series around $\mathbf{x} = 0$, we get

$$d\mathbf{x}/dt \;=\; A\,\mathbf{x} \;+\; \sum_{k=1}^{\infty} f_k(\mathbf{x}) \qquad (*)$$

with f_k homogeneous of degree $k+1$.

Problem: find coordinates in which the (lower order) nonlinear terms cancel out (or at least are simplified).

Idea: do it step by step.

• Not surprising: Killing all nonlinear terms is not always possible.

• Nice surprise: The obstacle can be explicitly determined.

• Reason: Transformation at each step is controlled by a linear operator.

2.2. The linear part

The linear part of our system (*) is identified by the matrix A.

This is decomposed as

$$A \;=\; A_s \;+\; A_n \;,$$

its semisimple and nilpotent parts; in Jordan normal form,

$$A_s \;=\; \mathrm{diag}(\lambda_1, ..., \lambda_n) \;.$$

In the following $A_n = 0$ (this is always the case if $f = -\nabla\Phi$).

The criteria for eliminating (or reducing) the nonlinear terms can be stated in terms of the spectrum $\{\lambda_1, ..., \lambda_n\}$ of A.

2.3. Poincaré's result

Poincaré shows that one can (at least formally) eliminate nonlinear terms by a sequence of near-identity changes of coordinates [Poincaré transformations] if and only if the eigenvalues λ_i satisfy a **non-resonance condition**:

There are no non-negative integers m_j (with $|m| = \sum_j m_j > 1$) such that

$$\lambda_i \;=\; \sum_j m_j \lambda_j \;:=\; (m \cdot \lambda) \;.$$

2.4. Poincaré's trick

Consider $|x| \simeq \varepsilon$, and $x^i \to x^i + h^i_m(\mathbf{x})$ (with h_m homogeneous). Then f_k and $\dot{x}$ change according to

$$\begin{aligned} f_k(x) &\to f_k(x + h_m) = f_k(x) + (\partial f_k/\partial x^i)\, h^i_m(x) + \texttt{h.o.t.}\ ; \\ \dot{x}^i &\to \dot{x}^i + (\partial h^i_m/\partial x^j)\, \dot{x}^j + \texttt{h.o.t.}\ . \end{aligned}$$

Thus $\dot{x}^i = \sum_k f^i_k(x)$ goes into $\dot{x}^i = \sum_k \widehat{f}^i_k(x)$ with

$$\begin{cases} \widehat{f}_k = f_k & \text{for } k < m, \\ \widehat{f}_m = f_m - \mathcal{L}_0(h_m) & (k = m) \\ \widehat{f}_k = f_k + \text{ some complex expression} & \text{for } k > m \end{cases}$$

2.5. Poincaré normalizing procedure.

Proceeding sequentially for $m = 1, 2, 3, ...$ at each step lower orders are not touched, and the action at order m is controlled by the **homological operator***

$$[\mathcal{L}_0(h)] \ := \ (f_0 \cdot \nabla)\, h \ - \ (h \cdot \nabla)\, f_0 \ .$$

- All terms f_k in the **range** of $\mathcal{L}_0$ can be killed off;

- We can always choose freely a term δh_m in the **kernel** of $\mathcal{L}_0$.

*At each step we have to solve the *homological equation* $\mathcal{L}_0(h_m) = \pi_m \widetilde{f}_m$.

2.6. Proper coordinates.

In the proper (Jordan) coordinates, all monomials

$$h^i = c^i_{m_1 \dots m_n} x_1^{m_1} \dots x_n^{m_n} := c^i_{\mathbf{m}} \mathbf{x}^{\mathbf{m}} \ , \quad |m| = m_1 + \dots + m_n$$

are eigenfunctions of $\mathcal{L}_0$ with eigenvector

$$\sigma^i_{\mathbf{m}} \ = \ - \left[\lambda_i \ - \ (\lambda \cdot m) \right] \ .$$

This explains the origin of the non-resonance condition.

Resonant terms are in the kernel – and in the complementary to the range – of $\mathcal{L}_0$ and could not be eliminated in this way.

2.7. The resonant case

Dulac studied what happens when A is *resonant*. In this case one can eliminate all nonlinear terms except the resonant ones, reducing (*) to a fully resonant system

$$dy^i/dt \;=\; A\,y \;+\; \sum_{k=1}^{\infty} g_k(\mathbf{y}) \qquad (**)$$

where all the nonlinear terms g_k are resonant.

Resonant also means that the flows of $X_k = g_k^i(\mathbf{x})(\partial/\partial x^i)$ and $X_0 = (A\mathbf{x})^i(\partial/\partial x^i)$ commute,

$$[X_0, X_k] \;=\; 0\ .$$

I do not want to enter in the technical detail of this, but observe that there is a relevant consequence:

The linear part commutes with the full dynamics.

2.8. Convergence?

This shows at once that the Poincaré's procedure cannot converge unless the original problem had a symmetry (Moser).

On the other hand, a relatively recent theory (developed by Bryuno, Ito, Rüssmann, Walcher, Cicogna) shows that symmetry can guarantee the convergence of the normalizing procedure.*

In concrete applications (finitely many steps plus truncation), one is able to explicitly determine the convergence properties.

*See G. Cicogna & S. Walcher, *Acta Appl. Math.* **70** (2002), 95-111.

3. EXTENSIONS

3.1. Hamiltonian systems

A few decades later (!), Birkhoff observed that if the dynamical system under study is Hamiltonian, one can deal directly directly with the Hamiltonian rather than with the vector field.

Advantages:

(1) deal with a *scalar* quantity rather than with vector ones (n components).

(2) guarantee to preserve the Hamiltonian character of the dynamical system.

Now we always have "trivial" resonances due to Hamiltonian symmetries (near a stable equilibrium $\lambda_j = \pm i\omega_j$), and the non-resonance condition should not take these into account.

• In the non-resonant case, the Hamiltonian can be reduced (formally) to its quadratic part (Birkhoff);

• In the resonant case, the Hamiltonian can be modified so that only resonant terms are present (Gustavsson).

Again this means that H_0 is a constant of motion for the full Hamiltonian; by Moser remark, convergence is possible only if H had an additional constant of motion.

3.2. Further normalization

One can use "higher order effects" in the Poincaré procedure to obtain a better control on resonant terms.*

In particular, in the Hamiltonian case one can retain only resonant terms commuting among themselves,

$$\{\widehat{H}_k, \widehat{H}_m\} \;=\; 0 \;.$$

As usual the Moser remark shows that this will be only formal, unless the original system had enough symmetries.

*For a review, see GG, *Acta Appl. Math.* **70** (2002), 113-131; or article in *Mathematics of Complexity and Dynamical Systems*, Springer 2011.

4. INVARIANT POTENTIALS

Let us turn to considering the problem of simplifying (in the Poincaré's spirit) a G-invariant potential $\Phi(x)$.

Assume $x \in M \subseteq R^n$ and that G is a compact group which leaves M invariant and acts orthogonally in R^n.
(Could do without this assumption, but this way things are simpler, and assumption natural in the Landau theory context.)

Theory based on many results, but key names (in my approach) are Gufan and Sartori. [Plus L.D. Landau and L. Michel.]

4.1. The Hilbert theorem.

First problem: *determine the most general invariant potential*

$$\Phi(gx) \;=\; \Phi(x) \quad \forall g \in G \ .$$

Answer provided by the *Hilbert basis theorem*: there are

$$\{J_1(x), ..., J_r(x)\} \ ,$$

G-invariant homogeneous polynomials of degrees $\{d_1, ..., d_r\}$, such that any G-invariant polynomial $\Phi(x)$ can be written as a polynomial in the $\{J_1, ..., J_r\}$, i.e.

$$\Phi(x) \;=\; \Psi\left[J_1(x), ..., J_r(x)\right]$$

with Ψ a polynomial in $(J_1, ..., J_r)$.

With our hypotheses on G, the basis is finite.

4.2. Minimal integrity basis

When the J_α are chosen so that:
(i) none of them can be written as a polynomial of the others;
(ii) r has the smallest possible value,
we say that they are a *minimal integrity basis (MIB)*, and that the $\{J_\alpha\}$ 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).

Assume from now on we have chosen a MIB $\{J_1, ..., J_r\}$ (with degrees $\{d_1, ..., d_r\}$ in x, $d_1 \leq d_2 \leq ... \leq d_r$).

4.3. The orbit space.

Denote by $\Omega \subseteq \mathbf{R}^r$ the target space for $\mathbf{J} = (J_1, ..., J_r)$. The space $\Omega \simeq M/G$ is the **orbit space** for the G action on M: its points are in correspondence with the G-orbits in M.*

If the MIB is regular Ω is a full measure region in $\mathbf{R}^r$, while in general Ω is an algebraic submanifold of $\mathbf{R}^r$.

An invariant polynomial Φ can be written in terms of the basic invariants. Thus the evaluation of $\Phi : M \to \mathbf{R}$ is in principles substituted by evaluation of $\mathbf{J} : M \to \Omega$ and $\Psi : \Omega \to \mathbf{R}$.

*The geometry of orbit space is discussed e.g. in Abud & Sartori *Ann. Phys. (NY)* **150** (1983), Michel & al. *Phys. Rep.* **341** (2001); for applications in dynamics see Chossat *Acta Appl. Math.* **70** (2002).

4.4. The Landau-Michel principle.

If – as in Landau theory – we have to consider the most general G-invariant polynomial, we only have to deal with the map $\Psi : \Omega \to \mathbf{R}$. Thus we come to the

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

4.5. Stability (thermodynamic)

How is the request of thermodynamic stability (i.e. convexity) of Φ reflected in the polynomial $\Psi(J)$?

(a) The regular case. Now $\Psi : \mathbf{R}_0^r \to \mathbf{R}$, and the J_a can be considered as independent variables. The minimal Landau polynomial $\Phi(x) = \Psi[J(x)]$ will be quadratic in the J; stability is ensured by requiring that $D_{ih} = [\partial^2\Psi/(\partial J_i \partial J_h)]$ is positive definite.

The prescription in this case is to *consider a polynomial of order* $N = 2\text{max}(d_1, ..., d_r) = 2d_r$ [and of course *choose coefficients so that* D *is positive definite* for large $|x|$].

Reason: allow symmetry breaking along all directions in Ω.

(b) The non-regular case. This prescription also works here: 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.

Two remarks are in order here:

(1) The prescription is *not* to write Ψ 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.

(2) The coefficients of (at least some of) the polynomials will depend on the external parameters; in particular, this will be the case for the quadratic terms, which control the loss of stability of the critical point $x = 0$ and thus the onset of the phase transition.

4.6. The Sartori $\mathcal{P}$-matrix

The Sartori $\mathcal{P}$-matrix* is built with the gradients of basic invariants; with $\langle .,. \rangle$ the standard scalar product in $M = \mathbf{R}^m$, this is defined as

$$\mathcal{P}_{\alpha\beta}(x) \ := \ \langle \nabla J_\alpha(x), \nabla J_\beta(x) \rangle \ .$$

The gradient of an invariant is a covariant; the scalar product of two covariants is an invariant, and hence *the $\mathcal{P}$-matrix can always be written in terms of the J themselves*.

The $\mathcal{P}$-matrix will control transformations of Φ.

*See G. Sartori, *Acta Appl. Math.* **70** (2002)

5. REDUCTION OF INVARIANT POLYNOMIALS

Consider (Poincaré) changes of coordinates of the form

$$x^i \;\rightarrow\; x^i \;+\; h^i_m(x)$$

We want h to (i) preserve the symmetry of Φ and (ii) be gradient functions; thus

$$h(T_g x) \;=\; T_g\, h(x)\;; \qquad h^i(x) \;=\; [\partial H(x)/\partial x^i]\;.$$

As H is G-invariant, we can write $H(x) = \chi[J_1(x), ..., J_r(x)]$;

$$h^i \;=\; (\partial H/\partial x^i) = (\partial\chi/\partial J_\beta)\cdot(\partial J_\beta/\partial x^i)\;.$$

To know how the change of variables acts on the Φ_k,
it suffices to know how it acts on the basic invariants J_α.

Dropping h.o.t. we get

$$\begin{aligned} J_\alpha(x) &\rightarrow J_\alpha(x) + (\partial J_\alpha/\partial x^p)\delta^{pq}(\partial H/\partial x^q) \\ &= J_\alpha(x) + ((\partial J_\alpha/\partial x^i)(\partial\chi/\partial J_\beta)\cdot(\partial J_\beta/\partial x^i) \\ &= J_\alpha(x) + \mathcal{P}_{\alpha\beta}\,(\partial H/\partial J_\beta) \\ &= J_\alpha(x) + \mathcal{P}_{\alpha\beta}\,Q_\beta\ . \end{aligned}$$

Note: $Q_\alpha = \partial_\alpha H(J)$ implies

$$\partial_\alpha Q_\beta = \partial_\beta Q_\alpha\ .$$

5.1. Reduction of invariant polynomials

We can apply the above discussion to the reduction of an invariant polynomial

$$\Phi(x) = \Psi(J_1, ..., J_r) \ ; \quad \Phi(x) = \sum_k \Phi_k[J(x)] \ , \quad \Psi = \sum_k \Psi_k(J) \ .$$

Under $x \to x + \nabla H_m$, the Ψ_k with $k \leq m$ are not changed, while the terms Ψ_{m+p} change according to

$$\Psi_{m+p} \ \to \ \Psi_{m+p} + (D_\alpha \Psi_p) \mathcal{P}_{\alpha\beta} (D_\beta H_m) \ + \ \text{h.o.t.} \ .$$

In particular (up to h.o.t.),

$$\begin{aligned} \Psi_m &\rightarrow \Psi_m + (D_\alpha \Psi_0)\mathcal{P}_{\alpha\beta}(D_\beta H_m) \\ &= \Psi_m + \mathcal{L}_0(H_m) \ , \end{aligned}$$

where now

$$\begin{aligned} \mathcal{L}_0(H) &= (\partial \Psi_0/\partial J_\alpha)\mathcal{P}_{\alpha\beta}(\partial H/\partial J_\beta) \\ &= U_\beta Q_\beta \ . \end{aligned}$$

We can thus operate sequentially with $H_1, H_2, ...$; at each stage (generator H_m) we are not affecting the terms Ψ_k with $k \leq m$.

- terms in $\mathtt{Ran}(\mathcal{L}_0)$ can be eliminated;

- adding a term in $\mathtt{Ker}(\mathcal{L}_0)$ to H_m is inessential.

Ψ_0 corresponds to the quadratic part of the potential; thus

$$\Psi_0 \;=\; \sum_{\alpha=1}^{s} \gamma_\alpha \; J_\alpha \;, \quad \gamma_\alpha \in \mathbf{R} \;;$$

and hence (defining $\gamma_\alpha = 0$ for $\alpha > s$)

$$\mathcal{L}_0 \;=\; \gamma_\alpha \, \mathcal{P}_{\alpha\beta} \, \frac{\partial}{\partial J_\beta} \;.$$

With notation introduced above,

$$U_\beta \;=\; \gamma_\alpha \; \mathcal{P}_{\alpha\beta} \;.$$

5.2. Dynamic Landau theory

Had we been studying

$$dx/dt \;=\; f(x) \;=\; -\nabla\Phi(x) \;,$$

there would have been a term coming from the transformation of dx/dt as well.

In this case it is convenient to write

$$\Phi_0 \;=\; \frac{1}{2}A_{ij}x^i x^j \;;$$

the change in f_k under $x \to x + h_m(x)$ $(h_m = \nabla H)$ is given by

$$\delta f^i_m \;=\; -\,A^{i\ell}(\partial_\ell H) \;.$$

5.3. Example 1.

Consider $M = \mathbf{R}^2 = \{x, y\}$ and $G = Z_2 \times Z_2$ generated by

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

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

$$\nabla J_1 = \begin{pmatrix} 2x \\ 0 \end{pmatrix} \ , \quad \nabla J_2 = \begin{pmatrix} 0 \\ 2y \end{pmatrix} \ ; \quad \mathcal{P} = \begin{pmatrix} 4J_1 & 0 \\ 0 & 4J_2 \end{pmatrix} \ .$$

In this case we choose $N = 4$ and $\Phi = \Phi_0 + \Phi_2$ with

$$\Phi_0 = a_1 J_1 + a_2 J_2 \ , \quad \Phi_2 = b_1 J_1^2 + b_2 J_2^2 + c J_1 J_2 \ .$$

Now

$$H_2 \;=\; p_1\, J_1^2 \;+\; p_2\, J_2 \;+\; q\, J_1\, J_2$$

and

$$\mathcal{L}_0(H_2) \;=\; (8a_1p_1)\, J_1^2 \;+\; (8a_2p_2)\, J_2^2 \;+\; [4(a_1+a_2)\, q]\, J_1\, J_2$$

Thus we can eliminate Φ_2 provided we choose

$$p_1 \;=\; -\frac{b_1}{8a_1}\;,\quad p_2 \;=\; -\frac{b_2}{8a_2}\;;\quad q \;=\; -\frac{c}{4(a_1+a_2)}\;.$$

5.4. Example 2.

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

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

Again $N = 4$. In this case the basis is *not* regular: $J_1 J_2 = J_3^2$.

Now $J_1 \in \mathbf{R}_+$, $J_2 \in \mathbf{R}_+$, and $J_3 \in \mathbf{R}$; as (x, y) varies in $\mathbf{R}^2$, the point (J_1, J_2, J_3) varies on the manifold $J_3^2 = J_1 J_2$.

$$\nabla J_1 = (2x, 0) \ , \quad \nabla J_2 = (0, 2y) \ , \quad \nabla J_3 = (y, x) \ ;$$

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

Here again $d_1 = d_2 = d_3 = 2$, hence $N = 4$ and $\Phi = \Phi_0 + \Phi_2$;

$$\Phi_0 = (a_1 J_1 + a_2 J_2 + a_3 J_3) \ ,$$
$$\Phi_2 = \Big[(b_1 J_1^2 + b_2 J_2^2 + b_3 J_3^2) \ + \ (c_1 J_1 J_3 + c_2 J_2 J_3) \Big] \ .$$

Thus 3+5 coefficients.

Note: I have not included terms of the form $c_0 J_1 J_2$ in Φ_2: as $J_1 J_2 = J_3^2$, these can be absorbed in $b_3 J_3^2$.

Change of variables generated by

$$H_2 \;=\; p_1 J_1^2 + p_2 J_2^2 + p_3 J_3^2 + q_1 J_1 J_3 + q_2 J_2 J_3 \ .$$

Under this, $\Phi_2 \to \widetilde{\Phi}_2 = \Phi_2 + \delta\Phi_2$, with (using $J_3^2 = J_1 J_2$)

$$\begin{aligned}\delta\Phi_2 \;=\;& (8a_1h_1 + a_3k_1)J_1^2 + (8a_2h_2 + a_3k_2)J_2^2 + [4(a_1+a_2)h_3 \\ & +3a_3(k_1+k_2)]J_3^2 + [4a_3h_1 + 2a_3h_3 + (6a_1+2a_2)k_1]J_1J_3 \\ & +[4a_3h_2 + 2a_3h_3 + (2a_1+6a_2)k_2]J_2J_3 \ .\end{aligned}$$

With obvious notation, $\widetilde{\Phi}_2 = A(\mathbf{p}, \mathbf{q}) + (\mathbf{b}, \mathbf{c})$, where

$$A = \begin{pmatrix} 8a_1 & 0 & 0 & a_3 & 0 \\ 0 & 8a_2 & 0 & 0 & a_3 \\ 0 & 0 & 4(a_1+a_2) & 3a_3 & 3a_3 \\ 4a_3 & 0 & 2a_3 & (6a_1+2a_2) & 0 \\ 0 & 4a_3 & 2a_3 & 0 & (2a_1+6a_2) \end{pmatrix}.$$

Thus we can invert and solve if A has non-vanishing determinant. This cancels the 5 coefficients of quartic terms.

I won't discuss this is detail, but just remark that all formulas can be made completely explicit.

5.5. Example 3 (SGU)*

Consider $M = \mathbf{R}^3$ and $G = Z_2 \times Z_2 \times Z_2$ generated by

$$\begin{aligned} g_x &: (x, y, z) \ \rightarrow \ (-x, y, z) \ , \\ g_y &: (x, y, z) \ \rightarrow \ (x, -y, z) \ , \\ g_z &: (x, y, z) \ \rightarrow \ (x, y, -z) \ . \end{aligned}$$

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

in this case $d_1 = 2$, $d_2 = 4$, $d_3 = 6$. Thus $N = 12$ and Φ depends on 22 coefficients.

*Sergienko, Gufan & Urazhdin, "Phenomenological theory of phase transitions in highly piezoelectric perovskites", *Phys. Rev. B* **65** (2002), 144104.

$$
\begin{aligned}
\Phi_0 &= c_1 J_1 \\
\Phi_2 &= c_2 J_2 + c_3 J_1^2 \\
\Phi_4 &= c_4 J_3 + c_5 J_1^3 + c_6 J_1 J_2 \\
\Phi_6 &= c_7 J_1^4 + c_8 J_1^2 J_2 + c_9 J_1 J_3 + c_{10} J_2^2 \\
\Phi_8 &= c_{11} J_1^5 + c_{12} J_1^3 J_2 + c_{13} J_1^2 J_3 + c_{14} J_1 J_2^2 + c_{15} J_2 J_3 \\
\Phi_{10} &= c_{16} J_1^6 + c_{17} J_1^4 J_2 + c_{18} J_1^3 J_3 + c_{19} J_1^2 J_2^2 + c_{20} J_1 J_2 J_3 \\
&\quad + c_{21} J_2^3 + c_{22} J_3^2 \ .
\end{aligned}
$$

Note: The group D_{2h} has the same basic invariants and hence the same general Landau expansion.*

*See: E.F. Gramsbergen, L. Longa & W.H. de Jeua, "Landau theory of the nematic-isotropic phase transition", *Physics Reports* **135** (1986), 195-257.

Sergienko, Gufan and Urazhdin argue that one can consider the reduced Landau polynomial

$$\widehat{\Phi} \;=\; \beta_1 J_1 + \beta_2 J_2 + \beta_3 J_3 + \gamma_1 J_1^2 + \gamma_2 J_2^2 + \gamma_3 J_3^2 \;;$$

in our present notation this means setting all coefficients to zero at the exception of the following 3+3 ones:

$$\{a_1, a_2, a_3, b_1, b_2, b_4\} \;.$$

Their statement can be justified based on the observation that all the other terms lie in the range of the $\mathcal{L}_0$ operator.

In this case we have

$$\nabla J_1 = 2\begin{pmatrix} x \\ y \\ z \end{pmatrix} \ , \quad \nabla J_2 = 2\begin{pmatrix} x(y^2+z^2) \\ y(x^2+z^2) \\ z(x^2+y^2) \end{pmatrix} \ , \quad \nabla J_3 = 2\begin{pmatrix} x(y^2z^2) \\ y(x^2z^2) \\ z(x^2y^2) \end{pmatrix} \ ;$$

and hence

$$\mathcal{P} \ = \ 4 \begin{pmatrix} J_1 & 2J_2 & 3J_3 \\ 2J_2 & (J_1J_2+3J_3) & 2J_1J_3 \\ 3J_3 & 2J_1J_3 & J_2J_3 \end{pmatrix} \ .$$

6. VARYING PARAMETERS

So far we have worked with a given Landau polynomial, i.e. with *fixed* values of the parameters (maybe near the phase transition).

These parameter (at least some of them) will depend on the external "control" parameter (temperature, pressure, magnetic field, etc);
some extra care is needed if we want to work on a full interval of values of the control parameter(s).

In particular, in Landau theory one is considering phase transitions; that is, the coefficients of the polynomial $\Phi(x)$ depend on external control parameters λ, and *necessarily pass through critical values*.

If we want to explore a range of values, we are allowed to consider only those Poincaré transformations which are *smooth and well defined in a full neighborhood of the critical point, and in particular at the critical point itself*.

The SGU example is quite involved if we want to work in this framework; see GG 2004 for this analysis.

We finally summarize our discussion in the following reduction criterion. (If one works at a fixed (noncritical) value λ_0 of the control parameter, the set Λ reduces to the single point λ_0.)

The reduction criterion.

1 (notation). Let G be a compact Lie group, acting in $\mathbf{R}^n$ through a linear representation; let $\{J_1, ..., J_r\}$ be a minimal integrity basis for G, and let $\Phi(\lambda; J_1, ..., J_r) : \Lambda \times \mathbf{R}^n \to \mathbf{R}$ be a potential depending on the control parameters $\lambda \in \Lambda \subseteq \mathbf{R}^p$.
Define, for $i = 1, ..., r$ and with $\langle ., . \rangle$ the scalar product in $\mathbf{R}^n$, the quantities

$$U_\alpha(\lambda; J_1, ..., J_r) \ := \ \sum_{k=1}^{r} \frac{\partial \Phi_0}{\partial J_k} \ \langle \nabla J_k, \nabla J_\alpha \rangle \ .$$

Let $B \subseteq \mathbf{R}^n$ be a sufficiently small neighborhood of 0 in $\mathbf{R}^n$.

2 (result). Then there is a sequence of Poincaré changes of coordinates in B, such that the potential Φ is expressed in an equivalent form $\widetilde{\Phi}$ in a neighborhood $\Lambda_0 \subseteq \Lambda$ of the critical value $\lambda = \lambda_0$; terms of Φ which can be written uniformly in Λ, as

$$\sum_{\alpha=1}^{r} Q_\alpha(J_1, ..., J_r)\ U_\alpha(\lambda; J_1, ..., J_r) \ + \ \text{h.o.t.}$$

where Q_α are polynomials in $J_1, ..., J_r$ satisfying the compatibility condition $(\partial Q_\alpha/\partial J_\beta) = (\partial Q_\beta/\partial J_\alpha)$, can be eliminated in $\widetilde{\Phi}$.

Notes

Here "sufficiently small" means that the overall change of coordinates described by the combination of the different ones at each order $k = 2, ..., 2d_r$ should define a convergent series in this domain. In general – for a given finite order d_r – this will be the case only in some neighborhood B of the origin; the convergence is also related to symmetry properties, i.e. to G.

Don't worry: When one performs a concrete computation, the radius of convergence will always be computable from the concrete inversion formulas.

Recall also here we consider just changes of coordinates: that is, we eliminate terms by choosing suitable coordinates, but we are *not* changing the 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, the transformations considered here are surely allowed, and actually can be easily implemented (algorithmically) via a symbolic manipulation language.

CONCLUSION

• The Poincaré approach is useful and constructive also in the realm of Landau theory; it should be employed to reduce the complexity of the Landau polynomial.

• Presumably, work has still to be done to fully put to use the power of Poincaré's approach in this realm.

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