The Landau Theory of Second-Order Phase Transitions and the Invariant Theory

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The following discussion is along the lines of a paper by Gufan¹ who, more than ten years ago, started to apply invariant theory to study the Landau theory of second-order phase transitions. Since that work was completed new results have been obtained for the structure of the computation of the ring of G-invariant polynomials, when G is a finite group. For a survey of this mathematical topic, see the excellent review by Stanley.² I used these results in a work³ not very accessible in this country. In it I studied two physical problems of symmetry breaking very similar from the mathematical point of view: the Landau theory and the Higgs mechanism in unified theories of fundamental interactions. I have only little progress to report since Ref. 3 was published. However, I will give here a self-contained account.

Allow me to start with a few mathematical definitions and theorems. We consider a linear representation $g \rightarrow \mathcal{D}(g)$ of a group Γ acting on a vector space \mathscr{E} . The Γ -orbit $\mathcal{D}(\Gamma)\phi$ of a vector $\phi \in \mathscr{E}$ is the set of transformed ϕ by Γ

$$\mathcal{D}(\Gamma)\phi = \{\mathcal{D}(g)\phi, g\in\Gamma\} \tag{1}$$

The isotropic group Γ_{ϕ} (physicists often say the "little group") is the set of elements $g \in \Gamma$ leaving ϕ invariant

$$\Gamma_{\phi} = \{ g \in \Gamma, \mathcal{D}(g)\phi = \phi \} \tag{2}$$

One shows easily that the isotropy group of $\mathcal{D}(g)\phi$ is the conjugate of Γ_{ϕ} by g

$$\Gamma_{\mathcal{L}(g)\phi} = g\Gamma_{\phi}g^{-1}$$

So the isotropic groups of a Γ -orbit form a conjugation class of Γ -subgroups. We denote by $\lceil \Lambda \rceil$ the conjugation class of the subgroup Λ

 $<\Gamma$. All orbits with the same conjugation class[Λ] of isotropic groups are said to be of the same type, and their union is called a *stratum*.

A Γ -covariant vector field on \mathscr{E} is a function $\mathscr{E} \xrightarrow{\nu} \mathscr{E}$, which commutes with the group representation

$$\forall g \in \Gamma \qquad \mathcal{D}(g)v(\phi) = v(\mathcal{D}(g)\phi) \tag{14}$$

Such a covariant vector field is tangential at ϕ to the stratum $S(\phi)$ of ϕ . The *kernel* of the representation $\mathcal{D}(g)$ of Γ is the set of elements of Γ represented by the matrix I, denoted by ker \mathcal{D} . It is an invariant subgroup of Γ and the quotient group

$$\operatorname{Im} \mathscr{D} = \Gamma/\ker \mathscr{D} \tag{5}$$

is called the *image* of \mathcal{D} . It is the set of matrices $\{\mathcal{D}(g), g \in \Gamma\}$. The decomposition of \mathscr{E} into Γ orbits and strata depends only on Im \mathscr{D} , which we denote by G, i.e., $G = \mathcal{D}(\Gamma)$. To each conjugate class [H] of Gsubgroups corresponds a unique conjugate class $\mathcal{D}^{-1}([H])$ of Γ subgroups. If G is a compact (or, as a particular case, a finite) group, there is a natural order on the set of its conjugate classes of subgroups: [H] < [H'] to any $H' \in [H']$ there is a subgroup H of H' belonging to [H]. We denote by \mathcal{K} the set of conjugate classes of isotropic groups of G acting on $\mathscr{E} - \{0\}$. There is a minimal class⁴; when G is finite, this is the class of the identity, so it corresponds to ker $\mathcal{D} < \Gamma$. In all cases, the corresponding stratum is open dense. We will call it generic. The crystallographic space group Γ of a crystal is discrete but infinite, so it is not compact. Let \mathcal{D} be a representation of Γ , irreducible on the real. acting on the real vector space \mathscr{E} of dimension n. It is known from the representation theory of space groups that n divides 48 and that \mathcal{D} is equivalent to an orthogonal representation, so we assume ("<" reads here "subgroup")

$$\operatorname{Im} \mathscr{D} < \operatorname{O}(n) \tag{6}$$

Let $[\Lambda] \in \mathcal{K}$, that is, let $[\Lambda]$ be the conjugated class of isotropic groups of an orbit of Γ , and let $K_{[\Lambda]}$ be the common intersection of all subgroups $\Lambda \in [\Lambda]$. Then $K_{[\Lambda]} \triangleleft \Gamma$ (\triangleleft reads "invariant subgroup"); moreover $K_{[\Lambda]}$ leaves invariant every point of the orbit and therefore its linear space as well, which must be the whole space \mathscr{E} since \mathscr{D} is irreducible. So

 $K_{[\Lambda]} = \ker \mathcal{D}$. But by definition of the kernel: $\ker \mathcal{D} = \bigcap_{v \in \mathcal{E}} \Gamma_v$ so $K_{[\Lambda]} = \ker \mathcal{D}$, and this result is independent of the class $[\Lambda] \in \mathcal{K}$ we started from. In other words, $\ker \mathcal{D}$ is the largest invariant subgroup of Γ contained in any isotropic group.

Landau theory⁵ is probably so well known to the reader that I will need only to recall here the mathematical computation it leads to. To study a second-order phase transition in a crystal one has to choose an irreducible (in the real) orthogonal representation \mathcal{D} of its space group Γ . (The choice of \mathcal{D} is usually guided by the experimental data, e.g., by the existence of zero modes.) This representation must be *active*, i.e., it must not admit third-degree homogeneous polynomial on \mathcal{E} invariant by Γ . At the phase transition, the symmetry Γ is spontaneously broken into a subgroup $\Lambda < \Gamma$, which is the isotropic group of an absolute minimum of a Γ -invariant polynomial that is bounded below and possesses a local maximum at the origin. We call such a polynomial a generalized Landau polynomial. Its lowest possible degree is four. When this is the case, we simply call it a "Landau polynomial."

In a second-order phase transition from crystal to crystal Λ is also a crystallographic group; its largest Γ -invariant subgroup contains a three-dimensional lattice of translations so $\ker \mathcal{D}$ is also a crystallographic group and $\operatorname{Im} \mathcal{D} = G$ is finite. When the transition is to a incommensurable structure, the Lifschits condition is not satisfied; $\operatorname{Im} \mathcal{D}$ is infinite and therefore it is not a closed subgroup of $\operatorname{O}(n)$. We call G its closure in $\operatorname{O}(n)$: then G is compact. The Γ -invariants on $\mathscr E$ depends only on the image of $\mathscr D$; if, moreover, we exclude distributions and consider only smooth invariant functions, they depend only on the closure of $\operatorname{Im} \mathscr D$.

From this point on we need only to consider the effective orthogonal representation of the compact (or finite) group G on \mathscr{E}_0 . For such a representation, Schwarz has shown that every G-invariant smooth (i.e., C^{∞}) function is a smooth function of invariant polynomials. We could even consider "Landau functions." For this it is convenient to build \mathscr{E}_c , the compactified function of \mathscr{E} , by adding the point Ω at infinity (Ω is G-invariant). A Landau function is a smooth G-invariant function with only two local maxima, at Ω and at Ω . These are the only two G-invariant points of \mathscr{E}_c . † Let $\mathscr{K}' = \mathscr{K} - [G]$, i.e., \mathscr{K}' is the set of classes of isotropic

[†] In the same paper counterexamples have also been given for reducible representations. This is interesting in the actual applications of Higgs polynomials in high-energy physics and also in some cases of the application of Landau theory.

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groups on \mathscr{E}_c minus 0 and Ω . Let [H] be a maximal element of \mathscr{K}' and $\mathscr{E}_c^{[H]}$ the set of points whose isotropic group contains a group of [H]: $\mathscr{E}_c^{[H]}$ is the union of the strata larger than [H], that is, the two strata defined by [H] and [G] (i.e., the points 0 and Ω). It is easy to show that $\mathscr{E}_c^{[H]}$ its closed and therefore compact. Let Φ be a Landau function and $\Phi/\mathscr{E}_c^{[H]}$ its restriction on this compact space. It has two maxima on it, at 0 and Ω . It must also have at least a minimum elsewhere (by definition, it is not constant!) and the isotropic groups of these absolute minima belong to [H]. The gradient of Φ is G-covariant and, as we have seen in Eq. (4), it is tangent at each point to its stratum, so it vanishes at the minima of $\Phi/\mathscr{E}_c^{[H]}$; these are therefore extrema of Φ . By a standard trick (due to Morse) this result also applies to generalized Landau polynomials and, as a particular case, to Landau polynomials. That is, we have proven

Theorem 1. Any Landau function or (generalized) Landau polynomial has an extremum on each maximal stratum of \mathcal{K}' , that is, every maximal, isotropically strict subgroup of G is the isotropic group of an extremum of any Landau function or (generalized) polynomial. Are the absolute minima among those extrema with maximal isotropic subgroups? Not necessarily for the Landau function of generalized polynomials: it is easy to give counterexamples (e.g., see Ref. 3).† There is even a known counterexample for the (degree four) Landau polynomial given by the Toledano brothers. It is based on the four-dimensional irreducible representation of the space group $I4_1 = C_4^6$, built with the wave vector N of the Brillouin zone.

However, there is an important remark to be made here on this example: The invariance group of the Landau polynomial is a group \tilde{G} < O(4), which is larger than $G = \operatorname{Im} \mathcal{D} = \mathcal{D}(\Gamma)$. A mathematical theorem on the symmetry of the minima of Landau polynomials can be based only on the exact symmetry group \tilde{G} of the polynomial P, i.e., the isotropy group $O(n)_P$ of P for the action of O(n) on \mathscr{E} . For example, the only quartic harmonic polynomial $\neq (\phi, \phi)^2$ (up to an orthogonal transformation of coordinates) invariant by an irreducible subgroup of O(3) is $\phi_1^4 + \phi_2^4 + \phi_3^4$. It could be obtained as invariant of any point group of the cubic system T, T_h , T_d , O, O_h , but its maximal invariance group is $\tilde{G} = O_h$. This is the only possible \tilde{G} (i.e., irreducible isotropic

[†]For Theorem 1, we need only this hypothesis and not the irreducibility of the representation.

subgroups of O(n) for a non-O(n)-invariant quartic polynomial) for n=3 just as C_{4v} is the only possible \tilde{G} for n=2. For n=4 it has been found in Ref. 9 that the \tilde{G} 's fall into 13 conjugate classes of O(n).

In the Toledanos' counterexample, the isotropic group of the minima is a maximal isotropic subgroup for the action of \tilde{G} . Is that always sure for Landau polynomials? I have been able to prove it only of some families of \tilde{G} .³ But no counterexample is known.

Let me explain now some results of invariant theory. The representation \mathcal{D} of the compact (or finite) group G on \mathscr{E} defines also a linear action of G in the vector space \mathscr{P} of polynomials on \mathscr{E} (i.e., of n-variable polynomials). This vector space is the direct sum

$$\mathscr{P} = \bigoplus_{m=0}^{\infty} \mathscr{P}_m \tag{7}$$

where \mathscr{P}_m is the set of all homogeneous polynomials of degree $m(\mathscr{P}_0 = \mathbb{R}, \mathscr{P}_1 = \mathscr{E})$. The linear representation of G on \mathscr{P}_m is the completely symmetricized mth tensor power of the representation \mathscr{D} . Its character χ_m is given by the generating function

$$C(g,t) = \sum_{m=0}^{\infty} \chi_m(g) t^m = \det[I - t\mathcal{D}(g)]^{-1}$$
 (8)

Let \mathscr{P}^G the set of G-invariant polynomials: since the sum and the product of invariant polynomials are again invariant polynomials, \mathscr{P}^G is a ring, and also an algebra on the real, whose vector space decomposes into

$$\mathscr{P}^G = \bigoplus_{m=0}^{\infty} \mathscr{P}_m^G \quad \text{with} \quad \mathscr{P}_m^G = \mathscr{P}_m \cap \mathscr{P}^G \tag{9}$$

Using the orthogonal property of characters, $c_m = \dim \mathscr{P}_m^G$ is given by the generating function, when G is finite

$$M(t) = \sum_{m=0}^{\infty} c_m t^m = \frac{1}{|G|} \sum_{g \in G} \det[I - t\mathcal{D}(g)]^{-1}$$
 (10)

For a compact group, the finite sum $1/|G|\sum_g$ is to be replaced by $\int_G d\mu(g)$, where integration over the G-invariant measure is normalized

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to 1 for the whole group. The M(t) function of Eq. (10) was found last century by Molien. ¹⁰ It is a rational fraction in t, which can be written as the ratio of two polynomials

$$M(t) = \frac{N(t)}{D(t)}, \quad D(t) = \prod_{i=1}^{n'} (1 - t^{d_i}), \quad N(t) = \sum_{\alpha=0}^{\nu-1} t^{\delta_{\alpha}}, \quad \delta_0 = 0,$$
 (11)

For finite groups n'=n; for compact groups n' < n. Such a form translates exactly the nature of the ring \mathcal{P}^G , as was recently proven (see Ref. 2): \mathcal{P}^G is a free module of finite dimension v over a polymonial ring of n' variables. (It was known from Hilbert 11 that \mathcal{P}^G has a finite number of generators when G is finite.) This means more explicitly that there exists n' algebraically independent G-invariant homogeneous polynomials θ_i of degree d_i and v-1 G-invariant homogeneous polynomials φ_α of degree δ_α such that any G-invariant polynomial $p \in \mathcal{P}^G$ has a unique decomposition into the sum

$$p(\phi) = \sum_{\alpha=0}^{\nu-1} q_{\alpha} [\theta_1(\phi), \dots, \theta_{n'}(\phi)] \varphi_{\alpha}(\phi), \qquad \varphi_0 = 1$$
 (12)

where the q_{α} are arbitrary n'-variable polynomials. For each φ_{α} there is a smallest positive integer v_{α} such that

$$\varphi_{\alpha}^{v_{\alpha}} = \Phi_{\alpha}(\theta_1, \dots, \theta_{n'}) \tag{13}$$

a polynomial in the θ_i 's.

For groups generated by reflections, whose list was established by Coxeter, v = 1 and the θ 's are tabulated. For some subgroups of Coxeter groups, there are methods for finding the θ 's and φ 's. ¹² For other finite groups and for most compact groups this is partly an art.

From now on, we consider only Landau polynomials over irreducible $[c_2=1, \text{ i.e.}, \theta_1=(\phi,\phi) \text{ the invariant orthogonal scalar product on } \mathcal{E}]$ active $(c_3=0)$ representations. For a given image $G=\mathcal{D}(\Gamma)$ of the symmetry group one computes, e.g., from Eq. (10), $c_4=\dim \mathcal{P}_4^G=N$. One also determines $\mathscr{C}(\mathcal{P}_4^G)$, the centralizer of \mathcal{P}_4^G , i.e., the intersection of all isotropic groups of the polynomials in \mathcal{P}_4^G , for the action of O(n) on \mathcal{P}_4 . Then the most general Landau polynomial can be written

$$P(\phi) = \frac{1}{4} [(\phi, \phi)^2 + \omega(\phi)] - \frac{\mu^2}{2} (\phi, \phi) = \frac{1}{4} \rho(\phi) - \frac{\mu^2}{2} (\phi, \phi)$$
 (14)

where

$$\omega[\mathcal{D}(g)\phi] = \omega(\phi), \qquad \omega(\lambda\phi) = \lambda^4\omega(\phi)$$
 (15)

$$\Delta\omega(\phi) = \sum_{i=1}^{n} \frac{\partial^2}{\partial \phi_i^2} \omega(\phi) = 0 \qquad \text{(harmonicity)}$$
 (15')

$$(\hat{\phi}, \hat{\phi}) = 1 \Rightarrow \rho(\hat{\phi}) = 1 + \omega(\hat{\phi}) > 0 \tag{15''}$$

The most general quartic harmonic invariant can be written as a linear combination of N-1 harmonic invariants

$$\omega(\phi) = \sum_{\alpha=i}^{N-1} \lambda_{\alpha} \omega_{\alpha}(\phi)$$
 (16)

The conditions of Eq. (15") imposes a domain in the space of the λ 's.

The polynomials ω_{α} are θ_i 's (i>1) or φ_{α} 's. If these polynomials are algebraically independent (this will generally be the case when $N \leq n$) then $P(\phi)$ has no extrema on the open dense generic stratum.†

 $\omega(\hat{\phi})$ reaches its maximum ω_M and its minimum ω_m in the unit sphere S_{n-1} ; from Eq. (15") and the harmonicity of ω (which is assumed nonconstant)

$$-1 < \omega_m < 0 < \omega_M \tag{17}$$

By means of polarization¹⁴ $P(\phi)$ can be written as a quadrilinear form $\tilde{\rho}(\phi_1, \phi_2, \phi_3, \phi_4)$, completely symmetrical into its arguments. This form defines a map

$$\mathscr{E} \times \mathscr{E} \xrightarrow{R} \mathscr{L}(\mathscr{E}) \tag{18}$$

that is, R_{ϕ_1,ϕ_2} is a linear operator on \mathscr{E} depending bilinearly on two vectors of \mathscr{E} . This operator is covariant and symmetrical, i.e.,

$$R_{\mathscr{D}(y)\phi_1,\mathscr{D}(g)\phi_2} = \mathscr{D}(g)R_{\phi_1,\phi_2}\mathscr{D}(g)^{-1}, \qquad R^T = R$$
(19)

[†] This was established in Ref. 3 and by Jaric in Ref. 13.

and, moreover,

$$\tilde{\rho}(\phi_1, \phi_2, \phi_3, \phi_4) = (\phi_1, R_{\phi_2, \phi_3} \phi_4)$$
 (20)

We can therefore write

$$\rho(\phi) = (\phi, R_{\phi,\phi}\phi) = (\phi, S_{\phi\phi}\phi) + (\phi, T_{\phi\phi}\phi) \equiv (\phi, \phi)^2 + \omega(\phi)$$
 (21)

with

$$S_{\phi\phi} = \frac{1}{3}(\phi, \phi)(I + 2P_{\phi})$$
 (22)

where P_{ϕ} is the orthogonal projector on ϕ and

$$\operatorname{Tr} T_{\phi,\phi} = \frac{1}{12} \Delta \omega(\phi) = 0 \tag{23}$$

An easy computation yields

$$\frac{dP}{d\phi} = (R_{\phi\phi} - \mu^2 I)\phi \equiv \{T_{\phi\phi} + [(\phi, \phi) - \mu^2]I\}\phi$$
 (24)

$$\frac{\mathrm{d}^{2}P}{\mathrm{d}\phi^{2}} = 3R_{\phi\phi} - \mu^{2}I \equiv 3T_{\phi\phi} + [(\phi,\phi) - \mu^{2}]I + 2(\phi,\phi)P_{\phi}$$
 (25)

If $u = \xi \hat{u}$, with $(\hat{u}, \hat{u}) = 1$, $\xi > 0$ is an extremum:

$$\frac{d^2 P}{d\phi^2}(u)u = 2\mu^2 u, \qquad \xi^2 = \frac{\mu^2}{1 + \omega(\hat{u})}$$
 (26)

$$P(u) = -\frac{\mu^2}{4} \, \xi^2 \equiv -\frac{\mu^2}{4} (u, u) \tag{27}$$

This shows that the absolute minima of P are the farthest extrema from the origin.

$$\xi = \frac{\mu}{(1 + \omega_m)^{1/2}} \tag{28}$$

Other local minima, if they exist, require the value $\omega_0 = \omega(\hat{u})$ to be

negative. Indeed from Eqs. (23), (25), and (26) the trace of $d^2p/d\phi^2(u)$ restricted to the space u^{\perp} is $-\mu^2n\omega_0/1+\omega_0$.

If the conjecture were true one would only have to verify, among the extrema of maximal strata (i.e., corresponding to maximal isotropic subgroups) which ones were minima. The answer to this question depends on the values of the λ_{α} and leads generally to phase diagram with several phases. However, it is always useful to determine the isotropic groups and the strata of the group of matrices G. For compact (or finite) groups this problem is studied in Ref. 15. For finite groups G the problem is simpler. An explicit procedure has been given (without proof) in Ref. 16. The matrix group G acting on \mathscr{E} defines a representation for all its subgroups. Let c(H) be the multiplicity of the trivial representation of the subgroup H of G. It is the same for all subgroups of the conjugation class [H]. The subgroup H is an isotropy group if and only if for all H' > H, c(H') < c(H). Moreover c(H) is the dimension of the stratum of H. We have already seen that $I \in G$ is the smallest isotropy subgroup $\lceil c(I) = \dim \mathscr{E} \rceil$ and the corresponding statum is open dense. Finally, the intersection of isotropic subgroups are isotropic subgroups (when G is finite!). And for groups generated by reflections, the isotropic subgroups are also generated by reflections.

Jaric et al.¹⁷ have shown how to write for each stratum a covariant set of equations for the zero of covariant vector fields. One only needs to study the Hessian of Eq. (25) for each found zero of the gradient in Eq. (24).

Here we just give a small remark that may help to find new extrema from already known ones. Assume that $\pm u$ and $\pm v$ are extrema and have the same length (which will occur if they belong to the same G-orbit)

$$R_{uu}u = \mu^2 u, \qquad R_{vv}v = \mu^2 v, \qquad (u, u) = (v, v)$$
 (29)

We define

$$(u,v) = (u,u)\cos\theta, \qquad \frac{\tilde{\rho}(u,u,v,v)}{\mu^2(u,u)} = K$$
 (29')

That $\rho(\alpha u + \beta v) > 0$ for all α, β implies

$$3(K-1)\gamma^2 + 2(1+2\gamma\cos\theta) > 0, \qquad -1 \le \gamma = \frac{2\alpha\beta}{\alpha^2 + \beta^2} \le 1$$
 (30)

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We define

$$w_{\varepsilon} = u + \varepsilon v \tag{31}$$

Then

$$R_{w,w}W_{\varepsilon} = \mu^{2}W_{\varepsilon} + 3\varepsilon R_{uv}W_{\varepsilon} \tag{32}$$

From

$$(w_{\varepsilon}, w_{-\varepsilon}) = 0 \tag{33}$$

and Eq. (29) we deduce to be

$$(w_{-\varepsilon}, R_{w_{\varepsilon}w_{\varepsilon}}w_{\varepsilon}) = 0 \tag{34}$$

We see that the vectors w_+ and w_- are directions of extrema if $R_{uv}w_{\varepsilon}$ is in the two-plane spanned by u and v. This happens for instance if u and v are on an orbit in a maximal stratum and $c(G_u \cap G_v) = 2$, $(G_x$ is the isotropic group of x). It also happens that if $G_u = G_v = H$ with c(H) = 2, the normalizer of H in G (i.e., the largest subgroup of G which contains H as an invariant subgroup) acts on the two-plane spanned by u and v, and it exchanges them. Since c(H) = 2, H may be a nonmaximal isotropic group. With this hypothesis on $R_{uv}w_{\varepsilon}$, the four new extrema are

$$\pm \alpha_{\varepsilon} w_{\varepsilon}$$
 with $\alpha_{\varepsilon}^2 = (1 + \cos \theta)(1 + 4\varepsilon \cos \theta + 3K)^{-1}$ (35)

We remark that

$$\frac{(\alpha_{\varepsilon} w_{\varepsilon}, \alpha_{\varepsilon} w_{\varepsilon}) - (u, u)}{(u, u)} = \frac{1 - 3K + 2\cos^2 \theta}{1 + 3K + 4\varepsilon\cos\theta}$$
(36)

From Eq. (30) with $\gamma^2 = 1$ we deduce that the sign of this expression is independent from ε , so the two extrema $\alpha_{\pm}w_{\pm}$ are both either longer or shorter than the extrema u and v. Note that if $\cos\theta \neq 0$, $\alpha_{+}w_{+}$ and $\alpha_{-}w_{-}$ have different length and therefore are not on the same orbit. As we have seen, the absolute minimum of $P(\phi)$ corresponds to the longest extremum. Finally, the application of Morse theory may also be very helpful.^{3,18}

As is well known, one has to complete Landau theory by a renormalization group computation for comparing its prediction with an actual possible second-order phase transition. Then the second-order transition occurs only if there is a stable fixed point under the renormalization group. I have recently proven¹⁹ that stable fixed points, when they exist, are unique. As recalled in Eq. (16), the quartic term of the Landau polynomial may depend on N parameters. No stable fixed points were known when N > 3. This led Dzyaloshinskii²⁰ to conjecture that this result is a topological theorem; I gave counterexamples in Ref. 19, independently from Grinstein and Mukamel who published the first counterexample.²¹

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Latest news (March 1983): Jarić and Mukamel²² have found a counter-example to the hypothesis of maximality of isotropic subgroups for the minimum of Landau polynomials in six dimensions.

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